



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 04:17 PM GMT

PDB ID : 4A0C
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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

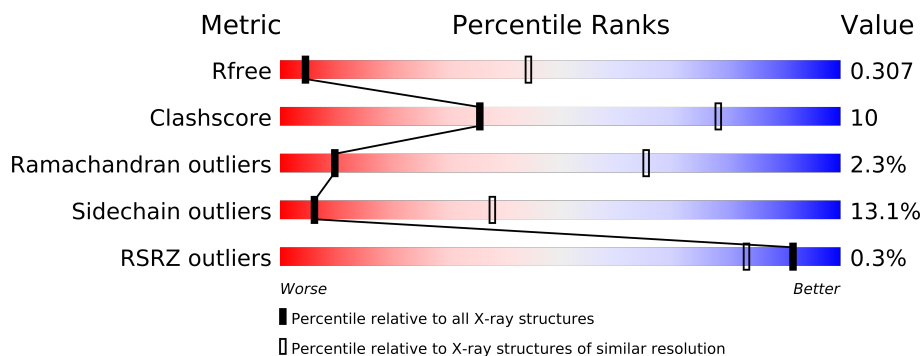
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1162 (4.20-3.40)
Clashscore	79885	1100 (4.10-3.50)
Ramachandran outliers	78287	1050 (4.10-3.50)
Sidechain outliers	78261	1042 (4.10-3.50)
RSRZ outliers	66119	1163 (4.20-3.40)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	1253	
1	B	1253	
2	C	741	
2	E	741	
3	D	98	
3	F	98	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 30804 atoms, of which 0 are hydrogen and 0 are deuterium.

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 (three-letter code: ZN) (formula: Zn).

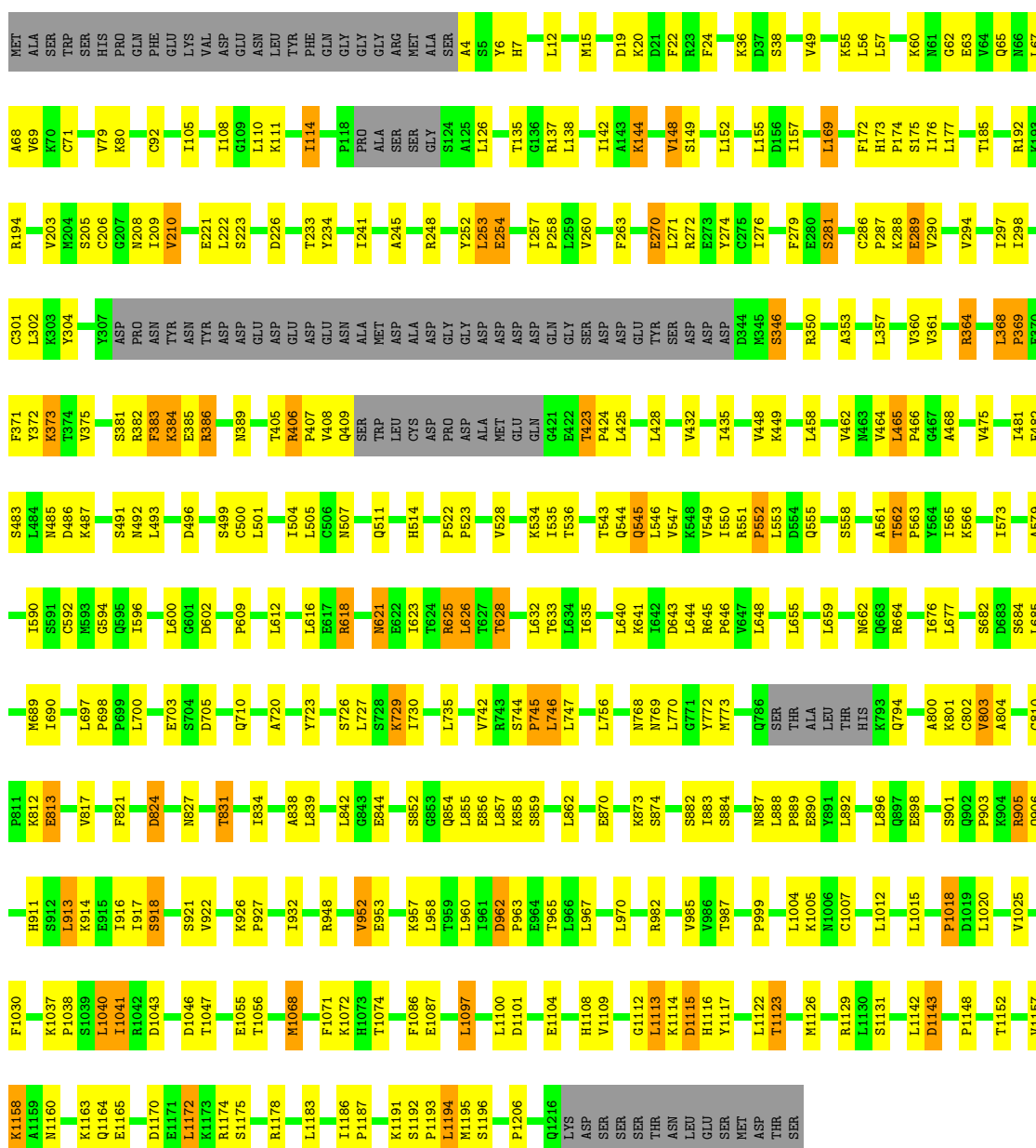
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	3	Total 3	Zn 3	0	0
4	F	3	Total 3	Zn 3	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

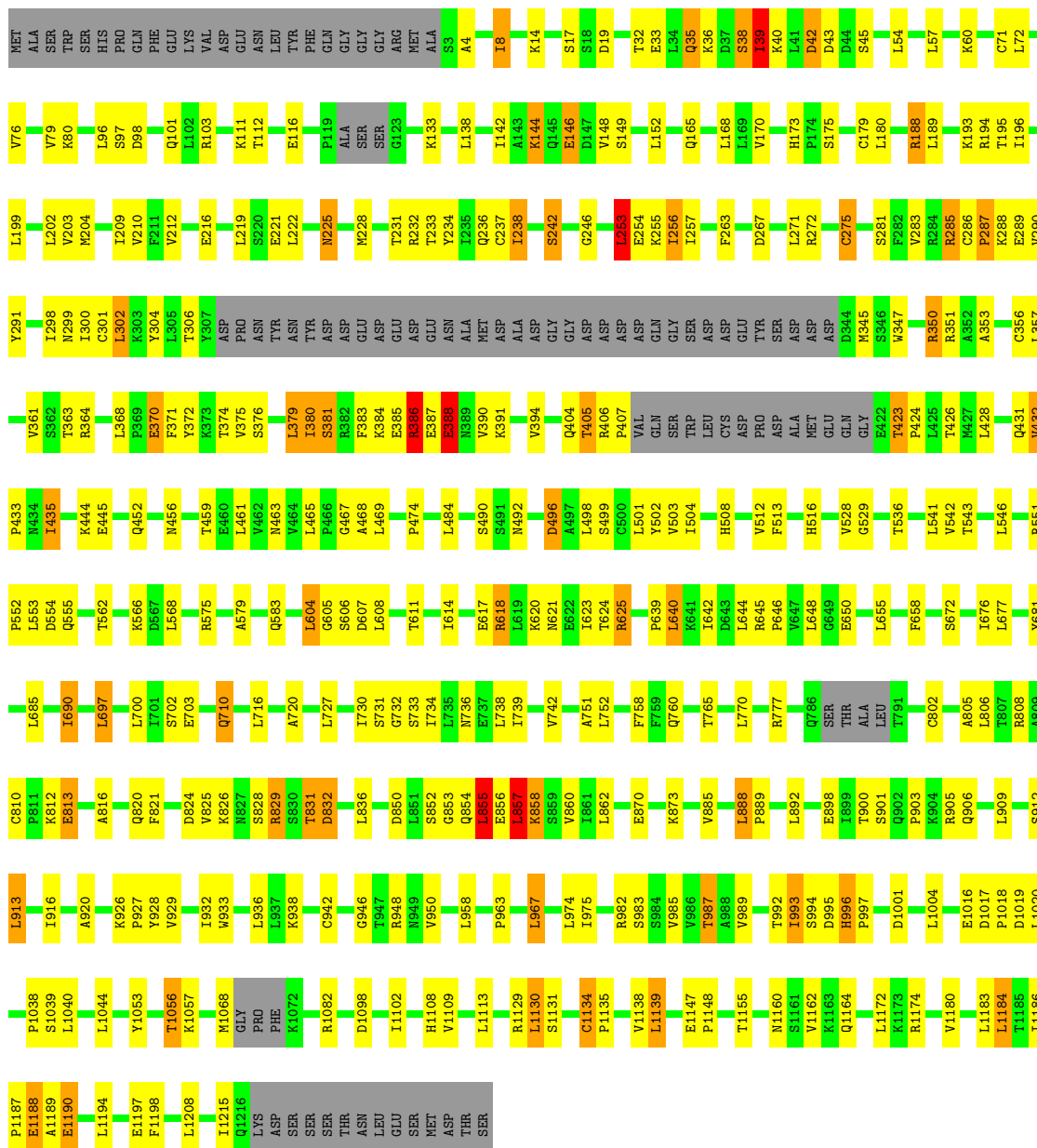
• Molecule 1: CULLIN-ASSOCIATED NEDD8-DISSOCIATED PROTEIN 1

