



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 28, 2025 – 10:40 PM EDT

PDB ID : 4R7D / pdb_00004r7d
Title : Fab Hu 15C1
Authors : Loyau, J.; Didelot, G.; Malinge, P.; Ravn, U.; Magistrelli, G.; Depoisier, J.F.;
Kosco-Vilbois, M.; Fischer, N.; Thore, S.; Rousseau, F.
Deposited on : 2014-08-27
Resolution : 2.75 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
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

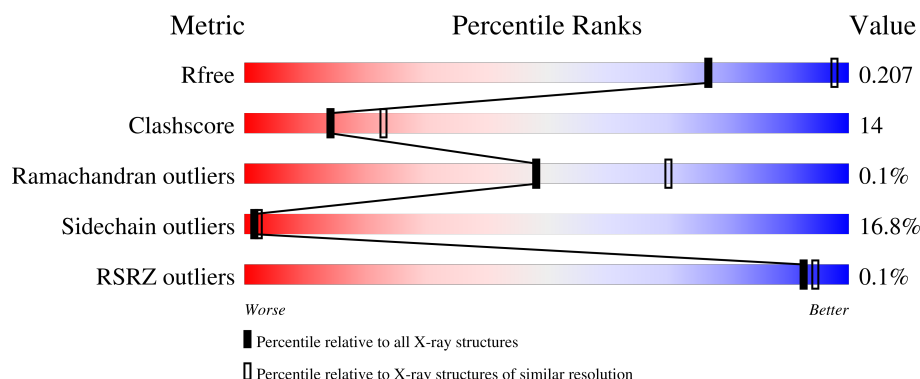
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

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	225	
1	C	225	
1	E	225	
1	G	225	
1	I	225	

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Mol	Chain	Length	Quality of chain
1	K	225	
1	M	225	
1	O	225	
2	B	214	
2	D	214	
2	F	214	
2	H	214	
2	J	214	
2	L	214	
2	N	214	
2	P	214	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 26033 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 Fab Hu 15C1 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1641	1042	272	322	5			
1	C	210	Total	C	N	O	S	0	0	0
			1593	1016	263	309	5			
1	E	209	Total	C	N	O	S	0	0	0
			1584	1011	261	307	5			
1	G	190	Total	C	N	O	S	0	0	0
			1445	927	236	277	5			
1	I	218	Total	C	N	O	S	0	0	0
			1641	1042	272	322	5			
1	K	201	Total	C	N	O	S	0	0	0
			1533	980	253	295	5			
1	M	201	Total	C	N	O	S	0	0	0
			1533	980	253	295	5			
1	O	209	Total	C	N	O	S	0	0	0
			1584	1011	261	307	5			

- Molecule 2 is a protein called Fab Hu 15C1 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1631	1023	275	329	4			
2	D	211	Total	C	N	O	S	0	0	0
			1626	1020	275	327	4			
2	F	211	Total	C	N	O	S	0	0	0
			1626	1020	275	327	4			
2	H	212	Total	C	N	O	S	0	0	0
			1635	1025	276	330	4			
2	J	212	Total	C	N	O	S	0	0	0
			1635	1025	276	330	4			
2	L	211	Total	C	N	O	S	0	0	0
			1631	1023	275	329	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	211	Total	C	N	O	S	0	0	0
			1626	1020	275	327	4			
2	P	211	Total	C	N	O	S	0	0	0
			1626	1020	275	327	4			

- Molecule 3 is water.

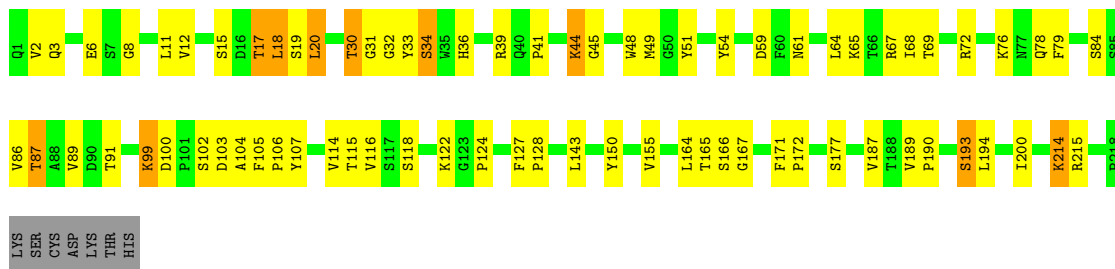
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total	O	0	0
			35	35		
3	B	25	Total	O	0	0
			25	25		
3	C	29	Total	O	0	0
			29	29		
3	D	23	Total	O	0	0
			23	23		
3	E	18	Total	O	0	0
			18	18		
3	F	22	Total	O	0	0
			22	22		
3	G	42	Total	O	0	0
			42	42		
3	H	21	Total	O	0	0
			21	21		
3	I	37	Total	O	0	0
			37	37		
3	J	28	Total	O	0	0
			28	28		
3	K	33	Total	O	0	0
			33	33		
3	L	24	Total	O	0	0
			24	24		
3	M	29	Total	O	0	0
			29	29		
3	N	32	Total	O	0	0
			32	32		
3	O	19	Total	O	0	0
			19	19		
3	P	26	Total	O	0	0
			26	26		

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

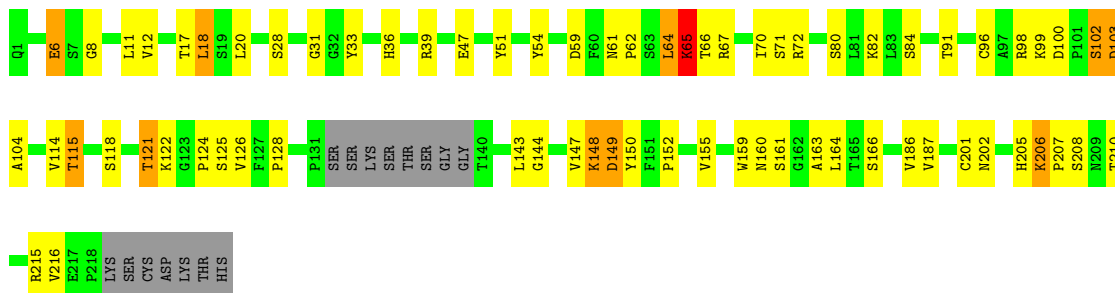
- Molecule 1: Fab Hu 15C1 Heavy chain

Chain A: 



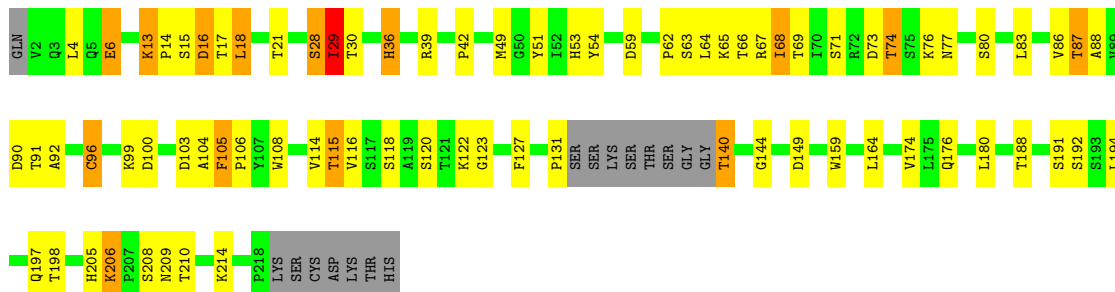
- Molecule 1: Fab Hu 15C1 Heavy chain

Chain C: 

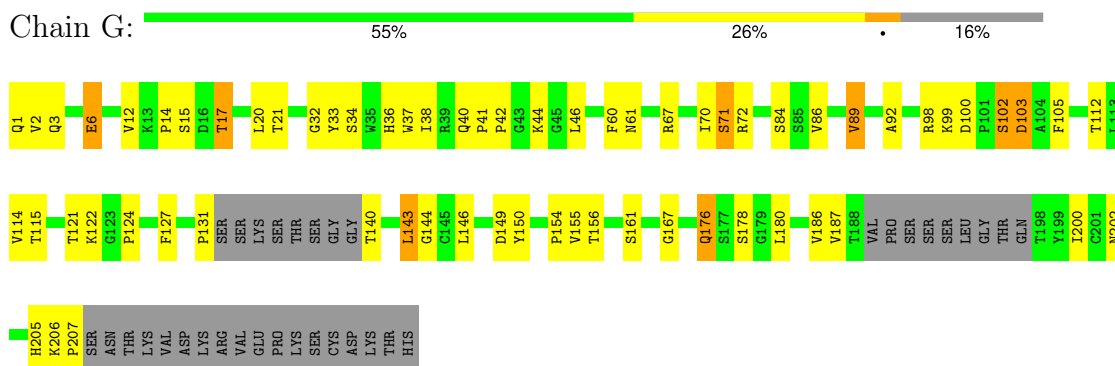


- Molecule 1: Fab Hu 15C1 Heavy chain

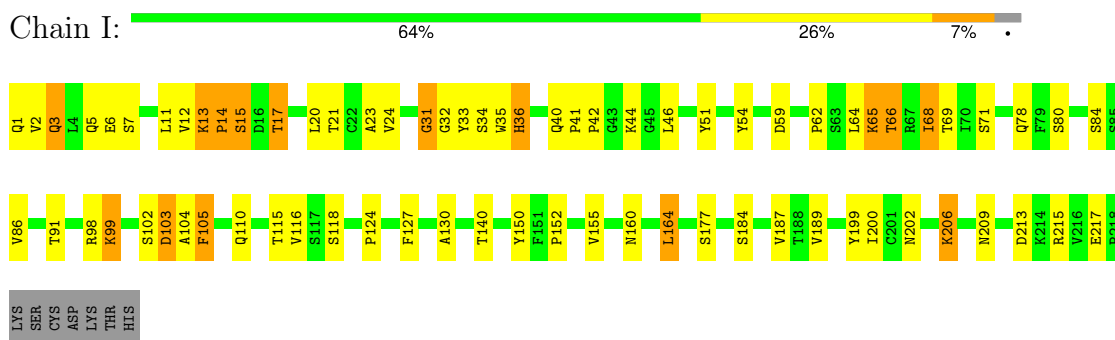
Chain E: 



