



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:13 PM UTC

PDB ID : 4A0C / pdb_00004a0c
Title : Structure of the CAND1-CUL4B-RBX1 complex
Authors : Scrima, A.; Fischer, E.S.; Faty, M.; Gut, H.; Thoma, N.H.
Deposited on : 2011-09-08
Resolution : 3.80 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

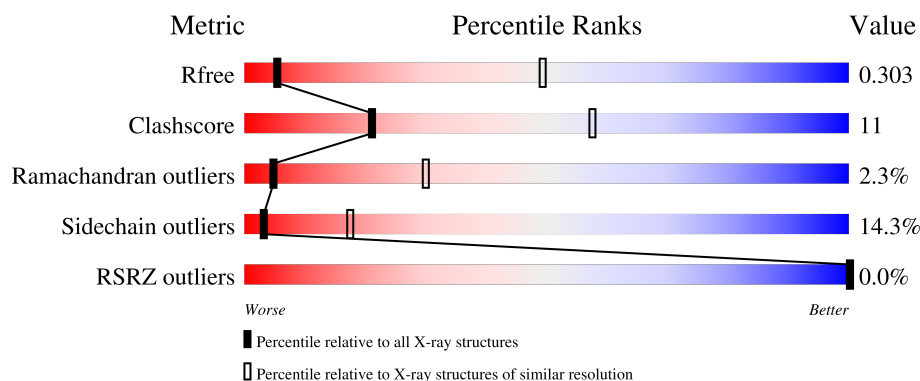
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1065 (3.96-3.64)
Clashscore	190562	1012 (3.94-3.66)
Ramachandran outliers	187476	1048 (3.96-3.64)
Sidechain outliers	187428	1043 (3.96-3.64)
RSRZ outliers	180081	1064 (3.96-3.64)

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	1253	
1	B	1253	
2	C	741	
2	E	741	
3	D	98	

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Mol	Chain	Length	Quality of chain
3	F	98	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: green (51%), yellow (27%), orange (1%), and grey (18%). The percentages are labeled below the bar segments. 51% 27% • 18%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30804 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 CULLIN-ASSOCIATED NEDD8-DISSOCIATED PROTEIN 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1155	Total	C	N	O	S	0	0	0
			8963	5708	1517	1682	56			
1	B	1154	Total	C	N	O	S	0	0	0
			8975	5713	1519	1687	56			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-22	MET	-	expression tag	UNP Q86VP6
A	-21	ALA	-	expression tag	UNP Q86VP6
A	-20	SER	-	expression tag	UNP Q86VP6
A	-19	TRP	-	expression tag	UNP Q86VP6
A	-18	SER	-	expression tag	UNP Q86VP6
A	-17	HIS	-	expression tag	UNP Q86VP6
A	-16	PRO	-	expression tag	UNP Q86VP6
A	-15	GLN	-	expression tag	UNP Q86VP6
A	-14	PHE	-	expression tag	UNP Q86VP6
A	-13	GLU	-	expression tag	UNP Q86VP6
A	-12	LYS	-	expression tag	UNP Q86VP6
A	-11	VAL	-	expression tag	UNP Q86VP6
A	-10	ASP	-	expression tag	UNP Q86VP6
A	-9	GLU	-	expression tag	UNP Q86VP6
A	-8	ASN	-	expression tag	UNP Q86VP6
A	-7	LEU	-	expression tag	UNP Q86VP6
A	-6	TYR	-	expression tag	UNP Q86VP6
A	-5	PHE	-	expression tag	UNP Q86VP6
A	-4	GLN	-	expression tag	UNP Q86VP6
A	-3	GLY	-	expression tag	UNP Q86VP6
A	-2	GLY	-	expression tag	UNP Q86VP6
A	-1	GLY	-	expression tag	UNP Q86VP6
A	0	ARG	-	expression tag	UNP Q86VP6
A	952	VAL	ALA	variant	UNP Q86VP6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	MET	-	expression tag	UNP Q86VP6
B	-21	ALA	-	expression tag	UNP Q86VP6
B	-20	SER	-	expression tag	UNP Q86VP6
B	-19	TRP	-	expression tag	UNP Q86VP6
B	-18	SER	-	expression tag	UNP Q86VP6
B	-17	HIS	-	expression tag	UNP Q86VP6
B	-16	PRO	-	expression tag	UNP Q86VP6
B	-15	GLN	-	expression tag	UNP Q86VP6
B	-14	PHE	-	expression tag	UNP Q86VP6
B	-13	GLU	-	expression tag	UNP Q86VP6
B	-12	LYS	-	expression tag	UNP Q86VP6
B	-11	VAL	-	expression tag	UNP Q86VP6
B	-10	ASP	-	expression tag	UNP Q86VP6
B	-9	GLU	-	expression tag	UNP Q86VP6
B	-8	ASN	-	expression tag	UNP Q86VP6
B	-7	LEU	-	expression tag	UNP Q86VP6
B	-6	TYR	-	expression tag	UNP Q86VP6
B	-5	PHE	-	expression tag	UNP Q86VP6
B	-4	GLN	-	expression tag	UNP Q86VP6
B	-3	GLY	-	expression tag	UNP Q86VP6
B	-2	GLY	-	expression tag	UNP Q86VP6
B	-1	GLY	-	expression tag	UNP Q86VP6
B	0	ARG	-	expression tag	UNP Q86VP6
B	952	VAL	ALA	variant	UNP Q86VP6

- Molecule 2 is a protein called CULLIN-4B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	692	Total	C	N	O	S	0	0	0
			5702	3636	973	1062	31			
2	E	696	Total	C	N	O	S	0	0	0
			5744	3663	978	1071	32			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	173	MET	-	expression tag	UNP Q13620
C	174	HIS	-	expression tag	UNP Q13620
C	175	HIS	-	expression tag	UNP Q13620
C	176	HIS	-	expression tag	UNP Q13620
C	177	HIS	-	expression tag	UNP Q13620
C	178	HIS	-	expression tag	UNP Q13620

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Chain	Residue	Modelled	Actual	Comment	Reference
C	179	HIS	-	expression tag	UNP Q13620
C	180	VAL	-	expression tag	UNP Q13620
C	181	ASP	-	expression tag	UNP Q13620
C	182	GLU	-	expression tag	UNP Q13620
C	183	ASN	-	expression tag	UNP Q13620
C	184	LEU	-	expression tag	UNP Q13620
C	185	TYR	-	expression tag	UNP Q13620
C	186	PHE	-	expression tag	UNP Q13620
C	187	GLN	-	expression tag	UNP Q13620
C	188	GLY	-	expression tag	UNP Q13620
C	189	GLY	-	expression tag	UNP Q13620
C	190	GLY	-	expression tag	UNP Q13620
C	191	ARG	-	expression tag	UNP Q13620
E	173	MET	-	expression tag	UNP Q13620
E	174	HIS	-	expression tag	UNP Q13620
E	175	HIS	-	expression tag	UNP Q13620
E	176	HIS	-	expression tag	UNP Q13620
E	177	HIS	-	expression tag	UNP Q13620
E	178	HIS	-	expression tag	UNP Q13620
E	179	HIS	-	expression tag	UNP Q13620
E	180	VAL	-	expression tag	UNP Q13620
E	181	ASP	-	expression tag	UNP Q13620
E	182	GLU	-	expression tag	UNP Q13620
E	183	ASN	-	expression tag	UNP Q13620
E	184	LEU	-	expression tag	UNP Q13620
E	185	TYR	-	expression tag	UNP Q13620
E	186	PHE	-	expression tag	UNP Q13620
E	187	GLN	-	expression tag	UNP Q13620
E	188	GLY	-	expression tag	UNP Q13620
E	189	GLY	-	expression tag	UNP Q13620
E	190	GLY	-	expression tag	UNP Q13620
E	191	ARG	-	expression tag	UNP Q13620

- Molecule 3 is a protein called E3 UBIQUITIN-PROTEIN LIGASE RBX1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	89	Total	C	N	O	S	0	0	0
			737	466	135	127	9			
3	F	80	Total	C	N	O	S	0	0	0
			677	434	125	109	9			

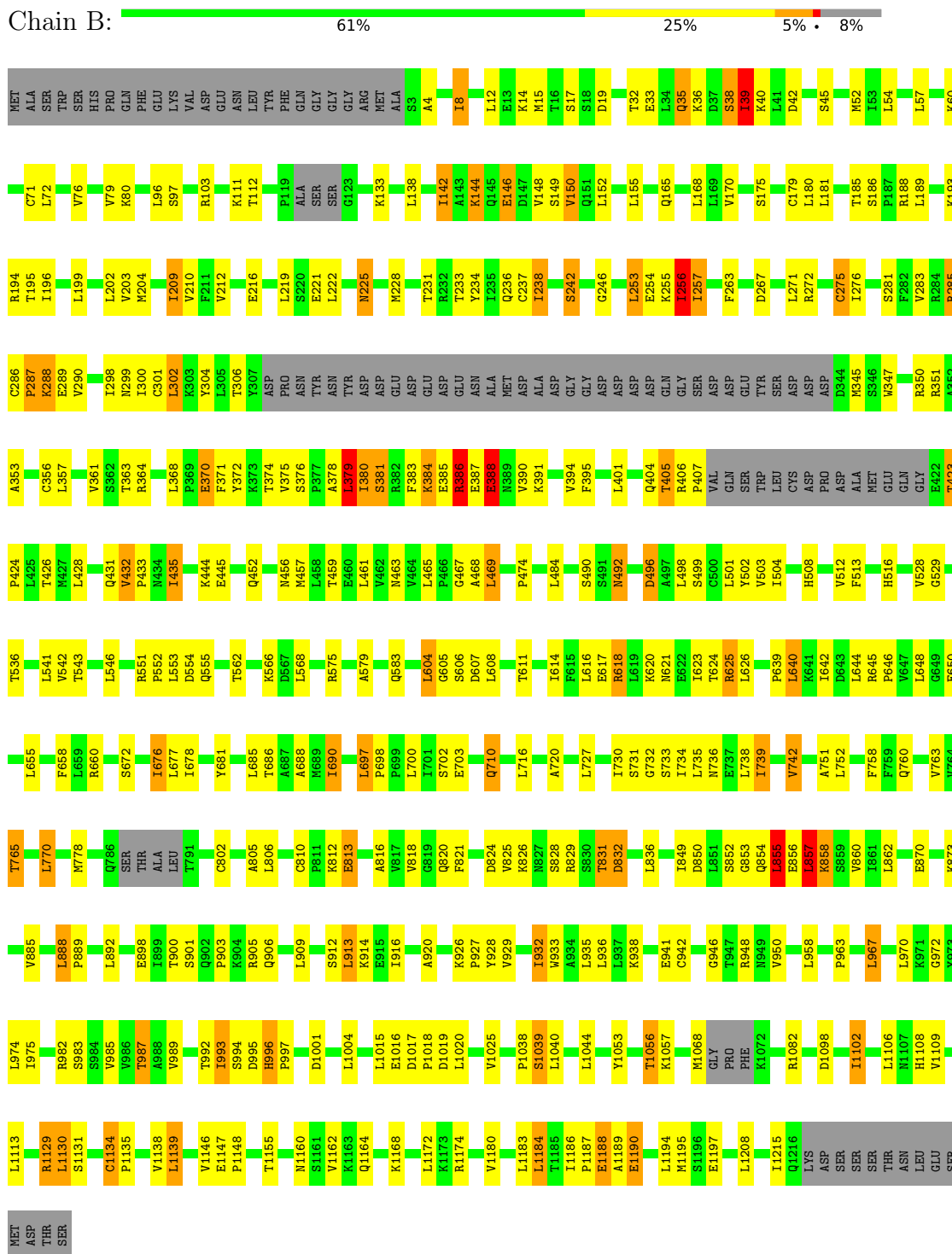
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	11	MET	-	expression tag	UNP P62878
F	11	MET	-	expression tag	UNP P62878