Chain A:



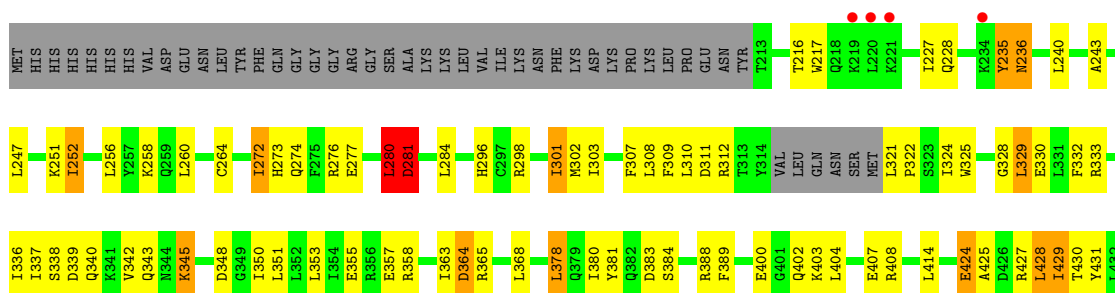
• Molecule 1: CULLIN-ASSOCIATED NEDD8-DISSOCIATED PROTEIN 1

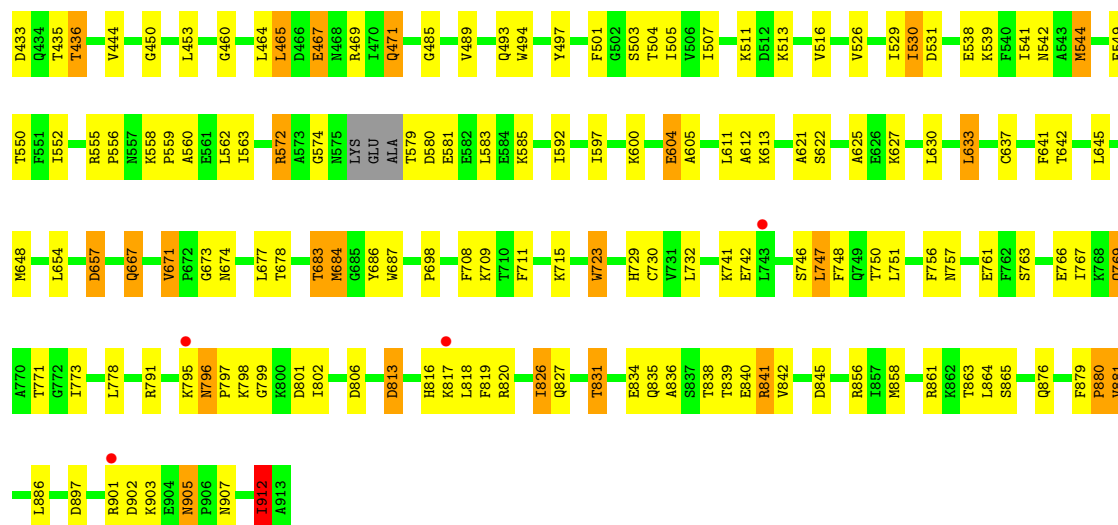
Chain B:



• Molecule 2: CULLIN-4B

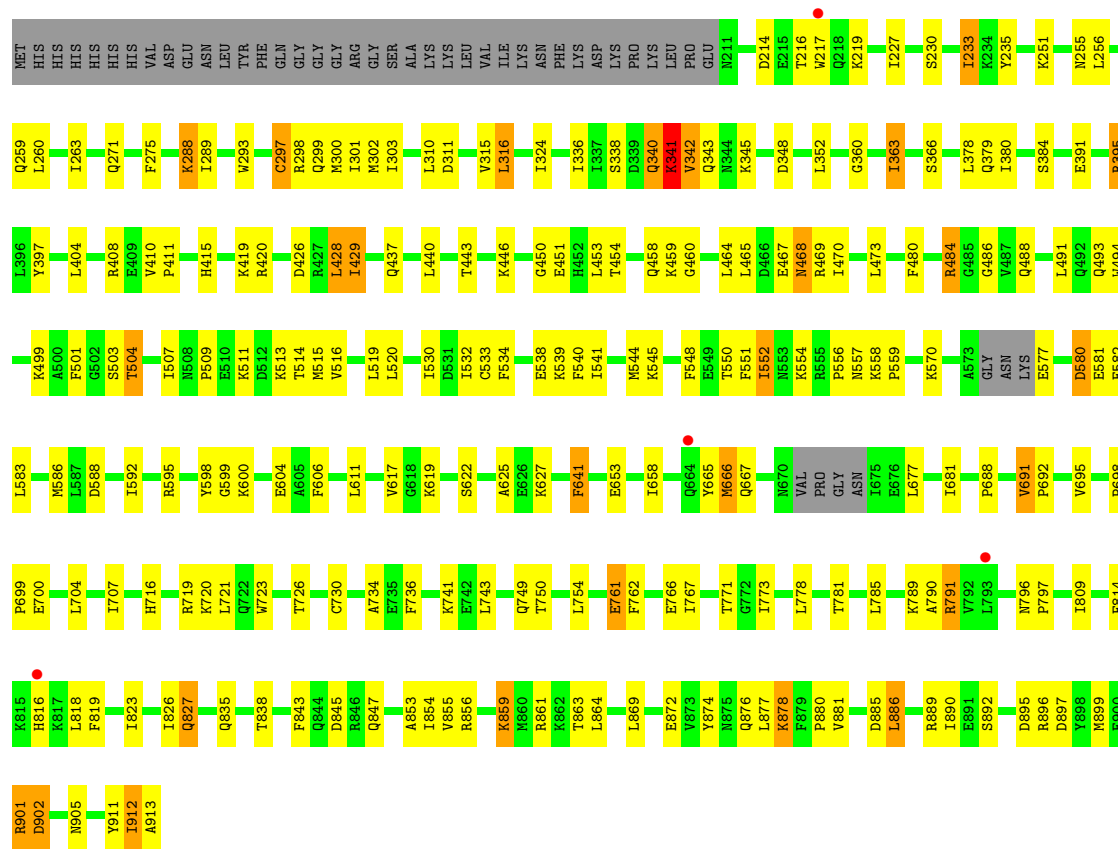
Chain C:





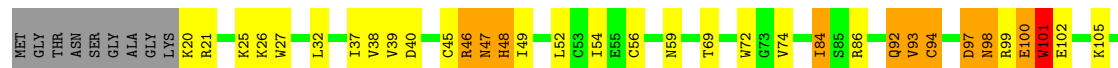
• Molecule 2: CULLIN-4B

Chain E:



• Molecule 3: E3 UBIQUITIN-PROTEIN LIGASE RBX1

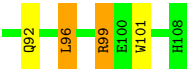
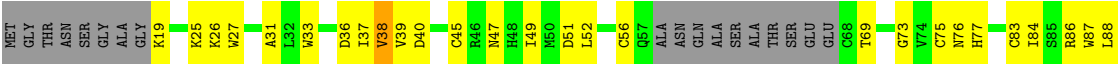
Chain D:



H108

● Molecule 3: E3 UBIQUITIN-PROTEIN LIGASE RBX1

Chain F: 



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 0.231 , 0.307	Depositor DCC
R_{free} test set	2990 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	119.1	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 57.7	EDS
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 59850 reflections	Xtriage
F_o, F_c correlation	0.93	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.

