



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:09 am BST

PDB ID : 2GIF
Title : Asymmetric structure of trimeric AcrB from Escherichia coli
Authors : Seeger, M.A.; Schiefner, A.; Eicher, T.; Verrey, F.; Diederichs, K.; Pos, K.M.
Deposited on : 2006-03-28
Resolution : 2.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

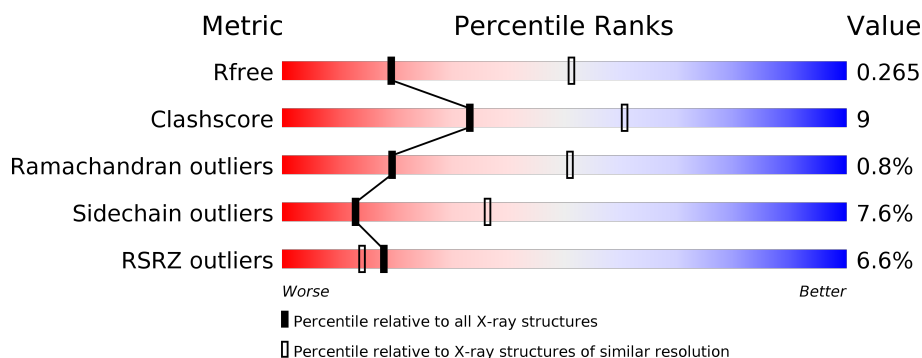
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	1057	<div> <div>7%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>••</div> </div> </div>
1	B	1057	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>20%</div> <div>••</div> </div> </div>
1	C	1057	<div> <div>5%</div> <div> <div></div> <div>73%</div> <div>22%</div> <div>••</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 23650 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 Acriflavine resistance protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1032	Total	C	N	O	S	0	0	0
			7841	5047	1294	1457	43			
1	B	1044	Total	C	N	O	S	0	0	0
			7942	5105	1315	1479	43			
1	C	1032	Total	C	N	O	S	0	0	0
			7841	5047	1294	1457	43			

There are 24 discrepancies between the modelled and reference sequences:

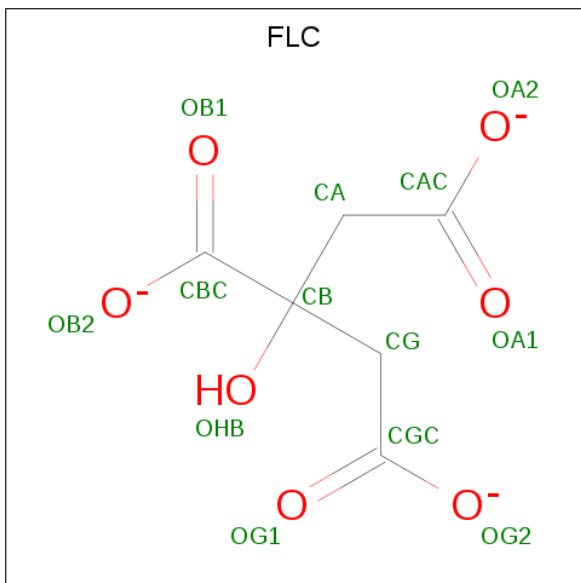
Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	LEU	-	CLONING ARTIFACT	UNP P31224
A	1051	GLU	-	CLONING ARTIFACT	UNP P31224
A	1052	HIS	-	EXPRESSION TAG	UNP P31224
A	1053	HIS	-	EXPRESSION TAG	UNP P31224
A	1054	HIS	-	EXPRESSION TAG	UNP P31224
A	1055	HIS	-	EXPRESSION TAG	UNP P31224
A	1056	HIS	-	EXPRESSION TAG	UNP P31224
A	1057	HIS	-	EXPRESSION TAG	UNP P31224
B	1050	LEU	-	CLONING ARTIFACT	UNP P31224
B	1051	GLU	-	CLONING ARTIFACT	UNP P31224
B	1052	HIS	-	EXPRESSION TAG	UNP P31224
B	1053	HIS	-	EXPRESSION TAG	UNP P31224
B	1054	HIS	-	EXPRESSION TAG	UNP P31224
B	1055	HIS	-	EXPRESSION TAG	UNP P31224
B	1056	HIS	-	EXPRESSION TAG	UNP P31224
B	1057	HIS	-	EXPRESSION TAG	UNP P31224
C	1050	LEU	-	CLONING ARTIFACT	UNP P31224
C	1051	GLU	-	CLONING ARTIFACT	UNP P31224
C	1052	HIS	-	EXPRESSION TAG	UNP P31224
C	1053	HIS	-	EXPRESSION TAG	UNP P31224
C	1054	HIS	-	EXPRESSION TAG	UNP P31224
C	1055	HIS	-	EXPRESSION TAG	UNP P31224
C	1056	HIS	-	EXPRESSION TAG	UNP P31224

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1057	HIS	-	EXPRESSION TAG	UNP P31224

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).

