



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 10:25 AM UTC

PDB ID : 5H7D / pdb_00005h7d
Title : Crystal structure of the YgjG-protein A-Zpa963-calmodulin complex
Authors : Youn, S.J.; Kwon, N.Y.; Lee, J.H.; Kim, J.H.; Lee, H.; Lee, J.O.
Deposited on : 2016-11-17
Resolution : 2.57 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

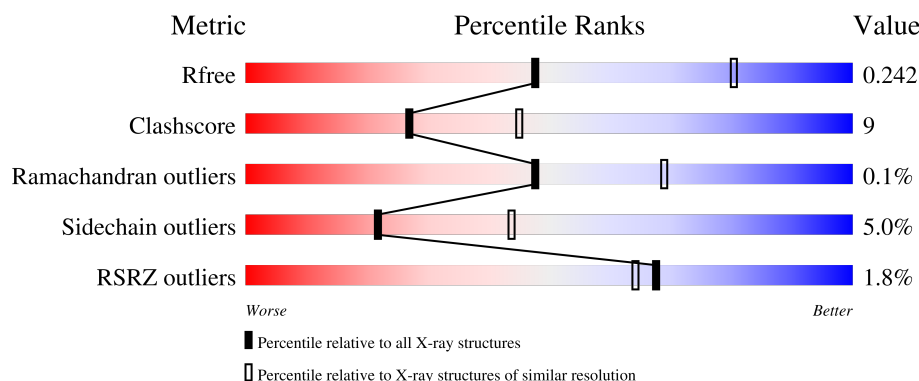
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	499	 81% 17% ..
1	B	499	 81% 17% ..
1	C	499	 81% 17% ..
1	D	499	 81% 16% ..
1	I	499	 82% 16% ..

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Mol	Chain	Length	Quality of chain
1	J	499	81%17%..
1	M	499	83%15%..
1	N	499	82%15%..
2	E	120	2% 20%62%25%7%6%
2	F	120	62%23%8%7%
2	G	120	% 61%26%8%6%
2	H	120	10% 63%27%.7%
2	K	120	62%27%6%6%
2	L	120	16% 68%19%6%7%
2	O	120	3% 63%23%8%6%
2	P	120	15% 62%23%8%7%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 37132 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 Putrescine aminotransferase,Immunoglobulin G-binding protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			3775	2396	651	706	22			
1	B	495	Total	C	N	O	S	0	0	0
			3775	2396	651	706	22			
1	C	495	Total	C	N	O	S	0	0	0
			3775	2396	651	706	22			
1	D	495	Total	C	N	O	S	0	0	0
			3775	2396	651	706	22			
1	I	495	Total	C	N	O	S	0	0	0
			3775	2396	651	706	22			
1	J	495	Total	C	N	O	S	0	0	0
			3775	2396	651	706	22			
1	M	495	Total	C	N	O	S	0	0	0
			3775	2396	651	706	22			
1	N	495	Total	C	N	O	S	0	0	0
			3775	2396	651	706	22			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLY	-	expression tag	UNP P42588
A	4	SER	-	expression tag	UNP P42588
A	5	HIS	-	expression tag	UNP P42588
A	6	MET	-	expression tag	UNP P42588
A	456	VAL	ASN	engineered mutation	UNP P38507
A	474	ALA	GLY	engineered mutation	UNP P38507
B	3	GLY	-	expression tag	UNP P42588
B	4	SER	-	expression tag	UNP P42588
B	5	HIS	-	expression tag	UNP P42588
B	6	MET	-	expression tag	UNP P42588
B	456	VAL	ASN	engineered mutation	UNP P38507
B	474	ALA	GLY	engineered mutation	UNP P38507

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Chain	Residue	Modelled	Actual	Comment	Reference
C	3	GLY	-	expression tag	UNP P42588
C	4	SER	-	expression tag	UNP P42588
C	5	HIS	-	expression tag	UNP P42588
C	6	MET	-	expression tag	UNP P42588
C	456	VAL	ASN	engineered mutation	UNP P38507
C	474	ALA	GLY	engineered mutation	UNP P38507
D	3	GLY	-	expression tag	UNP P42588
D	4	SER	-	expression tag	UNP P42588
D	5	HIS	-	expression tag	UNP P42588
D	6	MET	-	expression tag	UNP P42588
D	456	VAL	ASN	engineered mutation	UNP P38507
D	474	ALA	GLY	engineered mutation	UNP P38507
I	3	GLY	-	expression tag	UNP P42588
I	4	SER	-	expression tag	UNP P42588
I	5	HIS	-	expression tag	UNP P42588
I	6	MET	-	expression tag	UNP P42588
I	456	VAL	ASN	engineered mutation	UNP P38507
I	474	ALA	GLY	engineered mutation	UNP P38507
J	3	GLY	-	expression tag	UNP P42588
J	4	SER	-	expression tag	UNP P42588
J	5	HIS	-	expression tag	UNP P42588
J	6	MET	-	expression tag	UNP P42588
J	456	VAL	ASN	engineered mutation	UNP P38507
J	474	ALA	GLY	engineered mutation	UNP P38507
M	3	GLY	-	expression tag	UNP P42588
M	4	SER	-	expression tag	UNP P42588
M	5	HIS	-	expression tag	UNP P42588
M	6	MET	-	expression tag	UNP P42588
M	456	VAL	ASN	engineered mutation	UNP P38507
M	474	ALA	GLY	engineered mutation	UNP P38507
N	3	GLY	-	expression tag	UNP P42588
N	4	SER	-	expression tag	UNP P42588
N	5	HIS	-	expression tag	UNP P42588
N	6	MET	-	expression tag	UNP P42588
N	456	VAL	ASN	engineered mutation	UNP P38507
N	474	ALA	GLY	engineered mutation	UNP P38507

- Molecule 2 is a protein called Zpa963, Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	113	Total	C	N	O	S	0	0	0
			872	544	143	181	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	112	Total	C	N	O	S	0	0	0
			857	536	139	178	4			
2	G	113	Total	C	N	O	S	0	0	0
			872	544	143	181	4			
2	H	112	Total	C	N	O	S	0	0	0
			857	536	139	178	4			
2	K	113	Total	C	N	O	S	0	0	0
			872	544	143	181	4			
2	L	112	Total	C	N	O	S	0	0	0
			857	536	139	178	4			
2	O	113	Total	C	N	O	S	0	0	0
			872	544	143	181	4			
2	P	112	Total	C	N	O	S	0	0	0
			857	536	139	178	4			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	2	Total	Ca	0	0
			2	2		
3	F	2	Total	Ca	0	0
			2	2		
3	G	2	Total	Ca	0	0
			2	2		
3	H	2	Total	Ca	0	0
			2	2		
3	K	2	Total	Ca	0	0
			2	2		
3	L	2	Total	Ca	0	0
			2	2		
3	O	2	Total	Ca	0	0
			2	2		
3	P	2	Total	Ca	0	0
			2	2		

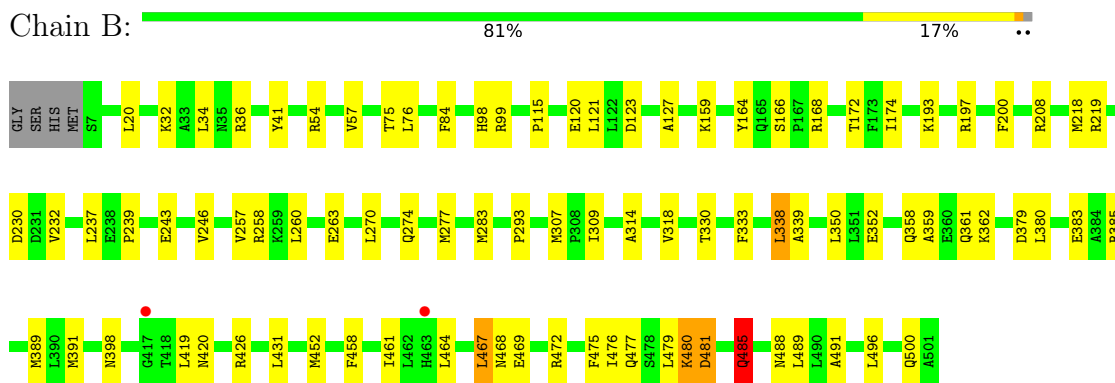
3 Residue-property plots [i](#)

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.

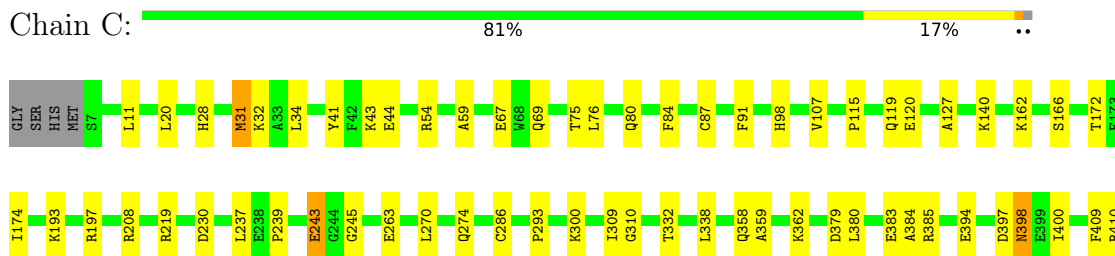
- Molecule 1: Putrescine aminotransferase,Immunoglobulin G-binding protein A



- Molecule 1: Putrescine aminotransferase,Immunoglobulin G-binding protein A



- Molecule 1: Putrescine aminotransferase,Immunoglobulin G-binding protein A





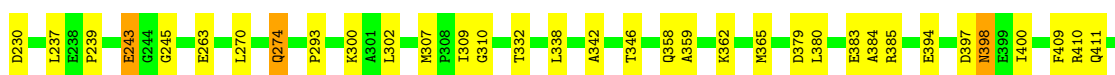
- Molecule 1: Putrescine aminotransferase,Immunoglobulin G-binding protein A

Chain D: 81% 16% ..



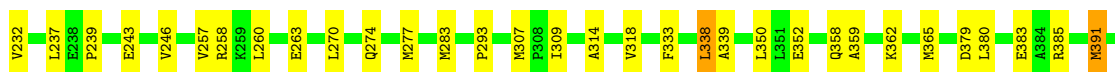
- Molecule 1: Putrescine aminotransferase,Immunoglobulin G-binding protein A

Chain I: 82% 16% ..



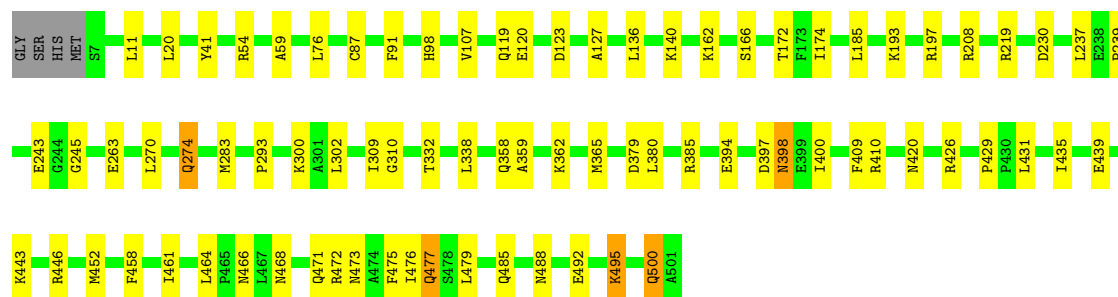
- Molecule 1: Putrescine aminotransferase,Immunoglobulin G-binding protein A

Chain J: 81% 17% ..



