



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:59 PM UTC

PDB ID : 5AWG / pdb_00005awg
Title : Crystal structure of Hg-bound SufB-SufC-SufD complex from Escherichia coli
Authors : Hirabayashi, K.; Wada, K.
Deposited on : 2015-07-03
Resolution : 4.28 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 Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

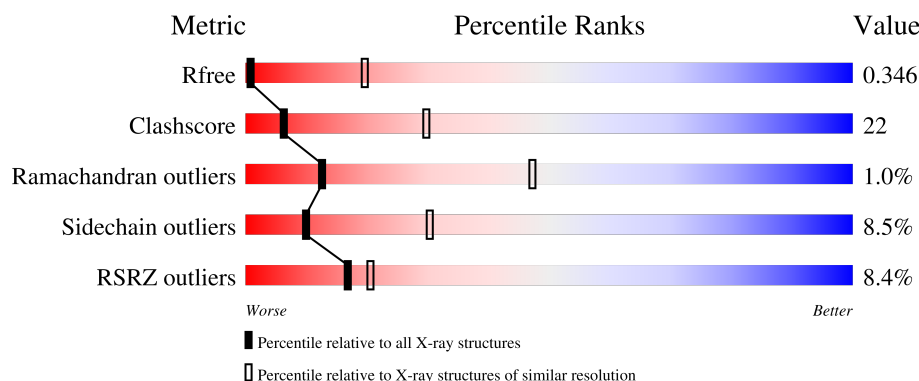
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.28 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}	180053	1036 (4.66-3.90)
Clashscore	190562	1081 (4.66-3.90)
Ramachandran outliers	187476	1007 (4.68-3.88)
Sidechain outliers	187428	1034 (4.70-3.86)
RSRZ outliers	180081	1033 (4.66-3.90)

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	495	
1	E	495	
2	B	423	
2	F	423	
3	C	248	

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Mol	Chain	Length	Quality of chain
3	D	248	6% 56% 33% 6% 5%
3	G	248	4% 58% 33% 5% •
3	H	248	8% 51% 38% 6% 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 18808 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 FeS cluster assembly protein SufB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			2968	1869	509	572	18			
1	E	372	Total	C	N	O	S	0	0	0
			2910	1833	498	561	18			

- Molecule 2 is a protein called FeS cluster assembly protein SufD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	361	Total	C	N	O	S	0	0	0
			2798	1743	514	533	8			
2	F	355	Total	C	N	O	S	0	0	0
			2752	1712	507	525	8			

- Molecule 3 is a protein called Probable ATP-dependent transporter SufC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	237	Total	C	N	O	S	0	0	0
			1846	1169	312	358	7			
3	D	235	Total	C	N	O	S	0	0	0
			1829	1158	310	354	7			
3	G	239	Total	C	N	O	S	0	0	0
			1864	1179	315	363	7			
3	H	236	Total	C	N	O	S	0	0	0
			1837	1164	311	355	7			

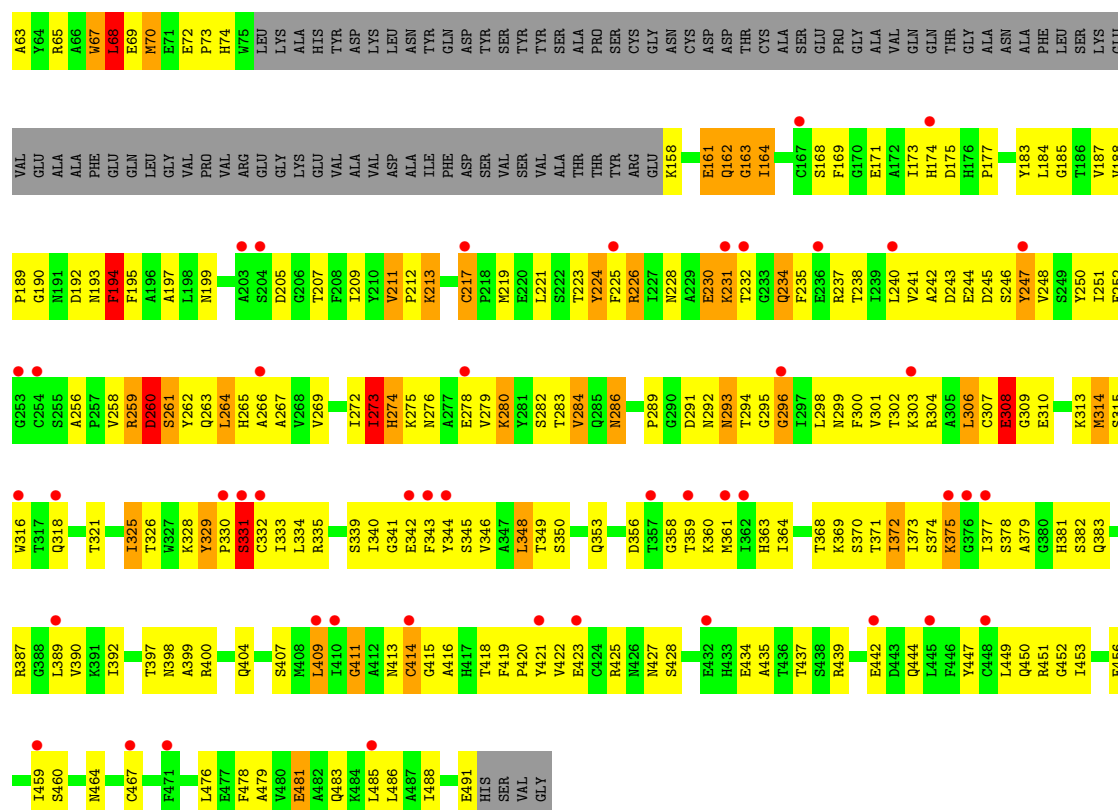
- Molecule 4 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Hg	0	0
			1	1		
4	B	1	Total	Hg	0	0
			1	1		

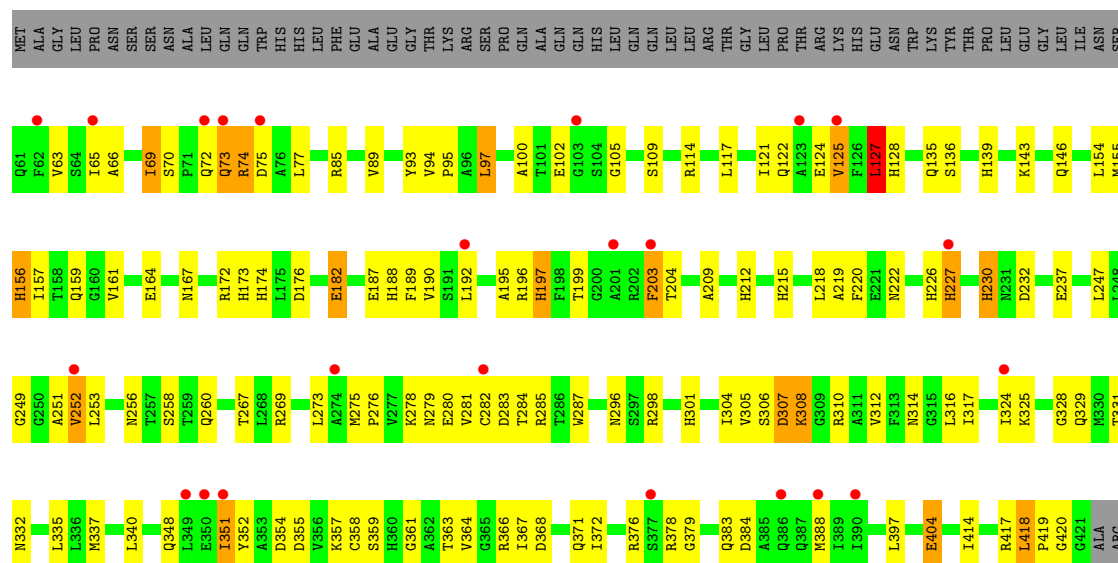
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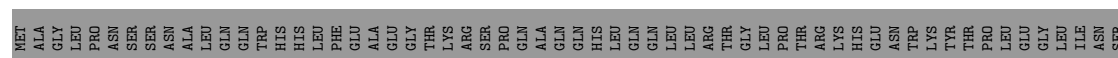
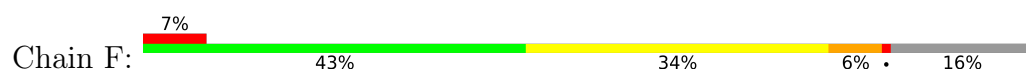
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	E	1	Total	Hg	0	0
			1	1		
4	F	1	Total	Hg	0	0
			1	1		

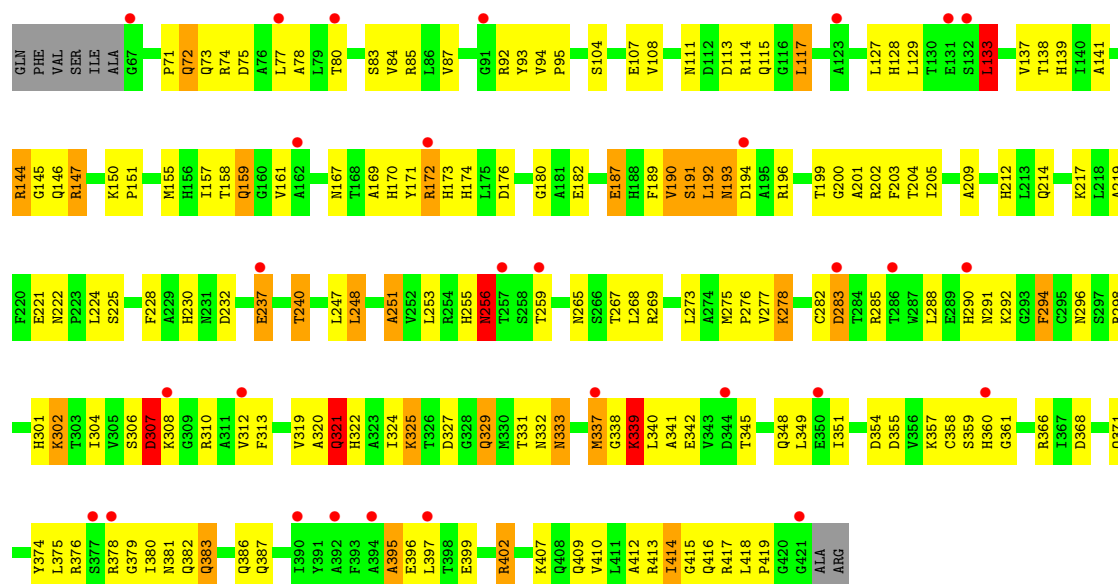


• Molecule 2: FeS cluster assembly protein SufD

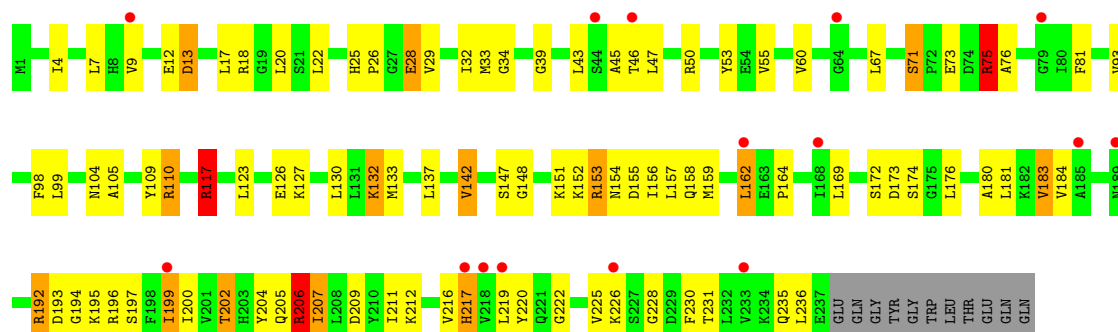


• Molecule 2: FeS cluster assembly protein SufD

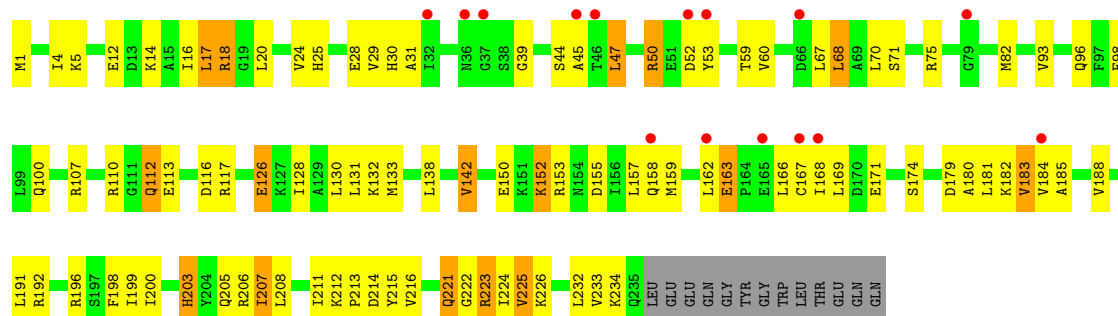




• Molecule 3: Probable ATP-dependent transporter SufC

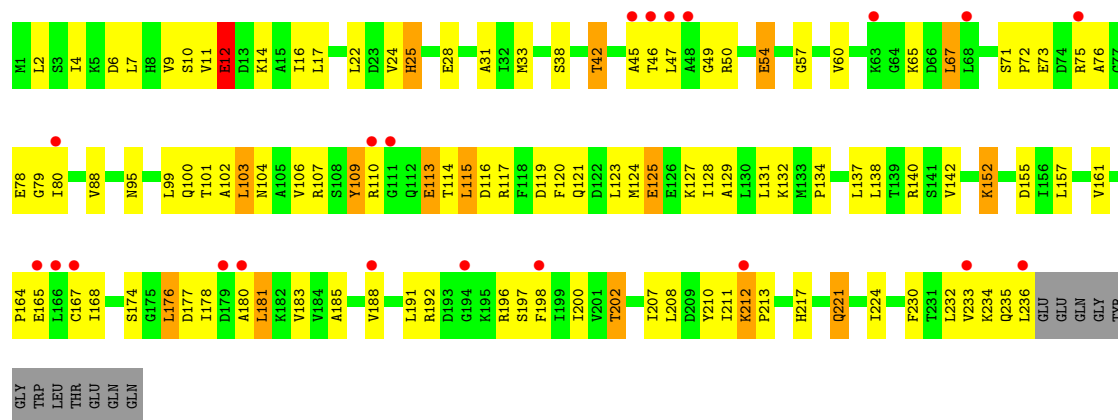


• Molecule 3: Probable ATP-dependent transporter SufC



• Molecule 3: Probable ATP-dependent transporter SufC





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.85Å 139.38Å 124.41Å 90.00° 113.55° 90.00°	Depositor
Resolution (Å)	43.94 – 4.28 43.94 – 4.28	Depositor EDS
% Data completeness (in resolution range)	98.4 (43.94-4.28) 92.8 (43.94-4.28)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 4.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.295 , 0.340 0.300 , 0.346	Depositor DCC
R_{free} test set	1291 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	94.9	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 56.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.025 for l,-k,h	Xtriage
F_o, F_c correlation	0.81	EDS
Total number of atoms	18808	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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: HG

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	0.47	0/3031	1.23	21/4104 (0.5%)
1	E	0.51	0/2972	1.34	38/4025 (0.9%)
2	B	0.44	0/2847	1.10	19/3858 (0.5%)
2	F	0.48	0/2800	1.25	27/3794 (0.7%)
3	C	0.46	0/1875	1.28	16/2529 (0.6%)
3	D	0.43	0/1858	1.19	11/2506 (0.4%)
3	G	0.43	0/1893	1.10	9/2553 (0.4%)
3	H	0.48	0/1866	1.37	27/2517 (1.1%)
All	All	0.47	0/19142	1.24	168/25886 (0.6%)

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	E	0	2
2	F	0	1
3	D	0	1
3	G	0	2
3	H	0	1
All	All	0	7

There are no bond length outliers.