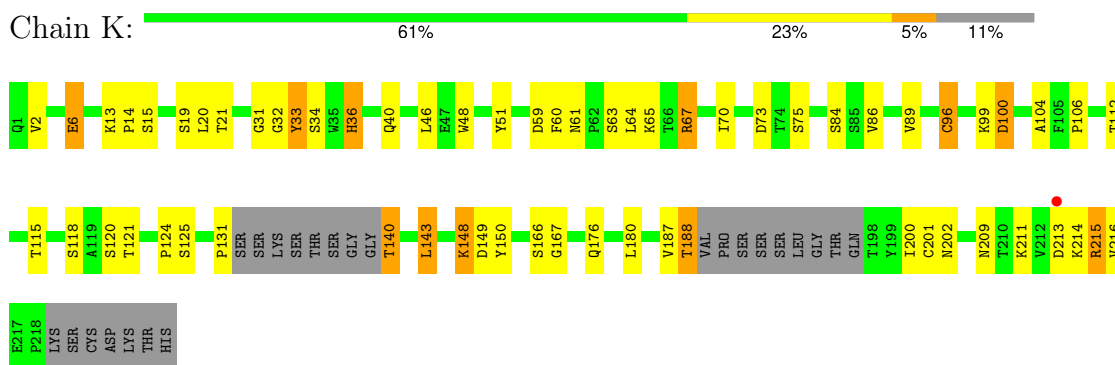
- Molecule 1: Fab Hu 15C1 Heavy chain



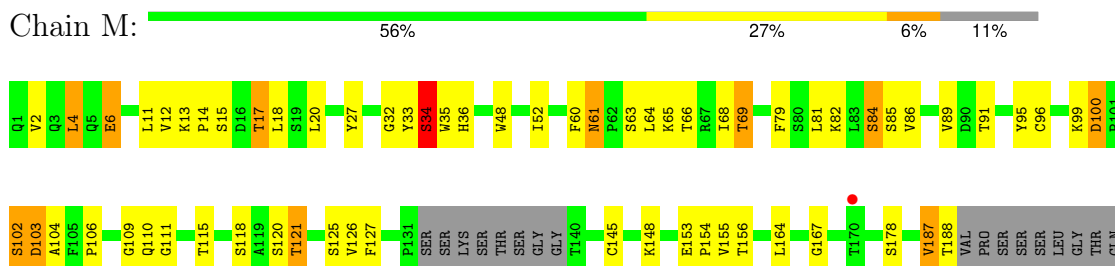
- Molecule 1: Fab Hu 15C1 Heavy chain



- Molecule 1: Fab Hu 15C1 Heavy chain



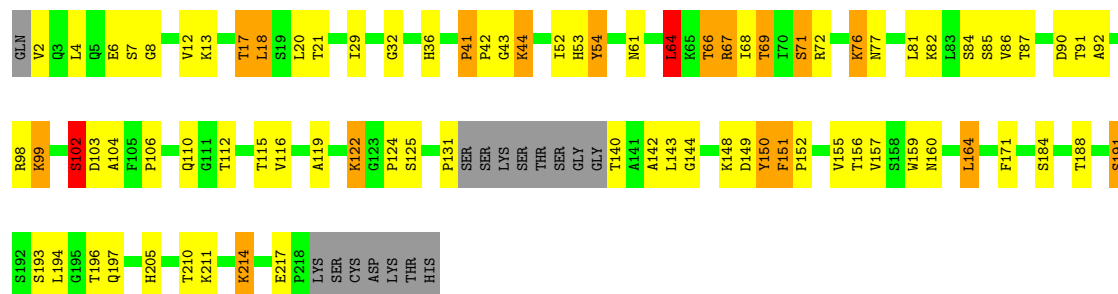
- Molecule 1: Fab Hu 15C1 Heavy chain





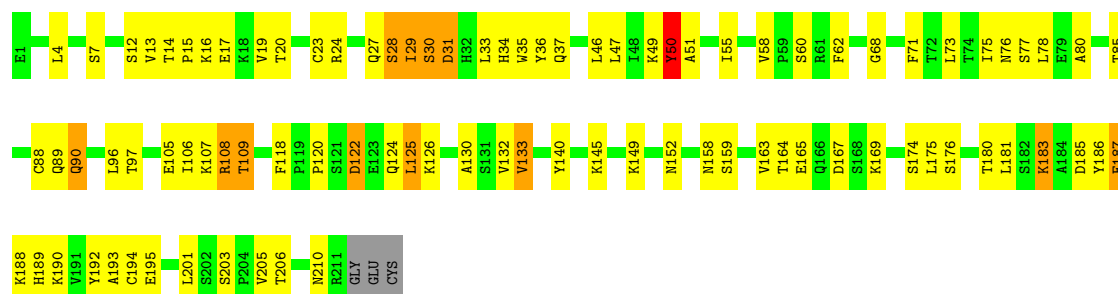
• Molecule 1: Fab Hu 15C1 Heavy chain

Chain O: 56% 28% 8% 7%



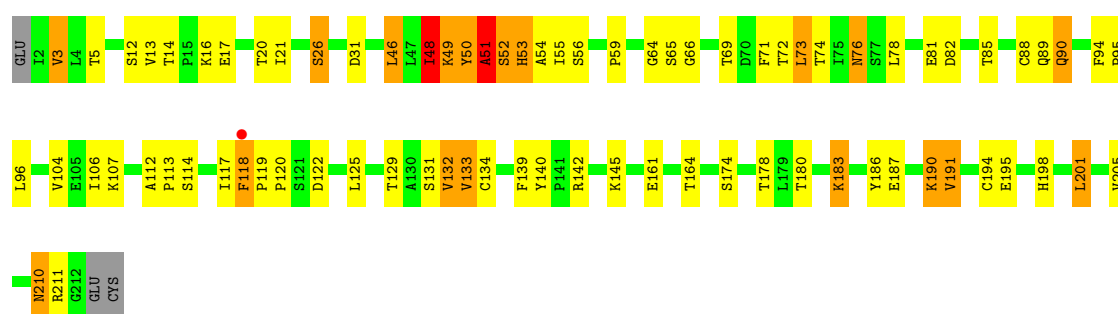
• Molecule 2: Fab Hu 15C1 Light chain

Chain B: 56% 36% 6%



• Molecule 2: Fab Hu 15C1 Light chain

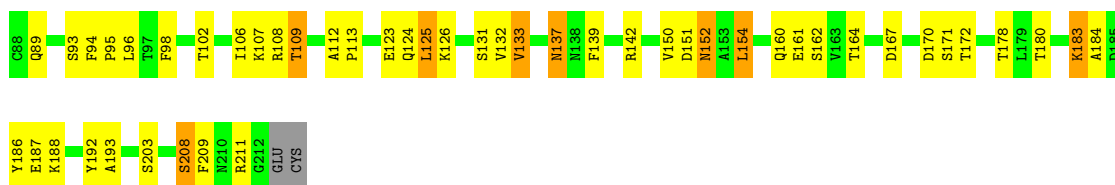
Chain D: 62% 28% 8% 2%



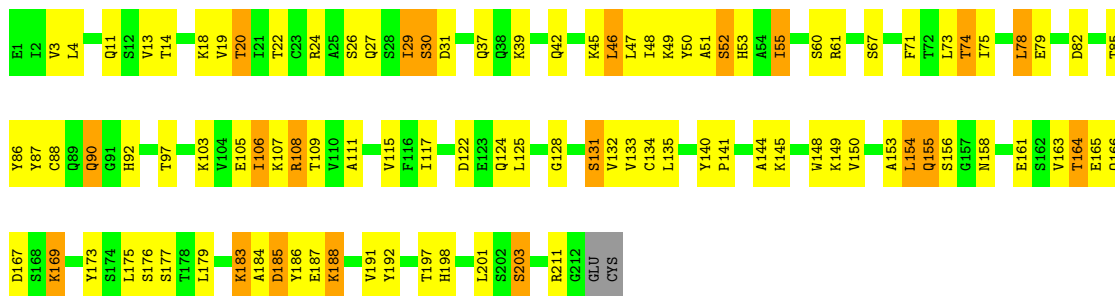
• Molecule 2: Fab Hu 15C1 Light chain

Chain F: 60% 31% 7%





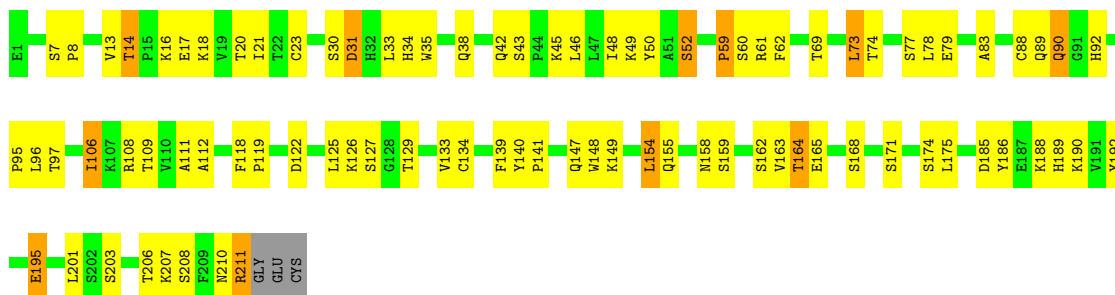
• Molecule 2: Fab Hu 15C1 Light chain



• Molecule 2: Fab Hu 15C1 Light chain



• Molecule 2: Fab Hu 15C1 Light chain

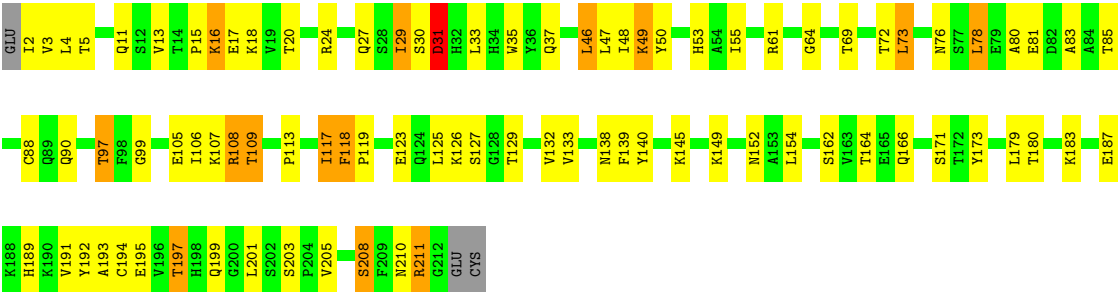


• Molecule 2: Fab Hu 15C1 Light chain





● Molecule 2: Fab Hu 15C1 Light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.82Å 82.51Å 261.57Å 90.00° 101.21° 90.00°	Depositor
Resolution (Å)	15.00 – 2.75 15.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.8 (15.00-2.75) 98.8 (15.00-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.177 , 0.209 0.179 , 0.207	Depositor DCC
R_{free} test set	5475 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	54.3	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 29.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.377 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	26033	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.11% 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

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	0.76	1/1687 (0.1%)	0.98	3/2307 (0.1%)
1	C	0.60	0/1638	1.00	6/2241 (0.3%)
1	E	0.63	2/1629 (0.1%)	1.02	9/2229 (0.4%)
1	G	0.64	0/1487	0.95	4/2034 (0.2%)
1	I	0.73	3/1687 (0.2%)	1.06	7/2307 (0.3%)
1	K	0.71	3/1576 (0.2%)	1.04	5/2154 (0.2%)
1	M	0.64	2/1576 (0.1%)	1.03	8/2154 (0.4%)
1	O	0.63	1/1629 (0.1%)	1.00	10/2229 (0.4%)
2	B	0.62	2/1668 (0.1%)	0.98	4/2265 (0.2%)
2	D	0.61	3/1663 (0.2%)	0.97	9/2258 (0.4%)
2	F	0.55	0/1663	0.94	4/2258 (0.2%)
2	H	0.60	2/1672 (0.1%)	0.99	4/2270 (0.2%)
2	J	0.83	3/1672 (0.2%)	1.12	12/2270 (0.5%)
2	L	0.58	0/1668	0.97	3/2265 (0.1%)
2	N	0.67	0/1663	1.00	3/2258 (0.1%)
2	P	0.62	0/1663	1.00	6/2258 (0.3%)
All	All	0.65	22/26241 (0.1%)	1.00	97/35757 (0.3%)

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	C	0	1
1	O	0	1
2	D	0	2
All	All	0	4

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	33	TYR	N-CA	-7.22	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	30	SER	C-O	-6.71	1.17	1.24
2	D	51	ALA	CA-C	-6.58	1.43	1.52
1	O	151	PHE	C-O	-6.23	1.17	1.24
2	J	140	TYR	CA-C	-6.09	1.46	1.52
1	I	34	SER	C-O	-5.93	1.16	1.23
2	B	30	SER	C-O	-5.81	1.19	1.24
1	I	33	TYR	C-O	-5.69	1.19	1.24
2	H	52	SER	CA-C	-5.60	1.44	1.52
1	E	13	LYS	C-N	5.49	1.40	1.33
1	K	13	LYS	C-N	5.47	1.40	1.33
1	M	33	TYR	C-O	-5.47	1.19	1.23
1	E	16	ASP	CA-C	-5.47	1.46	1.53
2	J	138	ASN	CA-C	5.32	1.58	1.53
2	D	54	ALA	CA-C	-5.25	1.46	1.52
1	K	32	GLY	C-O	-5.23	1.18	1.23
2	D	48	ILE	C-O	-5.21	1.18	1.24
1	I	31	GLY	C-O	-5.21	1.17	1.23
1	A	45	GLY	C-O	-5.17	1.17	1.23
2	J	140	TYR	C-O	-5.14	1.18	1.24
2	B	28	SER	CA-C	-5.01	1.46	1.52
1	K	33	TYR	C-O	-5.01	1.17	1.24