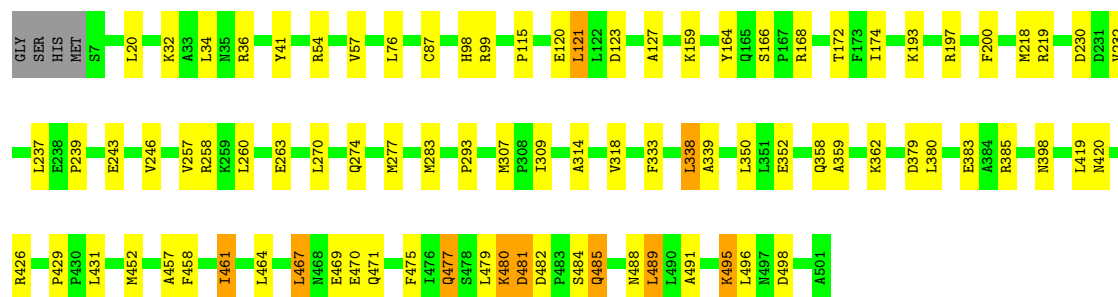
- Molecule 1: Putrescine aminotransferase,Immunoglobulin G-binding protein A

Chain M: 83% 15% ..



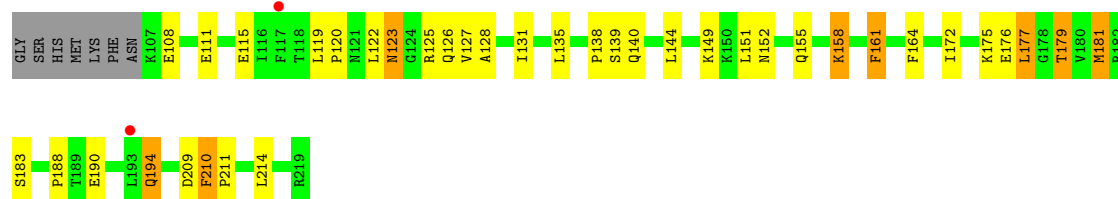
- Molecule 1: Putrescine aminotransferase,Immunoglobulin G-binding protein A

Chain N: 82% 15% ..



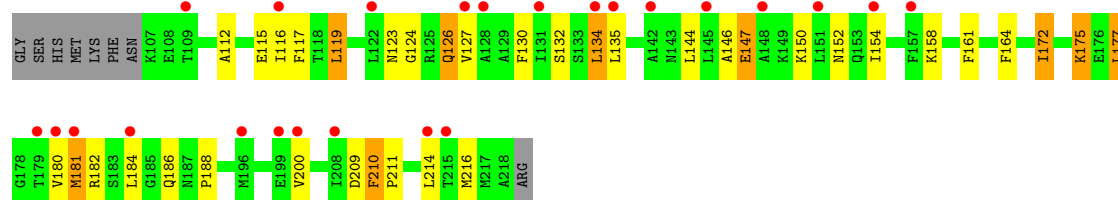
- Molecule 2: Zpa963,Calmodulin

Chain E: 2% 62% 25% 7% 6%



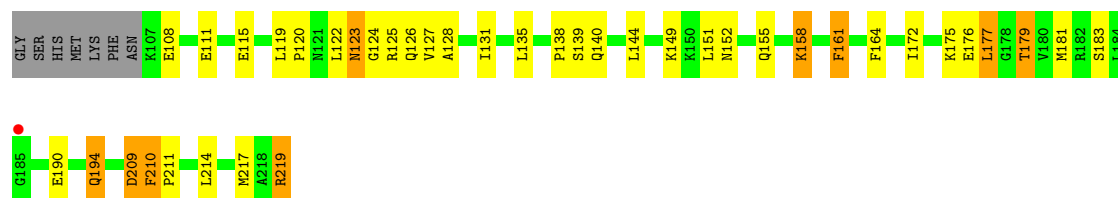
- Molecule 2: Zpa963,Calmodulin

Chain F: 20% 62% 23% 8% 7%

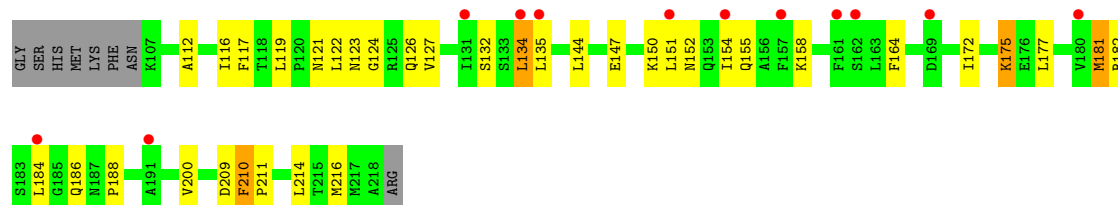


- Molecule 2: Zpa963,Calmodulin

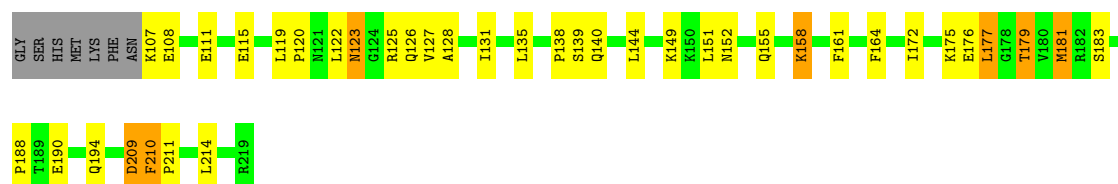
Chain G: 61% 26% 8% 6%



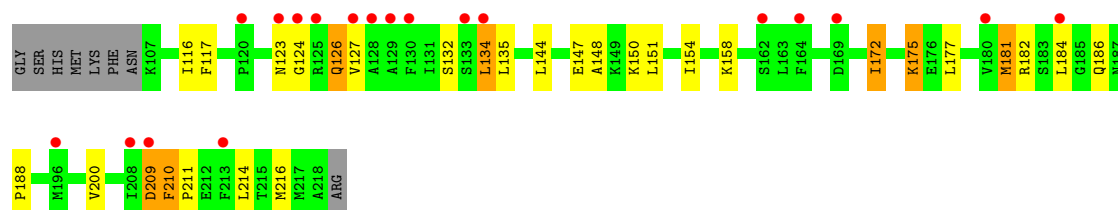
• Molecule 2: Zpa963,Calmodulin



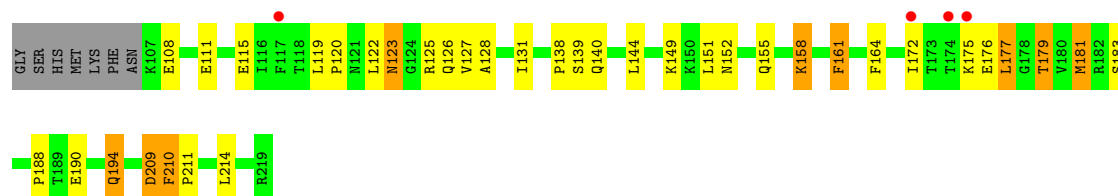
• Molecule 2: Zpa963,Calmodulin



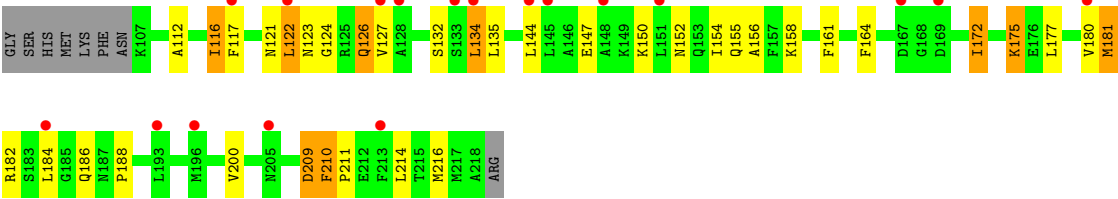
• Molecule 2: Zpa963,Calmodulin



• Molecule 2: Zpa963,Calmodulin



• Molecule 2: Zpa963,Calmodulin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.49Å 155.38Å 155.49Å 84.84° 89.68° 89.56°	Depositor
Resolution (Å)	50.00 – 2.57 50.00 – 2.57	Depositor EDS
% Data completeness (in resolution range)	89.5 (50.00-2.57) 89.4 (50.00-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.58Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.204 , 0.241 0.204 , 0.242	Depositor DCC
R_{free} test set	21075 reflections (8.95%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.397 for h,-k,-l 0.387 for -h,l,k 0.439 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	37132	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.49	0/3845	0.54	0/5203
1	B	0.54	0/3845	0.57	0/5203
1	C	0.50	0/3845	0.55	1/5203 (0.0%)
1	D	0.53	0/3845	0.57	0/5203
1	I	0.50	0/3845	0.54	0/5203
1	J	0.53	0/3845	0.58	0/5203
1	M	0.50	0/3845	0.54	0/5203
1	N	0.53	0/3845	0.56	0/5203
2	E	0.70	0/884	0.73	0/1194
2	F	0.85	0/869	0.91	0/1175
2	G	0.72	0/884	0.75	0/1194
2	H	0.79	0/869	0.87	0/1175
2	K	0.70	0/884	0.71	0/1194
2	L	0.76	0/869	0.87	0/1175
2	O	0.69	0/884	0.74	0/1194
2	P	0.80	0/869	0.86	0/1175
All	All	0.57	0/37772	0.61	1/51100 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	31	MET	CG-SD-CE	-5.94	87.83	100.90

There are no chirality outliers.

There are no planarity outliers.

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	3775	0	3801	64	0
1	B	3775	0	3801	67	0
1	C	3775	0	3801	65	0
1	D	3775	0	3801	66	0
1	I	3775	0	3801	60	0
1	J	3775	0	3801	65	0
1	M	3775	0	3801	57	0
1	N	3775	0	3801	58	0
2	E	872	0	846	33	0
2	F	857	0	829	36	0
2	G	872	0	846	34	0
2	H	857	0	829	30	0
2	K	872	0	846	32	0
2	L	857	0	829	23	0
2	O	872	0	846	35	0
2	P	857	0	829	34	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
3	O	2	0	0	0	0
3	P	2	0	0	0	0
All	All	37132	0	37108	682	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 9.