5 Model quality

5.1 Standard geometry

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	0.37	0/9101	0.56	0/12327
1	B	0.38	0/9113	0.58	2/12340 (0.0%)
2	C	0.39	0/5794	0.57	1/7776 (0.0%)
2	E	0.38	0/5836	0.55	0/7832
3	D	0.40	0/759	0.52	0/1029
3	F	0.37	0/698	0.50	0/943
All	All	0.38	0/31301	0.56	3/42247 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	280	LEU	CA-CB-CG	5.98	129.06	115.30
1	B	857	LEU	CA-CB-CG	5.68	128.36	115.30
1	B	253	LEU	CA-CB-CG	5.59	128.16	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8963	0	9308	208	0
1	B	8975	0	9328	192	0
2	C	5702	0	5801	137	0
2	E	5744	0	5841	110	0
3	D	737	0	687	17	0
3	F	677	0	642	13	0
4	D	3	0	0	0	0
4	F	3	0	0	1	0
All	All	30804	0	31607	653	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (653) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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
1:B:1129:ARG:HG3	1:B:1129:ARG:HH11	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:HD13	2:E:363:ILE:H	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:B:376:SER:HA	1:B:380:ILE:CD1	2.18	0.73
2:C:345:LYS:HA	2:C:348:ASP:HB2	1.68	0.73
2:C:858:MET:HE1	2:C:864:LEU:HB3	1.70	0.73
1:A:350:ARG:NH2	1:A:386:ARG:HH22	1.87	0.72