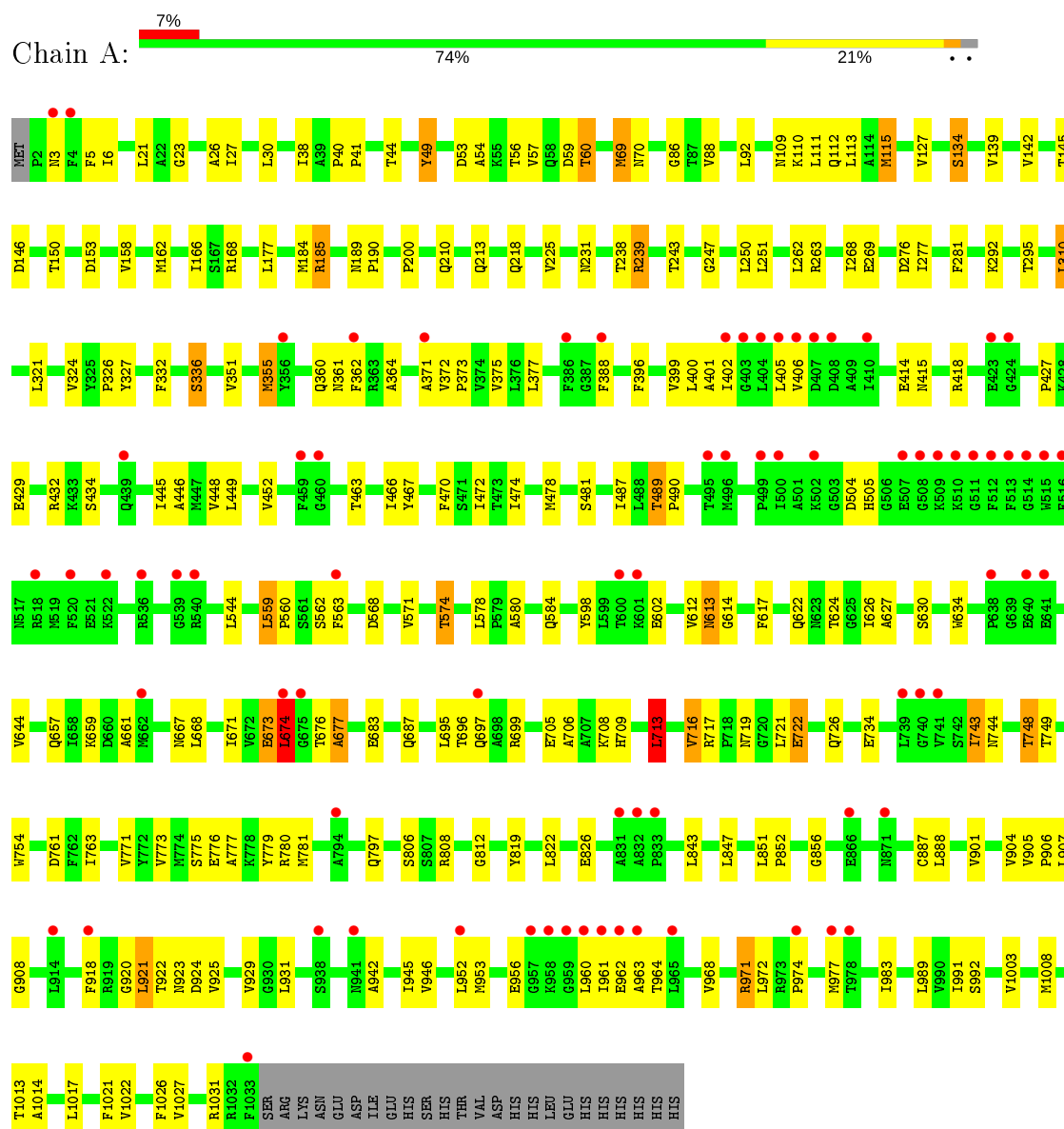


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		

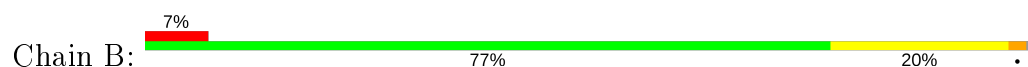