All (682) 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:461:ILE:HD11	1:A:475:PHE:HB3	1.28	1.14
1:C:31:MET:HE1	1:C:80:GLN:HG2	1.22	1.14
1:M:461:ILE:HD11	1:M:475:PHE:HB3	1.30	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:485:GLN:HB2	1:D:489:LEU:HG	1.30	1.11
1:B:461:ILE:HD11	1:B:475:PHE:HB3	1.26	1.08
1:N:485:GLN:HB2	1:N:489:LEU:HG	1.35	1.07
2:F:175:LYS:HE2	2:F:175:LYS:H	1.22	1.04
1:C:274:GLN:HE22	1:C:426:ARG:HH21	1.05	0.95
2:O:161:PHE:HE2	2:O:210:PHE:HA	1.34	0.92
2:E:158:LYS:HG2	2:E:210:PHE:HZ	1.35	0.92
2:O:161:PHE:CE2	2:O:210:PHE:HA	2.05	0.92
2:E:161:PHE:CE2	2:E:210:PHE:HA	2.05	0.91
2:O:158:LYS:HG2	2:O:210:PHE:HZ	1.35	0.90
2:G:158:LYS:HG2	2:G:210:PHE:HZ	1.36	0.90
1:M:245:GLY:O	1:M:385:ARG:NH1	2.05	0.90
1:C:245:GLY:O	1:C:385:ARG:NH1	2.05	0.90
1:I:245:GLY:O	1:I:385:ARG:NH1	2.05	0.90
1:A:245:GLY:O	1:A:385:ARG:NH1	2.05	0.89
2:K:158:LYS:HG2	2:K:210:PHE:HZ	1.36	0.89
2:G:161:PHE:CE2	2:G:210:PHE:HA	2.12	0.84
2:L:177:LEU:HB3	2:L:181:MET:HE3	1.60	0.84
2:P:177:LEU:HB3	2:P:181:MET:HE3	1.60	0.84
2:H:177:LEU:HB3	2:H:181:MET:HE3	1.60	0.83
2:E:161:PHE:HE2	2:E:210:PHE:HA	1.39	0.83
1:B:481:ASP:OD1	1:B:481:ASP:N	2.13	0.82
1:C:274:GLN:HE22	1:C:426:ARG:NH2	1.77	0.82
2:F:177:LEU:HB3	2:F:181:MET:HE3	1.60	0.81
1:I:274:GLN:OE1	1:I:426:ARG:NH2	2.13	0.81
1:J:218:MET:HE1	1:J:257:VAL:HG13	1.63	0.80
1:N:218:MET:HE1	1:N:257:VAL:HG13	1.64	0.79
1:D:218:MET:HE1	1:D:257:VAL:HG13	1.64	0.78
1:M:274:GLN:OE1	1:M:426:ARG:NH2	2.17	0.78
1:J:485:GLN:O	1:J:489:LEU:HB2	1.82	0.78
1:B:218:MET:HE1	1:B:257:VAL:HG13	1.64	0.78
1:I:243:GLU:OE1	1:I:426:ARG:NH1	2.17	0.77
1:A:274:GLN:OE1	1:A:426:ARG:NH2	2.17	0.77
1:M:119:GLN:NE2	1:M:332:THR:O	2.17	0.77
1:I:119:GLN:NE2	1:I:332:THR:O	2.17	0.77
2:L:175:LYS:HE2	2:L:175:LYS:H	1.48	0.77
2:H:175:LYS:H	2:H:175:LYS:HE2	1.50	0.76
1:A:119:GLN:NE2	1:A:332:THR:O	2.16	0.76
1:N:481:ASP:OD1	1:N:481:ASP:N	2.18	0.75
2:F:175:LYS:HE2	2:F:175:LYS:N	2.00	0.75
1:C:243:GLU:OE1	1:C:426:ARG:NH1	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:GLN:NE2	1:C:332:THR:O	2.17	0.74
1:I:59:ALA:HB2	1:I:410:ARG:HH21	1.53	0.73
1:M:59:ALA:HB2	1:M:410:ARG:HH21	1.53	0.73
2:P:123:ASN:H	2:P:126:GLN:HE21	1.37	0.73
2:G:211:PRO:O	2:G:214:LEU:N	2.21	0.72
1:A:59:ALA:HB2	1:A:410:ARG:HH21	1.53	0.72
1:B:277:MET:HA	1:B:283:MET:HE3	1.71	0.72
1:D:277:MET:HA	1:D:283:MET:HE3	1.71	0.72
2:P:134:LEU:HG	2:P:144:LEU:HD23	1.70	0.72
1:C:59:ALA:HB2	1:C:410:ARG:HH21	1.53	0.72
1:J:277:MET:HA	1:J:283:MET:HE3	1.70	0.72
2:O:158:LYS:HG2	2:O:210:PHE:CZ	2.24	0.71
2:K:211:PRO:O	2:K:214:LEU:N	2.23	0.71
1:N:277:MET:HA	1:N:283:MET:HE3	1.71	0.71
1:J:458:PHE:HB2	1:J:479:LEU:HD21	1.70	0.71
2:L:134:LEU:HG	2:L:144:LEU:HD23	1.70	0.71
2:G:158:LYS:HG2	2:G:210:PHE:CZ	2.25	0.71
1:M:464:LEU:O	1:M:472:ARG:NH2	2.24	0.71
1:I:464:LEU:O	1:I:472:ARG:NH2	2.24	0.70
2:K:158:LYS:HG2	2:K:210:PHE:CZ	2.24	0.70
1:A:464:LEU:O	1:A:472:ARG:NH2	2.24	0.70
1:I:342:ALA:O	1:I:346:THR:HG23	1.92	0.70
1:M:492:GLU:HA	1:M:495:LYS:HE3	1.74	0.70
1:C:464:LEU:O	1:C:472:ARG:NH2	2.24	0.70
1:C:492:GLU:HA	1:C:495:LYS:HE3	1.73	0.70
1:I:492:GLU:HA	1:I:495:LYS:HE3	1.74	0.70
2:K:123:ASN:OD1	2:K:126:GLN:NE2	2.24	0.70
2:P:211:PRO:O	2:P:214:LEU:N	2.24	0.70
1:A:342:ALA:O	1:A:346:THR:HG23	1.92	0.70
2:H:211:PRO:O	2:H:214:LEU:N	2.25	0.69
2:G:123:ASN:OD1	2:G:126:GLN:NE2	2.24	0.69
1:D:461:ILE:HD11	1:D:475:PHE:CG	2.26	0.69
2:H:117:PHE:HA	2:H:127:VAL:HG21	1.73	0.69
2:O:123:ASN:OD1	2:O:126:GLN:NE2	2.24	0.69
2:O:211:PRO:O	2:O:214:LEU:N	2.25	0.69
2:F:211:PRO:O	2:F:214:LEU:N	2.26	0.69
1:A:492:GLU:HA	1:A:495:LYS:HE3	1.74	0.69
2:E:123:ASN:OD1	2:E:126:GLN:NE2	2.24	0.69
2:L:211:PRO:O	2:L:214:LEU:N	2.25	0.69
2:E:211:PRO:O	2:E:214:LEU:N	2.26	0.68
1:A:59:ALA:HB3	1:A:410:ARG:HE	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:117:PHE:HA	2:L:127:VAL:HG21	1.76	0.68
1:C:59:ALA:HB3	1:C:410:ARG:HE	1.59	0.67
1:B:461:ILE:HD11	1:B:475:PHE:CB	2.16	0.67
1:I:59:ALA:HB3	1:I:410:ARG:HE	1.58	0.67
1:M:59:ALA:HB3	1:M:410:ARG:HE	1.58	0.67
1:B:481:ASP:CG	2:F:124:GLY:H	2.03	0.67
2:P:123:ASN:OD1	2:P:126:GLN:NE2	2.28	0.66
2:F:134:LEU:HG	2:F:144:LEU:HD23	1.77	0.66
2:P:117:PHE:HA	2:P:127:VAL:HG21	1.78	0.65
2:F:200:VAL:HG21	2:F:216:MET:HG3	1.78	0.65
2:H:164:PHE:CD2	2:H:172:ILE:HD13	2.32	0.65
1:C:385:ARG:NH2	1:C:394:GLU:OE1	2.29	0.65
2:H:200:VAL:HG21	2:H:216:MET:HG3	1.78	0.65
1:A:385:ARG:NH2	1:A:394:GLU:OE1	2.29	0.65
1:C:28:HIS:O	1:C:31:MET:HG3	1.96	0.65
2:P:200:VAL:HG21	2:P:216:MET:HG3	1.79	0.64
2:L:200:VAL:HG21	2:L:216:MET:HG3	1.78	0.64
1:D:485:GLN:HB2	1:D:489:LEU:CG	2.18	0.64
1:I:385:ARG:NH2	1:I:394:GLU:OE1	2.29	0.64
1:I:409:PHE:HE1	1:J:121:LEU:HD11	1.63	0.64
1:M:385:ARG:NH2	1:M:394:GLU:OE1	2.30	0.64
1:N:457:ALA:O	1:N:461:ILE:HG22	1.98	0.64
2:H:121:ASN:OD1	2:H:152:ASN:ND2	2.29	0.64
2:E:158:LYS:HG2	2:E:210:PHE:CZ	2.24	0.63
1:C:409:PHE:HE1	1:D:121:LEU:HD21	1.62	0.63
1:J:258:ARG:HH21	1:J:293:PRO:HA	1.63	0.63
1:N:115:PRO:HA	1:N:338:LEU:HD13	1.80	0.63
1:N:485:GLN:HB2	1:N:489:LEU:CG	2.20	0.63
1:A:435:ILE:HD12	1:A:435:ILE:H	1.64	0.62
1:D:258:ARG:HH21	1:D:293:PRO:HA	1.64	0.62
1:N:258:ARG:HH21	1:N:293:PRO:HA	1.64	0.62
1:B:258:ARG:HH21	1:B:293:PRO:HA	1.64	0.62
2:F:117:PHE:HA	2:F:127:VAL:HG21	1.80	0.62
2:H:122:LEU:HD21	2:H:151:LEU:HD23	1.81	0.62
2:F:164:PHE:HD2	2:F:172:ILE:HD12	1.64	0.62
1:C:435:ILE:HD12	1:C:435:ILE:H	1.65	0.62
1:I:485:GLN:OE1	1:I:488:ASN:ND2	2.32	0.62
1:I:307:MET:HE1	1:J:307:MET:SD	2.40	0.61
1:M:485:GLN:OE1	1:M:488:ASN:ND2	2.32	0.61
1:B:477:GLN:HA	2:F:124:GLY:HA3	1.81	0.61
1:I:435:ILE:HD12	1:I:435:ILE:H	1.66	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:398:ASN:N	1:M:398:ASN:OD1	2.33	0.61
2:P:175:LYS:HE2	2:P:175:LYS:H	1.65	0.61
1:C:398:ASN:N	1:C:398:ASN:OD1	2.33	0.61
1:A:127:ALA:HB1	1:B:41:TYR:HB2	1.83	0.60
1:A:398:ASN:N	1:A:398:ASN:OD1	2.33	0.60
2:H:112:ALA:O	2:H:116:ILE:HG12	2.01	0.60
2:G:190:GLU:OE1	2:G:194:GLN:NE2	2.34	0.60
1:I:398:ASN:OD1	1:I:398:ASN:N	2.33	0.60
1:J:218:MET:HE2	1:J:260:LEU:HD23	1.83	0.60
1:M:435:ILE:HD12	1:M:435:ILE:H	1.67	0.60
1:N:477:GLN:HA	2:P:124:GLY:HA3	1.84	0.60
2:E:190:GLU:OE1	2:E:194:GLN:NE2	2.34	0.60
1:C:127:ALA:HB1	1:D:41:TYR:HB2	1.83	0.60
1:B:309:ILE:HD12	1:B:339:ALA:HB1	1.84	0.60
1:N:218:MET:HE2	1:N:260:LEU:HD23	1.83	0.60
1:B:218:MET:HE2	1:B:260:LEU:HD23	1.83	0.60
2:H:150:LYS:O	2:H:154:ILE:HD12	2.02	0.60
2:O:190:GLU:OE1	2:O:194:GLN:NE2	2.34	0.60
1:C:485:GLN:OE1	1:C:488:ASN:ND2	2.32	0.60
1:D:309:ILE:HD12	1:D:339:ALA:HB1	1.84	0.60
1:M:54:ARG:HD3	1:N:120:GLU:O	2.02	0.59
1:I:127:ALA:HB1	1:J:41:TYR:HB2	1.82	0.59
1:B:464:LEU:O	1:B:472:ARG:NH2	2.34	0.59
2:G:161:PHE:HE2	2:G:210:PHE:HA	1.62	0.59
1:A:54:ARG:HD3	1:B:120:GLU:O	2.02	0.59
1:M:107:VAL:HG13	1:M:338:LEU:HD22	1.84	0.59
1:A:107:VAL:HG13	1:A:338:LEU:HD22	1.84	0.59
1:A:485:GLN:OE1	1:A:488:ASN:ND2	2.33	0.59
2:H:158:LYS:HG2	2:H:210:PHE:CE2	2.37	0.59
2:E:126:GLN:HE22	2:E:155:GLN:HE22	1.51	0.59
1:C:107:VAL:HG13	1:C:338:LEU:HD22	1.84	0.59
2:E:123:ASN:H	2:E:126:GLN:HE21	1.51	0.59
1:D:496:LEU:O	1:D:500:GLN:HG2	2.03	0.59
1:D:218:MET:HE2	1:D:260:LEU:HD23	1.84	0.59
2:P:158:LYS:HG2	2:P:210:PHE:CE2	2.37	0.59
1:A:307:MET:HE1	1:B:307:MET:SD	2.42	0.59
2:G:123:ASN:H	2:G:126:GLN:HE21	1.51	0.59
1:I:107:VAL:HG13	1:I:338:LEU:HD22	1.84	0.59
1:J:481:ASP:OD1	1:J:481:ASP:N	2.33	0.59
2:G:126:GLN:HE22	2:G:155:GLN:HE22	1.51	0.58
1:D:461:ILE:CD1	1:D:475:PHE:HB3	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:309:ILE:HD12	1:J:339:ALA:HB1	1.84	0.58
1:N:309:ILE:HD12	1:N:339:ALA:HB1	1.84	0.58
1:C:31:MET:HG3	1:C:32:LYS:N	2.18	0.58
2:F:115:GLU:O	2:F:119:LEU:HD23	2.03	0.58
1:C:274:GLN:NE2	1:C:428:GLU:OE2	2.37	0.58
1:N:458:PHE:HB2	1:N:479:LEU:HD21	1.86	0.58
1:B:485:GLN:HB2	1:B:489:LEU:HD23	1.85	0.57
2:O:126:GLN:HE22	2:O:155:GLN:HE22	1.51	0.57
1:B:32:LYS:HE2	1:B:36:ARG:HH11	1.69	0.57
1:D:32:LYS:HE2	1:D:36:ARG:HH11	1.70	0.57
2:K:126:GLN:HE22	2:K:155:GLN:HE22	1.51	0.57
1:D:464:LEU:O	1:D:472:ARG:NH2	2.38	0.57
1:C:41:TYR:HB2	1:D:127:ALA:HB1	1.87	0.57
1:N:32:LYS:HE2	1:N:36:ARG:HH11	1.69	0.57
2:O:123:ASN:H	2:O:126:GLN:HE21	1.51	0.57
2:H:134:LEU:HG	2:H:144:LEU:HD23	1.85	0.57
1:J:464:LEU:O	1:J:472:ARG:NH2	2.38	0.57
1:A:409:PHE:HE1	1:B:121:LEU:HD11	1.68	0.57
1:I:359:ALA:HB2	1:I:431:LEU:HG	1.87	0.57
1:I:54:ARG:HD3	1:J:120:GLU:O	2.04	0.57
2:K:123:ASN:H	2:K:126:GLN:HE21	1.51	0.57
2:E:172:ILE:HG21	2:E:177:LEU:HD13	1.87	0.56
1:C:466:ASN:ND2	1:C:500:GLN:O	2.38	0.56
1:I:243:GLU:HG3	1:I:419:LEU:HB2	1.87	0.56
1:J:477:GLN:HA	2:L:124:GLY:HA3	1.86	0.56
1:A:466:ASN:ND2	1:A:500:GLN:O	2.38	0.56
2:G:126:GLN:OE1	2:G:155:GLN:NE2	2.38	0.56
2:O:172:ILE:HG21	2:O:177:LEU:HD13	1.87	0.56
1:I:466:ASN:ND2	1:I:500:GLN:O	2.39	0.56
1:I:466:ASN:HD21	1:I:500:GLN:HB2	1.70	0.56
2:K:126:GLN:OE1	2:K:155:GLN:NE2	2.38	0.56
1:M:466:ASN:ND2	1:M:500:GLN:O	2.39	0.56
1:A:120:GLU:O	1:B:54:ARG:HD2	2.05	0.56
2:E:126:GLN:OE1	2:E:155:GLN:NE2	2.39	0.56
1:C:243:GLU:HG3	1:C:419:LEU:HB2	1.88	0.56
1:J:32:LYS:HE2	1:J:36:ARG:HH11	1.70	0.56
2:L:150:LYS:O	2:L:154:ILE:HD12	2.04	0.56
1:M:127:ALA:HB1	1:N:41:TYR:HB2	1.86	0.56
1:M:466:ASN:HD21	1:M:500:GLN:HB2	1.71	0.56
1:I:41:TYR:HB2	1:J:127:ALA:HB1	1.87	0.56
2:O:126:GLN:OE1	2:O:155:GLN:NE2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:150:LYS:O	2:P:154:ILE:HD12	2.06	0.56
1:C:54:ARG:HD3	1:D:120:GLU:O	2.05	0.56
1:A:41:TYR:HB2	1:B:127:ALA:HB1	1.88	0.56
1:D:472:ARG:O	1:D:475:PHE:N	2.39	0.55
1:A:466:ASN:HD21	1:A:500:GLN:HB2	1.71	0.55
2:F:126:GLN:O	2:F:130:PHE:HD1	1.90	0.55
1:C:466:ASN:HD21	1:C:500:GLN:HB2	1.71	0.55
2:F:150:LYS:O	2:F:154:ILE:HD12	2.05	0.55
1:D:461:ILE:HD11	1:D:475:PHE:HB3	1.87	0.55
1:D:461:ILE:HD11	1:D:475:PHE:CB	2.36	0.55
1:B:274:GLN:HE22	1:B:426:ARG:NH2	2.05	0.55
1:B:208:ARG:NH1	1:C:208:ARG:HD3	2.22	0.54
2:H:172:ILE:HG21	2:H:177:LEU:HD23	1.89	0.54
1:N:274:GLN:HE22	1:N:426:ARG:NH2	2.06	0.54
2:P:116:ILE:HD12	2:P:134:LEU:HD11	1.88	0.54
1:J:208:ARG:NH1	1:M:208:ARG:HD3	2.23	0.54
1:D:274:GLN:HE22	1:D:426:ARG:NH2	2.06	0.54
1:M:41:TYR:HB2	1:N:127:ALA:HB1	1.88	0.54
1:M:120:GLU:O	1:N:54:ARG:HD2	2.08	0.54
2:P:161:PHE:CZ	2:P:172:ILE:HG13	2.42	0.54
1:B:461:ILE:CD1	1:B:475:PHE:HB3	2.19	0.54
2:G:108:GLU:N	2:G:108:GLU:OE1	2.41	0.54
2:G:161:PHE:CZ	2:G:210:PHE:HA	2.42	0.54
2:O:108:GLU:N	2:O:108:GLU:OE1	2.41	0.54
1:B:480:LYS:HE2	2:F:117:PHE:O	2.07	0.54