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:E:530:ILE:HA	2:E:534:PHE:HB2	1.74	0.69
1:A:690:ILE:HG21	1:A:726:SER:HB3	1.73	0.69
1:B:299:ASN:HA	1:B:379:LEU:CD2	2.23	0.69
2:E:762:PHE:HB3	2:E:766:GLU:HG3	1.76	0.68
1:A:381:SER:HA	1:A:384:LYS:HE3	1.74	0.68
1:A:298:ILE:HG23	1:A:353:ALA:HB1	1.75	0.68
2:C:467:GLU:HB3	2:C:469:ARG:HG2	1.74	0.68
1:A:903:PRO:HA	1:A:906:GLN:HB2	1.76	0.68
1:A:855:LEU:C	1:A:857:LEU:H	1.94	0.68
1:B:385:GLU:O	1:B:386:ARG:HB2	1.93	0.67
1:A:831:THR:H	1:A:834:ILE:HD12	1.59	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
2:C:604:GLU:HB3	2:C:641:PHE:CZ	2.30	0.67
1:B:942:CYS:HB3	1:B:948:ARG:HD3	1.77	0.67
1:B:372:TYR:HA	1:B:376:SER:HB3	1.77	0.66
2:C:471:GLN:HA	2:C:471:GLN:HE21	1.60	0.66
2:C:817:LYS:HG3	2:C:818:LEU:H	1.59	0.66
2:C:604:GLU:HG3	2:C:605:ALA:N	2.09	0.66
1:A:1113:LEU:HD12	1:A:1148:PRO:HB2	1.76	0.66
1:A:144:LYS:H	1:A:144:LYS:HD2	1.60	0.66
1:B:302:LEU:HD12	1:B:379:LEU:HG	1.76	0.66
2:E:299:GLN:HA	2:E:302:MET:HE2	1.78	0.66
1:A:192:ARG:HB3	1:A:233:THR:HG21	1.75	0.66
2:C:340:GLN:CB	2:C:342:VAL:HB	2.26	0.66
1:B:380:ILE:HG22	1:B:394:VAL:HG13	1.78	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:879:PHE:HB2	2:C:880:PRO:HD2	1.77	0.65
1:B:926:LYS:HB3	1:B:927:PRO:HD3	1.79	0.65
1:B:903:PRO:HA	1:B:906:GLN:HB2	1.78	0.65
1:B:193:LYS:HE3	2:C:581:GLU:HG2	1.78	0.65
1:A:862:LEU:HB3	1:A:905:ARG:NH2	2.12	0.65
2:C:796:ASN:CB	2:C:797:PRO:HD3	2.27	0.65
2:C:424:GLU:HG2	2:C:444:VAL:HG21	1.79	0.65
1:B:386:ARG:HH11	1:B:386:ARG:HG3	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
3:D:72:TRP:HB2	3:D:105:LYS:CB	2.25	0.64
2:C:280:LEU:CD1	2:C:281:ASP:H	2.09	0.64
2:E:911:TYR:O	2:E:912:ILE:HG13	1.96	0.64
1:B:553:LEU:HB3	1:B:639:PRO:HG2	1.78	0.64
2:E:397:TYR:CE1	2:E:420:ARG:HD2	2.33	0.64
2:C:227:ILE:CD1	2:C:303:ILE:HG13	2.25	0.64
1:A:625:ARG:HG2	1:A:626:LEU:N	2.13	0.63
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
2:C:905:ASN:HB2	2:C:907:ASN:HD22	1.64	0.63
2:C:235:TYR:H	2:C:235:TYR:HD1	1.47	0.63
2:E:363:ILE:CD1	2:E:363:ILE:H	2.11	0.63
1:B:242:SER:HB3	1:B:281:SER:HB3	1.80	0.63
1:B:298:ILE:HG23	1:B:353:ALA:HB1	1.80	0.63
1:B:97:SER:HB2	1:B:103:ARG:HB2	1.79	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:952:VAL:HG11	1:A:987:THR:HB	1.81	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
2:C:597:ILE:O	2:C:600:LYS:HE3	2.01	0.61
1:A:4:ALA:HB3	1:A:7:HIS:HB3	1.81	0.61
1:A:855:LEU:C	1:A:857:LEU:N	2.54	0.61
2:C:276:ARG:HE	2:C:340:GLN:NE2	1.98	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:465:LEU:HB2	1:B:468:ALA:HB2	1.84	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:361:VAL:HA	1:B:371:PHE:CE2	2.36	0.60
1:B:42:ASP:HB2	1:B:45:SER:H	1.66	0.60
2:C:450:GLY:HA2	2:C:453:LEU:CD2	2.31	0.60
2:C:380:ILE:HG23	2:C:384:SER:HB2	1.82	0.60
2:C:485:GLY:O	2:C:489:VAL:HG23	2.01	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:A:590:ILE:HD13	1:A:628:THR:HG22	1.83	0.60
1:B:283:VAL:O	1:B:363:THR:HG21	2.02	0.60
1:B:1138:VAL:HG11	1:B:1183:LEU:HD12	1.84	0.59
1:B:299:ASN:HA	1:B:379:LEU:HD22	1.83	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
2:C:280:LEU:HD23	2:C:345:LYS:HD3	1.83	0.59
1:A:15:MET:HG2	1:A:56:LEU:HD11	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
2:C:303:ILE:HG21	2:C:324:ILE:HG21	1.84	0.58
1:B:1129:ARG:NH1	1:B:1129:ARG:HG3	2.14	0.58
1:A:952:VAL:CG1	1:A:987:THR:HB	2.33	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
2:C:902:ASP:CG	2:C:903:LYS:H	2.07	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:E:730:CYS:HB2	3:F:26:LYS:O	2.03	0.58
2:C:427:ARG:HD2	2:C:431:TYR:OH	2.03	0.58
1:A:297:ILE:O	1:A:297:ILE:HG22	2.04	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:A:562:THR:N	1:A:563:PRO:HD2	2.18	0.57
1:A:492:ASN:HD22	2:E:514:THR:HG21	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:B:347:TRP:HA	1:B:350:ARG:CZ	2.34	0.57
1:A:458:LEU:O	1:A:462:VAL:HG23	2.05	0.57
2:C:494:TRP:HE1	2:C:529:ILE:HD11	1.70	0.57
2:E:519:LEU:HD21	2:E:552:ILE:HD11	1.85	0.56
1:A:1101:ASP:OD2	1:A:1104:GLU:HB2	2.04	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:B:383:PHE:HE2	1:B:386:ARG:HE	1.53	0.56
1:A:368:LEU:N	1:A:369:PRO:HD2	2.20	0.56
2:E:771:THR:HG23	2:E:773:ILE:HG12	1.86	0.56
2:E:658:ILE:HG21	2:E:716:HIS:HE1	1.71	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
1:B:298:ILE:HD11	1:B:356:CYS:HB3	1.87	0.56
2:C:329:LEU:HD13	2:C:378:LEU:HD22	1.88	0.56
2:C:309:PHE:HA	2:C:312:ARG:HB2	1.87	0.56
1:A:703:GLU:OE1	1:A:746:LEU:HD21	2.05	0.56
1:B:821:PHE:HA	1:B:824:ASP:HB3	1.86	0.56
2:C:358:ARG:NE	2:C:427:ARG:HH12	2.03	0.56
1:A:1097:LEU:HA	1:A:1100:LEU:HD12	1.88	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
2:E:734:ALA:HB1	2:E:736:PHE:CE2	2.42	0.55
1:B:913:LEU:HA	1:B:916:ILE:HD12	1.88	0.55
3:F:45:CYS:HG	4:F:4001:ZN:ZN	1.18	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:982:ARG:HA	1:B:985:VAL:HG12	1.88	0.55
1:B:39:ILE:HD13	1:B:40:LYS:HG2	1.87	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:338:SER:O	2:C:340:GLN:HG2	2.06	0.55
1:B:272:ARG:NH1	1:B:301:CYS:SG	2.80	0.55
1:A:645:ARG:N	1:A:646:PRO:HD2	2.22	0.55
1:B:644:LEU:HD12	1:B:681:TYR:HE2	1.72	0.55
2:E:730:CYS:HB3	3:F:27:TRP:HA	1.87	0.54
1:A:111:LYS:O	1:A:114:ILE:HG22	2.07	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:B:1183:LEU:O	1:B:1187:PRO:HG3	2.08	0.54
1:A:1142:LEU:HD21	1:A:1195:MET:HG3	1.87	0.54
1:B:231:THR:HG21	1:B:263:PHE:HE2	1.72	0.54
2:C:858:MET:CE	2:C:864:LEU:HB3	2.35	0.54
2:C:425:ALA:O	2:C:429:ILE:HG23	2.07	0.54
1:B:165:GLN:HG3	1:B:168:LEU:HD12	1.90	0.54
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
2:C:796:ASN:HB2	2:C:797:PRO:HD3	1.88	0.54
2:C:460:GLY:O	2:C:464:LEU:HG	2.07	0.54
2:C:333:ARG:O	2:C:338:SER:HB2	2.08	0.54
1:B:375:VAL:O	1:B:380:ILE:HD11	2.08	0.54
2:C:351:LEU:HD21	2:C:389:PHE:HA	1.89	0.54
1:A:481:ILE:HG23	1:A:523:PRO:HG3	1.89	0.54
1:B:225:ASN:HD22	1:B:225:ASN:H	1.56	0.54
1:B:604:LEU:HD22	1:B:608:LEU:HB2	1.90	0.53
1:A:756:LEU:HD22	1:A:802:CYS:HA	1.90	0.53
2:E:340:GLN:NE2	2:E:342:VAL:HG22	2.23	0.53
1:B:870:GLU:HA	1:B:873:LYS:HE3	1.89	0.53
1:B:298:ILE:CD1	1:B:356:CYS:HB3	2.39	0.53
1:A:1157:VAL:HG23	1:A:1158:LYS:HE3	1.90	0.53
2:C:856:ARG:HH11	2:C:876:GLN:NE2	2.07	0.53
1:B:8:ILE:HD13	1:B:45:SER:HB3	1.90	0.53
2:E:677:LEU:HD13	3:F:27:TRP:CE3	2.43	0.53
1:A:19:ASP:HB3	1:A:22:PHE:HB2	1.91	0.53
2:E:665:TYR:HD2	2:E:666:MET:SD	2.31	0.53
2:E:767:ILE:O	2:E:771:THR:HG22	2.09	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:789:LYS:HB2	2:E:791:ARG:HH12	1.73	0.53
1:B:386:ARG:HG3	1:B:387:GLU:N	2.14	0.53
2:E:600:LYS:HG3	2:E:878:LYS:HG3	1.91	0.53
2:C:767:ILE:O	2:C:771:THR:HG22	2.09	0.53
1:B:888:LEU:N	1:B:889:PRO:HD2	2.23	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:376:SER:CA	1:B:380:ILE:HD11	2.38	0.53
1:A:1174:ARG:O	1:A:1178:ARG:HB2	2.09	0.53
1:A:67:LEU:O	1:A:71:CYS:HB2	2.08	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
2:E:428:LEU:HD11	2:E:437:GLN:HB2	1.92	0.52
1:A:1115:ASP:CG	1:A:1116:HIS:H	2.13	0.52
2:C:501:PHE:O	2:C:504:THR:HB	2.10	0.52
1:B:271:LEU:O	1:B:275:CYS:HB2	2.10	0.52
1:B:1186:ILE:N	1:B:1187:PRO:HD2	2.24	0.52
1:B:432:VAL:HA	1:B:435:ILE:HG22	1.91	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:1147:GLU:HB3	1:B:1148:PRO:HD3	1.91	0.52
1:B:640:LEU:O	1:B:642:ILE:HG13	2.09	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:B:1138:VAL:CG1	1:B:1183:LEU:HD12	2.39	0.51
1:A:381:SER:O	1:A:384:LYS:HB2	2.09	0.51
2:C:307:PHE:HD2	2:C:310:LEU:HD22	1.75	0.51
1:B:898:GLU:HB3	1:B:909:LEU:HD13	1.92	0.51
1:B:386:ARG:CG	1:B:387:GLU:H	2.07	0.51