3 Residue-property plots

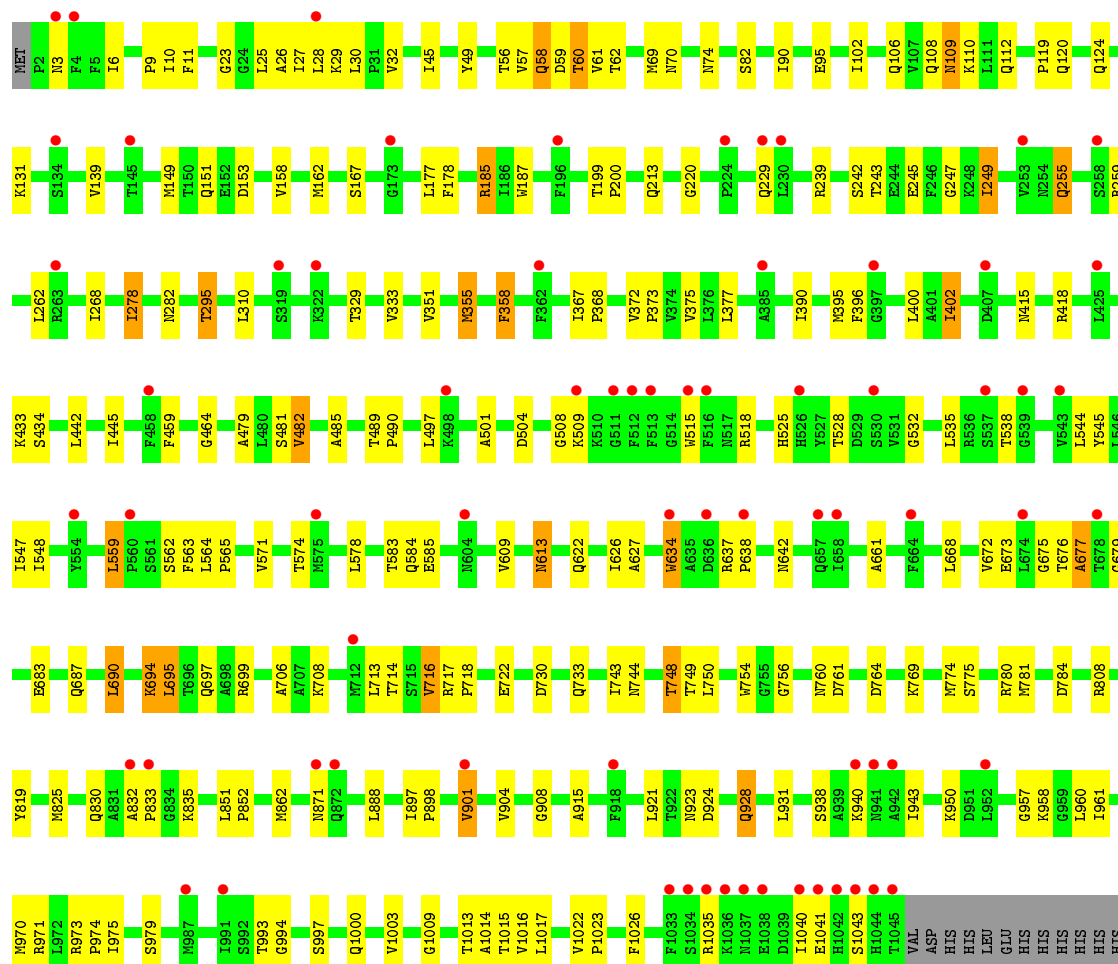
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

