



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2025 – 11:03 AM EDT

PDB ID : 1T6P / pdb_00001t6p
Title : Crystal Structure of Phenylalanine Ammonia Lyase from *Rhodospiridium toruloides*
Authors : Calabrese, J.C.; Jordan, D.B.
Deposited on : 2004-05-06
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

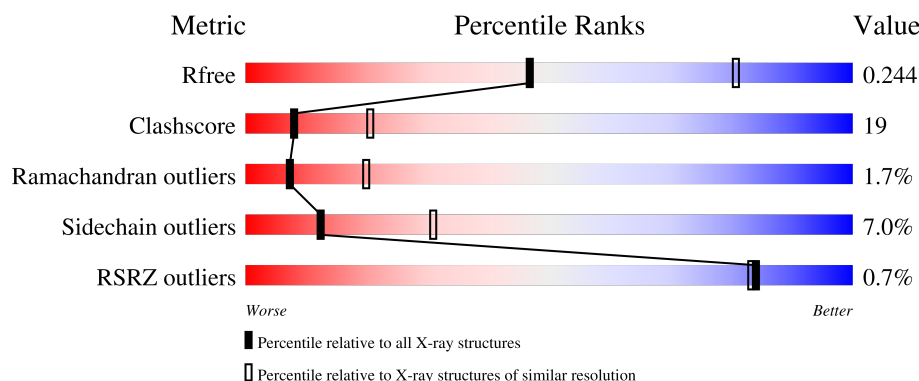
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	714	
1	B	714	
1	C	714	
1	D	714	
1	E	714	

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Mol	Chain	Length	Quality of chain
1	F	714	
1	G	714	
1	H	714	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	175	A	211	X	-	-	-
1	175	B	211	X	-	-	-
1	175	C	211	X	-	-	-
1	175	D	211	X	-	-	-
1	175	E	211	X	-	-	-
1	175	F	211	X	-	-	-
1	175	G	211	X	-	-	-
1	175	H	211	X	-	-	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 40380 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called phenylalanine ammonia-lyase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	654	Total	C	N	O	S	Se	0	0	0
			4978	3131	884	946	4	13			
1	B	660	Total	C	N	O	S	Se	0	0	0
			5019	3153	893	956	4	13			
1	C	650	Total	C	N	O	S	Se	0	0	0
			4946	3110	882	937	4	13			
1	D	650	Total	C	N	O	S	Se	0	0	0
			4948	3111	880	940	4	13			
1	E	655	Total	C	N	O	S	Se	0	0	0
			4982	3133	886	946	4	13			
1	F	650	Total	C	N	O	S	Se	0	0	0
			4951	3113	882	939	4	13			
1	G	656	Total	C	N	O	S	Se	0	0	0
			4995	3140	890	948	4	13			
1	H	644	Total	C	N	O	S	Se	0	0	0
			4910	3088	872	933	4	13			

There are 144 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P11544
A	51	MSE	MET	modified residue	UNP P11544
A	107	MSE	MET	modified residue	UNP P11544
A	169	MSE	MET	modified residue	UNP P11544
A	211	175	ALA	SEE REMARK 999	UNP P11544
A	211	175	SER	SEE REMARK 999	UNP P11544
A	211	175	GLY	SEE REMARK 999	UNP P11544
A	250	MSE	MET	modified residue	UNP P11544
A	278	MSE	MET	modified residue	UNP P11544
A	288	MSE	MET	modified residue	UNP P11544
A	299	MSE	MET	modified residue	UNP P11544
A	304	MSE	MET	modified residue	UNP P11544
A	422	MSE	MET	modified residue	UNP P11544

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Chain	Residue	Modelled	Actual	Comment	Reference
A	443	MSE	MET	modified residue	UNP P11544
A	448	MSE	MET	modified residue	UNP P11544
A	497	MSE	MET	modified residue	UNP P11544
A	564	MSE	MET	modified residue	UNP P11544
A	714	MSE	MET	modified residue	UNP P11544
B	1	MSE	MET	modified residue	UNP P11544
B	51	MSE	MET	modified residue	UNP P11544
B	107	MSE	MET	modified residue	UNP P11544
B	169	MSE	MET	modified residue	UNP P11544
B	211	175	ALA	SEE REMARK 999	UNP P11544
B	211	175	SER	SEE REMARK 999	UNP P11544
B	211	175	GLY	SEE REMARK 999	UNP P11544
B	250	MSE	MET	modified residue	UNP P11544
B	278	MSE	MET	modified residue	UNP P11544
B	288	MSE	MET	modified residue	UNP P11544
B	299	MSE	MET	modified residue	UNP P11544
B	304	MSE	MET	modified residue	UNP P11544
B	422	MSE	MET	modified residue	UNP P11544
B	443	MSE	MET	modified residue	UNP P11544
B	448	MSE	MET	modified residue	UNP P11544
B	497	MSE	MET	modified residue	UNP P11544
B	564	MSE	MET	modified residue	UNP P11544
B	714	MSE	MET	modified residue	UNP P11544
C	1	MSE	MET	modified residue	UNP P11544
C	51	MSE	MET	modified residue	UNP P11544
C	107	MSE	MET	modified residue	UNP P11544
C	169	MSE	MET	modified residue	UNP P11544
C	211	175	ALA	SEE REMARK 999	UNP P11544
C	211	175	SER	SEE REMARK 999	UNP P11544
C	211	175	GLY	SEE REMARK 999	UNP P11544
C	250	MSE	MET	modified residue	UNP P11544
C	278	MSE	MET	modified residue	UNP P11544
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C	448	MSE	MET	modified residue	UNP P11544
C	497	MSE	MET	modified residue	UNP P11544
C	564	MSE	MET	modified residue	UNP P11544
C	714	MSE	MET	modified residue	UNP P11544
D	1	MSE	MET	modified residue	UNP P11544

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Chain	Residue	Modelled	Actual	Comment	Reference
D	51	MSE	MET	modified residue	UNP P11544
D	107	MSE	MET	modified residue	UNP P11544
D	169	MSE	MET	modified residue	UNP P11544
D	211	175	ALA	SEE REMARK 999	UNP P11544
D	211	175	SER	SEE REMARK 999	UNP P11544
D	211	175	GLY	SEE REMARK 999	UNP P11544
D	250	MSE	MET	modified residue	UNP P11544
D	278	MSE	MET	modified residue	UNP P11544
D	288	MSE	MET	modified residue	UNP P11544
D	299	MSE	MET	modified residue	UNP P11544
D	304	MSE	MET	modified residue	UNP P11544
D	422	MSE	MET	modified residue	UNP P11544
D	443	MSE	MET	modified residue	UNP P11544
D	448	MSE	MET	modified residue	UNP P11544
D	497	MSE	MET	modified residue	UNP P11544
D	564	MSE	MET	modified residue	UNP P11544
D	714	MSE	MET	modified residue	UNP P11544
E	1	MSE	MET	modified residue	UNP P11544
E	51	MSE	MET	modified residue	UNP P11544
E	107	MSE	MET	modified residue	UNP P11544
E	169	MSE	MET	modified residue	UNP P11544
E	211	175	ALA	SEE REMARK 999	UNP P11544
E	211	175	SER	SEE REMARK 999	UNP P11544
E	211	175	GLY	SEE REMARK 999	UNP P11544
E	250	MSE	MET	modified residue	UNP P11544
E	278	MSE	MET	modified residue	UNP P11544
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E	299	MSE	MET	modified residue	UNP P11544
E	304	MSE	MET	modified residue	UNP P11544
E	422	MSE	MET	modified residue	UNP P11544
E	443	MSE	MET	modified residue	UNP P11544
E	448	MSE	MET	modified residue	UNP P11544
E	497	MSE	MET	modified residue	UNP P11544
E	564	MSE	MET	modified residue	UNP P11544
E	714	MSE	MET	modified residue	UNP P11544
F	1	MSE	MET	modified residue	UNP P11544
F	51	MSE	MET	modified residue	UNP P11544
F	107	MSE	MET	modified residue	UNP P11544
F	169	MSE	MET	modified residue	UNP P11544
F	211	175	ALA	SEE REMARK 999	UNP P11544
F	211	175	SER	SEE REMARK 999	UNP P11544
F	211	175	GLY	SEE REMARK 999	UNP P11544

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Chain	Residue	Modelled	Actual	Comment	Reference
F	250	MSE	MET	modified residue	UNP P11544
F	278	MSE	MET	modified residue	UNP P11544
F	288	MSE	MET	modified residue	UNP P11544
F	299	MSE	MET	modified residue	UNP P11544
F	304	MSE	MET	modified residue	UNP P11544
F	422	MSE	MET	modified residue	UNP P11544
F	443	MSE	MET	modified residue	UNP P11544
F	448	MSE	MET	modified residue	UNP P11544
F	497	MSE	MET	modified residue	UNP P11544
F	564	MSE	MET	modified residue	UNP P11544
F	714	MSE	MET	modified residue	UNP P11544
G	1	MSE	MET	modified residue	UNP P11544
G	51	MSE	MET	modified residue	UNP P11544
G	107	MSE	MET	modified residue	UNP P11544
G	169	MSE	MET	modified residue	UNP P11544
G	211	175	ALA	SEE REMARK 999	UNP P11544
G	211	175	SER	SEE REMARK 999	UNP P11544
G	211	175	GLY	SEE REMARK 999	UNP P11544
G	250	MSE	MET	modified residue	UNP P11544
G	278	MSE	MET	modified residue	UNP P11544
G	288	MSE	MET	modified residue	UNP P11544
G	299	MSE	MET	modified residue	UNP P11544
G	304	MSE	MET	modified residue	UNP P11544
G	422	MSE	MET	modified residue	UNP P11544
G	443	MSE	MET	modified residue	UNP P11544
G	448	MSE	MET	modified residue	UNP P11544
G	497	MSE	MET	modified residue	UNP P11544
G	564	MSE	MET	modified residue	UNP P11544
G	714	MSE	MET	modified residue	UNP P11544
H	1	MSE	MET	modified residue	UNP P11544
H	51	MSE	MET	modified residue	UNP P11544
H	107	MSE	MET	modified residue	UNP P11544
H	169	MSE	MET	modified residue	UNP P11544
H	211	175	ALA	SEE REMARK 999	UNP P11544
H	211	175	SER	SEE REMARK 999	UNP P11544
H	211	175	GLY	SEE REMARK 999	UNP P11544
H	250	MSE	MET	modified residue	UNP P11544
H	278	MSE	MET	modified residue	UNP P11544
H	288	MSE	MET	modified residue	UNP P11544
H	299	MSE	MET	modified residue	UNP P11544
H	304	MSE	MET	modified residue	UNP P11544
H	422	MSE	MET	modified residue	UNP P11544

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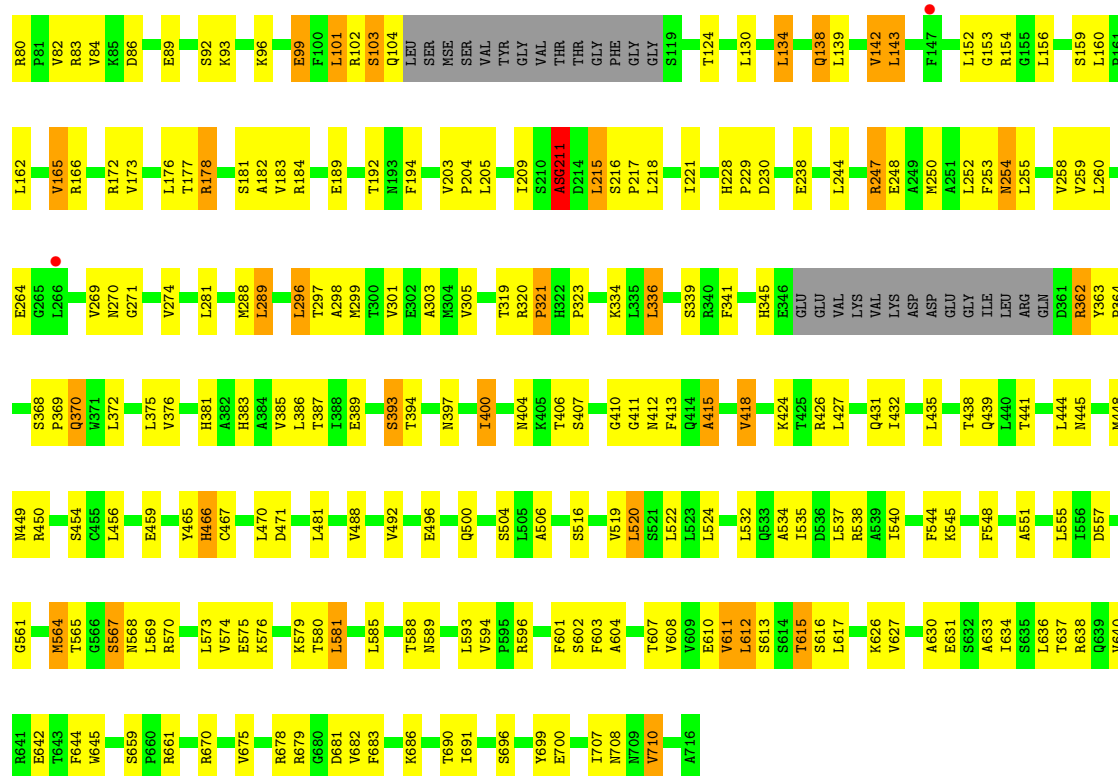
Chain	Residue	Modelled	Actual	Comment	Reference
H	443	MSE	MET	modified residue	UNP P11544
H	448	MSE	MET	modified residue	UNP P11544
H	497	MSE	MET	modified residue	UNP P11544
H	564	MSE	MET	modified residue	UNP P11544
H	714	MSE	MET	modified residue	UNP P11544

- Molecule 2 is water.

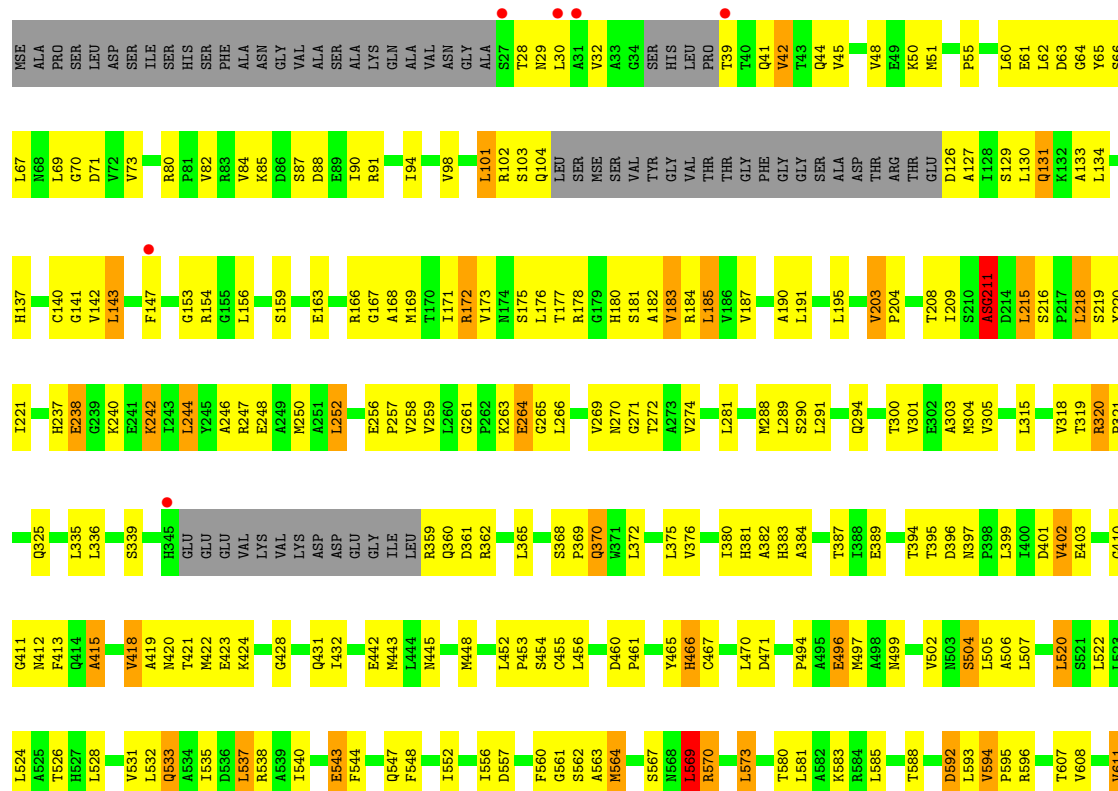
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	84	Total O 84 84	0	0
2	B	79	Total O 79 79	0	0
2	C	72	Total O 72 72	0	0
2	D	101	Total O 101 101	0	0
2	E	64	Total O 64 64	0	0
2	F	83	Total O 83 83	0	0
2	G	96	Total O 96 96	0	0
2	H	72	Total O 72 72	0	0