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

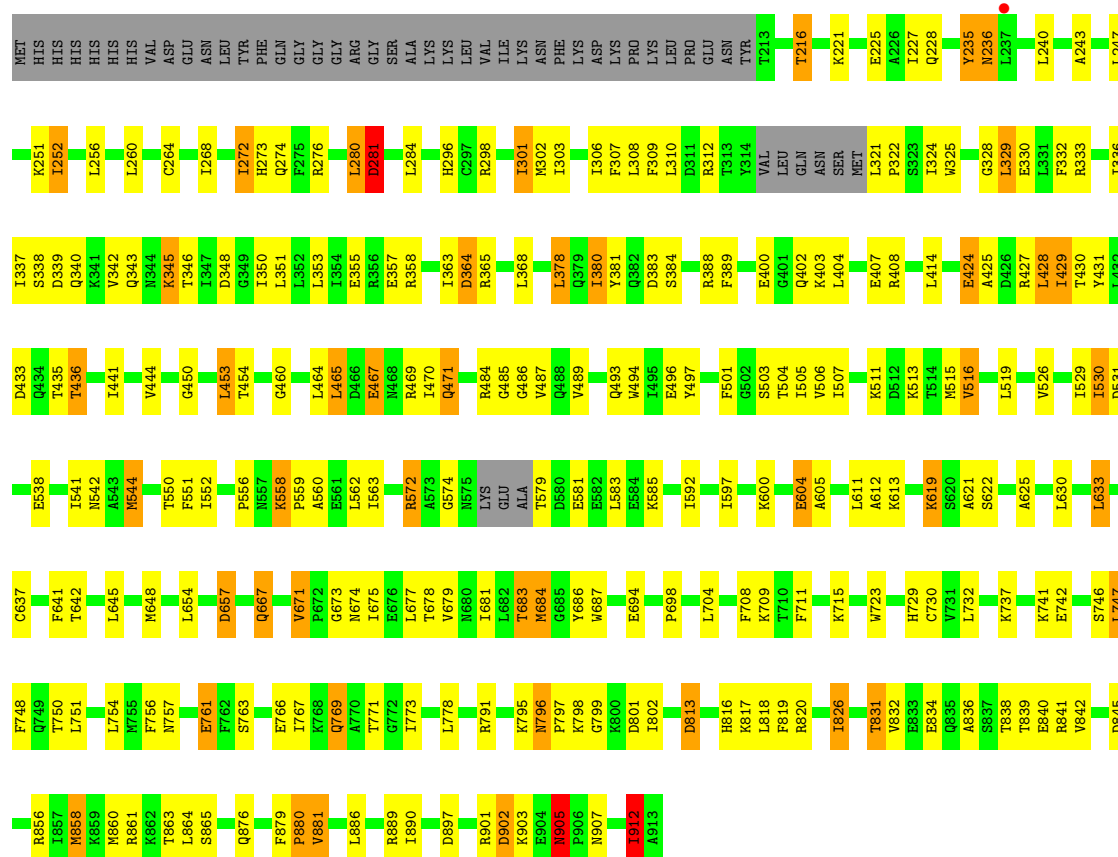
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total 3	Zn 3	0	0
4	F	3	Total 3	Zn 3	0	0

- Molecule 1: CULLIN-ASSOCIATED NEDD8-DISSOCIATED PROTEIN 1



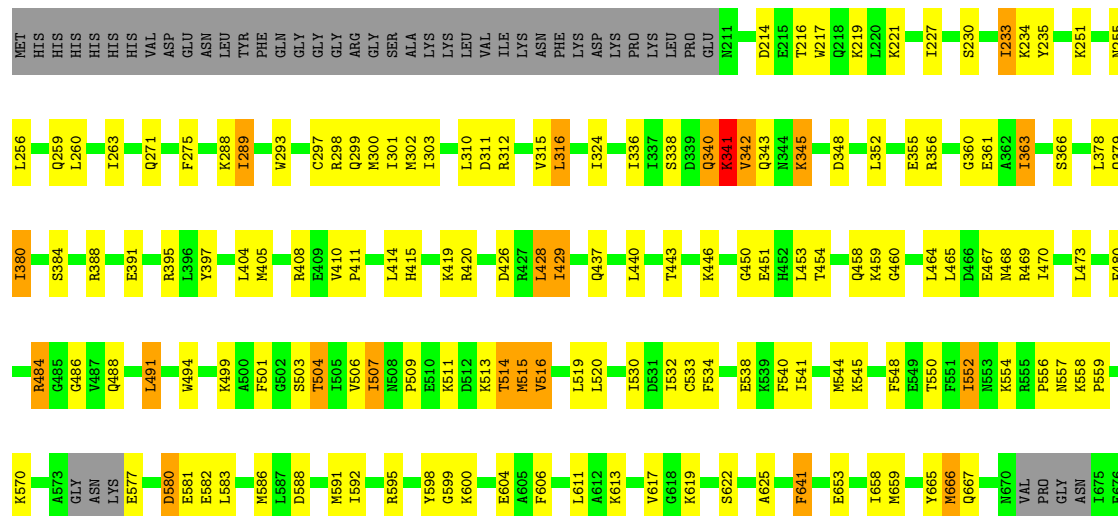
• Molecule 2: CULLIN-4B

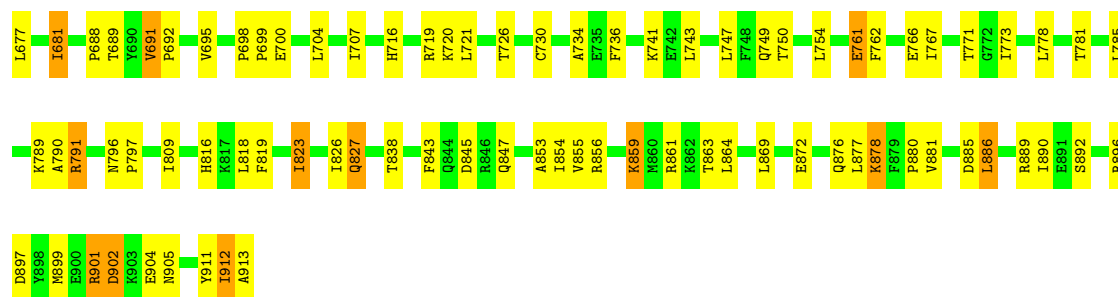
Chain C:  59% 28% 6% 7%



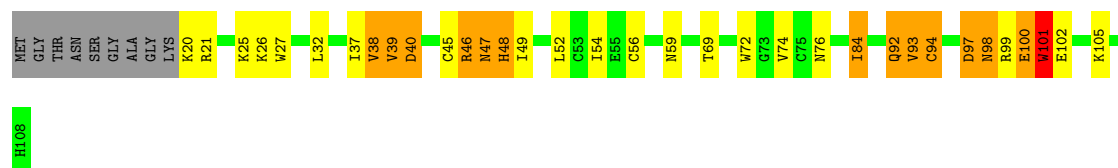
• Molecule 2: CULLIN-4B

Chain E:  62% 27% 6%

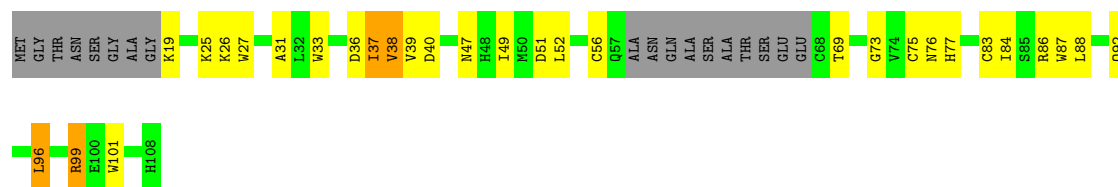




• Molecule 3: E3 UBIQUITIN-PROTEIN LIGASE RBX1



• Molecule 3: E3 UBIQUITIN-PROTEIN LIGASE RBX1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.09Å 152.36Å 263.01Å 90.00° 89.37° 90.00°	Depositor
Resolution (Å)	47.76 – 3.80 47.76 – 3.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.76-3.80) 99.7 (47.76-3.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.238 , 0.319 0.230 , 0.303	Depositor DCC
R_{free} test set	2990 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	119.1	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30804	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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: ZN

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	0.50	0/9101	0.91	2/12327 (0.0%)
1	B	0.52	1/9113 (0.0%)	0.93	10/12340 (0.1%)
2	C	0.49	0/5794	0.86	5/7776 (0.1%)
2	E	0.48	0/5836	0.85	1/7832 (0.0%)
3	D	0.56	0/759	0.75	0/1029
3	F	0.49	0/698	0.69	0/943
All	All	0.50	1/31301 (0.0%)	0.89	18/42247 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	257	ILE	CA-CB	7.18	1.58	1.53

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	698	PRO	N-CA-C	6.43	118.55	110.70
2	C	216	THR	N-CA-C	-6.03	107.75	114.62
1	B	1020	LEU	N-CA-C	5.97	117.39	108.31
1	B	551	ARG	CA-C-N	5.95	125.43	119.24
1	B	551	ARG	C-N-CA	5.95	125.43	119.24
1	B	698	PRO	N-CA-C	5.93	117.94	110.70
1	B	150	VAL	N-CA-C	-5.90	104.37	113.16
1	B	857	LEU	N-CA-C	5.84	117.65	111.28
2	C	902	ASP	N-CA-C	5.72	115.57	108.19
1	B	256	ILE	CA-C-N	5.59	123.76	120.24
1	B	256	ILE	C-N-CA	5.59	123.76	120.24
1	B	288	LYS	N-CA-C	5.51	119.17	112.23
2	E	666	MET	N-CA-C	5.43	119.17	112.54
2	C	484	ARG	N-CA-C	5.42	118.02	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	619	LYS	N-CA-C	5.36	117.01	110.41
1	B	378	ALA	CA-C-O	5.34	121.04	117.94
1	A	522	PRO	N-CA-C	5.34	117.21	110.70
2	C	905	ASN	N-CA-C	5.21	114.30	108.25

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	8963	0	9308	215	0
1	B	8975	0	9328	204	0
2	C	5702	0	5801	142	0
2	E	5744	0	5841	117	0
3	D	737	0	687	19	0
3	F	677	0	642	12	0
4	D	3	0	0	0	0
4	F	3	0	0	0	0
All	All	30804	0	31607	685	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 11.