2:E:341:LYS:HD2	2:E:341:LYS:H	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
1:B:38:SER:O	1:B:39:ILE:HB	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:HG13	2:C:671:VAL:O	2.11	0.50
1:B:368:LEU:HD11	1:B:405:THR:HG23	1.91	0.50
2:E:340:GLN:HG2	2:E:341:LYS:CD	2.42	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:494:TRP:CH2	2:E:530:ILE:HG21	2.46	0.50
1:A:253:LEU:HD21	1:A:289:GLU:HB2	1.93	0.50
2:E:216:THR:HA	2:E:219:LYS:HB2	1.93	0.50
2:C:831:THR:OG1	2:C:834:GLU:HB2	2.12	0.50
1:B:38:SER:OG	1:B:39:ILE:N	2.44	0.50
1:A:1068:MET:HG3	2:E:302:MET:HE3	1.93	0.50
1:A:270:GLU:HG3	1:A:274:TYR:CE2	2.45	0.50
1:B:996:HIS:HB2	1:B:997:PRO:HD2	1.92	0.50
1:A:257:ILE:N	1:A:258:PRO:HD2	2.27	0.50
1:B:35:GLN:O	1:B:36:LYS:HG2	2.12	0.50
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:1152:THR:HG23	1:A:1172:LEU:HD13	1.94	0.49
2:E:598:TYR:HD1	2:E:878:LYS:O	1.95	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:716:LEU:HB3	1:B:758:PHE:CE1	2.47	0.49
1:B:625:ARG:HG3	1:B:658:PHE:CE1	2.47	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:E:886:LEU:O	2:E:890:ILE:HG12	2.12	0.49
2:C:538:GLU:O	2:C:542:ASN:HB2	2.13	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
2:E:340:GLN:O	2:E:342:VAL:N	2.45	0.49
2:E:796:ASN:HB2	2:E:797:PRO:HD3	1.94	0.49
1:A:648:LEU:HD21	1:A:677:LEU:HD22	1.95	0.49
2:E:761:GLU:HB3	2:E:809:ILE:HG22	1.94	0.49
2:C:633:LEU:O	2:C:637:CYS:HB2	2.13	0.49
2:E:233:ILE:H	2:E:233:ILE:HD13	1.78	0.49
1:A:350:ARG:HE	1:A:386:ARG:CZ	2.25	0.49
2:C:516:VAL:HG13	2:C:563:ILE:HD13	1.93	0.49
1:A:1158:LYS:CD	1:A:1158:LYS:H	2.26	0.49
2:E:557:ASN:ND2	2:E:843:PHE:HZ	2.10	0.49
1:A:169:LEU:HB3	1:A:172:PHE:HB2	1.94	0.49
2:E:681:ILE:HD11	2:E:721:LEU:HD22	1.95	0.49
2:E:345:LYS:HA	2:E:348:ASP:HB2	1.94	0.49
1:B:528:VAL:O	1:B:536:THR:HG23	2.13	0.49
2:C:742:GLU:HG3	2:C:820:ARG:HB3	1.94	0.49
1:B:946:GLY:O	1:B:950:VAL:HG23	2.12	0.49
2:C:351:LEU:O	2:C:355:GLU:HB2	2.13	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:B:180:LEU:HD22	1:B:195:THR:HG23	1.95	0.48
1:A:465:LEU:HD22	1:A:468:ALA:HB2	1.95	0.48
1:A:260:VAL:HB	1:A:279:PHE:HE1	1.78	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:A:142:ILE:HD12	1:A:155:LEU:HG	1.94	0.48
2:C:307:PHE:CD1	2:C:307:PHE:N	2.81	0.48
2:C:698:PRO:HD3	2:C:751:LEU:HD21	1.95	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: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
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:149:SER:HA	1:A:152:LEU:HB2	1.96	0.48
2:E:340:GLN:HE22	2:E:342:VAL:HG22	1.79	0.48
1:A:1086:PHE:CZ	1:A:1112:GLY:HA3	2.48	0.48
3:F:73:GLY:HA3	3:F:101:TRP:CH2	2.49	0.48
1:A:855:LEU:CD1	1:A:858:LYS:HE3	2.44	0.48
1:A:659:LEU:HD22	1:A:700:LEU:HD11	1.96	0.48
1:B:543:THR:HG23	1:B:568:LEU:HD22	1.94	0.48
1:A:547:VAL:HG11	1:A:596:ILE:HA	1.94	0.47
1:B:467:GLY:HA2	1:B:508:HIS:CE1	2.49	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:A:62:GLY:O	1:A:65:GLN:HB2	2.14	0.47
1:B:4:ALA:C	1:B:40:LYS:HG3	2.34	0.47
2:E:622:SER:HB3	2:E:625:ALA:HB2	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
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
2:C:622:SER:HB3	2:C:625:ALA:HB3	1.96	0.47
1:B:850:ASP:OD1	1:B:852:SER:HB2	2.14	0.47
2:C:340:GLN:HB3	2:C:342:VAL:H	1.80	0.47
1:B:347:TRP:HA	1:B:350:ARG:NE	2.29	0.47
1:A:350:ARG:HE	1:A:386:ARG:NH2	2.13	0.47
2:C:450:GLY:HA2	2:C:453:LEU:HD22	1.95	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
3:D:94:CYS:HB2	3:D:101:TRP:HB2	1.96	0.47
2:C:674:ASN:OD1	2:C:674:ASN:N	2.47	0.47
1:B:928:TYR:O	1:B:932:ILE:HG12	2.14	0.47
1:B:386:ARG:HH11	1:B:386:ARG:CG	2.27	0.47
1:B:376:SER:HA	1:B:380:ILE:HD13	1.95	0.47
2:C:505:ILE:HA	2:C:511:LYS:HD2	1.96	0.47
1:B:388:GLU:O	1:B:391:LYS:HB3	2.15	0.47
1:A:550:ILE:C	1:A:552:PRO:HD2	2.34	0.47
1:A:948:ARG:O	1:A:952:VAL:HG23	2.14	0.47
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:69:VAL:HG11	1:A:108:ILE:HG22	1.96	0.46
1:A:596:ILE:HG23	1:A:600:LEU:HD12	1.97	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:E:411:PRO:HG3	2:E:464:LEU:HD21	1.97	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
1:B:1180:VAL:O	1:B:1183:LEU:HD23	2.15	0.46
1:A:987:THR:OG1	1:A:1025:VAL:HG11	2.15	0.46
2:C:748:PHE:CD2	2:C:773:ILE:HD12	2.50	0.46
1:B:813:GLU:HA	1:B:813:GLU:OE1	2.15	0.46
1:A:813:GLU:O	1:A:817:VAL:HG23	2.15	0.46
1:A:1109:VAL:HG22	1:A:1126:MET:HE2	1.98	0.46
1:B:617:GLU:HA	1:B:620:LYS:HD2	1.96	0.46
1:A:838:ALA:O	1:A:842:LEU:HG	2.16	0.46
1:B:828:SER:O	1:B:829:ARG:HB2	2.16	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
2:C:530:ILE:HG13	2:C:531:ASP:N	2.30	0.46
1:B:1056:THR:HA	1:B:1082:ARG:HG3	1.98	0.46
2:E:720:LYS:HB3	3:F:36:ASP:HB2	1.98	0.46
1:A:357:LEU:O	1:A:361:VAL:HG23	2.16	0.46
1:B:552:PRO:C	1:B:554:ASP:H	2.19	0.46
1:B:857:LEU:HD12	1:B:858:LYS:N	2.31	0.46
1:A:346:SER:HB2	1:A:350:ARG:HH12	1.80	0.46
2:E:340:GLN:HG2	2:E:341:LYS:HD2	1.97	0.46
1:B:499:SER:O	1:B:503:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
2:E:698:PRO:O	2:E:700:GLU:N	2.48	0.46
1:A:633:THR:HA	1:A:676:ILE:HD11	1.97	0.46
1:B:529:GLY:HA2	1:B:575:ARG:HH21	1.81	0.46
1:B:209:ILE:O	1:B:212:VAL:HG12	2.16	0.46
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
2:C:905:ASN:C	2:C:907:ASN:H	2.20	0.45
1:B:35:GLN:O	1:B:36:LYS:CG	2.64	0.45
1:A:914:LYS:O	1:A:918:SER:HB2	2.16	0.45
1:B:831:THR:HG22	1:B:832:ASP:H	1.80	0.45
1:B:456:ASN:ND2	1:B:496:ASP:OD1	2.46	0.45
1:B:929:VAL:HG13	1:B:958:LEU:HD22	1.98	0.45
1:A:854:GLN:NE2	1:A:854:GLN:H	2.13	0.45
1:A:957:LYS:HA	1:A:960:LEU:HD23	1.98	0.45
2:E:491:LEU:HG	2:E:540:PHE:CZ	2.51	0.45
2:E:847:GLN:HE22	2:E:885:ASP:HB3	1.80	0.45
1:A:253:LEU:HD13	1:A:254:GLU:N	2.31	0.45
1:A:24:PHE:HE2	1:A:63:GLU:HB3	1.80	0.45
2:C:465:LEU:HB3	2:C:497:TYR:CZ	2.51	0.45
1:B:605:GLY:C	1:B:607:ASP:H	2.19	0.45
2:E:580:ASP:HA	2:E:583:LEU:HB3	1.99	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:795:LYS:HE2	2:C:802:ILE:HG12	1.98	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
1:A:804:ALA:HB2	1:A:844:GLU:HB3	1.99	0.45
1:A:286:CYS:C	1:A:288:LYS:H	2.20	0.45
2:C:756:PHE:HB3	3:D:21:ARG:HD2	1.98	0.45
2:E:428:LEU:HD23	2:E:440:LEU:HD23	1.99	0.45
1:B:655:LEU:HA	1:B:658:PHE:HD2	1.82	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:768:ASN:O	1:A:769:ASN:HB2	2.16	0.45
1:B:380:ILE:N	1:B:380:ILE:HD12	2.32	0.45
1:A:1068:MET:HG3	2:E:302:MET:CE	2.47	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
2:E:854:ILE:HD13	2:E:890:ILE:HD13	2.00	0.44
1:A:1012:LEU:HD11	1:A:1030:PHE:HB2	1.98	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:D:37:ILE:HG22	3:D:37:ILE:O	2.16	0.44
1:B:993:ILE:HG13	1:B:993:ILE:H	1.64	0.44
2:C:235:TYR:O	2:C:236:ASN:CB	2.65	0.44
3:F:88:LEU:HD21	3:F:101:TRP:HD1	1.82	0.44
2:E:275:PHE:CE2	2:E:289:ILE:HD13	2.53	0.44
1:A:428:LEU:HD23	1:A:465:LEU:HD12	1.99	0.44
1:B:253:LEU:HA	1:B:256:ILE:HG13	2.00	0.44
3:F:37:ILE:O	3:F:38:VAL:C	2.56	0.44
1:A:500:CYS:O	1:A:504:ILE:HG13	2.17	0.44
1:B:885:VAL:HG13	1:B:920:ALA:HA	1.99	0.44
2:E:391:GLU:HG2	2:E:395:ARG:HH22	1.81	0.44
2:C:667:GLN:HE21	2:C:667:GLN:HB3	1.61	0.44
2:E:719:ARG:HD3	3:F:33:TRP:CE3	2.53	0.44
1:B:1188:GLU:CG	1:B:1189:ALA:N	2.80	0.44
2:C:560:ALA:HB2	2:C:597:ILE:HG21	1.99	0.44
2:C:559:PRO:O	2:C:563:ILE:HG12	2.17	0.44
2:E:743:LEU:HD22	2:E:823:ILE:HD11	2.00	0.44
1:B:1001:ASP:HA	1:B:1004:LEU:HB2	1.99	0.44
1:B:146:GLU:HG2	1:B:146:GLU:H	1.57	0.44
1:A:466:PRO:HB3	1:A:507:ASN:HD22	1.83	0.44
1:A:742:VAL:HA	1:A:747:LEU:HD22	2.00	0.44
2:C:730:CYS:HB2	3:D:26:LYS:O	2.18	0.44
1:B:231:THR:HG21	1:B:263:PHE:CE2	2.52	0.44
2:E:507:ILE:HD11	2:E:554:LYS:HB3	2.00	0.44
2:C:404:LEU:HD22	2:C:408:ARG:HE	1.83	0.44