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	52	SER	N-CA-C	11.95	124.39	111.36
1	K	31	GLY	N-CA-C	11.62	126.55	112.49
1	M	102	SER	N-CA-C	10.05	122.31	111.36
2	J	138	ASN	N-CA-C	9.00	121.44	110.91
2	B	50	TYR	N-CA-C	8.65	123.51	111.92
1	G	102	SER	N-CA-C	8.41	122.04	111.69
1	O	102	SER	N-CA-C	8.20	119.99	111.14
1	E	28	SER	N-CA-C	8.15	119.79	111.07
1	C	102	SER	N-CA-C	7.79	120.45	111.11
2	J	127	SER	CA-C-N	-7.71	115.13	123.30
2	J	127	SER	C-N-CA	-7.71	115.13	123.30
2	J	58	VAL	CA-C-N	7.43	127.47	119.90
2	J	58	VAL	C-N-CA	7.43	127.47	119.90
2	B	30	SER	CA-C-N	7.42	130.96	120.28
2	B	30	SER	C-N-CA	7.42	130.96	120.28
2	J	128	GLY	N-CA-C	7.35	121.44	113.58
2	D	76	ASN	N-CA-C	7.17	119.95	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	16	ASP	N-CA-C	-7.01	100.67	110.35
1	K	13	LYS	CA-C-N	-6.95	112.60	119.76
1	K	13	LYS	C-N-CA	-6.95	112.60	119.76
1	C	149	ASP	N-CA-C	6.92	121.19	111.92
2	H	52	SER	N-CA-C	-6.90	105.41	114.31
2	F	58	VAL	CA-C-N	6.84	128.39	119.84
2	F	58	VAL	C-N-CA	6.84	128.39	119.84
1	A	31	GLY	N-CA-C	6.80	121.47	112.77
2	N	29	ILE	N-CA-C	-6.77	100.85	109.58
1	C	65	LYS	N-CA-C	6.72	120.51	111.24
2	J	123	GLU	N-CA-C	-6.58	104.03	111.07
2	N	49	LYS	N-CA-C	6.50	121.32	112.68
2	P	31	ASP	N-CA-C	6.43	119.28	111.82
1	E	13	LYS	CA-C-N	-6.33	113.25	119.76
1	E	13	LYS	C-N-CA	-6.33	113.25	119.76
2	P	118	PHE	CA-C-N	6.33	126.89	120.38
2	P	118	PHE	C-N-CA	6.33	126.89	120.38
2	J	50	TYR	N-CA-C	6.30	124.23	110.80
1	M	61	ASN	CA-C-N	6.25	127.65	119.84
1	M	61	ASN	C-N-CA	6.25	127.65	119.84
1	E	36	HIS	N-CA-C	6.23	119.69	109.85
1	O	150	TYR	N-CA-C	6.20	118.61	109.24
1	O	61	ASN	CA-C-N	6.20	127.59	119.84
1	O	61	ASN	C-N-CA	6.20	127.59	119.84
1	I	31	GLY	N-CA-C	6.16	120.65	112.77
1	I	13	LYS	CA-C-N	-6.09	113.48	119.76
1	I	13	LYS	C-N-CA	-6.09	113.48	119.76
1	M	33	TYR	N-CA-CB	-6.09	105.93	111.59
2	H	191	VAL	N-CA-C	6.08	116.63	107.75
2	L	112	ALA	CA-C-N	5.91	126.21	119.83
2	L	112	ALA	C-N-CA	5.91	126.21	119.83
2	P	208	SER	N-CA-C	5.88	116.86	108.74
1	M	100	ASP	CA-C-N	-5.86	114.85	120.83
1	M	100	ASP	C-N-CA	-5.86	114.85	120.83
2	J	32	HIS	N-CA-C	5.86	118.40	109.62
1	E	123	GLY	CA-C-N	5.81	126.30	120.14
1	E	123	GLY	C-N-CA	5.81	126.30	120.14
2	J	53	HIS	N-CA-C	5.81	118.42	109.07
2	D	53	HIS	N-CA-C	5.77	118.61	109.96
1	M	199	TYR	N-CA-C	5.73	118.30	109.07
1	I	105	PHE	CA-C-N	5.68	125.21	119.19
1	I	105	PHE	C-N-CA	5.68	125.21	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	191	VAL	N-CA-C	5.67	116.11	108.17
1	O	32	GLY	N-CA-C	5.67	118.86	110.42
2	F	87	TYR	N-CA-C	5.56	118.28	109.50
1	M	34	SER	N-CA-C	-5.55	100.73	109.50
1	K	36	HIS	N-CA-C	5.54	118.60	109.85
2	D	52	SER	N-CA-C	5.51	126.43	111.00
1	O	8	GLY	CA-C-N	5.50	125.82	119.93
1	O	8	GLY	C-N-CA	5.50	125.82	119.93
2	D	51	ALA	CA-C-N	5.49	131.59	121.70
2	D	51	ALA	C-N-CA	5.49	131.59	121.70
2	N	87	TYR	N-CA-C	5.47	117.81	108.90
1	G	61	ASN	CA-C-N	5.46	125.55	119.32
1	G	61	ASN	C-N-CA	5.46	125.55	119.32
2	D	104	VAL	N-CA-C	5.46	115.75	108.11
1	A	30	THR	CA-C-N	5.44	125.98	120.00
1	A	30	THR	C-N-CA	5.44	125.98	120.00
1	I	130	ALA	N-CA-C	5.43	116.54	109.64
2	J	124	GLN	N-CA-C	5.43	117.27	111.36
1	I	36	HIS	N-CA-C	5.40	118.38	109.85
1	K	32	GLY	N-CA-C	-5.40	101.60	110.56
2	F	137	ASN	N-CA-C	5.34	117.67	109.07
2	H	87	TYR	N-CA-C	5.31	117.56	108.90
1	O	157	VAL	N-CA-C	5.27	115.71	108.12
2	J	156	SER	N-CA-C	5.25	117.73	108.75
1	O	41	PRO	CA-C-N	5.19	126.32	119.84
1	O	41	PRO	C-N-CA	5.19	126.32	119.84
2	B	50	TYR	CB-CA-C	-5.17	104.59	111.63
1	G	200	ILE	N-CA-C	5.16	115.91	108.48
1	E	105	PHE	CA-C-N	5.10	124.76	119.56
1	E	105	PHE	C-N-CA	5.10	124.76	119.56
2	P	138	ASN	N-CA-C	5.07	118.13	111.28
2	H	29	ILE	N-CA-C	5.05	117.23	111.88
1	C	8	GLY	CA-C-N	5.05	125.33	119.93
1	C	8	GLY	C-N-CA	5.05	125.33	119.93
1	C	31	GLY	N-CA-C	5.03	119.20	112.77
2	P	191	VAL	N-CA-C	5.02	115.20	108.17
2	D	118	PHE	CA-C-N	5.02	125.55	120.38
2	D	118	PHE	C-N-CA	5.02	125.55	120.38

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	64	LEU	Peptide
2	D	50	TYR	Peptide
2	D	51	ALA	Peptide
1	O	64	LEU	Peptide

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	1641	0	1609	45	0
1	C	1593	0	1562	39	0
1	E	1584	0	1551	47	0
1	G	1445	0	1409	30	0
1	I	1641	0	1609	43	0
1	K	1533	0	1501	36	0
1	M	1533	0	1501	37	0
1	O	1584	0	1551	48	0
2	B	1631	0	1586	48	0
2	D	1626	0	1580	46	0
2	F	1626	0	1580	46	0
2	H	1635	0	1589	55	0
2	J	1635	0	1587	65	0
2	L	1631	0	1586	46	0
2	N	1626	0	1580	52	0
2	P	1626	0	1580	47	1
3	A	35	0	0	4	0
3	B	25	0	0	2	0
3	C	29	0	0	3	0
3	D	23	0	0	4	0
3	E	18	0	0	4	0
3	F	22	0	0	4	0
3	G	42	0	0	4	0
3	H	21	0	0	4	1
3	I	37	0	0	4	0
3	J	28	0	0	6	0
3	K	33	0	0	5	0
3	L	24	0	0	4	0
3	M	29	0	0	3	0
3	N	32	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	19	0	0	6	0
3	P	26	0	0	4	0
All	All	26033	0	24961	707	1

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 14.