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	211	VAL	CA-C-N	13.68	135.43	120.11
1	A	211	VAL	C-N-CA	13.68	135.43	120.11
1	E	232	THR	N-CA-C	11.46	127.17	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	192	LEU	N-CA-C	11.30	123.67	111.36
3	C	207	ILE	N-CA-C	10.92	124.70	111.05
1	E	217	CYS	CA-C-N	10.84	131.09	119.05
1	E	217	CYS	C-N-CA	10.84	131.09	119.05
3	H	212	LYS	CA-C-N	10.60	130.70	120.31
3	H	212	LYS	C-N-CA	10.60	130.70	120.31
3	C	206	ARG	CA-C-N	10.35	136.82	120.47
3	C	206	ARG	C-N-CA	10.35	136.82	120.47
3	D	203	HIS	N-CA-C	-9.46	99.31	112.45
3	D	16	ILE	N-CA-C	9.42	120.33	111.48
3	D	205	GLN	N-CA-C	9.11	124.19	112.89
1	E	256	ALA	N-CA-C	8.98	116.22	108.13
2	F	414	ILE	N-CA-C	-8.94	101.84	110.42
3	C	235	GLN	N-CA-C	8.84	120.91	111.28
1	E	256	ALA	CA-C-N	8.78	129.32	119.92
1	E	256	ALA	C-N-CA	8.78	129.32	119.92
2	B	94	VAL	CA-C-N	8.71	128.30	119.24
2	B	94	VAL	C-N-CA	8.71	128.30	119.24
3	G	86	TYR	CA-C-N	8.53	128.60	119.90
3	G	86	TYR	C-N-CA	8.53	128.60	119.90
1	E	211	VAL	CA-C-N	8.22	128.17	120.03
1	E	211	VAL	C-N-CA	8.22	128.17	120.03
2	F	94	VAL	CA-C-N	8.20	127.77	119.24
2	F	94	VAL	C-N-CA	8.20	127.77	119.24
3	H	109	TYR	N-CA-C	-8.20	99.69	110.43
2	F	192	LEU	CB-CA-C	-8.19	96.93	110.85
3	D	16	ILE	CB-CA-C	-8.12	104.81	111.71
3	D	71	SER	CA-C-N	7.88	127.44	119.24
3	D	71	SER	C-N-CA	7.88	127.44	119.24
1	A	308	GLU	N-CA-C	7.57	119.31	111.14
3	H	233	VAL	N-CA-C	7.56	119.23	110.62
1	E	74	HIS	N-CA-C	7.49	121.53	110.30
1	A	258	VAL	N-CA-C	7.46	119.57	108.46
1	E	273	ILE	N-CA-C	7.34	118.47	107.75
3	H	100	GLN	N-CA-C	7.33	118.91	111.07
2	F	150	LYS	CA-C-N	7.27	127.19	119.85
2	F	150	LYS	C-N-CA	7.27	127.19	119.85
3	G	118	PHE	N-CA-C	7.26	122.54	112.45
1	A	198	LEU	N-CA-C	7.12	119.90	111.71
1	A	72	GLU	CA-C-N	7.11	126.87	119.76
1	A	72	GLU	C-N-CA	7.11	126.87	119.76
3	H	232	LEU	N-CA-C	6.96	119.71	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	194	GLY	N-CA-C	-6.95	105.73	115.32
1	A	215	VAL	N-CA-C	6.89	118.05	107.99
1	E	67	TRP	N-CA-C	6.89	119.81	111.82
2	F	379	GLY	N-CA-C	6.84	124.08	114.85
3	H	117	ARG	N-CA-C	6.79	119.26	111.11
1	E	231	LYS	N-CA-C	-6.75	97.73	108.73
2	F	395	ALA	N-CA-C	6.71	119.16	111.11
1	E	286	ASN	N-CA-C	6.67	119.34	107.80
2	F	387	GLN	N-CA-C	6.64	118.52	111.28
3	H	16	ILE	N-CA-C	6.63	116.73	110.30
2	B	127	LEU	N-CA-C	6.62	118.57	111.36
1	E	161	GLU	CA-C-N	6.53	133.45	121.70
1	E	161	GLU	C-N-CA	6.53	133.45	121.70
1	A	273	ILE	N-CA-C	6.44	117.15	107.75
2	F	194	ASP	N-CA-C	-6.43	105.40	113.18
3	H	202	THR	N-CA-C	6.38	119.72	110.28
2	B	105	GLY	N-CA-C	-6.37	106.28	115.27
2	B	70	SER	CA-C-N	6.32	126.23	119.28
2	B	70	SER	C-N-CA	6.32	126.23	119.28
3	H	197	SER	N-CA-C	6.29	119.28	109.52
1	E	228	ASN	N-CA-C	-6.29	104.82	113.18
1	E	52	GLU	CA-C-N	6.25	127.65	119.84
1	E	52	GLU	C-N-CA	6.25	127.65	119.84
3	G	203	HIS	N-CA-C	-6.24	103.78	112.45
1	E	329	TYR	CA-C-N	-6.22	112.07	119.84
1	E	329	TYR	C-N-CA	-6.22	112.07	119.84
1	E	411	GLY	N-CA-C	-6.13	104.91	112.33
2	B	307	ASP	N-CA-C	6.10	123.80	110.80
3	C	205	GLN	N-CA-C	-6.08	104.77	111.82
1	E	306	LEU	CA-C-N	6.05	131.31	122.41
1	E	306	LEU	C-N-CA	6.05	131.31	122.41
3	G	111	GLY	N-CA-C	6.01	127.42	113.18
3	H	103	LEU	N-CA-C	-6.00	104.65	111.07
2	B	222	ASN	CA-C-N	6.00	125.68	119.56
2	B	222	ASN	C-N-CA	6.00	125.68	119.56
3	H	132	LYS	CA-CB-CG	5.99	126.08	114.10
3	H	101	THR	N-CA-C	5.95	117.77	111.28
3	H	67	LEU	N-CA-C	5.95	117.85	111.36
1	A	286	ASN	N-CA-C	5.95	118.09	107.80
2	F	94	VAL	N-CA-C	5.93	114.02	108.15
3	C	209	ASP	N-CA-C	-5.89	105.58	112.89
3	H	221	GLN	CB-CA-C	5.88	120.78	111.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	133	LEU	N-CA-C	5.87	120.44	113.28
1	E	372	ILE	N-CA-C	5.86	116.31	108.11
1	A	439	ARG	N-CA-C	5.85	117.14	108.60
1	E	190	GLY	N-CA-C	-5.85	105.09	113.86
3	D	17	LEU	N-CA-C	5.83	119.13	109.46
3	C	7	LEU	N-CA-C	5.82	118.15	109.59
2	F	410	VAL	N-CA-C	-5.82	104.84	110.72
3	G	117	ARG	N-CA-C	5.79	118.34	111.33
3	H	42	THR	N-CA-C	5.71	118.44	111.82
3	H	12	GLU	CA-CB-CG	5.68	125.46	114.10
3	H	7	LEU	N-CA-C	5.67	117.92	109.59
1	E	296	GLY	N-CA-C	5.65	123.61	114.90
3	H	132	LYS	N-CA-C	5.65	119.19	111.39
2	F	248	LEU	N-CA-C	5.64	117.27	109.54
3	G	75	ARG	N-CA-C	5.64	117.43	111.28
3	D	207	ILE	N-CA-C	5.64	118.10	111.05
1	A	232	THR	N-CA-C	5.63	117.11	110.97
1	A	492	HIS	CB-CA-C	-5.62	100.24	110.63
3	D	222	GLY	N-CA-C	5.61	123.54	114.90
2	F	191	SER	N-CA-C	5.60	118.94	109.76
2	B	164	GLU	N-CA-C	-5.58	106.14	113.17
1	A	226	ARG	CA-C-N	5.56	128.08	120.35
1	A	226	ARG	C-N-CA	5.56	128.08	120.35
3	C	75	ARG	N-CA-C	5.55	117.33	111.28
2	F	321	GLN	N-CA-CB	5.53	118.17	110.04
2	F	128	HIS	N-CA-C	-5.53	105.26	111.28
1	E	331	SER	N-CA-C	5.50	118.60	110.46
1	E	217	CYS	N-CA-C	5.50	117.40	109.48
3	D	200	ILE	N-CA-C	5.50	115.24	106.88
1	E	163	GLY	N-CA-C	5.50	126.21	113.18
1	E	194	PHE	CB-CA-C	5.49	119.65	110.92
3	H	129	ALA	N-CA-C	5.49	117.07	111.14
3	H	76	ALA	N-CA-C	-5.41	105.46	111.36
3	H	124	MET	N-CA-C	5.41	116.87	110.97
3	C	181	LEU	N-CA-C	5.40	117.17	111.28
1	E	479	ALA	N-CA-C	5.39	116.84	111.07
3	H	132	LYS	N-CA-CB	-5.38	103.74	111.70
1	A	422	VAL	N-CA-C	5.38	115.83	107.28
2	F	256	ASN	N-CA-C	5.38	118.16	109.40
1	A	390	VAL	N-CA-C	5.37	115.32	107.37
2	F	144	ARG	N-CA-C	5.37	118.13	110.24
3	G	151	LYS	N-CA-C	5.35	117.19	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	200	ILE	N-CA-C	5.32	114.96	106.88
1	E	224	TYR	N-CA-C	5.32	118.06	110.24
3	H	230	PHE	N-CA-C	5.28	118.51	111.75
2	F	351	ILE	N-CA-C	5.27	115.44	107.80
1	E	260	ASP	N-CA-C	-5.25	99.63	110.80
3	C	200	ILE	N-CA-C	5.23	114.83	106.88
3	C	71	SER	CA-C-N	5.22	125.27	119.32
3	C	71	SER	C-N-CA	5.22	125.27	119.32
2	B	379	GLY	N-CA-C	5.22	121.90	114.85
2	F	307	ASP	N-CA-C	5.21	121.90	110.80
2	B	66	ALA	N-CA-C	5.21	117.16	107.99
2	B	305	VAL	N-CA-C	5.20	115.34	107.80
2	F	147	ARG	CA-C-N	5.20	125.21	119.90
2	F	147	ARG	C-N-CA	5.20	125.21	119.90
2	F	159	GLN	CA-CB-CG	5.20	124.50	114.10
2	F	339	LYS	N-CA-C	5.16	119.21	113.01
2	F	251	ALA	N-CA-C	-5.16	105.73	111.36
2	B	69	ILE	N-CA-C	5.15	116.28	108.96
3	C	157	LEU	N-CA-C	-5.15	105.67	111.28
2	B	227	HIS	N-CA-C	5.13	117.16	108.02
1	E	308	GLU	N-CA-C	5.13	117.67	111.40
1	A	160	ALA	N-CA-C	5.12	117.08	108.73
1	A	413	ASN	CB-CA-C	5.12	118.90	109.99
3	H	57	GLY	N-CA-C	5.12	117.95	110.38
1	E	68	LEU	N-CA-C	5.11	116.93	111.36
1	A	161	GLU	CA-C-N	5.11	130.89	121.70
1	A	161	GLU	C-N-CA	5.11	130.89	121.70
1	E	49	LYS	CA-C-N	5.10	129.56	122.77
1	E	49	LYS	C-N-CA	5.10	129.56	122.77
3	H	161	VAL	N-CA-C	5.10	116.56	111.00
1	E	50	ARG	N-CA-C	-5.09	100.44	108.73
2	B	418	LEU	CA-C-N	-5.07	113.50	119.84
2	B	418	LEU	C-N-CA	-5.07	113.50	119.84
3	H	200	ILE	N-CA-C	5.07	114.59	106.88
2	B	125	VAL	N-CA-C	5.06	119.87	109.34
3	C	117	ARG	CA-C-N	5.02	127.26	120.38
3	C	117	ARG	C-N-CA	5.02	127.26	120.38
2	B	230	HIS	N-CA-C	5.01	116.33	107.61
3	D	112	GLN	N-CA-C	-5.00	102.07	109.18

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	113	GLU	Peptide
1	E	231	LYS	Peptide
1	E	61	LEU	Peptide
2	F	321	GLN	Sidechain
3	G	115	LEU	Peptide
3	G	116	ASP	Peptide
3	H	115	LEU	Peptide

5.2 Too-close contacts [i](#)

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	2968	0	2876	158	0
1	E	2910	0	2816	192	0
2	B	2798	0	2754	94	0
2	F	2752	0	2707	153	0
3	C	1846	0	1857	74	0
3	D	1829	0	1840	60	0
3	G	1864	0	1871	61	0
3	H	1837	0	1851	83	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	18808	0	18572	828	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 22.