All (685) 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:982:ARG:HH21	1:A:1018:PRO:HB3	1.25	1.00
1:A:423:THR:HG22	1:A:424:PRO:HD2	1.45	0.99
1:B:386:ARG:HG3	1:B:387:GLU:H	1.35	0.90
3:D:72:TRP:HB2	3:D:105:LYS:HB3	1.52	0.89
1:A:862:LEU:HB3	1:A:905:ARG:HH21	1.40	0.86
2:C:227:ILE:HD11	2:C:303:ILE:HG13	1.55	0.86
1:A:385:GLU:O	1:A:386:ARG:HB2	1.78	0.84
1:A:350:ARG:HH21	1:A:386:ARG:HH22	1.23	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1129:ARG:HH11	1:B:1129:ARG:HG3	1.45	0.82
2:E:617:VAL:HG11	2:E:827:GLN:HB3	1.62	0.81
2:C:791:ARG:HG2	2:C:813:ASP:HB3	1.62	0.80
1:A:383:PHE:HE2	1:A:386:ARG:HD2	1.46	0.80
1:A:92:CYS:HB3	1:A:137:ARG:HG2	1.61	0.80
2:C:280:LEU:HD13	2:C:281:ASP:H	1.47	0.80
2:E:363:ILE:H	2:E:363:ILE:HD13	1.47	0.79
1:A:276:ILE:HG21	1:A:353:ALA:HA	1.66	0.77
2:C:276:ARG:HE	2:C:340:GLN:HE22	1.32	0.76
2:E:901:ARG:O	2:E:902:ASP:HB2	1.84	0.75
1:A:621:ASN:HD22	1:A:623:ILE:H	1.31	0.75
1:B:376:SER:HA	1:B:380:ILE:HD11	1.68	0.75
2:C:307:PHE:HB3	2:C:310:LEU:HB2	1.68	0.74
2:C:353:LEU:HB3	2:C:363:ILE:HD11	1.69	0.74
1:B:19:ASP:HA	3:D:92:GLN:HE22	1.52	0.74
1:B:982:ARG:NH2	1:B:1018:PRO:HB3	2.02	0.74
1:A:1068:MET:HG3	2:E:302:MET:HE1	1.69	0.73
1:B:376:SER:HA	1:B:380:ILE:CD1	2.18	0.73
1:A:855:LEU:C	1:A:857:LEU:H	1.94	0.73
2:C:345:LYS:HA	2:C:348:ASP:HB2	1.68	0.73
2:E:299:GLN:HA	2:E:302:MET:HE2	1.68	0.73
1:A:350:ARG:NH2	1:A:386:ARG:HH22	1.87	0.72
1:A:79:VAL:HG22	1:A:80:LYS:H	1.53	0.72
2:C:526:VAL:HG11	2:C:544:MET:HG3	1.71	0.72
2:E:847:GLN:HB3	2:E:889:ARG:HD2	1.72	0.71
1:A:982:ARG:NH2	1:A:1018:PRO:HB3	2.04	0.71
1:A:720:ALA:HA	1:A:727:LEU:HD11	1.73	0.71
1:A:221:GLU:HG2	1:A:234:TYR:CE2	2.26	0.70
1:B:621:ASN:HD22	1:B:623:ILE:H	1.36	0.70
1:A:545:GLN:HE21	1:A:545:GLN:HA	1.56	0.70
1:A:423:THR:CG2	1:A:424:PRO:HD2	2.21	0.70
1:A:245:ALA:HB1	1:A:248:ARG:HB2	1.73	0.69
1:A:1192:SER:HB2	1:A:1193:PRO:HD2	1.73	0.69
1:A:690:ILE:HG21	1:A:726:SER:HB3	1.73	0.69
2:E:530:ILE:HA	2:E:534:PHE:HB2	1.74	0.69
1:B:299:ASN:HA	1:B:379:LEU:CD2	2.23	0.69
1:A:381:SER:HA	1:A:384:LYS:HE3	1.74	0.68
2:E:762:PHE:HB3	2:E:766:GLU:HG3	1.76	0.68
1:A:298:ILE:HG23	1:A:353:ALA:HB1	1.75	0.68
1:A:903:PRO:HA	1:A:906:GLN:HB2	1.76	0.68
2:C:467:GLU:HB3	2:C:469:ARG:HG2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:831:THR:H	1:A:834:ILE:HD12	1.59	0.67
1:B:385:GLU:O	1:B:386:ARG:HB2	1.93	0.67
2:C:530:ILE:HD13	2:C:541:ILE:HB	1.75	0.67
2:C:747:LEU:HA	2:C:750:THR:HG22	1.75	0.67
1:B:1068:MET:HB3	2:C:227:ILE:HG22	1.76	0.67
1:A:1143:ASP:HA	1:A:1194:LEU:HD21	1.77	0.67
1:B:942:CYS:HB3	1:B:948:ARG:HD3	1.77	0.67
2:C:604:GLU:HB3	2:C:641:PHE:CZ	2.30	0.67
1:B:372:TYR:HA	1:B:376:SER:HB3	1.77	0.66
2:C:471:GLN:HE21	2:C:471:GLN:HA	1.60	0.66
2:C:817:LYS:HG3	2:C:818:LEU:H	1.59	0.66
1:A:144:LYS:H	1:A:144:LYS:HD2	1.60	0.66
1:A:1113:LEU:HD12	1:A:1148:PRO:HB2	1.76	0.66
2:C:604:GLU:HG3	2:C:605:ALA:N	2.09	0.66
1:B:302:LEU:HD12	1:B:379:LEU:HG	1.76	0.66
2:C:506:VAL:HA	2:C:515:MET:HE2	1.77	0.66
1:A:192:ARG:HB3	1:A:233:THR:HG21	1.75	0.66
1:B:380:ILE:HG22	1:B:394:VAL:HG13	1.78	0.66
2:C:340:GLN:CB	2:C:342:VAL:HB	2.26	0.66
1:A:110:LEU:HD23	1:A:157:ILE:HD13	1.78	0.66
2:C:340:GLN:HB2	2:C:342:VAL:HB	1.79	0.65
1:A:511:GLN:HA	1:A:514:HIS:CD2	2.31	0.65
1:B:926:LYS:HB3	1:B:927:PRO:HD3	1.79	0.65
2:C:879:PHE:HB2	2:C:880:PRO:HD2	1.77	0.65
1:B:193:LYS:HE3	2:C:581:GLU:HG2	1.78	0.65
1:B:903:PRO:HA	1:B:906:GLN:HB2	1.78	0.65
1:A:862:LEU:HB3	1:A:905:ARG:NH2	2.12	0.65
2:C:424:GLU:HG2	2:C:444:VAL:HG21	1.79	0.65
2:C:796:ASN:CB	2:C:797:PRO:HD3	2.27	0.65
1:B:386:ARG:HG3	1:B:386:ARG:HH11	1.62	0.64
2:C:730:CYS:HB3	3:D:27:TRP:HD1	1.62	0.64
2:E:415:HIS:O	2:E:419:LYS:HG2	1.97	0.64
2:C:280:LEU:CD1	2:C:281:ASP:H	2.09	0.64
3:D:72:TRP:HB2	3:D:105:LYS:CB	2.25	0.64
1:B:553:LEU:HB3	1:B:639:PRO:HG2	1.78	0.64
2:E:911:TYR:O	2:E:912:ILE:HG13	1.96	0.64
2:E:397:TYR:CE1	2:E:420:ARG:HD2	2.33	0.64
1:A:855:LEU:C	1:A:857:LEU:N	2.54	0.64
2:C:227:ILE:CD1	2:C:303:ILE:HG13	2.25	0.64
2:E:599:GLY:H	2:E:878:LYS:HG2	1.63	0.63
2:C:357:GLU:HB2	2:C:363:ILE:HD12	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:905:ASN:HB2	2:C:907:ASN:HD22	1.64	0.63
1:A:625:ARG:HG2	1:A:626:LEU:N	2.13	0.63
2:C:235:TYR:HD1	2:C:235:TYR:H	1.47	0.63
2:E:363:ILE:H	2:E:363:ILE:CD1	2.11	0.63
1:B:242:SER:HB3	1:B:281:SER:HB3	1.80	0.63
2:C:902:ASP:CG	2:C:903:LYS:H	2.07	0.63
1:B:298:ILE:HG23	1:B:353:ALA:HB1	1.80	0.63
2:C:858:MET:HE1	2:C:864:LEU:HB3	1.80	0.63
1:B:97:SER:HB2	1:B:103:ARG:HB2	1.79	0.62
1:A:952:VAL:HG11	1:A:987:THR:HB	1.81	0.62
1:B:1187:PRO:O	1:B:1188:GLU:HB3	1.99	0.62
2:C:503:SER:HB3	2:C:507:ILE:HD12	1.82	0.62
1:A:383:PHE:CE2	1:A:386:ARG:HD2	2.32	0.62
1:A:304:TYR:H	1:A:350:ARG:HD2	1.64	0.62
1:A:547:VAL:HG21	1:A:596:ILE:HG12	1.80	0.62
1:A:1178:ARG:NH1	2:E:429:ILE:HG13	2.15	0.61
1:B:386:ARG:HG2	1:B:390:VAL:HB	1.82	0.61
1:A:4:ALA:HB3	1:A:7:HIS:HB3	1.81	0.61
2:C:597:ILE:O	2:C:600:LYS:HE3	2.01	0.61
2:C:276:ARG:HE	2:C:340:GLN:NE2	1.98	0.60
2:E:405:MET:HE3	2:E:405:MET:HA	1.83	0.60
1:A:870:GLU:HA	1:A:873:LYS:HE2	1.82	0.60
1:A:528:VAL:O	1:A:536:THR:HG23	2.00	0.60
2:E:501:PHE:O	2:E:504:THR:HG22	2.01	0.60
1:A:970:LEU:HB3	1:A:985:VAL:HG23	1.84	0.60
1:B:361:VAL:HA	1:B:371:PHE:CE2	2.36	0.60
1:B:465:LEU:HB2	1:B:468:ALA:HB2	1.84	0.60
1:B:42:ASP:HB2	1:B:45:SER:H	1.66	0.60
2:C:380:ILE:HG23	2:C:384:SER:HB2	1.82	0.60
2:C:450:GLY:HA2	2:C:453:LEU:CD2	2.31	0.60
2:C:485:GLY:O	2:C:489:VAL:HG23	2.01	0.60
1:A:590:ILE:HD13	1:A:628:THR:HG22	1.83	0.60
1:B:982:ARG:HH21	1:B:1018:PRO:HB3	1.64	0.60
2:C:897:ASP:O	2:C:912:ILE:HD11	2.02	0.60
1:B:283:VAL:O	1:B:363:THR:HG21	2.02	0.60
1:B:299:ASN:HA	1:B:379:LEU:HD22	1.83	0.59
1:B:1138:VAL:HG11	1:B:1183:LEU:HD12	1.84	0.59
2:C:816:HIS:HD2	2:C:818:LEU:O	1.85	0.59
1:A:304:TYR:HB3	1:A:350:ARG:HH11	1.66	0.59
1:B:504:ILE:O	1:B:508:HIS:HD2	1.84	0.59
1:A:15:MET:HG2	1:A:56:LEU:HD11	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:280:LEU:HD23	2:C:345:LYS:HD3	1.83	0.59
1:A:270:GLU:HG3	1:A:274:TYR:HE2	1.67	0.59
1:B:963:PRO:O	1:B:967:LEU:HB2	2.02	0.59
1:B:386:ARG:HG3	1:B:386:ARG:NH1	2.16	0.59
1:B:1188:GLU:HG2	1:B:1189:ALA:N	2.17	0.59
1:A:952:VAL:CG1	1:A:987:THR:HB	2.33	0.58
1:B:1129:ARG:HG3	1:B:1129:ARG:NH1	2.14	0.58
2:C:303:ILE:HG21	2:C:324:ILE:HG21	1.84	0.58
3:F:75:CYS:HB2	3:F:99:ARG:HH11	1.68	0.58
1:A:892:LEU:HD21	1:A:932:ILE:HD11	1.84	0.58
2:C:332:PHE:HD2	2:C:378:LEU:HD11	1.67	0.58
1:A:546:LEU:O	1:A:550:ILE:HD12	2.02	0.58
1:B:469:LEU:H	1:B:508:HIS:HE1	1.51	0.58
1:B:474:PRO:HA	1:B:516:HIS:CE1	2.39	0.58
1:B:196:ILE:HG12	1:B:237:CYS:HB2	1.85	0.58
2:E:604:GLU:HB2	2:E:641:PHE:CE2	2.38	0.58
1:B:996:HIS:HB2	1:B:997:PRO:CD	2.33	0.58
2:C:427:ARG:HD2	2:C:431:TYR:OH	2.03	0.58
2:E:730:CYS:HB2	3:F:26:LYS:O	2.03	0.58
1:A:492:ASN:HD22	2:E:514:THR:HG21	1.69	0.57
1:A:562:THR:N	1:A:563:PRO:HD2	2.18	0.57
2:C:307:PHE:HB3	2:C:310:LEU:CB	2.35	0.57
2:E:467:GLU:HG2	2:E:469:ARG:HE	1.69	0.57
1:B:645:ARG:N	1:B:646:PRO:HD2	2.19	0.57
1:B:286:CYS:O	1:B:288:LYS:N	2.35	0.57
1:A:896:LEU:HD21	1:A:932:ILE:HD13	1.87	0.57
1:A:350:ARG:HE	1:A:386:ARG:NH1	2.03	0.57
2:E:506:VAL:HA	2:E:515:MET:HE2	1.87	0.57
1:A:458:LEU:O	1:A:462:VAL:HG23	2.05	0.57
1:B:347:TRP:HA	1:B:350:ARG:CZ	2.34	0.57
1:A:1115:ASP:CG	1:A:1116:HIS:H	2.13	0.57
2:C:494:TRP:HE1	2:C:529:ILE:HD11	1.70	0.57
1:A:297:ILE:O	1:A:297:ILE:HG22	2.04	0.57
1:A:1101:ASP:OD2	1:A:1104:GLU:HB2	2.04	0.56
2:E:519:LEU:HD21	2:E:552:ILE:HD11	1.85	0.56
1:B:299:ASN:HA	1:B:379:LEU:HD21	1.87	0.56
2:C:604:GLU:HB3	2:C:641:PHE:CE2	2.40	0.56
2:C:671:VAL:HG22	2:C:673:GLY:O	2.06	0.56
2:E:734:ALA:HB3	2:E:741:LYS:O	2.04	0.56
1:B:14:LYS:HA	1:B:17:SER:HB2	1.87	0.56
1:A:368:LEU:N	1:A:369:PRO:HD2	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:PHE:HE2	1:B:386:ARG:HE	1.53	0.56
2:E:771:THR:HG23	2:E:773:ILE:HG12	1.86	0.56
1:A:173:HIS:HB2	1:A:174:PRO:HD3	1.86	0.56
1:A:373:LYS:HE3	1:A:428:LEU:HB2	1.88	0.56
2:E:658:ILE:HG21	2:E:716:HIS:HE1	1.71	0.56
1:A:703:GLU:OE1	1:A:746:LEU:HD21	2.05	0.56
1:B:298:ILE:HD11	1:B:356:CYS:HB3	1.87	0.56
1:B:821:PHE:HA	1:B:824:ASP:HB3	1.86	0.56
2:C:309:PHE:HA	2:C:312:ARG:HB2	1.87	0.56
2:C:329:LEU:HD13	2:C:378:LEU:HD22	1.88	0.56
1:A:1097:LEU:HA	1:A:1100:LEU:HD12	1.88	0.56
2:C:358:ARG:NE	2:C:427:ARG:HH12	2.03	0.56
2:C:858:MET:CE	2:C:864:LEU:HB3	2.35	0.56
2:C:741:LYS:HB2	2:C:819:PHE:O	2.06	0.56
1:B:238:ILE:HD11	1:B:256:ILE:HD12	1.86	0.56
1:A:565:ILE:HG12	1:A:600:LEU:HD13	1.88	0.55
1:A:579:ALA:HB2	1:A:618:ARG:NH2	2.21	0.55
1:B:504:ILE:HG22	1:B:513:PHE:HZ	1.71	0.55
2:C:558:LYS:N	2:C:559:PRO:HD2	2.21	0.55
1:B:298:ILE:HG21	1:B:357:LEU:HG	1.88	0.55
1:A:551:ARG:N	1:A:552:PRO:HD2	2.22	0.55
2:E:446:LYS:HG3	2:E:484:ARG:HH22	1.71	0.55
1:B:350:ARG:HH21	1:B:386:ARG:HH12	1.55	0.55
1:B:913:LEU:HA	1:B:916:ILE:HD12	1.88	0.55
2:E:734:ALA:HB1	2:E:736:PHE:CE2	2.42	0.55
1:A:12:LEU:HD11	1:A:49:VAL:HG22	1.89	0.55
1:B:79:VAL:HG22	1:B:80:LYS:H	1.72	0.55
1:B:39:ILE:HD13	1:B:40:LYS:HG2	1.87	0.55
1:B:982:ARG:HA	1:B:985:VAL:HG12	1.88	0.55
1:A:645:ARG:N	1:A:646:PRO:HD2	2.22	0.55
1:B:272:ARG:NH1	1:B:301:CYS:SG	2.80	0.55
1:B:644:LEU:HD12	1:B:681:TYR:HE2	1.72	0.55
2:C:338:SER:O	2:C:340:GLN:HG2	2.06	0.55
1:A:111:LYS:O	1:A:114:ILE:HG22	2.07	0.54
2:E:730:CYS:HB3	3:F:27:TRP:HA	1.87	0.54
1:A:279:PHE:HD2	1:A:294:VAL:HG13	1.71	0.54
1:A:1191:LYS:HD2	1:A:1196:SER:HB3	1.90	0.54
1:A:1142:LEU:HD21	1:A:1195:MET:HG3	1.87	0.54
1:B:1183:LEU:O	1:B:1187:PRO:HG3	2.08	0.54
1:B:231:THR:HG21	1:B:263:PHE:HE2	1.72	0.54
2:C:425:ALA:O	2:C:429:ILE:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:505:LEU:HD22	1:A:549:VAL:HG21	1.89	0.54
1:B:148:VAL:HG21	1:B:188:ARG:HD3	1.90	0.54
1:B:165:GLN:HG3	1:B:168:LEU:HD12	1.90	0.54
2:E:659:MET:HE2	2:E:659:MET:HA	1.90	0.54
2:C:460:GLY:O	2:C:464:LEU:HG	2.07	0.54
2:C:796:ASN:HB2	2:C:797:PRO:HD3	1.88	0.54
1:A:481:ILE:HG23	1:A:523:PRO:HG3	1.89	0.54
1:B:375:VAL:O	1:B:380:ILE:HD11	2.08	0.54
2:C:333:ARG:O	2:C:338:SER:HB2	2.08	0.54
2:C:351:LEU:HD21	2:C:389:PHE:HA	1.89	0.54
1:B:225:ASN:H	1:B:225:ASN:HD22	1.56	0.54
1:A:756:LEU:HD22	1:A:802:CYS:HA	1.90	0.53
1:B:604:LEU:HD22	1:B:608:LEU:HB2	1.90	0.53
1:B:870:GLU:HA	1:B:873:LYS:HE3	1.89	0.53
2:E:340:GLN:NE2	2:E:342:VAL:HG22	2.23	0.53
1:A:1157:VAL:HG23	1:A:1158:LYS:HE3	1.90	0.53