All (707) 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:E:28:SER:O	1:E:77:ASN:ND2	1.65	1.30
1:O:149:ASP:OD2	3:O:304:HOH:O	1.76	1.04
1:M:6:GLU:OE2	1:M:109:GLY:HA3	1.66	0.96
1:I:32:GLY:HA3	1:I:54:TYR:HB3	1.48	0.95
1:O:99:LYS:HD2	1:O:103:ASP:HB2	1.45	0.95
1:A:41:PRO:HB2	1:A:44:LYS:HG3	1.48	0.93
1:I:127:PHE:CD1	2:J:123:GLU:OE1	2.22	0.92
2:J:31:ASP:OD1	2:J:50:TYR:O	1.85	0.92
2:N:34:HIS:ND1	2:N:49:LYS:O	2.02	0.91
1:O:64:LEU:O	1:O:66:THR:N	2.04	0.90
1:G:176:GLN:NE2	1:G:180:LEU:O	2.06	0.89
1:O:91:THR:HG23	1:O:115:THR:HA	1.52	0.88
2:J:122:ASP:O	2:J:126:LYS:HG2	1.73	0.88
2:L:190:LYS:HE2	2:L:210:ASN:HB3	1.53	0.88
1:I:32:GLY:HA3	1:I:54:TYR:CB	2.05	0.87
1:E:14:PRO:O	1:E:15:SER:OG	1.92	0.86
1:G:124:PRO:HB3	1:G:150:TYR:HB3	1.58	0.86
1:E:131:PRO:O	3:E:307:HOH:O	1.94	0.85
2:F:125:LEU:O	2:F:183:LYS:NZ	2.10	0.84
2:N:202:SER:O	3:N:316:HOH:O	1.97	0.83
1:M:6:GLU:OE2	1:M:109:GLY:CA	2.25	0.82
2:H:184:ALA:O	2:H:188:LYS:NZ	2.10	0.82
1:G:131:PRO:HG3	1:G:143:LEU:HB3	1.62	0.82
2:J:24:ARG:NH2	2:N:17:GLU:OE2	2.14	0.81
2:J:105:GLU:OE2	2:J:140:TYR:OH	1.97	0.81
1:K:188:THR:O	3:K:333:HOH:O	1.97	0.81
2:N:37:GLN:HB2	2:N:47:LEU:HD11	1.62	0.81
1:K:14:PRO:O	1:K:15:SER:OG	1.98	0.81
2:F:46:LEU:HD13	2:F:55:ILE:HD11	1.61	0.80
1:E:16:ASP:OD2	3:E:311:HOH:O	2.00	0.80
1:I:5:GLN:OE1	3:I:316:HOH:O	1.98	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:127:PHE:CE1	2:J:123:GLU:OE1	2.35	0.80
1:I:127:PHE:HD1	2:J:123:GLU:OE1	1.66	0.79
2:H:49:LYS:O	2:H:53:HIS:HB2	1.82	0.78
2:P:46:LEU:HD13	2:P:55:ILE:HD11	1.66	0.78
1:K:48:TRP:O	1:K:61:ASN:ND2	2.14	0.78
2:D:190:LYS:HD3	2:D:210:ASN:HB3	1.65	0.78
2:H:39:LYS:NZ	3:H:321:HOH:O	2.15	0.78
1:G:34:SER:OG	1:G:36:HIS:NE2	2.17	0.78
2:J:170:ASP:OD2	3:J:311:HOH:O	2.03	0.76
2:B:164:THR:HG22	2:B:174:SER:H	1.51	0.76
1:O:2:VAL:N	3:O:309:HOH:O	2.17	0.76
1:I:66:THR:OG1	3:I:317:HOH:O	2.03	0.75
2:J:50:TYR:N	2:J:51:ALA:HA	2.00	0.75
2:J:49:LYS:O	2:J:53:HIS:HB2	1.86	0.74
2:J:30:SER:OG	2:J:31:ASP:N	2.14	0.74
1:A:34:SER:HB3	1:A:36:HIS:HE2	1.51	0.74
2:D:187:GLU:O	2:D:211:ARG:NH2	2.19	0.74
1:E:87:THR:OG1	1:E:90:ASP:OD2	2.04	0.74
1:I:23:ALA:HA	1:I:78:GLN:HG2	1.68	0.74
1:M:4:LEU:N	1:M:4:LEU:HD12	2.02	0.74
2:F:108:ARG:NH1	2:F:109:THR:O	2.20	0.73
2:L:59:PRO:O	3:L:304:HOH:O	2.06	0.73
2:B:37:GLN:HB2	2:B:47:LEU:HD11	1.70	0.73
2:D:142:ARG:NH2	3:D:310:HOH:O	2.22	0.73
1:K:34:SER:OG	1:K:36:HIS:NE2	2.20	0.73
2:L:171:SER:OG	3:L:306:HOH:O	2.06	0.73
1:O:68:ILE:HD11	1:O:81:LEU:CD1	2.19	0.72
1:A:64:LEU:O	1:A:68:ILE:HG22	1.89	0.72
2:N:128:GLY:HA2	2:N:183:LYS:HD2	1.71	0.72
1:A:18:LEU:HD21	1:A:114:VAL:HG21	1.72	0.72
2:D:13:VAL:O	2:D:107:LYS:N	2.22	0.72
2:B:4:LEU:O	3:B:315:HOH:O	2.08	0.71
2:L:147:GLN:HB3	2:L:195:GLU:HB3	1.71	0.71
1:A:34:SER:HB3	1:A:36:HIS:NE2	2.06	0.71
2:N:149:LYS:HB2	2:N:193:ALA:HB3	1.71	0.70
2:P:2:ILE:N	3:P:317:HOH:O	2.22	0.70
2:P:37:GLN:HB2	2:P:47:LEU:HD11	1.73	0.70
1:I:40:GLN:HB2	1:I:46:LEU:HD23	1.74	0.70
2:J:90:GLN:NE2	2:J:97:THR:OG1	2.25	0.70
2:D:48:ILE:HG23	2:D:53:HIS:O	1.91	0.69
1:C:124:PRO:HD2	1:C:210:THR:HG21	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:136:LEU:HD11	2:J:196:VAL:HG21	1.73	0.69
2:D:95:PRO:O	3:D:301:HOH:O	2.09	0.69
1:M:60:PHE:HB2	1:M:65:LYS:HD2	1.75	0.69
1:C:54:TYR:O	1:C:72:ARG:NH1	2.24	0.69
1:A:8:GLY:HA3	1:A:20:LEU:HD12	1.73	0.69
2:P:61:ARG:O	2:P:76:ASN:ND2	2.23	0.69
2:P:166:GLN:NE2	2:P:171:SER:O	2.26	0.69
2:H:47:LEU:HB3	2:H:48:ILE:HD12	1.74	0.69
1:K:202:ASN:ND2	1:K:213:ASP:OD2	2.26	0.68
2:L:20:THR:HG22	2:L:74:THR:HG22	1.73	0.68
1:M:6:GLU:OE2	1:M:109:GLY:C	2.36	0.68
1:A:87:THR:OG1	3:A:303:HOH:O	2.10	0.68
1:A:124:PRO:HB3	1:A:150:TYR:HB3	1.74	0.68
2:J:37:GLN:HB2	2:J:47:LEU:HD11	1.75	0.68
1:M:6:GLU:OE2	1:M:110:GLN:N	2.26	0.68
2:N:78:LEU:HD11	2:N:106:ILE:HG12	1.75	0.68
2:D:48:ILE:HG21	2:D:51:ALA:CB	2.24	0.67
1:K:120:SER:O	3:K:302:HOH:O	2.11	0.67
1:E:91:THR:HG23	1:E:115:THR:HA	1.76	0.67
2:L:108:ARG:NH1	2:L:109:THR:O	2.27	0.67
1:G:149:ASP:OD1	3:G:327:HOH:O	2.12	0.67
2:H:185:ASP:HA	2:H:188:LYS:HZ3	1.60	0.67
1:I:41:PRO:HB2	1:I:44:LYS:HD2	1.76	0.67
1:I:64:LEU:O	1:I:68:ILE:HG22	1.95	0.66
1:O:71:SER:OG	3:O:314:HOH:O	2.13	0.66
2:J:61:ARG:NH2	3:J:322:HOH:O	2.28	0.66
1:K:104:ALA:O	1:K:106:PRO:HD3	1.96	0.66
2:J:57:GLY:O	3:J:317:HOH:O	2.13	0.66
1:E:42:PRO:HD3	1:E:92:ALA:HA	1.76	0.66
2:H:103:LYS:NZ	3:H:307:HOH:O	2.26	0.66
1:C:128:PRO:HB2	1:C:216:VAL:HG13	1.77	0.66
1:O:131:PRO:O	3:O:302:HOH:O	2.13	0.66
2:D:78:LEU:HD11	2:D:106:ILE:HD12	1.77	0.66
2:H:52:SER:HB2	2:H:53:HIS:ND1	2.11	0.66
1:E:140:THR:N	3:E:313:HOH:O	2.29	0.66
2:J:138:ASN:OD1	3:J:314:HOH:O	2.13	0.66
2:P:108:ARG:NH2	3:P:310:HOH:O	2.29	0.66
1:C:144:GLY:HA3	1:C:186:VAL:HG12	1.78	0.65
2:F:133:VAL:HG12	2:F:178:THR:HG23	1.78	0.65
1:C:100:ASP:OD2	3:C:303:HOH:O	2.14	0.65
2:D:133:VAL:HG12	2:D:178:THR:HG23	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:6:GLU:HG3	1:K:112:THR:HG22	1.78	0.65
1:O:4:LEU:O	3:O:303:HOH:O	2.14	0.65
2:F:78:LEU:HD13	2:F:106:ILE:HG13	1.78	0.65
2:L:139:PHE:HZ	2:L:175:LEU:HB2	1.61	0.65
1:E:86:VAL:HG11	1:E:116:VAL:HG21	1.77	0.65
1:M:120:SER:OG	3:M:308:HOH:O	2.13	0.65
1:O:69:THR:HG23	1:O:82:LYS:HB3	1.79	0.65
2:J:49:LYS:O	2:J:50:TYR:HB2	1.97	0.64
2:N:197:THR:HG23	2:N:204:PRO:HG3	1.78	0.64
2:H:124:GLN:HE22	2:H:131:SER:HB2	1.61	0.64
2:L:33:LEU:HD21	2:L:88:CYS:SG	2.38	0.64
2:H:188:LYS:HB2	2:H:188:LYS:HZ2	1.63	0.64
2:N:61:ARG:HD2	2:N:77:SER:HB3	1.78	0.64
2:J:189:HIS:O	2:J:211:ARG:NE	2.25	0.64
2:F:98:PHE:O	3:F:304:HOH:O	2.15	0.64
1:C:6:GLU:OE1	1:C:96:CYS:N	2.31	0.63
1:A:15:SER:O	3:A:329:HOH:O	2.16	0.63
2:H:108:ARG:HD3	2:H:109:THR:O	1.98	0.63
1:A:30:THR:HG22	1:A:72:ARG:NH1	2.14	0.63
1:A:51:TYR:CE1	1:A:59:ASP:HB3	2.34	0.62
2:P:80:ALA:HA	2:P:106:ILE:HD13	1.80	0.62
1:A:72:ARG:NH1	3:A:301:HOH:O	2.32	0.62
1:C:206:LYS:O	1:C:208:SER:HA	1.99	0.62
2:D:49:LYS:O	2:D:50:TYR:HB2	1.98	0.62
2:F:50:TYR:HB2	2:F:53:HIS:HD2	1.64	0.62
1:K:131:PRO:HG3	1:K:143:LEU:HB3	1.81	0.62
2:N:50:TYR:C	2:N:52:SER:H	2.06	0.62
1:G:99:LYS:HD2	1:G:103:ASP:HB3	1.80	0.62
1:M:204:ASN:ND2	1:M:210:THR:O	2.33	0.62
2:F:61:ARG:NH2	2:F:82:ASP:OD1	2.33	0.62
2:H:108:ARG:NH1	2:H:111:ALA:HB2	2.15	0.62
2:H:30:SER:OG	2:H:31:ASP:N	2.33	0.62
2:J:48:ILE:HG21	2:J:51:ALA:O	2.00	0.62
1:C:102:SER:HB2	1:C:104:ALA:H	1.63	0.62
2:F:154:LEU:HB2	2:L:154:LEU:HB2	1.81	0.62
1:E:86:VAL:HG12	1:E:87:THR:N	2.15	0.62
2:N:89:GLN:HG3	2:N:98:PHE:CE2	2.34	0.61
1:I:99:LYS:HB2	1:I:105:PHE:CE1	2.35	0.61
2:J:61:ARG:O	2:J:76:ASN:ND2	2.34	0.61
2:J:149:LYS:HG2	2:J:154:LEU:HD22	1.82	0.61
1:A:200:ILE:HD11	1:A:215:ARG:HD3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:205:HIS:CD2	1:G:207:PRO:HD2	2.36	0.61
1:E:99:LYS:HE2	1:E:103:ASP:HA	1.83	0.61
1:I:14:PRO:HG3	1:I:116:VAL:HG12	1.82	0.61
1:O:102:SER:N	1:O:103:ASP:HA	2.15	0.61
1:G:155:VAL:HG22	1:G:205:HIS:HB2	1.83	0.61
1:A:102:SER:HB2	1:A:104:ALA:N	2.16	0.60
2:H:46:LEU:HD13	2:H:55:ILE:HD11	1.83	0.60
2:L:201:LEU:O	3:L:313:HOH:O	2.17	0.60
2:P:4:LEU:HD11	2:P:90:GLN:HB2	1.82	0.60
2:B:29:ILE:C	2:B:30:SER:HG	2.08	0.60
2:B:80:ALA:HA	2:B:106:ILE:HD12	1.83	0.60
2:N:2:ILE:N	3:N:309:HOH:O	2.34	0.60
1:G:102:SER:N	1:G:103:ASP:HA	2.17	0.60
1:I:1:GLN:OE1	1:I:3:GLN:NE2	2.35	0.60
1:O:68:ILE:HD11	1:O:81:LEU:HD12	1.83	0.60
2:H:184:ALA:C	2:H:188:LYS:HZ1	2.08	0.60
2:F:50:TYR:HB2	2:F:53:HIS:CD2	2.37	0.60
2:F:170:ASP:OD2	2:F:172:THR:OG1	2.20	0.60
2:B:49:LYS:HG3	2:B:55:ILE:HD11	1.84	0.59
1:E:86:VAL:HG13	1:E:90:ASP:HB2	1.84	0.59
2:L:186:TYR:O	2:L:192:TYR:OH	2.19	0.59
1:E:86:VAL:HG13	1:E:90:ASP:CB	2.32	0.59
1:O:68:ILE:CD1	1:O:81:LEU:CD1	2.81	0.59
1:G:60:PHE:HE2	1:G:70:ILE:HG13	1.67	0.59
2:F:112:ALA:O	3:F:312:HOH:O	2.16	0.59
1:E:28:SER:O	1:E:29:ILE:HG22	2.03	0.59
1:O:54:TYR:O	1:O:72:ARG:NH1	2.29	0.59
1:E:86:VAL:CG1	1:E:116:VAL:HG21	2.33	0.59
2:N:90:GLN:O	2:N:90:GLN:NE2	2.36	0.58
1:E:208:SER:OG	1:E:210:THR:OG1	2.18	0.58
1:M:34:SER:HB3	1:M:36:HIS:HE2	1.68	0.58
2:H:125:LEU:HD12	2:H:183:LYS:HE3	1.84	0.58
2:P:187:GLU:O	2:P:211:ARG:NH2	2.35	0.58
2:D:59:PRO:O	3:D:313:HOH:O	2.16	0.58
2:B:120:PRO:HG3	2:B:130:ALA:HB1	1.86	0.58
2:P:30:SER:OG	2:P:31:ASP:N	2.35	0.58
1:A:102:SER:HB2	1:A:104:ALA:H	1.69	0.58
2:D:113:PRO:HD3	2:D:198:HIS:ND1	2.19	0.58
1:C:102:SER:N	1:C:103:ASP:HA	2.18	0.57
2:B:14:THR:O	2:B:17:GLU:HB2	2.04	0.57
2:N:161:GLU:HG2	2:N:175:LEU:HD21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:131:PRO:HG3	1:O:143:LEU:HB3	1.86	0.57
2:F:113:PRO:HB3	2:F:139:PHE:CD2	2.40	0.57
2:B:30:SER:H	2:B:68:GLY:HA2	1.69	0.57
2:F:13:VAL:O	2:F:107:LYS:N	2.31	0.57
2:H:18:LYS:NZ	3:H:305:HOH:O	2.37	0.57
2:N:3:VAL:H	2:N:26:SER:HB2	1.70	0.57
2:B:90:GLN:NE2	2:B:97:THR:OG1	2.34	0.57
2:N:150:VAL:HG22	2:N:192:TYR:CD2	2.40	0.57
1:M:102:SER:N	1:M:103:ASP:HA	2.20	0.57
2:J:49:LYS:C	2:J:51:ALA:HA	2.30	0.56
1:I:124:PRO:HB3	1:I:150:TYR:HB3	1.87	0.56
1:A:30:THR:HG22	1:A:72:ARG:HH12	1.69	0.56
2:J:123:GLU:O	2:J:126:LYS:HG3	2.06	0.56
2:B:186:TYR:O	2:B:192:TYR:OH	2.24	0.56
2:F:89:GLN:HB2	2:F:98:PHE:CE1	2.41	0.56
2:F:61:ARG:HH21	2:F:82:ASP:CG	2.14	0.56
2:J:33:LEU:O	2:J:51:ALA:HB2	2.06	0.56
1:O:142:ALA:HB2	1:O:188:THR:HG22	1.86	0.56
1:C:102:SER:HB2	1:C:104:ALA:N	2.20	0.56
2:H:49:LYS:HG3	2:H:55:ILE:HD11	1.87	0.56
2:P:108:ARG:NH1	2:P:109:THR:HG22	2.21	0.56
2:F:12:SER:O	3:F:302:HOH:O	2.17	0.55
1:G:72:ARG:NH1	3:G:307:HOH:O	2.32	0.55
2:L:149:LYS:HG2	2:L:154:LEU:HD22	1.87	0.55
1:M:91:THR:HG23	1:M:115:THR:HA	1.89	0.55
1:E:62:PRO:HA	1:E:65:LYS:HB2	1.89	0.55
2:J:115:VAL:HG22	2:J:136:LEU:HD12	1.88	0.55
1:I:14:PRO:O	1:I:15:SER:HB3	2.07	0.55
2:J:48:ILE:HD13	2:J:73:LEU:HD23	1.88	0.55
1:K:140:THR:N	3:K:305:HOH:O	2.40	0.55
2:B:108:ARG:HD3	2:B:109:THR:O	2.07	0.55
1:C:18:LEU:HD11	1:C:114:VAL:HG11	1.88	0.55
2:F:193:ALA:HB2	2:F:208:SER:HB3	1.89	0.55
1:M:85:SER:OG	3:M:309:HOH:O	2.15	0.55
2:N:170:ASP:OD1	2:N:172:THR:OG1	2.23	0.55
1:O:12:VAL:HG11	1:O:18:LEU:HD23	1.89	0.55
1:C:215:ARG:NH2	3:C:310:HOH:O	2.40	0.54
2:B:13:VAL:HG21	2:B:19:VAL:HG22	1.89	0.54
2:H:185:ASP:HA	2:H:188:LYS:NZ	2.21	0.54
1:I:14:PRO:HG3	1:I:116:VAL:CG1	2.37	0.54
2:D:48:ILE:CG2	2:D:51:ALA:CB	2.85	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:102:SER:HB2	1:I:104:ALA:H	1.72	0.54
2:H:186:TYR:O	2:H:192:TYR:OH	2.26	0.54
2:J:122:ASP:O	2:J:126:LYS:CG	2.51	0.54
1:M:104:ALA:O	1:M:106:PRO:HD3	2.06	0.54
1:M:167:GLY:O	1:M:187:VAL:HA	2.07	0.54
2:N:43:SER:OG	3:N:303:HOH:O	2.19	0.54
2:L:49:LYS:HB3	2:L:50:TYR:CD2	2.43	0.54
2:B:164:THR:HG23	2:B:165:GLU:O	2.08	0.54
1:C:11:LEU:HB2	1:C:152:PRO:HG3	1.89	0.54
2:H:39:LYS:O	2:H:42:GLN:HB2	2.07	0.54
2:H:78:LEU:HD13	2:H:106:ILE:HG13	1.90	0.54
2:J:164:THR:HG22	2:J:174:SER:H	1.73	0.54
1:E:105:PHE:O	1:E:108:TRP:NE1	2.41	0.53
1:A:17:THR:HB	1:A:84:SER:HA	1.89	0.53
1:G:6:GLU:HG3	1:G:112:THR:HG22	1.90	0.53
2:J:48:ILE:CG2	2:J:51:ALA:O	2.55	0.53
2:B:118:PHE:HD2	2:B:133:VAL:HG22	1.74	0.53
2:D:164:THR:HG22	2:D:174:SER:H	1.72	0.53
1:K:36:HIS:CE1	1:K:51:TYR:HB3	2.44	0.53
2:J:125:LEU:HD11	2:J:130:ALA:HB2	1.90	0.53
2:P:90:GLN:NE2	2:P:97:THR:OG1	2.41	0.53
1:C:36:HIS:CE1	1:C:51:TYR:HB3	2.43	0.53
2:N:209:PHE:CD1	2:N:209:PHE:C	2.87	0.53
2:D:117:ILE:HD12	2:D:194:CYS:HB2	1.91	0.53
1:M:34:SER:HB3	1:M:36:HIS:NE2	2.24	0.53
2:B:122:ASP:OD1	2:B:126:LYS:NZ	2.34	0.52
1:G:2:VAL:HG21	1:G:98:ARG:NH1	2.24	0.52
2:H:187:GLU:HB3	1:K:118:SER:HB3	1.90	0.52
2:N:122:ASP:O	2:N:126:LYS:HD2	2.09	0.52
2:L:13:VAL:HG13	2:L:17:GLU:CD	2.34	0.52
1:C:148:LYS:O	1:C:149:ASP:HB2	2.09	0.52
2:J:115:VAL:HG22	2:J:136:LEU:CD1	2.39	0.52
1:E:149:ASP:O	1:E:180:LEU:HD13	2.09	0.52
1:I:17:THR:HG22	3:I:303:HOH:O	2.10	0.52
2:N:90:GLN:HE22	2:N:96:LEU:HA	1.75	0.52
1:O:151:PHE:CD1	1:O:152:PRO:HA	2.44	0.52
2:D:190:LYS:O	2:D:210:ASN:HA	2.09	0.52
1:E:64:LEU:O	1:E:68:ILE:HG22	2.10	0.52
1:E:68:ILE:HG12	1:E:69:THR:N	2.23	0.52
2:H:128:GLY:HA2	2:H:183:LYS:HB3	1.90	0.52
1:C:11:LEU:HD23	1:C:121:THR:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:89:VAL:O	3:G:313:HOH:O	2.18	0.52
1:C:65:LYS:N	1:C:66:THR:HA	2.25	0.52
2:F:184:ALA:O	2:F:188:LYS:HG3	2.10	0.51
2:J:164:THR:HG23	2:J:165:GLU:O	2.09	0.51
1:I:91:THR:O	3:I:310:HOH:O	2.19	0.51
2:D:48:ILE:HG21	2:D:51:ALA:HB1	1.92	0.51
1:E:99:LYS:HB2	1:E:105:PHE:CE2	2.46	0.51
1:O:193:SER:HB2	1:O:197:GLN:HG2	1.90	0.51
1:E:28:SER:OG	1:E:29:ILE:N	2.43	0.51
2:H:11:GLN:HE21	2:H:19:VAL:HG13	1.75	0.51
2:J:11:GLN:HG3	2:N:8:PRO:HG3	1.90	0.51
1:K:19:SER:OG	3:K:317:HOH:O	2.19	0.51
1:K:33:TYR:CZ	3:K:331:HOH:O	2.54	0.51
2:N:158:ASN:ND2	2:N:179:LEU:HD11	2.25	0.51
2:F:13:VAL:HG13	2:F:17:GLU:HB3	1.92	0.51
2:H:19:VAL:HB	2:H:75:ILE:HB	1.93	0.51
1:M:153:GLU:OE2	1:M:154:PRO:HA	2.11	0.51
2:P:47:LEU:HB3	2:P:48:ILE:HD12	1.92	0.51
1:K:99:LYS:HE3	1:K:100:ASP:O	2.10	0.51
1:A:32:GLY:O	1:A:33:TYR:HB2	2.10	0.51
1:E:86:VAL:HG11	1:E:116:VAL:CG2	2.41	0.51
2:H:45:LYS:NZ	3:H:321:HOH:O	2.44	0.51
2:B:158:ASN:N	2:B:158:ASN:OD1	2.43	0.51
1:I:31:GLY:N	1:I:32:GLY:HA2	2.25	0.51
2:D:107:LYS:HA	2:D:140:TYR:OH	2.11	0.51
1:A:32:GLY:HA2	1:A:54:TYR:CD2	2.45	0.50
2:L:108:ARG:NH1	2:L:111:ALA:HB2	2.26	0.50
2:N:50:TYR:O	2:N:52:SER:N	2.44	0.50
2:N:203:SER:O	3:N:317:HOH:O	2.18	0.50
2:P:193:ALA:HB2	2:P:208:SER:HB3	1.92	0.50
1:A:102:SER:N	1:A:103:ASP:HA	2.26	0.50
2:L:50:TYR:O	2:L:52:SER:N	2.41	0.50
1:M:48:TRP:O	1:M:61:ASN:ND2	2.40	0.50
2:F:187:GLU:O	2:F:211:ARG:NH2	2.45	0.50
2:J:30:SER:HG	2:J:31:ASP:H	1.53	0.50
2:L:23:CYS:HB2	2:L:35:TRP:CH2	2.47	0.50
2:N:108:ARG:NH1	2:N:109:THR:O	2.44	0.50
1:O:140:THR:N	1:O:191:SER:HG	2.10	0.50
1:C:91:THR:HG23	1:C:115:THR:HA	1.94	0.50
1:G:42:PRO:HD3	1:G:92:ALA:HA	1.93	0.50
2:J:120:PRO:HD3	2:J:132:VAL:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:17:GLU:OE1	2:N:7:SER:OG	2.30	0.49
2:L:158:ASN:OD1	2:L:158:ASN:N	2.42	0.49
2:P:201:LEU:HD13	2:P:205:VAL:HG23	1.92	0.49
2:P:149:LYS:HZ1	2:P:195:GLU:CD	2.19	0.49
2:D:48:ILE:CG2	2:D:51:ALA:HB2	2.42	0.49
2:H:149:LYS:HA	2:H:153:ALA:O	2.12	0.49
2:N:148:TRP:CE2	2:N:179:LEU:HB2	2.47	0.49
1:C:70:ILE:HG23	1:C:80:SER:O	2.13	0.49
2:B:120:PRO:HD3	2:B:132:VAL:HG22	1.94	0.49
2:N:92:HIS:HD2	2:N:93:SER:HB2	1.78	0.49
1:O:68:ILE:CD1	1:O:81:LEU:HD12	2.42	0.49
2:B:30:SER:OG	2:B:31:ASP:N	2.42	0.49
1:A:86:VAL:HG12	1:A:116:VAL:HG11	1.94	0.49
1:E:127:PHE:CE1	2:F:124:GLN:HA	2.48	0.49
2:H:201:LEU:HB3	2:H:203:SER:O	2.12	0.49
1:K:167:GLY:O	1:K:187:VAL:HA	2.13	0.49
2:P:117:ILE:HD12	2:P:194:CYS:HB2	1.95	0.49
1:A:41:PRO:HB2	1:A:44:LYS:CG	2.34	0.49
2:D:122:ASP:HA	2:D:125:LEU:HB2	1.94	0.49
1:G:41:PRO:HB2	1:G:44:LYS:HD3	1.95	0.49
2:J:18:LYS:NZ	3:J:301:HOH:O	2.45	0.49
2:F:49:LYS:O	2:F:53:HIS:HB2	2.12	0.49
2:F:94:PHE:HA	2:F:95:PRO:C	2.38	0.49
2:H:82:ASP:O	2:H:86:TYR:OH	2.20	0.49
1:K:201:CYS:O	1:K:213:ASP:HA	2.13	0.49
1:O:36:HIS:NE2	1:O:99:LYS:HB2	2.28	0.49
2:F:123:GLU:HA	2:F:126:LYS:HG3	1.95	0.48
2:H:13:VAL:HB	2:H:78:LEU:HD12	1.95	0.48
1:K:124:PRO:HB3	1:K:150:TYR:HB3	1.94	0.48
1:K:202:ASN:HD22	1:K:213:ASP:CG	2.21	0.48
1:M:6:GLU:OE1	1:M:95:TYR:HA	2.13	0.48
2:B:105:GLU:HG2	2:B:106:ILE:N	2.27	0.48
1:O:102:SER:HB2	1:O:104:ALA:H	1.79	0.48
2:D:64:GLY:HA2	2:D:72:THR:O	2.14	0.48
2:B:14:THR:HB	2:B:17:GLU:CD	2.38	0.48
1:I:99:LYS:HE2	1:I:103:ASP:HB2	1.94	0.48
1:A:106:PRO:HB2	1:A:107:TYR:CD2	2.48	0.48
1:E:21:THR:HA	1:E:80:SER:HA	1.96	0.48
2:H:175:LEU:HD23	2:H:176:SER:N	2.28	0.48
1:I:160:ASN:HB2	1:I:164:LEU:HB2	1.94	0.48
2:B:35:TRP:NE1	3:B:310:HOH:O	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:105:GLU:OE2	2:H:173:TYR:OH	2.31	0.48
1:K:6:GLU:OE1	1:K:96:CYS:N	2.47	0.48
1:M:6:GLU:CD	1:M:111:GLY:H	2.22	0.48
1:M:99:LYS:HD2	1:M:103:ASP:HB3	1.96	0.48
2:N:164:THR:HG23	2:N:165:GLU:O	2.13	0.48
1:C:122:LYS:HG2	1:C:149:ASP:O	2.13	0.48
1:O:87:THR:O	1:O:116:VAL:HG11	2.13	0.48
2:P:13:VAL:HG13	2:P:17:GLU:HB3	1.94	0.48
2:P:113:PRO:HB3	2:P:139:PHE:CD1	2.49	0.48
2:D:31:ASP:O	2:D:50:TYR:HD1	1.96	0.48
2:D:48:ILE:CG2	2:D:51:ALA:HA	2.43	0.48
2:L:164:THR:HG23	2:L:165:GLU:O	2.14	0.48
1:A:99:LYS:HB2	1:A:105:PHE:CE1	2.48	0.48
2:D:66:GLY:HA3	2:D:71:PHE:HA	1.96	0.48
1:G:14:PRO:O	1:G:15:SER:OG	2.27	0.48
2:J:47:LEU:O	2:J:55:ILE:HG12	2.14	0.48
2:J:107:LYS:HE2	2:J:107:LYS:HB2	1.66	0.48
1:O:193:SER:O	1:O:197:GLN:HG2	2.14	0.48
1:E:18:LEU:N	1:E:83:LEU:O	2.39	0.47
2:J:201:LEU:HD13	2:J:205:VAL:HG23	1.94	0.47
2:L:83:ALA:HB2	2:L:106:ILE:HD11	1.96	0.47
1:E:39:ARG:HB3	1:E:49:MET:SD	2.55	0.47
1:E:188:THR:HG21	2:F:137:ASN:ND2	2.28	0.47
2:H:144:ALA:HB2	2:H:198:HIS:HD2	1.79	0.47
1:I:164:LEU:CD1	1:I:187:VAL:HG21	2.44	0.47
1:K:6:GLU:OE1	1:K:96:CYS:HB2	2.13	0.47
2:D:112:ALA:HB1	2:D:201:LEU:HD23	1.96	0.47
1:I:51:TYR:CE1	1:I:59:ASP:HB3	2.49	0.47
2:N:108:ARG:HG3	2:N:109:THR:O	2.14	0.47
1:O:119:ALA:HB3	1:O:151:PHE:CE2	2.49	0.47
2:F:124:GLN:HE22	2:F:131:SER:N	2.12	0.47
2:J:194:CYS:O	2:J:206:THR:HA	2.14	0.47
2:P:24:ARG:HD3	3:P:320:HOH:O	2.15	0.47
2:P:105:GLU:OE2	2:P:173:TYR:OH	2.20	0.47
1:C:160:ASN:HB2	1:C:163:ALA:HB3	1.96	0.47
1:O:171:PHE:HB3	2:P:162:SER:OG	2.15	0.47
2:B:30:SER:O	2:B:71:PHE:CZ	2.67	0.47
2:F:192:TYR:HB2	2:F:209:PHE:CZ	2.50	0.47
2:F:49:LYS:HG3	2:F:53:HIS:HB2	1.96	0.47
2:F:61:ARG:NH1	3:F:303:HOH:O	2.48	0.47
2:F:66:GLY:HA3	2:F:71:PHE:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:61:ARG:NE	2:H:82:ASP:OD2	2.41	0.47
2:H:164:THR:HG23	2:H:165:GLU:O	2.15	0.47
1:M:103:ASP:OD1	1:M:103:ASP:N	2.48	0.47
2:N:61:ARG:HA	2:N:61:ARG:HD3	1.62	0.47
1:A:39:ARG:HD3	1:A:49:MET:SD	2.55	0.47
1:I:32:GLY:CA	1:I:54:TYR:HB3	2.31	0.47
2:J:33:LEU:HD22	2:J:89:GLN:O	2.15	0.47
2:L:90:GLN:HG2	2:L:92:HIS:H	1.80	0.47
2:J:19:VAL:HB	2:J:75:ILE:HB	1.97	0.47
2:L:148:TRP:HB2	2:L:155:GLN:HB2	1.96	0.47
2:N:50:TYR:C	2:N:52:SER:N	2.72	0.47
1:O:76:LYS:HA	3:O:316:HOH:O	2.15	0.47
2:H:145:LYS:HB3	2:H:197:THR:HB	1.96	0.47
1:M:11:LEU:HD23	1:M:121:THR:HG22	1.97	0.47
2:B:167:ASP:OD1	2:B:169:LYS:N	2.37	0.46
1:C:54:TYR:HA	3:C:308:HOH:O	2.14	0.46
2:L:7:SER:HA	2:L:8:PRO:C	2.40	0.46
2:N:47:LEU:C	2:N:48:ILE:HD12	2.40	0.46
2:N:66:GLY:HA3	2:N:71:PHE:HA	1.97	0.46
2:P:118:PHE:HA	2:P:119:PRO:HD2	1.74	0.46
1:A:34:SER:HB2	1:A:99:LYS:HZ3	1.79	0.46
1:E:174:VAL:HG11	2:F:160:GLN:HB3	1.97	0.46
1:I:189:VAL:HG11	1:I:199:TYR:CE2	2.50	0.46
2:J:1:GLU:N	3:J:305:HOH:O	2.48	0.46
2:J:139:PHE:CD1	2:J:139:PHE:N	2.82	0.46
2:L:33:LEU:HD22	2:L:89:GLN:O	2.15	0.46
2:B:30:SER:HA	2:B:68:GLY:H	1.80	0.46
1:E:73:ASP:CG	1:E:76:LYS:HE2	2.41	0.46
1:A:11:LEU:HD12	1:A:115:THR:O	2.16	0.46
1:A:99:LYS:HE2	1:A:100:ASP:O	2.16	0.46
2:B:180:THR:O	2:B:181:LEU:HD23	2.15	0.46
2:D:210:ASN:ND2	3:D:311:HOH:O	2.22	0.46
1:E:88:ALA:C	1:E:90:ASP:H	2.23	0.46
2:H:4:LEU:HD13	2:H:88:CYS:HB3	1.97	0.46
1:I:62:PRO:HA	1:I:65:LYS:HG3	1.96	0.46
1:O:2:VAL:HG21	1:O:98:ARG:NH1	2.31	0.46
1:O:17:THR:HA	1:O:84:SER:HA	1.98	0.46
1:E:86:VAL:CG1	1:E:87:THR:N	2.77	0.46
1:G:38:ILE:HD11	1:G:105:PHE:CE2	2.50	0.46
2:H:148:TRP:CE2	2:H:179:LEU:HB2	2.51	0.46
1:I:91:THR:HG23	1:I:115:THR:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:34:HIS:CE1	2:N:49:LYS:O	2.66	0.46
2:P:37:GLN:HB2	2:P:47:LEU:CD1	2.44	0.46
1:E:36:HIS:CE1	1:E:51:TYR:HB3	2.51	0.46
1:M:204:ASN:HD22	1:M:205:HIS:N	2.14	0.46
2:P:27:GLN:O	2:P:29:ILE:HG23	2.15	0.46
2:B:125:LEU:O	2:B:183:LYS:NZ	2.30	0.46
1:C:51:TYR:CE1	1:C:59:ASP:HB3	2.51	0.46
1:G:122:LYS:HD2	1:G:180:LEU:HD13	1.97	0.46
2:H:166:GLN:HB2	2:H:173:TYR:CZ	2.50	0.46
1:M:126:VAL:O	1:M:214:LYS:NZ	2.49	0.46
1:O:68:ILE:HD12	1:O:82:LYS:O	2.16	0.46
1:E:91:THR:O	3:E:309:HOH:O	2.21	0.46
2:H:20:THR:HG23	2:H:74:THR:HG23	1.97	0.46
2:J:8:PRO:HG2	2:J:11:GLN:HB2	1.98	0.46
2:L:38:GLN:HG3	2:L:42:GLN:O	2.15	0.46
2:L:185:ASP:N	2:L:185:ASP:OD1	2.48	0.46
1:M:17:THR:HB	1:M:84:SER:HA	1.97	0.46
1:M:127:PHE:HB3	2:N:121:SER:OG	2.16	0.46
2:N:62:PHE:CE2	2:N:75:ILE:HG12	2.50	0.46
1:O:122:LYS:HD2	1:O:149:ASP:O	2.15	0.46
1:C:103:ASP:OD1	1:C:103:ASP:N	2.49	0.45
2:J:3:VAL:H	2:J:26:SER:HB2	1.82	0.45
1:K:200:ILE:HG12	1:K:215:ARG:HB2	1.98	0.45
1:M:27:TYR:HE2	1:M:32:GLY:HA2	1.81	0.45
2:P:108:ARG:HD3	2:P:109:THR:O	2.17	0.45
2:D:3:VAL:N	2:D:26:SER:OG	2.49	0.45
2:J:78:LEU:HD23	2:J:78:LEU:HA	1.82	0.45
1:K:73:ASP:OD1	1:K:75:SER:OG	2.33	0.45
2:N:116:PHE:HA	3:N:315:HOH:O	2.16	0.45
2:D:190:LYS:CD	2:D:210:ASN:HB3	2.42	0.45
2:J:107:LYS:HD3	2:N:9:ASP:CG	2.41	0.45
1:M:178:SER:OG	3:M:320:HOH:O	2.19	0.45
1:I:206:LYS:H	1:I:206:LYS:HG3	1.60	0.45
1:O:67:ARG:NH2	1:O:90:ASP:OD1	2.49	0.45
2:H:149:LYS:HG2	2:H:154:LEU:HD22	1.99	0.45
2:J:33:LEU:HD21	2:J:88:CYS:SG	2.57	0.45
1:M:200:ILE:HD13	1:M:215:ARG:HB2	1.98	0.45
1:O:41:PRO:HA	1:O:42:PRO:HD3	1.88	0.45
1:A:127:PHE:CD1	2:B:124:GLN:HB2	2.51	0.45
1:M:35:TRP:HB3	1:M:79:PHE:CZ	2.52	0.45
2:N:45:LYS:HB2	2:N:45:LYS:HE3	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:TRP:CE2	2:B:96:LEU:HD13	2.51	0.45
2:D:94:PHE:HA	2:D:95:PRO:C	2.42	0.45
2:J:145:LYS:HG2	2:J:146:VAL:N	2.32	0.45
2:J:159:SER:HA	2:J:178:THR:O	2.17	0.45
2:L:108:ARG:HG3	2:L:109:THR:O	2.16	0.45
2:P:15:PRO:C	2:P:16:LYS:HD2	2.40	0.45
1:A:128:PRO:HD3	1:A:214:LYS:HE2	1.99	0.45
2:D:78:LEU:HD11	2:D:106:ILE:CD1	2.47	0.45
2:D:131:SER:OG	2:D:180:THR:HG22	2.17	0.45
1:G:17:THR:HB	1:G:84:SER:HA	1.98	0.45
2:H:128:GLY:C	2:H:183:LYS:HB3	2.41	0.45
1:K:148:LYS:HD3	1:K:149:ASP:OD2	2.17	0.45
1:K:200:ILE:HD11	1:K:215:ARG:NH2	2.32	0.45
2:P:50:TYR:OH	3:P:301:HOH:O	2.05	0.45
1:A:17:THR:HG23	3:A:308:HOH:O	2.16	0.45
1:K:60:PHE:HE1	1:K:70:ILE:HG13	1.81	0.45
2:P:4:LEU:HB2	2:P:99:GLY:HA2	1.99	0.45
1:A:99:LYS:HG2	1:A:100:ASP:O	2.17	0.44
1:E:30:THR:HG21	1:E:74:THR:HG22	1.98	0.44
1:I:102:SER:N	1:I:103:ASP:HA	2.32	0.44
2:N:64:GLY:HA2	2:N:72:THR:O	2.17	0.44
1:O:214:LYS:NZ	2:P:123:GLU:OE1	2.45	0.44
1:E:14:PRO:C	1:E:15:SER:HG	2.03	0.44
2:P:108:ARG:H	2:P:108:ARG:HG3	1.60	0.44
1:A:91:THR:HG23	1:A:115:THR:HA	1.98	0.44
2:D:14:THR:O	2:D:17:GLU:HB3	2.17	0.44
1:E:99:LYS:HG2	1:E:100:ASP:O	2.18	0.44
2:F:193:ALA:CB	2:F:208:SER:HB3	2.47	0.44
2:L:14:THR:O	2:L:17:GLU:HB3	2.18	0.44
2:D:89:GLN:HG2	2:D:90:GLN:N	2.31	0.44
2:H:37:GLN:HG3	2:H:86:TYR:CE2	2.53	0.44
1:I:71:SER:OG	1:I:80:SER:HB2	2.17	0.44
1:M:198:THR:HG21	1:M:215:ARG:NH2	2.33	0.44
1:O:43:GLY:C	1:O:44:LYS:HG2	2.42	0.44
2:P:132:VAL:HB	2:P:179:LEU:HB3	2.00	0.44
1:E:53:HIS:CE1	1:E:54:TYR:CE1	3.05	0.44
2:F:73:LEU:HD22	2:F:74:THR:H	1.83	0.44
2:F:85:THR:HA	2:F:102:THR:O	2.17	0.44
1:A:167:GLY:O	1:A:187:VAL:HA	2.17	0.44
2:L:206:THR:O	2:L:207:LYS:HD2	2.16	0.44
1:O:68:ILE:HD12	1:O:69:THR:H	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:31:ASP:O	2:D:50:TYR:HA	2.18	0.44
2:D:125:LEU:O	2:D:183:LYS:HE3	2.18	0.44
2:N:194:CYS:O	2:N:206:THR:HA	2.18	0.44
2:P:108:ARG:HG2	2:P:171:SER:HB2	1.99	0.44
2:B:24:ARG:HH21	2:D:17:GLU:HA	1.83	0.44
2:N:117:ILE:HG13	2:N:118:PHE:N	2.32	0.44
1:O:29:ILE:HG23	1:O:77:ASN:OD1	2.18	0.44
2:J:22:THR:HG22	2:J:72:THR:OG1	2.18	0.44
2:P:189:HIS:HB2	2:P:192:TYR:OH	2.18	0.44
2:B:163:VAL:HG22	2:B:175:LEU:HD12	1.99	0.43
2:F:63:SER:O	2:F:74:THR:N	2.46	0.43
2:J:140:TYR:CG	2:J:141:PRO:HA	2.53	0.43
2:B:47:LEU:O	2:B:55:ILE:HG12	2.17	0.43
2:L:34:HIS:ND1	2:L:49:LYS:HA	2.32	0.43
1:M:99:LYS:CD	1:M:103:ASP:HB3	2.48	0.43
2:N:18:LYS:HG2	2:N:76:ASN:HA	2.00	0.43
2:B:50:TYR:N	2:B:51:ALA:HA	2.33	0.43
1:E:86:VAL:CG1	1:E:90:ASP:HB2	2.46	0.43
2:P:2:ILE:HB	2:P:90:GLN:NE2	2.32	0.43
2:P:13:VAL:HG12	2:P:78:LEU:HD12	1.98	0.43
2:F:46:LEU:HD13	2:F:55:ILE:CD1	2.41	0.43
1:I:36:HIS:ND1	1:I:51:TYR:HB3	2.33	0.43
1:O:87:THR:C	1:O:116:VAL:HG11	2.43	0.43
2:B:149:LYS:HB2	2:B:193:ALA:HB3	2.01	0.43
1:C:6:GLU:CD	1:C:96:CYS:H	2.27	0.43
1:E:144:GLY:HA2	1:E:159:TRP:CZ2	2.54	0.43
2:L:62:PHE:HD1	3:L:304:HOH:O	2.01	0.43
2:P:46:LEU:HD13	2:P:55:ILE:CD1	2.44	0.43
1:A:104:ALA:O	1:A:106:PRO:HD3	2.19	0.43
1:K:215:ARG:HG3	1:K:216:VAL:N	2.31	0.43
2:P:18:LYS:HG3	2:P:76:ASN:HA	2.00	0.43
2:B:201:LEU:HD13	2:B:205:VAL:HG23	2.01	0.43
2:F:35:TRP:CE2	2:F:73:LEU:HB2	2.53	0.43
2:H:158:ASN:ND2	2:H:179:LEU:HD11	2.34	0.43
1:A:48:TRP:CE3	1:A:61:ASN:HB2	2.54	0.43
1:E:6:GLU:OE1	1:E:96:CYS:N	2.51	0.43
1:E:205:HIS:HB3	1:E:210:THR:HB	2.00	0.43
1:I:11:LEU:HB2	1:I:152:PRO:HG3	1.99	0.43
1:A:171:PHE:HA	1:A:172:PRO:HD2	1.75	0.43
2:H:11:GLN:HE22	2:H:20:THR:H	1.67	0.43
2:H:115:VAL:HA	2:H:135:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:32:GLY:HA3	1:I:54:TYR:HB2	1.95	0.43
1:I:202:ASN:ND2	1:I:213:ASP:OD2	2.51	0.43
2:D:113:PRO:HD2	2:D:201:LEU:HD21	2.00	0.43
2:F:17:GLU:HG2	2:L:7:SER:HB3	2.00	0.43
2:H:90:GLN:HG2	2:H:92:HIS:H	1.84	0.43
2:B:55:ILE:HB	2:B:58:VAL:HG21	2.01	0.42
1:C:124:PRO:HB3	1:C:150:TYR:HB3	1.99	0.42
2:H:50:TYR:O	2:H:51:ALA:HB3	2.19	0.42
1:I:2:VAL:HG21	1:I:98:ARG:NH1	2.34	0.42
2:L:30:SER:O	2:L:30:SER:OG	2.28	0.42
1:O:205:HIS:HB3	1:O:210:THR:HB	2.01	0.42
2:P:83:ALA:HB2	2:P:106:ILE:HD12	1.99	0.42
1:A:36:HIS:ND1	1:A:51:TYR:HB3	2.33	0.42
1:I:36:HIS:CE1	1:I:99:LYS:HD3	2.54	0.42
1:A:72:ARG:HA	1:A:79:PHE:HA	2.01	0.42
2:B:89:GLN:HG2	2:B:90:GLN:N	2.33	0.42
1:C:67:ARG:HD2	1:C:84:SER:O	2.19	0.42
2:F:151:ASP:O	2:F:152:ASN:HB2	2.19	0.42
2:L:33:LEU:HD13	2:L:34:HIS:N	2.34	0.42
1:O:124:PRO:HA	1:O:150:TYR:HB3	2.01	0.42
1:A:106:PRO:HB2	1:A:107:TYR:CE2	2.54	0.42
1:C:33:TYR:CE2	1:C:98:ARG:CZ	3.02	0.42
1:C:64:LEU:HA	1:C:64:LEU:HD23	1.75	0.42
1:C:161:SER:H	1:C:202:ASN:ND2	2.17	0.42
1:E:206:LYS:HB3	1:E:206:LYS:HE3	1.56	0.42
2:H:150:VAL:HG12	2:H:155:GLN:OE1	2.19	0.42
2:J:161:GLU:HA	2:J:176:SER:O	2.19	0.42
1:K:51:TYR:CE1	1:K:59:ASP:HB3	2.54	0.42
1:K:67:ARG:HD2	1:K:84:SER:O	2.19	0.42
2:L:21:ILE:HD12	2:L:73:LEU:HD12	2.01	0.42
1:O:144:GLY:HA2	1:O:159:TRP:CZ2	2.55	0.42
2:P:107:LYS:HA	2:P:140:TYR:CZ	2.54	0.42
1:C:99:LYS:NZ	1:C:103:ASP:HB3	2.34	0.42
2:J:34:HIS:O	2:J:89:GLN:N	2.33	0.42
2:J:149:LYS:HG2	2:J:154:LEU:CD2	2.47	0.42
1:O:29:ILE:HG23	1:O:77:ASN:CG	2.45	0.42
2:B:14:THR:HG23	2:B:15:PRO:HD2	2.01	0.42
2:L:189:HIS:O	2:L:211:ARG:HD3	2.18	0.42
2:B:187:GLU:C	2:B:189:HIS:H	2.28	0.42
1:C:159:TRP:CZ3	1:C:201:CYS:HB3	2.55	0.42
1:O:160:ASN:HB2	1:O:164:LEU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:64:GLY:HA2	2:P:72:THR:O	2.20	0.42
1:C:61:ASN:HA	1:C:62:PRO:HD3	1.87	0.42
1:G:100:ASP:HB2	1:G:102:SER:OG	2.20	0.42
1:K:40:GLN:HB2	1:K:46:LEU:HD23	2.01	0.42
1:I:41:PRO:HA	1:I:42:PRO:HD3	1.95	0.42
2:B:195:GLU:HG3	2:B:206:THR:OG1	2.20	0.42
1:C:6:GLU:H	1:C:6:GLU:HG2	1.43	0.42
1:C:18:LEU:O	1:C:82:LYS:HA	2.20	0.42
2:D:125:LEU:HD21	2:D:186:TYR:CD2	2.55	0.42
2:H:67:SER:HA	2:H:71:PHE:CE2	2.55	0.42
2:L:140:TYR:CG	2:L:141:PRO:HA	2.54	0.42
2:B:30:SER:O	2:B:71:PHE:CE2	2.73	0.41
1:C:126:VAL:HG22	1:C:147:VAL:HG13	2.00	0.41
1:E:51:TYR:CE2	1:E:59:ASP:HB3	2.55	0.41
2:F:50:TYR:O	2:F:52:SER:N	2.48	0.41
1:I:127:PHE:HE1	2:J:123:GLU:OE1	1.95	0.41
1:O:53:HIS:CE1	1:O:54:TYR:HE1	2.38	0.41
2:P:49:LYS:N	2:P:53:HIS:O	2.51	0.41
1:G:127:PHE:HD2	1:G:146:LEU:HD23	1.85	0.41
1:G:154:PRO:O	1:G:205:HIS:HD2	2.03	0.41
2:L:90:GLN:NE2	2:L:97:THR:OG1	2.53	0.41
2:P:35:TRP:CE2	2:P:73:LEU:HB2	2.55	0.41
2:H:161:GLU:HA	2:H:176:SER:O	2.20	0.41
2:J:160:GLN:O	2:J:177:SER:HA	2.21	0.41
2:L:49:LYS:HB3	2:L:50:TYR:HD2	1.86	0.41
2:N:115:VAL:O	2:N:207:LYS:HD3	2.21	0.41
1:O:42:PRO:HD3	1:O:92:ALA:HA	2.02	0.41
1:A:189:VAL:HG21	1:A:194:LEU:HD21	2.01	0.41
1:G:144:GLY:HA3	1:G:186:VAL:HA	2.02	0.41
2:N:37:GLN:HG3	2:N:86:TYR:CE2	2.55	0.41
2:P:13:VAL:C	2:P:107:LYS:HG2	2.45	0.41
1:A:36:HIS:NE2	1:A:99:LYS:HD3	2.36	0.41
1:C:205:HIS:HB3	1:C:210:THR:HB	2.02	0.41
2:D:118:PHE:HA	2:D:119:PRO:HD3	1.94	0.41
1:E:104:ALA:O	1:E:106:PRO:HD3	2.21	0.41
2:F:3:VAL:HG23	2:F:26:SER:HB3	2.03	0.41
1:G:71:SER:OG	3:G:318:HOH:O	2.10	0.41
1:K:176:GLN:HG3	1:K:180:LEU:O	2.21	0.41
2:N:211:ARG:HE	2:N:211:ARG:HB3	1.61	0.41
2:D:78:LEU:HD22	2:D:82:ASP:HB2	2.02	0.41
1:G:40:GLN:HB2	1:G:46:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:3:VAL:H	2:H:26:SER:HG	1.63	0.41
2:L:17:GLU:HG2	2:L:18:LYS:N	2.35	0.41
2:L:95:PRO:O	2:L:97:THR:HG23	2.21	0.41
2:L:122:ASP:O	2:L:126:LYS:HG2	2.21	0.41
1:M:14:PRO:O	1:M:15:SER:OG	2.33	0.41
1:M:95:TYR:CE2	2:N:43:SER:HB3	2.55	0.41
2:P:24:ARG:HG2	2:P:69:THR:HG22	2.02	0.41
2:B:190:LYS:O	2:B:210:ASN:HA	2.21	0.41
2:F:150:VAL:HG22	2:F:192:TYR:CD2	2.56	0.41
2:F:167:ASP:O	2:F:171:SER:HA	2.21	0.41
1:G:32:GLY:O	1:G:33:TYR:HB2	2.21	0.41
1:I:17:THR:HB	1:I:84:SER:HA	2.02	0.41
1:I:32:GLY:O	1:I:35:TRP:NE1	2.53	0.41
1:K:167:GLY:C	1:K:187:VAL:HG23	2.46	0.41
1:A:200:ILE:CD1	1:A:215:ARG:HD3	2.49	0.41
2:D:21:ILE:HD12	2:D:73:LEU:HD13	2.03	0.41
2:D:120:PRO:HD3	2:D:132:VAL:HG13	2.03	0.41
2:H:134:CYS:HB3	2:H:177:SER:OG	2.20	0.41
2:J:89:GLN:HG2	2:J:90:GLN:N	2.35	0.41
1:K:14:PRO:C	1:K:15:SER:HG	2.14	0.41
1:K:48:TRP:HZ2	1:K:51:TYR:HD1	1.68	0.41
2:L:31:ASP:O	2:L:50:TYR:HA	2.20	0.41
2:L:139:PHE:CE1	2:L:174:SER:HA	2.55	0.41
1:M:69:THR:OG1	1:M:82:LYS:HB2	2.21	0.41
2:B:34:HIS:O	2:B:88:CYS:HA	2.21	0.41
2:D:46:LEU:HD13	2:D:55:ILE:HD11	2.02	0.41
2:F:7:SER:HB3	2:L:17:GLU:OE1	2.21	0.41
1:G:161:SER:N	1:G:202:ASN:OD1	2.50	0.41
2:J:122:ASP:HA	2:J:125:LEU:HB2	2.03	0.41
1:K:14:PRO:HD2	1:K:118:SER:OG	2.21	0.41
2:N:89:GLN:HG3	2:N:98:PHE:CZ	2.55	0.41
1:O:104:ALA:O	1:O:106:PRO:HD3	2.21	0.41
1:C:39:ARG:O	1:C:47:GLU:N	2.50	0.40
2:D:125:LEU:HD23	2:D:183:LYS:HG3	2.03	0.40
2:D:139:PHE:HB2	2:D:198:HIS:CE1	2.56	0.40
2:J:33:LEU:HD13	2:J:34:HIS:N	2.36	0.40
2:J:50:TYR:N	2:J:51:ALA:CA	2.79	0.40
2:B:62:PHE:CD2	2:B:75:ILE:HG12	2.56	0.40
2:B:108:ARG:NH1	2:B:109:THR:HG23	2.36	0.40
2:F:186:TYR:CZ	2:F:211:ARG:HD3	2.57	0.40
2:J:13:VAL:HG22	2:N:8:PRO:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:3:VAL:HG12	3:N:320:HOH:O	2.21	0.40
2:P:13:VAL:CG1	2:P:17:GLU:HB3	2.51	0.40
2:P:145:LYS:HD2	2:P:197:THR:OG1	2.21	0.40
2:B:33:LEU:HD22	2:B:89:GLN:O	2.21	0.40
2:D:201:LEU:HD22	2:D:205:VAL:HG21	2.02	0.40
1:E:21:THR:HG23	1:E:80:SER:OG	2.22	0.40
2:H:167:ASP:OD1	2:H:169:LYS:N	2.49	0.40
1:I:164:LEU:HD23	1:I:164:LEU:HA	1.92	0.40
1:O:64:LEU:C	1:O:66:THR:H	2.17	0.40
2:B:36:TYR:HE1	2:B:89:GLN:HB3	1.86	0.40
2:B:107:LYS:HA	2:B:140:TYR:OH	2.21	0.40
1:G:167:GLY:O	1:G:187:VAL:HA	2.22	0.40
2:H:140:TYR:CG	2:H:141:PRO:HA	2.56	0.40
1:K:200:ILE:CG2	1:K:213:ASP:HB3	2.52	0.40
1:A:190:PRO:O	1:A:193:SER:OG	2.39	0.40
1:C:115:THR:HG21	1:C:152:PRO:HB2	2.04	0.40
1:G:37:TRP:C	1:G:38:ILE:HG13	2.45	0.40
2:L:118:PHE:HA	2:L:119:PRO:HD3	1.97	0.40
1:M:64:LEU:O	1:M:68:ILE:HG22	2.22	0.40
1:M:99:LYS:HG2	1:M:100:ASP:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:17:GLU:OE2	3:H:303:HOH:O[1_455]	2.01	0.19