• Molecule 1: Acriflavine resistance protein B

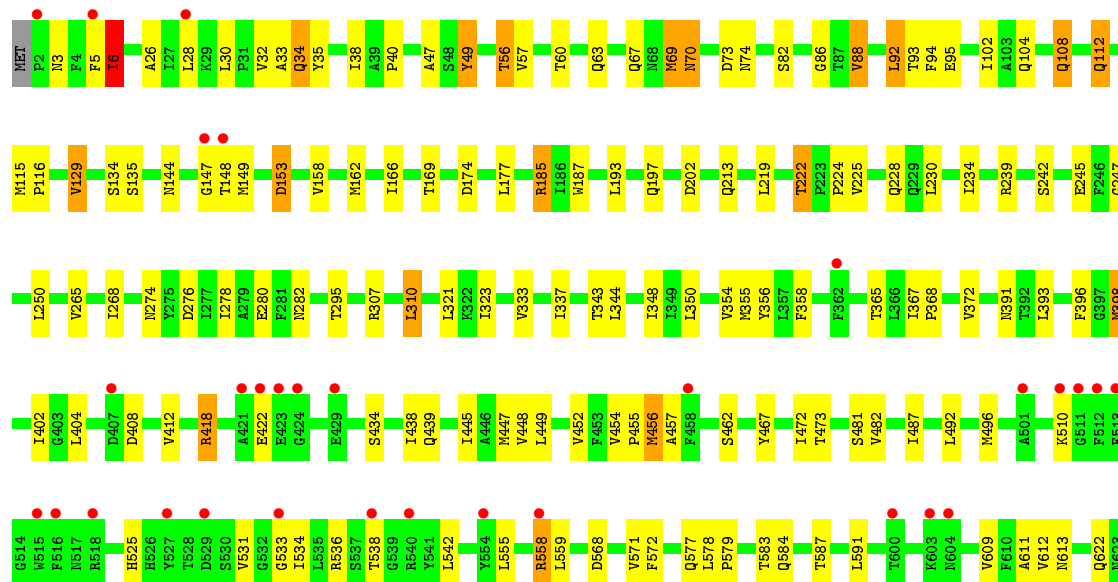
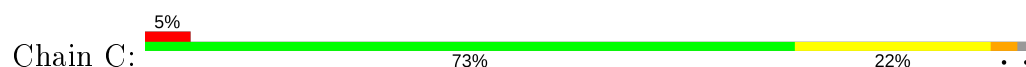


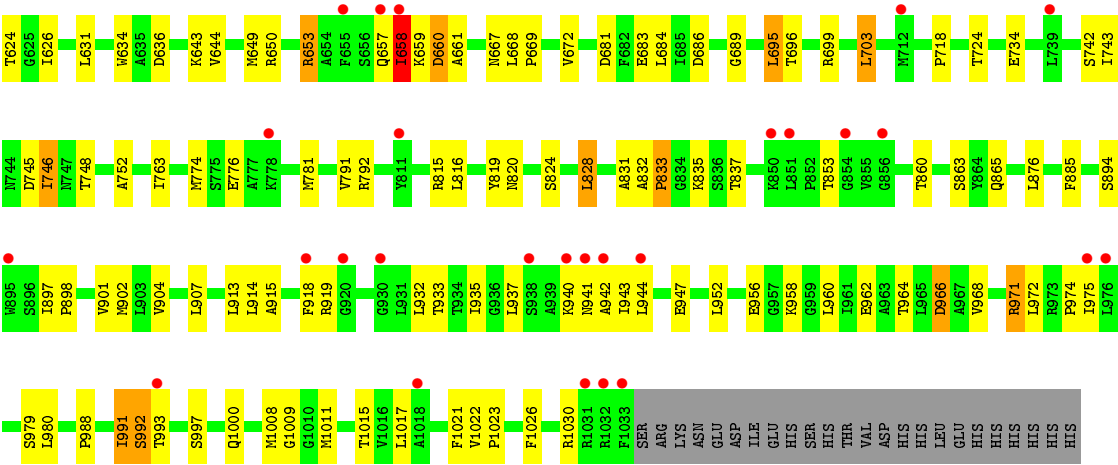
• Molecule 1: Acriflavine resistance protein B





• Molecule 1: Acriflavine resistance protein B





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	222.80Å 134.10Å 161.01Å 90.00° 98.21° 90.00°	Depositor
Resolution (Å)	29.51 – 2.90 29.22 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.51-2.90) 99.8 (29.22-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.226 , 0.267 0.226 , 0.265	Depositor DCC
R_{free} test set	5177 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	89.1	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 87.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	23650	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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: FLC