1:B:298:ILE:CD1	1:B:356:CYS:HB3	2.39	0.53
2:C:856:ARG:HH11	2:C:876:GLN:NE2	2.07	0.53
1:A:19:ASP:HB3	1:A:22:PHE:HB2	1.91	0.53
1:B:8:ILE:HD13	1:B:45:SER:HB3	1.90	0.53
2:E:665:TYR:HD2	2:E:666:MET:SD	2.31	0.53
2:E:677:LEU:HD13	3:F:27:TRP:CE3	2.43	0.53
1:B:710:GLN:HB2	1:B:751:ALA:HA	1.90	0.53
1:B:810:CYS:HB3	1:B:812:LYS:HG2	1.91	0.53
2:E:767:ILE:O	2:E:771:THR:HG22	2.09	0.53
2:E:789:LYS:HB2	2:E:791:ARG:HH12	1.73	0.53
1:A:263:PHE:HB3	1:A:271:LEU:HD21	1.90	0.53
1:B:816:ALA:O	1:B:820:GLN:HB2	2.09	0.53
1:B:888:LEU:N	1:B:889:PRO:HD2	2.23	0.53
2:C:767:ILE:O	2:C:771:THR:HG22	2.09	0.53
2:E:600:LYS:HG3	2:E:878:LYS:HG3	1.91	0.53
1:A:67:LEU:O	1:A:71:CYS:HB2	2.08	0.53
1:A:1174:ARG:O	1:A:1178:ARG:HB2	2.09	0.53
1:B:376:SER:CA	1:B:380:ILE:HD11	2.38	0.53
1:B:149:SER:HA	1:B:152:LEU:HB2	1.91	0.53
1:B:148:VAL:HG12	1:B:149:SER:N	2.24	0.52
2:C:348:ASP:OD1	2:C:388:ARG:NH2	2.42	0.52
1:A:855:LEU:HD11	1:A:858:LYS:HE3	1.91	0.52
1:B:4:ALA:C	1:B:40:LYS:HG3	2.34	0.52
2:E:428:LEU:HD11	2:E:437:GLN:HB2	1.92	0.52
1:B:271:LEU:O	1:B:275:CYS:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:501:PHE:O	2:C:504:THR:HB	2.10	0.52
2:E:854:ILE:HG21	2:E:899:MET:HE1	1.91	0.52
1:B:432:VAL:HA	1:B:435:ILE:HG22	1.91	0.52
1:B:1186:ILE:N	1:B:1187:PRO:HD2	2.24	0.52
2:E:704:LEU:HA	2:E:707:ILE:HG22	1.91	0.52
1:A:1056:THR:HG23	1:A:1086:PHE:CE1	2.45	0.52
1:B:395:PHE:HD1	1:B:457:MET:HE2	1.74	0.52
1:B:640:LEU:O	1:B:642:ILE:HG13	2.09	0.52
1:B:1147:GLU:HB3	1:B:1148:PRO:HD3	1.91	0.52
1:A:1068:MET:HA	2:E:230:SER:HA	1.92	0.52
2:E:271:GLN:HB3	2:E:336:ILE:HD11	1.91	0.52
3:F:83:CYS:HA	3:F:86:ARG:HD2	1.92	0.52
1:A:381:SER:O	1:A:384:LYS:HB2	2.09	0.51
1:B:1138:VAL:CG1	1:B:1183:LEU:HD12	2.39	0.51
1:B:898:GLU:HB3	1:B:909:LEU:HD13	1.92	0.51
2:C:307:PHE:HD2	2:C:310:LEU:HD22	1.75	0.51
1:A:550:ILE:C	1:A:552:PRO:HD2	2.34	0.51
1:B:386:ARG:CG	1:B:387:GLU:H	2.07	0.51
2:E:341:LYS:H	2:E:341:LYS:HD2	1.75	0.51
2:C:572:ARG:O	2:C:621:ALA:HB2	2.10	0.51
1:A:625:ARG:HG2	1:A:626:LEU:H	1.74	0.51
1:B:1162:VAL:HG11	2:C:325:TRP:CG	2.45	0.51
2:E:311:ASP:O	2:E:316:LEU:HB2	2.10	0.51
1:A:206:CYS:SG	1:A:210:VAL:HG12	2.51	0.51
1:B:912:SER:O	1:B:916:ILE:HG13	2.10	0.51
2:E:450:GLY:O	2:E:451:GLU:HB2	2.10	0.51
1:B:370:GLU:O	1:B:374:THR:HG22	2.11	0.51
2:E:864:LEU:HD23	2:E:869:LEU:HD12	1.92	0.51
1:B:225:ASN:HD22	1:B:225:ASN:N	2.06	0.51
2:C:671:VAL:O	2:C:671:VAL:HG13	2.11	0.50
1:B:552:PRO:C	1:B:554:ASP:H	2.19	0.50
1:B:368:LEU:HD11	1:B:405:THR:HG23	1.91	0.50
2:C:905:ASN:C	2:C:907:ASN:H	2.20	0.50
2:E:340:GLN:HG2	2:E:341:LYS:CD	2.42	0.50
1:A:253:LEU:HD21	1:A:289:GLU:HB2	1.93	0.50
2:E:494:TRP:CH2	2:E:530:ILE:HG21	2.46	0.50
2:C:831:THR:OG1	2:C:834:GLU:HB2	2.12	0.50
2:E:216:THR:HA	2:E:219:LYS:HB2	1.93	0.50
1:B:38:SER:OG	1:B:39:ILE:N	2.44	0.50
1:B:605:GLY:C	1:B:607:ASP:H	2.19	0.50
1:A:257:ILE:N	1:A:258:PRO:HD2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLU:HG3	1:A:274:TYR:CE2	2.45	0.50
1:A:286:CYS:C	1:A:288:LYS:H	2.20	0.50
1:B:35:GLN:O	1:B:36:LYS:HG2	2.12	0.50
1:B:996:HIS:HB2	1:B:997:PRO:HD2	1.92	0.50
1:A:1152:THR:HG23	1:A:1172:LEU:HD13	1.94	0.49
2:C:637:CYS:HB3	2:C:641:PHE:HB3	1.93	0.49
2:E:380:ILE:HG22	2:E:384:SER:HB2	1.94	0.49
1:A:19:ASP:HB3	1:A:22:PHE:HD2	1.77	0.49
1:A:609:PRO:HA	1:A:612:LEU:HD12	1.94	0.49
1:B:38:SER:O	1:B:39:ILE:HB	2.11	0.49
1:B:625:ARG:HG3	1:B:658:PHE:CE1	2.47	0.49
1:B:716:LEU:HB3	1:B:758:PHE:CE1	2.47	0.49
2:E:598:TYR:HD1	2:E:878:LYS:O	1.95	0.49
1:A:360:VAL:HG12	1:A:372:TYR:OH	2.12	0.49
1:A:272:ARG:NH2	1:A:301:CYS:SG	2.83	0.49
2:C:538:GLU:O	2:C:542:ASN:HB2	2.13	0.49
2:E:886:LEU:O	2:E:890:ILE:HG12	2.12	0.49
1:B:304:TYR:O	1:B:350:ARG:HD2	2.13	0.49
2:C:298:ARG:HA	2:C:301:ILE:HB	1.94	0.49
1:A:645:ARG:N	1:A:646:PRO:CD	2.76	0.49
1:A:648:LEU:HD21	1:A:677:LEU:HD22	1.95	0.49
2:E:340:GLN:O	2:E:342:VAL:N	2.45	0.49
2:E:761:GLU:HB3	2:E:809:ILE:HG22	1.94	0.49
2:E:796:ASN:HB2	2:E:797:PRO:HD3	1.94	0.49
2:C:633:LEU:O	2:C:637:CYS:HB2	2.13	0.49
2:E:233:ILE:HD13	2:E:233:ILE:H	1.78	0.49
1:A:169:LEU:HB3	1:A:172:PHE:HB2	1.94	0.49
1:A:350:ARG:HE	1:A:386:ARG:CZ	2.25	0.49
1:A:1158:LYS:H	1:A:1158:LYS:CD	2.26	0.49
2:C:516:VAL:HG13	2:C:563:ILE:HD13	1.93	0.49
2:E:345:LYS:HA	2:E:348:ASP:HB2	1.94	0.49
2:E:557:ASN:ND2	2:E:843:PHE:HZ	2.10	0.49
2:E:681:ILE:HD11	2:E:721:LEU:HD22	1.95	0.49
1:B:528:VAL:O	1:B:536:THR:HG23	2.13	0.49
1:B:946:GLY:O	1:B:950:VAL:HG23	2.12	0.49
2:C:742:GLU:HG3	2:C:820:ARG:HB3	1.94	0.49
2:C:351:LEU:O	2:C:355:GLU:HB2	2.13	0.49
2:C:798:LYS:HG2	2:C:799:GLY:H	1.77	0.49
2:C:841:ARG:O	2:C:845:ASP:HB2	2.13	0.49
3:F:37:ILE:O	3:F:38:VAL:C	2.56	0.49
1:B:180:LEU:HD22	1:B:195:THR:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:591:MET:HA	2:E:591:MET:HE2	1.95	0.48
1:A:260:VAL:HB	1:A:279:PHE:HE1	1.78	0.48
1:A:465:LEU:HD22	1:A:468:ALA:HB2	1.95	0.48
1:A:142:ILE:HD12	1:A:155:LEU:HG	1.94	0.48
1:A:522:PRO:HB2	1:A:523:PRO:HD3	1.96	0.48
1:A:913:LEU:O	1:A:917:ILE:HG12	2.12	0.48
1:B:285:ARG:C	1:B:287:PRO:HD3	2.38	0.48
1:B:375:VAL:C	1:B:380:ILE:HD11	2.38	0.48
2:C:307:PHE:N	2:C:307:PHE:CD1	2.81	0.48
2:C:698:PRO:HD3	2:C:751:LEU:HD21	1.95	0.48
1:A:1038:PRO:C	1:A:1040:LEU:H	2.21	0.48
1:A:643:ASP:OD1	1:A:645:ARG:HG2	2.13	0.48
1:A:1056:THR:HG21	1:A:1108:HIS:HB3	1.95	0.48
1:B:432:VAL:N	1:B:433:PRO:HD2	2.28	0.48
2:C:381:TYR:C	2:C:383:ASP:H	2.21	0.48
2:E:582:GLU:O	2:E:586:MET:HG2	2.14	0.48
1:B:459:THR:HG23	1:B:503:VAL:HG21	1.96	0.48
1:B:648:LEU:HD21	1:B:677:LEU:HD22	1.95	0.48
2:E:300:MET:C	2:E:302:MET:H	2.22	0.48
1:A:149:SER:HA	1:A:152:LEU:HB2	1.96	0.48
1:B:720:ALA:HB2	1:B:727:LEU:HD21	1.95	0.48
2:E:781:THR:HG22	2:E:826:ILE:HD13	1.94	0.48
1:A:854:GLN:CD	1:A:854:GLN:H	2.21	0.48
1:A:1086:PHE:CZ	1:A:1112:GLY:HA3	2.48	0.48
2:E:340:GLN:HE22	2:E:342:VAL:HG22	1.79	0.48
3:F:73:GLY:HA3	3:F:101:TRP:CH2	2.49	0.48
1:A:659:LEU:HD22	1:A:700:LEU:HD11	1.96	0.48
1:A:727:LEU:C	1:A:729:LYS:H	2.22	0.48
1:A:855:LEU:CD1	1:A:858:LYS:HE3	2.44	0.48
1:B:543:THR:HG23	1:B:568:LEU:HD22	1.94	0.48
1:A:62:GLY:O	1:A:65:GLN:HB2	2.14	0.47
1:A:547:VAL:HG11	1:A:596:ILE:HA	1.94	0.47
1:A:913:LEU:HA	1:A:916:ILE:HD12	1.95	0.47
1:B:423:THR:HG23	1:B:426:THR:HG23	1.97	0.47
1:B:467:GLY:HA2	1:B:508:HIS:CE1	2.49	0.47
1:B:778:MET:HE2	1:B:778:MET:HA	1.95	0.47
2:E:622:SER:HB3	2:E:625:ALA:HB2	1.96	0.47
1:A:24:PHE:HE1	2:E:876:GLN:HE21	1.61	0.47
1:A:406:ARG:HG3	1:A:407:PRO:HD2	1.96	0.47
1:B:350:ARG:HE	1:B:386:ARG:NH1	2.12	0.47
1:B:380:ILE:HD12	1:B:380:ILE:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:850:ASP:OD1	1:B:852:SER:HB2	2.14	0.47
2:C:622:SER:HB3	2:C:625:ALA:HB3	1.96	0.47
2:C:340:GLN:HB3	2:C:342:VAL:H	1.80	0.47
2:E:468:ASN:C	2:E:468:ASN:HD22	2.21	0.47
1:A:350:ARG:HE	1:A:386:ARG:NH2	2.13	0.47
1:B:347:TRP:HA	1:B:350:ARG:NE	2.29	0.47
2:C:450:GLY:HA2	2:C:453:LEU:HD22	1.95	0.47
2:C:836:ALA:O	2:C:840:GLU:HB2	2.14	0.47
1:A:1112:GLY:HA2	1:A:1115:ASP:HB2	1.95	0.47
1:B:928:TYR:O	1:B:932:ILE:HG12	2.14	0.47
2:C:674:ASN:OD1	2:C:674:ASN:N	2.47	0.47
3:D:94:CYS:HB2	3:D:101:TRP:HB2	1.96	0.47
1:B:376:SER:HA	1:B:380:ILE:HD13	1.95	0.47
1:B:386:ARG:HH11	1:B:386:ARG:CG	2.27	0.47
2:C:505:ILE:HA	2:C:511:LYS:HD2	1.96	0.47
1:A:644:LEU:C	1:A:646:PRO:HD2	2.40	0.47
1:B:388:GLU:O	1:B:391:LYS:HB3	2.15	0.47
1:A:948:ARG:O	1:A:952:VAL:HG23	2.14	0.47
2:E:509:PRO:C	2:E:511:LYS:H	2.22	0.47
1:A:69:VAL:HG11	1:A:108:ILE:HG22	1.96	0.46
1:B:685:LEU:HD22	1:B:690:ILE:HD11	1.97	0.46
2:C:648:MET:HG2	2:C:687:TRP:CE2	2.50	0.46
1:A:596:ILE:HG23	1:A:600:LEU:HD12	1.97	0.46
1:B:1129:ARG:C	1:B:1131:SER:H	2.23	0.46
2:C:428:LEU:HD21	2:C:436:THR:HB	1.97	0.46
2:E:892:SER:O	2:E:896:ARG:HD3	2.14	0.46
1:B:32:THR:HA	1:B:35:GLN:HE22	1.81	0.46
2:C:350:ILE:HG23	2:C:368:LEU:HD22	1.97	0.46
2:C:838:THR:O	2:C:842:VAL:HG23	2.15	0.46
2:E:411:PRO:HG3	2:E:464:LEU:HD21	1.97	0.46
1:A:987:THR:OG1	1:A:1025:VAL:HG11	2.15	0.46
1:B:813:GLU:OE1	1:B:813:GLU:HA	2.15	0.46
1:B:1180:VAL:O	1:B:1183:LEU:HD23	2.15	0.46
2:C:748:PHE:CD2	2:C:773:ILE:HD12	2.50	0.46
1:A:813:GLU:O	1:A:817:VAL:HG23	2.15	0.46
1:A:838:ALA:O	1:A:842:LEU:HG	2.16	0.46
1:B:617:GLU:HA	1:B:620:LYS:HD2	1.96	0.46
1:B:54:LEU:HA	1:B:57:LEU:HD13	1.98	0.46
1:A:817:VAL:HG12	1:A:821:PHE:CE2	2.51	0.46
1:B:1053:TYR:O	1:B:1056:THR:HG23	2.15	0.46
1:A:357:LEU:O	1:A:361:VAL:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1056:THR:HA	1:B:1082:ARG:HG3	1.98	0.46
2:C:530:ILE:HG13	2:C:531:ASP:N	2.30	0.46
2:E:720:LYS:HB3	3:F:36:ASP:HB2	1.98	0.46
1:B:857:LEU:HD12	1:B:858:LYS:N	2.31	0.46
1:B:1038:PRO:C	1:B:1040:LEU:H	2.24	0.46
1:A:346:SER:HB2	1:A:350:ARG:HH12	1.80	0.46
1:A:633:THR:HA	1:A:676:ILE:HD11	1.97	0.46
1:A:887:ASN:ND2	1:A:890:GLU:HG3	2.30	0.46
1:B:138:LEU:O	1:B:142:ILE:HG13	2.15	0.46
1:B:209:ILE:O	1:B:212:VAL:HG12	2.16	0.46
1:B:499:SER:O	1:B:503:VAL:HG23	2.15	0.46
1:B:529:GLY:HA2	1:B:575:ARG:HH21	1.81	0.46
2:E:340:GLN:HG2	2:E:341:LYS:HD2	1.97	0.46
2:E:698:PRO:O	2:E:700:GLU:N	2.48	0.46
1:A:914:LYS:O	1:A:918:SER:HB2	2.16	0.45
1:B:35:GLN:O	1:B:36:LYS:CG	2.64	0.45
1:B:456:ASN:ND2	1:B:496:ASP:OD1	2.46	0.45
1:B:828:SER:O	1:B:829:ARG:HB2	2.16	0.45
1:B:831:THR:HG22	1:B:832:ASP:H	1.80	0.45
1:B:929:VAL:HG13	1:B:958:LEU:HD22	1.98	0.45
2:C:303:ILE:CG2	2:C:324:ILE:HG21	2.45	0.45
2:E:911:TYR:CE2	2:E:913:ALA:HB2	2.50	0.45
1:A:854:GLN:H	1:A:854:GLN:NE2	2.13	0.45
1:A:957:LYS:HA	1:A:960:LEU:HD23	1.98	0.45
1:B:386:ARG:HG3	1:B:387:GLU:N	2.14	0.45
1:B:15:MET:HE3	1:B:52:MET:HG2	1.99	0.45
2:C:272:ILE:C	2:C:274:GLN:H	2.24	0.45
2:E:491:LEU:HG	2:E:540:PHE:CZ	2.51	0.45
1:A:24:PHE:HE2	1:A:63:GLU:HB3	1.80	0.45
1:A:253:LEU:HD13	1:A:254:GLU:N	2.31	0.45
1:A:926:LYS:N	1:A:927:PRO:HD2	2.31	0.45
1:B:199:LEU:O	1:B:203:VAL:HG23	2.15	0.45
2:C:465:LEU:HB3	2:C:497:TYR:CZ	2.51	0.45
2:E:580:ASP:HA	2:E:583:LEU:HB3	1.99	0.45
2:E:847:GLN:HE22	2:E:885:ASP:HB3	1.80	0.45
2:C:630:LEU:HD23	2:C:630:LEU:HA	1.81	0.45
2:C:654:LEU:HA	2:C:657:ASP:HB2	1.97	0.45
2:C:795:LYS:HE2	2:C:802:ILE:HG12	1.98	0.45
1:A:804:ALA:HB2	1:A:844:GLU:HB3	1.99	0.45
2:C:756:PHE:HB3	3:D:21:ARG:HD2	1.98	0.45
1:A:768:ASN:O	1:A:769:ASN:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:LEU:HA	1:B:658:PHE:HD2	1.82	0.45
2:E:428:LEU:HD23	2:E:440:LEU:HD23	1.99	0.45
2:E:558:LYS:N	2:E:559:PRO:HD2	2.32	0.45