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	216/225 (96%)	205 (95%)	11 (5%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	206/225 (92%)	192 (93%)	13 (6%)	1 (0%)	25	41
1	E	205/225 (91%)	194 (95%)	10 (5%)	1 (0%)	25	41
1	G	184/225 (82%)	172 (94%)	12 (6%)	0	100	100
1	I	216/225 (96%)	203 (94%)	13 (6%)	0	100	100
1	K	195/225 (87%)	183 (94%)	12 (6%)	0	100	100
1	M	195/225 (87%)	185 (95%)	10 (5%)	0	100	100
1	O	205/225 (91%)	193 (94%)	12 (6%)	0	100	100
2	B	209/214 (98%)	202 (97%)	7 (3%)	0	100	100
2	D	209/214 (98%)	200 (96%)	9 (4%)	0	100	100
2	F	209/214 (98%)	194 (93%)	15 (7%)	0	100	100
2	H	210/214 (98%)	199 (95%)	11 (5%)	0	100	100
2	J	210/214 (98%)	198 (94%)	12 (6%)	0	100	100
2	L	209/214 (98%)	197 (94%)	11 (5%)	1 (0%)	25	41
2	N	209/214 (98%)	196 (94%)	13 (6%)	0	100	100
2	P	209/214 (98%)	200 (96%)	9 (4%)	0	100	100
All	All	3296/3512 (94%)	3113 (94%)	180 (6%)	3 (0%)	48	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	29	ILE
1	C	207	PRO
2	L	59	PRO