All (828) 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:A:332:CYS:HB2	1:A:361:MET:HE3	1.45	0.98
2:F:85:ARG:HB2	2:F:155:MET:HE1	1.41	0.98
1:E:161:GLU:HA	1:E:162:GLN:HG3	1.46	0.98
3:C:133:MET:HE2	3:C:154:ASN:HD22	1.29	0.97
2:F:230:HIS:HA	2:F:256:ASN:ND2	1.81	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:314:MET:SD	1:E:314:MET:N	2.43	0.91
2:B:249:GLY:HA2	2:B:417:ARG:HH22	1.36	0.91
1:A:316:TRP:HB3	1:A:318:GLN:HE22	1.34	0.90
1:E:301:VAL:HG23	1:E:328:LYS:HD3	1.55	0.89
1:A:448:CYS:HB3	1:A:453:ILE:HD11	1.54	0.88
1:E:435:ALA:HB3	2:F:360:HIS:CD2	2.10	0.87
2:F:92:ARG:NH1	2:F:93:TYR:O	2.09	0.86
2:F:230:HIS:HA	2:F:256:ASN:HD21	1.39	0.84
1:A:216:ARG:NH1	1:A:217:CYS:O	2.10	0.83
1:E:328:LYS:HG3	1:E:330:PRO:HD3	1.58	0.83
3:H:176:LEU:HD21	3:H:181:LEU:HB2	1.61	0.83
3:C:193:ASP:HB2	3:C:195:LYS:HG2	1.61	0.82
1:E:409:LEU:HG	1:E:414:CYS:SG	2.20	0.81
3:G:171:GLU:HB2	3:G:203:HIS:HB2	1.63	0.80
2:B:276:PRO:HG3	2:B:282:CYS:HB2	1.60	0.80
3:G:233:VAL:HA	3:G:236:LEU:HD23	1.63	0.79
1:E:335:ARG:HA	1:E:364:ILE:HB	1.65	0.79
3:C:195:LYS:HG3	3:C:196:ARG:H	1.48	0.79
2:B:89:VAL:HG22	2:B:157:ILE:HD11	1.65	0.78
1:E:321:THR:HG22	1:E:348:LEU:HB3	1.64	0.78
1:E:286:ASN:HD21	1:E:485:LEU:HD13	1.48	0.78
2:F:296:ASN:OD1	2:F:298:ARG:NH1	2.18	0.77
2:F:248:LEU:HD21	2:F:275:MET:HB2	1.66	0.76
3:C:133:MET:HE2	3:C:154:ASN:ND2	2.00	0.76
3:D:67:LEU:O	3:D:75:ARG:NH1	2.15	0.76
3:C:207:ILE:HD11	3:C:211:ILE:HD12	1.67	0.76
1:A:451:ARG:NH1	3:C:158:GLN:OE1	2.19	0.76
1:E:289:PRO:HG3	1:E:294:THR:HA	1.66	0.76
1:E:303:LYS:H	1:E:328:LYS:HZ1	1.30	0.76
1:E:350:SER:H	1:E:353:GLN:HE21	1.32	0.76
3:C:133:MET:CE	3:C:154:ASN:HD22	1.99	0.75
1:E:437:THR:HG21	2:F:358:CYS:H	1.52	0.75
2:F:378:ARG:NH1	3:H:99:LEU:HA	2.02	0.75
3:H:79:GLY:O	3:H:165:GLU:N	2.21	0.74
1:E:381:HIS:CD2	1:E:413:ASN:HD22	2.05	0.74
2:F:283:ASP:HB2	2:F:312:VAL:HB	1.69	0.74
3:D:179:ASP:OD1	3:D:180:ALA:N	2.21	0.74
3:D:1:MET:N	3:D:24:VAL:O	2.21	0.73
1:E:414:CYS:SG	1:E:415:GLY:N	2.61	0.73
1:E:234:GLN:NE2	1:E:263:GLN:OE1	2.22	0.73
2:F:77:LEU:HD13	2:F:190:VAL:HG21	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:68:LEU:HD12	1:E:69:GLU:HG2	1.71	0.73
2:F:147:ARG:HH21	2:F:147:ARG:HG3	1.52	0.73
3:C:17:LEU:HD21	3:C:39:GLY:HA3	1.69	0.72
1:E:292:ASN:OD1	1:E:293:ASN:N	2.21	0.72
1:A:254:CYS:N	1:A:285:GLN:OE1	2.23	0.72
3:C:123:LEU:HD11	3:C:127:LYS:HE3	1.70	0.72
1:E:343:PHE:HB3	1:E:372:ILE:HG12	1.71	0.72
3:D:191:LEU:HB3	3:D:198:PHE:HZ	1.55	0.71
2:B:189:PHE:HB2	2:B:219:ALA:HA	1.71	0.71
3:H:11:VAL:O	3:H:12:GLU:HG2	1.91	0.71
3:H:60:VAL:HG23	3:H:67:LEU:HB3	1.73	0.71
1:E:329:TYR:OH	1:E:387:ARG:NH1	2.24	0.70
2:F:247:LEU:HB3	2:F:253:LEU:HD11	1.73	0.70
2:F:133:LEU:HD21	2:F:170:HIS:CD2	2.25	0.70
1:A:331:SER:OG	1:A:360:LYS:O	2.08	0.70
2:F:191:SER:HB3	2:F:222:ASN:H	1.56	0.70
3:C:148:GLY:HA2	3:C:151:LYS:HE3	1.72	0.70
3:G:67:LEU:HD11	3:G:75:ARG:HG3	1.72	0.70
1:E:356:ASP:OD2	1:E:387:ARG:NH2	2.25	0.70
2:B:159:GLN:O	2:B:167:ASN:ND2	2.23	0.69
3:H:47:LEU:HB3	3:H:75:ARG:HH12	1.57	0.69
2:B:182:GLU:HB2	2:B:212:HIS:HB2	1.73	0.69
1:E:316:TRP:HZ3	1:E:332:CYS:HG	1.40	0.69
1:E:418:THR:HG22	1:E:420:PRO:HD3	1.74	0.69
1:E:428:SER:O	2:F:366:ARG:NH2	2.25	0.69
2:F:324:ILE:HG23	2:F:355:ASP:HB3	1.72	0.69
1:A:446:PHE:HA	1:A:449:LEU:HG	1.75	0.69
3:H:177:ASP:OD1	3:H:178:ILE:N	2.23	0.69
1:E:293:ASN:O	1:E:294:THR:OG1	2.10	0.69
2:B:378:ARG:HE	3:D:98:PHE:HZ	1.41	0.68
2:F:256:ASN:HA	2:F:285:ARG:O	1.92	0.68
2:B:324:ILE:HD11	2:B:355:ASP:HB3	1.75	0.68
2:F:333:ASN:HD22	2:F:333:ASN:N	1.91	0.68
2:B:203:PHE:O	2:B:232:ASP:N	2.25	0.68
3:D:208:LEU:HD22	3:D:213:PRO:HG3	1.74	0.68
1:E:361:MET:SD	1:E:390:VAL:HG22	2.34	0.68
1:A:419:PHE:HB3	2:B:348:GLN:HG3	1.75	0.68
1:E:189:PRO:HD2	1:E:192:ASP:HB2	1.74	0.68
1:E:243:ASP:HA	1:E:274:HIS:CE1	2.28	0.67
3:H:11:VAL:HG12	3:H:12:GLU:OE1	1.93	0.67
1:E:488:ILE:HA	1:E:491:GLU:HG2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:399:GLU:OE1	2:F:407:LYS:NZ	2.25	0.67
2:B:308:LYS:HB2	2:B:340:LEU:HD22	1.77	0.67
3:D:47:LEU:HD23	3:D:168:ILE:HD13	1.76	0.66
1:E:251:ILE:HG13	1:E:478:PHE:HE2	1.61	0.66
2:F:157:ILE:O	2:F:171:TYR:OH	2.14	0.66
3:H:45:ALA:HB1	3:H:50:ARG:HD3	1.77	0.66
2:F:114:ARG:HG3	2:F:117:LEU:HB2	1.75	0.66
3:H:2:LEU:HB3	3:H:24:VAL:HB	1.77	0.66
2:F:225:SER:O	2:F:251:ALA:N	2.26	0.65
1:A:196:ALA:HA	1:A:199:ASN:HD21	1.62	0.65
1:A:418:THR:HG22	1:A:420:PRO:HD3	1.77	0.65
2:F:192:LEU:O	2:F:193:ASN:ND2	2.27	0.65
2:B:143:LYS:HG3	2:B:146:GLN:HG3	1.79	0.65
2:F:381:ASN:OD1	2:F:382:GLN:N	2.30	0.65
2:F:189:PHE:HB2	2:F:219:ALA:HA	1.76	0.65
1:A:451:ARG:HH22	3:C:155:ASP:HB2	1.61	0.65
1:E:326:THR:O	1:E:356:ASP:N	2.30	0.65
2:F:275:MET:HG2	2:F:304:ILE:HB	1.78	0.65
3:C:225:VAL:HG23	3:C:226:LYS:HG2	1.79	0.65
3:C:104:ASN:OD1	3:C:105:ALA:N	2.29	0.65
1:A:291:ASP:HA	1:A:492:HIS:HE1	1.62	0.64
2:F:174:HIS:NE2	2:F:176:ASP:OD1	2.30	0.64
1:A:391:LYS:HE3	1:A:423:GLU:HB2	1.80	0.64
3:C:217:HIS:N	3:C:217:HIS:CD2	2.66	0.64
3:D:185:ALA:HA	3:D:211:ILE:HD11	1.80	0.64
3:H:191:LEU:HD13	3:H:196:ARG:CZ	2.28	0.64
2:F:277:VAL:HG12	2:F:278:LYS:H	1.62	0.64
2:F:269:ARG:HG2	2:F:298:ARG:HB2	1.79	0.64
3:C:22:LEU:HD13	3:C:217:HIS:CE1	2.33	0.64
1:E:58:GLU:HG3	1:E:62:ASN:OD1	1.97	0.64
2:B:368:ASP:HB3	2:B:371:GLN:HE21	1.63	0.63
3:C:47:LEU:O	3:C:75:ARG:NH2	2.29	0.63
1:A:344:TYR:HB3	1:A:470:VAL:HG13	1.81	0.63
2:F:277:VAL:HA	2:F:306:SER:HB2	1.81	0.63
1:A:335:ARG:HA	1:A:364:ILE:HB	1.80	0.63
3:D:221:GLN:OE1	3:D:221:GLN:N	2.32	0.63
1:E:459:ILE:HD12	1:E:460:SER:N	2.14	0.62
2:F:310:ARG:HG3	2:F:342:GLU:HB3	1.80	0.62
1:A:61:LEU:O	1:A:65:ARG:HG3	1.98	0.62
2:B:204:THR:HA	2:B:232:ASP:HB2	1.80	0.62
1:A:372:ILE:HB	1:A:403:THR:HG23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:390:VAL:N	1:E:421:TYR:O	2.29	0.62
2:F:113:ASP:OD2	2:F:115:GLN:NE2	2.32	0.62
3:C:33:MET:HG2	3:C:34:GLY:H	1.64	0.62
3:C:17:LEU:HD13	3:C:20:LEU:HD21	1.80	0.62
2:F:329:GLN:HA	2:F:359:SER:O	1.99	0.62
3:G:7:LEU:HA	3:G:58:GLY:HA3	1.80	0.62
2:B:173:HIS:HB2	2:B:203:PHE:CE1	2.35	0.62
1:E:435:ALA:O	2:F:359:SER:OG	2.12	0.62
2:F:204:THR:HG22	2:F:232:ASP:HB2	1.81	0.62
1:E:291:ASP:CG	1:E:292:ASN:HB2	2.24	0.61
2:F:301:HIS:O	2:F:332:ASN:HA	2.00	0.61
1:A:62:ASN:OD1	1:A:63:ALA:N	2.33	0.61
3:H:152:LYS:NZ	3:H:174:SER:O	2.29	0.61
1:E:199:ASN:ND2	1:E:266:ALA:O	2.34	0.61
2:F:308:LYS:HE2	2:F:340:LEU:HD23	1.81	0.61
3:G:4:ILE:HD12	3:G:22:LEU:HB3	1.83	0.61
2:F:196:ARG:HG3	2:F:224:LEU:O	1.99	0.61
1:A:409:LEU:HD23	2:B:354:ASP:HB3	1.83	0.61
1:A:477:GLU:OE1	1:A:477:GLU:N	2.33	0.61
3:D:1:MET:HE3	3:D:166:LEU:HB2	1.82	0.61
2:B:74:ARG:HG2	2:B:75:ASP:N	2.16	0.61
3:C:22:LEU:HD13	3:C:217:HIS:HE1	1.66	0.61
2:F:111:ASN:O	2:F:137:VAL:N	2.31	0.61
2:F:137:VAL:HG13	2:F:172:ARG:CZ	2.31	0.61
3:G:45:ALA:HB2	3:G:50:ARG:HH21	1.66	0.61
1:A:459:ILE:HD12	1:A:460:SER:N	2.17	0.60
3:C:216:VAL:O	3:C:228:GLY:N	2.33	0.60
1:E:251:ILE:HD12	1:E:282:SER:HB2	1.84	0.60
1:E:350:SER:H	1:E:353:GLN:NE2	2.00	0.60
3:C:152:LYS:HD2	3:C:172:SER:O	2.02	0.60
2:F:277:VAL:HG21	2:F:417:ARG:HG2	1.83	0.60
2:B:174:HIS:NE2	2:B:176:ASP:OD1	2.34	0.60
2:B:187:GLU:O	2:B:218:LEU:N	2.28	0.60
1:E:313:LYS:HG2	1:E:340:ILE:HD11	1.81	0.60
2:F:374:TYR:OH	3:H:155:ASP:OD1	2.16	0.60
1:A:358:GLY:HA3	1:A:387:ARG:O	2.02	0.60
3:D:25:HIS:HB2	3:D:28:GLU:CD	2.25	0.60
1:A:62:ASN:HA	1:A:65:ARG:HE	1.67	0.60
3:D:181:LEU:HD11	3:D:207:ILE:HD12	1.83	0.60
2:F:302:LYS:HE3	2:F:333:ASN:HB2	1.82	0.60
1:A:283:THR:HB	1:A:318:GLN:HG3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:316:TRP:HZ3	1:E:332:CYS:SG	2.24	0.59
3:G:136:ASP:O	3:G:140:ARG:HG3	2.02	0.59
3:C:25:HIS:O	3:C:28:GLU:HG3	2.02	0.59
1:E:350:SER:O	1:E:353:GLN:HG2	2.01	0.59
2:F:324:ILE:HD12	2:F:355:ASP:HB3	1.85	0.59
3:G:220:TYR:CD1	3:G:221:GLN:HG2	2.37	0.59
1:E:280:LYS:HD2	1:E:315:SER:HB3	1.84	0.59
1:A:192:ASP:OD1	1:A:193:ASN:N	2.35	0.59
1:A:42:VAL:O	1:A:46:ILE:HG13	2.02	0.59
1:E:70:MET:SD	1:E:194:PHE:HA	2.42	0.59
2:F:382:GLN:HG2	2:F:383:GLN:N	2.18	0.59
2:B:209:ALA:HA	2:B:237:GLU:O	2.02	0.59
3:C:9:VAL:HG21	3:C:46:THR:HG21	1.83	0.59
1:A:477:GLU:CD	1:A:477:GLU:H	2.11	0.59
2:F:158:THR:HG23	2:F:169:ALA:HB3	1.84	0.59
1:E:303:LYS:HG3	1:E:328:LYS:HZ1	1.67	0.59
3:H:115:LEU:HD21	3:H:120:PHE:N	2.18	0.59
3:H:185:ALA:HA	3:H:211:ILE:HD11	1.84	0.59
3:C:206:ARG:NH1	3:C:207:ILE:HB	2.18	0.59
2:F:173:HIS:HB2	2:F:203:PHE:CD1	2.38	0.59
2:F:173:HIS:HB2	2:F:203:PHE:HD1	1.68	0.59
3:G:100:GLN:HE22	3:G:115:LEU:HD11	1.68	0.59
1:A:252:GLU:OE1	1:A:281:TYR:OH	2.17	0.58
1:E:308:GLU:N	1:E:309:GLY:HA3	2.17	0.58
1:E:349:THR:HA	1:E:353:GLN:HE21	1.66	0.58
2:F:265:ASN:H	2:F:294:PHE:HB2	1.67	0.58
2:B:187:GLU:OE2	2:B:215:HIS:NE2	2.33	0.58
2:F:248:LEU:HB3	2:F:413:ARG:HD3	1.85	0.58
1:A:161:GLU:HA	1:A:162:GLN:HB2	1.85	0.58
1:A:387:ARG:HB2	1:A:419:PHE:HD1	1.68	0.58
1:E:404:GLN:NE2	1:E:434:GLU:OE1	2.36	0.58
3:C:155:ASP:OD1	3:C:156:ILE:N	2.37	0.58
2:F:331:THR:HG22	2:F:333:ASN:HD21	1.67	0.58
3:D:167:CYS:HB2	3:D:198:PHE:CD1	2.39	0.58
1:E:447:TYR:OH	3:G:155:ASP:OD1	2.22	0.58
2:F:137:VAL:HG13	2:F:172:ARG:NH2	2.18	0.58
2:F:331:THR:HG22	2:F:333:ASN:ND2	2.19	0.58
2:F:331:THR:HA	2:F:361:GLY:O	2.03	0.58
3:G:40:LYS:HG3	3:G:41:SER:N	2.19	0.58