- Molecule 1: phenylalanine ammonia-lyase



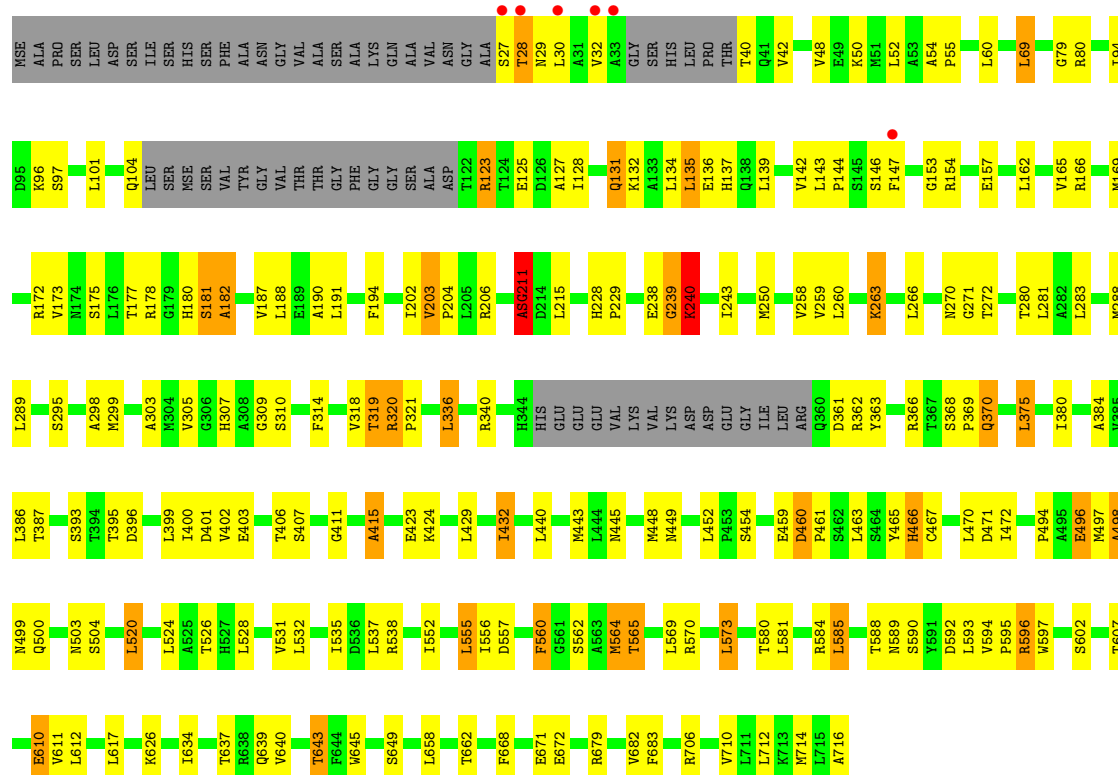


• Molecule 1: phenylalanine ammonia-lyase

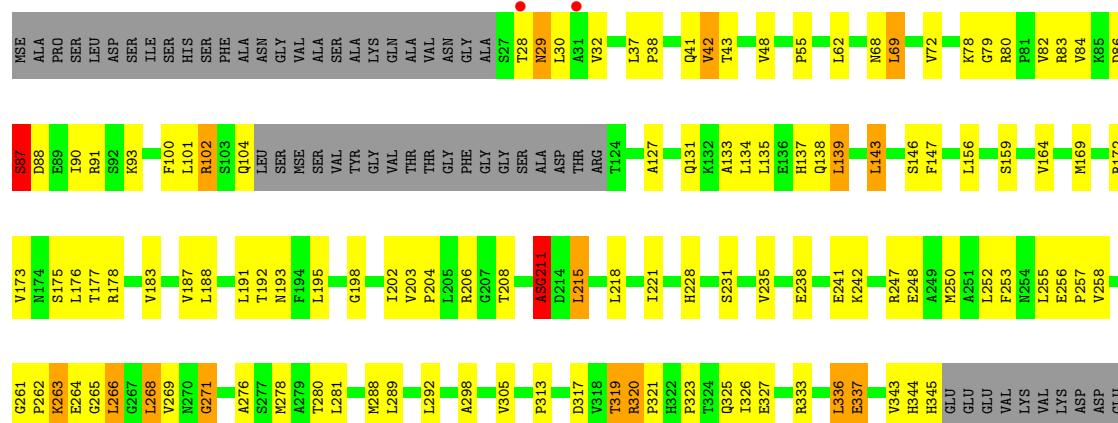


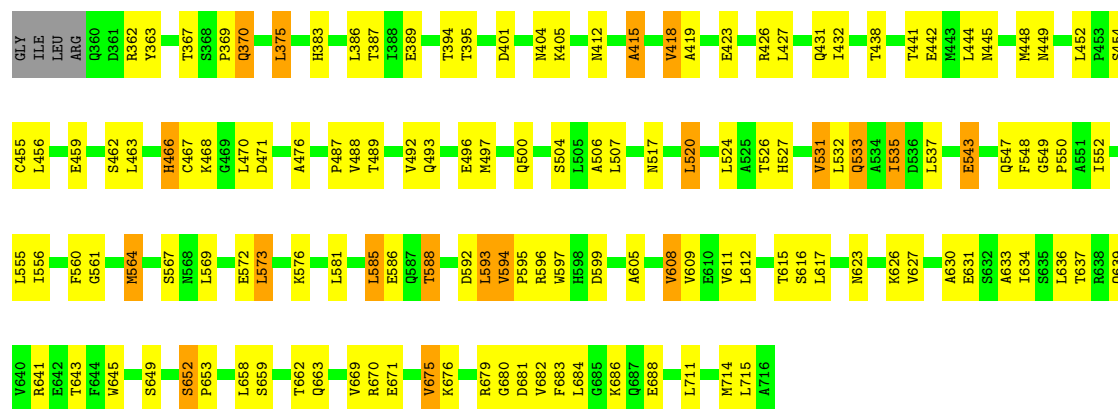


- Molecule 1: phenylalanine ammonia-lyase

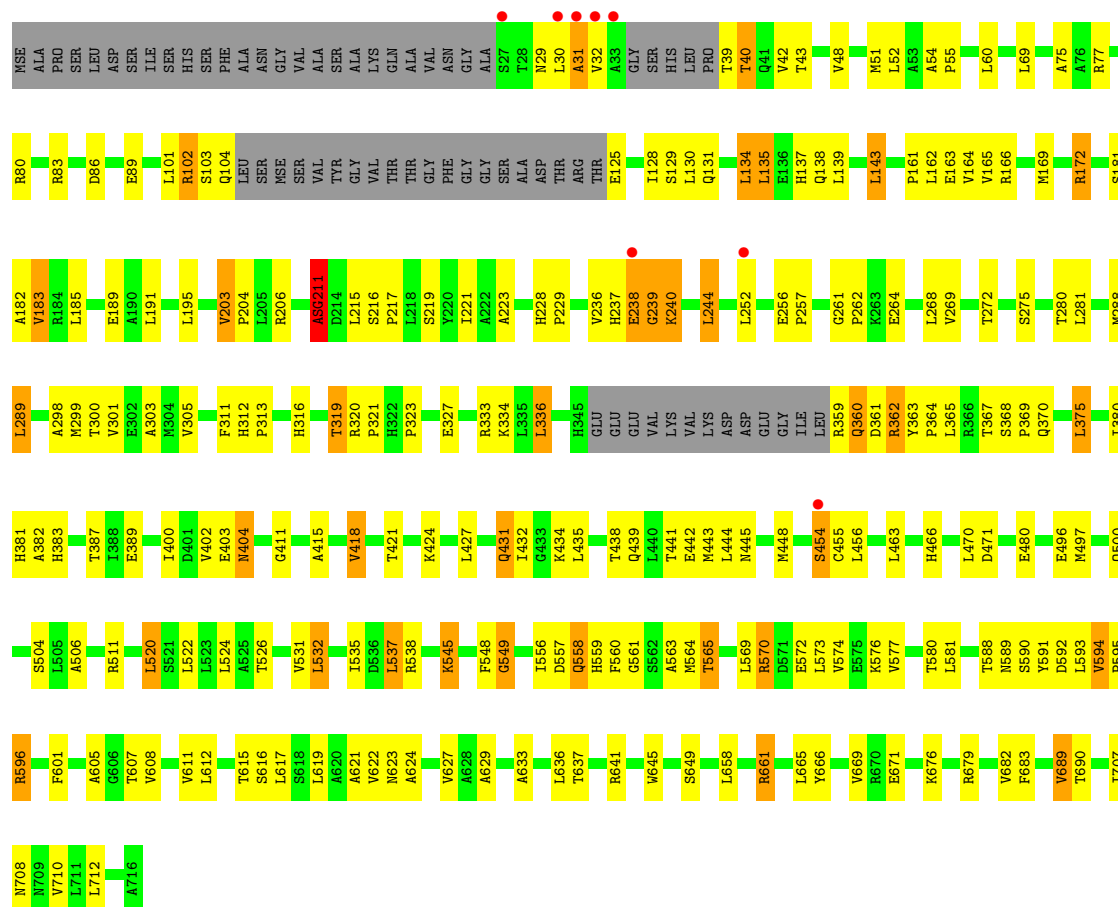


- Molecule 1: phenylalanine ammonia-lyase



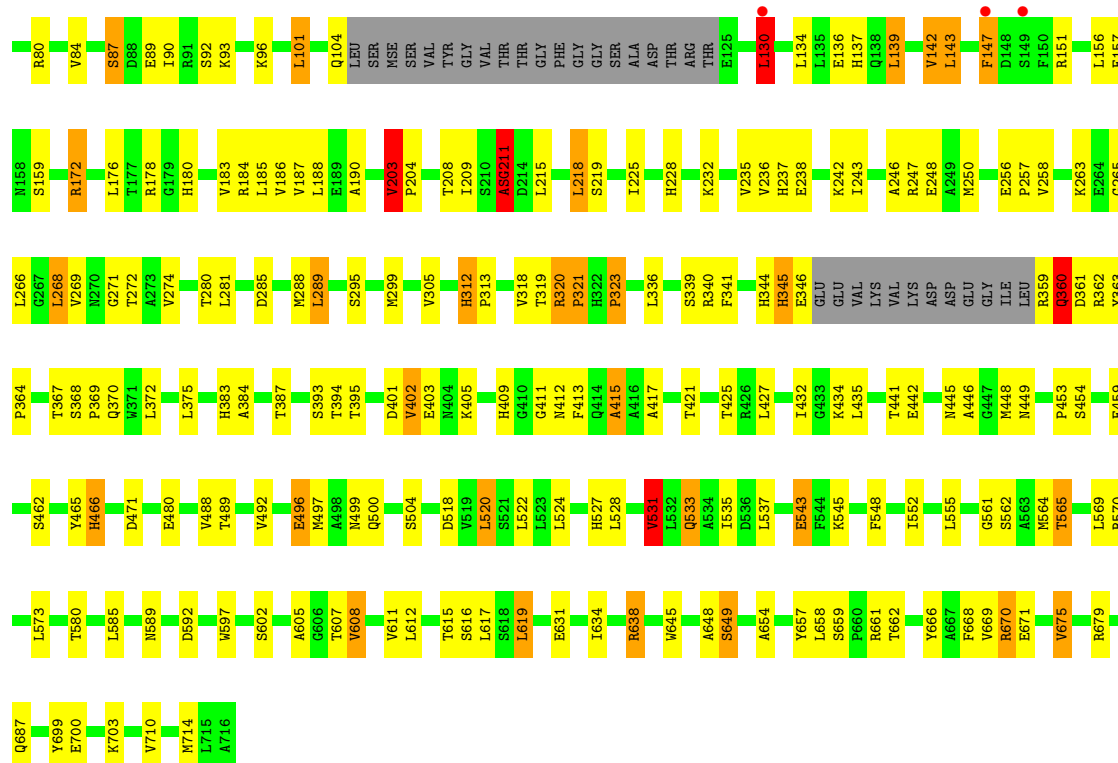


• Molecule 1: phenylalanine ammonia-lyase

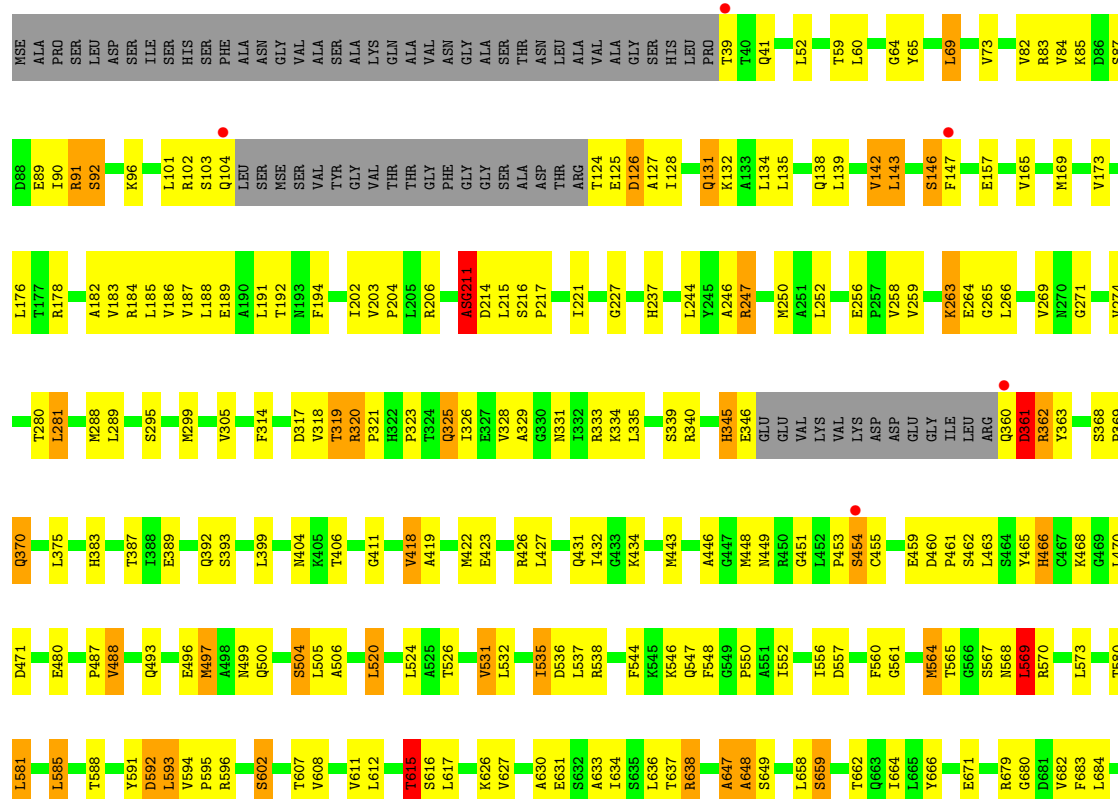


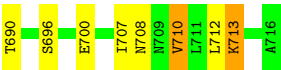
• Molecule 1: phenylalanine ammonia-lyase





• Molecule 1: phenylalanine ammonia-lyase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.19Å 180.97Å 149.22Å 90.00° 96.95° 90.00°	Depositor
Resolution (Å)	25.10 – 2.70 25.10 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.10-2.70) 96.8 (25.10-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.64 (at 2.72Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.194 , 0.253 0.189 , 0.244	Depositor DCC
R_{free} test set	3693 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å ²)	36.3	Xtriage
Anisotropy	0.796	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	40380	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.05% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 175

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.48	2/5036 (0.0%)	1.01	14/6815 (0.2%)
1	B	0.48	1/5077 (0.0%)	1.03	17/6871 (0.2%)
1	C	0.47	1/5001 (0.0%)	1.01	16/6764 (0.2%)
1	D	0.49	2/5002 (0.0%)	1.04	16/6766 (0.2%)
1	E	0.47	2/5040 (0.0%)	1.02	17/6821 (0.2%)
1	F	0.48	0/5006	1.02	12/6771 (0.2%)
1	G	0.48	0/5053	1.04	21/6837 (0.3%)
1	H	0.47	2/4966 (0.0%)	1.02	19/6718 (0.3%)
All	All	0.48	10/40181 (0.0%)	1.02	132/54363 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	2	2
1	B	2	2
1	C	2	2
1	D	2	2
1	E	2	2
1	F	2	2
1	G	2	2
1	H	2	2
All	All	16	16

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	564	MSE	SE-CE	-5.87	1.77	1.95
1	D	564	MSE	SE-CE	-5.57	1.78	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	564	MSE	SE-CE	-5.51	1.78	1.95
1	H	564	MSE	SE-CE	-5.49	1.78	1.95
1	H	564	MSE	CG-SE	-5.36	1.79	1.95
1	C	564	MSE	SE-CE	-5.11	1.80	1.95
1	D	564	MSE	CG-SE	-5.08	1.80	1.95
1	E	564	MSE	SE-CE	-5.05	1.80	1.95
1	A	564	MSE	CG-SE	-5.01	1.80	1.95
1	E	564	MSE	CG-SE	-5.00	1.80	1.95

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	320	ARG	CA-C-N	10.04	132.39	119.84
1	G	320	ARG	C-N-CA	10.04	132.39	119.84
1	B	124	THR	N-CA-C	-9.55	102.13	113.88
1	C	320	ARG	CA-C-N	7.94	129.76	119.84
1	C	320	ARG	C-N-CA	7.94	129.76	119.84
1	E	319	THR	N-CA-C	7.89	122.17	112.23
1	F	504	SER	N-CA-C	7.84	120.73	111.71
1	D	560	PHE	N-CA-C	7.81	122.33	111.56
1	H	592	ASP	N-CA-C	7.79	119.40	111.07
1	C	504	SER	N-CA-C	7.77	119.83	111.36
1	C	570	ARG	N-CA-C	-7.75	103.67	113.43
1	B	567	SER	N-CA-C	7.73	123.39	113.88
1	H	504	SER	N-CA-C	7.43	119.46	111.36
1	B	504	SER	N-CA-C	7.38	120.38	111.82
1	E	215	LEU	N-CA-C	7.35	118.94	111.07
1	F	319	THR	N-CA-C	7.31	119.15	111.03
1	H	271	GLY	N-CA-C	7.26	119.44	112.04
1	C	562	SER	N-CA-C	-7.06	104.13	112.89
1	G	504	SER	N-CA-C	6.86	119.60	111.71
1	H	318	VAL	N-CA-C	6.86	117.47	110.82
1	E	320	ARG	CA-C-N	6.79	128.32	119.84
1	E	320	ARG	C-N-CA	6.79	128.32	119.84
1	B	320	ARG	CA-C-N	6.76	128.28	119.84
1	B	320	ARG	C-N-CA	6.76	128.28	119.84
1	D	602	SER	N-CA-C	-6.74	104.01	111.36
1	E	432	ILE	N-CA-C	-6.71	104.22	110.53
1	A	504	SER	N-CA-C	6.68	118.35	111.14
1	H	488	VAL	N-CA-C	-6.67	106.50	111.90
1	A	215	LEU	N-CA-C	6.64	118.52	111.28
1	H	320	ARG	CA-C-N	6.48	127.94	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	320	ARG	C-N-CA	6.48	127.94	119.84
1	A	602	SER	N-CA-C	-6.47	104.31	111.36
1	F	689	VAL	N-CA-C	6.42	122.70	109.34
1	D	504	SER	N-CA-C	6.29	120.16	112.23
1	B	602	SER	N-CA-C	-6.28	104.31	112.23
1	D	432	ILE	N-CA-C	-6.28	104.38	110.72
1	A	320	ARG	CA-C-N	6.27	127.67	119.84
1	A	320	ARG	C-N-CA	6.27	127.67	119.84
1	B	319	THR	N-CA-C	6.18	120.56	112.89
1	A	319	THR	N-CA-C	6.06	119.86	112.23
1	D	180	HIS	N-CA-C	-6.04	106.88	114.56
1	E	133	ALA	N-CA-C	-5.97	106.13	113.41
1	B	400	ILE	N-CA-C	5.96	116.69	107.99
1	G	602	SER	N-CA-C	-5.95	104.88	111.36
1	H	569	LEU	N-CA-C	5.92	120.20	112.92
1	B	36	HIS	N-CA-C	-5.92	101.77	110.52
1	D	592	ASP	N-CA-C	5.89	120.73	112.72
1	D	319	THR	N-CA-C	5.88	119.63	112.23
1	G	130	LEU	N-CA-C	-5.86	106.26	113.41
1	H	602	SER	N-CA-C	-5.84	105.04	111.82
1	G	228	HIS	CA-C-N	5.81	125.94	119.32
1	G	228	HIS	C-N-CA	5.81	125.94	119.32
1	H	560	PHE	N-CA-C	5.79	120.85	113.55
1	C	318	VAL	N-CA-C	5.79	116.79	111.81
1	E	504	SER	N-CA-C	5.78	118.52	111.82
1	A	308	ALA	N-CA-C	-5.75	105.76	112.89
1	D	320	ARG	CA-C-N	5.74	127.02	119.84
1	D	320	ARG	C-N-CA	5.74	127.02	119.84
1	H	319	THR	N-CA-C	5.72	120.41	113.38
1	G	319	THR	N-CA-C	5.70	119.42	112.23
1	B	393	SER	N-CA-C	5.70	118.76	109.59
1	H	92	SER	N-CA-C	-5.65	105.42	112.93
1	D	94	ILE	N-CA-C	-5.61	105.38	110.82
1	E	467	CYS	N-CA-C	5.61	119.75	113.02
1	G	139	LEU	N-CA-C	-5.60	102.90	110.68
1	E	325	GLN	N-CA-C	-5.60	105.18	111.28
1	D	135	LEU	N-CA-C	-5.59	107.00	113.88
1	F	203	VAL	CA-C-N	5.58	125.53	119.78
1	F	203	VAL	C-N-CA	5.58	125.53	119.78
1	C	180	HIS	N-CA-C	-5.58	107.13	114.04
1	A	209	ILE	N-CA-C	-5.54	106.00	111.77
1	G	488	VAL	N-CA-C	-5.53	107.05	111.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	THR	N-CA-C	5.52	122.56	110.80
1	F	261	GLY	CA-C-N	5.52	126.74	119.84
1	F	261	GLY	C-N-CA	5.52	126.74	119.84
1	F	102	ARG	N-CA-C	-5.51	105.17	111.07
1	H	247	ARG	N-CA-C	-5.49	99.10	110.80
1	C	325	GLN	N-CA-C	-5.49	105.22	111.14
1	F	31	ALA	N-CA-C	-5.48	106.57	113.20
1	E	87	SER	N-CA-C	5.46	122.55	114.09
1	C	669	VAL	N-CA-C	5.42	115.62	110.53
1	C	215	LEU	N-CA-C	5.40	117.61	111.02
1	G	562	SER	N-CA-C	-5.40	105.40	111.28
1	A	530	CYS	N-CA-C	5.38	116.83	111.07
1	F	40	THR	N-CA-C	-5.38	106.69	113.20
1	B	37	LEU	CA-C-N	5.36	126.54	119.84
1	B	37	LEU	C-N-CA	5.36	126.54	119.84
1	B	103	SER	N-CA-C	-5.31	106.57	113.16
1	G	454	SER	N-CA-C	5.30	120.11	111.37
1	G	318	VAL	N-CA-C	5.30	116.38	111.45
1	A	467	CYS	N-CA-C	5.29	119.43	112.92
1	H	325	GLN	N-CA-C	-5.28	105.69	111.82
1	G	360	GLN	N-CA-C	5.26	122.00	110.80
1	G	35	SER	N-CA-C	5.24	117.04	108.55
1	D	460	ASP	CA-C-N	5.23	124.95	119.82
1	D	460	ASP	C-N-CA	5.23	124.95	119.82
1	E	271	GLY	N-CA-C	5.22	118.39	111.70
1	D	318	VAL	N-CA-C	5.19	116.60	111.67
1	B	209	ILE	N-CA-C	-5.17	106.39	111.77
1	G	203	VAL	CA-C-N	5.17	125.09	119.76
1	G	203	VAL	C-N-CA	5.17	125.09	119.76
1	D	467	CYS	N-CA-C	5.16	118.60	112.72
1	E	276	ALA	N-CA-C	-5.16	105.34	111.69
1	C	569	LEU	N-CA-C	5.16	116.43	109.11
1	B	166	ARG	N-CA-C	-5.15	105.74	111.36
1	E	715	LEU	N-CA-C	5.15	119.62	113.23
1	C	261	GLY	CA-C-N	5.14	125.38	119.83
1	C	261	GLY	C-N-CA	5.14	125.38	119.83
1	C	467	CYS	N-CA-C	5.13	118.57	112.72
1	H	362	ARG	N-CA-C	5.13	117.30	110.53
1	D	318	VAL	CB-CA-C	-5.11	105.77	111.80
1	A	162	LEU	N-CA-C	5.11	116.84	111.28
1	E	517	ASN	N-CA-C	-5.10	105.61	111.07
1	C	209	ILE	N-CA-C	-5.09	107.51	112.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	321	PRO	N-CA-C	5.08	122.94	112.47
1	G	619	LEU	N-CA-C	-5.08	105.92	111.82
1	A	558	GLN	N-CA-C	5.08	116.50	111.07
1	H	659	SER	CA-C-N	5.08	125.11	119.32
1	H	659	SER	C-N-CA	5.08	125.11	119.32
1	C	592	ASP	N-CA-C	-5.07	103.70	110.55
1	E	78	LYS	N-CA-C	5.07	118.30	112.57
1	E	652	SER	CA-C-N	5.06	124.78	119.82
1	E	652	SER	C-N-CA	5.06	124.78	119.82
1	A	321	PRO	N-CA-C	5.05	122.88	112.47
1	H	451	GLY	N-CA-C	5.05	122.29	115.32
1	G	312	HIS	CA-C-N	5.05	125.33	119.47
1	G	312	HIS	C-N-CA	5.05	125.33	119.47
1	G	531	VAL	CB-CA-C	-5.04	105.33	112.14
1	H	499	ASN	N-CA-C	-5.04	106.30	112.90
1	F	549	GLY	CA-C-N	5.01	126.10	119.84
1	F	549	GLY	C-N-CA	5.01	126.10	119.84
1	B	467	CYS	N-CA-C	5.00	119.36	113.16

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	211	175	C3,C2
1	B	211	175	C3,C2
1	C	211	175	C3,C2
1	D	211	175	C3,C2
1	E	211	175	C3,C2
1	F	211	175	C3,C2
1	G	211	175	C3,C2
1	H	211	175	C3,C2