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	188/195 (96%)	160 (85%)	28 (15%)	2	3
1	C	182/195 (93%)	162 (89%)	20 (11%)	5	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	181/195 (93%)	151 (83%)	30 (17%)	2	2
1	G	163/195 (84%)	142 (87%)	21 (13%)	3	5
1	I	188/195 (96%)	158 (84%)	30 (16%)	2	2
1	K	174/195 (89%)	150 (86%)	24 (14%)	3	4
1	M	174/195 (89%)	139 (80%)	35 (20%)	1	1
1	O	181/195 (93%)	146 (81%)	35 (19%)	1	1
2	B	187/189 (99%)	154 (82%)	33 (18%)	1	2
2	D	186/189 (98%)	152 (82%)	34 (18%)	1	2
2	F	186/189 (98%)	151 (81%)	35 (19%)	1	1
2	H	187/189 (99%)	152 (81%)	35 (19%)	1	2
2	J	187/189 (99%)	157 (84%)	30 (16%)	2	2
2	L	187/189 (99%)	154 (82%)	33 (18%)	1	2
2	N	186/189 (98%)	153 (82%)	33 (18%)	1	2
2	P	186/189 (98%)	152 (82%)	34 (18%)	1	2
All	All	2923/3072 (95%)	2433 (83%)	490 (17%)	1	2