2:E:861:ARG:NH1	2:E:872:GLU:OE2	2.50	0.44
2:C:757:ASN:HD22	3:D:20:LYS:HD2	1.83	0.44
1:A:697:LEU:N	1:A:698:PRO:CD	2.81	0.44
1:B:386:ARG:CG	1:B:387:GLU:N	2.78	0.44
1:A:350:ARG:HH21	1:A:386:ARG:NH2	2.04	0.44
1:A:551:ARG:NE	1:A:553:LEU:HB2	2.33	0.44
1:A:368:LEU:HD11	1:A:405:THR:HG23	2.00	0.44
1:B:381:SER:HA	1:B:384:LYS:HE2	1.99	0.44
2:C:227:ILE:HD11	2:C:303:ILE:CG1	2.37	0.44
1:A:855:LEU:HG	1:A:855:LEU:O	2.17	0.44
1:B:285:ARG:C	1:B:287:PRO:HD3	2.38	0.44
2:E:859:LYS:HE3	2:E:859:LYS:HB3	1.80	0.44
1:A:1037:LYS:HB3	1:A:1040:LEU:HD12	1.99	0.44
1:B:375:VAL:C	1:B:380:ILE:HD11	2.38	0.43
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:B:231:THR:HA	1:B:234:TYR:HB2	1.99	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:622:SER:HB3	2:E:625:ALA:CB	2.48	0.43
2:E:293:TRP:O	2:E:297:CYS:HB2	2.18	0.43
2:C:338:SER:O	2:C:340:GLN:N	2.51	0.43
1:A:727:LEU:C	1:A:729:LYS:H	2.22	0.43
1:A:1117:TYR:HE1	1:A:1172:LEU:HB2	1.83	0.43
1:A:406:ARG:HD2	1:A:464:VAL:HG22	2.00	0.43
1:A:276:ILE:HG21	1:A:353:ALA:CA	2.44	0.43
2:E:300:MET:C	2:E:302:MET:H	2.22	0.43
2:C:332:PHE:CE1	2:C:336:ILE:HD12	2.54	0.43
1:B:996:HIS:CB	1:B:997:PRO:CD	2.96	0.43
1:B:730:ILE:HA	1:B:734:ILE:HD12	2.01	0.43
1:A:543:THR:O	1:A:547:VAL:HG23	2.18	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:B:144:LYS:HA	1:B:144:LYS:NZ	2.34	0.43
1:B:385:GLU:HA	1:B:391:LYS:HE2	2.00	0.43
1:A:144:LYS:CD	1:A:144:LYS:H	2.28	0.43
1:A:854:GLN:CD	1:A:854:GLN:H	2.21	0.43
2:C:630:LEU:HD21	2:C:645:LEU:HB3	2.01	0.43
1:A:1038:PRO:C	1:A:1040:LEU:H	2.21	0.43
1:A:962:ASP:HA	1:A:963:PRO:HD3	1.92	0.43
1:B:1057:LYS:HE2	1:B:1108:HIS:HE1	1.83	0.43
1:A:800:ALA:O	1:A:803:VAL:HG12	2.18	0.43
1:A:1068:MET:HB2	2:E:227:ILE:HA	1.99	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
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
1:B:731:SER:HB2	1:B:770:LEU:HD11	2.00	0.43
1:A:448:VAL:HG13	1:A:493:LEU:HD22	2.01	0.43
2:C:763:SER:O	2:C:766:GLU:HG2	2.19	0.43
3:D:52:LEU:HD12	3:D:56:CYS:HB3	2.00	0.43
2:E:741:LYS:HG2	2:E:818:LEU:O	2.19	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
1:A:544:GLN:HG3	1:A:592:CYS:HA	2.01	0.43
1:A:203:VAL:HG11	1:A:241:ILE:HG12	2.01	0.43
2:C:381:TYR:C	2:C:383:ASP:H	2.21	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:138:LEU:O	1:A:142:ILE:HG12	2.19	0.43
1:A:839:LEU:HA	1:A:842:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:697:LEU:HA	1:B:700:LEU:HD12	2.00	0.43
1:A:744:SER:HA	1:A:745:PRO:HD3	1.80	0.43
2:C:424:GLU:OE1	2:C:424:GLU:HA	2.18	0.42
1:A:501:LEU:HA	1:A:504:ILE:HD12	2.00	0.42
3:D:47:ASN:O	3:D:48:HIS:HB2	2.18	0.42
1:B:350:ARG:HD3	1:B:350:ARG:H	1.84	0.42
1:A:276:ILE:HD13	1:A:353:ALA:HB2	2.01	0.42
1:B:553:LEU:HD22	1:B:639:PRO:HB2	2.01	0.42
1:A:485:ASN:HD22	1:A:523:PRO:HB3	1.84	0.42
1:B:739:ILE:HA	1:B:742:VAL:HG23	2.01	0.42
1:A:952:VAL:O	1:A:952:VAL:HG12	2.19	0.42
1:A:491:SER:HA	1:A:535:ILE:HD11	2.01	0.42
2:E:853:ALA:HA	2:E:856:ARG:HG2	2.00	0.42
3:D:84:ILE:HD13	3:D:84:ILE:O	2.19	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
2:E:311:ASP:HA	2:E:315:VAL:HG23	2.00	0.42
2:E:750:THR:O	2:E:754:LEU:HB2	2.19	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
1:B:821:PHE:HB2	1:B:860:VAL:HG11	2.02	0.42
1:A:253:LEU:HD13	1:A:254:GLU:H	1.84	0.42
2:E:298:ARG:HB3	2:E:298:ARG:CZ	2.50	0.42
1:A:110:LEU:HD23	1:A:157:ILE:HG21	2.01	0.42
1:A:644:LEU:C	1:A:646:PRO:HD2	2.40	0.42
2:C:732:LEU:O	2:C:742:GLU:HB2	2.19	0.42
2:E:855:VAL:O	2:E:859:LYS:HB2	2.20	0.42
2:C:228:GLN:HE22	2:C:264:CYS:HA	1.85	0.42
2:E:509:PRO:C	2:E:511:LYS:H	2.22	0.42
2:E:606:PHE:CZ	2:E:838:THR:HG23	2.55	0.42
1:A:408:VAL:O	1:A:409:GLN:HB2	2.19	0.42
2:E:453:LEU:HD12	2:E:480:PHE:CE2	2.55	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
1:B:233:THR:HA	1:B:236:GLN:HE21	1.85	0.42
2:E:468:ASN:HD22	2:E:468:ASN:C	2.21	0.42
1:A:898:GLU:HA	1:A:901:SER:HB3	2.02	0.42
1:B:484:LEU:HD21	1:B:498:LEU:HG	2.01	0.42
2:E:749:GLN:HG2	2:E:785:LEU:HD11	2.00	0.42
2:E:545:LYS:HE2	2:E:545:LYS:HB3	1.82	0.42
1:A:1117:TYR:HD1	1:A:1172:LEU:HG	1.85	0.42
1:A:409:GLN:HE21	1:A:409:GLN:HB2	1.70	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:E:691:VAL:HA	2:E:692:PRO:HD3	1.85	0.42
1:B:1129:ARG:C	1:B:1131:SER:H	2.23	0.42
2:C:642:THR:HA	2:C:645:LEU:HD12	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
1:A:594:GLY:HA2	1:A:635:ILE:HD11	2.02	0.42
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:1113:LEU:HA	1:A:1113:LEU:HD22	1.97	0.41
2:E:533:CYS:HB2	2:E:534:PHE:HD1	1.85	0.41
1:B:821:PHE:HA	1:B:824:ASP:CB	2.49	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
2:C:708:PHE:O	2:C:711:PHE:HB3	2.20	0.41
2:C:363:ILE:HG22	2:C:365:ARG:HG2	2.01	0.41
1:A:1194:LEU:HD13	1:A:1194:LEU:H	1.85	0.41
2:E:397:TYR:HE1	2:E:420:ARG:HD2	1.82	0.41
2:C:572:ARG:HB3	2:C:574:GLY:H	1.85	0.41
1:B:246:GLY:HA3	1:B:285:ARG:CG	2.50	0.41
2:E:499:LYS:HE2	2:E:550:THR:HG21	2.02	0.41
1:A:57:LEU:HD12	1:A:68:ALA:HB1	2.02	0.41
1:B:1180:VAL:HG12	1:B:1184:LEU:HD11	2.02	0.41
1:B:1017:ASP:N	1:B:1018:PRO:HD2	2.35	0.41
2:C:235:TYR:O	2:C:236:ASN:HB2	2.21	0.41
1:A:579:ALA:HB2	1:A:618:ARG:HH22	1.85	0.41
1:A:1131:SER:HB3	1:A:1183:LEU:HD23	2.01	0.41
1:B:502:TYR:HB2	1:B:542:VAL:HG22	2.01	0.41
1:B:1102:ILE:H	1:B:1102:ILE:HG12	1.69	0.41
1:A:135:THR:CG2	1:A:176:ILE:HD11	2.51	0.41
1:B:933:TRP:HA	1:B:936:LEU:HD12	2.02	0.41
2:E:681:ILE:HD12	3:F:31:ALA:HB3	2.03	0.41
1:A:685:LEU:HA	1:A:689:MET:SD	2.60	0.41
1:A:664:ARG:NH1	1:A:705:ASP:OD2	2.53	0.41
3:D:97:ASP:OD1	3:D:97:ASP:N	2.54	0.41
1:B:72:LEU:O	1:B:76:VAL:HG23	2.20	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
2:E:468:ASN:HD21	2:E:470:ILE:HG23	1.86	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
1:A:824:ASP:N	1:A:824:ASP:OD1	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1038:PRO:C	1:B:1040:LEU:H	2.24	0.41
1:A:561:ALA:C	1:A:563:PRO:HD2	2.41	0.41
1:B:855:LEU:HD23	1:B:856:GLU:H	1.86	0.41
1:A:857:LEU:HD21	1:A:883:ILE:HD13	2.02	0.41
2:E:899:MET:HA	2:E:911:TYR:O	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:371:PHE:O	1:A:375:VAL:HG22	2.21	0.41
2:C:769:GLN:HB3	2:C:769:GLN:HE21	1.69	0.41
1:B:452:GLN:HE22	1:B:492:ASN:HD22	1.69	0.41
2:C:816:HIS:CD2	2:C:818:LEU:O	2.69	0.41
2:E:494:TRP:CE3	2:E:540:PHE:HD2	2.38	0.41
2:E:404:LEU:HD22	2:E:408:ARG:HH21	1.86	0.41
1:B:760:GLN:HE21	1:B:805:ALA:HB1	1.85	0.41
1:A:888:LEU:N	1:A:889:PRO:HD2	2.36	0.41
1:A:602:ASP:OD1	1:A:640:LEU:HD11	2.21	0.41
2:C:791:ARG:CZ	2:C:816:HIS:HB2	2.51	0.40
1:A:645:ARG:HD2	1:A:684:SER:OG	2.21	0.40
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
3:D:45:CYS:HB2	3:D:54:ILE:HG12	2.04	0.40
2:E:741:LYS:HA	2:E:819:PHE:CE1	2.56	0.40
2:E:464:LEU:HB3	2:E:473:LEU:CD2	2.51	0.40
2:C:321:LEU:HA	2:C:322:PRO:HD2	1.85	0.40
2:C:272:ILE:C	2:C:274:GLN:H	2.24	0.40
1:B:406:ARG:HA	1:B:407:PRO:HD3	1.90	0.40
1:B:19:ASP:HA	3:D:92:GLN:NE2	2.30	0.40
1:A:65:GLN:HB3	1:A:105:ILE:HD11	2.02	0.40
2:C:612:ALA:HA	2:C:687:TRP:HZ3	1.86	0.40
1:B:611:THR:O	1:B:614:ILE:HB	2.21	0.40
1:A:772:TYR:CD2	1:A:812:LYS:HG3	2.57	0.40
1:B:733:SER:HA	1:B:736:ASN:HB2	2.03	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:1160:ASN:OD1	2:C:308:LEU:HD13	2.22	0.40
1:B:1134:CYS:HA	1:B:1135:PRO:HD2	1.99	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%)	12	69
1	B	1142/1253 (91%)	991 (87%)	129 (11%)	22 (2%)	12	69
2	C	686/741 (93%)	589 (86%)	83 (12%)	14 (2%)	11	68
2	E	690/741 (93%)	611 (89%)	63 (9%)	16 (2%)	10	65
3	D	87/98 (89%)	62 (71%)	16 (18%)	9 (10%)	1	19
3	F	76/98 (78%)	48 (63%)	23 (30%)	5 (7%)	2	36
All	All	3826/4184 (91%)	3302 (86%)	436 (11%)	88 (2%)	10	65