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	211	175	Peptide,Mainchain
1	B	211	175	Peptide,Mainchain
1	C	211	175	Peptide,Mainchain
1	D	211	175	Peptide,Mainchain
1	E	211	175	Peptide,Mainchain
1	F	211	175	Peptide,Mainchain
1	G	211	175	Peptide,Mainchain
1	H	211	175	Peptide,Mainchain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4978	0	5037	204	0
1	B	5019	0	5077	211	0
1	C	4946	0	5014	264	0
1	D	4948	0	5017	164	0
1	E	4982	0	5045	197	0
1	F	4951	0	5017	209	0
1	G	4995	0	5057	209	0
1	H	4910	0	4970	196	0
2	A	84	0	0	4	0
2	B	79	0	0	3	0
2	C	72	0	0	5	0
2	D	101	0	0	4	0
2	E	64	0	0	5	0
2	F	83	0	0	2	0
2	G	96	0	0	8	0
2	H	72	0	0	4	0
All	All	40380	0	40234	1541	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1541) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:594:VAL:HG23	1:F:595:PRO:HD3	1.26	1.09
1:B:247:ARG:HH11	1:B:247:ARG:HB3	1.13	1.08
1:A:244:LEU:HD11	1:A:249:ALA:HB2	1.31	1.07
1:F:334:LYS:HD3	1:F:661:ARG:HH21	1.21	1.04
1:H:615:THR:HG23	1:H:617:LEU:H	1.24	1.02
1:F:591:TYR:HB2	1:F:596:ARG:HG2	1.40	1.00
1:F:319:THR:HG23	1:G:394:THR:HG23	1.43	1.00
1:D:594:VAL:HG23	1:D:595:PRO:HD3	1.38	1.00
1:E:615:THR:HG22	1:E:617:LEU:H	1.27	0.99
1:E:594:VAL:HG13	1:E:595:PRO:HD3	1.44	0.98
1:C:185:LEU:HD12	1:C:185:LEU:H	1.27	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:ASN:HD21	1:C:397:ASN:H	1.08	0.97
1:D:202:ILE:HD11	1:D:243:ILE:HD12	1.45	0.94
1:B:567:SER:HB2	1:B:569:LEU:HD23	1.49	0.94
1:E:29:ASN:HB3	1:E:32:VAL:HG12	1.50	0.93
1:A:261:GLY:H	1:A:264:GLU:HG3	1.33	0.93
1:A:594:VAL:HG12	1:A:595:PRO:HD3	1.52	0.92
1:C:300:THR:HG23	1:C:443:MSE:HE3	1.52	0.91
1:C:679:ARG:HB3	1:C:684:LEU:HD11	1.53	0.91
1:F:364:PRO:HB3	1:F:438:THR:HG23	1.51	0.90
1:A:615:THR:HG22	1:A:617:LEU:H	1.37	0.90
1:E:102:ARG:HH11	1:E:102:ARG:HB3	1.33	0.90
1:B:615:THR:HG23	1:B:617:LEU:H	1.36	0.90
1:F:580:THR:HG21	1:F:607:THR:HG21	1.51	0.89
1:C:588:THR:HG22	1:C:596:ARG:HG3	1.54	0.89
1:D:580:THR:HG21	1:D:607:THR:HG21	1.54	0.89
1:F:611:VAL:HG23	1:F:612:LEU:HD13	1.54	0.89
1:B:611:VAL:HG23	1:B:612:LEU:HD13	1.55	0.89
1:F:301:VAL:HG21	1:F:336:LEU:HD21	1.56	0.87
1:F:573:LEU:HD23	1:F:611:VAL:HG21	1.55	0.87
1:B:645:TRP:CD1	1:B:679:ARG:HE	1.92	0.87
1:C:69:LEU:HG	1:C:387:THR:HG22	1.55	0.87
1:C:169:MSE:HE3	1:C:221:ILE:HG23	1.55	0.86
1:H:142:VAL:C	1:H:143:LEU:HD12	2.01	0.86
1:C:615:THR:HG22	1:C:616:SER:H	1.40	0.85
1:F:69:LEU:HD13	1:F:387:THR:HG22	1.56	0.85
1:D:594:VAL:CG2	1:D:595:PRO:HD3	2.07	0.85
1:D:611:VAL:HG23	1:D:612:LEU:HD13	1.57	0.85
1:C:270:ASN:HD21	1:C:397:ASN:N	1.75	0.85
1:F:431:GLN:HE21	1:F:431:GLN:HA	1.42	0.85
1:H:178:ARG:HH22	1:H:393:SER:N	1.75	0.85
1:B:247:ARG:HB3	1:B:247:ARG:NH1	1.91	0.84
1:F:594:VAL:CG2	1:F:595:PRO:HD3	2.09	0.83
1:C:270:ASN:ND2	1:C:397:ASN:H	1.76	0.82
1:B:588:THR:HG22	1:B:596:ARG:HH11	1.41	0.82
1:H:496:GLU:HA	1:H:497:MSE:HE3	1.60	0.82
1:A:244:LEU:CD1	1:A:249:ALA:HB2	2.09	0.82
1:A:633:ALA:O	1:A:637:THR:HG22	1.80	0.81
1:F:522:LEU:HD22	1:H:142:VAL:HG11	1.62	0.81
1:D:305:VAL:HG23	1:D:538:ARG:HD3	1.61	0.81
1:C:528:LEU:HD11	1:C:669:VAL:HG21	1.63	0.81
1:F:615:THR:HG22	1:F:617:LEU:H	1.44	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:592:ASP:O	1:E:595:PRO:HD2	1.81	0.80
1:C:588:THR:CG2	1:C:596:ARG:HG3	2.11	0.80
1:G:101:LEU:HD21	1:G:263:LYS:HD3	1.62	0.80
1:B:33:ALA:HB2	2:B:764:HOH:O	1.81	0.80
1:A:270:ASN:OD1	1:A:396:ASP:HA	1.82	0.80
1:F:216:SER:HB3	1:F:217:PRO:HD3	1.62	0.79
1:B:250:MSE:HB3	1:B:255:LEU:HB2	1.64	0.79
1:B:471:ASP:OD2	1:C:496:GLU:HA	1.81	0.79
1:H:679:ARG:HD3	1:H:683:PHE:CD2	2.17	0.79
1:G:232:LYS:HE3	1:G:243:ILE:HG22	1.63	0.79
1:C:445:ASN:ND2	1:C:448:MSE:HE3	1.98	0.79
1:A:535:ILE:HD11	1:A:666:TYR:CD1	2.18	0.79
1:C:248:GLU:O	1:C:252:LEU:HD13	1.84	0.78
1:A:37:LEU:HD21	1:C:380:ILE:HG22	1.65	0.78
1:F:29:ASN:HB3	1:F:32:VAL:HG12	1.64	0.78
1:B:570:ARG:O	1:B:574:VAL:HG23	1.84	0.77
1:H:633:ALA:O	1:H:637:THR:HG23	1.84	0.77
1:E:593:LEU:HD11	1:E:637:THR:HG21	1.65	0.77
1:F:305:VAL:HG12	1:F:305:VAL:O	1.83	0.77
1:F:435:LEU:O	1:F:438:THR:HG22	1.85	0.77
1:A:612:LEU:O	1:A:615:THR:HB	1.84	0.77
1:C:615:THR:HG22	1:C:616:SER:N	1.99	0.77
1:C:30:LEU:O	1:C:42:VAL:HG21	1.83	0.77
1:E:492:VAL:CG2	1:H:434:LYS:HE2	2.15	0.77
1:E:567:SER:HB2	1:E:569:LEU:HD13	1.67	0.77
1:G:69:LEU:HD13	1:G:387:THR:HG22	1.66	0.77
1:A:248:GLU:O	1:A:252:LEU:HD13	1.84	0.76
1:B:184:ARG:HG3	1:B:184:ARG:HH11	1.49	0.76
1:E:470:LEU:HD22	1:E:526:THR:HG23	1.67	0.76
1:B:375:LEU:HD21	1:B:431:GLN:HB2	1.66	0.76
1:E:588:THR:HG23	1:E:596:ARG:HE	1.49	0.76
1:H:39:THR:HG22	1:H:41:GLN:H	1.49	0.76
1:A:39:THR:HG21	1:A:380:ILE:HD13	1.67	0.76
1:E:248:GLU:O	1:E:252:LEU:HD13	1.85	0.76
1:F:615:THR:HG22	1:F:616:SER:N	1.99	0.76
1:D:48:VAL:HG13	1:D:288:MSE:HE1	1.68	0.76
1:B:247:ARG:HG2	1:B:248:GLU:H	1.51	0.76
1:D:239:GLY:O	1:D:240:LYS:HB3	1.86	0.75
1:C:360:GLN:HG2	1:C:361:ASP:N	2.02	0.75
1:D:79:GLY:HA2	1:D:166:ARG:HH12	1.51	0.75
1:A:615:THR:HG21	1:A:617:LEU:HD12	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:362:ARG:NH2	1:F:448:MSE:HB2	2.01	0.75
1:A:561:GLY:H	1:A:564:MSE:HG3	1.51	0.75
1:G:611:VAL:HG23	1:G:612:LEU:HD13	1.69	0.74
1:B:633:ALA:O	1:B:637:THR:HG22	1.87	0.74
1:C:247:ARG:HA	1:C:250:MSE:HE3	1.69	0.74
1:E:90:ILE:HD13	1:E:93:LYS:HE2	1.69	0.74
1:C:131:GLN:HE21	1:C:131:GLN:HA	1.52	0.73
1:B:383:HIS:O	1:B:387:THR:HG23	1.88	0.73
1:G:45:VAL:HG23	2:G:803:HOH:O	1.88	0.73
1:A:570:ARG:HG3	1:A:570:ARG:HH11	1.51	0.73
1:D:581:LEU:O	1:D:585:LEU:HB2	1.88	0.73
1:F:470:LEU:HD22	1:F:526:THR:HG23	1.70	0.73
1:F:615:THR:CG2	1:F:616:SER:H	2.02	0.73
1:G:215:LEU:H	1:G:215:LEU:HD22	1.54	0.73
1:E:611:VAL:HG23	1:E:612:LEU:HD13	1.69	0.73
1:H:649:SER:HB3	1:H:671:GLU:OE2	1.88	0.73
1:D:520:LEU:HD22	1:D:524:LEU:HG	1.69	0.73
1:A:125:GLU:O	1:A:128:ILE:HG22	1.88	0.72
1:F:320:ARG:HG3	1:G:393:SER:HB3	1.69	0.72
1:H:138:GLN:HG3	1:H:216:SER:HA	1.70	0.72
1:C:588:THR:HG22	1:C:588:THR:O	1.90	0.72
1:A:128:ILE:O	1:A:128:ILE:HD13	1.89	0.72
1:D:594:VAL:HG12	1:D:634:ILE:HD13	1.70	0.72
1:C:55:PRO:O	1:C:80:ARG:HD2	1.89	0.72
1:C:272:THR:HG21	1:C:415:ALA:HB2	1.71	0.72
1:C:594:VAL:HG22	1:C:595:PRO:HD3	1.70	0.72
1:D:97:SER:HB2	1:D:400:ILE:HD11	1.71	0.72
1:A:176:LEU:HD22	1:A:183:VAL:HG11	1.71	0.72
1:A:535:ILE:HD11	1:A:666:TYR:CE1	2.24	0.72
1:C:713:LYS:NZ	1:C:713:LYS:HB3	2.04	0.72
1:F:319:THR:HG23	1:G:394:THR:CG2	2.19	0.72
1:F:143:LEU:HD13	1:F:204:PRO:HG3	1.72	0.71
1:G:176:LEU:HD13	1:G:183:VAL:HG21	1.72	0.71
1:B:593:LEU:HD11	1:B:637:THR:HG21	1.73	0.71
1:C:496:GLU:HG2	1:C:499:ASN:HD22	1.56	0.71
1:G:48:VAL:HG22	1:G:288:MSE:HE1	1.72	0.71
1:A:594:VAL:CG1	1:A:595:PRO:HD3	2.20	0.71
1:E:564:MSE:SE	1:E:573:LEU:HD12	2.41	0.71
1:H:214:ASP:O	1:H:217:PRO:HD2	1.90	0.71
1:B:39:THR:HG22	1:B:41:GLN:H	1.55	0.71
1:C:237:HIS:HB3	1:C:242:LYS:HD3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:52:LEU:HD12	1:H:712:LEU:HD22	1.73	0.71
1:A:615:THR:CG2	1:A:617:LEU:H	2.04	0.70
1:F:359:ARG:O	1:F:360:GLN:HB2	1.89	0.70
1:G:615:THR:HG22	1:G:617:LEU:H	1.55	0.70
1:H:143:LEU:HD11	1:H:204:PRO:HB3	1.73	0.70
1:D:240:LYS:HB2	1:D:240:LYS:NZ	2.07	0.70
1:E:615:THR:HG22	1:E:617:LEU:N	2.05	0.70
1:F:300:THR:HG23	1:F:443:MSE:HE3	1.72	0.70
1:F:496:GLU:HA	1:H:471:ASP:OD2	1.91	0.70
1:F:301:VAL:HG12	1:F:365:LEU:HD13	1.72	0.70
1:B:69:LEU:HD13	1:B:387:THR:HG22	1.73	0.70
1:E:615:THR:HG22	1:E:616:SER:N	2.06	0.70
1:H:169:MSE:HE3	1:H:221:ILE:HG23	1.73	0.70
1:A:244:LEU:HD11	1:A:249:ALA:CB	2.15	0.69
1:E:615:THR:CG2	1:E:616:SER:N	2.55	0.69
1:C:218:LEU:O	1:C:269:VAL:HG12	1.91	0.69
1:C:240:LYS:HB2	2:C:775:HOH:O	1.92	0.69
1:B:184:ARG:HG3	1:B:184:ARG:NH1	2.06	0.69
1:B:588:THR:HG22	1:B:596:ARG:HG3	1.75	0.69
1:C:91:ARG:HG3	1:C:185:LEU:HD21	1.73	0.69
1:F:572:GLU:O	1:F:572:GLU:HG2	1.92	0.69
1:G:520:LEU:HD22	1:G:524:LEU:HG	1.74	0.69
1:B:567:SER:CB	1:B:569:LEU:HD23	2.22	0.69
1:F:500:GLN:HG2	1:G:363:TYR:CE2	2.28	0.69
1:H:345:HIS:ND1	1:H:346:GLU:N	2.40	0.69
1:H:594:VAL:HB	1:H:595:PRO:HD3	1.75	0.69
1:D:594:VAL:HG23	1:D:595:PRO:CD	2.19	0.69
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.58	0.68
1:A:339:SER:HB2	1:A:659:SER:OG	1.92	0.68
1:G:250:MSE:HE1	1:G:257:PRO:HB3	1.73	0.68
1:E:241:GLU:O	1:E:242:LYS:HG3	1.94	0.68
1:G:184:ARG:NH1	1:G:184:ARG:HB2	2.08	0.68
1:B:362:ARG:HD2	1:D:499:ASN:HA	1.74	0.68
1:E:496:GLU:HA	1:G:471:ASP:OD2	1.94	0.68
1:F:143:LEU:HD11	1:F:204:PRO:HA	1.76	0.68
1:G:30:LEU:HD12	1:G:42:VAL:HB	1.75	0.68
1:G:178:ARG:HH22	1:G:393:SER:C	2.01	0.68
1:E:29:ASN:HB3	1:E:32:VAL:CG1	2.22	0.68
1:F:558:GLN:HG3	1:F:559:HIS:N	2.09	0.68
1:F:707:ILE:O	1:F:710:VAL:HG12	1.94	0.68
1:D:639:GLN:O	1:D:643:THR:HG23	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:345:HIS:HA	2:E:741:HOH:O	1.93	0.68
1:G:634:ILE:O	1:G:638:ARG:HG3	1.94	0.68
1:G:256:GLU:HG3	1:G:257:PRO:HD2	1.76	0.68
1:F:522:LEU:CD2	1:H:142:VAL:HG11	2.23	0.68
1:G:445:ASN:ND2	1:G:448:MSE:HE3	2.09	0.68
1:H:615:THR:CG2	1:H:617:LEU:H	2.05	0.68
1:G:237:HIS:HB3	1:G:242:LYS:HE3	1.75	0.67
1:A:593:LEU:H	1:A:595:PRO:HD2	1.60	0.67
1:F:239:GLY:O	1:F:240:LYS:HB2	1.95	0.67
1:G:645:TRP:CE2	1:G:679:ARG:HG3	2.28	0.67
1:F:615:THR:CG2	1:F:616:SER:N	2.57	0.67
1:G:362:ARG:HD2	1:G:442:GLU:OE1	1.93	0.67
1:A:339:SER:HB2	1:A:659:SER:HG	1.59	0.67
1:H:567:SER:OG	1:H:569:LEU:HG	1.95	0.67
1:G:48:VAL:O	1:G:52:LEU:HD23	1.94	0.67
1:B:247:ARG:HG2	1:B:248:GLU:N	2.08	0.67
1:C:359:ARG:HH11	1:C:360:GLN:HB2	1.58	0.67
1:C:470:LEU:HD22	1:C:526:THR:HG23	1.77	0.67
1:E:662:THR:HA	1:E:714:MSE:HE3	1.77	0.67
1:E:588:THR:CG2	1:E:596:ARG:HE	2.08	0.67
1:F:380:ILE:HG22	1:G:37:LEU:HD21	1.77	0.67
1:H:462:SER:C	1:H:463:LEU:HD12	2.20	0.67
1:F:615:THR:HG22	1:F:616:SER:H	1.57	0.66
1:C:48:VAL:HG13	1:C:288:MSE:HE1	1.78	0.66
1:H:596:ARG:HG3	1:H:596:ARG:HH11	1.59	0.66
1:A:368:SER:OG	1:A:369:PRO:HD3	1.95	0.66
1:C:82:VAL:HG21	1:C:195:LEU:HD13	1.77	0.66
1:D:314:PHE:O	1:D:319:THR:HG22	1.95	0.66
1:E:615:THR:CG2	1:E:616:SER:H	2.08	0.66
1:G:55:PRO:O	1:G:80:ARG:HD2	1.95	0.66
1:H:87:SER:N	1:H:91:ARG:HH12	1.93	0.66
1:F:605:ALA:O	1:F:608:VAL:HG12	1.94	0.66
1:A:40:THR:HG23	2:A:784:HOH:O	1.95	0.66
1:F:556:ILE:HD13	1:F:573:LEU:CD1	2.26	0.66
1:G:143:LEU:HD11	1:G:204:PRO:HA	1.77	0.66
1:G:247:ARG:HA	1:G:250:MSE:HE2	1.77	0.66
1:A:573:LEU:HD23	1:A:611:VAL:HG21	1.78	0.66
1:E:627:VAL:O	1:E:631:GLU:HG3	1.95	0.66
1:G:219:SER:HA	1:G:269:VAL:HG11	1.77	0.65
1:C:45:VAL:HG23	2:C:723:HOH:O	1.96	0.65
1:F:556:ILE:HG21	1:F:573:LEU:HD12	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:87:SER:H	1:H:91:ARG:HH12	1.44	0.65
1:A:399:LEU:HD13	1:C:319:THR:HG21	1.77	0.65
1:F:364:PRO:HB3	1:F:438:THR:CG2	2.25	0.65
1:F:573:LEU:HD23	1:F:611:VAL:CG2	2.27	0.65
1:B:470:LEU:HD21	1:C:140:CYS:HB2	1.79	0.65
1:G:178:ARG:HH22	1:G:393:SER:CA	2.09	0.65
1:G:362:ARG:HD2	1:G:442:GLU:CD	2.21	0.65
1:C:421:THR:HG22	2:C:732:HOH:O	1.95	0.65
1:D:470:LEU:HD22	1:D:526:THR:HG23	1.79	0.65
1:F:569:LEU:HD12	1:F:569:LEU:O	1.97	0.65
1:C:535:ILE:HD11	1:C:666:TYR:CD1	2.31	0.65
1:E:363:TYR:CE2	1:H:500:GLN:HG2	2.31	0.65
1:A:418:VAL:HG22	1:A:506:ALA:HB1	1.79	0.65
1:C:580:THR:OG1	1:C:607:THR:HG21	1.95	0.65
1:A:180:HIS:ND1	1:A:394:THR:HG21	2.12	0.65
1:C:269:VAL:HG23	1:C:269:VAL:O	1.94	0.64
1:F:298:ALA:O	1:F:301:VAL:HG22	1.96	0.64
1:G:518:ASP:OD1	1:G:703:LYS:HE3	1.97	0.64
1:B:194:PHE:HE1	1:B:250:MSE:HE3	1.62	0.64
1:B:450:ARG:HH11	1:B:450:ARG:HG2	1.61	0.64
1:F:161:PRO:HB2	1:F:164:VAL:HG23	1.79	0.64
1:H:375:LEU:HD23	1:H:432:ILE:HG13	1.79	0.64
1:G:383:HIS:O	1:G:387:THR:HG23	1.97	0.64
1:H:592:ASP:O	1:H:593:LEU:HB2	1.96	0.64
1:H:612:LEU:O	1:H:615:THR:HB	1.98	0.64
1:C:370:GLN:H	1:C:370:GLN:NE2	1.96	0.64
1:D:178:ARG:HH12	1:D:393:SER:N	1.96	0.64
1:F:305:VAL:HG23	1:F:538:ARG:HD3	1.80	0.64
1:G:172:ARG:HH21	1:G:176:LEU:HD21	1.62	0.64
1:B:588:THR:CG2	1:B:596:ARG:HG3	2.28	0.64
1:D:305:VAL:CG2	1:D:538:ARG:HD3	2.27	0.64
1:G:184:ARG:NH1	1:G:186:VAL:HG12	2.12	0.64
1:A:166:ARG:O	1:A:170:THR:HG23	1.98	0.64
1:E:412:ASN:HD21	1:H:319:THR:HG23	1.63	0.64
1:E:594:VAL:HG13	1:E:595:PRO:CD	2.23	0.64
1:A:661:ARG:HD3	1:A:714:MSE:O	1.98	0.64
1:C:60:LEU:HB3	1:C:82:VAL:HG12	1.79	0.64
1:H:126:ASP:OD2	1:H:126:ASP:N	2.31	0.64
1:H:426:ARG:NH2	1:H:488:VAL:HG23	2.12	0.64
1:A:36:HIS:O	1:A:37:LEU:HB2	1.98	0.63
1:C:547:GLN:HB2	1:C:636:LEU:HD11	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:SER:O	1:B:700:GLU:HG3	1.97	0.63
1:D:362:ARG:NE	1:D:448:MSE:HE2	2.14	0.63
1:F:415:ALA:HB1	1:F:418:VAL:HG13	1.80	0.63
1:A:43:THR:HB	1:A:327:GLU:OE1	1.98	0.63
1:D:263:LYS:HD2	1:D:263:LYS:O	1.98	0.63
1:H:679:ARG:HD3	1:H:683:PHE:CE2	2.32	0.63
1:D:69:LEU:HD13	1:D:387:THR:HG22	1.79	0.63
1:E:449:ASN:ND2	1:E:452:LEU:HB2	2.13	0.63
1:H:73:VAL:HG22	1:H:281:LEU:HD12	1.81	0.63
1:H:588:THR:O	1:H:588:THR:HG22	1.99	0.63
1:A:669:VAL:HG12	1:A:675:VAL:HG13	1.79	0.63
1:B:153:GLY:HA2	1:C:154:ARG:O	1.98	0.63
1:B:573:LEU:HD23	1:B:611:VAL:HG21	1.78	0.63
1:E:649:SER:HB2	1:E:671:GLU:OE2	1.98	0.63
1:B:444:LEU:HD23	1:B:471:ASP:HB2	1.81	0.63
1:C:520:LEU:HD22	1:C:524:LEU:HG	1.81	0.63
1:G:48:VAL:HG13	1:G:288:MSE:HE1	1.79	0.63
1:G:615:THR:HG22	1:G:616:SER:N	2.14	0.63
1:H:535:ILE:HD11	1:H:666:TYR:CE1	2.34	0.63
1:A:411:GLY:O	1:C:370:GLN:HG3	1.98	0.63
1:A:570:ARG:HG3	1:A:570:ARG:NH1	2.14	0.63
1:F:573:LEU:CD2	1:F:611:VAL:HG21	2.27	0.63
1:B:410:GLY:O	1:D:366:ARG:HD2	1.98	0.62
1:B:427:LEU:O	1:B:431:GLN:HG2	1.98	0.62
1:C:679:ARG:HG2	1:C:679:ARG:HH11	1.64	0.62
1:E:438:THR:O	1:E:442:GLU:HG3	1.99	0.62
1:E:459:GLU:HG3	1:E:683:PHE:CD1	2.34	0.62
1:F:288:MSE:HE2	1:F:708:ASN:HA	1.81	0.62
1:F:334:LYS:HD3	1:F:661:ARG:NH2	2.04	0.62
1:A:37:LEU:HD23	1:C:381:HIS:HA	1.80	0.62
1:A:471:ASP:OD2	1:D:496:GLU:HA	1.99	0.62
1:H:375:LEU:HD21	1:H:431:GLN:HB2	1.82	0.62
1:F:303:ALA:O	1:F:538:ARG:NH1	2.32	0.62
1:A:33:ALA:O	1:A:384:ALA:HA	1.98	0.62
1:C:126:ASP:N	1:C:129:SER:HG	1.97	0.62
1:C:184:ARG:HG3	1:C:264:GLU:OE1	1.99	0.62
1:C:303:ALA:HB3	1:C:443:MSE:HE2	1.80	0.62
1:F:362:ARG:HH22	1:F:448:MSE:HB2	1.62	0.62
1:C:369:PRO:HD2	1:C:370:GLN:NE2	2.15	0.62
1:C:615:THR:HG21	1:C:617:LEU:HG	1.82	0.62
1:E:633:ALA:O	1:E:637:THR:HG22	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:ASN:HD22	1:B:271:GLY:H	1.47	0.62
1:C:678:ARG:HD2	2:C:728:HOH:O	2.00	0.62
1:A:419:ALA:O	1:A:423:GLU:HG2	1.99	0.62
1:B:362:ARG:CZ	1:B:448:MSE:HE2	2.30	0.62
1:F:605:ALA:HA	1:F:608:VAL:HG12	1.80	0.62
1:E:449:ASN:HD22	1:E:452:LEU:HB2	1.65	0.62
1:B:576:LYS:O	1:B:580:THR:HG23	1.99	0.62
1:C:29:ASN:HB3	1:C:32:VAL:HG12	1.81	0.62
1:G:402:VAL:HG23	1:G:403:GLU:H	1.64	0.62
1:D:662:THR:HA	1:D:714:MSE:HE3	1.81	0.62
1:F:55:PRO:O	1:F:80:ARG:HD2	1.99	0.62
1:A:261:GLY:N	1:A:264:GLU:HG3	2.12	0.61
1:B:573:LEU:HD23	1:B:611:VAL:CG2	2.29	0.61
1:C:335:LEU:HD22	1:C:714:MSE:HE2	1.81	0.61
1:E:138:GLN:NE2	1:E:215:LEU:HD23	2.15	0.61
1:H:419:ALA:O	1:H:423:GLU:HG2	2.00	0.61
1:H:634:ILE:O	1:H:638:ARG:HG3	2.00	0.61
1:A:370:GLN:H	1:A:370:GLN:NE2	1.96	0.61
1:F:206:ARG:NH1	1:H:480:GLU:OE2	2.32	0.61
1:E:127:ALA:O	1:E:131:GLN:HG2	2.00	0.61
1:H:320:ARG:HD3	1:H:325:GLN:HE22	1.64	0.61
1:B:561:GLY:O	1:B:565:THR:HG23	2.00	0.61
1:D:202:ILE:CD1	1:D:243:ILE:HD12	2.25	0.61
1:D:716:ALA:HA	2:D:797:HOH:O	2.01	0.61
1:G:402:VAL:HG23	1:G:403:GLU:N	2.15	0.61
1:F:594:VAL:HG23	1:F:595:PRO:CD	2.18	0.61
1:A:520:LEU:HD22	1:A:524:LEU:HG	1.82	0.61
1:F:30:LEU:O	1:F:42:VAL:HG21	2.00	0.61
1:G:265:GLY:O	1:G:269:VAL:HG22	2.00	0.61
1:A:62:LEU:HD21	1:A:82:VAL:HG13	1.82	0.61
1:C:368:SER:HB3	1:C:369:PRO:HD3	1.82	0.61
1:E:82:VAL:HG21	1:E:195:LEU:HD13	1.82	0.61
1:G:459:GLU:OE1	1:G:679:ARG:NH1	2.34	0.61
1:G:535:ILE:HD11	1:G:666:TYR:CE1	2.36	0.61
1:A:448:MSE:HE2	2:B:773:HOH:O	2.01	0.61
1:C:305:VAL:HG12	1:C:305:VAL:O	2.01	0.61
1:C:634:ILE:HG13	1:C:635:SER:N	2.16	0.61
1:H:520:LEU:HD22	1:H:524:LEU:HG	1.83	0.61
1:A:588:THR:HG23	1:A:596:ARG:HE	1.65	0.60
1:B:183:VAL:HG23	1:B:264:GLU:HG3	1.82	0.60
1:D:203:VAL:HG23	1:D:204:PRO:HD2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:669:VAL:HG12	1:E:675:VAL:HG13	1.83	0.60
1:B:611:VAL:CG2	1:B:612:LEU:HD13	2.30	0.60
1:C:339:SER:HB2	1:C:659:SER:HB3	1.84	0.60
1:C:375:LEU:HD21	1:C:431:GLN:HB2	1.83	0.60
1:B:690:THR:HA	2:B:755:HOH:O	2.01	0.60
1:E:419:ALA:O	1:E:423:GLU:HG2	2.02	0.60
1:G:359:ARG:O	1:G:360:GLN:HB2	2.00	0.60
1:G:369:PRO:HD2	1:G:370:GLN:NE2	2.16	0.60
1:D:239:GLY:O	1:D:240:LYS:CB	2.49	0.60
1:F:435:LEU:O	1:F:439:GLN:HG3	2.00	0.60
1:G:237:HIS:HB3	1:G:242:LYS:CE	2.32	0.60
1:C:402:VAL:HG23	1:C:403:GLU:N	2.17	0.60
1:G:172:ARG:HG2	1:G:172:ARG:HH11	1.67	0.60
1:G:453:PRO:HD2	1:G:537:LEU:HD23	1.83	0.60
1:D:645:TRP:CE2	1:D:679:ARG:HG3	2.36	0.60
2:E:778:HOH:O	1:G:497:MSE:HG3	2.00	0.60
1:G:247:ARG:HG2	1:G:250:MSE:HE2	1.82	0.60
1:A:459:GLU:OE1	1:A:679:ARG:NH1	2.35	0.60
1:G:285:ASP:O	1:G:289:LEU:HD22	2.01	0.60
1:H:143:LEU:CD1	1:H:204:PRO:HB3	2.31	0.60
1:B:247:ARG:H	1:B:247:ARG:HD2	1.67	0.59
1:C:401:ASP:O	1:C:402:VAL:HG22	2.01	0.59
1:F:125:GLU:O	1:F:128:ILE:HG22	2.02	0.59
1:H:557:ASP:OD1	1:H:570:ARG:HD2	2.02	0.59
1:C:593:LEU:HD11	1:C:637:THR:HG21	1.83	0.59
1:D:463:LEU:HD13	1:D:682:VAL:HG11	1.84	0.59
1:C:418:VAL:CG2	1:C:506:ALA:HB1	2.31	0.59
1:A:678:ARG:HH21	1:D:136:GLU:HG3	1.67	0.59
1:B:216:SER:HB3	1:B:217:PRO:HD3	1.84	0.59
1:C:178:ARG:HH21	1:C:394:THR:CB	2.14	0.59
1:C:631:GLU:O	1:C:634:ILE:HG12	2.03	0.59
1:D:305:VAL:HG12	1:D:305:VAL:O	2.02	0.59