All (490) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	VAL
1	A	3	GLN
1	A	6	GLU
1	A	12	VAL
1	A	17	THR
1	A	18	LEU
1	A	19	SER
1	A	20	LEU
1	A	34	SER
1	A	44	LYS
1	A	65	LYS
1	A	67	ARG
1	A	69	THR
1	A	76	LYS
1	A	78	GLN
1	A	87	THR
1	A	89	VAL
1	A	99	LYS

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Mol	Chain	Res	Type
1	A	118	SER
1	A	122	LYS
1	A	143	LEU
1	A	155	VAL
1	A	164	LEU
1	A	165	THR
1	A	166	SER
1	A	177	SER
1	A	193	SER
1	A	214	LYS
2	B	7	SER
2	B	12	SER
2	B	16	LYS
2	B	20	THR
2	B	23	CYS
2	B	27	GLN
2	B	28	SER
2	B	29	ILE
2	B	31	ASP
2	B	46	LEU
2	B	50	TYR
2	B	60	SER
2	B	73	LEU
2	B	76	ASN
2	B	77	SER
2	B	78	LEU
2	B	85	THR
2	B	90	GLN
2	B	108	ARG
2	B	109	THR
2	B	122	ASP
2	B	125	LEU
2	B	133	VAL
2	B	145	LYS
2	B	152	ASN
2	B	159	SER
2	B	176	SER
2	B	183	LYS
2	B	185	ASP
2	B	187	GLU
2	B	188	LYS
2	B	194	CYS