3:F:77:HIS:CD2	3:F:96:LEU:HD13	2.52	0.45
1:A:561:ALA:C	1:A:563:PRO:HD2	2.41	0.45
1:B:380:ILE:HD12	1:B:380:ILE:N	2.32	0.45
1:A:1041:ILE:HD13	1:A:1041:ILE:HA	1.85	0.45
1:A:432:VAL:HA	1:A:435:ILE:HD12	1.98	0.45
1:B:970:LEU:C	1:B:972:GLY:H	2.24	0.45
1:A:1012:LEU:HD11	1:A:1030:PHE:HB2	1.98	0.44
1:B:993:ILE:H	1:B:993:ILE:HG13	1.64	0.44
3:D:37:ILE:O	3:D:37:ILE:HG22	2.16	0.44
2:E:854:ILE:HD13	2:E:890:ILE:HD13	2.00	0.44
2:C:235:TYR:O	2:C:236:ASN:CB	2.65	0.44
2:E:275:PHE:CE2	2:E:289:ILE:HD13	2.53	0.44
3:F:88:LEU:HD21	3:F:101:TRP:HD1	1.82	0.44
1:A:428:LEU:HD23	1:A:465:LEU:HD12	1.99	0.44
1:A:500:CYS:O	1:A:504:ILE:HG13	2.17	0.44
1:B:253:LEU:HA	1:B:256:ILE:HG13	2.00	0.44
2:E:514:THR:O	2:E:515:MET:C	2.60	0.44
1:B:885:VAL:HG13	1:B:920:ALA:HA	1.99	0.44
2:C:667:GLN:HE21	2:C:667:GLN:HB3	1.61	0.44
2:E:391:GLU:HG2	2:E:395:ARG:HH22	1.81	0.44
2:E:719:ARG:HD3	3:F:33:TRP:CE3	2.53	0.44
1:A:466:PRO:HB3	1:A:507:ASN:HD22	1.83	0.44
1:B:146:GLU:H	1:B:146:GLU:HG2	1.57	0.44
1:B:1001:ASP:HA	1:B:1004:LEU:HB2	1.99	0.44
1:B:1188:GLU:CG	1:B:1189:ALA:N	2.80	0.44
2:C:559:PRO:O	2:C:563:ILE:HG12	2.17	0.44
2:C:560:ALA:HB2	2:C:597:ILE:HG21	1.99	0.44
2:E:743:LEU:HD22	2:E:823:ILE:HD11	2.00	0.44
1:A:742:VAL:HA	1:A:747:LEU:HD22	2.00	0.44
1:A:697:LEU:N	1:A:698:PRO:CD	2.81	0.44
1:B:231:THR:HG21	1:B:263:PHE:CE2	2.52	0.44
2:C:404:LEU:HD22	2:C:408:ARG:HE	1.83	0.44
2:C:730:CYS:HB2	3:D:26:LYS:O	2.18	0.44
2:C:757:ASN:HD22	3:D:20:LYS:HD2	1.83	0.44
2:E:507:ILE:HD11	2:E:554:LYS:HB3	2.00	0.44
2:E:861:ARG:NH1	2:E:872:GLU:OE2	2.50	0.44
1:A:350:ARG:HH21	1:A:386:ARG:NH2	2.04	0.44
1:A:368:LEU:HD11	1:A:405:THR:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:ARG:NE	1:A:553:LEU:HB2	2.33	0.44
1:B:381:SER:HA	1:B:384:LYS:HE2	1.99	0.44
1:B:386:ARG:CG	1:B:387:GLU:N	2.78	0.44
1:A:1037:LYS:HB3	1:A:1040:LEU:HD12	1.99	0.44
2:C:227:ILE:HD11	2:C:303:ILE:CG1	2.37	0.44
2:E:859:LYS:HB3	2:E:859:LYS:HE3	1.80	0.44
1:A:364:ARG:HE	1:A:364:ARG:HA	1.83	0.43
1:A:368:LEU:HD11	1:A:405:THR:CG2	2.48	0.43
1:A:855:LEU:HG	1:A:855:LEU:O	2.17	0.43
1:B:231:THR:HA	1:B:234:TYR:HB2	1.99	0.43
2:E:293:TRP:O	2:E:297:CYS:HB2	2.18	0.43
2:E:622:SER:HB3	2:E:625:ALA:CB	2.48	0.43
1:A:406:ARG:HD2	1:A:464:VAL:HG22	2.00	0.43
1:A:1117:TYR:HE1	1:A:1172:LEU:HB2	1.83	0.43
2:C:338:SER:O	2:C:340:GLN:N	2.51	0.43
1:A:276:ILE:HG21	1:A:353:ALA:CA	2.44	0.43
1:B:730:ILE:HA	1:B:734:ILE:HD12	2.01	0.43
1:B:996:HIS:CB	1:B:997:PRO:CD	2.96	0.43
2:C:332:PHE:CE1	2:C:336:ILE:HD12	2.54	0.43
1:A:543:THR:O	1:A:547:VAL:HG23	2.18	0.43
1:A:685:LEU:HD23	1:A:689:MET:HE2	2.00	0.43
1:B:144:LYS:NZ	1:B:144:LYS:HA	2.34	0.43
2:C:683:THR:HB	2:C:686:TYR:CD1	2.54	0.43
2:C:826:ILE:H	2:C:826:ILE:HG13	1.47	0.43
1:A:144:LYS:H	1:A:144:LYS:CD	2.28	0.43
1:A:962:ASP:HA	1:A:963:PRO:HD3	1.92	0.43
1:B:385:GLU:HA	1:B:391:LYS:HE2	2.00	0.43
2:C:630:LEU:HD21	2:C:645:LEU:HB3	2.01	0.43
1:A:800:ALA:O	1:A:803:VAL:HG12	2.18	0.43
1:B:1057:LYS:HE2	1:B:1108:HIS:HE1	1.83	0.43
1:A:448:VAL:HG13	1:A:493:LEU:HD22	2.01	0.43
1:A:1068:MET:HB2	2:E:227:ILE:HA	1.99	0.43
1:B:731:SER:HB2	1:B:770:LEU:HD11	2.00	0.43
2:C:450:GLY:HA2	2:C:453:LEU:HD21	2.00	0.43
2:C:709:LYS:HD2	2:C:723:TRP:HZ3	1.83	0.43
2:C:763:SER:O	2:C:766:GLU:HG2	2.19	0.43
2:C:860:MET:HA	2:C:860:MET:HE3	2.01	0.43
3:D:52:LEU:HD12	3:D:56:CYS:HB3	2.00	0.43
2:E:227:ILE:HD11	2:E:303:ILE:HG13	2.01	0.43
2:E:426:ASP:O	2:E:429:ILE:HG23	2.18	0.43
1:A:203:VAL:HG11	1:A:241:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:GLN:HG3	1:A:592:CYS:HA	2.01	0.43
1:B:246:GLY:HA3	1:B:285:ARG:HG3	2.01	0.43
3:D:93:VAL:HG12	3:D:100:GLU:HA	2.01	0.43
2:E:741:LYS:HG2	2:E:818:LEU:O	2.19	0.43
1:A:138:LEU:O	1:A:142:ILE:HG12	2.19	0.43
1:A:744:SER:HA	1:A:745:PRO:HD3	1.80	0.43
1:A:839:LEU:HA	1:A:842:LEU:HD12	2.01	0.43
1:B:697:LEU:HA	1:B:700:LEU:HD12	2.00	0.43
2:C:330:GLU:HG3	2:C:333:ARG:NH1	2.33	0.43
2:C:579:THR:HG22	2:C:581:GLU:H	1.84	0.43
1:A:501:LEU:HA	1:A:504:ILE:HD12	2.00	0.42
1:B:686:THR:C	1:B:688:ALA:H	2.27	0.42
2:C:486:GLY:O	2:C:487:VAL:C	2.61	0.42
3:D:47:ASN:O	3:D:48:HIS:HB2	2.18	0.42
1:A:276:ILE:HD13	1:A:353:ALA:HB2	2.01	0.42
1:A:485:ASN:HD22	1:A:523:PRO:HB3	1.84	0.42
1:B:350:ARG:H	1:B:350:ARG:HD3	1.84	0.42
1:B:553:LEU:HD22	1:B:639:PRO:HB2	2.01	0.42
1:B:739:ILE:HA	1:B:742:VAL:HG23	2.01	0.42
2:C:424:GLU:OE1	2:C:424:GLU:HA	2.18	0.42
1:A:491:SER:HA	1:A:535:ILE:HD11	2.01	0.42
1:A:952:VAL:HG12	1:A:952:VAL:O	2.19	0.42
1:A:1121:MET:HE2	1:A:1172:LEU:HD23	2.00	0.42
3:D:84:ILE:HD13	3:D:84:ILE:O	2.19	0.42
2:E:853:ALA:HA	2:E:856:ARG:HG2	2.00	0.42
1:A:350:ARG:HE	1:A:386:ARG:HH12	1.67	0.42
1:B:983:SER:O	1:B:987:THR:OG1	2.34	0.42
1:B:618:ARG:HG3	1:B:624:THR:HG21	2.01	0.42
2:C:729:HIS:HA	2:C:746:SER:HA	2.01	0.42
2:E:311:ASP:HA	2:E:315:VAL:HG23	2.00	0.42
2:E:356:ARG:HD2	2:E:361:GLU:CD	2.44	0.42
2:E:750:THR:O	2:E:754:LEU:HB2	2.19	0.42
1:A:253:LEU:HD13	1:A:254:GLU:H	1.84	0.42
1:A:998:GLN:C	1:A:1000:ILE:H	2.28	0.42
1:B:821:PHE:HB2	1:B:860:VAL:HG11	2.02	0.42
2:E:298:ARG:CZ	2:E:298:ARG:HB3	2.50	0.42
1:A:110:LEU:HD23	1:A:157:ILE:HG21	2.01	0.42
1:A:408:VAL:O	1:A:409:GLN:HB2	2.19	0.42
2:C:228:GLN:HE22	2:C:264:CYS:HA	1.85	0.42
2:C:732:LEU:O	2:C:742:GLU:HB2	2.19	0.42
2:E:453:LEU:HD12	2:E:480:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:606:PHE:CZ	2:E:838:THR:HG23	2.55	0.42
2:E:855:VAL:O	2:E:859:LYS:HB2	2.20	0.42
1:A:898:GLU:HA	1:A:901:SER:HB3	2.02	0.42
1:A:1109:VAL:HG22	1:A:1126:MET:HE2	2.00	0.42
1:B:233:THR:HA	1:B:236:GLN:HE21	1.85	0.42
1:B:484:LEU:HD21	1:B:498:LEU:HG	2.01	0.42
1:B:1131:SER:HB2	1:B:1186:ILE:HD12	2.01	0.42
2:C:796:ASN:CB	2:C:797:PRO:CD	2.97	0.42
2:E:545:LYS:HB3	2:E:545:LYS:HE2	1.82	0.42
2:E:749:GLN:HG2	2:E:785:LEU:HD11	2.00	0.42
1:A:409:GLN:HB2	1:A:409:GLN:HE21	1.70	0.42
1:A:1117:TYR:HD1	1:A:1172:LEU:HG	1.85	0.42
1:B:17:SER:C	1:B:19:ASP:H	2.27	0.42
2:E:691:VAL:HA	2:E:692:PRO:HD3	1.85	0.42
1:A:280:GLU:C	1:A:282:PHE:H	2.28	0.42
1:A:594:GLY:HA2	1:A:635:ILE:HD11	2.02	0.42
1:B:1139:LEU:HD21	1:B:1190:GLU:HB3	2.01	0.42
2:C:296:HIS:NE2	2:C:328:GLY:O	2.51	0.42
2:C:642:THR:HA	2:C:645:LEU:HD12	2.02	0.42
3:D:39:VAL:O	3:D:40:ASP:C	2.62	0.42
1:A:1113:LEU:HD22	1:A:1113:LEU:HA	1.97	0.41
1:B:350:ARG:HE	1:B:386:ARG:CZ	2.33	0.41
2:C:363:ILE:O	2:C:364:ASP:HB3	2.20	0.41
1:A:177:LEU:HD22	1:A:210:VAL:HG22	2.03	0.41
1:B:368:LEU:CD2	1:B:424:PRO:HB3	2.50	0.41
1:B:821:PHE:HA	1:B:824:ASP:CB	2.49	0.41
2:C:708:PHE:O	2:C:711:PHE:HB3	2.20	0.41
2:E:533:CYS:HB2	2:E:534:PHE:HD1	1.85	0.41
1:A:57:LEU:HD12	1:A:68:ALA:HB1	2.02	0.41
1:A:144:LYS:O	1:A:145:GLN:C	2.64	0.41
1:A:1194:LEU:HD13	1:A:1194:LEU:H	1.85	0.41
1:B:246:GLY:HA3	1:B:285:ARG:CG	2.50	0.41
2:C:363:ILE:HG22	2:C:365:ARG:HG2	2.01	0.41
2:C:572:ARG:HB3	2:C:574:GLY:H	1.85	0.41
2:E:397:TYR:HE1	2:E:420:ARG:HD2	1.82	0.41
2:E:499:LYS:HE2	2:E:550:THR:HG21	2.02	0.41
1:A:135:THR:CG2	1:A:176:ILE:HD11	2.51	0.41
1:A:579:ALA:HB2	1:A:618:ARG:HH22	1.85	0.41
1:A:605:GLY:C	1:A:607:ASP:H	2.28	0.41
1:A:1131:SER:HB3	1:A:1183:LEU:HD23	2.01	0.41
1:B:185:THR:O	1:B:186:SER:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:502:TYR:HB2	1:B:542:VAL:HG22	2.01	0.41
1:B:933:TRP:HA	1:B:936:LEU:HD12	2.02	0.41
1:B:1017:ASP:N	1:B:1018:PRO:HD2	2.35	0.41
1:B:1102:ILE:H	1:B:1102:ILE:HG12	1.69	0.41
1:B:1180:VAL:HG12	1:B:1184:LEU:HD11	2.02	0.41
2:C:235:TYR:O	2:C:236:ASN:HB2	2.21	0.41
2:C:683:THR:HG22	3:D:76:ASN:CG	2.45	0.41
1:A:289:GLU:O	1:A:290:VAL:C	2.63	0.41
1:A:664:ARG:NH1	1:A:705:ASP:OD2	2.53	0.41
1:A:685:LEU:HA	1:A:689:MET:SD	2.60	0.41
1:B:72:LEU:O	1:B:76:VAL:HG23	2.20	0.41
1:B:763:VAL:C	1:B:765:THR:N	2.76	0.41
3:D:97:ASP:OD1	3:D:97:ASP:N	2.54	0.41
2:E:681:ILE:HD12	3:F:31:ALA:HB3	2.03	0.41
1:B:148:VAL:CG1	1:B:149:SER:N	2.82	0.41
2:E:288:LYS:HD3	2:E:288:LYS:HA	1.88	0.41
1:A:423:THR:HG22	1:A:424:PRO:CD	2.33	0.41
1:A:824:ASP:OD1	1:A:824:ASP:N	2.54	0.41
1:B:1109:VAL:O	1:B:1113:LEU:HD12	2.20	0.41
2:C:240:LEU:HA	2:C:243:ALA:HB3	2.02	0.41
2:E:468:ASN:HD21	2:E:470:ILE:HG23	1.86	0.41
1:B:855:LEU:HD23	1:B:856:GLU:H	1.86	0.41
1:A:371:PHE:O	1:A:375:VAL:HG22	2.21	0.41
1:A:551:ARG:HG2	1:A:553:LEU:N	2.36	0.41
1:A:562:THR:N	1:A:563:PRO:CD	2.84	0.41
1:A:857:LEU:HD21	1:A:883:ILE:HD13	2.02	0.41
1:B:452:GLN:HE22	1:B:492:ASN:HD22	1.69	0.41
2:C:769:GLN:HE21	2:C:769:GLN:HB3	1.69	0.41
2:E:899:MET:HA	2:E:911:TYR:O	2.21	0.41
1:A:602:ASP:OD1	1:A:640:LEU:HD11	2.21	0.41
1:A:888:LEU:N	1:A:889:PRO:HD2	2.36	0.41
1:B:760:GLN:HE21	1:B:805:ALA:HB1	1.85	0.41
2:C:816:HIS:CD2	2:C:818:LEU:O	2.69	0.41
2:E:404:LEU:HD22	2:E:408:ARG:HH21	1.86	0.41
2:E:494:TRP:CE3	2:E:540:PHE:HD2	2.38	0.41
1:A:645:ARG:HD2	1:A:684:SER:OG	2.21	0.40
1:A:1186:ILE:O	1:A:1187:PRO:C	2.64	0.40
1:B:148:VAL:C	1:B:150:VAL:H	2.28	0.40
1:B:1146:VAL:HG21	1:B:1195:MET:HE2	2.03	0.40
2:C:791:ARG:CZ	2:C:816:HIS:HB2	2.51	0.40
3:D:45:CYS:HB2	3:D:54:ILE:HG12	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:410:VAL:HG21	2:E:460:GLY:HA3	2.02	0.40
2:E:538:GLU:HA	2:E:541:ILE:HG22	2.03	0.40
1:B:406:ARG:HA	1:B:407:PRO:HD3	1.90	0.40
2:C:321:LEU:HA	2:C:322:PRO:HD2	1.85	0.40
2:C:551:PHE:CD1	2:C:551:PHE:C	2.99	0.40
2:E:464:LEU:HB3	2:E:473:LEU:CD2	2.51	0.40
2:E:741:LYS:HA	2:E:819:PHE:CE1	2.56	0.40
1:A:65:GLN:HB3	1:A:105:ILE:HD11	2.02	0.40
1:A:772:TYR:CD2	1:A:812:LYS:HG3	2.57	0.40
1:B:19:ASP:HA	3:D:92:GLN:NE2	2.30	0.40
1:B:611:THR:O	1:B:614:ILE:HB	2.21	0.40
1:B:733:SER:HA	1:B:736:ASN:HB2	2.03	0.40
2:C:612:ALA:HA	2:C:687:TRP:HZ3	1.86	0.40
2:C:684:MET:HG2	3:D:32:LEU:HB3	2.04	0.40
1:A:1123:THR:HA	1:A:1126:MET:HB2	2.03	0.40
1:B:763:VAL:C	1:B:765:THR:H	2.28	0.40
1:B:1134:CYS:HA	1:B:1135:PRO:HD2	1.99	0.40
1:B:1160:ASN:OD1	2:C:308:LEU:HD13	2.22	0.40
2:E:515:MET:O	2:E:516:VAL:C	2.63	0.40
1:B:12:LEU:HD23	1:B:15:MET:HE3	2.03	0.40
1:B:368:LEU:HD12	1:B:404:GLN:HB3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1145/1253 (91%)	1001 (87%)	122 (11%)	22 (2%)	6	32
1	B	1142/1253 (91%)	991 (87%)	129 (11%)	22 (2%)	6	32
2	C	686/741 (93%)	589 (86%)	83 (12%)	14 (2%)	6	32
2	E	690/741 (93%)	611 (89%)	63 (9%)	16 (2%)	5	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	87/98 (89%)	62 (71%)	16 (18%)	9 (10%)	0	6
3	F	76/98 (78%)	48 (63%)	23 (30%)	5 (7%)	1	13
All	All	3826/4184 (91%)	3302 (86%)	436 (11%)	88 (2%)	5	30