2:B:331:THR:HA	2:B:361:GLY:O	2.04	0.58
3:D:70:LEU:HB2	3:D:75:ARG:NH1	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:217:HIS:HB3	3:H:224:ILE:HD12	1.86	0.57
2:B:122:GLN:O	2:B:122:GLN:HG3	2.03	0.57
1:E:464:ASN:CG	1:E:483:GLN:HE21	2.12	0.57
3:H:45:ALA:HB1	3:H:50:ARG:CD	2.35	0.57
1:A:304:ARG:HG2	1:A:331:SER:CB	2.35	0.57
1:A:383:GLN:HA	1:A:415:GLY:O	2.04	0.57
1:A:304:ARG:HG2	1:A:331:SER:HB3	1.86	0.57
3:H:31:ALA:O	3:H:217:HIS:N	2.32	0.57
1:A:294:THR:OG1	1:A:296:GLY:HA3	2.04	0.57
1:E:349:THR:OG1	1:E:382:SER:OG	2.19	0.57
1:A:188:VAL:HG23	1:A:270:GLU:HG3	1.86	0.57
2:F:196:ARG:NH1	2:F:224:LEU:O	2.38	0.57
1:E:260:ASP:N	1:E:260:ASP:OD1	2.38	0.56
3:H:65:LYS:NZ	3:H:78:GLU:OE2	2.38	0.56
3:D:44:SER:HB3	3:D:82:MET:SD	2.45	0.56
3:H:9:VAL:HG13	3:H:54:GLU:O	2.05	0.56
1:A:35:ALA:HB1	1:A:36:LYS:HA	1.88	0.56
1:A:67:TRP:CZ3	1:A:198:LEU:HB2	2.40	0.56
1:E:184:LEU:HD11	1:E:237:ARG:NH1	2.21	0.56
1:E:174:HIS:HA	1:E:177:PRO:HG3	1.86	0.56
1:E:398:ASN:HA	1:E:428:SER:O	2.05	0.56
2:F:108:VAL:HA	2:F:139:HIS:O	2.06	0.56
3:H:71:SER:OG	3:H:73:GLU:OE1	2.18	0.56
3:D:126:GLU:O	3:D:130:LEU:HD13	2.05	0.56
1:E:283:THR:HB	1:E:318:GLN:OE1	2.06	0.56
2:F:327:ASP:HA	2:F:357:LYS:O	2.06	0.56
3:H:78:GLU:CD	3:H:110:ARG:HH12	2.13	0.56
2:F:415:GLY:O	2:F:418:LEU:HG	2.06	0.56
2:B:125:VAL:HA	2:B:128:HIS:NE2	2.21	0.55
1:E:265:HIS:HB2	1:E:299:ASN:HA	1.88	0.55
1:A:71:GLU:N	1:A:71:GLU:OE1	2.39	0.55
1:A:291:ASP:HA	1:A:492:HIS:CE1	2.41	0.55
1:E:161:GLU:CD	1:E:164:ILE:HG12	2.30	0.55
1:E:251:ILE:HG13	1:E:478:PHE:CE2	2.41	0.55
1:A:182:LYS:HE3	1:A:183:TYR:CE2	2.42	0.55
3:C:73:GLU:OE1	3:C:73:GLU:N	2.34	0.55
2:F:248:LEU:HD22	2:F:417:ARG:HD2	1.87	0.55
3:G:84:PHE:HD2	3:G:86:TYR:H	1.55	0.55
1:E:234:GLN:HG3	1:E:264:LEU:O	2.06	0.55
2:F:80:THR:HG22	2:F:409:GLN:NE2	2.21	0.55
2:B:329:GLN:HA	2:B:359:SER:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:56:MET:O	1:E:60:ARG:HG3	2.07	0.55
1:E:195:PHE:CE2	1:E:300:PHE:HD2	2.24	0.55
1:E:209:ILE:HD13	1:E:221:LEU:HD13	1.89	0.55
3:G:167:CYS:HB2	3:G:198:PHE:CD1	2.42	0.55
3:H:12:GLU:HG3	3:H:14:LYS:HE2	1.88	0.55
1:A:380:GLY:O	1:A:414:CYS:HB3	2.06	0.55
2:B:306:SER:HB3	2:B:337:MET:HE3	1.88	0.55
1:A:296:GLY:HA2	1:A:324:ALA:HB2	1.89	0.55
1:A:303:LYS:HZ1	1:A:318:GLN:HG2	1.71	0.55
3:C:99:LEU:HD21	3:C:158:GLN:HG2	1.88	0.55
2:F:209:ALA:HA	2:F:237:GLU:O	2.07	0.54
3:G:33:MET:HE1	3:G:236:LEU:HD22	1.87	0.54
2:F:171:TYR:O	2:F:201:ALA:HA	2.08	0.54
1:A:67:TRP:CH2	1:A:198:LEU:HD22	2.41	0.54
1:E:427:ASN:HB3	2:F:338:GLY:O	2.07	0.54
1:E:450:GLN:HE22	1:E:451:ARG:HH11	1.56	0.54
3:H:181:LEU:HD21	3:H:210:TYR:CD2	2.43	0.54
2:B:340:LEU:HD23	2:B:340:LEU:O	2.07	0.54
1:E:318:GLN:HB3	1:E:345:SER:HA	1.90	0.54
1:E:161:GLU:HG3	1:E:164:ILE:HG12	1.90	0.54
1:E:303:LYS:HG3	1:E:328:LYS:NZ	2.23	0.54
1:E:439:ARG:NH1	2:F:354:ASP:OD2	2.40	0.54
2:F:368:ASP:HB3	2:F:371:GLN:HB3	1.90	0.54
2:F:386:GLN:OE1	2:F:419:PRO:HG3	2.08	0.54
3:G:96:GLN:HB2	3:G:138:LEU:HD12	1.90	0.54
3:H:10:SER:OG	3:H:14:LYS:O	2.23	0.54
1:A:389:LEU:HD11	1:A:391:LYS:HD2	1.89	0.54
2:B:283:ASP:CB	2:B:312:VAL:HB	2.38	0.54
1:A:343:PHE:HD2	1:A:372:ILE:HG23	1.73	0.54
1:A:356:ASP:OD1	1:A:387:ARG:NH1	2.41	0.54
1:A:413:ASN:OD1	1:A:413:ASN:O	2.25	0.54
1:E:435:ALA:CB	2:F:360:HIS:CD2	2.90	0.54
1:A:435:ALA:O	2:B:359:SER:HB2	2.08	0.53
1:E:187:VAL:HG22	1:E:306:LEU:HB3	1.90	0.53
1:E:313:LYS:HG2	1:E:340:ILE:CG1	2.37	0.53
1:E:398:ASN:N	1:E:428:SER:OG	2.31	0.53
1:E:300:PHE:HE1	1:E:325:ILE:HG23	1.71	0.53
3:G:148:GLY:O	3:G:151:LYS:HG2	2.08	0.53
2:F:291:ASN:HA	2:F:320:ALA:HB3	1.90	0.53
1:E:247:TYR:HB2	1:E:278:GLU:HB3	1.90	0.53
1:E:286:ASN:ND2	1:E:485:LEU:HD13	2.22	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:GLU:N	1:A:309:GLY:HA3	2.24	0.53
2:B:328:GLY:O	2:B:358:CYS:SG	2.66	0.53
1:E:262:TYR:HA	1:E:296:GLY:O	2.09	0.53
1:E:450:GLN:OE1	1:E:451:ARG:HD3	2.09	0.53
3:H:67:LEU:HD21	3:H:75:ARG:CZ	2.39	0.53
1:A:321:THR:HG23	1:A:348:LEU:HD23	1.90	0.53
3:D:131:LEU:HD22	3:D:157:LEU:HB2	1.91	0.53
1:E:299:ASN:C	1:E:300:PHE:HD1	2.15	0.53
1:A:300:PHE:HA	1:A:327:TRP:HB3	1.91	0.53
1:A:403:THR:O	1:A:404:GLN:NE2	2.41	0.53
1:E:213:LYS:O	1:E:213:LYS:HG2	2.07	0.53
2:F:378:ARG:HH11	3:H:99:LEU:HA	1.70	0.53
3:C:202:THR:HG23	3:C:204:TYR:O	2.09	0.53
3:H:192:ARG:HH12	3:H:198:PHE:HD2	1.56	0.53
1:A:199:ASN:ND2	1:A:268:VAL:HG23	2.24	0.53
2:B:173:HIS:HB2	2:B:203:PHE:CD1	2.44	0.53
2:F:200:GLY:HA2	2:F:228:PHE:O	2.09	0.53
3:G:230:PHE:O	3:G:233:VAL:HG22	2.08	0.53
1:A:183:TYR:CZ	1:A:241:VAL:HG11	2.43	0.53
1:A:234:GLN:O	1:A:265:HIS:HA	2.08	0.53
3:D:24:VAL:HG22	3:D:30:HIS:ND1	2.24	0.53
1:E:313:LYS:HG2	1:E:340:ILE:CD1	2.38	0.53
1:E:481:GLU:O	1:E:485:LEU:HG	2.09	0.53
1:E:298:LEU:HD22	1:E:325:ILE:HG22	1.89	0.52
2:F:201:ALA:O	2:F:230:HIS:N	2.37	0.52
1:A:67:TRP:CE3	1:A:198:LEU:HB2	2.45	0.52
2:F:173:HIS:O	2:F:203:PHE:HA	2.08	0.52
2:F:378:ARG:NH2	2:F:380:ILE:HD11	2.24	0.52
3:H:164:PRO:O	3:H:196:ARG:NE	2.42	0.52
2:B:124:GLU:HG2	2:B:127:LEU:HD11	1.91	0.52
1:E:437:THR:CG2	2:F:358:CYS:H	2.21	0.52
2:F:74:ARG:NH2	2:F:75:ASP:OD2	2.42	0.52
3:G:127:LYS:NZ	3:G:160:ALA:HB1	2.24	0.52
1:A:242:ALA:HB1	1:A:246:SER:OG	2.09	0.52
3:D:53:TYR:CG	3:D:53:TYR:O	2.63	0.52
1:E:65:ARG:HA	1:E:68:LEU:HD21	1.91	0.52
2:F:324:ILE:C	2:F:325:LYS:HG3	2.34	0.52
3:C:219:LEU:HD23	3:C:220:TYR:N	2.25	0.52
3:H:80:ILE:HD11	3:H:168:ILE:HD11	1.91	0.52
3:H:113:GLU:HG3	3:H:114:THR:N	2.25	0.52
2:B:324:ILE:CD1	2:B:355:ASP:HB3	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:330:PRO:HB2	1:E:343:PHE:HE1	1.74	0.52
2:F:73:GLN:N	2:F:73:GLN:OE1	2.43	0.52
3:H:38:SER:OG	3:H:221:GLN:N	2.42	0.52
2:B:72:GLN:OE1	2:B:72:GLN:HA	2.09	0.52
1:A:41:GLU:O	1:A:45:ALA:N	2.43	0.52
1:A:236:GLU:HG3	1:A:237:ARG:N	2.25	0.52
3:C:126:GLU:O	3:C:130:LEU:HG	2.10	0.52
1:E:63:ALA:HB1	1:E:197:ALA:O	2.10	0.52
1:E:259:ARG:O	1:E:261:SER:N	2.43	0.52
3:H:4:ILE:O	3:H:22:LEU:N	2.33	0.52
3:D:133:MET:HG3	3:D:157:LEU:HD12	1.92	0.51
1:A:212:PRO:HG2	1:A:215:VAL:HG11	1.90	0.51
1:E:267:ALA:N	1:E:301:VAL:HG12	2.26	0.51
1:E:331:SER:HB3	1:E:360:LYS:HG2	1.92	0.51
1:E:343:PHE:HD2	1:E:372:ILE:HG23	1.75	0.51
3:H:42:THR:O	3:H:46:THR:N	2.41	0.51
1:E:234:GLN:HB3	1:E:235:PHE:CD2	2.45	0.51
1:E:358:GLY:HA3	1:E:387:ARG:O	2.10	0.51
2:B:281:VAL:HG22	2:B:310:ARG:HB3	1.91	0.51
1:E:370:SER:N	1:E:400:ARG:O	2.37	0.51
1:A:226:ARG:HA	1:A:255:SER:OG	2.11	0.51
3:H:131:LEU:HD21	3:H:157:LEU:HB2	1.91	0.51
1:E:350:SER:N	1:E:353:GLN:HE21	2.04	0.51
3:D:191:LEU:HD12	3:D:196:ARG:HH11	1.76	0.51
1:E:330:PRO:HB2	1:E:343:PHE:CE1	2.45	0.51
1:E:363:HIS:HB2	1:E:392:ILE:HG13	1.92	0.51
2:F:237:GLU:H	2:F:237:GLU:CD	2.18	0.51
2:F:380:ILE:O	3:H:73:GLU:HG2	2.11	0.51
1:A:416:ALA:HB3	2:B:351:ILE:HD11	1.93	0.51
3:C:217:HIS:N	3:C:217:HIS:HD2	2.09	0.51
2:F:306:SER:OG	2:F:337:MET:HE3	2.10	0.51
1:A:46:ILE:HD12	1:A:202:VAL:HA	1.93	0.51
1:A:378:SER:HB3	1:A:409:LEU:HD12	1.93	0.51
3:C:12:GLU:C	3:C:13:ASP:OD1	2.53	0.51
3:C:219:LEU:HD21	3:C:222:GLY:HA2	1.93	0.51
1:E:55:TRP:CZ3	1:E:56:MET:HG2	2.46	0.51
2:F:214:GLN:OE1	2:F:402:ARG:NH2	2.43	0.51
1:A:334:LEU:HB3	1:A:339:SER:OG	2.12	0.50
1:A:385:SER:HB2	1:A:417:HIS:HB2	1.93	0.50
3:C:60:VAL:HG12	3:C:67:LEU:HD21	1.93	0.50
1:E:224:TYR:HE1	1:E:252:GLU:C	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:349:THR:O	1:E:379:ALA:N	2.42	0.50
2:F:276:PRO:HG3	2:F:282:CYS:HB3	1.92	0.50
1:A:205:ASP:OD1	1:A:206:GLY:N	2.44	0.50
1:A:485:LEU:HD12	1:A:486:LEU:N	2.26	0.50
2:B:258:SER:HA	2:B:287:TRP:O	2.11	0.50
2:B:368:ASP:HB3	2:B:371:GLN:HG2	1.94	0.50
1:E:407:SER:HB3	1:E:416:ALA:HB1	1.93	0.50
1:A:316:TRP:CD1	1:A:332:CYS:HG	2.30	0.50
1:E:444:GLN:HG2	3:G:88:VAL:HG11	1.92	0.50
3:H:234:LYS:HG3	3:H:235:GLN:HA	1.92	0.50
3:D:225:VAL:C	3:D:226:LYS:HG2	2.37	0.50
1:E:259:ARG:O	1:E:260:ASP:C	2.54	0.50
1:E:273:ILE:HG21	1:E:279:VAL:HG23	1.94	0.50
1:A:161:GLU:HB3	1:A:162:GLN:C	2.37	0.50
2:B:307:ASP:O	2:B:308:LYS:HG2	2.12	0.50
3:D:29:VAL:HG12	3:D:198:PHE:HB2	1.92	0.50
1:A:479:ALA:O	1:A:483:GLN:HG3	2.11	0.50
3:D:4:ILE:HG22	3:D:60:VAL:HG13	1.93	0.50
1:E:230:GLU:OE1	1:E:259:ARG:NH1	2.45	0.50
1:E:409:LEU:HD22	2:F:354:ASP:N	2.26	0.50
1:E:238:THR:OG1	1:E:252:GLU:OE2	2.29	0.50
1:E:331:SER:CB	1:E:360:LYS:HG2	2.42	0.50
2:F:138:THR:H	2:F:172:ARG:HH21	1.59	0.50
3:H:79:GLY:C	3:H:165:GLU:H	2.20	0.50
3:H:107:ARG:CD	3:H:114:THR:HG23	2.42	0.50
3:G:93:VAL:O	3:G:142:VAL:HG23	2.12	0.50
2:B:388:MET:HE1	3:D:98:PHE:HD1	1.77	0.49
3:D:50:ARG:O	3:D:53:TYR:CD2	2.65	0.49
3:D:110:ARG:NH2	3:D:163:GLU:OE2	2.45	0.49
1:E:313:LYS:HG2	1:E:340:ILE:HG12	1.94	0.49
3:G:103:LEU:HD23	3:G:115:LEU:HD23	1.94	0.49
3:G:110:ARG:O	3:G:112:GLN:NE2	2.45	0.49
3:G:203:HIS:O	3:G:204:TYR:HD1	1.94	0.49
2:B:195:ALA:O	2:B:197:HIS:CE1	2.66	0.49
3:G:107:ARG:HG2	3:G:114:THR:HA	1.94	0.49
3:H:119:ASP:O	3:H:123:LEU:N	2.43	0.49
1:A:159:LEU:HD23	1:A:161:GLU:OE2	2.12	0.49
2:B:65:ILE:HD11	2:B:161:VAL:HG11	1.95	0.49
2:B:73:GLN:HG2	2:B:192:LEU:HD11	1.94	0.49
3:D:30:HIS:NE2	3:D:215:TYR:HD2	2.10	0.49
3:D:60:VAL:HB	3:D:68:LEU:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:110:ARG:HG2	3:D:112:GLN:NE2	2.27	0.49
1:A:431:LEU:N	2:B:364:VAL:O	2.36	0.49
1:E:192:ASP:CG	1:E:304:ARG:HH21	2.20	0.49