2:G:172:ILE:HG21	2:G:177:LEU:HD13	1.90	0.54
2:K:108:GLU:OE1	2:K:108:GLU:N	2.41	0.54
1:J:274:GLN:HE22	1:J:426:ARG:NH2	2.06	0.54
1:D:383:GLU:OE2	1:D:385:ARG:NH1	2.42	0.53
1:A:174:ILE:HD13	1:A:208:ARG:HB2	1.91	0.53
2:E:108:GLU:N	2:E:108:GLU:OE1	2.41	0.53
1:C:174:ILE:HD13	1:C:208:ARG:HB2	1.91	0.53
2:K:126:GLN:NE2	2:K:155:GLN:HE22	2.06	0.53
2:G:126:GLN:NE2	2:G:155:GLN:HE22	2.06	0.53
1:I:174:ILE:HD13	1:I:208:ARG:HB2	1.90	0.53
2:O:126:GLN:NE2	2:O:155:GLN:HE22	2.06	0.53
1:B:383:GLU:OE2	1:B:385:ARG:NH1	2.42	0.53
1:I:473:ASN:O	1:I:477:GLN:HB2	2.08	0.53
1:B:464:LEU:HB2	1:B:467:LEU:HD21	1.89	0.53
1:J:379:ASP:OD1	1:J:379:ASP:N	2.41	0.53
2:L:158:LYS:HG2	2:L:210:PHE:CZ	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:379:ASP:OD1	1:N:379:ASP:N	2.41	0.53
2:F:146:ALA:O	2:F:150:LYS:HG3	2.09	0.53
2:L:209:ASP:OD1	2:L:209:ASP:N	2.40	0.53
1:I:120:GLU:O	1:J:54:ARG:HD2	2.10	0.52
1:M:174:ILE:HD13	1:M:208:ARG:HB2	1.91	0.52
2:E:126:GLN:NE2	2:E:155:GLN:HE22	2.06	0.52
1:C:120:GLU:O	1:D:54:ARG:HD2	2.08	0.52
1:C:439:GLU:O	1:C:443:LYS:HG3	2.10	0.52
1:A:208:ARG:HD3	1:D:208:ARG:NH1	2.24	0.52
1:C:473:ASN:O	1:C:477:GLN:HB2	2.09	0.52
1:C:31:MET:HE1	1:C:80:GLN:CG	2.16	0.52
2:E:120:PRO:HD2	2:E:152:ASN:HD21	1.75	0.52
1:J:391:MET:HG3	1:J:427:ILE:HB	1.92	0.52
2:K:172:ILE:HG21	2:K:177:LEU:HD13	1.91	0.52
2:G:120:PRO:HD2	2:G:152:ASN:HD21	1.75	0.51
2:K:120:PRO:HD2	2:K:152:ASN:HD21	1.75	0.51
1:C:359:ALA:HB2	1:C:431:LEU:HG	1.91	0.51
2:L:182:ARG:HA	2:L:186:GLN:O	2.11	0.51
2:P:182:ARG:HA	2:P:186:GLN:O	2.11	0.51
1:A:439:GLU:O	1:A:443:LYS:HG3	2.11	0.51
1:C:397:ASP:OD1	1:C:400:ILE:N	2.36	0.51
2:H:151:LEU:O	2:H:155:GLN:HG2	2.10	0.51
1:M:439:GLU:O	1:M:443:LYS:HG3	2.10	0.51
2:O:120:PRO:HD2	2:O:152:ASN:HD21	1.75	0.51
1:D:307:MET:HE2	1:D:338:LEU:HB3	1.92	0.51
1:I:439:GLU:O	1:I:443:LYS:HG3	2.11	0.51
2:H:182:ARG:HA	2:H:186:GLN:O	2.11	0.51
2:K:161:PHE:CE2	2:K:210:PHE:HA	2.46	0.51
1:A:359:ALA:HB2	1:A:431:LEU:HG	1.92	0.51
1:C:409:PHE:CE1	1:D:121:LEU:HD21	2.45	0.51
2:O:127:VAL:O	2:O:131:ILE:HG12	2.11	0.51
2:G:127:VAL:O	2:G:131:ILE:HG12	2.11	0.50
1:J:383:GLU:OE2	1:J:385:ARG:NH1	2.41	0.50
2:K:127:VAL:O	2:K:131:ILE:HG12	2.11	0.50
2:L:181:MET:HB2	2:L:188:PRO:HG3	1.94	0.50
1:C:434:THR:HG22	1:C:437:GLN:HG3	1.94	0.50
1:J:164:TYR:O	1:J:168:ARG:NH1	2.44	0.50
1:M:380:LEU:HD13	1:M:452:MET:HE2	1.93	0.50
1:A:397:ASP:OD1	1:A:400:ILE:N	2.36	0.50
2:H:181:MET:HB2	2:H:188:PRO:HG3	1.94	0.50
1:M:473:ASN:O	1:M:477:GLN:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:383:GLU:OE2	1:N:385:ARG:NH1	2.42	0.50
1:A:473:ASN:O	1:A:477:GLN:HB2	2.11	0.50
1:D:172:THR:HG21	1:D:230:ASP:HB3	1.93	0.50
1:J:486:SER:O	1:J:489:LEU:HB3	2.11	0.50
1:N:164:TYR:O	1:N:168:ARG:NH1	2.45	0.50
2:P:181:MET:HB2	2:P:188:PRO:HG3	1.94	0.50
1:A:434:THR:HG22	1:A:437:GLN:HG3	1.94	0.50
1:J:464:LEU:HB2	1:J:467:LEU:HD21	1.94	0.50
2:H:123:ASN:OD1	2:H:126:GLN:NE2	2.45	0.50
2:L:158:LYS:HE2	2:L:210:PHE:CZ	2.47	0.50
2:F:182:ARG:HA	2:F:186:GLN:O	2.11	0.49
1:I:380:LEU:HD13	1:I:452:MET:HE2	1.94	0.49
2:E:122:LEU:HD23	2:E:155:GLN:OE1	2.12	0.49
2:G:122:LEU:HD23	2:G:155:GLN:OE1	2.12	0.49
2:O:158:LYS:HE3	2:O:210:PHE:CE1	2.47	0.49
2:E:127:VAL:O	2:E:131:ILE:HG12	2.11	0.49
2:F:181:MET:HB2	2:F:188:PRO:HG3	1.94	0.49
2:E:111:GLU:O	2:E:115:GLU:HG2	2.13	0.49
2:G:111:GLU:O	2:G:115:GLU:HG2	2.13	0.49
2:O:122:LEU:HD23	2:O:155:GLN:OE1	2.12	0.49
2:E:119:LEU:HD22	2:E:152:ASN:HD22	1.76	0.49
2:E:158:LYS:HE3	2:E:210:PHE:CE1	2.47	0.49
1:C:380:LEU:HD13	1:C:452:MET:HE2	1.93	0.49
2:O:119:LEU:HD22	2:O:152:ASN:HD22	1.77	0.49
1:B:164:TYR:O	1:B:168:ARG:NH1	2.45	0.49
1:C:20:LEU:HD11	1:C:34:LEU:HD22	1.94	0.49
2:K:122:LEU:HD23	2:K:155:GLN:OE1	2.12	0.49
1:A:380:LEU:HD13	1:A:452:MET:HE2	1.93	0.49
1:A:468:ASN:H	1:A:471:GLN:HE22	1.60	0.49
1:D:164:TYR:O	1:D:168:ARG:NH1	2.45	0.49
1:I:193:LYS:HD2	1:I:420:ASN:HA	1.95	0.49
1:I:300:LYS:HA	1:J:333:PHE:CZ	2.47	0.49
2:P:121:ASN:H	2:P:152:ASN:HD21	1.59	0.49
1:M:11:LEU:HD11	1:N:352:GLU:HG3	1.95	0.49
2:L:172:ILE:CG2	2:L:177:LEU:HD23	2.43	0.49
1:M:193:LYS:HD2	1:M:420:ASN:HA	1.95	0.49
1:B:172:THR:HG21	1:B:230:ASP:HB3	1.95	0.48
2:F:164:PHE:CD1	2:F:180:VAL:HG21	2.48	0.48
2:G:119:LEU:HD22	2:G:152:ASN:HD22	1.77	0.48
1:J:172:THR:HG21	1:J:230:ASP:HB3	1.94	0.48
2:K:111:GLU:O	2:K:115:GLU:HG2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:119:LEU:HD22	2:K:152:ASN:HD22	1.77	0.48
1:A:193:LYS:HD2	1:A:420:ASN:HA	1.96	0.48
2:F:164:PHE:HD2	2:F:172:ILE:CD1	2.26	0.48
1:D:454:GLN:HG3	1:D:479:LEU:HD21	1.95	0.48
1:N:172:THR:HG21	1:N:230:ASP:HB3	1.95	0.48
2:O:111:GLU:O	2:O:115:GLU:HG2	2.13	0.48
1:A:476:ILE:HD11	2:E:128:ALA:HA	1.95	0.48
2:H:172:ILE:CG2	2:H:177:LEU:HD23	2.43	0.48
1:I:172:THR:HG21	1:I:230:ASP:HB3	1.95	0.48
2:O:209:ASP:OD1	2:O:209:ASP:N	2.40	0.48
2:P:122:LEU:HD23	2:P:126:GLN:CD	2.38	0.48
2:F:172:ILE:CG2	2:F:177:LEU:HD23	2.44	0.48
1:C:468:ASN:H	1:C:471:GLN:HE22	1.60	0.48
1:B:20:LEU:HD11	1:B:34:LEU:HD13	1.96	0.48
1:B:230:ASP:OD1	1:C:197:ARG:NH2	2.47	0.48
1:I:309:ILE:HG13	1:I:310:GLY:N	2.28	0.48
1:M:172:THR:HG21	1:M:230:ASP:HB3	1.95	0.48
1:M:468:ASN:H	1:M:471:GLN:HE22	1.60	0.48
1:D:482:ASP:C	1:D:484:SER:H	2.22	0.48
1:I:307:MET:CE	1:J:338:LEU:HD23	2.43	0.48
1:I:468:ASN:H	1:I:471:GLN:HE22	1.60	0.48
1:D:20:LEU:HD11	1:D:34:LEU:HD13	1.96	0.48
1:J:20:LEU:HD11	1:J:34:LEU:HD13	1.95	0.48
1:M:309:ILE:HG13	1:M:310:GLY:N	2.28	0.48
1:M:458:PHE:O	1:M:461:ILE:HG22	2.13	0.47
1:A:20:LEU:HD11	1:A:34:LEU:HD22	1.96	0.47
1:D:283:MET:HE1	1:D:350:LEU:HD13	1.97	0.47
1:N:243:GLU:HG2	1:N:419:LEU:HB2	1.97	0.47
2:O:158:LYS:HE3	2:O:210:PHE:HE1	1.79	0.47
1:B:115:PRO:HA	1:B:338:LEU:HD13	1.96	0.47
1:C:193:LYS:HD2	1:C:420:ASN:HA	1.97	0.47
1:M:492:GLU:O	1:M:495:LYS:HB2	2.14	0.47
1:A:172:THR:HG21	1:A:230:ASP:HB3	1.95	0.47
1:C:309:ILE:HG13	1:C:310:GLY:N	2.28	0.47
1:J:243:GLU:HG2	1:J:419:LEU:HB2	1.97	0.47
1:M:359:ALA:HB2	1:M:431:LEU:HG	1.96	0.47
1:N:20:LEU:HD11	1:N:34:LEU:HD13	1.96	0.47
1:D:473:ASN:O	1:D:477:GLN:HB3	2.15	0.47
1:C:172:THR:HG21	1:C:230:ASP:HB3	1.96	0.47
1:D:243:GLU:HG2	1:D:419:LEU:HB2	1.97	0.47
1:I:411:GLN:OE1	1:I:447:LYS:HE3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:172:ILE:CG2	2:P:177:LEU:HD23	2.45	0.47
1:D:481:ASP:OD1	1:D:481:ASP:N	2.41	0.47
2:H:123:ASN:H	2:H:126:GLN:HE21	1.63	0.47
1:M:300:LYS:HA	1:N:333:PHE:CZ	2.49	0.47
1:N:219:ARG:NH2	1:N:263:GLU:OE2	2.47	0.47
1:A:162:LYS:HE3	1:B:200:PHE:O	2.15	0.47
1:A:309:ILE:HG13	1:A:310:GLY:N	2.29	0.47
1:C:162:LYS:HE3	1:D:200:PHE:O	2.15	0.47
1:D:473:ASN:ND2	2:H:132:SER:OG	2.42	0.47
1:D:479:LEU:HD22	2:H:117:PHE:CZ	2.49	0.47
1:J:283:MET:HE1	1:J:350:LEU:HD13	1.96	0.47
1:J:307:MET:HE2	1:J:338:LEU:HB3	1.96	0.47
2:K:209:ASP:OD1	2:K:209:ASP:N	2.40	0.47
1:A:492:GLU:O	1:A:495:LYS:HB2	2.16	0.46
1:C:379:ASP:OD1	1:C:379:ASP:N	2.41	0.46
1:C:492:GLU:O	1:C:495:LYS:HB2	2.16	0.46
1:B:243:GLU:HG2	1:B:419:LEU:HB2	1.97	0.46
1:D:219:ARG:NH2	1:D:263:GLU:OE2	2.48	0.46
1:D:482:ASP:N	1:D:483:PRO:HD3	2.30	0.46
1:I:492:GLU:O	1:I:495:LYS:HB2	2.15	0.46
2:L:172:ILE:HG21	2:L:177:LEU:HD23	1.95	0.46
1:B:307:MET:HE2	1:B:338:LEU:HB3	1.97	0.46
1:C:91:PHE:HD1	1:C:426:ARG:CZ	2.29	0.46
1:I:162:LYS:HE3	1:J:200:PHE:O	2.16	0.46
1:J:482:ASP:C	1:J:484:SER:H	2.24	0.46
1:A:379:ASP:OD1	1:A:379:ASP:N	2.41	0.46
2:F:112:ALA:O	2:F:116:ILE:HG12	2.16	0.46
1:I:300:LYS:HA	1:J:333:PHE:HZ	1.81	0.46
1:N:461:ILE:CD1	1:N:475:PHE:HB3	2.46	0.46
1:A:358:GLN:HB3	1:A:362:LYS:HE3	1.98	0.46
1:B:488:ASN:O	1:B:491:ALA:HB3	2.15	0.46
1:M:358:GLN:HB3	1:M:362:LYS:HE3	1.98	0.46
1:N:480:LYS:HE3	2:P:117:PHE:O	2.16	0.46
1:A:270:LEU:HD12	1:A:293:PRO:HG3	1.98	0.46
1:I:397:ASP:OD1	1:I:400:ILE:N	2.36	0.46
1:A:411:GLN:OE1	1:A:447:LYS:HE3	2.16	0.46
1:B:283:MET:HE1	1:B:350:LEU:HD13	1.98	0.46
2:F:130:PHE:HE2	2:F:147:GLU:OE1	1.98	0.46
1:C:300:LYS:HA	1:D:333:PHE:CZ	2.51	0.46
2:G:126:GLN:CD	2:G:155:GLN:HE22	2.24	0.46
2:H:119:LEU:HB3	2:H:152:ASN:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:409:PHE:HE1	1:N:121:LEU:HD11	1.81	0.46
1:N:307:MET:HE2	1:N:338:LEU:HB3	1.97	0.46
1:C:358:GLN:HB3	1:C:362:LYS:HE3	1.98	0.46
1:I:20:LEU:HD11	1:I:34:LEU:HD22	1.98	0.46
1:M:162:LYS:HE3	1:N:200:PHE:O	2.16	0.46
1:A:300:LYS:HA	1:B:333:PHE:CZ	2.51	0.45
1:B:219:ARG:NH2	1:B:263:GLU:OE2	2.48	0.45
1:B:389:MET:HA	1:B:391:MET:HE2	1.99	0.45
2:E:161:PHE:CZ	2:E:210:PHE:HA	2.51	0.45
1:I:11:LEU:HD11	1:J:352:GLU:HG3	1.98	0.45
1:M:397:ASP:OD1	1:M:400:ILE:N	2.36	0.45
1:B:380:LEU:HD13	1:B:452:MET:HE2	1.98	0.45
1:C:243:GLU:CG	1:C:419:LEU:HB2	2.46	0.45
2:G:219:ARG:HB3	2:G:219:ARG:HH11	1.81	0.45
1:I:243:GLU:CG	1:I:419:LEU:HB2	2.45	0.45
1:J:219:ARG:NH2	1:J:263:GLU:OE2	2.47	0.45
1:J:488:ASN:O	1:J:491:ALA:HB3	2.16	0.45
1:N:283:MET:HE1	1:N:350:LEU:HD13	1.97	0.45
1:B:361:GLN:HG3	1:J:365:MET:HE3	1.98	0.45
2:E:158:LYS:HE3	2:E:210:PHE:HE1	1.81	0.45
1:C:476:ILE:HD11	2:G:128:ALA:HA	1.99	0.45
2:H:172:ILE:HG21	2:H:177:LEU:CD2	2.46	0.45
1:A:307:MET:CE	1:B:338:LEU:HD23	2.47	0.45
1:B:461:ILE:HD13	1:B:476:ILE:HD13	1.98	0.45
2:F:116:ILE:HD13	2:F:134:LEU:HD13	1.98	0.45
1:C:270:LEU:HD12	1:C:293:PRO:HG3	1.98	0.45
1:I:358:GLN:HB3	1:I:362:LYS:HE3	1.98	0.45
2:K:138:PRO:C	2:K:140:GLN:H	2.25	0.45
2:K:123:ASN:H	2:K:126:GLN:NE2	2.15	0.45
1:A:183:LYS:HD2	1:B:330:THR:H	1.82	0.45
2:E:126:GLN:CD	2:E:155:GLN:HE22	2.25	0.45
1:D:193:LYS:HD2	1:D:420:ASN:HA	1.98	0.45
2:G:209:ASP:OD1	2:G:209:ASP:N	2.40	0.45
1:J:193:LYS:HD2	1:J:420:ASN:HA	1.98	0.45
2:O:123:ASN:H	2:O:126:GLN:NE2	2.15	0.45
2:O:138:PRO:C	2:O:140:GLN:H	2.25	0.45
2:P:126:GLN:HE22	2:P:155:GLN:HE21	1.65	0.45
1:A:11:LEU:HD11	1:B:352:GLU:HG3	1.97	0.45
2:E:190:GLU:O	2:E:194:GLN:HB2	2.17	0.45
2:F:123:ASN:ND2	2:F:126:GLN:OE1	2.50	0.45
2:F:154:ILE:O	2:F:158:LYS:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:158:LYS:HE3	2:G:210:PHE:CE1	2.52	0.45
2:G:190:GLU:O	2:G:194:GLN:HB2	2.17	0.45
2:E:138:PRO:C	2:E:140:GLN:H	2.25	0.45
1:J:482:ASP:N	1:J:483:PRO:HD3	2.31	0.45
1:M:219:ARG:NH2	1:M:263:GLU:OE1	2.50	0.45
2:O:126:GLN:CD	2:O:155:GLN:HE22	2.24	0.45
2:O:211:PRO:HA	2:O:214:LEU:HG	1.99	0.45
1:D:76:LEU:HD21	1:D:98:HIS:CE1	2.52	0.45
1:D:380:LEU:HD13	1:D:452:MET:HE2	1.99	0.45
1:I:76:LEU:HD21	1:I:98:HIS:CE1	2.52	0.45
1:J:464:LEU:HD11	1:J:493:ALA:HB1	1.99	0.45
2:K:126:GLN:CD	2:K:155:GLN:HE22	2.24	0.45
1:M:123:ASP:OD1	1:M:123:ASP:N	2.40	0.45
1:N:76:LEU:HD21	1:N:98:HIS:CE1	2.52	0.45