All (88) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	208	ASN
1	A	226	ASP
1	A	290	VAL
1	A	386	ARG
1	A	552	PRO
1	B	39	ILE
1	B	379	LEU
1	B	386	ARG
1	B	855	LEU
2	C	235	TYR
2	C	236	ASN
2	C	881	VAL
2	E	341	LYS
2	E	515	MET
2	E	902	ASP
3	F	38	VAL
3	F	40	ASP
3	F	76	ASN
1	A	641	LYS
1	A	662	ASN
1	A	794	GLN
1	B	388	GLU
1	B	1188	GLU
2	C	339	ASP
3	D	38	VAL
3	D	94	CYS
2	E	338	SER
2	E	761	GLU
2	E	880	PRO
2	E	912	ILE
1	A	482	PHE
1	A	856	GLU
1	A	953	GLU
1	A	1018	PRO

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Mol	Chain	Res	Type
1	B	287	PRO
1	B	289	GLU
1	B	579	ALA
1	B	606	SER
1	B	995	ASP
1	B	1130	LEU
2	C	273	HIS
2	C	364	ASP
2	C	556	PRO
2	C	912	ILE
1	A	38	SER
1	B	290	VAL
1	B	901	SER
1	B	1039	SER
1	B	1134	CYS
2	C	281	ASP
3	D	46	ARG
3	D	97	ASP
3	D	98	ASN
2	E	699	PRO
1	A	148	VAL
1	A	287	PRO
1	A	369	PRO
1	A	999	PRO
1	A	1115	ASP
1	B	38	SER
1	B	267	ASP
1	B	732	GLY
2	C	251	LYS
2	C	761	GLU
3	D	48	HIS
3	D	92	GLN
3	D	101	TRP
2	E	360	GLY
2	E	556	PRO
2	E	790	ALA
3	F	47	ASN
1	A	281	SER
1	A	952	VAL
1	B	1098	ASP
3	D	40	ASP
2	E	301	ILE