2:F:147:ARG:HG3	2:F:147:ARG:NH2	2.26	0.49
3:H:95:ASN:HB2	3:H:138:LEU:HA	1.93	0.49
3:H:115:LEU:HD21	3:H:120:PHE:H	1.77	0.49
1:A:417:HIS:HE1	2:B:352:TYR:CE1	2.31	0.49
1:A:468:LYS:O	1:A:472:SER:OG	2.30	0.49
3:C:4:ILE:HG12	3:C:60:VAL:HG13	1.93	0.49
3:G:193:ASP:O	3:G:195:LYS:HD2	2.13	0.49
3:G:236:LEU:C	3:G:238:GLU:H	2.21	0.49
3:H:123:LEU:O	3:H:127:LYS:HG2	2.11	0.49
1:A:251:ILE:HG13	1:A:282:SER:HB2	1.94	0.49
2:F:170:HIS:ND1	2:F:200:GLY:HA3	2.27	0.49
3:G:132:LYS:HG3	3:G:132:LYS:O	2.13	0.49
1:A:432:GLU:HG3	2:B:363:THR:HG22	1.95	0.49
2:B:279:ASN:OD1	2:B:308:LYS:HD3	2.13	0.49
3:C:204:TYR:HB2	3:C:206:ARG:HG3	1.94	0.49
1:E:260:ASP:HA	1:E:295:GLY:HA3	1.94	0.49
3:C:132:LYS:HE3	3:C:153:ARG:NH1	2.28	0.49
3:D:18:ARG:HD3	3:D:223:ARG:HB2	1.94	0.49
1:E:359:THR:HG21	1:E:372:ILE:HD13	1.95	0.49
1:E:374:SER:C	1:E:375:LYS:HD2	2.38	0.49
1:A:182:LYS:HE3	1:A:183:TYR:HE2	1.77	0.48
1:A:300:PHE:HE1	1:A:325:ILE:HG22	1.78	0.48
2:B:154:LEU:HD12	2:B:203:PHE:HZ	1.78	0.48
3:C:132:LYS:HE3	3:C:153:ARG:HH11	1.77	0.48
2:F:275:MET:HA	2:F:304:ILE:O	2.13	0.48
3:H:104:ASN:HA	3:H:107:ARG:HD2	1.95	0.48
3:C:164:PRO:O	3:C:196:ARG:NE	2.46	0.48
2:F:129:LEU:O	2:F:133:LEU:HB3	2.13	0.48
3:H:164:PRO:HG2	3:H:196:ARG:HH21	1.78	0.48
3:H:176:LEU:HG	3:H:180:ALA:HB3	1.94	0.48
3:G:117:ARG:HG3	3:G:118:PHE:CD2	2.48	0.48
3:G:189:ASN:O	3:G:192:ARG:HB2	2.13	0.48
2:B:287:TRP:CZ3	2:B:316:LEU:HD23	2.49	0.48
3:H:207:ILE:HG23	3:H:208:LEU:HD12	1.93	0.48
2:B:199:THR:HG22	2:B:226:HIS:O	2.13	0.48
1:E:192:ASP:OD1	1:E:193:ASN:ND2	2.45	0.48
1:E:194:PHE:CE2	1:E:195:PHE:CE2	3.02	0.48
1:A:389:LEU:HD21	1:A:391:LYS:HD3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:132:LYS:HZ1	3:C:180:ALA:HA	1.78	0.48
1:A:303:LYS:HE2	1:A:330:PRO:HG3	1.95	0.48
1:E:389:LEU:HA	1:E:421:TYR:HB2	1.95	0.48
2:B:267:THR:OG1	2:B:296:ASN:ND2	2.45	0.48
3:G:67:LEU:HA	3:G:70:LEU:HD12	1.95	0.48
2:B:283:ASP:HB2	2:B:312:VAL:HB	1.95	0.48
3:C:109:TYR:O	3:C:110:ARG:HB2	2.13	0.48
2:F:212:HIS:CD2	2:F:240:THR:HG21	2.49	0.48
2:F:212:HIS:HA	2:F:240:THR:HG23	1.96	0.48
3:H:109:TYR:HE1	3:H:110:ARG:HH11	1.62	0.48
1:A:161:GLU:HG3	1:A:164:ILE:HB	1.96	0.47
1:A:448:CYS:O	1:A:453:ILE:HG13	2.14	0.47
2:B:251:ALA:HA	2:B:280:GLU:HG2	1.96	0.47
3:H:167:CYS:HB2	3:H:198:PHE:CD1	2.48	0.47
2:B:404:GLU:N	2:B:404:GLU:OE1	2.47	0.47
3:C:18:ARG:O	3:C:18:ARG:HG2	2.14	0.47
3:D:206:ARG:HG3	3:D:206:ARG:HH11	1.79	0.47
1:E:353:GLN:O	1:E:382:SER:HB2	2.14	0.47
3:D:150:GLU:HA	3:D:153:ARG:NH1	2.29	0.47
2:F:71:PRO:HG2	2:F:72:GLN:OE1	2.14	0.47
2:F:277:VAL:HG12	2:F:278:LYS:N	2.26	0.47
2:F:412:ALA:O	2:F:416:GLN:N	2.46	0.47
1:A:39:ASN:OD1	1:A:42:VAL:N	2.26	0.47
2:F:376:ARG:NE	3:H:73:GLU:OE2	2.39	0.47
3:D:107:ARG:HD3	3:D:112:GLN:HG2	1.97	0.47
2:F:83:SER:HB2	2:F:151:PRO:O	2.14	0.47
1:A:170:GLY:HA2	1:A:173:ILE:HD12	1.95	0.47
2:F:74:ARG:O	2:F:78:ALA:N	2.47	0.47
2:F:187:GLU:OE2	2:F:217:LYS:HD2	2.15	0.47
1:A:196:ALA:HA	1:A:199:ASN:ND2	2.28	0.47
1:A:450:GLN:O	3:C:76:ALA:HB2	2.15	0.47
3:C:206:ARG:HB2	3:C:207:ILE:H	1.15	0.47
3:D:20:LEU:HD11	3:D:224:ILE:HG13	1.97	0.47
1:E:344:TYR:HA	1:E:373:ILE:O	2.15	0.47
2:F:199:THR:OG1	2:F:221:GLU:OE2	2.29	0.47
3:G:96:GLN:O	3:G:100:GLN:HB2	2.14	0.47
3:H:80:ILE:HD11	3:H:168:ILE:CD1	2.44	0.47
3:H:125:GLU:O	3:H:128:ILE:HG12	2.14	0.47
3:D:31:ALA:HB3	3:D:216:VAL:HG22	1.96	0.47
3:D:155:ASP:O	3:D:158:GLN:HB2	2.14	0.47
1:E:39:ASN:O	1:E:42:VAL:HG12	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:VAL:HG22	1:E:46:ILE:HD11	1.96	0.47
1:E:261:SER:O	1:E:263:GLN:N	2.48	0.47
2:F:276:PRO:HG3	2:F:282:CYS:CB	2.45	0.47
2:F:339:LYS:HB2	2:F:339:LYS:HE3	1.63	0.47
1:A:387:ARG:HB2	1:A:419:PHE:CD1	2.50	0.47
1:A:465:GLY:HA3	3:C:93:VAL:HG22	1.97	0.47
3:C:147:SER:O	3:C:151:LYS:HG2	2.15	0.47
2:F:107:GLU:HB3	2:F:141:ALA:HB3	1.97	0.47
3:G:9:VAL:HG22	3:G:17:LEU:HB2	1.96	0.47
3:G:18:ARG:CG	3:G:18:ARG:O	2.63	0.47
2:B:368:ASP:CB	2:B:371:GLN:HE21	2.26	0.47
1:E:275:LYS:HG2	1:E:276:ASN:OD1	2.14	0.47
2:F:290:HIS:HB2	2:F:319:VAL:HG22	1.97	0.47
3:G:18:ARG:O	3:G:18:ARG:HG3	2.15	0.47
1:A:398:ASN:HA	1:A:428:SER:O	2.15	0.46
1:A:417:HIS:CE1	2:B:352:TYR:HE1	2.31	0.46
2:B:275:MET:SD	2:B:414:ILE:HG23	2.55	0.46
3:C:173:ASP:HA	3:C:176:LEU:HD12	1.96	0.46
3:D:45:ALA:HB3	3:D:50:ARG:NH2	2.30	0.46
1:E:286:ASN:ND2	1:E:485:LEU:HB3	2.30	0.46
1:E:450:GLN:NE2	3:G:82:MET:H	2.13	0.46
2:F:127:LEU:HD22	2:F:202:ARG:NH2	2.29	0.46
3:G:36:ASN:OD1	3:G:40:LYS:NZ	2.28	0.46
3:G:119:ASP:OD1	3:G:119:ASP:N	2.48	0.46
1:A:417:HIS:HE1	2:B:352:TYR:HE1	1.63	0.46
3:C:155:ASP:O	3:C:158:GLN:HB2	2.15	0.46
2:F:191:SER:CB	2:F:222:ASN:H	2.27	0.46
3:H:115:LEU:CD2	3:H:120:PHE:HB2	2.45	0.46
3:H:180:ALA:O	3:H:183:VAL:HG22	2.15	0.46
1:A:192:ASP:OD1	1:A:196:ALA:HB3	2.16	0.46
1:A:293:ASN:OD1	1:A:294:THR:N	2.48	0.46
2:B:301:HIS:O	2:B:332:ASN:HA	2.15	0.46
2:B:335:LEU:HD21	2:B:367:ILE:HD11	1.97	0.46
3:C:159:MET:HE1	3:C:169:LEU:HD21	1.97	0.46
2:F:277:VAL:HG12	2:F:278:LYS:HG3	1.96	0.46
2:F:339:LYS:O	2:F:339:LYS:HG3	2.14	0.46
3:G:112:GLN:N	3:G:112:GLN:OE1	2.49	0.46
1:A:449:LEU:HA	1:A:453:ILE:O	2.15	0.46
1:A:449:LEU:HD12	1:A:450:GLN:N	2.31	0.46
1:A:461:MET:HE1	3:C:98:PHE:HA	1.98	0.46
1:E:169:PHE:O	1:E:173:ILE:HG13	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:459:ILE:HD12	1:E:460:SER:H	1.81	0.46
3:G:33:MET:HG2	3:G:202:THR:OG1	2.16	0.46
3:G:67:LEU:HG	3:G:75:ARG:HE	1.80	0.46
1:A:162:GLN:O	1:A:164:ILE:HG13	2.14	0.46
1:A:409:LEU:HG	1:A:414:CYS:SG	2.56	0.46
3:C:32:ILE:HD13	3:C:199:ILE:HG13	1.98	0.46
3:C:132:LYS:HE2	3:C:183:VAL:HG11	1.98	0.46
1:E:339:SER:HB3	1:E:368:THR:HG22	1.97	0.46
1:E:349:THR:HA	1:E:353:GLN:NE2	2.30	0.46
2:F:375:LEU:HD22	2:F:380:ILE:HD13	1.98	0.46
1:A:39:ASN:OD1	1:A:42:VAL:HG23	2.16	0.46
2:B:230:HIS:CD2	2:B:256:ASN:ND2	2.84	0.46
3:C:93:VAL:O	3:C:142:VAL:HG23	2.16	0.46
1:A:212:PRO:O	1:A:215:VAL:HG12	2.16	0.46
1:A:346:VAL:HG23	1:A:470:VAL:HG11	1.97	0.46
2:B:74:ARG:NH1	2:B:75:ASP:OD2	2.48	0.46
1:A:50:ARG:NH2	1:A:204:SER:HB2	2.31	0.46
1:E:303:LYS:H	1:E:328:LYS:NZ	2.04	0.46
2:F:72:GLN:OE1	2:F:72:GLN:N	2.49	0.46
2:F:259:THR:HB	2:F:288:LEU:CD1	2.46	0.46
3:D:191:LEU:HD23	3:D:198:PHE:CZ	2.51	0.46
3:G:35:PRO:O	3:G:38:SER:OG	2.33	0.46
1:A:222:SER:HB2	1:A:251:ILE:HB	1.98	0.45
2:B:227:HIS:CD2	2:B:253:LEU:HG	2.50	0.45
1:E:292:ASN:CG	1:E:293:ASN:N	2.74	0.45
2:F:267:THR:HA	2:F:296:ASN:HB3	1.97	0.45
2:F:333:ASN:N	2:F:333:ASN:ND2	2.62	0.45
3:H:49:GLY:HA3	3:H:72:PRO:HG3	1.96	0.45
1:A:303:LYS:HZ1	1:A:318:GLN:CG	2.29	0.45
1:E:161:GLU:HB3	1:E:162:GLN:C	2.41	0.45
1:E:171:GLU:O	1:E:175:ASP:HB2	2.17	0.45
1:E:356:ASP:OD1	1:E:387:ARG:NH1	2.49	0.45
2:B:109:SER:HB2	2:B:139:HIS:HB2	1.99	0.45
1:E:72:GLU:HA	1:E:73:PRO:HD3	1.68	0.45
1:E:245:ASP:HA	1:E:276:ASN:O	2.16	0.45
3:C:206:ARG:HH12	3:C:207:ILE:HD12	1.81	0.45
3:D:93:VAL:O	3:D:142:VAL:HG23	2.16	0.45
3:D:132:LYS:O	3:D:132:LYS:HG3	2.17	0.45
2:F:93:TYR:CE2	2:F:95:PRO:HG3	2.52	0.45
3:H:95:ASN:ND2	3:H:137:LEU:O	2.44	0.45
1:A:359:THR:O	1:A:389:LEU:N	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:ARG:HA	1:A:430:GLN:O	2.16	0.45
2:B:269:ARG:HG3	2:B:298:ARG:HB2	1.99	0.45
1:E:67:TRP:O	1:E:70:MET:HG3	2.16	0.45
1:E:224:TYR:CE2	1:E:284:VAL:HG13	2.51	0.45
1:E:265:HIS:N	1:E:298:LEU:O	2.38	0.45
3:G:91:PRO:HA	3:G:144:VAL:HG21	1.99	0.45
1:A:66:ALA:O	1:A:69:GLU:HG2	2.16	0.45
2:B:85:ARG:HB2	2:B:155:MET:HE2	1.98	0.45
2:B:316:LEU:O	2:B:317:ILE:HD13	2.17	0.45
3:C:17:LEU:HD13	3:C:20:LEU:CD2	2.44	0.45
3:C:132:LYS:CG	3:C:132:LYS:O	2.65	0.45
1:E:329:TYR:HA	1:E:358:GLY:O	2.16	0.45
1:E:453:ILE:HD11	3:G:102:ALA:HB2	1.98	0.45
2:F:217:LYS:HD3	2:F:255:HIS:CE1	2.51	0.45
2:F:268:LEU:N	2:F:296:ASN:O	2.40	0.45
1:A:187:VAL:O	1:A:304:ARG:NH2	2.50	0.45
1:A:394:PRO:HG2	1:A:425:ARG:HH21	1.82	0.45
2:B:114:ARG:HB3	2:B:117:LEU:HD21	1.98	0.45
2:B:114:ARG:O	2:B:117:LEU:HG	2.17	0.45
2:B:383:GLN:HG3	2:B:384:ASP:OD2	2.17	0.45
2:F:324:ILE:HG22	2:F:325:LYS:HG2	1.98	0.45
1:A:290:GLY:HA2	1:A:291:ASP:HA	1.73	0.45
1:A:316:TRP:HB2	1:A:343:PHE:HD1	1.82	0.45
2:B:156:HIS:ND1	2:B:156:HIS:N	2.65	0.45
2:F:203:PHE:CE2	2:F:205:ILE:HD11	2.52	0.45
1:A:47:SER:O	1:A:48:ALA:HB3	2.17	0.44
1:A:243:ASP:O	1:A:246:SER:OG	2.32	0.44
3:D:18:ARG:HB3	3:D:223:ARG:HB2	1.98	0.44
1:E:67:TRP:HA	1:E:70:MET:SD	2.57	0.44
1:E:238:THR:HG21	1:E:250:TYR:CE1	2.52	0.44
2:F:371:GLN:HB2	3:H:88:VAL:HG21	1.99	0.44
3:H:121:GLN:OE1	3:H:138:LEU:HD11	2.17	0.44
1:A:454:SER:HA	3:C:73:GLU:CG	2.48	0.44
2:F:278:LYS:HB2	2:F:278:LYS:HE3	1.72	0.44
3:G:152:LYS:HD3	3:G:172:SER:O	2.18	0.44
3:H:191:LEU:HD21	3:H:198:PHE:HZ	1.83	0.44
1:A:269:VAL:HG11	1:A:281:TYR:CE1	2.52	0.44
1:A:392:ILE:HG23	1:A:396:ALA:HB3	1.99	0.44
1:E:390:VAL:HB	1:E:422:VAL:HA	2.00	0.44
1:A:428:SER:HA	2:B:366:ARG:HD3	2.00	0.44
3:C:152:LYS:HE2	3:C:174:SER:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:173:ASP:OD2	3:C:206:ARG:NE	2.50	0.44
1:E:211:VAL:HA	1:E:212:PRO:HD3	1.63	0.44
1:E:242:ALA:HB3	1:E:273:ILE:HG22	1.99	0.44
1:E:316:TRP:CH2	1:E:331:SER:O	2.70	0.44
1:E:340:ILE:HG22	1:E:369:LYS:HG3	1.99	0.44
2:F:382:GLN:HG2	2:F:383:GLN:H	1.82	0.44
3:G:7:LEU:HD12	3:G:7:LEU:O	2.18	0.44
3:G:132:LYS:HE3	3:G:153:ARG:CZ	2.47	0.44
3:H:234:LYS:HD2	3:H:234:LYS:HA	1.66	0.44