1:N:193:LYS:HD2	1:N:420:ASN:HA	1.98	0.45
1:B:477:GLN:HA	2:F:124:GLY:CA	2.46	0.44
1:I:123:ASP:OD1	1:I:123:ASP:N	2.40	0.44
1:N:380:LEU:HD13	1:N:452:MET:HE2	1.98	0.44
1:D:489:LEU:HD23	1:D:489:LEU:HA	1.75	0.44
1:J:76:LEU:HD21	1:J:98:HIS:CE1	2.53	0.44
2:L:200:VAL:HG21	2:L:216:MET:CG	2.46	0.44
2:P:158:LYS:HE2	2:P:210:PHE:CZ	2.53	0.44
2:P:175:LYS:H	2:P:175:LYS:CE	2.29	0.44
1:B:76:LEU:HD21	1:B:98:HIS:CE1	2.52	0.44
1:C:219:ARG:NH2	1:C:263:GLU:OE1	2.49	0.44
2:G:138:PRO:C	2:G:140:GLN:H	2.24	0.44
1:I:219:ARG:NH2	1:I:263:GLU:OE1	2.49	0.44
1:B:193:LYS:HD2	1:B:420:ASN:HA	1.99	0.44
2:F:119:LEU:HD12	2:F:152:ASN:HB2	2.00	0.44
1:D:358:GLN:HB3	1:D:362:LYS:HE3	1.99	0.44
1:J:123:ASP:OD1	1:J:123:ASP:N	2.40	0.44
1:B:358:GLN:HB3	1:B:362:LYS:HE3	1.99	0.44
1:I:270:LEU:HD12	1:I:293:PRO:HG3	1.98	0.44
2:K:175:LYS:O	2:K:179:THR:HG22	2.18	0.44
1:M:274:GLN:HE21	1:M:274:GLN:HB2	1.54	0.44
2:O:190:GLU:O	2:O:194:GLN:HB2	2.17	0.44
2:P:112:ALA:O	2:P:116:ILE:HG13	2.17	0.44
2:P:200:VAL:HG21	2:P:216:MET:CG	2.46	0.44
1:B:123:ASP:OD1	1:B:123:ASP:N	2.40	0.44
2:F:158:LYS:HA	2:F:210:PHE:HE2	1.81	0.44
1:M:76:LEU:HD21	1:M:98:HIS:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:243:GLU:OE2	1:M:274:GLN:NE2	2.50	0.44
2:O:172:ILE:HG21	2:O:172:ILE:HD13	1.67	0.44
1:J:358:GLN:HB3	1:J:362:LYS:HE3	1.99	0.44
2:K:164:PHE:O	2:K:176:GLU:HB3	2.18	0.44
1:A:219:ARG:NH2	1:A:263:GLU:OE1	2.50	0.44
1:B:485:GLN:C	1:B:489:LEU:HB2	2.43	0.44
1:C:461:ILE:HD12	1:C:479:LEU:HD12	1.99	0.44
1:M:270:LEU:HD12	1:M:293:PRO:HG3	1.99	0.44
1:N:123:ASP:OD1	1:N:123:ASP:N	2.41	0.44
1:N:358:GLN:HB3	1:N:362:LYS:HE3	1.99	0.44
1:J:314:ALA:HB1	1:J:318:VAL:CG2	2.48	0.44
2:O:175:LYS:O	2:O:179:THR:HG22	2.18	0.44
2:F:200:VAL:HG21	2:F:216:MET:CG	2.47	0.43
1:D:246:VAL:O	1:D:385:ARG:HD2	2.18	0.43
2:H:181:MET:O	2:H:186:GLN:HB2	2.18	0.43
1:J:115:PRO:HA	1:J:338:LEU:HD13	2.00	0.43
1:N:314:ALA:HB1	1:N:318:VAL:CG2	2.48	0.43
2:P:132:SER:O	2:P:135:LEU:HG	2.18	0.43
1:B:193:LYS:O	1:B:197:ARG:HG3	2.18	0.43
1:B:481:ASP:OD2	2:F:123:ASN:HB2	2.18	0.43
1:C:76:LEU:HD21	1:C:98:HIS:CE1	2.52	0.43
1:D:193:LYS:O	1:D:197:ARG:HG3	2.18	0.43
2:F:119:LEU:HD12	2:F:152:ASN:CB	2.48	0.43
1:J:193:LYS:O	1:J:197:ARG:HG3	2.18	0.43
1:N:239:PRO:HG3	1:N:270:LEU:HD22	2.00	0.43
1:C:11:LEU:HD11	1:D:352:GLU:HG3	2.00	0.43
1:D:123:ASP:OD1	1:D:123:ASP:N	2.41	0.43
1:D:239:PRO:HG3	1:D:270:LEU:HD22	2.01	0.43
2:G:175:LYS:O	2:G:179:THR:HG22	2.18	0.43
1:J:475:PHE:O	1:J:478:SER:OG	2.25	0.43
1:N:193:LYS:O	1:N:197:ARG:HG3	2.18	0.43
1:A:76:LEU:HD21	1:A:98:HIS:CE1	2.53	0.43
1:A:243:GLU:OE2	1:A:274:GLN:NE2	2.50	0.43
1:D:115:PRO:HA	1:D:338:LEU:HD13	2.00	0.43
2:G:164:PHE:O	2:G:176:GLU:HB3	2.18	0.43
1:I:461:ILE:HD12	1:I:479:LEU:HD12	1.99	0.43
1:J:230:ASP:OD1	1:M:197:ARG:NH2	2.49	0.43
1:J:239:PRO:HG3	1:J:270:LEU:HD22	2.01	0.43
1:J:246:VAL:O	1:J:385:ARG:HD2	2.18	0.43
1:N:174:ILE:HD11	1:N:232:VAL:HG21	2.01	0.43
1:N:464:LEU:CB	1:N:467:LEU:HD21	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:488:ASN:O	1:N:491:ALA:HB3	2.18	0.43
1:I:302:LEU:HD23	1:I:309:ILE:HG21	2.01	0.43
1:I:476:ILE:HD11	2:K:128:ALA:HA	2.01	0.43
1:M:302:LEU:HD23	1:M:309:ILE:HG21	2.00	0.43
1:N:270:LEU:HD12	1:N:293:PRO:HG3	2.01	0.43
2:O:164:PHE:O	2:O:176:GLU:HB3	2.18	0.43
1:B:314:ALA:HB1	1:B:318:VAL:CG2	2.48	0.43
1:M:458:PHE:HB2	1:M:479:LEU:HD21	1.99	0.43
1:B:54:ARG:HA	1:B:57:VAL:HG22	2.00	0.43
2:E:164:PHE:O	2:E:176:GLU:HB3	2.18	0.43
2:F:177:LEU:HB3	2:F:181:MET:CE	2.40	0.43
1:D:54:ARG:HA	1:D:57:VAL:HG22	2.00	0.43
1:I:91:PHE:HD1	1:I:426:ARG:CZ	2.32	0.43
1:J:54:ARG:HA	1:J:57:VAL:HG22	2.00	0.43
2:K:190:GLU:O	2:K:194:GLN:HB2	2.19	0.43
1:B:174:ILE:HD11	1:B:232:VAL:HG21	2.01	0.43
1:D:174:ILE:HD11	1:D:232:VAL:HG21	2.01	0.43
1:D:314:ALA:HB1	1:D:318:VAL:CG2	2.48	0.43
1:D:359:ALA:HB2	1:D:431:LEU:HD22	2.00	0.43
1:D:390:LEU:C	1:D:391:MET:HG3	2.44	0.43
1:J:380:LEU:HD13	1:J:452:MET:HE2	1.99	0.43
2:L:126:GLN:CD	2:L:126:GLN:H	2.18	0.43
2:L:132:SER:O	2:L:135:LEU:HG	2.19	0.43
1:M:379:ASP:OD1	1:M:379:ASP:N	2.41	0.43
1:B:359:ALA:HB2	1:B:431:LEU:HD22	2.00	0.43
1:B:379:ASP:OD1	1:B:379:ASP:N	2.41	0.43
1:B:461:ILE:HD13	1:B:461:ILE:HG21	1.74	0.43
2:F:132:SER:O	2:F:135:LEU:HG	2.19	0.43
1:D:270:LEU:HD12	1:D:293:PRO:HG3	2.01	0.43
1:I:379:ASP:OD1	1:I:379:ASP:N	2.41	0.43
1:J:270:LEU:HD12	1:J:293:PRO:HG3	2.01	0.43
2:L:181:MET:O	2:L:186:GLN:HB2	2.19	0.43
1:N:246:VAL:O	1:N:385:ARG:HD2	2.18	0.43
1:A:239:PRO:HG3	1:A:270:LEU:HD22	2.00	0.42
1:A:458:PHE:O	1:A:461:ILE:HG22	2.18	0.42
1:B:246:VAL:O	1:B:385:ARG:HD2	2.19	0.42
1:C:193:LYS:O	1:C:197:ARG:HG3	2.19	0.42
1:I:274:GLN:HE21	1:I:274:GLN:HB2	1.55	0.42
1:B:270:LEU:HD12	1:B:293:PRO:HG3	2.01	0.42
1:B:458:PHE:C	1:B:461:ILE:HG22	2.44	0.42
1:I:193:LYS:O	1:I:197:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:174:ILE:HD11	1:J:232:VAL:HG21	2.01	0.42
2:K:149:LYS:O	2:K:152:ASN:HB3	2.19	0.42
1:M:193:LYS:O	1:M:197:ARG:HG3	2.19	0.42
1:N:485:GLN:H	1:N:485:GLN:HG3	1.36	0.42
1:A:193:LYS:O	1:A:197:ARG:HG3	2.19	0.42
1:A:302:LEU:HD23	1:A:309:ILE:HG21	2.00	0.42
1:B:239:PRO:HG3	1:B:270:LEU:HD22	2.01	0.42
1:B:468:ASN:ND2	1:B:468:ASN:H	2.17	0.42
1:B:475:PHE:HD1	1:B:489:LEU:HD11	1.84	0.42
2:H:164:PHE:HD2	2:H:172:ILE:HD13	1.83	0.42
1:J:414:LEU:HD12	1:J:414:LEU:HA	1.92	0.42
1:M:91:PHE:HD1	1:M:426:ARG:CZ	2.32	0.42
1:M:300:LYS:HA	1:N:333:PHE:HZ	1.84	0.42
1:A:91:PHE:HD1	1:A:426:ARG:CZ	2.33	0.42
2:F:181:MET:O	2:F:186:GLN:HB2	2.19	0.42
1:C:383:GLU:HG2	1:C:384:ALA:N	2.35	0.42
1:D:464:LEU:N	1:D:472:ARG:HH22	2.18	0.42
1:J:480:LYS:HB3	2:L:124:GLY:HA2	2.02	0.42
1:M:461:ILE:HD13	1:M:461:ILE:HG21	1.83	0.42
2:P:172:ILE:HG21	2:P:177:LEU:HD23	2.00	0.42
2:E:149:LYS:O	2:E:152:ASN:HB3	2.20	0.42
2:E:175:LYS:O	2:E:179:THR:HG22	2.18	0.42
2:G:149:LYS:O	2:G:152:ASN:HB3	2.19	0.42
1:I:197:ARG:NH2	1:N:230:ASP:OD1	2.50	0.42
1:I:462:LEU:HD11	2:K:135:LEU:HD21	2.01	0.42
1:J:464:LEU:CB	1:J:467:LEU:HD21	2.49	0.42
1:N:482:ASP:C	1:N:484:SER:H	2.27	0.42
2:O:149:LYS:O	2:O:152:ASN:HB3	2.20	0.42
2:K:181:MET:HB2	2:K:188:PRO:HG3	2.02	0.42
2:F:161:PHE:CE1	2:F:172:ILE:HD12	2.54	0.42
1:D:379:ASP:OD1	1:D:379:ASP:N	2.41	0.42
2:H:200:VAL:HG21	2:H:216:MET:CG	2.46	0.42
1:J:114:GLN:HA	1:J:115:PRO:HD3	1.96	0.42
2:K:158:LYS:HE3	2:K:210:PHE:HE1	1.84	0.42
2:L:148:ALA:O	2:L:151:LEU:HB3	2.19	0.42
1:M:59:ALA:HB1	2:O:115:GLU:CD	2.45	0.42
2:P:181:MET:O	2:P:186:GLN:HB2	2.19	0.42
2:H:132:SER:O	2:H:135:LEU:HG	2.20	0.42
1:A:462:LEU:HD11	2:E:135:LEU:HD21	2.02	0.42
1:C:43:LYS:HG2	1:C:44:GLU:HG2	2.02	0.42
2:L:116:ILE:HG13	2:L:117:PHE:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:54:ARG:HA	1:N:57:VAL:HG22	2.01	0.42
1:C:239:PRO:HG3	1:C:270:LEU:HD22	2.01	0.42
1:A:197:ARG:NH2	1:D:230:ASP:OD1	2.49	0.41
1:J:485:GLN:H	1:J:485:GLN:HG3	1.41	0.41
2:K:172:ILE:CG2	2:K:177:LEU:HD13	2.50	0.41
2:K:177:LEU:HD12	2:K:177:LEU:HA	1.84	0.41
2:G:158:LYS:HE3	2:G:210:PHE:HE1	1.83	0.41
2:P:121:ASN:N	2:P:152:ASN:HD21	2.17	0.41
1:B:477:GLN:O	1:B:481:ASP:OD1	2.38	0.41
2:E:181:MET:HB2	2:E:188:PRO:HG3	2.01	0.41
1:C:477:GLN:HG2	2:G:124:GLY:C	2.46	0.41
2:O:177:LEU:HD12	2:O:177:LEU:HA	1.84	0.41
2:P:164:PHE:CD2	2:P:172:ILE:HD12	2.55	0.41
1:A:383:GLU:HG2	1:A:384:ALA:N	2.36	0.41
1:M:185:LEU:HD21	1:N:159:LYS:HG2	2.02	0.41
2:E:123:ASN:H	2:E:126:GLN:NE2	2.15	0.41
2:K:158:LYS:HE3	2:K:210:PHE:CE1	2.55	0.41
1:C:67:GLU:HG3	1:D:121:LEU:HB2	2.02	0.41
1:M:239:PRO:HG3	1:M:270:LEU:HD22	2.01	0.41
1:M:476:ILE:HD11	2:O:128:ALA:HA	2.03	0.41
2:P:164:PHE:HD1	2:P:180:VAL:HG21	1.86	0.41
1:A:185:LEU:HD21	1:B:159:LYS:HG2	2.02	0.41
1:C:462:LEU:HD11	2:G:135:LEU:HD21	2.02	0.41
2:O:172:ILE:CG2	2:O:177:LEU:HD13	2.51	0.41
2:O:181:MET:HB2	2:O:188:PRO:HG3	2.03	0.41
2:P:209:ASP:OD1	2:P:209:ASP:N	2.40	0.41
1:A:59:ALA:HB1	2:E:115:GLU:CD	2.46	0.41
1:J:87:CYS:HA	1:J:429:PRO:HB3	2.03	0.41
1:J:359:ALA:HB2	1:J:431:LEU:HD22	2.01	0.41
1:J:468:ASN:H	1:J:468:ASN:ND2	2.18	0.41
1:N:359:ALA:HB2	1:N:431:LEU:HD22	2.02	0.41
1:N:458:PHE:O	1:N:461:ILE:HG23	2.20	0.41
1:A:43:LYS:HG2	1:A:44:GLU:HG2	2.03	0.41
1:D:479:LEU:HD22	2:H:117:PHE:HZ	1.84	0.41
1:I:239:PRO:HG3	1:I:270:LEU:HD22	2.01	0.41
2:P:121:ASN:CG	2:P:156:ALA:HB2	2.46	0.41
1:D:477:GLN:O	2:H:124:GLY:HA3	2.21	0.41
1:N:495:LYS:HA	1:N:498:ASP:OD2	2.21	0.41
1:A:461:ILE:HD13	1:A:461:ILE:HG21	1.85	0.40
1:C:87:CYS:HA	1:C:429:PRO:HB3	2.03	0.40
2:G:172:ILE:CG2	2:G:177:LEU:HD13	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:481:ASP:OD2	2:L:123:ASN:HB3	2.22	0.40
2:K:119:LEU:HA	2:K:120:PRO:HD3	1.90	0.40
1:N:87:CYS:HA	1:N:429:PRO:HB3	2.03	0.40
1:B:75:THR:HA	1:B:84:PHE:O	2.21	0.40
1:D:423:LYS:HB2	1:D:423:LYS:HE3	2.00	0.40
1:D:488:ASN:O	1:D:491:ALA:HB3	2.21	0.40
1:I:383:GLU:HG2	1:I:384:ALA:N	2.35	0.40
2:F:126:GLN:H	2:F:126:GLN:CD	2.28	0.40
1:D:480:LYS:HG3	2:H:127:VAL:HG11	2.03	0.40
2:G:123:ASN:H	2:G:126:GLN:NE2	2.15	0.40
1:I:43:LYS:HG2	1:I:44:GLU:HG2	2.02	0.40
1:I:87:CYS:HA	1:I:429:PRO:HB3	2.03	0.40
1:N:480:LYS:HG3	2:P:127:VAL:HG11	2.03	0.40
1:A:69:GLN:HE21	1:A:69:GLN:HB3	1.75	0.40
1:A:75:THR:HA	1:A:84:PHE:O	2.22	0.40
1:C:270:LEU:HD13	1:C:286:CYS:HB3	2.04	0.40
1:M:136:LEU:HD11	1:M:283:MET:HE3	2.03	0.40
2:P:126:GLN:HE22	2:P:155:GLN:NE2	2.20	0.40
1:A:87:CYS:HA	1:A:429:PRO:HB3	2.03	0.40
2:E:172:ILE:CG2	2:E:177:LEU:HD13	2.51	0.40
1:C:75:THR:HA	1:C:84:PHE:O	2.22	0.40
1:M:87:CYS:HA	1:M:429:PRO:HB3	2.03	0.40
1:N:461:ILE:HD12	1:N:475:PHE:HB3	2.04	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	493/499 (99%)	472 (96%)	21 (4%)	0	100	100
1	B	493/499 (99%)	470 (95%)	22 (4%)	1 (0%)	43	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	493/499 (99%)	473 (96%)	19 (4%)	1 (0%)	43	63
1	D	493/499 (99%)	470 (95%)	23 (5%)	0	100	100
1	I	493/499 (99%)	472 (96%)	21 (4%)	0	100	100
1	J	493/499 (99%)	469 (95%)	24 (5%)	0	100	100
1	M	493/499 (99%)	472 (96%)	21 (4%)	0	100	100
1	N	493/499 (99%)	470 (95%)	23 (5%)	0	100	100
2	E	111/120 (92%)	105 (95%)	5 (4%)	1 (1%)	14	29
2	F	110/120 (92%)	103 (94%)	7 (6%)	0	100	100
2	G	111/120 (92%)	104 (94%)	6 (5%)	1 (1%)	14	29
2	H	110/120 (92%)	102 (93%)	8 (7%)	0	100	100
2	K	111/120 (92%)	105 (95%)	5 (4%)	1 (1%)	14	29
2	L	110/120 (92%)	103 (94%)	7 (6%)	0	100	100
2	O	111/120 (92%)	104 (94%)	6 (5%)	1 (1%)	14	29
2	P	110/120 (92%)	103 (94%)	7 (6%)	0	100	100
All	All	4828/4952 (98%)	4597 (95%)	225 (5%)	6 (0%)	48	69