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	904 (88%)	124 (12%)	7	42
1	B	1033/1118 (92%)	893 (86%)	140 (14%)	5	36
2	C	632/675 (94%)	548 (87%)	84 (13%)	6	37
2	E	637/675 (94%)	556 (87%)	81 (13%)	6	39
3	D	78/83 (94%)	62 (80%)	16 (20%)	2	14
3	F	72/83 (87%)	60 (83%)	12 (17%)	3	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	3480/3752 (93%)	3023 (87%)	457 (13%)	6 38

All (457) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	TYR
1	A	20	LYS
1	A	36	LYS
1	A	55	LYS
1	A	60	LYS
1	A	114	ILE
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	205	SER
1	A	209	ILE
1	A	210	VAL
1	A	222	LEU
1	A	223	SER
1	A	252	TYR
1	A	253	LEU
1	A	254	GLU
1	A	270	GLU
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	383	PHE
1	A	384	LYS
1	A	389	ASN
1	A	406	ARG
1	A	423	THR
1	A	425	LEU
1	A	449	LYS

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Mol	Chain	Res	Type
1	A	465	LEU
1	A	475	VAL
1	A	483	SER
1	A	486	ASP
1	A	487	LYS
1	A	496	ASP
1	A	499	SER
1	A	534	LYS
1	A	545	GLN
1	A	555	GLN
1	A	558	SER
1	A	562	THR
1	A	566	LYS
1	A	573	ILE
1	A	616	LEU
1	A	618	ARG
1	A	621	ASN
1	A	625	ARG
1	A	626	LEU
1	A	628	THR
1	A	632	LEU
1	A	655	LEU
1	A	682	SER
1	A	710	GLN
1	A	723	TYR
1	A	729	LYS
1	A	730	ILE
1	A	735	LEU
1	A	745	PRO
1	A	746	LEU
1	A	770	LEU
1	A	773	MET
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	874	SER

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Mol	Chain	Res	Type
1	A	882	SER
1	A	884	SER
1	A	905	ARG
1	A	911	HIS
1	A	913	LEU
1	A	918	SER
1	A	921	SER
1	A	922	VAL
1	A	958	LEU
1	A	962	ASP
1	A	965	THR
1	A	967	LEU
1	A	1004	LEU
1	A	1005	LYS
1	A	1007	CYS
1	A	1015	LEU
1	A	1020	LEU
1	A	1040	LEU
1	A	1041	ILE
1	A	1043	ASP
1	A	1046	ASP
1	A	1047	THR
1	A	1055	GLU
1	A	1068	MET
1	A	1071	PHE
1	A	1072	LYS
1	A	1074	THR
1	A	1087	GLU
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	1165	GLU
1	A	1170	ASP
1	A	1172	LEU

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Mol	Chain	Res	Type
1	A	1175	SER
1	A	1186	ILE
1	A	1194	LEU
1	B	8	ILE
1	B	33	GLU
1	B	35	GLN
1	B	39	ILE
1	B	42	ASP
1	B	43	ASP
1	B	60	LYS
1	B	71	CYS
1	B	96	LEU
1	B	98	ASP
1	B	101	GLN
1	B	111	LYS
1	B	112	THR
1	B	116	GLU
1	B	133	LYS
1	B	144	LYS
1	B	146	GLU
1	B	170	VAL
1	B	173	HIS
1	B	175	SER
1	B	179	CYS
1	B	188	ARG
1	B	189	LEU
1	B	194	ARG
1	B	202	LEU
1	B	204	MET
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	232	ARG
1	B	238	ILE
1	B	242	SER
1	B	253	LEU
1	B	254	GLU
1	B	255	LYS