1:A:299:ASN:ND2	1:A:320:GLU:OE2	2.50	0.44
1:A:316:TRP:NE1	1:A:331:SER:O	2.48	0.44
1:A:365:GLY:O	1:A:396:ALA:HA	2.18	0.44
3:C:156:ILE:HD13	3:C:184:VAL:HG22	2.00	0.44
1:E:329:TYR:O	1:E:330:PRO:C	2.60	0.44
3:H:191:LEU:HD11	3:H:198:PHE:CE2	2.53	0.44
3:D:50:ARG:O	3:D:50:ARG:HG2	2.18	0.44
1:E:240:LEU:HD21	1:E:248:VAL:HG11	1.99	0.44
1:E:409:LEU:HD23	1:E:411:GLY:O	2.18	0.44
2:F:161:VAL:HG12	2:F:167:ASN:HB2	1.99	0.44
2:F:371:GLN:HA	3:H:88:VAL:HG11	2.00	0.44
2:F:395:ALA:O	2:F:399:GLU:HG2	2.17	0.44
2:B:173:HIS:HB2	2:B:203:PHE:HE1	1.81	0.43
3:C:29:VAL:HG21	3:C:192:ARG:HH21	1.84	0.43
3:C:45:ALA:HB1	3:C:53:TYR:HE2	1.83	0.43
1:E:419:PHE:CD1	2:F:348:GLN:HB3	2.53	0.43
2:F:383:GLN:HB3	2:F:419:PRO:HB2	2.00	0.43
2:B:378:ARG:HD2	3:D:162:LEU:HD11	2.00	0.43
3:C:29:VAL:CG2	3:C:192:ARG:HH21	2.32	0.43
3:G:170:ASP:O	3:G:171:GLU:HG2	2.18	0.43
1:A:275:LYS:HG2	1:A:276:ASN:OD1	2.18	0.43
2:B:247:LEU:HD12	2:B:284:THR:HB	1.99	0.43
1:E:450:GLN:NE2	1:E:451:ARG:HH11	2.14	0.43
2:F:189:PHE:CE2	2:F:217:LYS:HE3	2.53	0.43
3:H:9:VAL:H	3:H:17:LEU:HB2	1.83	0.43
3:D:18:ARG:HG3	3:D:18:ARG:HH11	1.83	0.43
3:D:110:ARG:HG2	3:D:112:GLN:HE22	1.84	0.43
1:E:223:THR:OG1	1:E:252:GLU:HA	2.19	0.43
2:F:247:LEU:HB3	2:F:253:LEU:CD1	2.46	0.43
3:G:44:SER:HB3	3:G:82:MET:SD	2.58	0.43
2:B:69:ILE:HD13	2:B:157:ILE:HD13	2.01	0.43
3:G:2:LEU:HB3	3:G:24:VAL:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:134:PRO:HG2	3:H:140:ARG:HH12	1.83	0.43
1:A:271:VAL:HG11	1:A:279:VAL:HG11	2.01	0.43
1:E:168:SER:OG	1:E:169:PHE:N	2.52	0.43
2:F:324:ILE:HG22	2:F:325:LYS:CG	2.48	0.43
3:G:66:ASP:O	3:G:70:LEU:HD12	2.18	0.43
1:A:60:ARG:HG2	1:A:201:ALA:HA	2.01	0.43
1:A:303:LYS:HD2	1:A:316:TRP:CZ3	2.52	0.43
2:B:316:LEU:HD12	2:B:348:GLN:O	2.18	0.43
1:E:183:TYR:HB3	1:E:272:ILE:HD13	2.01	0.43
2:F:273:LEU:HB2	2:F:397:LEU:HD21	1.99	0.43
2:F:275:MET:SD	2:F:414:ILE:HG23	2.59	0.43
3:G:133:MET:HA	3:G:133:MET:HE2	1.99	0.43
3:H:78:GLU:HA	3:H:110:ARG:NH1	2.33	0.43
3:C:13:ASP:OD1	3:C:13:ASP:N	2.52	0.43
3:C:22:LEU:CD1	3:C:217:HIS:HE1	2.31	0.43
3:D:17:LEU:HD21	3:D:39:GLY:HA3	2.00	0.43
3:D:29:VAL:HG23	3:D:214:ASP:H	1.84	0.43
1:E:265:HIS:O	1:E:300:PHE:N	2.34	0.43
1:A:330:PRO:HD2	1:A:358:GLY:O	2.19	0.43
3:D:29:VAL:HG11	3:D:192:ARG:HH21	1.84	0.43
3:D:45:ALA:HB3	3:D:50:ARG:HH21	1.83	0.43
1:E:161:GLU:CG	1:E:164:ILE:HG12	2.48	0.43
1:A:237:ARG:HD3	1:A:239:ILE:HD11	2.00	0.43
1:A:344:TYR:HE1	1:A:373:ILE:HD12	1.84	0.43
1:A:398:ASN:OD1	1:A:428:SER:HB2	2.19	0.43
3:C:81:PHE:HB2	3:C:164:PRO:HB3	2.00	0.43
3:D:153:ARG:HG3	3:D:183:VAL:HG21	2.00	0.43
1:E:334:LEU:HD12	1:E:363:HIS:CD2	2.53	0.43
1:E:368:THR:C	1:E:369:LYS:HG2	2.44	0.43
2:B:97:LEU:HD12	2:B:97:LEU:O	2.19	0.42
2:B:285:ARG:HB3	2:B:314:ASN:HB3	2.00	0.42
2:F:396:GLU:H	2:F:396:GLU:HG3	1.59	0.42
3:G:108:SER:OG	3:G:109:TYR:N	2.52	0.42
3:H:73:GLU:H	3:H:73:GLU:CD	2.23	0.42
1:A:188:VAL:H	1:A:270:GLU:CD	2.27	0.42
2:F:418:LEU:HD12	2:F:419:PRO:C	2.45	0.42
2:B:418:LEU:C	2:B:420:GLY:H	2.27	0.42
1:E:307:CYS:SG	1:E:314:MET:HE3	2.60	0.42
1:A:213:LYS:HD3	1:A:244:GLU:HG2	2.01	0.42
1:E:207:THR:O	1:E:238:THR:HA	2.19	0.42
1:E:286:ASN:HD22	1:E:485:LEU:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:313:PHE:HD2	2:F:345:THR:OG1	2.03	0.42
2:F:172:ARG:C	2:F:172:ARG:HE	2.27	0.42
1:A:163:GLY:C	1:A:212:PRO:HG3	2.45	0.42
2:B:156:HIS:N	2:B:188:HIS:O	2.32	0.42
2:B:273:LEU:HB2	2:B:397:LEU:HD13	2.01	0.42
3:D:116:ASP:O	3:D:117:ARG:C	2.62	0.42
1:E:42:VAL:O	1:E:46:ILE:HD12	2.20	0.42
1:E:68:LEU:H	1:E:68:LEU:HG	1.49	0.42
1:E:158:LYS:HD2	1:E:158:LYS:HA	1.79	0.42
1:E:399:ALA:C	1:E:400:ARG:HG3	2.44	0.42
3:G:159:MET:HE1	3:G:169:LEU:CD2	2.49	0.42
3:H:67:LEU:HD11	3:H:75:ARG:CD	2.49	0.42
3:H:176:LEU:HD23	3:H:176:LEU:C	2.45	0.42
1:A:52:GLU:OE1	1:A:60:ARG:NH2	2.52	0.42
2:B:189:PHE:O	2:B:220:PHE:N	2.41	0.42
1:E:300:PHE:CZ	1:E:325:ILE:HD13	2.55	0.42
2:F:380:ILE:HD11	3:H:102:ALA:HB2	2.01	0.42
3:H:188:VAL:HG13	3:H:198:PHE:CZ	2.55	0.42
1:A:50:ARG:O	1:A:52:GLU:N	2.52	0.42
1:A:161:GLU:HG3	1:A:164:ILE:O	2.19	0.42
1:A:213:LYS:HG2	1:A:244:GLU:OE2	2.20	0.42
1:A:352:HIS:O	1:A:352:HIS:CG	2.72	0.42
1:E:341:GLY:O	1:E:370:SER:HA	2.20	0.42
1:E:169:PHE:CE2	1:E:237:ARG:HG2	2.55	0.42
1:E:302:THR:O	1:E:302:THR:OG1	2.33	0.42
2:B:93:TYR:CE2	2:B:95:PRO:HG3	2.55	0.42
3:C:60:VAL:O	3:C:67:LEU:HG	2.20	0.42
2:F:182:GLU:CD	2:F:212:HIS:HB2	2.45	0.42
3:G:106:VAL:HB	3:G:110:ARG:NH2	2.35	0.42
1:A:439:ARG:NE	2:B:355:ASP:HA	2.35	0.41
3:D:166:LEU:HD11	3:D:199:ILE:HG13	2.02	0.41
1:E:304:ARG:HD2	1:E:333:ILE:HD11	2.01	0.41
1:E:449:LEU:HD21	3:G:73:GLU:CD	2.45	0.41
2:F:259:THR:HB	2:F:288:LEU:HD12	2.02	0.41
3:G:62:PHE:CD2	3:G:63:LYS:HG3	2.55	0.41
3:G:94:SER:HB2	3:G:138:LEU:O	2.19	0.41
3:H:191:LEU:HD11	3:H:198:PHE:CZ	2.55	0.41
1:E:211:VAL:N	1:E:241:VAL:O	2.35	0.41
1:E:234:GLN:HB3	1:E:235:PHE:CE2	2.55	0.41
1:E:383:GLN:OE1	1:E:415:GLY:HA3	2.21	0.41
2:F:87:VAL:HG22	2:F:155:MET:SD	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:103:LEU:HA	3:H:106:VAL:HG22	2.02	0.41
1:A:293:ASN:OD1	1:A:293:ASN:C	2.64	0.41
1:A:334:LEU:HD12	1:A:363:HIS:CE1	2.55	0.41
2:F:248:LEU:HA	2:F:248:LEU:HD23	1.85	0.41
2:F:331:THR:CG2	2:F:333:ASN:HD21	2.31	0.41
3:H:167:CYS:HB2	3:H:198:PHE:CE1	2.54	0.41
1:A:157:GLU:C	1:A:158:LYS:HG3	2.45	0.41
1:A:291:ASP:CG	1:A:292:ASN:H	2.28	0.41
1:E:42:VAL:C	1:E:46:ILE:HD12	2.45	0.41
3:G:40:LYS:HG3	3:G:41:SER:H	1.84	0.41
3:H:25:HIS:CE1	3:H:28:GLU:OE1	2.73	0.41
3:H:42:THR:HA	3:H:45:ALA:HB3	2.03	0.41
3:H:47:LEU:O	3:H:75:ARG:NH1	2.51	0.41
1:A:62:ASN:O	1:A:66:ALA:N	2.45	0.41
1:A:325:ILE:HA	1:A:354:GLN:O	2.20	0.41
2:B:267:THR:HG23	2:B:296:ASN:OD1	2.21	0.41
3:D:152:LYS:NZ	3:D:174:SER:O	2.49	0.41
3:D:188:VAL:HG13	3:D:198:PHE:CE1	2.56	0.41
1:E:275:LYS:N	1:E:309:GLY:HA2	2.34	0.41
1:E:346:VAL:HG21	1:E:467:CYS:SG	2.60	0.41
1:E:348:LEU:HA	1:E:377:ILE:O	2.20	0.41
1:E:425:ARG:HA	2:F:341:ALA:O	2.21	0.41
2:F:298:ARG:CZ	2:F:329:GLN:NE2	2.84	0.41
2:F:321:GLN:O	2:F:322:HIS:HB2	2.21	0.41
1:A:231:LYS:NZ	1:A:254:CYS:SG	2.94	0.41
1:E:226:ARG:H	1:E:226:ARG:HG3	1.48	0.41
2:F:277:VAL:CG1	2:F:278:LYS:H	2.31	0.41
3:H:164:PRO:HG2	3:H:196:ARG:NH2	2.36	0.41
1:A:325:ILE:HG12	1:A:354:GLN:HG3	2.03	0.41
1:A:403:THR:HB	1:A:433:HIS:ND1	2.36	0.41
2:B:226:HIS:ND1	2:B:252:VAL:HG22	2.34	0.41
2:B:249:GLY:HA2	2:B:417:ARG:NH2	2.19	0.41
2:F:111:ASN:ND2	2:F:113:ASP:HB3	2.35	0.41
2:F:145:GLY:H	2:F:180:GLY:HA3	1.86	0.41
2:F:418:LEU:HB2	2:F:419:PRO:HD2	2.02	0.41
3:H:188:VAL:HG13	3:H:198:PHE:CE1	2.55	0.41
1:A:59:PHE:CE2	1:A:200:ALA:HB1	2.55	0.41
1:A:301:VAL:N	1:A:327:TRP:O	2.54	0.41
2:B:100:ALA:HB1	2:B:102:GLU:OE1	2.20	0.41
3:C:9:VAL:HG22	3:C:55:VAL:HG22	2.03	0.41
3:D:50:ARG:HG3	3:D:52:ASP:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:THR:O	1:E:269:VAL:HG13	2.21	0.41
3:H:109:TYR:HD1	3:H:110:ARG:CD	2.34	0.41
1:A:275:LYS:HA	1:A:310:GLU:O	2.21	0.41
1:A:316:TRP:HB3	1:A:318:GLN:NE2	2.17	0.41
2:B:304:ILE:CG2	2:B:337:MET:HE2	2.51	0.41
3:D:159:MET:HE1	3:D:169:LEU:HD21	2.02	0.41
3:D:171:GLU:OE1	3:D:203:HIS:ND1	2.34	0.41
1:E:279:VAL:O	1:E:280:LYS:HD3	2.20	0.41
1:E:342:GLU:HA	1:E:371:THR:O	2.21	0.41
1:E:418:THR:O	2:F:348:GLN:HA	2.21	0.41
1:E:422:VAL:HB	2:F:345:THR:HG23	2.03	0.41
3:H:109:TYR:HD1	3:H:110:ARG:HD2	1.86	0.41
1:A:178:GLU:CD	1:A:178:GLU:H	2.28	0.41
2:F:84:VAL:HG21	2:F:104:SER:OG	2.21	0.41
2:F:127:LEU:HD21	2:F:230:HIS:CG	2.56	0.41
3:H:31:ALA:HB1	3:H:33:MET:CE	2.51	0.41
1:A:62:ASN:CA	1:A:65:ARG:HE	2.31	0.40
2:B:136:SER:O	2:B:172:ARG:HB3	2.21	0.40
2:B:372:ILE:O	2:B:376:ARG:HG2	2.20	0.40
3:C:4:ILE:HG23	3:C:60:VAL:HG22	2.02	0.40
3:C:26:PRO:HA	3:C:197:SER:OG	2.21	0.40
3:C:132:LYS:NZ	3:C:180:ALA:HA	2.36	0.40
3:D:96:GLN:HB2	3:D:138:LEU:HD22	2.03	0.40
1:E:301:VAL:C	1:E:328:LYS:HZ2	2.28	0.40
2:F:133:LEU:HD12	2:F:133:LEU:O	2.20	0.40
3:G:17:LEU:HD21	3:G:39:GLY:HA3	2.03	0.40
1:A:226:ARG:HG2	1:A:481:GLU:OE2	2.21	0.40
3:C:158:GLN:O	3:C:162:LEU:HD13	2.21	0.40
3:D:128:ILE:HG23	3:D:133:MET:HB2	2.03	0.40
1:E:40:GLU:O	1:E:44:ARG:HG3	2.21	0.40
1:E:185:GLY:HA2	1:E:188:VAL:O	2.20	0.40
3:G:181:LEU:HA	3:G:181:LEU:HD12	1.83	0.40
2:B:121:ILE:HD13	2:B:260:GLN:HG3	2.03	0.40
2:B:418:LEU:HB3	2:B:419:PRO:HD2	2.03	0.40
3:C:230:PHE:CD1	3:C:231:THR:N	2.89	0.40
2:F:278:LYS:HG2	2:F:307:ASP:HB2	2.03	0.40
3:H:103:LEU:O	3:H:107:ARG:HG3	2.22	0.40
3:H:212:LYS:HA	3:H:213:PRO:HD2	1.86	0.40
1:A:224:TYR:OH	1:A:255:SER:HB3	2.22	0.40
1:A:294:THR:CB	1:A:296:GLY:HA3	2.51	0.40
1:E:378:SER:HB3	1:E:414:CYS:SG	2.61	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:467:CYS:SG	1:E:467:CYS:O	2.79	0.40
3:C:71:SER:O	3:C:75:ARG:HG2	2.22	0.40
1:E:452:GLY:HA3	3:G:106:VAL:CG1	2.51	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	376/495 (76%)	350 (93%)	18 (5%)	8 (2%)	5	30
1	E	368/495 (74%)	339 (92%)	26 (7%)	3 (1%)	16	52
2	B	359/423 (85%)	344 (96%)	14 (4%)	1 (0%)	36	71
2	F	353/423 (84%)	337 (96%)	14 (4%)	2 (1%)	21	58
3	C	235/248 (95%)	221 (94%)	11 (5%)	3 (1%)	9	41
3	D	233/248 (94%)	222 (95%)	10 (4%)	1 (0%)	30	66
3	G	237/248 (96%)	222 (94%)	12 (5%)	3 (1%)	9	41
3	H	234/248 (94%)	222 (95%)	10 (4%)	2 (1%)	14	49
All	All	2395/2828 (85%)	2257 (94%)	115 (5%)	23 (1%)	12	47