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	485	GLN
2	E	139	SER
2	G	139	SER
2	K	139	SER
2	O	139	SER
1	C	115	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	396/399 (99%)	383 (97%)	13 (3%)	33	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	396/399 (99%)	383 (97%)	13 (3%)	33	59
1	C	396/399 (99%)	385 (97%)	11 (3%)	38	64
1	D	396/399 (99%)	381 (96%)	15 (4%)	29	54
1	I	396/399 (99%)	384 (97%)	12 (3%)	36	62
1	J	396/399 (99%)	383 (97%)	13 (3%)	33	59
1	M	396/399 (99%)	385 (97%)	11 (3%)	38	64
1	N	396/399 (99%)	378 (96%)	18 (4%)	24	47
2	E	95/101 (94%)	82 (86%)	13 (14%)	3	6
2	F	93/101 (92%)	82 (88%)	11 (12%)	5	10
2	G	95/101 (94%)	80 (84%)	15 (16%)	2	4
2	H	93/101 (92%)	86 (92%)	7 (8%)	12	26
2	K	95/101 (94%)	83 (87%)	12 (13%)	4	8
2	L	93/101 (92%)	84 (90%)	9 (10%)	8	16
2	O	95/101 (94%)	82 (86%)	13 (14%)	3	6
2	P	93/101 (92%)	82 (88%)	11 (12%)	5	10
All	All	3920/4000 (98%)	3723 (95%)	197 (5%)	22	44