1:A:399:LEU:HD12	1:C:315:LEU:HD23	1.83	0.59
1:A:557:ASP:OD1	1:A:570:ARG:NH1	2.35	0.59
1:A:588:THR:CG2	1:A:596:ARG:HE	2.16	0.59
1:F:359:ARG:HG2	1:G:409:HIS:CB	2.32	0.59
1:F:535:ILE:HD11	1:F:666:TYR:HD1	1.67	0.59
1:H:679:ARG:HD2	1:H:684:LEU:HD21	1.83	0.59
1:A:175:SER:O	1:A:178:ARG:HD3	2.02	0.59
1:B:520:LEU:HD22	1:B:524:LEU:HG	1.84	0.59
1:C:178:ARG:HH21	1:C:394:THR:HB	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:LEU:CD2	1:D:386:LEU:HD12	2.32	0.59
1:C:290:SER:O	1:C:294:GLN:HG3	2.02	0.59
1:C:359:ARG:HD2	1:C:359:ARG:C	2.28	0.59
1:D:368:SER:HB3	1:D:369:PRO:HD3	1.82	0.59
1:G:580:THR:OG1	1:G:607:THR:HG21	2.03	0.59
1:H:531:VAL:O	1:H:535:ILE:HG23	2.03	0.59
1:H:548:PHE:O	1:H:552:ILE:HG13	2.03	0.59
1:D:194:PHE:HE1	1:D:250:MSE:HE3	1.68	0.59
1:D:588:THR:OG1	1:D:596:ARG:NH1	2.36	0.59
1:F:75:ALA:O	1:F:166:ARG:NH1	2.36	0.59
1:F:564:MSE:SE	1:F:570:ARG:HG2	2.53	0.59
1:A:375:LEU:HD21	1:A:431:GLN:HB2	1.85	0.59
1:B:176:LEU:HD22	1:B:183:VAL:HG11	1.84	0.59
1:C:266:LEU:O	1:C:270:ASN:HB2	2.03	0.59
1:C:615:THR:CG2	1:C:616:SER:H	2.12	0.59
1:F:577:VAL:O	1:F:581:LEU:HB2	2.03	0.59
1:B:389:GLU:OE1	1:D:320:ARG:NH1	2.35	0.59
1:B:567:SER:O	1:B:568:ASN:HB3	2.03	0.59
1:C:300:THR:HA	1:C:443:MSE:HE1	1.85	0.59
1:G:446:ALA:HA	1:G:449:ASN:ND2	2.18	0.59
1:C:126:ASP:CG	1:C:127:ALA:H	2.11	0.58
1:D:128:ILE:O	1:D:132:LYS:HG3	2.02	0.58
1:E:463:LEU:HB3	1:E:682:VAL:HG21	1.84	0.58
1:B:247:ARG:HH11	1:B:247:ARG:CB	2.04	0.58
1:G:669:VAL:HG12	1:G:675:VAL:HG13	1.84	0.58
1:F:289:LEU:HG	1:F:520:LEU:HD13	1.85	0.58
1:G:446:ALA:HA	1:G:449:ASN:HD21	1.68	0.58
1:B:481:LEU:HD21	1:B:519:VAL:HG23	1.83	0.58
1:D:178:ARG:HH12	1:D:393:SER:C	2.11	0.58
1:F:320:ARG:HG3	1:G:393:SER:CB	2.33	0.58
1:A:445:ASN:ND2	1:A:448:MSE:HE3	2.18	0.58
1:D:679:ARG:HH11	1:D:679:ARG:HG2	1.68	0.58
1:B:593:LEU:HD21	1:B:637:THR:HG23	1.84	0.58
1:A:183:VAL:HG13	1:A:188:LEU:HD11	1.85	0.58
1:B:305:VAL:CG2	1:B:538:ARG:HD3	2.34	0.58
1:E:459:GLU:HG3	1:E:683:PHE:CG	2.38	0.58
1:G:232:LYS:HE3	1:G:243:ILE:CG2	2.34	0.58
1:H:143:LEU:HD12	1:H:143:LEU:N	2.17	0.58
1:H:185:LEU:O	1:H:189:GLU:HG3	2.03	0.58
1:D:29:ASN:HB3	1:D:32:VAL:HG12	1.86	0.57
1:H:561:GLY:O	1:H:565:THR:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:548:PHE:CZ	1:B:633:ALA:HB2	2.39	0.57
1:B:682:VAL:HG12	1:B:682:VAL:O	2.04	0.57
1:E:581:LEU:O	1:E:585:LEU:HD22	2.04	0.57
1:H:608:VAL:HG13	1:H:612:LEU:HD22	1.86	0.57
1:A:283:LEU:HD22	1:A:386:LEU:HD12	1.86	0.57
1:C:372:LEU:O	1:C:376:VAL:HG23	2.03	0.57
1:E:615:THR:HG21	1:E:617:LEU:HD12	1.85	0.57
1:F:29:ASN:O	1:F:30:LEU:HB2	2.03	0.57
1:G:184:ARG:HB2	1:G:184:ARG:HH11	1.69	0.57
1:A:567:SER:HB2	1:A:569:LEU:HD22	1.87	0.57
1:C:185:LEU:H	1:C:185:LEU:CD1	2.05	0.57
1:F:471:ASP:OD2	1:H:497:MSE:HE2	2.04	0.57
1:F:645:TRP:CE2	1:F:679:ARG:HG3	2.40	0.57
1:H:404:ASN:O	1:H:406:THR:HG23	2.03	0.57
1:A:449:ASN:HB2	1:A:452:LEU:HD12	1.85	0.57
1:B:37:LEU:HD21	1:D:380:ILE:HG22	1.86	0.57
1:C:359:ARG:O	1:C:360:GLN:HB3	2.03	0.57
1:E:88:ASP:H	1:E:91:ARG:HD3	1.69	0.57
1:G:548:PHE:CE2	1:G:552:ILE:HD11	2.39	0.57
1:H:134:LEU:HD21	1:H:269:VAL:HG21	1.86	0.57
1:C:528:LEU:HD12	1:C:698:ILE:HD13	1.86	0.57
1:A:134:LEU:HD21	1:A:269:VAL:HG21	1.85	0.57
1:A:266:LEU:HD23	1:A:266:LEU:O	2.04	0.57
1:B:89:GLU:CD	1:B:89:GLU:H	2.12	0.57
1:C:176:LEU:HD13	1:C:183:VAL:HG11	1.87	0.57
1:F:601:PHE:CZ	1:F:629:ALA:HB1	2.39	0.57
1:B:438:THR:HA	1:B:441:THR:HG22	1.87	0.57
1:E:415:ALA:HB1	1:E:418:VAL:HG13	1.87	0.57
1:E:426:ARG:NH2	1:E:488:VAL:HG23	2.20	0.57
1:A:298:ALA:HB1	1:A:336:LEU:HD13	1.87	0.57
1:D:270:ASN:HD22	1:D:396:ASP:HA	1.69	0.57
1:E:679:ARG:HD2	1:E:683:PHE:CD2	2.39	0.57
1:H:588:THR:HG22	1:H:596:ARG:HH11	1.70	0.57
1:A:50:LYS:O	1:A:50:LYS:HD3	2.04	0.57
1:A:206:ARG:HH11	1:A:511:ARG:HH22	1.53	0.57
1:F:560:PHE:HB2	1:F:564:MSE:HE2	1.86	0.57
1:A:59:THR:HG21	1:A:83:ARG:HD3	1.87	0.56
1:A:319:THR:HG21	1:C:399:LEU:HD13	1.86	0.56
1:C:87:SER:OG	1:C:90:ILE:HG12	2.05	0.56
1:D:178:ARG:HH12	1:D:393:SER:CA	2.18	0.56
1:E:466:HIS:HE1	1:E:533:GLN:HG3	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:52:LEU:HD12	1:F:712:LEU:HD22	1.87	0.56
1:F:418:VAL:HG22	1:F:506:ALA:HB1	1.87	0.56
1:G:497:MSE:HB2	1:G:499:ASN:ND2	2.20	0.56
1:B:139:LEU:HD23	1:C:690:THR:HG21	1.86	0.56
1:B:160:LEU:HD12	1:B:205:LEU:HD12	1.86	0.56
1:B:459:GLU:HG3	1:B:683:PHE:CD1	2.40	0.56
1:D:101:LEU:HD21	1:D:263:LYS:CB	2.35	0.56
1:G:36:HIS:O	1:G:37:LEU:HB2	2.06	0.56
1:G:266:LEU:N	1:G:266:LEU:HD12	2.19	0.56
1:H:422:MSE:HA	1:H:422:MSE:HE2	1.87	0.56
1:A:69:LEU:HG	1:A:280:THR:HG23	1.86	0.56
1:A:206:ARG:NH1	1:A:511:ARG:NH2	2.53	0.56
1:D:585:LEU:HD21	1:D:597:TRP:CH2	2.41	0.56
1:E:169:MSE:HE3	1:E:221:ILE:HG23	1.87	0.56
1:E:630:ALA:O	1:E:634:ILE:HG12	2.05	0.56
1:F:29:ASN:C	1:F:31:ALA:H	2.13	0.56
1:F:143:LEU:CD1	1:F:204:PRO:HA	2.35	0.56
1:F:593:LEU:HD11	1:F:637:THR:HG21	1.87	0.56
1:G:48:VAL:CG2	1:G:288:MSE:HE1	2.35	0.56
1:G:615:THR:CG2	1:G:616:SER:N	2.69	0.56
1:H:548:PHE:CZ	1:H:633:ALA:HB2	2.40	0.56
1:H:556:ILE:HD13	1:H:573:LEU:CD1	2.36	0.56
1:E:383:HIS:O	1:E:387:THR:HG23	2.06	0.56
1:B:588:THR:HG22	1:B:596:ARG:NH1	2.17	0.56
1:G:662:THR:HA	1:G:714:MSE:HE3	1.87	0.56
1:B:339:SER:HB2	1:B:659:SER:HB3	1.87	0.56
1:B:707:ILE:O	1:B:710:VAL:HG13	2.05	0.56
1:E:532:LEU:HD23	1:E:535:ILE:HD11	1.86	0.56
1:F:588:THR:C	1:F:590:SER:H	2.14	0.56
1:C:39:THR:HG22	1:C:41:GLN:H	1.70	0.56
1:D:173:VAL:O	1:D:177:THR:HG23	2.05	0.56
1:F:605:ALA:C	1:F:608:VAL:HG12	2.31	0.56
1:G:405:LYS:HE3	2:G:766:HOH:O	2.06	0.56
1:H:535:ILE:HD11	1:H:666:TYR:CD1	2.41	0.56
1:A:615:THR:CG2	1:A:616:SER:N	2.69	0.56
1:B:101:LEU:HD22	1:B:400:ILE:HD11	1.86	0.56
1:D:238:GLU:HA	1:D:238:GLU:OE2	2.06	0.56
1:G:235:VAL:HG12	1:G:236:VAL:N	2.21	0.56
1:F:438:THR:O	1:F:442:GLU:HG3	2.06	0.56
1:F:445:ASN:HA	1:H:497:MSE:HG2	1.87	0.56
1:G:33:ALA:O	1:G:384:ALA:HA	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:217:PRO:HB2	1:H:274:VAL:HG21	1.88	0.56
1:A:28:THR:HG22	1:A:29:ASN:N	2.21	0.56
1:F:359:ARG:HG2	1:G:409:HIS:CG	2.41	0.56
1:H:237:HIS:CE1	1:H:252:LEU:HD21	2.41	0.56
1:B:588:THR:C	1:B:596:ARG:NH1	2.64	0.55
1:B:611:VAL:HG23	1:B:612:LEU:CD1	2.34	0.55
1:B:645:TRP:CD1	1:B:679:ARG:NE	2.71	0.55
1:C:607:THR:O	1:C:611:VAL:HG12	2.06	0.55
1:E:137:HIS:CE1	1:E:138:GLN:HE21	2.24	0.55
1:F:137:HIS:CE1	1:F:138:GLN:HE21	2.24	0.55
1:B:679:ARG:NH1	1:B:683:PHE:CE2	2.75	0.55
1:D:535:ILE:HD13	1:D:658:LEU:HD21	1.87	0.55
1:A:244:LEU:C	1:A:244:LEU:HD12	2.31	0.55
1:B:30:LEU:HA	1:B:33:ALA:O	2.05	0.55
1:B:152:LEU:HD11	1:C:147:PHE:CE2	2.42	0.55
1:B:540:ILE:HD11	1:B:644:PHE:CD2	2.41	0.55
1:C:242:LYS:HD2	1:C:242:LYS:N	2.21	0.55
1:A:169:MSE:HE3	1:A:221:ILE:HG23	1.89	0.55
1:A:362:ARG:HD2	1:A:442:GLU:CD	2.31	0.55
1:E:317:ASP:HA	1:E:326:ILE:HD11	1.88	0.55
1:F:319:THR:HG21	1:G:412:ASN:HD22	1.71	0.55
1:F:334:LYS:HG2	1:F:661:ARG:HE	1.72	0.55
1:B:270:ASN:ND2	1:B:271:GLY:H	2.03	0.55
1:C:359:ARG:NH1	1:C:360:GLN:HB2	2.19	0.55
1:E:156:LEU:O	1:E:159:SER:HB3	2.06	0.55
1:E:623:ASN:O	1:E:627:VAL:HG23	2.07	0.55
1:C:557:ASP:OD2	1:C:570:ARG:NH1	2.40	0.55
1:C:561:GLY:H	1:C:564:MSE:HG3	1.71	0.55
1:D:181:SER:O	1:D:182:ALA:HB3	2.05	0.55
1:E:247:ARG:HA	1:E:250:MSE:CE	2.36	0.55
1:B:296:LEU:HD23	1:B:524:LEU:HD22	1.89	0.55
1:C:167:GLY:O	1:C:171:ILE:HG13	2.07	0.55
1:C:422:MSE:HA	1:C:422:MSE:HE2	1.89	0.55
1:C:583:LYS:HE2	1:D:584:ARG:NH2	2.22	0.55
1:C:645:TRP:CE2	1:C:679:ARG:HG3	2.41	0.55
1:D:298:ALA:HB1	1:D:336:LEU:HD13	1.87	0.55
1:E:375:LEU:HD11	1:E:431:GLN:OE1	2.07	0.55
1:G:605:ALA:HA	1:G:608:VAL:HG13	1.89	0.55
1:H:265:GLY:O	1:H:269:VAL:HG22	2.07	0.55
1:H:368:SER:OG	1:H:369:PRO:HD3	2.07	0.55
1:C:94:ILE:O	1:C:98:VAL:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:531:VAL:O	1:G:535:ILE:HG23	2.06	0.55
1:B:545:LYS:HD2	1:B:545:LYS:O	2.06	0.55
1:A:32:VAL:HG12	1:A:50:LYS:HG3	1.89	0.54
1:B:615:THR:HG23	1:B:616:SER:N	2.21	0.54
1:D:258:VAL:HG12	1:D:259:VAL:N	2.22	0.54
1:D:362:ARG:CZ	1:D:448:MSE:HE2	2.37	0.54
1:E:594:VAL:CG1	1:E:595:PRO:HD3	2.29	0.54
1:C:270:ASN:HD22	1:C:396:ASP:HB3	1.72	0.54
1:A:91:ARG:O	1:A:95:ASP:OD1	2.25	0.54
1:B:670:ARG:HD3	1:B:675:VAL:O	2.07	0.54
1:C:237:HIS:CB	1:C:242:LYS:HD3	2.36	0.54
1:H:454:SER:OG	1:H:455:CYS:N	2.40	0.54
1:B:303:ALA:O	1:B:538:ARG:NH1	2.40	0.54
1:B:412:ASN:HB3	1:D:320:ARG:HD2	1.90	0.54
1:G:272:THR:HG21	1:G:415:ALA:HB2	1.88	0.54
1:H:184:ARG:HD3	1:H:264:GLU:OE1	2.06	0.54
1:A:143:LEU:CD1	1:A:204:PRO:HA	2.37	0.54
1:H:178:ARG:HH12	1:H:392:GLN:C	2.15	0.54
1:B:363:TYR:CE2	1:D:500:GLN:HG2	2.42	0.54
1:C:219:SER:HA	1:C:269:VAL:HG11	1.89	0.54
1:D:496:GLU:O	1:D:497:MSE:HB2	2.08	0.54
1:G:238:GLU:O	1:G:238:GLU:HG3	2.07	0.54
1:H:696:SER:O	1:H:700:GLU:HG3	2.08	0.54
1:B:250:MSE:HE2	1:B:255:LEU:HB3	1.89	0.54
1:B:608:VAL:HG13	1:B:612:LEU:HD22	1.89	0.54
1:D:135:LEU:O	1:D:139:LEU:HG	2.07	0.54
1:E:271:GLY:HA2	1:E:395:THR:O	2.07	0.54
1:E:401:ASP:CG	1:E:404:ASN:HD22	2.16	0.54
1:E:626:LYS:HD3	1:E:626:LYS:C	2.33	0.54
1:G:417:ALA:O	1:G:421:THR:HG23	2.08	0.54
1:B:270:ASN:OD1	1:B:397:ASN:N	2.39	0.54
1:C:497:MSE:HB2	1:C:499:ASN:ND2	2.22	0.54
1:H:131:GLN:HG3	1:H:265:GLY:HA3	1.89	0.54
1:G:184:ARG:NH1	1:G:186:VAL:CG1	2.71	0.54
1:G:184:ARG:HH11	1:G:184:ARG:CB	2.21	0.54
1:C:103:SER:O	1:C:104:GLN:C	2.51	0.54
1:C:271:GLY:HA2	1:C:395:THR:O	2.07	0.54
1:E:266:LEU:HD13	1:E:266:LEU:C	2.33	0.54
1:F:244:LEU:HD12	1:F:244:LEU:N	2.22	0.54
1:F:404:ASN:N	1:F:404:ASN:HD22	2.06	0.54
1:F:592:ASP:O	1:F:596:ARG:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:527:HIS:O	1:G:531:VAL:HG22	2.07	0.54
1:H:588:THR:HG22	1:H:596:ARG:HG3	1.90	0.54
1:A:608:VAL:HG21	1:A:622:VAL:HG13	1.90	0.53
1:C:181:SER:O	1:C:182:ALA:HB3	2.08	0.53
1:C:419:ALA:O	1:C:423:GLU:HG2	2.09	0.53
1:C:455:CYS:O	1:C:456:LEU:HB2	2.07	0.53
1:E:298:ALA:HB1	1:E:336:LEU:HD13	1.90	0.53
1:F:561:GLY:HA2	1:F:564:MSE:HE3	1.89	0.53
1:B:557:ASP:OD1	1:B:570:ARG:HD2	2.08	0.53
1:E:30:LEU:O	1:E:42:VAL:HG21	2.07	0.53
1:E:262:PRO:O	1:E:264:GLU:N	2.39	0.53
1:G:143:LEU:CD1	1:G:204:PRO:HA	2.38	0.53
1:G:151:ARG:HG2	1:G:151:ARG:HH11	1.73	0.53
1:A:35:SER:N	1:A:384:ALA:HB2	2.24	0.53
1:E:548:PHE:CE2	1:E:552:ILE:HD11	2.43	0.53
1:B:130:LEU:O	1:B:134:LEU:HD13	2.09	0.53
1:E:28:THR:O	1:E:29:ASN:HB2	2.07	0.53
1:H:345:HIS:CG	1:H:346:GLU:H	2.27	0.53
1:A:446:ALA:HA	1:A:449:ASN:HD21	1.73	0.53
1:B:394:THR:HB	1:D:319:THR:OG1	2.07	0.53
1:C:669:VAL:HG12	1:C:675:VAL:HG13	1.90	0.53
1:F:593:LEU:HD21	1:F:637:THR:CG2	2.38	0.53
1:H:383:HIS:O	1:H:387:THR:HG23	2.09	0.53
1:E:176:LEU:HD22	1:E:183:VAL:HG11	1.89	0.53
1:E:343:VAL:HG12	1:E:345:HIS:H	1.72	0.53
1:F:535:ILE:HD11	1:F:666:TYR:CD1	2.42	0.53
1:H:187:VAL:HG22	1:H:258:VAL:HG11	1.90	0.53
1:H:535:ILE:HG13	1:H:536:ASP:N	2.23	0.53
1:B:593:LEU:HD21	1:B:637:THR:CG2	2.38	0.53
1:C:639:GLN:HE21	1:C:643:THR:HG22	1.74	0.53
1:H:615:THR:HG23	1:H:616:SER:N	2.24	0.53
1:A:659:SER:O	1:A:663:GLN:HB2	2.08	0.53
1:G:172:ARG:HG2	1:G:172:ARG:NH1	2.22	0.53
1:H:85:LYS:HB3	1:H:90:ILE:CD1	2.39	0.53
1:B:411:GLY:HA2	1:B:413:PHE:CE2	2.43	0.53
1:C:567:SER:OG	1:C:569:LEU:HD22	2.09	0.53
1:D:406:THR:HG22	1:D:407:SER:N	2.24	0.53
1:H:124:THR:O	1:H:127:ALA:HB3	2.09	0.53
1:A:160:LEU:HD12	1:A:205:LEU:HD12	1.89	0.53
1:A:504:SER:O	1:A:505:LEU:HB2	2.07	0.53
1:C:237:HIS:HB3	1:C:242:LYS:NZ	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:262:PRO:C	1:E:264:GLU:H	2.17	0.53
1:F:633:ALA:O	1:F:637:THR:HG22	2.08	0.53
1:G:619:LEU:HD12	1:H:615:THR:HG22	1.90	0.53
1:H:360:GLN:O	1:H:361:ASP:HB2	2.09	0.53
1:H:588:THR:HG23	1:H:591:TYR:CG	2.44	0.53
1:A:546:LYS:HE2	1:A:657:TYR:OH	2.09	0.52
1:C:237:HIS:HB3	1:C:242:LYS:CD	2.38	0.52
1:C:637:THR:HG23	1:C:638:ARG:N	2.24	0.52
1:F:500:GLN:HG2	1:G:363:TYR:CZ	2.44	0.52
1:B:160:LEU:HB2	1:B:203:VAL:HG23	1.91	0.52
1:B:173:VAL:O	1:B:177:THR:HG23	2.10	0.52
1:H:496:GLU:CD	1:H:500:GLN:HE21	2.18	0.52
1:A:418:VAL:CG2	1:A:506:ALA:HB1	2.39	0.52
1:A:594:VAL:CG1	1:A:595:PRO:CD	2.88	0.52
1:C:300:THR:HG23	1:C:443:MSE:CE	2.34	0.52
1:E:228:HIS:HB3	1:E:231:SER:OG	2.09	0.52
1:B:456:LEU:HD21	1:B:534:ALA:HB2	1.90	0.52
1:B:588:THR:HG22	1:B:588:THR:O	2.09	0.52
1:D:429:LEU:HD22	1:D:520:LEU:HD12	1.91	0.52
1:D:562:SER:O	1:D:565:THR:HG22	2.09	0.52
1:G:462:SER:HB2	1:G:592:ASP:OD1	2.09	0.52
1:D:260:LEU:HD22	1:D:260:LEU:H	1.72	0.52
1:F:463:LEU:HD13	1:F:682:VAL:HG11	1.90	0.52
1:G:187:VAL:HG22	1:G:258:VAL:HG11	1.92	0.52
1:G:237:HIS:O	1:G:238:GLU:HG2	2.09	0.52
1:G:246:ALA:O	1:G:250:MSE:HG2	2.09	0.52
1:E:131:GLN:NE2	1:E:265:GLY:H	2.07	0.52
1:E:247:ARG:HA	1:E:250:MSE:HE3	1.90	0.52
1:F:319:THR:HG21	1:G:412:ASN:ND2	2.25	0.52
1:A:169:MSE:HE2	1:A:191:LEU:HD22	1.91	0.52
1:A:319:THR:HB	1:C:394:THR:HG23	1.90	0.52
1:B:594:VAL:HA	1:B:634:ILE:HD13	1.91	0.52
1:D:97:SER:OG	1:D:182:ALA:HA	2.09	0.52
1:F:535:ILE:HD12	1:F:658:LEU:HD21	1.92	0.52
1:G:190:ALA:HB2	1:G:258:VAL:HG21	1.90	0.52
1:G:219:SER:HA	1:G:269:VAL:CG1	2.39	0.52
1:H:314:PHE:O	1:H:319:THR:HG22	2.10	0.52
1:H:418:VAL:CG2	1:H:506:ALA:HB1	2.40	0.52
1:C:623:ASN:O	1:C:627:VAL:HG23	2.10	0.52
1:C:709:ASN:O	1:C:713:LYS:HG3	2.10	0.52
1:E:615:THR:HG23	1:E:616:SER:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:30:LEU:O	1:G:42:VAL:HG21	2.10	0.52
1:G:367:THR:HA	1:G:370:GLN:NE2	2.25	0.52
1:B:375:LEU:HD23	1:B:432:ILE:HG13	1.91	0.52
1:B:470:LEU:HD11	1:B:691:ILE:HG21	1.92	0.52
1:C:466:HIS:HE1	1:C:533:GLN:HG3	1.74	0.52
1:H:339:SER:HB2	1:H:659:SER:HB3	1.91	0.52
1:C:540:ILE:HD11	1:C:644:PHE:CG	2.45	0.52
1:D:406:THR:HG22	1:D:407:SER:H	1.75	0.52
1:D:528:LEU:O	1:D:531:VAL:HG12	2.10	0.52
1:D:101:LEU:HD21	1:D:263:LYS:HB2	1.92	0.51
1:F:103:SER:O	1:F:104:GLN:C	2.53	0.51
1:H:647:ALA:O	1:H:648:ALA:HB2	2.10	0.51
1:C:304:MSE:O	1:C:305:VAL:HB	2.09	0.51
1:E:394:THR:HB	1:H:319:THR:OG1	2.09	0.51
1:E:468:LYS:HE2	1:G:496:GLU:CD	2.35	0.51
1:H:459:GLU:OE1	1:H:679:ARG:NH1	2.42	0.51
1:A:399:LEU:HD11	1:A:412:ASN:HD22	1.75	0.51
1:G:269:VAL:HG23	1:G:269:VAL:O	2.10	0.51
1:H:128:ILE:O	1:H:132:LYS:HG3	2.09	0.51
1:A:263:LYS:O	1:A:264:GLU:C	2.53	0.51
1:B:363:TYR:CZ	1:D:500:GLN:HG2	2.45	0.51
1:B:637:THR:O	1:B:640:VAL:HG12	2.10	0.51
1:C:176:LEU:HD22	1:C:183:VAL:HG11	1.91	0.51
1:C:237:HIS:HB3	1:C:242:LYS:CE	2.41	0.51
1:C:588:THR:CG2	1:C:588:THR:O	2.58	0.51
1:C:634:ILE:O	1:C:637:THR:HG22	2.09	0.51
1:E:612:LEU:O	1:E:615:THR:HB	2.11	0.51
1:F:561:GLY:CA	1:F:564:MSE:HE3	2.41	0.51
1:G:48:VAL:HG22	1:G:288:MSE:CE	2.40	0.51
1:H:101:LEU:HD11	1:H:263:LYS:HB3	1.92	0.51
1:H:690:THR:HA	2:H:750:HOH:O	2.10	0.51
1:B:142:VAL:HG11	1:C:522:LEU:HD22	1.92	0.51
1:B:176:LEU:HD22	1:B:183:VAL:CG1	2.40	0.51
1:G:48:VAL:CG1	1:G:288:MSE:HE1	2.41	0.51
1:G:266:LEU:H	1:G:266:LEU:CD1	2.23	0.51
1:H:305:VAL:HG23	1:H:538:ARG:HD3	1.91	0.51
1:A:32:VAL:HG12	1:A:50:LYS:CD	2.39	0.51
1:B:575:GLU:O	1:B:579:LYS:HG3	2.10	0.51
1:C:104:GLN:CD	1:C:104:GLN:H	2.19	0.51
1:H:556:ILE:HG21	1:H:573:LEU:HD12	1.91	0.51
1:H:564:MSE:O	1:H:567:SER:HB3	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:VAL:O	1:A:535:ILE:HG23	2.11	0.51
1:B:64:GLY:O	1:B:178:ARG:NH1	2.32	0.51
1:C:178:ARG:HH21	1:C:394:THR:N	2.08	0.51
1:C:563:ALA:HB1	1:C:615:THR:CG2	2.40	0.51
1:D:52:LEU:HD12	1:D:712:LEU:HD22	1.93	0.51
1:D:266:LEU:O	1:D:270:ASN:HB2	2.10	0.51
1:E:389:GLU:CD	1:H:320:ARG:HH21	2.19	0.51
1:F:129:SER:HB3	1:H:463:LEU:HD23	1.93	0.51
1:F:162:LEU:HD13	2:F:749:HOH:O	2.09	0.51
1:G:203:VAL:HG23	1:G:204:PRO:HD2	1.91	0.51
1:A:206:ARG:HH11	1:A:511:ARG:NH2	2.08	0.51
1:B:297:THR:O	1:B:301:VAL:HG23	2.11	0.51
1:D:340:ARG:HG2	1:D:340:ARG:HH11	1.74	0.51
1:E:131:GLN:HE22	1:E:265:GLY:H	1.59	0.51
1:F:130:LEU:HD23	1:F:130:LEU:O	2.11	0.51
1:G:401:ASP:O	1:G:403:GLU:N	2.44	0.51
1:A:183:VAL:HA	1:A:264:GLU:OE1	2.11	0.51
1:C:178:ARG:NH2	1:C:394:THR:N	2.58	0.51
1:C:187:VAL:HG22	1:C:258:VAL:HG11	1.92	0.51
1:E:187:VAL:HG22	1:E:258:VAL:HG11	1.93	0.51
1:E:253:PHE:HB2	1:E:255:LEU:HD23	1.93	0.51
1:F:101:LEU:HD11	1:F:400:ILE:CD1	2.41	0.51
1:G:87:SER:OG	1:G:90:ILE:HG12	2.11	0.51
1:H:176:LEU:HD22	1:H:183:VAL:HG11	1.93	0.51
1:B:450:ARG:HH11	1:B:450:ARG:CG	2.23	0.51
1:B:561:GLY:HA2	1:B:564:MSE:HE3	1.93	0.51
1:E:69:LEU:HD22	1:E:387:THR:HG22	1.93	0.51
1:E:263:LYS:HZ3	1:E:266:LEU:HD12	1.76	0.51
1:G:250:MSE:HE3	1:G:257:PRO:HD3	1.92	0.51
1:G:321:PRO:O	1:G:323:PRO:HD3	2.11	0.51
1:A:38:PRO:HB3	1:A:323:PRO:HD2	1.93	0.50
1:E:164:VAL:HG21	1:E:278:MSE:HE3	1.94	0.50
1:H:547:GLN:O	1:H:550:PRO:HD2	2.11	0.50
1:C:623:ASN:OD1	1:D:610:GLU:HG2	2.11	0.50
1:F:444:LEU:HD23	1:F:456:LEU:HD13	1.94	0.50
1:F:556:ILE:HD12	1:F:574:VAL:HG12	1.93	0.50
1:G:271:GLY:HA2	1:G:395:THR:O	2.11	0.50
1:H:288:MSE:HE2	1:H:708:ASN:HA	1.93	0.50
1:H:387:THR:HG22	2:H:786:HOH:O	2.11	0.50
1:A:394:THR:HG23	1:C:319:THR:HB	1.92	0.50
1:A:669:VAL:CG1	1:A:675:VAL:HG13	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ASN:HB3	1:B:32:VAL:HG12	1.93	0.50
1:C:552:ILE:O	1:C:556:ILE:HG13	2.12	0.50
1:C:713:LYS:HB3	1:C:713:LYS:HZ2	1.75	0.50
1:H:295:SER:O	1:H:299:MSE:HG3	2.11	0.50
1:B:418:VAL:HG22	1:B:506:ALA:HB1	1.93	0.50
1:C:573:LEU:HD23	1:C:611:VAL:HG11	1.92	0.50
1:D:240:LYS:HB2	1:D:240:LYS:HZ3	1.76	0.50
1:D:283:LEU:HD23	1:D:386:LEU:HD12	1.94	0.50
1:E:471:ASP:OD2	1:G:496:GLU:HA	2.11	0.50
1:E:560:PHE:HB2	1:E:564:MSE:HE2	1.92	0.50
1:B:412:ASN:OD1	1:D:320:ARG:HD3	2.11	0.50
1:C:190:ALA:HB2	1:C:258:VAL:HG21	1.94	0.50
1:C:301:VAL:HG22	1:C:365:LEU:HD13	1.93	0.50