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Mol	Chain	Res	Type
1	B	676	ILE
2	C	252	ILE
2	C	880	PRO
2	E	688	PRO
2	E	881	VAL
2	C	796	ASN
1	B	853	GLY
2	E	516	VAL
1	A	1187	PRO
3	F	39	VAL
1	A	1206	PRO
2	E	486	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1028/1118 (92%)	897 (87%)	131 (13%)	4	21
1	B	1033/1118 (92%)	877 (85%)	156 (15%)	3	16
2	C	632/675 (94%)	535 (85%)	97 (15%)	3	16
2	E	637/675 (94%)	552 (87%)	85 (13%)	4	19
3	D	78/83 (94%)	62 (80%)	16 (20%)	1	7
3	F	72/83 (87%)	59 (82%)	13 (18%)	2	12
All	All	3480/3752 (93%)	2982 (86%)	498 (14%)	3	17

All (498) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	TYR
1	A	8	ILE
1	A	20	LYS
1	A	36	LYS
1	A	39	ILE
1	A	41	LEU

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Mol	Chain	Res	Type
1	A	60	LYS
1	A	105	ILE
1	A	114	ILE
1	A	116	GLU
1	A	126	LEU
1	A	144	LYS
1	A	148	VAL
1	A	169	LEU
1	A	175	SER
1	A	185	THR
1	A	194	ARG
1	A	196	ILE
1	A	205	SER
1	A	209	ILE
1	A	210	VAL
1	A	222	LEU
1	A	252	TYR
1	A	253	LEU
1	A	254	GLU
1	A	257	ILE
1	A	260	VAL
1	A	281	SER
1	A	289	GLU
1	A	302	LEU
1	A	346	SER
1	A	364	ARG
1	A	368	LEU
1	A	373	LYS
1	A	382	ARG
1	A	384	LYS
1	A	389	ASN
1	A	423	THR
1	A	425	LEU
1	A	434	ASN
1	A	449	LYS
1	A	465	LEU
1	A	475	VAL
1	A	483	SER
1	A	486	ASP
1	A	534	LYS
1	A	541	LEU
1	A	545	GLN

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Mol	Chain	Res	Type
1	A	555	GLN
1	A	558	SER
1	A	562	THR
1	A	566	LYS
1	A	573	ILE
1	A	581	ILE
1	A	604	LEU
1	A	616	LEU
1	A	618	ARG
1	A	621	ASN
1	A	622	GLU
1	A	625	ARG
1	A	626	LEU
1	A	628	THR
1	A	632	LEU
1	A	640	LEU
1	A	655	LEU
1	A	678	ILE
1	A	682	SER
1	A	690	ILE
1	A	710	GLN
1	A	723	TYR
1	A	729	LYS
1	A	730	ILE
1	A	735	LEU
1	A	739	ILE
1	A	746	LEU
1	A	770	LEU
1	A	783	VAL
1	A	801	LYS
1	A	803	VAL
1	A	810	CYS
1	A	813	GLU
1	A	824	ASP
1	A	827	ASN
1	A	831	THR
1	A	852	SER
1	A	859	SER
1	A	861	ILE
1	A	874	SER
1	A	882	SER
1	A	884	SER

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Mol	Chain	Res	Type
1	A	911	HIS
1	A	913	LEU
1	A	918	SER
1	A	921	SER
1	A	922	VAL
1	A	938	LYS
1	A	958	LEU
1	A	961	ILE
1	A	962	ASP
1	A	965	THR
1	A	967	LEU
1	A	987	THR
1	A	1003	LEU
1	A	1004	LEU
1	A	1005	LYS
1	A	1007	CYS
1	A	1015	LEU
1	A	1040	LEU
1	A	1041	ILE
1	A	1044	LEU
1	A	1047	THR
1	A	1055	GLU
1	A	1068	MET
1	A	1072	LYS
1	A	1074	THR
1	A	1097	LEU
1	A	1113	LEU
1	A	1114	LYS
1	A	1122	LEU
1	A	1123	THR
1	A	1129	ARG
1	A	1143	ASP
1	A	1158	LYS
1	A	1160	ASN
1	A	1163	LYS
1	A	1164	GLN
1	A	1172	LEU
1	A	1175	SER
1	A	1186	ILE
1	A	1194	LEU
1	A	1216	GLN
1	B	8	ILE

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Mol	Chain	Res	Type
1	B	33	GLU
1	B	35	GLN
1	B	39	ILE
1	B	60	LYS
1	B	71	CYS
1	B	96	LEU
1	B	111	LYS
1	B	112	THR
1	B	133	LYS
1	B	142	ILE
1	B	144	LYS
1	B	146	GLU
1	B	155	LEU
1	B	170	VAL
1	B	175	SER
1	B	179	CYS
1	B	181	LEU
1	B	189	LEU
1	B	194	ARG
1	B	202	LEU
1	B	204	MET
1	B	209	ILE
1	B	210	VAL
1	B	216	GLU
1	B	219	LEU
1	B	221	GLU
1	B	222	LEU
1	B	225	ASN
1	B	228	MET
1	B	238	ILE
1	B	242	SER
1	B	253	LEU
1	B	254	GLU
1	B	255	LYS
1	B	256	ILE
1	B	257	ILE
1	B	275	CYS
1	B	276	ILE
1	B	285	ARG
1	B	300	ILE
1	B	302	LEU
1	B	306	THR