All (197) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	140	LYS
1	A	166	SER
1	A	237	LEU
1	A	274	GLN
1	A	365	MET
1	A	398	ASN
1	A	431	LEU
1	A	446	ARG
1	A	476	ILE
1	A	477	GLN
1	A	495	LYS
1	A	500	GLN
1	B	99	ARG
1	B	166	SER
1	B	237	LEU
1	B	338	LEU

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Mol	Chain	Res	Type
1	B	398	ASN
1	B	467	LEU
1	B	469	GLU
1	B	479	LEU
1	B	480	LYS
1	B	481	ASP
1	B	485	GLN
1	B	496	LEU
1	B	500	GLN
2	E	123	ASN
2	E	125	ARG
2	E	144	LEU
2	E	151	LEU
2	E	158	LYS
2	E	161	PHE
2	E	177	LEU
2	E	179	THR
2	E	181	MET
2	E	183	SER
2	E	194	GLN
2	E	209	ASP
2	E	210	PHE
2	F	119	LEU
2	F	126	GLN
2	F	134	LEU
2	F	147	GLU
2	F	172	ILE
2	F	175	LYS
2	F	177	LEU
2	F	181	MET
2	F	184	LEU
2	F	209	ASP
2	F	210	PHE
1	C	69	GLN
1	C	140	LYS
1	C	166	SER
1	C	237	LEU
1	C	243	GLU
1	C	398	ASN
1	C	431	LEU
1	C	446	ARG
1	C	477	GLN