1:E:532:LEU:HD12	1:E:669:VAL:HG11	1.92	0.50
1:H:535:ILE:CD1	1:H:658:LEU:HD11	2.41	0.50
1:H:679:ARG:HD3	1:H:683:PHE:HD2	1.74	0.50
1:D:96:LYS:HD2	1:D:402:VAL:HG11	1.93	0.50
1:H:194:PHE:HE1	1:H:250:MSE:HE3	1.77	0.50
1:C:291:LEU:HD22	1:C:715:LEU:HD13	1.93	0.50
1:F:305:VAL:O	1:F:305:VAL:CG1	2.56	0.50
1:H:707:ILE:O	1:H:710:VAL:HG13	2.11	0.50
1:B:389:GLU:CD	1:D:320:ARG:HH12	2.20	0.50
1:C:176:LEU:HD22	1:C:183:VAL:CG1	2.42	0.50
1:D:32:VAL:HA	1:D:50:LYS:HE2	1.94	0.50
1:D:172:ARG:HE	1:D:172:ARG:HA	1.76	0.50
1:F:305:VAL:CG2	1:F:538:ARG:HD3	2.40	0.50
1:G:64:GLY:O	1:G:178:ARG:HD2	2.10	0.50
1:G:615:THR:HG22	1:G:617:LEU:N	2.26	0.50
1:H:87:SER:H	1:H:91:ARG:NH1	2.09	0.50
1:H:87:SER:O	1:H:91:ARG:HG2	2.11	0.50
1:H:592:ASP:O	1:H:593:LEU:CB	2.59	0.50
1:B:435:LEU:O	1:B:439:GLN:HG3	2.12	0.50
1:B:645:TRP:CD2	1:B:679:ARG:HD2	2.47	0.50
1:C:237:HIS:ND1	1:C:238:GLU:HG2	2.27	0.50
1:D:552:ILE:O	1:D:556:ILE:HG13	2.11	0.50
1:D:637:THR:O	1:D:640:VAL:HG12	2.12	0.50
1:E:527:HIS:O	1:E:531:VAL:CG2	2.60	0.50
1:F:383:HIS:O	1:F:387:THR:HG23	2.12	0.50
1:G:533:GLN:O	1:G:537:LEU:HD13	2.12	0.50
1:H:90:ILE:C	1:H:92:SER:H	2.20	0.50
1:A:206:ARG:NH1	1:A:511:ARG:HH22	2.09	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:ARG:HG2	1:A:450:ARG:HH11	1.77	0.49
1:F:215:LEU:HD22	1:F:215:LEU:H	1.77	0.49
1:F:216:SER:O	1:F:219:SER:HB3	2.12	0.49
1:G:142:VAL:O	1:G:143:LEU:HD13	2.12	0.49
1:A:35:SER:H	1:A:384:ALA:HB2	1.77	0.49
1:A:470:LEU:HD22	1:A:526:THR:HG23	1.93	0.49
1:B:288:MSE:HE2	1:B:708:ASN:CB	2.42	0.49
1:E:412:ASN:ND2	1:H:319:THR:HG23	2.25	0.49
1:F:679:ARG:NH1	1:F:683:PHE:CE2	2.80	0.49
1:H:305:VAL:HG12	1:H:305:VAL:O	2.12	0.49
1:B:83:ARG:HH21	1:B:86:ASP:HB2	1.76	0.49
1:C:64:GLY:C	1:C:65:TYR:CD1	2.90	0.49
1:C:169:MSE:HE2	1:C:191:LEU:CD2	2.42	0.49
1:D:283:LEU:HD22	1:D:386:LEU:HD12	1.93	0.49
1:E:427:LEU:O	1:E:431:GLN:HG3	2.11	0.49
1:F:359:ARG:HG2	1:G:409:HIS:HB2	1.93	0.49
1:F:545:LYS:O	1:F:545:LYS:HE2	2.13	0.49
1:H:184:ARG:HB3	1:H:186:VAL:HG12	1.95	0.49
1:A:39:THR:O	1:A:40:THR:HB	2.12	0.49
1:A:362:ARG:HD2	1:A:442:GLU:OE1	2.12	0.49
1:A:466:HIS:HE1	1:A:533:GLN:HG3	1.77	0.49
1:D:50:LYS:HD2	1:D:50:LYS:C	2.37	0.49
1:E:462:SER:HB2	1:E:592:ASP:OD2	2.12	0.49
1:E:572:GLU:HG2	1:E:576:LYS:HD2	1.94	0.49
1:F:573:LEU:C	1:F:573:LEU:HD13	2.37	0.49
1:G:51:MSE:HE1	1:G:288:MSE:HE3	1.93	0.49
1:C:594:VAL:HG22	1:C:595:PRO:CD	2.41	0.49
1:E:43:THR:HB	1:E:327:GLU:OE1	2.13	0.49
1:E:463:LEU:CD2	1:G:130:LEU:HG	2.43	0.49
1:F:300:THR:CG2	1:F:365:LEU:HD21	2.42	0.49
1:G:184:ARG:HH12	1:G:186:VAL:CG1	2.26	0.49
1:B:580:THR:HG21	1:B:607:THR:OG1	2.12	0.49
1:B:615:THR:HG21	1:B:617:LEU:HD12	1.95	0.49
1:F:183:VAL:HA	1:F:264:GLU:HG2	1.95	0.49
1:G:180:HIS:ND1	1:G:394:THR:HG21	2.28	0.49
1:A:615:THR:HG21	1:A:617:LEU:CD1	2.39	0.49
1:B:217:PRO:HB2	1:B:274:VAL:HG21	1.95	0.49
1:C:244:LEU:HD12	1:C:248:GLU:HG2	1.95	0.49
1:D:596:ARG:HH11	1:D:596:ARG:CG	2.25	0.49
1:E:87:SER:O	1:E:88:ASP:HB2	2.12	0.49
1:E:500:GLN:HG2	1:H:363:TYR:CE2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:89:GLU:CD	1:F:89:GLU:H	2.21	0.49
1:G:31:ALA:O	1:G:47:ILE:HA	2.13	0.49
1:G:266:LEU:HD12	1:G:266:LEU:H	1.78	0.49
1:G:570:ARG:HG3	1:G:570:ARG:HH11	1.77	0.49
1:A:235:VAL:HG22	1:A:236:VAL:N	2.28	0.49
1:A:375:LEU:HD23	1:A:432:ILE:HG13	1.93	0.49
1:F:359:ARG:C	1:F:359:ARG:HD2	2.38	0.49
1:G:143:LEU:HD11	1:G:204:PRO:CA	2.42	0.49
1:H:427:LEU:O	1:H:431:GLN:HG2	2.13	0.49
1:A:402:VAL:HG23	1:A:403:GLU:N	2.26	0.49
1:C:615:THR:CG2	1:C:617:LEU:HG	2.42	0.49
1:E:264:GLU:O	1:E:268:LEU:HB2	2.12	0.49
1:F:52:LEU:HD12	1:F:712:LEU:CD2	2.43	0.49
1:F:272:THR:HG21	1:F:415:ALA:HB2	1.94	0.49
1:A:30:LEU:HD13	1:A:41:GLN:HG3	1.95	0.49
1:D:125:GLU:O	1:D:128:ILE:HG22	2.13	0.49
1:D:202:ILE:HD11	1:D:243:ILE:CD1	2.31	0.49
1:E:134:LEU:HD21	1:E:269:VAL:HG21	1.95	0.49
1:G:69:LEU:HG	1:G:280:THR:HG23	1.95	0.49
1:H:101:LEU:O	1:H:102:ARG:C	2.56	0.49
1:H:169:MSE:HE2	1:H:191:LEU:HD22	1.95	0.49
1:B:37:LEU:HD22	1:D:384:ALA:HB2	1.94	0.48
1:B:411:GLY:O	1:D:370:GLN:HG3	2.13	0.48
1:B:470:LEU:CD2	1:C:140:CYS:HB2	2.43	0.48
1:E:449:ASN:N	1:E:449:ASN:OD1	2.46	0.48
1:F:520:LEU:HD22	1:F:524:LEU:HG	1.95	0.48
1:G:535:ILE:HD12	1:G:535:ILE:C	2.38	0.48
1:B:299:MSE:HE2	1:B:535:ILE:CD1	2.43	0.48
1:B:406:THR:HG22	1:B:407:SER:N	2.28	0.48
1:E:69:LEU:HD22	1:E:387:THR:CG2	2.44	0.48
1:G:305:VAL:O	1:G:305:VAL:HG12	2.12	0.48
1:C:143:LEU:CD1	1:C:204:PRO:HA	2.43	0.48
1:E:193:ASN:HB3	1:E:255:LEU:HD11	1.96	0.48
1:E:362:ARG:NE	1:E:448:MSE:HE2	2.28	0.48
1:E:684:LEU:HD12	1:E:688:GLU:OE2	2.12	0.48
1:F:42:VAL:HG13	1:F:42:VAL:O	2.12	0.48
1:F:480:GLU:OE1	1:H:206:ARG:HD3	2.12	0.48
1:G:496:GLU:HG2	1:G:499:ASN:HD22	1.78	0.48
1:A:170:THR:HG22	1:A:195:LEU:CD1	2.43	0.48
1:C:169:MSE:HE2	1:C:191:LEU:HD23	1.96	0.48
1:C:713:LYS:HB3	1:C:713:LYS:HZ3	1.75	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:227:GLY:HA2	1:H:246:ALA:O	2.14	0.48
1:A:176:LEU:HD13	1:A:183:VAL:HG11	1.94	0.48
1:A:401:ASP:HB3	1:A:406:THR:HG23	1.94	0.48
1:B:601:PHE:O	1:B:626:LYS:HG3	2.13	0.48
1:C:50:LYS:O	1:C:50:LYS:HD3	2.14	0.48
1:C:359:ARG:HD2	1:C:360:GLN:N	2.29	0.48
1:C:630:ALA:O	1:C:634:ILE:HG23	2.12	0.48
1:D:611:VAL:HG23	1:D:612:LEU:CD1	2.38	0.48
1:F:166:ARG:NH2	1:F:195:LEU:O	2.46	0.48
1:F:532:LEU:HD21	1:F:669:VAL:HB	1.96	0.48
1:G:670:ARG:HG2	1:G:670:ARG:HH11	1.78	0.48
1:H:602:SER:HA	1:H:626:LYS:HD2	1.94	0.48
1:A:415:ALA:HB1	1:A:418:VAL:HG13	1.94	0.48
1:C:237:HIS:CE1	1:C:238:GLU:HG2	2.49	0.48
1:F:359:ARG:HD2	1:F:360:GLN:N	2.28	0.48
1:A:398:PRO:HG3	1:A:409:HIS:CE1	2.49	0.48
1:B:99:GLU:O	1:B:102:ARG:HB3	2.13	0.48
1:F:313:PRO:HG3	1:F:333:ARG:CZ	2.44	0.48
1:A:417:ALA:O	1:A:421:THR:HG23	2.14	0.48
1:B:545:LYS:HD2	1:B:545:LYS:C	2.38	0.48
1:D:299:MSE:HE2	1:D:535:ILE:CD1	2.43	0.48
1:E:492:VAL:HG23	1:H:434:LYS:HE2	1.94	0.48
1:F:564:MSE:O	1:F:565:THR:C	2.57	0.48
1:A:263:LYS:O	1:A:263:LYS:HD3	2.14	0.48
1:B:218:LEU:HD12	1:B:269:VAL:O	2.12	0.48
1:C:375:LEU:HD23	1:C:432:ILE:HG13	1.96	0.48
1:G:367:THR:HA	1:G:370:GLN:HE21	1.79	0.48
1:G:367:THR:C	1:G:370:GLN:HE21	2.22	0.48
1:H:188:LEU:O	1:H:192:THR:HG23	2.14	0.48
1:A:319:THR:HB	1:C:394:THR:CG2	2.44	0.47
1:B:270:ASN:ND2	1:B:271:GLY:N	2.62	0.47
1:A:37:LEU:HD22	1:C:384:ALA:HB2	1.95	0.47
1:A:360:GLN:N	2:A:800:HOH:O	2.48	0.47
1:B:138:GLN:HG3	1:B:216:SER:HA	1.96	0.47
1:C:563:ALA:HB1	1:C:615:THR:HG23	1.95	0.47
1:D:29:ASN:O	1:D:30:LEU:HB2	2.14	0.47
1:E:202:ILE:HA	2:E:747:HOH:O	2.14	0.47
1:E:588:THR:HG23	1:E:596:ARG:NE	2.24	0.47
1:G:375:LEU:HD23	1:G:432:ILE:HG13	1.97	0.47
1:A:218:LEU:HD13	1:A:274:VAL:HG23	1.96	0.47
1:A:573:LEU:CD2	1:A:611:VAL:HG21	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:588:THR:HG23	1:A:588:THR:O	2.14	0.47
1:B:372:LEU:O	1:B:376:VAL:HG23	2.14	0.47
1:C:94:ILE:HG21	1:C:185:LEU:HG	1.96	0.47
1:C:402:VAL:CG2	1:C:403:GLU:N	2.78	0.47
1:E:615:THR:HG21	1:E:617:LEU:CD1	2.44	0.47
1:G:363:TYR:HB2	1:G:364:PRO:HD3	1.97	0.47
1:A:370:GLN:HG3	1:C:411:GLY:O	2.14	0.47
1:C:581:LEU:C	1:C:585:LEU:HD23	2.39	0.47
1:E:188:LEU:O	1:E:192:THR:HG23	2.15	0.47
1:E:370:GLN:HE21	1:H:411:GLY:C	2.23	0.47
1:C:50:LYS:HD3	1:C:50:LYS:C	2.39	0.47
1:C:250:MSE:HE1	1:C:257:PRO:HB3	1.95	0.47
1:F:69:LEU:HG	1:F:280:THR:HG23	1.96	0.47
1:F:143:LEU:HD11	1:F:204:PRO:CA	2.43	0.47
1:F:593:LEU:HD21	1:F:637:THR:HG23	1.96	0.47
1:G:89:GLU:HG2	1:G:93:LYS:HE3	1.96	0.47
1:G:340:ARG:HB2	1:G:657:TYR:HA	1.97	0.47
1:A:147:PHE:O	1:A:147:PHE:CD1	2.68	0.47
1:B:645:TRP:NE1	1:B:679:ARG:HE	2.12	0.47
1:C:713:LYS:NZ	1:C:713:LYS:CB	2.76	0.47
1:D:101:LEU:HD21	1:D:263:LYS:HB3	1.95	0.47
1:E:135:LEU:O	1:E:139:LEU:HD22	2.15	0.47
1:E:317:ASP:HA	1:E:326:ILE:CD1	2.44	0.47
1:E:362:ARG:HD2	1:E:442:GLU:OE1	2.15	0.47
1:F:300:THR:HG23	1:F:443:MSE:CE	2.44	0.47
1:F:431:GLN:HA	1:F:431:GLN:NE2	2.20	0.47
1:G:564:MSE:HE3	1:G:570:ARG:HD3	1.97	0.47
1:G:631:GLU:HA	1:G:634:ILE:HG12	1.96	0.47
1:A:50:LYS:HD3	1:A:50:LYS:C	2.40	0.47
1:A:62:LEU:HD21	1:A:82:VAL:CG1	2.44	0.47
1:A:650:THR:O	1:A:650:THR:HG22	2.13	0.47
1:B:154:ARG:O	1:C:153:GLY:HA2	2.14	0.47
1:C:494:PRO:CG	1:D:494:PRO:HG3	2.44	0.47
1:C:535:ILE:HD11	1:C:666:TYR:HD1	1.79	0.47
1:C:670:ARG:HD3	1:C:676:LYS:HA	1.95	0.47
1:E:28:THR:O	1:E:29:ASN:CB	2.62	0.47
1:E:596:ARG:O	1:E:599:ASP:HB3	2.14	0.47
1:E:680:GLY:O	1:E:684:LEU:HG	2.14	0.47
1:F:381:HIS:HA	1:G:37:LEU:HD23	1.97	0.47
1:F:605:ALA:CA	1:F:608:VAL:HG12	2.42	0.47
1:G:50:LYS:C	1:G:50:LYS:HD3	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:69:LEU:CD1	1:G:387:THR:HA	2.44	0.47
1:G:543:GLU:OE1	1:G:543:GLU:HA	2.14	0.47
1:A:188:LEU:HD12	1:A:188:LEU:N	2.30	0.47
1:A:605:ALA:O	1:A:609:VAL:HG23	2.14	0.47
1:H:535:ILE:HD13	1:H:658:LEU:HD21	1.96	0.47
1:B:544:PHE:CE2	1:B:637:THR:HB	2.50	0.47
1:C:143:LEU:HD11	1:C:204:PRO:HA	1.96	0.47
1:C:370:GLN:H	1:C:370:GLN:CD	2.23	0.47
1:C:382:ALA:HA	2:C:732:HOH:O	2.15	0.47
1:C:561:GLY:HA2	1:C:564:MSE:HB2	1.96	0.47
1:D:401:ASP:OD1	1:D:403:GLU:HG3	2.14	0.47
1:F:172:ARG:NH1	1:F:268:LEU:O	2.48	0.47
1:F:605:ALA:HA	1:F:608:VAL:CG1	2.43	0.47
1:G:134:LEU:HD12	1:G:137:HIS:CE1	2.50	0.47
1:B:253:PHE:O	1:B:254:ASN:HB2	2.14	0.47
1:C:252:LEU:N	1:C:252:LEU:HD12	2.30	0.47
1:C:395:THR:HA	1:C:412:ASN:HB3	1.97	0.47
1:D:143:LEU:HB3	1:D:144:PRO:HD2	1.96	0.47
1:E:659:SER:O	1:E:663:GLN:HB2	2.13	0.47
1:F:135:LEU:O	1:F:139:LEU:HG	2.15	0.47
1:A:693:SER:HA	2:A:742:HOH:O	2.14	0.46
1:B:60:LEU:HD22	1:B:62:LEU:CD1	2.45	0.46
1:B:445:ASN:HA	1:C:497:MSE:HG2	1.97	0.46
1:C:219:SER:HA	1:C:269:VAL:CG1	2.45	0.46
1:C:401:ASP:O	1:C:403:GLU:N	2.47	0.46
1:C:497:MSE:HB2	1:C:499:ASN:HD21	1.79	0.46
1:D:320:ARG:HH11	1:D:320:ARG:HG3	1.80	0.46
1:D:459:GLU:HG3	1:D:683:PHE:CG	2.50	0.46
1:G:104:GLN:HG2	2:G:799:HOH:O	2.14	0.46
1:G:445:ASN:CG	1:G:448:MSE:HE3	2.39	0.46
1:H:266:LEU:O	1:H:266:LEU:HG	2.13	0.46
1:B:61:GLU:HA	1:B:83:ARG:O	2.15	0.46
1:B:103:SER:O	1:B:104:GLN:HB2	2.14	0.46
1:C:163:GLU:OE2	1:C:281:LEU:HD23	2.15	0.46
1:D:30:LEU:HB3	1:D:42:VAL:HB	1.98	0.46
1:D:375:LEU:HD23	1:D:432:ILE:HG13	1.97	0.46
1:E:38:PRO:HB2	1:E:323:PRO:HG2	1.97	0.46
1:E:102:ARG:HB3	1:E:102:ARG:NH1	2.15	0.46
1:A:32:VAL:HG12	1:A:50:LYS:HD2	1.98	0.46
1:B:228:HIS:ND1	1:B:229:PRO:HD2	2.30	0.46
1:B:594:VAL:HA	1:B:634:ILE:CD1	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:GLY:O	1:C:269:VAL:HG22	2.16	0.46
1:E:415:ALA:HB1	1:E:418:VAL:CG1	2.46	0.46
1:E:532:LEU:HA	1:E:535:ILE:HD11	1.96	0.46
1:F:560:PHE:CE1	1:F:608:VAL:HG21	2.50	0.46
1:G:218:LEU:HD13	1:G:274:VAL:HG23	1.96	0.46
1:G:535:ILE:CD1	1:G:654:ALA:HB1	2.45	0.46
1:H:504:SER:O	1:H:505:LEU:HB2	2.16	0.46
1:C:420:ASN:O	1:C:424:LYS:HG2	2.16	0.46
1:E:676:LYS:HB3	2:E:755:HOH:O	2.15	0.46
1:F:239:GLY:O	1:F:240:LYS:CB	2.60	0.46
1:G:648:ALA:O	1:G:649:SER:C	2.58	0.46
1:H:453:PRO:O	1:H:454:SER:C	2.59	0.46
1:A:101:LEU:HD11	1:A:263:LYS:HG3	1.98	0.46
1:A:178:ARG:HG2	1:A:178:ARG:HH11	1.80	0.46
1:A:608:VAL:O	1:A:612:LEU:HB2	2.16	0.46
1:C:69:LEU:HD12	1:C:383:HIS:NE2	2.31	0.46
1:C:203:VAL:HG23	1:C:204:PRO:HD2	1.97	0.46
1:D:368:SER:CB	1:D:369:PRO:HD3	2.45	0.46
1:D:396:ASP:C	1:D:399:LEU:HD21	2.41	0.46
1:D:588:THR:C	1:D:590:SER:H	2.24	0.46
1:D:668:PHE:CD1	1:D:710:VAL:HG21	2.51	0.46
1:F:102:ARG:HD3	1:F:102:ARG:C	2.40	0.46
1:G:497:MSE:HB2	1:G:499:ASN:HD21	1.78	0.46
1:G:608:VAL:HA	1:G:611:VAL:HG22	1.97	0.46
1:B:38:PRO:HB3	1:B:323:PRO:HG2	1.98	0.46
1:C:362:ARG:HD2	1:C:442:GLU:OE1	2.16	0.46
1:C:418:VAL:HG23	1:C:506:ALA:HB1	1.96	0.46
1:D:203:VAL:HG23	1:D:204:PRO:CD	2.44	0.46
1:D:626:LYS:HD3	1:D:626:LYS:C	2.41	0.46
1:E:169:MSE:HE3	1:E:221:ILE:CG2	2.45	0.46
1:E:627:VAL:HG12	1:E:631:GLU:OE2	2.16	0.46
1:E:645:TRP:CE2	1:E:679:ARG:HG3	2.50	0.46
1:B:42:VAL:O	1:B:42:VAL:HG13	2.16	0.46
1:B:634:ILE:O	1:B:638:ARG:HG3	2.16	0.46
1:C:504:SER:O	1:C:505:LEU:HB2	2.16	0.46
1:C:581:LEU:O	1:C:585:LEU:HD23	2.14	0.46
1:C:631:GLU:HA	1:C:634:ILE:HG12	1.98	0.46
1:D:340:ARG:HG2	1:D:340:ARG:NH1	2.31	0.46
1:D:662:THR:HA	1:D:714:MSE:CE	2.45	0.46
1:E:593:LEU:HG	1:E:634:ILE:HG22	1.97	0.46
1:E:681:ASP:OD1	1:G:136:GLU:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:561:GLY:C	1:F:563:ALA:H	2.23	0.46
1:G:215:LEU:H	1:G:215:LEU:CD2	2.27	0.46
1:H:648:ALA:O	1:H:649:SER:C	2.59	0.46
1:A:101:LEU:CD1	1:A:263:LYS:HG3	2.45	0.46
1:A:240:LYS:HG3	1:A:242:LYS:HE3	1.98	0.46
1:A:311:PHE:CD1	1:A:311:PHE:N	2.83	0.46
1:A:631:GLU:O	1:A:634:ILE:HG12	2.15	0.46
1:C:453:PRO:HG2	1:C:537:LEU:HD23	1.96	0.46
1:D:55:PRO:O	1:D:80:ARG:HD2	2.16	0.46
1:E:369:PRO:HD2	1:E:370:GLN:OE1	2.16	0.46
1:H:580:THR:HG21	1:H:607:THR:OG1	2.16	0.46
1:H:594:VAL:HA	1:H:634:ILE:CD1	2.46	0.46
1:A:59:THR:HG21	1:A:83:ARG:CD	2.46	0.46
1:A:283:LEU:CD2	1:A:386:LEU:HD12	2.45	0.46
1:A:631:GLU:HA	1:A:634:ILE:CD1	2.46	0.46
1:C:29:ASN:O	1:C:32:VAL:HG12	2.16	0.46
1:C:452:LEU:HG	1:C:538:ARG:NH2	2.31	0.46
1:C:631:GLU:C	1:C:634:ILE:HG12	2.40	0.46
1:E:639:GLN:O	1:E:643:THR:HG23	2.16	0.46
1:F:83:ARG:HH22	1:F:86:ASP:HB2	1.81	0.46
1:F:557:ASP:OD2	1:F:570:ARG:NH1	2.49	0.46
1:G:597:TRP:CD1	1:G:634:ILE:HG22	2.51	0.46
1:A:176:LEU:HD22	1:A:183:VAL:CG1	2.42	0.45
1:A:315:LEU:HD13	1:C:410:GLY:HA3	1.98	0.45
1:B:28:THR:HG23	1:B:28:THR:O	2.16	0.45
1:B:181:SER:O	1:B:182:ALA:HB3	2.15	0.45
1:B:496:GLU:HA	1:C:471:ASP:OD2	2.16	0.45
1:B:678:ARG:HD2	1:B:691:ILE:CD1	2.46	0.45
1:C:375:LEU:HD21	1:C:431:GLN:CB	2.46	0.45
1:E:87:SER:OG	1:E:90:ILE:HG12	2.16	0.45
1:E:319:THR:HG21	1:H:399:LEU:HD13	1.98	0.45
1:A:161:PRO:HG2	1:A:164:VAL:CG2	2.46	0.45
1:A:340:ARG:HB2	1:A:657:TYR:HA	1.98	0.45
1:B:152:LEU:HD11	1:C:147:PHE:HE2	1.80	0.45
1:C:178:ARG:NH1	1:C:178:ARG:HG2	2.32	0.45
1:E:137:HIS:HE1	1:E:138:GLN:HE21	1.63	0.45
1:E:634:ILE:HA	1:E:637:THR:CG2	2.46	0.45
1:F:336:LEU:HD12	1:F:336:LEU:HA	1.78	0.45
1:A:43:THR:HB	1:A:327:GLU:CD	2.41	0.45
1:B:522:LEU:HD23	1:B:699:TYR:CD1	2.51	0.45
1:C:173:VAL:O	1:C:177:THR:HG23	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:SER:O	1:C:178:ARG:HD3	2.16	0.45
1:D:127:ALA:O	1:D:131:GLN:NE2	2.50	0.45
1:D:295:SER:O	1:D:299:MSE:HG3	2.16	0.45
1:D:303:ALA:O	1:D:538:ARG:NH1	2.39	0.45
1:E:527:HIS:O	1:E:531:VAL:HG23	2.17	0.45
1:G:29:ASN:C	1:G:31:ALA:H	2.23	0.45
1:H:544:PHE:CE2	1:H:637:THR:HG22	2.51	0.45
1:A:86:ASP:OD1	1:A:91:ARG:NH2	2.46	0.45
1:A:367:THR:HG22	1:C:411:GLY:HA3	1.99	0.45
1:A:369:PRO:HD2	1:A:370:GLN:NE2	2.31	0.45
1:A:446:ALA:HA	1:A:449:ASN:ND2	2.31	0.45
1:B:603:PHE:HD2	1:B:603:PHE:O	1.99	0.45
1:C:592:ASP:O	1:C:595:PRO:HD2	2.17	0.45
1:E:69:LEU:HG	1:E:280:THR:HG23	1.98	0.45
1:E:611:VAL:HG23	1:E:612:LEU:CD1	2.40	0.45
1:G:266:LEU:N	1:G:266:LEU:CD1	2.79	0.45
1:H:568:ASN:CG	1:H:568:ASN:O	2.58	0.45
1:A:83:ARG:HG3	1:A:83:ARG:NH1	2.28	0.45
1:D:271:GLY:HA2	1:D:395:THR:O	2.17	0.45
1:D:497:MSE:HE3	1:D:497:MSE:H	1.82	0.45
1:D:649:SER:HB3	1:D:671:GLU:OE2	2.17	0.45
1:E:292:LEU:HB2	1:E:711:LEU:HD11	1.99	0.45
1:F:427:LEU:O	1:F:431:GLN:HG2	2.16	0.45
1:G:359:ARG:O	1:G:360:GLN:CB	2.64	0.45
1:G:375:LEU:H	1:G:375:LEU:CD1	2.29	0.45
1:H:89:GLU:H	1:H:89:GLU:CD	2.25	0.45
1:H:146:SER:OG	1:H:147:PHE:N	2.49	0.45
1:H:360:GLN:HG2	1:H:361:ASP:H	1.81	0.45
1:B:83:ARG:HH11	1:B:83:ARG:HG3	1.82	0.45
1:B:218:LEU:HD23	1:B:221:ILE:HD12	1.98	0.45
1:B:270:ASN:HD22	1:B:271:GLY:N	2.14	0.45
1:B:561:GLY:HA2	1:B:564:MSE:HB2	1.97	0.45
1:C:583:LYS:HE2	1:D:584:ARG:HH22	1.80	0.45
1:F:311:PHE:HA	1:F:316:HIS:HE2	1.81	0.45
1:H:143:LEU:HD23	1:H:202:ILE:HG22	1.98	0.45
1:A:560:PHE:HD2	1:A:617:LEU:CD1	2.29	0.45
1:C:28:THR:HG22	1:C:28:THR:O	2.17	0.45
1:F:434:LYS:NZ	1:H:493:GLN:OE1	2.46	0.45
1:G:208:THR:HA	2:G:743:HOH:O	2.16	0.45
1:B:341:PHE:CE1	1:B:538:ARG:HG2	2.52	0.45
1:E:531:VAL:O	1:E:535:ILE:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:362:ARG:NE	1:H:448:MSE:HE2	2.32	0.45
1:E:169:MSE:HE2	1:E:191:LEU:HD22	1.98	0.45
1:E:363:TYR:CZ	1:H:500:GLN:HG2	2.52	0.45
1:F:608:VAL:HG11	1:F:622:VAL:HG13	1.98	0.45
1:G:344:HIS:O	1:G:345:HIS:HB3	2.17	0.45
1:H:125:GLU:O	1:H:128:ILE:HG22	2.17	0.45
1:H:178:ARG:HH22	1:H:392:GLN:C	2.23	0.45
1:A:480:GLU:OE1	1:D:206:ARG:HD3	2.17	0.45
1:B:426:ARG:NH2	1:B:488:VAL:HG23	2.32	0.45
1:C:131:GLN:OE1	1:C:263:LYS:N	2.50	0.45
1:C:134:LEU:HD12	1:C:137:HIS:HE1	1.82	0.45
1:D:596:ARG:HH11	1:D:596:ARG:HG2	1.80	0.45
1:F:130:LEU:HD23	1:F:130:LEU:C	2.42	0.45
1:F:130:LEU:HD23	1:F:134:LEU:HD13	1.99	0.45
1:F:637:THR:O	1:F:641:ARG:HG3	2.17	0.45
1:C:63:ASP:OD1	1:C:66:SER:HB2	2.16	0.44
1:C:178:ARG:HG2	1:C:178:ARG:HH11	1.83	0.44
1:E:143:LEU:CD1	1:E:204:PRO:HA	2.47	0.44
1:H:561:GLY:HA2	1:H:564:MSE:HE3	1.99	0.44
1:C:218:LEU:HD13	1:C:274:VAL:CG2	2.47	0.44
1:C:258:VAL:HG12	1:C:259:VAL:N	2.32	0.44
1:C:411:GLY:HA2	1:C:413:PHE:CE2	2.52	0.44
1:C:633:ALA:O	1:C:637:THR:HG22	2.16	0.44
1:E:146:SER:OG	1:E:147:PHE:N	2.42	0.44
1:F:621:ALA:O	1:F:624:ALA:N	2.51	0.44
1:H:630:ALA:O	1:H:634:ILE:HG13	2.17	0.44
1:A:153:GLY:HA2	1:D:154:ARG:O	2.17	0.44
1:B:92:SER:O	1:B:96:LYS:HG3	2.17	0.44
1:B:588:THR:CG2	1:B:588:THR:O	2.65	0.44
1:H:588:THR:O	1:H:588:THR:CG2	2.65	0.44
1:A:55:PRO:O	1:A:80:ARG:HD2	2.16	0.44
1:A:181:SER:O	1:A:182:ALA:HB3	2.18	0.44
1:B:630:ALA:O	1:B:634:ILE:HG13	2.16	0.44
1:D:178:ARG:NH1	1:D:393:SER:C	2.75	0.44
1:E:305:VAL:HG12	1:E:305:VAL:O	2.18	0.44
1:G:29:ASN:HD22	1:G:31:ALA:HB3	1.82	0.44
1:H:92:SER:O	1:H:96:LYS:HG2	2.16	0.44
1:H:157:GLU:CD	1:H:157:GLU:H	2.25	0.44
1:A:29:ASN:C	1:A:31:ALA:H	2.26	0.44