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	HIS
1	A	163	GLY
1	A	202	VAL
1	A	259	ARG
1	A	289	PRO
3	C	117	ARG
3	C	206	ARG

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Mol	Chain	Res	Type
1	E	62	ASN
3	C	142	VAL
3	D	142	VAL
1	E	163	GLY
3	G	6	ASP
3	G	142	VAL
3	H	142	VAL
1	A	191	ASN
2	B	278	LYS
1	E	49	LYS
2	F	307	ASP
3	G	237	GLU
3	H	116	ASP
1	A	35	ALA
2	F	278	LYS
1	A	296	GLY

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	320/413 (78%)	298 (93%)	22 (7%)	14	37
1	E	314/413 (76%)	270 (86%)	44 (14%)	3	15
2	B	297/350 (85%)	278 (94%)	19 (6%)	16	38
2	F	292/350 (83%)	266 (91%)	26 (9%)	9	29
3	C	203/212 (96%)	185 (91%)	18 (9%)	9	29
3	D	201/212 (95%)	179 (89%)	22 (11%)	6	22
3	G	205/212 (97%)	194 (95%)	11 (5%)	20	43
3	H	202/212 (95%)	191 (95%)	11 (5%)	20	43
All	All	2034/2374 (86%)	1861 (92%)	173 (8%)	10	30