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Mol	Chain	Res	Type
1	B	345	MET
1	B	351	ARG
1	B	364	ARG
1	B	370	GLU
1	B	379	LEU
1	B	380	ILE
1	B	381	SER
1	B	384	LYS
1	B	386	ARG
1	B	388	GLU
1	B	401	LEU
1	B	405	THR
1	B	423	THR
1	B	428	LEU
1	B	431	GLN
1	B	432	VAL
1	B	435	ILE
1	B	444	LYS
1	B	445	GLU
1	B	461	LEU
1	B	463	ASN
1	B	469	LEU
1	B	490	SER
1	B	492	ASN
1	B	496	ASP
1	B	501	LEU
1	B	512	VAL
1	B	541	LEU
1	B	546	LEU
1	B	555	GLN
1	B	562	THR
1	B	566	LYS
1	B	583	GLN
1	B	604	LEU
1	B	616	LEU
1	B	618	ARG
1	B	625	ARG
1	B	626	LEU
1	B	640	LEU
1	B	650	GLU
1	B	660	ARG
1	B	672	SER

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Mol	Chain	Res	Type
1	B	676	ILE
1	B	678	ILE
1	B	690	ILE
1	B	697	LEU
1	B	702	SER
1	B	703	GLU
1	B	710	GLN
1	B	735	LEU
1	B	738	LEU
1	B	739	ILE
1	B	742	VAL
1	B	752	LEU
1	B	765	THR
1	B	770	LEU
1	B	802	CYS
1	B	806	LEU
1	B	813	GLU
1	B	818	VAL
1	B	825	VAL
1	B	826	LYS
1	B	831	THR
1	B	832	ASP
1	B	836	LEU
1	B	849	ILE
1	B	854	GLN
1	B	855	LEU
1	B	857	LEU
1	B	858	LYS
1	B	862	LEU
1	B	888	LEU
1	B	892	LEU
1	B	900	THR
1	B	905	ARG
1	B	913	LEU
1	B	914	LYS
1	B	932	ILE
1	B	935	LEU
1	B	938	LYS
1	B	941	GLU
1	B	967	LEU
1	B	974	LEU
1	B	975	ILE

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Mol	Chain	Res	Type
1	B	987	THR
1	B	989	VAL
1	B	992	THR
1	B	993	ILE
1	B	994	SER
1	B	996	HIS
1	B	1015	LEU
1	B	1016	GLU
1	B	1019	ASP
1	B	1025	VAL
1	B	1039	SER
1	B	1044	LEU
1	B	1056	THR
1	B	1102	ILE
1	B	1106	LEU
1	B	1129	ARG
1	B	1130	LEU
1	B	1139	LEU
1	B	1155	THR
1	B	1164	GLN
1	B	1168	LYS
1	B	1172	LEU
1	B	1174	ARG
1	B	1184	LEU
1	B	1190	GLU
1	B	1194	LEU
1	B	1197	GLU
1	B	1208	LEU
1	B	1215	ILE
2	C	216	THR
2	C	221	LYS
2	C	225	GLU
2	C	247	LEU
2	C	252	ILE
2	C	256	LEU
2	C	260	LEU
2	C	268	ILE
2	C	272	ILE
2	C	280	LEU
2	C	281	ASP
2	C	284	LEU
2	C	301	ILE

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Mol	Chain	Res	Type
2	C	302	MET
2	C	306	ILE
2	C	329	LEU
2	C	337	ILE
2	C	343	GLN
2	C	345	LYS
2	C	346	THR
2	C	378	LEU
2	C	380	ILE
2	C	400	GLU
2	C	402	GLN
2	C	403	LYS
2	C	407	GLU
2	C	414	LEU
2	C	424	GLU
2	C	428	LEU
2	C	429	ILE
2	C	430	THR
2	C	433	ASP
2	C	435	THR
2	C	436	THR
2	C	441	ILE
2	C	453	LEU
2	C	454	THR
2	C	465	LEU
2	C	467	GLU
2	C	470	ILE
2	C	471	GLN
2	C	493	GLN
2	C	496	GLU
2	C	513	LYS
2	C	516	VAL
2	C	519	LEU
2	C	530	ILE
2	C	544	MET
2	C	550	THR
2	C	552	ILE
2	C	558	LYS
2	C	562	LEU
2	C	572	ARG
2	C	583	LEU
2	C	585	LYS

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Mol	Chain	Res	Type
2	C	592	ILE
2	C	604	GLU
2	C	611	LEU
2	C	613	LYS
2	C	619	LYS
2	C	633	LEU
2	C	657	ASP
2	C	667	GLN
2	C	671	VAL
2	C	675	ILE
2	C	677	LEU
2	C	678	THR
2	C	679	VAL
2	C	681	ILE
2	C	683	THR
2	C	684	MET
2	C	694	GLU
2	C	704	LEU
2	C	715	LYS
2	C	737	LYS
2	C	747	LEU
2	C	754	LEU
2	C	761	GLU
2	C	769	GLN
2	C	778	LEU
2	C	801	ASP
2	C	813	ASP
2	C	826	ILE
2	C	831	THR
2	C	832	VAL
2	C	839	THR
2	C	858	MET
2	C	861	ARG
2	C	863	THR
2	C	865	SER
2	C	881	VAL
2	C	886	LEU
2	C	889	ARG
2	C	890	ILE
2	C	901	ARG
2	C	905	ASN
2	C	912	ILE

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Mol	Chain	Res	Type
3	D	25	LYS
3	D	38	VAL
3	D	39	VAL
3	D	46	ARG
3	D	47	ASN
3	D	49	ILE
3	D	59	ASN
3	D	69	THR
3	D	74	VAL
3	D	84	ILE
3	D	93	VAL
3	D	98	ASN
3	D	99	ARG
3	D	100	GLU
3	D	101	TRP
3	D	102	GLU
2	E	214	ASP
2	E	217	TRP
2	E	221	LYS
2	E	233	ILE
2	E	234	LYS
2	E	235	TYR
2	E	251	LYS
2	E	255	ASN
2	E	256	LEU
2	E	259	GLN
2	E	260	LEU
2	E	263	ILE
2	E	289	ILE
2	E	310	LEU
2	E	312	ARG
2	E	316	LEU
2	E	324	ILE
2	E	340	GLN
2	E	341	LYS
2	E	342	VAL
2	E	343	GLN
2	E	345	LYS
2	E	352	LEU
2	E	355	GLU
2	E	363	ILE
2	E	366	SER

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Mol	Chain	Res	Type
2	E	378	LEU
2	E	379	GLN
2	E	380	ILE
2	E	388	ARG
2	E	414	LEU
2	E	428	LEU
2	E	429	ILE
2	E	443	THR
2	E	454	THR
2	E	458	GLN
2	E	459	LYS
2	E	465	LEU
2	E	484	ARG
2	E	488	GLN
2	E	491	LEU
2	E	503	SER
2	E	504	THR
2	E	507	ILE
2	E	513	LYS
2	E	514	THR
2	E	520	LEU
2	E	532	ILE
2	E	544	MET
2	E	548	PHE
2	E	552	ILE
2	E	570	LYS
2	E	577	GLU
2	E	580	ASP
2	E	581	GLU
2	E	588	ASP
2	E	592	ILE
2	E	595	ARG
2	E	611	LEU
2	E	613	LYS
2	E	619	LYS
2	E	641	PHE
2	E	653	GLU
2	E	667	GLN
2	E	681	ILE
2	E	689	THR
2	E	691	VAL
2	E	695	VAL

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Mol	Chain	Res	Type
2	E	726	THR
2	E	747	LEU
2	E	778	LEU
2	E	791	ARG
2	E	816	HIS
2	E	823	ILE
2	E	827	GLN
2	E	845	ASP
2	E	859	LYS
2	E	863	THR
2	E	877	LEU
2	E	878	LYS
2	E	886	LEU
2	E	897	ASP
2	E	901	ARG
2	E	904	GLU
2	E	905	ASN
3	F	19	LYS
3	F	25	LYS
3	F	37	ILE
3	F	49	ILE
3	F	51	ASP
3	F	52	LEU
3	F	56	CYS
3	F	69	THR
3	F	84	ILE
3	F	87	TRP
3	F	92	GLN
3	F	96	LEU
3	F	99	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (105) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	66	ASN
1	A	83	GLN
1	A	151	GLN
1	A	236	GLN
1	A	404	GLN
1	A	409	GLN
1	A	429	GLN

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Mol	Chain	Res	Type
1	A	456	ASN
1	A	463	ASN
1	A	492	ASN
1	A	507	ASN
1	A	544	GLN
1	A	599	ASN
1	A	603	ASN
1	A	621	ASN
1	A	848	HIS
1	A	854	GLN
1	A	897	GLN
1	A	902	GLN
1	A	906	GLN
1	A	939	HIS
1	A	1107	ASN
1	A	1164	GLN
1	A	1201	GLN
1	A	1216	GLN
1	B	35	GLN
1	B	66	ASN
1	B	101	GLN
1	B	151	GLN
1	B	225	ASN
1	B	236	GLN
1	B	434	ASN
1	B	442	GLN
1	B	492	ASN
1	B	507	ASN
1	B	508	HIS
1	B	516	HIS
1	B	595	GLN
1	B	603	ASN
1	B	610	ASN
1	B	613	GLN
1	B	621	ASN
1	B	707	HIS
1	B	736	ASN
1	B	760	GLN
1	B	820	GLN
1	B	827	ASN
1	B	848	HIS
1	B	902	GLN

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Mol	Chain	Res	Type
1	B	939	HIS
1	B	1035	HIS
1	B	1036	ASN
1	B	1108	HIS
1	B	1201	GLN
2	C	228	GLN
2	C	259	GLN
2	C	340	GLN
2	C	359	ASN
2	C	387	GLN
2	C	458	GLN
2	C	471	GLN
2	C	661	GLN
2	C	667	GLN
2	C	729	HIS
2	C	744	GLN
2	C	769	GLN
2	C	796	ASN
2	C	811	ASN
2	C	816	HIS
2	C	824	ASN
2	C	835	GLN
2	C	847	GLN
2	C	876	GLN
2	C	905	ASN
2	C	907	ASN
2	C	910	ASN
3	D	92	GLN
3	D	98	ASN
3	D	104	GLN
2	E	246	ASN
2	E	255	ASN
2	E	296	HIS
2	E	318	ASN
2	E	379	GLN
2	E	402	GLN
2	E	418	ASN
2	E	434	GLN
2	E	468	ASN
2	E	542	ASN
2	E	557	ASN
2	E	716	HIS

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Mol	Chain	Res	Type
2	E	724	GLN
2	E	744	GLN
2	E	827	GLN
2	E	847	GLN
2	E	876	GLN
2	E	905	ASN
2	E	907	ASN
2	E	910	ASN
3	F	47	ASN
3	F	48	HIS
3	F	57	GLN
3	F	98	ASN
3	F	108	HIS

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 6 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1155/1253 (92%)	-0.46	0 100 100	103, 127, 153, 165	0
1	B	1154/1253 (92%)	-0.44	0 100 100	90, 115, 159, 179	0
2	C	692/741 (93%)	-0.35	1 (0%) 92 87	86, 129, 188, 201	0
2	E	696/741 (93%)	-0.41	0 100 100	98, 141, 173, 177	0
3	D	89/98 (90%)	-0.33	0 100 100	111, 132, 148, 149	0
3	F	80/98 (81%)	-0.21	0 100 100	141, 155, 168, 170	0
All	All	3866/4184 (92%)	-0.42	1 (0%) 100 100	86, 125, 170, 201	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	237	LEU	2.1

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
4	ZN	F	4003	1/1	0.98	0.03	144,144,144,144	0
4	ZN	F	4002	1/1	0.99	0.03	120,120,120,120	0
4	ZN	F	4001	1/1	0.99	0.02	113,113,113,113	0
4	ZN	D	4001	1/1	1.00	0.01	104,104,104,104	0
4	ZN	D	4002	1/1	1.00	0.04	92,92,92,92	0
4	ZN	D	4003	1/1	1.00	0.04	104,104,104,104	0

6.5 Other polymers [i](#)

There are no such residues in this entry.