1:A:218:LEU:HD12	1:A:218:LEU:HA	1.86	0.44
1:B:78:LYS:O	1:B:80:ARG:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ARG:HB3	1:B:364:PRO:HD2	1.99	0.44
1:F:165:VAL:HG23	1:F:221:ILE:HD11	2.00	0.44
1:F:454:SER:OG	1:F:455:CYS:N	2.51	0.44
1:F:576:LYS:O	1:F:580:THR:HG23	2.18	0.44
1:G:570:ARG:HH11	1:G:570:ARG:CG	2.30	0.44
1:B:610:GLU:O	1:B:613:SER:HB2	2.18	0.44
1:D:496:GLU:O	1:D:498:ALA:N	2.49	0.44
1:E:206:ARG:HD3	1:G:480:GLU:OE1	2.18	0.44
1:H:103:SER:O	1:H:104:GLN:HB2	2.18	0.44
1:A:169:MSE:HE2	1:A:191:LEU:CD2	2.48	0.44
1:A:228:HIS:HB3	1:A:231:SER:HB2	2.00	0.44
1:B:305:VAL:O	1:B:305:VAL:HG12	2.18	0.44
1:F:216:SER:HB3	1:F:217:PRO:CD	2.39	0.44
1:H:389:GLU:HG2	1:H:418:VAL:HG12	1.99	0.44
1:H:664:ILE:HD13	1:H:713:LYS:HE2	1.99	0.44
1:H:679:ARG:NH1	1:H:683:PHE:CE2	2.85	0.44
1:A:370:GLN:H	1:A:370:GLN:HE21	1.65	0.44
1:A:497:MSE:SE	2:A:739:HOH:O	2.86	0.44
1:B:36:HIS:O	1:B:37:LEU:O	2.36	0.44
1:C:69:LEU:O	1:C:73:VAL:HG23	2.18	0.44
1:F:588:THR:C	1:F:590:SER:N	2.75	0.44
1:G:250:MSE:CE	1:G:257:PRO:HD3	2.48	0.44
1:G:668:PHE:CD1	1:G:710:VAL:HG21	2.52	0.44
1:H:176:LEU:HD13	1:H:183:VAL:HG11	1.99	0.44
1:H:418:VAL:HG22	1:H:506:ALA:HB1	1.99	0.44
1:A:607:THR:O	1:A:611:VAL:HG22	2.17	0.44
1:B:228:HIS:CG	1:B:229:PRO:HD2	2.52	0.44
1:C:247:ARG:HH21	1:C:257:PRO:HG3	1.83	0.44
1:D:440:LEU:HD12	1:D:443:MSE:HE2	1.99	0.44
1:E:68:ASN:HB2	2:E:725:HOH:O	2.18	0.44
1:E:497:MSE:HG3	2:G:720:HOH:O	2.17	0.44
1:G:289:LEU:HD12	1:G:524:LEU:HD12	2.00	0.44
1:H:216:SER:HB3	1:H:217:PRO:HD3	1.99	0.44
1:H:328:VAL:HG11	1:H:369:PRO:HA	2.00	0.44
1:A:208:THR:CG2	1:A:507:LEU:HD23	2.48	0.43
1:A:418:VAL:HG22	1:A:506:ALA:CB	2.46	0.43
1:B:305:VAL:HG23	1:B:538:ARG:HD3	2.00	0.43
1:C:679:ARG:HH11	1:C:679:ARG:CG	2.31	0.43
1:E:69:LEU:HD23	1:E:383:HIS:CE1	2.53	0.43
1:E:487:PRO:HD3	1:H:487:PRO:HD3	2.00	0.43
1:F:77:ARG:HG2	1:F:163:GLU:OE1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:VAL:HG23	1:A:612:LEU:HD13	2.01	0.43
1:B:368:SER:OG	1:B:369:PRO:HD3	2.18	0.43
1:C:168:ALA:O	1:C:172:ARG:HB2	2.18	0.43
1:C:246:ALA:O	1:C:250:MSE:HG3	2.18	0.43
1:C:375:LEU:N	1:C:375:LEU:HD12	2.33	0.43
1:C:588:THR:HG21	1:C:596:ARG:HG3	1.95	0.43
1:E:634:ILE:HA	1:E:637:THR:HG22	1.99	0.43
1:F:367:THR:HG22	1:G:411:GLY:HA3	1.99	0.43
1:F:588:THR:OG1	1:F:596:ARG:HD3	2.19	0.43
1:H:69:LEU:HG	1:H:280:THR:HG23	2.00	0.43
1:H:581:LEU:O	1:H:585:LEU:HD22	2.18	0.43
1:A:311:PHE:CE2	1:A:332:ILE:HG21	2.53	0.43
1:B:230:ASP:O	1:B:230:ASP:OD2	2.35	0.43
1:B:259:VAL:O	1:B:259:VAL:HG23	2.18	0.43
1:B:450:ARG:CG	1:B:450:ARG:NH1	2.80	0.43
1:C:564:MSE:CE	1:C:570:ARG:HG3	2.48	0.43
1:D:157:GLU:H	1:D:157:GLU:CD	2.26	0.43
1:D:460:ASP:HA	1:D:461:PRO:HD3	1.81	0.43
1:D:562:SER:O	1:D:565:THR:CG2	2.67	0.43
1:E:520:LEU:HD22	1:E:524:LEU:HG	2.00	0.43
1:H:64:GLY:C	1:H:65:TYR:CD1	2.96	0.43
1:A:460:ASP:HA	1:A:461:PRO:HD3	1.86	0.43
1:E:93:LYS:HE3	1:E:177:THR:O	2.19	0.43
1:E:561:GLY:H	1:E:564:MSE:HE2	1.81	0.43
1:F:471:ASP:CG	1:H:497:MSE:HE2	2.44	0.43
1:F:671:GLU:OE1	1:F:671:GLU:HA	2.18	0.43
1:G:65:TYR:CZ	1:G:178:ARG:HG2	2.54	0.43
1:G:561:GLY:O	1:G:565:THR:HG23	2.17	0.43
1:H:258:VAL:CG1	1:H:259:VAL:N	2.82	0.43
1:A:209:ILE:CD1	1:D:472:ILE:HG23	2.49	0.43
1:A:496:GLU:HA	1:D:471:ASP:OD2	2.18	0.43
1:B:38:PRO:CB	1:B:323:PRO:HG2	2.49	0.43
1:B:83:ARG:HG3	1:B:83:ARG:NH1	2.33	0.43
1:B:142:VAL:CG1	1:C:522:LEU:HD22	2.48	0.43
1:B:156:LEU:O	1:B:159:SER:HB3	2.19	0.43
1:C:369:PRO:HD2	1:C:370:GLN:HE22	1.81	0.43
1:C:543:GLU:HA	1:C:543:GLU:OE1	2.17	0.43
1:C:631:GLU:O	1:C:634:ILE:CG1	2.65	0.43
1:C:683:PHE:HD2	1:C:684:LEU:HD12	1.82	0.43
1:E:55:PRO:O	1:E:80:ARG:HD2	2.18	0.43
1:E:543:GLU:OE1	1:E:543:GLU:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:THR:CG2	1:B:41:GLN:H	2.27	0.43
1:B:143:LEU:CD1	1:B:204:PRO:HA	2.48	0.43
1:B:465:TYR:O	1:B:466:HIS:C	2.62	0.43
1:D:146:SER:OG	1:D:147:PHE:N	2.51	0.43
1:D:465:TYR:O	1:D:466:HIS:C	2.62	0.43
1:F:135:LEU:HD12	1:F:223:ALA:HB2	2.01	0.43
1:F:557:ASP:CG	1:F:570:ARG:HH11	2.24	0.43
1:A:48:VAL:HG13	1:A:288:MSE:HE1	2.01	0.43
1:A:240:LYS:CG	1:A:242:LYS:HE3	2.48	0.43
1:A:413:PHE:CD1	1:A:413:PHE:C	2.97	0.43
1:C:547:GLN:CB	1:C:636:LEU:HD11	2.46	0.43
1:C:593:LEU:HD21	1:C:637:THR:CG2	2.48	0.43
1:D:187:VAL:HG22	1:D:258:VAL:HG11	2.00	0.43
1:E:444:LEU:HD23	1:E:456:LEU:HD13	2.00	0.43
1:G:339:SER:HB2	1:G:659:SER:HB3	2.00	0.43
1:G:528:LEU:O	1:G:531:VAL:HG23	2.19	0.43
1:H:323:PRO:O	1:H:326:ILE:HB	2.19	0.43
1:H:362:ARG:HG3	1:H:362:ARG:HH11	1.82	0.43
1:C:531:VAL:HG23	1:C:532:LEU:N	2.34	0.43
1:D:169:MSE:HE3	1:D:191:LEU:HD23	2.01	0.43
1:D:424:LYS:HB2	1:D:424:LYS:NZ	2.34	0.43
1:E:208:THR:CG2	1:E:507:LEU:HD23	2.49	0.43
1:E:492:VAL:HG21	1:H:434:LYS:HE2	2.00	0.43
1:F:443:MSE:HE1	1:F:531:VAL:HG23	2.00	0.43
1:G:38:PRO:HB3	1:G:323:PRO:HG2	2.00	0.43
1:A:393:SER:HB3	1:C:320:ARG:HG3	2.00	0.43
1:B:334:LYS:HD3	1:B:661:ARG:NH2	2.34	0.43
1:B:370:GLN:H	1:B:370:GLN:CD	2.27	0.43
1:C:428:GLY:O	1:C:432:ILE:HG13	2.18	0.43
1:D:400:ILE:O	1:D:400:ILE:HG13	2.18	0.43
1:E:169:MSE:O	1:E:173:VAL:HG23	2.19	0.43
1:E:344:HIS:O	1:E:345:HIS:C	2.61	0.43
1:E:543:GLU:OE2	1:E:653:PRO:HB3	2.18	0.43
1:F:548:PHE:O	1:F:549:GLY:C	2.61	0.43
1:F:623:ASN:O	1:F:627:VAL:HG23	2.19	0.43
1:A:36:HIS:O	1:A:37:LEU:CB	2.64	0.43
1:A:360:GLN:O	1:A:361:ASP:HB2	2.18	0.43
1:B:55:PRO:O	1:B:80:ARG:HD2	2.17	0.43
1:B:567:SER:O	1:B:568:ASN:CB	2.67	0.43
1:E:263:LYS:NZ	1:E:266:LEU:HD12	2.34	0.43
1:E:493:GLN:OE1	1:G:434:LYS:NZ	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:411:GLY:O	1:G:370:GLN:HG3	2.18	0.43
1:F:611:VAL:HG23	1:F:612:LEU:N	2.34	0.43
1:G:218:LEU:C	1:G:269:VAL:HG12	2.43	0.43
1:G:465:TYR:O	1:G:466:HIS:C	2.62	0.43
1:H:237:HIS:CG	1:H:252:LEU:HD21	2.54	0.43
1:H:463:LEU:HD23	1:H:682:VAL:HG11	1.99	0.43
1:A:214:ASP:O	1:A:218:LEU:HB2	2.19	0.42
1:B:69:LEU:HD11	1:B:387:THR:HA	2.01	0.42
1:B:189:GLU:HA	1:B:192:THR:OG1	2.18	0.42
1:B:211:175:H41	1:B:215:LEU:HD21	2.01	0.42
1:B:450:ARG:CZ	1:B:450:ARG:HB3	2.49	0.42
1:C:634:ILE:O	1:C:637:THR:CG2	2.67	0.42
1:D:272:THR:HG21	1:D:415:ALA:HB2	2.00	0.42
1:D:459:GLU:OE1	1:D:679:ARG:NH1	2.44	0.42
1:D:564:MSE:CE	1:D:570:ARG:HG3	2.49	0.42
1:E:198:GLY:O	1:E:235:VAL:HG23	2.18	0.42
1:E:320:ARG:HG3	1:H:393:SER:HB3	2.01	0.42
1:E:489:THR:O	1:E:492:VAL:HG13	2.18	0.42
1:F:236:VAL:HG23	1:F:236:VAL:O	2.19	0.42
1:F:300:THR:HA	1:F:443:MSE:HE1	2.01	0.42
1:F:363:TYR:CE2	1:G:500:GLN:HG2	2.54	0.42
1:G:312:HIS:HA	1:G:313:PRO:HD3	1.91	0.42
1:G:402:VAL:HG22	2:G:757:HOH:O	2.19	0.42
1:G:615:THR:CG2	1:G:616:SER:H	2.31	0.42
1:H:317:ASP:OD2	1:H:326:ILE:HG23	2.19	0.42
1:A:211:175:O6	1:A:215:LEU:HD13	2.19	0.42
1:A:497:MSE:HG3	1:D:445:ASN:HA	2.00	0.42
1:C:208:THR:CG2	1:C:507:LEU:HD23	2.49	0.42
1:C:544:PHE:CE2	1:C:637:THR:HB	2.53	0.42
1:E:178:ARG:HG2	1:E:178:ARG:HH11	1.84	0.42
1:F:237:HIS:O	1:F:238:GLU:C	2.62	0.42
1:G:178:ARG:HH22	1:G:393:SER:HA	1.81	0.42
1:G:679:ARG:HG2	1:G:679:ARG:HH11	1.83	0.42
1:B:375:LEU:HD12	2:D:816:HOH:O	2.20	0.42
1:C:87:SER:O	1:C:88:ASP:HB2	2.20	0.42
1:C:208:THR:HG21	1:C:507:LEU:HD23	2.02	0.42
1:C:548:PHE:O	1:C:552:ILE:HG13	2.18	0.42
1:D:580:THR:HG21	1:D:607:THR:CG2	2.39	0.42
1:E:652:SER:HA	1:E:653:PRO:HD3	1.86	0.42
1:G:36:HIS:O	1:G:37:LEU:CB	2.67	0.42
1:G:147:PHE:O	1:G:147:PHE:CD1	2.73	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:178:ARG:HH22	1:G:394:THR:N	2.17	0.42
1:B:38:PRO:HB3	1:B:323:PRO:HD2	2.00	0.42
1:B:298:ALA:HB1	1:B:336:LEU:HD13	2.01	0.42
1:B:642:GLU:HG3	1:F:252:LEU:O	2.20	0.42
1:F:601:PHE:CE1	1:F:629:ALA:HB1	2.55	0.42
1:G:649:SER:HB3	1:G:671:GLU:OE2	2.19	0.42
1:A:32:VAL:CG1	1:A:50:LYS:HG3	2.49	0.42
1:C:101:LEU:O	1:C:102:ARG:C	2.61	0.42
1:D:528:LEU:O	1:D:528:LEU:HD12	2.20	0.42
1:F:39:THR:CG2	1:F:323:PRO:HG2	2.50	0.42
1:F:611:VAL:HG23	1:F:612:LEU:CD1	2.37	0.42
1:H:362:ARG:HG3	1:H:362:ARG:NH1	2.34	0.42
1:A:596:ARG:O	1:A:599:ASP:HB3	2.19	0.42
1:B:500:GLN:HA	1:D:363:TYR:CD2	2.54	0.42
1:E:367:THR:HG22	1:H:411:GLY:HA3	2.02	0.42
1:F:368:SER:OG	1:F:369:PRO:HD3	2.20	0.42
1:H:535:ILE:HD13	1:H:658:LEU:HD11	2.02	0.42
1:A:459:GLU:HG3	1:A:683:PHE:CG	2.55	0.42
1:B:381:HIS:O	1:B:385:VAL:HG23	2.19	0.42
1:B:682:VAL:HG21	1:C:133:ALA:HB2	2.01	0.42
1:D:97:SER:CB	1:D:400:ILE:HD11	2.44	0.42
1:F:228:HIS:HA	1:F:229:PRO:HD3	1.91	0.42
1:F:375:LEU:HD23	1:F:432:ILE:HG13	2.00	0.42
1:F:588:THR:O	1:F:590:SER:N	2.53	0.42
1:G:411:GLY:HA2	1:G:413:PHE:CE2	2.55	0.42
1:H:82:VAL:C	1:H:83:ARG:HG2	2.44	0.42
1:H:370:GLN:H	1:H:370:GLN:HG2	1.40	0.42
1:A:32:VAL:HG12	1:A:50:LYS:CG	2.49	0.42
1:A:645:TRP:CE2	1:A:679:ARG:HG2	2.54	0.42
1:B:415:ALA:HB1	1:B:418:VAL:HG13	2.01	0.42
1:C:131:GLN:HE21	1:C:131:GLN:CA	2.25	0.42
1:C:143:LEU:HD12	1:C:143:LEU:HA	1.92	0.42
1:E:609:VAL:HG22	1:F:619:LEU:HD22	2.02	0.42
1:G:156:LEU:O	1:G:159:SER:HB3	2.20	0.42
1:B:68:ASN:OD1	1:B:68:ASN:C	2.63	0.42
1:B:296:LEU:CD2	1:B:524:LEU:HD22	2.49	0.42
1:C:61:GLU:HB3	1:C:85:LYS:HB2	2.02	0.42
1:D:555:LEU:HD12	1:D:555:LEU:HA	1.82	0.42
1:D:612:LEU:HD23	1:D:617:LEU:CD1	2.50	0.42
1:E:445:ASN:HA	1:G:497:MSE:HG2	2.02	0.42
1:E:527:HIS:CD2	1:E:531:VAL:HG22	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:545:LYS:HE2	1:F:545:LYS:CA	2.50	0.42
1:A:363:TYR:CD1	1:A:363:TYR:N	2.88	0.42
1:B:69:LEU:CD1	1:B:387:THR:HA	2.49	0.42
1:C:648:ALA:O	1:C:650:THR:N	2.53	0.42
1:D:401:ASP:OD1	1:D:403:GLU:CG	2.68	0.42
1:G:225:ILE:HD11	1:G:268:LEU:HD11	2.02	0.42
1:H:128:ILE:HG12	1:H:132:LYS:HE2	2.00	0.42
1:H:470:LEU:HD22	1:H:526:THR:HG23	2.01	0.42
1:A:94:ILE:O	1:A:98:VAL:HG23	2.20	0.41
1:A:489:THR:O	1:A:492:VAL:HG23	2.19	0.41
1:B:544:PHE:CD1	1:B:544:PHE:C	2.98	0.41
1:B:627:VAL:O	1:B:631:GLU:HG2	2.19	0.41
1:C:460:ASP:HA	1:C:461:PRO:HD3	1.89	0.41
1:D:134:LEU:HA	1:D:137:HIS:CE1	2.54	0.41
1:E:228:HIS:CD2	1:G:687:GLN:NE2	2.88	0.41
1:E:263:LYS:O	1:E:263:LYS:HG2	2.19	0.41
1:F:181:SER:O	1:F:182:ALA:HB3	2.20	0.41
1:F:256:GLU:CD	1:F:257:PRO:HD2	2.45	0.41
1:F:608:VAL:O	1:F:612:LEU:HB2	2.19	0.41
1:G:522:LEU:HD23	1:G:699:TYR:CD1	2.55	0.41
1:G:543:GLU:OE1	1:G:657:TYR:OH	2.37	0.41
1:H:169:MSE:O	1:H:173:VAL:HG23	2.20	0.41
1:H:331:ASN:O	1:H:335:LEU:HG	2.20	0.41
1:H:362:ARG:CZ	1:H:448:MSE:HE2	2.50	0.41
1:A:375:LEU:N	1:A:375:LEU:CD1	2.84	0.41
1:B:48:VAL:O	1:B:52:LEU:HG	2.20	0.41
1:B:89:GLU:O	1:B:93:LYS:HG2	2.20	0.41
1:C:593:LEU:HD21	1:C:637:THR:HG21	2.02	0.41
1:D:29:ASN:O	1:D:29:ASN:ND2	2.53	0.41
1:D:188:LEU:HD12	1:D:188:LEU:N	2.35	0.41
1:G:92:SER:OG	1:G:96:LYS:NZ	2.53	0.41
1:G:368:SER:OG	1:G:369:PRO:HD3	2.20	0.41
1:H:299:MSE:HE3	1:H:662:THR:HB	2.03	0.41
1:A:170:THR:HG22	1:A:195:LEU:HD13	2.02	0.41
1:A:178:ARG:HG2	1:A:178:ARG:NH1	2.35	0.41
1:B:162:LEU:O	1:B:165:VAL:HG13	2.19	0.41
1:B:252:LEU:HD23	1:B:253:PHE:CE1	2.56	0.41
1:B:564:MSE:SE	1:B:570:ARG:HA	2.69	0.41
1:C:270:ASN:ND2	1:C:396:ASP:HB3	2.34	0.41
1:D:69:LEU:HG	1:D:280:THR:HG23	2.01	0.41
1:E:455:CYS:O	1:E:456:LEU:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:552:ILE:O	1:E:556:ILE:HG13	2.19	0.41
1:F:43:THR:HB	1:F:327:GLU:CD	2.46	0.41
1:F:382:ALA:HB1	1:F:421:THR:HB	2.02	0.41
1:H:329:ALA:O	1:H:333:ARG:HB2	2.20	0.41
1:A:30:LEU:O	1:A:42:VAL:HG21	2.20	0.41
1:C:465:TYR:O	1:C:466:HIS:C	2.63	0.41
1:E:131:GLN:NE2	1:E:261:GLY:O	2.45	0.41
1:E:592:ASP:O	1:E:594:VAL:N	2.53	0.41
1:F:511:ARG:NH1	2:F:798:HOH:O	2.47	0.41
1:G:375:LEU:HD12	1:G:375:LEU:N	2.35	0.41
1:G:661:ARG:HG3	2:G:802:HOH:O	2.20	0.41
1:H:258:VAL:HG12	1:H:259:VAL:N	2.34	0.41
1:H:340:ARG:HD3	1:H:340:ARG:N	2.36	0.41
1:H:460:ASP:OD1	1:H:592:ASP:O	2.36	0.41
1:H:627:VAL:O	1:H:631:GLU:HG2	2.20	0.41
1:A:175:SER:HA	1:A:178:ARG:HD3	2.02	0.41
1:A:320:ARG:NH1	1:C:389:GLU:OE2	2.53	0.41
1:A:535:ILE:HG13	1:A:536:ASP:N	2.34	0.41
1:C:166:ARG:NH1	1:C:195:LEU:HD23	2.36	0.41
1:C:375:LEU:N	1:C:375:LEU:CD1	2.83	0.41
1:D:228:HIS:HA	1:D:229:PRO:HD3	1.94	0.41
1:D:557:ASP:OD1	1:D:570:ARG:HD2	2.21	0.41
1:E:48:VAL:HG13	1:E:288:MSE:HE1	2.01	0.41
1:E:101:LEU:O	1:E:104:GLN:N	2.53	0.41
1:E:547:GLN:O	1:E:550:PRO:HG2	2.20	0.41
1:E:670:ARG:HD3	1:E:676:LYS:HA	2.01	0.41
1:F:548:PHE:HD1	1:F:636:LEU:HD12	1.84	0.41
1:B:178:ARG:NH2	1:B:393:SER:C	2.79	0.41
1:B:289:LEU:HG	1:B:520:LEU:HD13	2.03	0.41
1:B:516:SER:HA	1:B:519:VAL:HG22	2.03	0.41
1:B:581:LEU:HD13	1:B:604:ALA:HB2	2.02	0.41
1:B:681:ASP:C	1:B:683:PHE:H	2.28	0.41
1:F:593:LEU:HD21	1:F:637:THR:HG21	2.01	0.41
1:F:649:SER:OG	1:F:676:LYS:HD2	2.21	0.41
1:G:40:THR:O	1:G:40:THR:HG22	2.19	0.41
1:G:84:VAL:HG12	2:G:808:HOH:O	2.19	0.41
1:H:135:LEU:O	1:H:139:LEU:HG	2.21	0.41
1:A:560:PHE:HD2	1:A:617:LEU:HD13	1.86	0.41
1:D:27:SER:O	1:D:28:THR:C	2.63	0.41
1:D:54:ALA:HA	1:D:55:PRO:HD3	1.85	0.41
1:D:270:ASN:HD22	1:D:396:ASP:CA	2.31	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:370:GLN:NE2	1:H:411:GLY:C	2.79	0.41
1:F:54:ALA:HA	1:F:55:PRO:HD3	1.91	0.41
1:F:169:MSE:HE2	1:F:191:LEU:HD23	2.01	0.41
1:F:319:THR:CG2	1:G:412:ASN:ND2	2.84	0.41
1:G:295:SER:O	1:G:299:MSE:HG3	2.21	0.41
1:G:446:ALA:HB1	1:G:589:ASN:ND2	2.35	0.41
1:H:465:TYR:O	1:H:466:HIS:C	2.63	0.41
1:A:143:LEU:HD13	1:A:204:PRO:HA	2.02	0.41
1:B:522:LEU:HD22	1:C:142:VAL:HG21	2.02	0.41
1:C:560:PHE:HB2	1:C:564:MSE:HE2	2.02	0.41
1:C:659:SER:O	1:C:663:GLN:HB2	2.20	0.41
1:D:573:LEU:HG	1:D:611:VAL:HG21	2.03	0.41
1:E:175:SER:HA	1:E:178:ARG:HD3	2.03	0.41
1:E:337:GLU:O	1:E:337:GLU:HG2	2.18	0.41
1:E:418:VAL:HG22	1:E:506:ALA:HB1	2.02	0.41
1:F:185:LEU:O	1:F:189:GLU:HG3	2.21	0.41
1:G:185:LEU:HA	1:G:188:LEU:HD13	2.02	0.41
1:G:375:LEU:CD1	1:G:375:LEU:N	2.84	0.41
1:G:421:THR:O	1:G:425:THR:OG1	2.38	0.41
1:A:168:ALA:O	1:A:172:ARG:HB2	2.21	0.41
1:A:427:LEU:O	1:A:431:GLN:HG2	2.21	0.41
1:A:548:PHE:O	1:A:552:ILE:HG13	2.21	0.41
1:C:141:GLY:HA3	1:C:204:PRO:HG2	2.02	0.41
1:C:244:LEU:HD23	1:C:244:LEU:N	2.36	0.41
1:C:466:HIS:CE1	1:C:533:GLN:HG3	2.54	0.41
1:C:648:ALA:C	1:C:650:THR:N	2.77	0.41
1:D:190:ALA:HA	2:D:748:HOH:O	2.19	0.41
1:E:256:GLU:HA	1:E:257:PRO:HD2	1.85	0.41
1:E:593:LEU:HD12	1:E:597:TRP:CD1	2.56	0.41
1:E:649:SER:HB2	1:E:671:GLU:CD	2.45	0.41
1:G:178:ARG:NH2	1:G:394:THR:N	2.69	0.41
1:H:59:THR:HG21	1:H:83:ARG:HG3	2.02	0.41
1:C:696:SER:O	1:C:700:GLU:HG3	2.21	0.41
1:D:169:MSE:CE	1:D:191:LEU:HD23	2.51	0.41
1:E:535:ILE:HG12	1:E:535:ILE:H	1.66	0.41
1:E:588:THR:HG23	1:E:596:ARG:HG3	2.03	0.41
1:F:48:VAL:HA	1:F:51:MSE:HE2	2.02	0.41
1:F:545:LYS:HE2	1:F:545:LYS:HA	2.03	0.41
1:F:561:GLY:C	1:F:563:ALA:N	2.79	0.41
1:G:341:PHE:CE2	1:G:657:TYR:HB2	2.55	0.41
1:H:548:PHE:CE1	1:H:633:ALA:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:VAL:HG13	1:A:183:VAL:O	2.21	0.40
1:A:465:TYR:O	1:A:466:HIS:C	2.64	0.40
1:C:126:ASP:CG	1:C:127:ALA:N	2.78	0.40
1:E:548:PHE:O	1:E:549:GLY:C	2.64	0.40
1:E:605:ALA:HA	1:E:608:VAL:HG13	2.02	0.40
1:F:312:HIS:HA	1:F:313:PRO:HD3	1.95	0.40
1:F:359:ARG:O	1:F:360:GLN:CB	2.65	0.40
1:G:372:LEU:HD21	1:G:435:LEU:HD23	2.03	0.40
1:G:561:GLY:HA2	1:G:564:MSE:HB3	2.02	0.40
1:H:142:VAL:HG12	2:H:718:HOH:O	2.20	0.40
1:H:169:MSE:HE2	1:H:191:LEU:CD2	2.51	0.40
1:H:680:GLY:O	1:H:684:LEU:HG	2.21	0.40
1:A:62:LEU:HD22	1:A:62:LEU:N	2.37	0.40
1:B:178:ARG:NH2	1:B:393:SER:O	2.54	0.40
1:B:551:ALA:O	1:B:555:LEU:HD13	2.21	0.40
1:D:307:HIS:C	1:D:309:GLY:H	2.28	0.40
1:E:176:LEU:HD22	1:E:183:VAL:CG1	2.51	0.40
1:F:299:MSE:SE	1:F:665:LEU:HD23	2.72	0.40
1:F:402:VAL:O	1:F:403:GLU:C	2.65	0.40
1:F:594:VAL:CB	1:F:595:PRO:HD3	2.52	0.40
1:G:489:THR:O	1:G:492:VAL:HG23	2.21	0.40
1:G:605:ALA:HA	1:G:608:VAL:CG1	2.50	0.40
1:B:142:VAL:HG11	1:C:522:LEU:CD2	2.51	0.40
1:D:123:ARG:HD2	1:D:123:ARG:C	2.46	0.40
1:E:476:ALA:HB2	1:G:209:ILE:HG23	2.04	0.40
1:E:637:THR:O	1:E:641:ARG:HG3	2.21	0.40
1:G:157:GLU:H	1:G:157:GLU:CD	2.29	0.40
1:G:597:TRP:HD1	1:G:634:ILE:HG22	1.86	0.40
1:B:370:GLN:HG3	1:D:411:GLY:O	2.21	0.40
1:B:448:MSE:C	1:B:450:ARG:H	2.29	0.40
1:B:575:GLU:HG2	1:B:579:LYS:HE3	2.03	0.40
1:C:44:GLN:O	1:C:48:VAL:HG23	2.21	0.40
1:C:67:LEU:HD12	1:C:71:ASP:HB2	2.02	0.40
1:C:216:SER:O	1:C:220:TYR:HD1	2.04	0.40
1:D:449:ASN:HB2	1:D:452:LEU:HD12	2.02	0.40
1:F:389:GLU:OE2	1:G:320:ARG:NH1	2.55	0.40
1:G:184:ARG:HH11	1:G:186:VAL:HG12	1.84	0.40
1:H:443:MSE:SE	1:H:531:VAL:HG23	2.71	0.40
1:H:462:SER:O	1:H:463:LEU:HD12	2.20	0.40
1:A:154:ARG:O	1:D:153:GLY:HA2	2.22	0.40
1:C:51:MSE:HG3	1:C:70:GLY:HA2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:LEU:HB3	1:C:159:SER:OG	2.22	0.40
1:C:634:ILE:C	1:C:637:THR:HG22	2.46	0.40
1:C:679:ARG:NH1	1:C:683:PHE:CE2	2.89	0.40
1:D:202:ILE:HA	2:D:732:HOH:O	2.21	0.40
1:E:100:PHE:CE1	1:E:405:LYS:HA	2.56	0.40
1:E:313:PRO:HD3	1:E:333:ARG:NE	2.36	0.40
1:F:431:GLN:HE21	1:F:431:GLN:CA	2.18	0.40
1:F:497:MSE:HG3	2:H:737:HOH:O	2.21	0.40
1:F:537:LEU:HD12	1:F:537:LEU:HA	1.88	0.40
1:H:143:LEU:CD1	1:H:143:LEU:N	2.82	0.40
1:H:178:ARG:HH12	1:H:393:SER:CA	2.35	0.40
1:H:446:ALA:HA	1:H:449:ASN:HD21	1.87	0.40
1:H:460:ASP:HA	1:H:461:PRO:HD3	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	647/714 (91%)	593 (92%)	46 (7%)	8 (1%)	11	28
1	B	653/714 (92%)	598 (92%)	41 (6%)	14 (2%)	5	15
1	C	641/714 (90%)	587 (92%)	45 (7%)	9 (1%)	9	24
1	D	641/714 (90%)	591 (92%)	38 (6%)	12 (2%)	6	17
1	E	648/714 (91%)	594 (92%)	43 (7%)	11 (2%)	7	20
1	F	641/714 (90%)	588 (92%)	41 (6%)	12 (2%)	6	17
1	G	649/714 (91%)	604 (93%)	34 (5%)	11 (2%)	7	20
1	H	637/714 (89%)	590 (93%)	34 (5%)	13 (2%)	6	16
All	All	5157/5712 (90%)	4745 (92%)	322 (6%)	90 (2%)	7	20