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Mol	Chain	Res	Type
1	C	495	LYS
1	C	500	GLN
1	D	99	ARG
1	D	166	SER
1	D	237	LEU
1	D	338	LEU
1	D	398	ASN
1	D	467	LEU
1	D	469	GLU
1	D	470	GLU
1	D	476	ILE
1	D	477	GLN
1	D	480	LYS
1	D	481	ASP
1	D	485	GLN
1	D	496	LEU
1	D	500	GLN
2	G	123	ASN
2	G	125	ARG
2	G	144	LEU
2	G	151	LEU
2	G	158	LYS
2	G	161	PHE
2	G	177	LEU
2	G	179	THR
2	G	181	MET
2	G	183	SER
2	G	194	GLN
2	G	209	ASP
2	G	210	PHE
2	G	217	MET
2	G	219	ARG
2	H	134	LEU
2	H	147	GLU
2	H	175	LYS
2	H	181	MET
2	H	184	LEU
2	H	209	ASP
2	H	210	PHE
1	I	69	GLN
1	I	140	LYS
1	I	166	SER

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Mol	Chain	Res	Type
1	I	237	LEU
1	I	243	GLU
1	I	274	GLN
1	I	365	MET
1	I	398	ASN
1	I	431	LEU
1	I	477	GLN
1	I	495	LYS
1	I	500	GLN
1	J	99	ARG
1	J	121	LEU
1	J	166	SER
1	J	237	LEU
1	J	338	LEU
1	J	391	MET
1	J	398	ASN
1	J	467	LEU
1	J	469	GLU
1	J	476	ILE
1	J	481	ASP
1	J	485	GLN
1	J	496	LEU
2	K	107	LYS
2	K	123	ASN
2	K	125	ARG
2	K	144	LEU
2	K	151	LEU
2	K	158	LYS
2	K	177	LEU
2	K	179	THR
2	K	181	MET
2	K	183	SER
2	K	209	ASP
2	K	210	PHE
2	L	126	GLN
2	L	134	LEU
2	L	147	GLU
2	L	172	ILE
2	L	175	LYS
2	L	181	MET
2	L	184	LEU
2	L	209	ASP

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Mol	Chain	Res	Type
2	L	210	PHE
1	M	20	LEU
1	M	140	LYS
1	M	166	SER
1	M	237	LEU
1	M	274	GLN
1	M	365	MET
1	M	398	ASN
1	M	446	ARG
1	M	477	GLN
1	M	495	LYS
1	M	500	GLN
1	N	99	ARG
1	N	121	LEU
1	N	166	SER
1	N	237	LEU
1	N	338	LEU
1	N	398	ASN
1	N	461	ILE
1	N	467	LEU
1	N	469	GLU
1	N	470	GLU
1	N	471	GLN
1	N	477	GLN
1	N	480	LYS
1	N	481	ASP
1	N	485	GLN
1	N	489	LEU
1	N	495	LYS
1	N	496	LEU
2	O	123	ASN
2	O	125	ARG
2	O	144	LEU
2	O	151	LEU
2	O	158	LYS
2	O	161	PHE
2	O	177	LEU
2	O	179	THR
2	O	181	MET
2	O	183	SER
2	O	194	GLN
2	O	209	ASP

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Mol	Chain	Res	Type
2	O	210	PHE
2	P	116	ILE
2	P	122	LEU
2	P	126	GLN
2	P	134	LEU
2	P	147	GLU
2	P	172	ILE
2	P	175	LYS
2	P	181	MET
2	P	184	LEU
2	P	209	ASP
2	P	210	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	74	ASN
1	A	114	GLN
1	A	353	GLN
1	B	74	ASN
1	B	274	GLN
1	B	353	GLN
1	B	468	ASN
1	B	471	GLN
1	B	473	ASN
2	E	126	GLN
2	E	152	ASN
2	E	155	GLN
2	F	155	GLN
2	F	194	GLN
1	C	69	GLN
1	C	74	ASN
1	C	114	GLN
1	C	274	GLN
1	C	353	GLN
1	D	74	ASN
1	D	274	GLN
1	D	353	GLN
1	D	454	GLN
1	D	468	ASN
1	D	471	GLN

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Mol	Chain	Res	Type
2	G	110	GLN
2	G	126	GLN
2	G	152	ASN
2	G	155	GLN
2	H	126	GLN
2	H	155	GLN
2	H	194	GLN
1	I	69	GLN
1	I	74	ASN
1	I	114	GLN
1	I	353	GLN
1	J	74	ASN
1	J	274	GLN
1	J	353	GLN
1	J	398	ASN
1	J	454	GLN
1	J	466	ASN
1	J	468	ASN
2	K	110	GLN
2	K	126	GLN
2	K	152	ASN
2	K	155	GLN
2	L	194	GLN
1	M	74	ASN
1	M	353	GLN
1	N	74	ASN
1	N	274	GLN
1	N	485	GLN
2	O	126	GLN
2	O	152	ASN
2	O	155	GLN
2	P	126	GLN
2	P	152	ASN
2	P	194	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 16 ligands modelled in this entry, 16 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	495/499 (99%)	-0.58	0 100 100	45, 69, 137, 163	0
1	B	495/499 (99%)	-0.59	2 (0%) 88 87	43, 62, 126, 159	0
1	C	495/499 (99%)	-0.71	0 100 100	42, 65, 86, 98	0
1	D	495/499 (99%)	-0.61	0 100 100	44, 62, 129, 162	0
1	I	495/499 (99%)	-0.62	3 (0%) 85 84	44, 68, 130, 155	0
1	J	495/499 (99%)	-0.64	1 (0%) 91 90	44, 61, 128, 162	0
1	M	495/499 (99%)	-0.59	0 100 100	46, 69, 137, 164	0
1	N	495/499 (99%)	-0.66	0 100 100	44, 63, 128, 160	0
2	E	113/120 (94%)	0.06	2 (1%) 67 64	103, 125, 147, 155	0
2	F	112/120 (93%)	1.26	24 (21%) 2 2	163, 203, 250, 261	0
2	G	113/120 (94%)	-0.15	1 (0%) 81 79	97, 119, 151, 160	0
2	H	112/120 (93%)	0.96	12 (10%) 11 9	147, 183, 233, 246	0
2	K	113/120 (94%)	-0.17	0 100 100	97, 117, 142, 153	0
2	L	112/120 (93%)	1.08	19 (16%) 4 3	166, 201, 241, 251	0
2	O	113/120 (94%)	0.12	4 (3%) 47 42	103, 127, 156, 162	0
2	P	112/120 (93%)	1.19	18 (16%) 4 4	170, 192, 227, 237	0
All	All	4860/4952 (98%)	-0.41	86 (1%) 67 64	42, 70, 188, 261	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	184	LEU	6.0
2	F	184	LEU	5.6
2	P	184	LEU	5.5
2	P	167	ASP	5.2
2	L	169	ASP	5.1

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Mol	Chain	Res	Type	RSRZ
2	F	180	VAL	5.1
2	F	122	LEU	5.1
2	H	134	LEU	4.8
2	F	157	PHE	4.8
2	F	127	VAL	4.6
2	P	169	ASP	4.2
2	L	128	ALA	4.1
2	L	184	LEU	3.9
2	L	180	VAL	3.9
2	F	200	VAL	3.9
2	H	180	VAL	3.6
2	F	145	LEU	3.4
2	P	148	ALA	3.2
2	O	174	THR	3.2
2	F	134	LEU	3.2
2	P	122	LEU	3.2
2	L	124	GLY	3.2
2	F	116	ILE	3.1
2	F	196	MET	3.1
1	B	417	GLY	3.1
2	F	154	ILE	3.0
2	L	209	ASP	3.0
2	P	196	MET	3.0
1	B	463	HIS	3.0
2	H	135	LEU	2.9
2	L	130	PHE	2.9
2	F	128	ALA	2.9
2	F	208	ILE	2.9
2	H	154	ILE	2.8
2	L	208	ILE	2.8
2	L	127	VAL	2.8
2	F	151	LEU	2.8
2	P	133	SER	2.7
2	H	162	SER	2.7
2	L	123	ASN	2.6
2	P	144	LEU	2.6
2	F	148	ALA	2.6
2	H	131	ILE	2.6
2	F	179	THR	2.6
2	P	213	PHE	2.6
2	F	214	LEU	2.6
2	P	128	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	117	PHE	2.5
2	F	135	LEU	2.5
2	F	181	MET	2.5
1	I	499	ALA	2.5
2	L	133	SER	2.5
2	P	151	LEU	2.4
2	F	131	ILE	2.4
2	H	157	PHE	2.4
2	H	191	ALA	2.4
2	P	117	PHE	2.4
1	I	478	SER	2.4
2	H	151	LEU	2.4
2	H	161	PHE	2.4
2	P	127	VAL	2.4
2	L	162	SER	2.3
1	I	82	GLN	2.3
2	O	172	ILE	2.3
2	P	134	LEU	2.3
2	L	125	ARG	2.3
2	H	169	ASP	2.3
1	J	481	ASP	2.2
2	L	196	MET	2.2
2	O	117	PHE	2.2
2	F	215	THR	2.2
2	L	134	LEU	2.2
2	L	213	PHE	2.2
2	F	109	THR	2.1
2	O	175	LYS	2.1
2	L	164	PHE	2.1
2	P	205	ASN	2.1
2	E	193	LEU	2.1
2	P	145	LEU	2.1
2	P	193	LEU	2.1
2	F	199	GLU	2.1
2	L	120	PRO	2.1
2	F	142	ALA	2.0
2	L	129	ALA	2.0
2	G	185	GLY	2.0
2	P	180	VAL	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($\text{\AA}^2$)	Q<0.9
3	CA	H	502	1/1	0.91	0.11	83,83,83,83	0
3	CA	P	502	1/1	0.91	0.07	84,84,84,84	0
3	CA	K	502	1/1	0.96	0.05	86,86,86,86	0
3	CA	F	501	1/1	0.96	0.06	91,91,91,91	0
3	CA	H	501	1/1	0.97	0.05	90,90,90,90	0
3	CA	P	501	1/1	0.97	0.07	89,89,89,89	0
3	CA	F	502	1/1	0.97	0.05	87,87,87,87	0
3	CA	L	501	1/1	0.98	0.07	88,88,88,88	0
3	CA	L	502	1/1	0.98	0.10	82,82,82,82	0
3	CA	G	501	1/1	0.99	0.02	82,82,82,82	0
3	CA	G	502	1/1	0.99	0.08	84,84,84,84	0
3	CA	E	501	1/1	0.99	0.04	82,82,82,82	0
3	CA	O	501	1/1	0.99	0.02	79,79,79,79	0
3	CA	O	502	1/1	0.99	0.03	88,88,88,88	0
3	CA	E	502	1/1	0.99	0.02	86,86,86,86	0
3	CA	K	501	1/1	0.99	0.02	80,80,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.