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Mol	Chain	Res	Type
2	B	203	SER
1	C	6	GLU
1	C	12	VAL
1	C	17	THR
1	C	18	LEU
1	C	20	LEU
1	C	28	SER
1	C	65	LYS
1	C	71	SER
1	C	103	ASP
1	C	115	THR
1	C	118	SER
1	C	121	THR
1	C	125	SER
1	C	143	LEU
1	C	148	LYS
1	C	155	VAL
1	C	164	LEU
1	C	166	SER
1	C	187	VAL
1	C	206	LYS
2	D	3	VAL
2	D	5	THR
2	D	12	SER
2	D	16	LYS
2	D	20	THR
2	D	26	SER
2	D	46	LEU
2	D	48	ILE
2	D	49	LYS
2	D	52	SER
2	D	56	SER
2	D	65	SER
2	D	69	THR
2	D	73	LEU
2	D	74	THR
2	D	76	ASN
2	D	81	GLU
2	D	85	THR
2	D	88	CYS
2	D	90	GLN
2	D	96	LEU

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Mol	Chain	Res	Type
2	D	114	SER
2	D	129	THR
2	D	132	VAL
2	D	133	VAL
2	D	134	CYS
2	D	145	LYS
2	D	161	GLU
2	D	183	LYS
2	D	190	LYS
2	D	191	VAL
2	D	195	GLU
2	D	201	LEU
2	D	210	ASN
1	E	4	LEU
1	E	6	GLU
1	E	13	LYS
1	E	17	THR
1	E	18	LEU
1	E	29	ILE
1	E	63	SER
1	E	66	THR
1	E	67	ARG
1	E	68	ILE
1	E	71	SER
1	E	74	THR
1	E	87	THR
1	E	96	CYS
1	E	114	VAL
1	E	115	THR
1	E	118	SER
1	E	120	SER
1	E	122	LYS
1	E	140	THR
1	E	164	LEU
1	E	176	GLN
1	E	191	SER
1	E	192	SER
1	E	194	LEU
1	E	197	GLN
1	E	198	THR
1	E	206	LYS
1	E	209	ASN

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Mol	Chain	Res	Type
1	E	214	LYS
2	F	7	SER
2	F	16	LYS
2	F	20	THR
2	F	28	SER
2	F	31	ASP
2	F	39	LYS
2	F	46	LEU
2	F	48	ILE
2	F	49	LYS
2	F	52	SER
2	F	60	SER
2	F	73	LEU
2	F	74	THR
2	F	76	ASN
2	F	77	SER
2	F	78	LEU
2	F	79	GLU
2	F	81	GLU
2	F	85	THR
2	F	93	SER
2	F	96	LEU
2	F	109	THR
2	F	125	LEU
2	F	132	VAL
2	F	133	VAL
2	F	142	ARG
2	F	152	ASN
2	F	154	LEU
2	F	161	GLU
2	F	162	SER
2	F	164	THR
2	F	180	THR
2	F	183	LYS
2	F	203	SER
2	F	208	SER
1	G	1	GLN
1	G	3	GLN
1	G	6	GLU
1	G	12	VAL
1	G	17	THR
1	G	20	LEU

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Mol	Chain	Res	Type
1	G	21	THR
1	G	67	ARG
1	G	71	SER
1	G	86	VAL
1	G	89	VAL
1	G	103	ASP
1	G	114	VAL
1	G	115	THR
1	G	121	THR
1	G	140	THR
1	G	143	LEU
1	G	156	THR
1	G	176	GLN
1	G	178	SER
1	G	206	LYS
2	H	14	THR
2	H	20	THR
2	H	22	THR
2	H	24	ARG
2	H	27	GLN
2	H	29	ILE
2	H	46	LEU
2	H	55	ILE
2	H	60	SER
2	H	73	LEU
2	H	74	THR
2	H	78	LEU
2	H	79	GLU
2	H	85	THR
2	H	90	GLN
2	H	97	THR
2	H	106	ILE
2	H	107	LYS
2	H	108	ARG
2	H	117	ILE
2	H	122	ASP
2	H	131	SER
2	H	132	VAL
2	H	133	VAL
2	H	154	LEU
2	H	155	GLN
2	H	156	SER

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Mol	Chain	Res	Type
2	H	163	VAL
2	H	164	THR
2	H	169	LYS
2	H	183	LYS
2	H	185	ASP
2	H	188	LYS
2	H	203	SER
2	H	211	ARG
1	I	3	GLN
1	I	6	GLU
1	I	7	SER
1	I	12	VAL
1	I	13	LYS
1	I	14	PRO
1	I	15	SER
1	I	17	THR
1	I	20	LEU
1	I	21	THR
1	I	24	VAL
1	I	65	LYS
1	I	66	THR
1	I	68	ILE
1	I	69	THR
1	I	86	VAL
1	I	99	LYS
1	I	103	ASP
1	I	110	GLN
1	I	118	SER
1	I	140	THR
1	I	155	VAL
1	I	164	LEU
1	I	177	SER
1	I	184	SER
1	I	200	ILE
1	I	206	LYS
1	I	209	ASN
1	I	215	ARG
1	I	217	GLU
2	J	14	THR
2	J	18	LYS
2	J	24	ARG
2	J	26	SER

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Mol	Chain	Res	Type
2	J	30	SER
2	J	46	LEU
2	J	48	ILE
2	J	50	TYR
2	J	73	LEU
2	J	78	LEU
2	J	85	THR
2	J	90	GLN
2	J	96	LEU
2	J	103	LYS
2	J	108	ARG
2	J	125	LEU
2	J	126	LYS
2	J	133	VAL
2	J	136	LEU
2	J	142	ARG
2	J	152	ASN
2	J	154	LEU
2	J	164	THR
2	J	176	SER
2	J	180	THR
2	J	181	LEU
2	J	183	LYS
2	J	194	CYS
2	J	199	GLN
2	J	211	ARG
1	K	2	VAL
1	K	6	GLU
1	K	20	LEU
1	K	21	THR
1	K	63	SER
1	K	64	LEU
1	K	65	LYS
1	K	67	ARG
1	K	86	VAL
1	K	89	VAL
1	K	96	CYS
1	K	100	ASP
1	K	115	THR
1	K	121	THR
1	K	125	SER
1	K	140	THR

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Mol	Chain	Res	Type
1	K	143	LEU
1	K	148	LYS
1	K	166	SER
1	K	188	THR
1	K	209	ASN
1	K	211	LYS
1	K	214	LYS
1	K	215	ARG
2	L	14	THR
2	L	16	LYS
2	L	31	ASP
2	L	43	SER
2	L	45	LYS
2	L	46	LEU
2	L	48	ILE
2	L	60	SER
2	L	61	ARG
2	L	69	THR
2	L	73	LEU
2	L	77	SER
2	L	78	LEU
2	L	79	GLU
2	L	90	GLN
2	L	96	LEU
2	L	106	ILE
2	L	125	LEU
2	L	127	SER
2	L	129	THR
2	L	133	VAL
2	L	134	CYS
2	L	154	LEU
2	L	159	SER
2	L	162	SER
2	L	163	VAL
2	L	164	THR
2	L	168	SER
2	L	188	LYS
2	L	195	GLU
2	L	203	SER
2	L	208	SER
2	L	211	ARG
1	M	2	VAL

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Mol	Chain	Res	Type
1	M	4	LEU
1	M	6	GLU
1	M	12	VAL
1	M	13	LYS
1	M	17	THR
1	M	18	LEU
1	M	20	LEU
1	M	34	SER
1	M	52	ILE
1	M	63	SER
1	M	66	THR
1	M	69	THR
1	M	81	LEU
1	M	84	SER
1	M	86	VAL
1	M	89	VAL
1	M	96	CYS
1	M	103	ASP
1	M	118	SER
1	M	121	THR
1	M	125	SER
1	M	145	CYS
1	M	148	LYS
1	M	155	VAL
1	M	156	THR
1	M	164	LEU
1	M	187	VAL
1	M	188	THR
1	M	200	ILE
1	M	208	SER
1	M	209	ASN
1	M	210	THR
1	M	213	ASP
1	M	214	LYS
2	N	7	SER
2	N	18	LYS
2	N	20	THR
2	N	26	SER
2	N	29	ILE
2	N	43	SER
2	N	46	LEU
2	N	50	TYR

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Mol	Chain	Res	Type
2	N	56	SER
2	N	73	LEU
2	N	76	ASN
2	N	78	LEU
2	N	85	THR
2	N	88	CYS
2	N	90	GLN
2	N	105	GLU
2	N	107	LYS
2	N	117	ILE
2	N	121	SER
2	N	125	LEU
2	N	126	LYS
2	N	133	VAL
2	N	142	ARG
2	N	163	VAL
2	N	164	THR
2	N	168	SER
2	N	180	THR
2	N	197	THR
2	N	199	GLN
2	N	203	SER
2	N	207	LYS
2	N	209	PHE
2	N	211	ARG
1	O	6	GLU
1	O	7	SER
1	O	13	LYS
1	O	17	THR
1	O	18	LEU
1	O	20	LEU
1	O	21	THR
1	O	44	LYS
1	O	52	ILE
1	O	54	TYR
1	O	64	LEU
1	O	66	THR
1	O	67	ARG
1	O	69	THR
1	O	71	SER
1	O	76	LYS
1	O	85	SER

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Mol	Chain	Res	Type
1	O	86	VAL
1	O	99	LYS
1	O	102	SER
1	O	110	GLN
1	O	112	THR
1	O	122	LYS
1	O	125	SER
1	O	148	LYS
1	O	155	VAL
1	O	156	THR
1	O	164	LEU
1	O	184	SER
1	O	191	SER
1	O	194	LEU
1	O	196	THR
1	O	211	LYS
1	O	214	LYS
1	O	217	GLU
2	P	3	VAL
2	P	5	THR
2	P	11	GLN
2	P	16	LYS
2	P	20	THR
2	P	29	ILE
2	P	31	ASP
2	P	33	LEU
2	P	46	LEU
2	P	49	LYS
2	P	73	LEU
2	P	78	LEU
2	P	81	GLU
2	P	85	THR
2	P	88	CYS
2	P	97	THR
2	P	108	ARG
2	P	109	THR
2	P	117	ILE
2	P	125	LEU
2	P	126	LYS
2	P	127	SER
2	P	129	THR
2	P	133	VAL

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Mol	Chain	Res	Type
2	P	152	ASN
2	P	154	LEU
2	P	164	THR
2	P	180	THR
2	P	183	LYS
2	P	197	THR
2	P	199	GLN
2	P	203	SER
2	P	210	ASN
2	P	211	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	197	GLN
2	B	124	GLN
2	B	138	ASN
1	C	176	GLN
2	D	124	GLN
1	E	169	HIS
2	F	11	GLN
2	F	53	HIS
2	F	138	ASN
2	F	160	GLN
2	F	189	HIS
1	G	3	GLN
2	H	11	GLN
2	H	90	GLN
2	H	124	GLN
1	I	1	GLN
1	I	3	GLN
1	I	5	GLN
2	J	11	GLN
2	J	32	HIS
2	J	34	HIS
2	J	42	GLN
2	J	76	ASN
2	J	147	GLN
1	K	160	ASN
1	K	176	GLN
2	L	147	GLN

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Mol	Chain	Res	Type
1	M	204	ASN
2	N	90	GLN
2	N	138	ASN
2	N	199	GLN
1	O	53	HIS
1	O	160	ASN
1	O	197	GLN
2	P	155	GLN
2	P	189	HIS

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](#)

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	218/225 (96%)	-1.24	0	100 100	29, 42, 55, 64	0
1	C	210/225 (93%)	-0.95	0	100 100	38, 55, 84, 97	0
1	E	209/225 (92%)	-0.95	0	100 100	43, 58, 70, 80	0
1	G	190/225 (84%)	-1.14	0	100 100	28, 43, 70, 81	0
1	I	218/225 (96%)	-1.22	0	100 100	27, 42, 53, 68	0
1	K	201/225 (89%)	-1.17	1 (0%)	87 89	30, 45, 62, 76	0
1	M	201/225 (89%)	-1.05	1 (0%)	87 89	36, 54, 74, 85	0
1	O	209/225 (92%)	-1.00	0	100 100	41, 56, 68, 74	0
2	B	211/214 (98%)	-1.19	0	100 100	36, 49, 66, 78	0
2	D	211/214 (98%)	-1.01	1 (0%)	87 89	36, 56, 75, 83	0
2	F	211/214 (98%)	-1.09	0	100 100	39, 52, 69, 79	0
2	H	212/214 (99%)	-1.09	0	100 100	32, 52, 78, 84	0
2	J	212/214 (99%)	-1.11	0	100 100	34, 48, 66, 72	0
2	L	211/214 (98%)	-1.17	0	100 100	32, 52, 74, 82	0
2	N	211/214 (98%)	-1.05	0	100 100	33, 54, 71, 81	0
2	P	211/214 (98%)	-1.13	0	100 100	35, 49, 67, 75	0
All	All	3346/3512 (95%)	-1.10	3 (0%)	92 94	27, 51, 72, 97	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	118	PHE	2.2
1	K	213	ASP	2.1
1	M	170	THR	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 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.