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	454	SER
1	A	466	HIS
1	B	39	THR
1	B	260	LEU
1	B	404	ASN
1	B	466	HIS
1	C	454	SER
1	D	28	THR
1	D	466	HIS
1	D	498	ALA
1	E	29	ASN
1	E	263	LYS
1	F	240	LYS
1	F	262	PRO
1	F	360	GLN
1	F	466	HIS
1	F	689	VAL
1	F	690	THR
1	G	38	PRO
1	G	39	THR
1	G	321	PRO
1	G	466	HIS
1	H	454	SER
1	H	466	HIS
1	H	593	LEU
1	H	647	ALA
1	H	648	ALA
1	A	415	ALA
1	A	593	LEU
1	B	34	GLY
1	B	79	GLY
1	B	415	ALA
1	C	466	HIS
1	D	454	SER
1	D	589	ASN
1	E	454	SER
1	E	466	HIS
1	E	593	LEU
1	G	402	VAL
1	H	247	ARG
1	H	345	HIS

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Mol	Chain	Res	Type
1	H	615	THR
1	A	40	THR
1	B	454	SER
1	B	589	ASN
1	C	496	GLU
1	D	321	PRO
1	D	415	ALA
1	D	496	GLU
1	E	415	ALA
1	F	565	THR
1	F	589	ASN
1	G	360	GLN
1	G	649	SER
1	A	321	PRO
1	B	321	PRO
1	B	345	HIS
1	C	252	LEU
1	C	321	PRO
1	C	649	SER
1	D	182	ALA
1	D	240	LYS
1	D	593	LEU
1	E	86	ASP
1	F	454	SER
1	G	345	HIS
1	G	496	GLU
1	H	91	ARG
1	H	321	PRO
1	H	361	ASP
1	B	38	PRO
1	B	449	ASN
1	C	415	ALA
1	D	239	GLY
1	E	42	VAL
1	F	238	GLU
1	F	239	GLY
1	F	321	PRO
1	G	147	PHE
1	G	415	ALA
1	H	146	SER
1	H	182	ALA
1	B	37	LEU