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Mol	Chain	Res	Type
1	B	256	ILE
1	B	257	ILE
1	B	275	CYS
1	B	285	ARG
1	B	291	TYR
1	B	300	ILE
1	B	302	LEU
1	B	306	THR
1	B	345	MET
1	B	350	ARG
1	B	351	ARG
1	B	364	ARG
1	B	370	GLU
1	B	380	ILE
1	B	381	SER
1	B	386	ARG
1	B	388	GLU
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	490	SER
1	B	496	ASP
1	B	501	LEU
1	B	512	VAL
1	B	541	LEU
1	B	546	LEU
1	B	551	ARG
1	B	555	GLN
1	B	562	THR
1	B	566	LYS
1	B	583	GLN
1	B	604	LEU
1	B	618	ARG
1	B	625	ARG
1	B	640	LEU

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Mol	Chain	Res	Type
1	B	650	GLU
1	B	672	SER
1	B	690	ILE
1	B	697	LEU
1	B	702	SER
1	B	703	GLU
1	B	710	GLN
1	B	738	LEU
1	B	752	LEU
1	B	765	THR
1	B	777	ARG
1	B	802	CYS
1	B	806	LEU
1	B	808	ARG
1	B	813	GLU
1	B	825	VAL
1	B	826	LYS
1	B	829	ARG
1	B	831	THR
1	B	832	ASP
1	B	836	LEU
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	938	LYS
1	B	967	LEU
1	B	974	LEU
1	B	975	ILE
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	1016	GLU

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Mol	Chain	Res	Type
1	B	1019	ASP
1	B	1020	LEU
1	B	1044	LEU
1	B	1056	THR
1	B	1130	LEU
1	B	1139	LEU
1	B	1155	THR
1	B	1164	GLN
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	1198	PHE
1	B	1208	LEU
1	B	1215	ILE
2	C	216	THR
2	C	217	TRP
2	C	247	LEU
2	C	252	ILE
2	C	256	LEU
2	C	258	LYS
2	C	260	LEU
2	C	272	ILE
2	C	277	GLU
2	C	280	LEU
2	C	281	ASP
2	C	284	LEU
2	C	301	ILE
2	C	302	MET
2	C	311	ASP
2	C	329	LEU
2	C	337	ILE
2	C	343	GLN
2	C	345	LYS
2	C	378	LEU
2	C	400	GLU
2	C	402	GLN
2	C	403	LYS
2	C	407	GLU
2	C	414	LEU

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Mol	Chain	Res	Type
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	465	LEU
2	C	467	GLU
2	C	471	GLN
2	C	493	GLN
2	C	513	LYS
2	C	530	ILE
2	C	539	LYS
2	C	544	MET
2	C	549	GLU
2	C	550	THR
2	C	552	ILE
2	C	555	ARG
2	C	562	LEU
2	C	572	ARG
2	C	580	ASP
2	C	583	LEU
2	C	585	LYS
2	C	592	ILE
2	C	604	GLU
2	C	611	LEU
2	C	613	LYS
2	C	627	LYS
2	C	633	LEU
2	C	657	ASP
2	C	667	GLN
2	C	671	VAL
2	C	677	LEU
2	C	678	THR
2	C	683	THR
2	C	684	MET
2	C	715	LYS
2	C	723	TRP
2	C	747	LEU
2	C	769	GLN
2	C	778	LEU

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Mol	Chain	Res	Type
2	C	801	ASP
2	C	806	ASP
2	C	813	ASP
2	C	826	ILE
2	C	827	GLN
2	C	831	THR
2	C	835	GLN
2	C	839	THR
2	C	841	ARG
2	C	861	ARG
2	C	863	THR
2	C	865	SER
2	C	881	VAL
2	C	886	LEU
2	C	901	ARG
2	C	905	ASN
2	C	912	ILE
3	D	25	LYS
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	86	ARG
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	233	ILE
2	E	235	TYR
2	E	251	LYS
2	E	255	ASN
2	E	256	LEU
2	E	259	GLN
2	E	260	LEU

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Mol	Chain	Res	Type
2	E	263	ILE
2	E	288	LYS
2	E	297	CYS
2	E	310	LEU
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	352	LEU
2	E	363	ILE
2	E	366	SER
2	E	378	LEU
2	E	379	GLN
2	E	395	ARG
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	468	ASN
2	E	484	ARG
2	E	488	GLN
2	E	493	GLN
2	E	503	SER
2	E	504	THR
2	E	513	LYS
2	E	520	LEU
2	E	532	ILE
2	E	539	LYS
2	E	544	MET
2	E	548	PHE
2	E	551	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

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Mol	Chain	Res	Type
2	E	592	ILE
2	E	595	ARG
2	E	611	LEU
2	E	619	LYS
2	E	627	LYS
2	E	641	PHE
2	E	653	GLU
2	E	666	MET
2	E	667	GLN
2	E	691	VAL
2	E	695	VAL
2	E	723	TRP
2	E	726	THR
2	E	778	LEU
2	E	791	ARG
2	E	814	PHE
2	E	816	HIS
2	E	827	GLN
2	E	835	GLN
2	E	845	ASP
2	E	859	LYS
2	E	863	THR
2	E	874	TYR
2	E	877	LEU
2	E	878	LYS
2	E	886	LEU
2	E	895	ASP
2	E	897	ASP
2	E	901	ARG
2	E	905	ASN
3	F	19	LYS
3	F	25	LYS
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (75) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	83	GLN
1	A	151	GLN
1	A	404	GLN
1	A	409	GLN
1	A	429	GLN
1	A	463	ASN
1	A	492	ASN
1	A	508	HIS
1	A	514	HIS
1	A	595	GLN
1	A	603	ASN
1	A	621	ASN
1	A	854	GLN
1	A	897	GLN
1	A	902	GLN
1	A	911	HIS
1	A	939	HIS
1	A	1036	ASN
1	A	1107	ASN
1	A	1160	ASN
1	A	1164	GLN
1	B	35	GLN
1	B	66	ASN
1	B	101	GLN
1	B	225	ASN
1	B	236	GLN
1	B	442	GLN
1	B	485	ASN
1	B	492	ASN
1	B	508	HIS
1	B	516	HIS
1	B	621	ASN
1	B	760	GLN
1	B	820	GLN
1	B	902	GLN
1	B	1035	HIS
1	B	1107	ASN
1	B	1108	HIS
1	B	1201	GLN
2	C	228	GLN

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Mol	Chain	Res	Type
2	C	340	GLN
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	769	GLN
2	C	816	HIS
2	C	824	ASN
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	255	ASN
2	E	259	GLN
2	E	343	GLN
2	E	379	GLN
2	E	402	GLN
2	E	418	ASN
2	E	434	GLN
2	E	468	ASN
2	E	557	ASN
2	E	716	HIS
2	E	744	GLN
2	E	827	GLN
2	E	847	GLN
2	E	849	GLN
2	E	905	ASN
2	E	910	ASN
3	F	98	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 carbohydrates 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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	1155/1253 (92%)	-0.04	0	100	100	103, 127, 153, 165	0
1	B	1154/1253 (92%)	-0.04	0	100	100	90, 115, 159, 179	0
2	C	692/741 (93%)	0.14	8 (1%)	75	54	86, 129, 188, 201	0
2	E	696/741 (93%)	0.14	4 (0%)	86	70	98, 141, 173, 177	0
3	D	89/98 (90%)	0.08	0	100	100	111, 132, 148, 149	0
3	F	80/98 (81%)	0.09	0	100	100	141, 155, 168, 170	0
All	All	3866/4184 (92%)	0.03	12 (0%)	91	83	86, 125, 170, 201	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	816	HIS	2.9
2	C	221	LYS	2.9
2	C	817	LYS	2.8
2	E	217	TRP	2.6
2	E	793	LEU	2.5
2	C	743	LEU	2.3
2	E	664	GLN	2.2
2	C	234	LYS	2.1
2	C	220	LEU	2.1
2	C	795	LYS	2.1
2	C	901	ARG	2.0
2	C	219	LYS	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	ZN	D	4003	1/1	0.12	-0.63	104,104,104,104	0
4	ZN	D	4002	1/1	0.12	-0.72	92,92,92,92	0
4	ZN	D	4001	1/1	0.11	-0.80	104,104,104,104	0
4	ZN	F	4002	1/1	0.07	-1.11	120,120,120,120	0
4	ZN	F	4001	1/1	0.10	-1.27	113,113,113,113	0
4	ZN	F	4003	1/1	0.05	-1.38	144,144,144,144	0

6.5 Other polymers

There are no such residues in this entry.