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ARG
1	A	55	TRP
1	A	68	LEU
1	A	71	GLU
1	A	176	HIS
1	A	213	LYS
1	A	226	ARG
1	A	236	GLU
1	A	240	LEU
1	A	254	CYS
1	A	273	ILE
1	A	328	LYS
1	A	335	ARG
1	A	354	GLN
1	A	357	THR
1	A	381	HIS
1	A	397	THR
1	A	400	ARG
1	A	409	LEU
1	A	413	ASN
1	A	419	PHE
1	A	477	GLU
2	B	63	VAL
2	B	73	GLN
2	B	74	ARG
2	B	77	LEU
2	B	97	LEU
2	B	127	LEU
2	B	135	GLN
2	B	156	HIS
2	B	182	GLU
2	B	190	VAL
2	B	196	ARG
2	B	197	HIS
2	B	203	PHE
2	B	252	VAL
2	B	308	LYS
2	B	325	LYS
2	B	351	ILE
2	B	357	LYS
2	B	404	GLU
3	C	13	ASP
3	C	28	GLU

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Mol	Chain	Res	Type
3	C	43	LEU
3	C	50	ARG
3	C	75	ARG
3	C	110	ARG
3	C	117	ARG
3	C	132	LYS
3	C	137	LEU
3	C	153	ARG
3	C	162	LEU
3	C	183	VAL
3	C	192	ARG
3	C	199	ILE
3	C	202	THR
3	C	212	LYS
3	C	217	HIS
3	C	236	LEU
3	D	5	LYS
3	D	12	GLU
3	D	14	LYS
3	D	18	ARG
3	D	47	LEU
3	D	50	ARG
3	D	59	THR
3	D	68	LEU
3	D	100	GLN
3	D	126	GLU
3	D	152	LYS
3	D	163	GLU
3	D	182	LYS
3	D	183	VAL
3	D	184	VAL
3	D	212	LYS
3	D	221	GLN
3	D	223	ARG
3	D	225	VAL
3	D	232	LEU
3	D	233	VAL
3	D	234	LYS
1	E	40	GLU
1	E	49	LYS
1	E	68	LEU
1	E	70	MET

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Mol	Chain	Res	Type
1	E	162	GLN
1	E	164	ILE
1	E	194	PHE
1	E	205	ASP
1	E	213	LYS
1	E	217	CYS
1	E	219	MET
1	E	225	PHE
1	E	226	ARG
1	E	230	GLU
1	E	234	GLN
1	E	244	GLU
1	E	246	SER
1	E	247	TYR
1	E	258	VAL
1	E	259	ARG
1	E	260	ASP
1	E	261	SER
1	E	264	LEU
1	E	273	ILE
1	E	274	HIS
1	E	280	LYS
1	E	284	VAL
1	E	293	ASN
1	E	308	GLU
1	E	310	GLU
1	E	314	MET
1	E	325	ILE
1	E	331	SER
1	E	348	LEU
1	E	375	LYS
1	E	397	THR
1	E	409	LEU
1	E	414	CYS
1	E	423	GLU
1	E	442	GLU
1	E	456	GLU
1	E	476	LEU
1	E	481	GLU
1	E	486	LEU
2	F	72	GLN
2	F	117	LEU

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Mol	Chain	Res	Type
2	F	133	LEU
2	F	144	ARG
2	F	146	GLN
2	F	159	GLN
2	F	172	ARG
2	F	187	GLU
2	F	190	VAL
2	F	193	ASN
2	F	237	GLU
2	F	240	THR
2	F	256	ASN
2	F	283	ASP
2	F	292	LYS
2	F	294	PHE
2	F	302	LYS
2	F	307	ASP
2	F	325	LYS
2	F	329	GLN
2	F	333	ASN
2	F	337	MET
2	F	339	LYS
2	F	349	LEU
2	F	383	GLN
2	F	402	ARG
3	G	1	MET
3	G	7	LEU
3	G	11	VAL
3	G	18	ARG
3	G	55	VAL
3	G	121	GLN
3	G	205	GLN
3	G	219	LEU
3	G	220	TYR
3	G	235	GLN
3	G	236	LEU
3	H	6	ASP
3	H	12	GLU
3	H	25	HIS
3	H	54	GLU
3	H	113	GLU
3	H	125	GLU
3	H	152	LYS

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Mol	Chain	Res	Type
3	H	176	LEU
3	H	181	LEU
3	H	202	THR
3	H	236	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	174	HIS
1	A	274	HIS
1	A	292	ASN
1	A	318	GLN
1	A	417	HIS
1	A	483	GLN
1	A	492	HIS
2	B	156	HIS
2	B	227	HIS
2	B	230	HIS
2	B	231	ASN
2	B	360	HIS
2	B	371	GLN
2	B	408	GLN
3	C	8	HIS
3	D	8	HIS
3	D	85	GLN
1	E	193	ASN
1	E	286	ASN
1	E	352	HIS
1	E	353	GLN
1	E	381	HIS
1	E	483	GLN
2	F	139	HIS
2	F	197	HIS
2	F	212	HIS
2	F	260	GLN
2	F	329	GLN
2	F	332	ASN
2	F	333	ASN
2	F	334	ASN
2	F	360	HIS
3	G	205	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	380/495 (76%)	1.06	43 (11%)	10 14	62, 101, 137, 154	0
1	E	372/495 (75%)	1.05	47 (12%)	8 12	77, 111, 147, 178	0
2	B	361/423 (85%)	0.86	23 (6%)	25 26	57, 96, 127, 142	0
2	F	355/423 (83%)	0.86	29 (8%)	17 21	73, 104, 132, 149	0
3	C	237/248 (95%)	0.78	15 (6%)	26 26	81, 110, 135, 156	0
3	D	235/248 (94%)	0.68	15 (6%)	25 26	74, 118, 149, 165	0
3	G	239/248 (96%)	0.60	10 (4%)	40 34	77, 108, 142, 162	0
3	H	236/248 (95%)	0.86	21 (8%)	15 18	85, 137, 166, 171	0
All	All	2415/2828 (85%)	0.87	203 (8%)	17 20	57, 108, 147, 178	0

All (203) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	332	CYS	6.4
1	E	332	CYS	6.2
1	E	254	CYS	5.7
2	B	65	ILE	5.2
1	E	330	PRO	5.1
3	G	162	LEU	4.8
2	F	132	SER	4.4
3	D	45	ALA	4.3
3	C	199	ILE	4.3
1	A	254	CYS	4.2
1	E	167	CYS	4.2
1	E	217	CYS	4.2
3	H	48	ALA	4.2
1	A	235	PHE	4.1
3	H	63	LYS	4.0
2	F	91	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
2	B	73	GLN	3.8
1	E	414	CYS	3.8
2	F	421	GLY	3.8
3	H	167	CYS	3.8
1	A	167	CYS	3.7
3	D	167	CYS	3.7
1	A	433	HIS	3.7
1	E	253	GLY	3.6
1	A	414	CYS	3.6
3	H	236	LEU	3.6
3	G	236	LEU	3.5
1	A	391	LYS	3.5
3	G	46	THR	3.5
2	B	390	ILE	3.5
3	H	46	THR	3.4
1	A	410	ILE	3.4
2	B	123	ALA	3.4
1	E	445	LEU	3.4
2	B	282	CYS	3.3
3	H	179	ASP	3.3
1	A	331	SER	3.3
2	F	194	ASP	3.3
2	F	344	ASP	3.3
3	C	168	ILE	3.3
1	A	409	LEU	3.3
1	E	232	THR	3.3
1	E	236	GLU	3.2
2	F	123	ALA	3.2
1	A	448	CYS	3.2
1	E	376	GLY	3.2
1	E	361	MET	3.2
1	E	52	GLU	3.1
1	E	203	ALA	3.1
2	F	392	ALA	3.1
1	E	409	LEU	3.1
3	H	47	LEU	3.1
1	E	342	GLU	3.0
1	A	360	LYS	2.9
3	C	226	LYS	2.9
2	B	274	ALA	2.9
3	H	165	GLU	2.9
3	H	233	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	E	375	LYS	2.9
1	A	223	THR	2.9
3	H	80	ILE	2.8
3	H	180	ALA	2.8
3	D	165	GLU	2.8
3	H	45	ALA	2.8
3	C	217	HIS	2.8
3	H	111	GLY	2.8
1	E	231	LYS	2.8
1	E	432	GLU	2.8
3	D	79	GLY	2.8
1	A	220	GLU	2.8
1	E	204	SER	2.8
3	C	162	LEU	2.8
1	E	225	PHE	2.8
2	B	351	ILE	2.8
2	F	337	MET	2.7
3	G	59	THR	2.7
3	G	54	GLU	2.7
3	G	56	THR	2.7
3	C	218	VAL	2.7
1	E	278	GLU	2.7
2	F	312	VAL	2.7
1	A	75	TRP	2.7
2	F	131	GLU	2.7
3	H	110	ARG	2.7
2	F	290	HIS	2.7
2	F	259	THR	2.7
1	E	421	TYR	2.7
2	F	172	ARG	2.7
2	F	77	LEU	2.6
2	F	350	GLU	2.6
1	A	361	MET	2.6
2	B	72	GLN	2.6
2	B	388	MET	2.6
3	D	46	THR	2.6
1	A	236	GLU	2.6
1	E	343	PHE	2.5
3	D	37	GLY	2.5
2	F	360	HIS	2.5
1	E	442	GLU	2.5
3	D	36	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	296	GLY	2.5
3	H	75	ARG	2.5
3	C	219	LEU	2.5
1	A	209	ILE	2.5
1	A	266	ALA	2.5
1	E	174	HIS	2.5
1	A	204	SER	2.5
1	A	202	VAL	2.5
2	F	162	ALA	2.5
2	B	386	GLN	2.5
2	F	378	ARG	2.5
3	C	64	GLY	2.5
2	B	227	HIS	2.5
1	A	444	GLN	2.4
1	E	423	GLU	2.4
3	H	194	GLY	2.4
3	C	185	ALA	2.4
1	E	485	LEU	2.4
1	E	266	ALA	2.4
2	B	201	ALA	2.4
1	E	344	TYR	2.4
2	B	192	LEU	2.4
1	A	216	ARG	2.3
1	E	467	CYS	2.3
2	F	394	ALA	2.3
3	G	129	ALA	2.3
1	E	389	LEU	2.3
1	E	448	CYS	2.3
2	F	80	THR	2.3
3	C	44	SER	2.3
1	A	421	TYR	2.3
2	F	67	GLY	2.3
1	A	404	GLN	2.3
2	F	377	SER	2.3
1	E	410	ILE	2.3
3	D	66	ASP	2.3
1	A	465	GLY	2.3
1	A	389	LEU	2.3
3	D	184	VAL	2.3
1	A	384	ASN	2.3
2	B	125	VAL	2.3
1	A	344	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	359	THR	2.2
1	E	362	ILE	2.2
2	F	286	THR	2.2
1	A	248	VAL	2.2
2	B	75	ASP	2.2
3	D	32	ILE	2.2
1	E	357	THR	2.2
3	D	162	LEU	2.2
1	A	285	GLN	2.2
3	D	52	ASP	2.2
2	B	324	ILE	2.2
1	A	179	LEU	2.2
2	B	103	GLY	2.2
1	E	459	ILE	2.2
2	B	62	PHE	2.2
3	G	58	GLY	2.2
1	A	240	LEU	2.2
1	E	240	LEU	2.2
3	C	233	VAL	2.2
2	B	377	SER	2.2
1	A	263	GLN	2.2
1	A	318	GLN	2.2
3	H	188	VAL	2.2
1	E	247	TYR	2.1
2	F	283	ASP	2.1
1	E	471	PHE	2.1
1	A	359	THR	2.1
3	D	53	TYR	2.1
1	E	318	GLN	2.1
2	F	237	GLU	2.1
1	E	316	TRP	2.1
1	A	218	PRO	2.1
3	D	168	ILE	2.1
3	H	166	LEU	2.1
3	H	212	LYS	2.1
1	A	55	TRP	2.1
1	E	377	ILE	2.1
3	G	72	PRO	2.1
3	C	9	VAL	2.1
1	A	250	TYR	2.1
2	F	257	THR	2.1
2	F	397	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	H	68	LEU	2.1
3	D	158	GLN	2.1
1	E	331	SER	2.1
2	B	350	GLU	2.1
2	F	308	LYS	2.1
1	A	323	SER	2.1
2	F	390	ILE	2.0
3	G	15	ALA	2.0
1	A	467	CYS	2.0
2	B	349	LEU	2.0
2	B	203	PHE	2.0
2	B	252	VAL	2.0
3	C	46	THR	2.0
3	C	189	ASN	2.0
1	A	34	LEU	2.0
1	A	203	ALA	2.0
3	C	79	GLY	2.0
1	E	303	LYS	2.0
3	H	198	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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
4	HG	F	600	1/1	0.88	0.12	176,176,176,176	0
4	HG	B	600	1/1	0.92	0.11	172,172,172,172	0
4	HG	E	600	1/1	0.98	0.06	117,117,117,117	0
4	HG	A	600	1/1	0.98	0.10	128,128,128,128	0

6.5 Other polymers [i](#)

There are no such residues in this entry.