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Mol	Chain	Res	Type
1	C	42	VAL
1	E	321	PRO
1	C	402	VAL
1	A	37	LEU
1	E	79	GLY
1	E	37	LEU

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	542/573 (95%)	502 (93%)	40 (7%)	11	28
1	B	547/573 (96%)	506 (92%)	41 (8%)	11	28
1	C	538/573 (94%)	502 (93%)	36 (7%)	13	33
1	D	539/573 (94%)	501 (93%)	38 (7%)	12	30
1	E	543/573 (95%)	501 (92%)	42 (8%)	10	26
1	F	539/573 (94%)	506 (94%)	33 (6%)	15	36
1	G	544/573 (95%)	506 (93%)	38 (7%)	12	31
1	H	535/573 (93%)	499 (93%)	36 (7%)	13	33
All	All	4327/4584 (94%)	4023 (93%)	304 (7%)	12	31

All (304) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	PRO
1	A	69	LEU
1	A	72	VAL
1	A	84	VAL
1	A	128	ILE
1	A	143	LEU
1	A	170	THR
1	A	172	ARG
1	A	203	VAL

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Mol	Chain	Res	Type
1	A	218	LEU
1	A	219	SER
1	A	256	GLU
1	A	268	LEU
1	A	289	LEU
1	A	320	ARG
1	A	336	LEU
1	A	366	ARG
1	A	370	GLN
1	A	375	LEU
1	A	394	THR
1	A	418	VAL
1	A	496	GLU
1	A	503	ASN
1	A	520	LEU
1	A	532	LEU
1	A	533	GLN
1	A	537	LEU
1	A	555	LEU
1	A	569	LEU
1	A	570	ARG
1	A	573	LEU
1	A	588	THR
1	A	599	ASP
1	A	608	VAL
1	A	615	THR
1	A	637	THR
1	A	656	SER
1	A	658	LEU
1	A	675	VAL
1	A	679	ARG
1	B	38	PRO
1	B	60	LEU
1	B	62	LEU
1	B	82	VAL
1	B	84	VAL
1	B	99	GLU
1	B	101	LEU
1	B	134	LEU
1	B	138	GLN
1	B	142	VAL
1	B	143	LEU

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Mol	Chain	Res	Type
1	B	165	VAL
1	B	172	ARG
1	B	178	ARG
1	B	215	LEU
1	B	238	GLU
1	B	244	LEU
1	B	247	ARG
1	B	254	ASN
1	B	258	VAL
1	B	281	LEU
1	B	289	LEU
1	B	296	LEU
1	B	336	LEU
1	B	362	ARG
1	B	370	GLN
1	B	386	LEU
1	B	418	VAL
1	B	424	LYS
1	B	492	VAL
1	B	520	LEU
1	B	532	LEU
1	B	537	LEU
1	B	581	LEU
1	B	585	LEU
1	B	611	VAL
1	B	612	LEU
1	B	615	THR
1	B	636	LEU
1	B	686	LYS
1	B	710	VAL
1	C	62	LEU
1	C	84	VAL
1	C	101	LEU
1	C	130	LEU
1	C	131	GLN
1	C	143	LEU
1	C	172	ARG
1	C	183	VAL
1	C	185	LEU
1	C	203	VAL
1	C	215	LEU
1	C	218	LEU

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Mol	Chain	Res	Type
1	C	238	GLU
1	C	242	LYS
1	C	244	LEU
1	C	256	GLU
1	C	264	GLU
1	C	289	LEU
1	C	336	LEU
1	C	370	GLN
1	C	418	VAL
1	C	502	VAL
1	C	520	LEU
1	C	533	GLN
1	C	537	LEU
1	C	543	GLU
1	C	569	LEU
1	C	573	LEU
1	C	594	VAL
1	C	608	VAL
1	C	611	VAL
1	C	612	LEU
1	C	636	LEU
1	C	643	THR
1	C	658	LEU
1	C	675	VAL
1	D	40	THR
1	D	60	LEU
1	D	69	LEU
1	D	104	GLN
1	D	123	ARG
1	D	131	GLN
1	D	142	VAL
1	D	162	LEU
1	D	165	VAL
1	D	175	SER
1	D	181	SER
1	D	203	VAL
1	D	215	LEU
1	D	240	LYS
1	D	263	LYS
1	D	281	LEU
1	D	289	LEU
1	D	310	SER

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Mol	Chain	Res	Type
1	D	336	LEU
1	D	361	ASP
1	D	370	GLN
1	D	375	LEU
1	D	423	GLU
1	D	503	ASN
1	D	520	LEU
1	D	532	LEU
1	D	537	LEU
1	D	555	LEU
1	D	560	PHE
1	D	565	THR
1	D	569	LEU
1	D	573	LEU
1	D	585	LEU
1	D	596	ARG
1	D	610	GLU
1	D	643	THR
1	D	672	GLU
1	D	706	ARG
1	E	41	GLN
1	E	62	LEU
1	E	69	LEU
1	E	72	VAL
1	E	83	ARG
1	E	84	VAL
1	E	87	SER
1	E	102	ARG
1	E	139	LEU
1	E	143	LEU
1	E	172	ARG
1	E	203	VAL
1	E	218	LEU
1	E	238	GLU
1	E	266	LEU
1	E	268	LEU
1	E	281	LEU
1	E	289	LEU
1	E	336	LEU
1	E	337	GLU
1	E	370	GLN
1	E	375	LEU

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Mol	Chain	Res	Type
1	E	386	LEU
1	E	418	VAL
1	E	441	THR
1	E	520	LEU
1	E	531	VAL
1	E	533	GLN
1	E	535	ILE
1	E	537	LEU
1	E	543	GLU
1	E	555	LEU
1	E	573	LEU
1	E	585	LEU
1	E	586	GLU
1	E	588	THR
1	E	594	VAL
1	E	608	VAL
1	E	636	LEU
1	E	658	LEU
1	E	675	VAL
1	E	686	LYS
1	F	40	THR
1	F	60	LEU
1	F	131	GLN
1	F	134	LEU
1	F	135	LEU
1	F	143	LEU
1	F	172	ARG
1	F	183	VAL
1	F	203	VAL
1	F	244	LEU
1	F	269	VAL
1	F	275	SER
1	F	281	LEU
1	F	289	LEU
1	F	336	LEU
1	F	361	ASP
1	F	362	ARG
1	F	370	GLN
1	F	375	LEU
1	F	404	ASN
1	F	418	VAL
1	F	424	LYS

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Mol	Chain	Res	Type
1	F	431	GLN
1	F	441	THR
1	F	520	LEU
1	F	532	LEU
1	F	537	LEU
1	F	545	LYS
1	F	558	GLN
1	F	570	ARG
1	F	594	VAL
1	F	596	ARG
1	F	661	ARG
1	G	30	LEU
1	G	38	PRO
1	G	62	LEU
1	G	87	SER
1	G	101	LEU
1	G	130	LEU
1	G	139	LEU
1	G	142	VAL
1	G	143	LEU
1	G	172	ARG
1	G	203	VAL
1	G	218	LEU
1	G	248	GLU
1	G	268	LEU
1	G	281	LEU
1	G	289	LEU
1	G	323	PRO
1	G	336	LEU
1	G	346	GLU
1	G	361	ASP
1	G	427	LEU
1	G	441	THR
1	G	520	LEU
1	G	531	VAL
1	G	533	GLN
1	G	543	GLU
1	G	545	LYS
1	G	555	LEU
1	G	565	THR
1	G	569	LEU
1	G	573	LEU

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Mol	Chain	Res	Type
1	G	585	LEU
1	G	608	VAL
1	G	638	ARG
1	G	658	LEU
1	G	670	ARG
1	G	675	VAL
1	G	700	GLU
1	H	60	LEU
1	H	69	LEU
1	H	84	VAL
1	H	126	ASP
1	H	131	GLN
1	H	142	VAL
1	H	143	LEU
1	H	165	VAL
1	H	203	VAL
1	H	215	LEU
1	H	244	LEU
1	H	256	GLU
1	H	263	LYS
1	H	281	LEU
1	H	289	LEU
1	H	334	LYS
1	H	361	ASP
1	H	370	GLN
1	H	418	VAL
1	H	468	LYS
1	H	497	MSE
1	H	520	LEU
1	H	531	VAL
1	H	532	LEU
1	H	535	ILE
1	H	537	LEU
1	H	546	LYS
1	H	569	LEU
1	H	581	LEU
1	H	585	LEU
1	H	611	VAL
1	H	615	THR
1	H	636	LEU
1	H	638	ARG
1	H	710	VAL

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Mol	Chain	Res	Type
1	H	713	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	36	HIS
1	A	137	HIS
1	A	254	ASN
1	A	370	GLN
1	A	412	ASN
1	A	436	ASN
1	A	483	HIS
1	A	499	ASN
1	A	623	ASN
1	A	639	GLN
1	A	663	GLN
1	B	36	HIS
1	B	137	HIS
1	B	138	GLN
1	B	420	ASN
1	B	483	HIS
1	B	499	ASN
1	B	558	GLN
1	B	559	HIS
1	B	623	ASN
1	B	663	GLN
1	B	709	ASN
1	C	29	ASN
1	C	137	HIS
1	C	138	GLN
1	C	234	HIS
1	C	270	ASN
1	C	345	HIS
1	C	370	GLN
1	C	383	HIS
1	C	408	HIS
1	C	499	ASN
1	C	639	GLN
1	C	663	GLN
1	C	709	ASN
1	D	29	ASN

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Mol	Chain	Res	Type
1	D	44	GLN
1	D	137	HIS
1	D	270	ASN
1	D	284	HIS
1	D	408	HIS
1	D	409	HIS
1	D	412	ASN
1	D	436	ASN
1	D	558	GLN
1	D	568	ASN
1	D	623	ASN
1	D	663	GLN
1	E	29	ASN
1	E	137	HIS
1	E	138	GLN
1	E	307	HIS
1	E	392	GLN
1	E	404	ASN
1	E	408	HIS
1	E	420	ASN
1	E	436	ASN
1	E	491	HIS
1	E	499	ASN
1	E	527	HIS
1	F	104	GLN
1	F	137	HIS
1	F	254	ASN
1	F	284	HIS
1	F	325	GLN
1	F	404	ASN
1	F	436	ASN
1	F	483	HIS
1	F	491	HIS
1	F	503	ASN
1	F	559	HIS
1	F	587	GLN
1	F	623	ASN
1	F	694	ASN
1	G	29	ASN
1	G	44	GLN
1	G	104	GLN
1	G	137	HIS

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Mol	Chain	Res	Type
1	G	138	GLN
1	G	331	ASN
1	G	344	HIS
1	G	360	GLN
1	G	370	GLN
1	G	397	ASN
1	G	408	HIS
1	G	436	ASN
1	G	466	HIS
1	G	499	ASN
1	G	623	ASN
1	G	687	GLN
1	H	44	GLN
1	H	137	HIS
1	H	174	ASN
1	H	237	HIS
1	H	294	GLN
1	H	325	GLN
1	H	331	ASN
1	H	370	GLN
1	H	383	HIS
1	H	404	ASN
1	H	420	ASN
1	H	436	ASN
1	H	500	GLN
1	H	578	ASN
1	H	587	GLN
1	H	623	ASN
1	H	708	ASN
1	H	709	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	175	B	211	1	13,14,15	1.58	3 (23%)	9,19,21	5.70	6 (66%)
1	175	D	211	1	13,14,15	1.84	3 (23%)	9,19,21	5.38	4 (44%)
1	175	E	211	1	13,14,15	1.52	2 (15%)	9,19,21	5.39	4 (44%)
1	175	F	211	1	13,14,15	1.68	2 (15%)	9,19,21	5.47	6 (66%)
1	175	C	211	1	13,14,15	1.48	2 (15%)	9,19,21	5.36	5 (55%)
1	175	G	211	1	13,14,15	1.52	2 (15%)	9,19,21	5.49	6 (66%)
1	175	A	211	1	13,14,15	1.63	3 (23%)	9,19,21	5.31	4 (44%)
1	175	H	211	1	13,14,15	1.48	2 (15%)	9,19,21	5.33	4 (44%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	175	B	211	1	2/2/5/7	0/3/25/26	0/1/1/1
1	175	D	211	1	2/2/5/7	0/3/25/26	0/1/1/1
1	175	E	211	1	2/2/5/7	0/3/25/26	0/1/1/1
1	175	F	211	1	2/2/5/7	0/3/25/26	0/1/1/1
1	175	C	211	1	2/2/5/7	0/3/25/26	0/1/1/1
1	175	G	211	1	2/2/5/7	0/3/25/26	0/1/1/1
1	175	A	211	1	2/2/5/7	0/3/25/26	0/1/1/1
1	175	H	211	1	2/2/5/7	0/3/25/26	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	211	175	C3-C5	-3.99	1.46	1.52
1	F	211	175	C4-C3	-3.80	1.45	1.53
1	D	211	175	C4-C3	-3.76	1.45	1.53
1	E	211	175	C4-C3	-3.63	1.46	1.53
1	B	211	175	C4-C3	-3.58	1.46	1.53
1	A	211	175	C4-C3	-3.48	1.46	1.53
1	F	211	175	C3-C5	-3.35	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	211	175	C4-C3	-3.26	1.47	1.53
1	C	211	175	C4-C3	-3.21	1.47	1.53
1	G	211	175	C4-C3	-3.21	1.47	1.53
1	G	211	175	C3-C5	-2.87	1.47	1.52
1	B	211	175	C3-C5	-2.82	1.48	1.52
1	A	211	175	C3-C5	-2.75	1.48	1.52
1	H	211	175	C3-C5	-2.49	1.48	1.52
1	E	211	175	C3-C5	-2.48	1.48	1.52
1	C	211	175	C3-C5	-2.43	1.48	1.52
1	D	211	175	C2-N0	-2.31	1.42	1.45
1	A	211	175	C2-N0	-2.19	1.42	1.45
1	B	211	175	C2-N0	-2.08	1.43	1.45

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	211	175	C4-C3-N2	13.48	131.29	114.04
1	F	211	175	C4-C3-N2	13.14	130.85	114.04
1	H	211	175	C4-C3-N2	13.03	130.72	114.04
1	B	211	175	C4-C3-N2	12.99	130.66	114.04
1	C	211	175	C4-C3-N2	12.94	130.60	114.04
1	A	211	175	C4-C3-N2	12.83	130.46	114.04
1	G	211	175	C4-C3-N2	12.79	130.41	114.04
1	E	211	175	C4-C3-N2	12.76	130.37	114.04
1	G	211	175	C4-C3-C5	7.84	131.02	111.84
1	E	211	175	C4-C3-C5	7.84	131.01	111.84
1	A	211	175	C4-C3-C5	7.84	131.01	111.84
1	C	211	175	C4-C3-C5	7.76	130.81	111.84
1	H	211	175	C4-C3-C5	7.69	130.65	111.84
1	B	211	175	C4-C3-C5	7.64	130.53	111.84
1	F	211	175	C4-C3-C5	7.63	130.50	111.84
1	D	211	175	C4-C3-C5	7.40	129.95	111.84
1	G	211	175	C-C0-N0	5.27	121.40	112.62
1	B	211	175	C0-N0-C5	5.19	129.60	122.70
1	B	211	175	C-C0-N0	5.00	120.94	112.62
1	E	211	175	C-C0-N0	4.76	120.55	112.62
1	F	211	175	C-C0-N0	4.41	119.95	112.62
1	A	211	175	C-C0-N0	4.06	119.39	112.62
1	C	211	175	C-C0-N0	3.96	119.21	112.62
1	H	211	175	C-C0-N0	3.92	119.14	112.62
1	D	211	175	C-C0-N0	3.51	118.46	112.62
1	F	211	175	C0-N0-C2	2.89	126.60	124.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	211	175	O6-C5-N0	-2.41	122.85	125.76
1	G	211	175	C0-N0-C2	2.27	126.10	124.24
1	B	211	175	C0-N0-C2	-2.27	122.39	124.24
1	C	211	175	C0-N0-C2	2.26	126.08	124.24
1	D	211	175	O6-C5-C3	-2.25	123.09	126.65
1	F	211	175	O6-C5-N0	-2.20	123.10	125.76
1	B	211	175	O6-C5-C3	-2.20	123.18	126.65
1	A	211	175	O6-C5-N0	-2.20	123.11	125.76
1	G	211	175	O6-C5-C3	-2.19	123.19	126.65
1	E	211	175	O6-C5-N0	-2.07	123.26	125.76
1	H	211	175	O6-C5-N0	-2.06	123.28	125.76
1	G	211	175	O6-C5-N0	-2.05	123.29	125.76
1	F	211	175	O6-C5-C3	-2.05	123.41	126.65

All (16) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	211	175	C3
1	A	211	175	C2
1	B	211	175	C3
1	B	211	175	C2
1	C	211	175	C3
1	C	211	175	C2
1	D	211	175	C3
1	D	211	175	C2
1	E	211	175	C3
1	E	211	175	C2
1	F	211	175	C3
1	F	211	175	C2
1	G	211	175	C3
1	G	211	175	C2
1	H	211	175	C3
1	H	211	175	C2

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	211	175	1	0
1	A	211	175	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	640/714 (89%)	-0.49	0 100 100	12, 36, 66, 87	0
1	B	646/714 (90%)	-0.39	5 (0%) 82 82	12, 37, 64, 78	0
1	C	636/714 (89%)	-0.37	6 (0%) 81 80	15, 36, 68, 92	0
1	D	636/714 (89%)	-0.49	6 (0%) 81 80	8, 33, 63, 113	0
1	E	641/714 (89%)	-0.37	2 (0%) 90 89	13, 39, 66, 94	0
1	F	636/714 (89%)	-0.38	8 (1%) 74 74	13, 36, 64, 98	0
1	G	642/714 (89%)	-0.48	6 (0%) 81 80	14, 35, 62, 94	0
1	H	630/714 (88%)	-0.47	5 (0%) 82 82	13, 36, 62, 91	0
All	All	5107/5712 (89%)	-0.43	38 (0%) 84 83	8, 36, 65, 113	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	33	ALA	4.1
1	D	33	ALA	4.0
1	F	238	GLU	3.6
1	B	266	LEU	3.1
1	D	30	LEU	3.0
1	F	32	VAL	2.8
1	H	39	THR	2.8
1	B	33	ALA	2.7
1	D	32	VAL	2.7
1	F	30	LEU	2.6
1	D	27	SER	2.6
1	G	39	THR	2.6
1	F	31	ALA	2.5
1	G	130	LEU	2.4
1	C	27	SER	2.4
1	C	345	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	G	147	PHE	2.3
1	F	454	SER	2.3
1	B	147	PHE	2.3
1	C	31	ALA	2.3
1	H	454	SER	2.3
1	G	32	VAL	2.2
1	B	34	GLY	2.2
1	B	35	SER	2.2
1	C	39	THR	2.2
1	D	147	PHE	2.1
1	F	27	SER	2.1
1	C	30	LEU	2.1
1	E	31	ALA	2.1
1	E	28	THR	2.1
1	H	104	GLN	2.1
1	G	38	PRO	2.0
1	C	147	PHE	2.0
1	F	252	LEU	2.0
1	D	28	THR	2.0
1	H	147	PHE	2.0
1	H	360	GLN	2.0
1	G	149	SER	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	175	D	211	14/15	0.89	0.10	31,35,37,37	0
1	175	C	211	14/15	0.90	0.09	30,35,36,37	0
1	175	E	211	14/15	0.90	0.08	30,37,38,38	0
1	175	H	211	14/15	0.91	0.08	24,32,35,35	0
1	175	F	211	14/15	0.94	0.07	25,31,34,36	0
1	175	G	211	14/15	0.94	0.07	25,31,35,36	0
1	175	B	211	14/15	0.94	0.07	23,29,32,32	0
1	175	A	211	14/15	0.95	0.06	27,32,34,35	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.