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	0/7991	0.54	1/10852 (0.0%)
1	B	0.37	0/8094	0.53	0/10990
1	C	0.36	1/7991 (0.0%)	0.53	1/10852 (0.0%)
All	All	0.37	1/24076 (0.0%)	0.53	2/32694 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	820	ASN	C-N	5.23	1.42	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	713	LEU	CA-CB-CG	5.82	128.69	115.30
1	C	92	LEU	CA-CB-CG	5.06	126.94	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7841	0	7990	152	0
1	B	7942	0	8080	124	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	7841	0	7990	154	0
2	A	13	0	5	0	0
2	B	13	0	5	0	0
All	All	23650	0	24070	410	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (410) 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:781:MET:HE2	1:C:225:VAL:H	1.06	1.12
1:A:239:ARG:HH11	1:A:239:ARG:HG3	1.24	1.03
1:B:185:ARG:HH11	1:B:185:ARG:HG3	1.24	1.00
1:A:225:VAL:H	1:B:781:MET:HE2	1.27	0.95
1:C:456:MET:HG3	1:C:467:TYR:HB3	1.49	0.94
1:C:578:LEU:HG	1:C:587:THR:HG22	1.49	0.93
1:A:213:GLN:HG2	1:A:239:ARG:HG2	1.55	0.87
1:A:781:MET:HE2	1:C:225:VAL:N	1.88	0.87
1:A:1013:THR:O	1:A:1017:LEU:HB2	1.75	0.86
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.58	0.85
1:B:971:ARG:O	1:B:975:ILE:HG12	1.80	0.82
1:C:894:SER:HB3	1:C:897:ILE:HG12	1.62	0.81
1:B:56:THR:O	1:B:60:THR:HB	1.82	0.79
1:B:109:ASN:HA	1:B:112:GLN:HB2	1.64	0.78
1:C:696:THR:HG23	1:C:699:ARG:HH12	1.48	0.77
1:C:445:ILE:HG23	1:C:940:LYS:HG3	1.66	0.76
1:A:49:TYR:HE1	1:A:60:THR:HG21	1.50	0.74
1:C:47:ALA:HB3	1:C:88:VAL:HG13	1.68	0.74
1:B:485:ALA:HA	1:B:489:THR:OG1	1.88	0.74
1:C:57:VAL:HG11	1:C:86:GLY:HA2	1.69	0.74
1:C:971:ARG:NH1	1:C:971:ARG:HB3	2.03	0.73
1:A:247:GLY:HA2	1:A:268:ILE:HD13	1.70	0.73
1:B:695:LEU:HD13	1:B:825:MET:HG3	1.68	0.73
1:C:971:ARG:CZ	1:C:971:ARG:HB3	2.19	0.72
1:B:396:PHE:O	1:B:400:LEU:HB2	1.90	0.72
1:B:32:VAL:HG12	1:B:390:ILE:HB	1.71	0.72
1:A:168:ARG:HG2	1:B:69:MET:O	1.90	0.71
1:C:831:ALA:HB3	1:C:835:LYS:HG3	1.71	0.71
1:A:734:GLU:HG2	1:C:250:LEU:HD22	1.71	0.70
1:B:185:ARG:NH1	1:B:185:ARG:HG3	2.00	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:463:THR:HG23	1:A:467:TYR:HE1	1.56	0.69
1:B:583:THR:HG22	1:B:585:GLU:H	1.55	0.69
1:A:23:GLY:HA3	1:A:377:LEU:O	1.93	0.69
1:B:400:LEU:HD13	1:B:1003:VAL:HG13	1.73	0.69
1:A:971:ARG:HB3	1:A:971:ARG:CZ	2.23	0.68
1:A:49:TYR:CE1	1:A:60:THR:HG21	2.28	0.68
1:B:372:VAL:HG23	1:B:373:PRO:HD3	1.76	0.67
1:B:60:THR:HG22	1:B:61:VAL:HG23	1.77	0.67
1:C:578:LEU:HB3	1:C:579:PRO:HD2	1.77	0.65
1:B:584:GLN:H	1:B:622:GLN:HE21	1.45	0.65
1:B:993:THR:HG22	1:B:994:GLY:H	1.62	0.65
1:A:26:ALA:O	1:A:30:LEU:HB2	1.96	0.64
1:C:74:ASN:HB3	1:C:95:GLU:HB2	1.78	0.64
1:B:139:VAL:HG13	1:B:178:PHE:HE1	1.62	0.64
1:A:673:GLU:O	1:A:674:LEU:HB2	1.96	0.64
1:C:832:ALA:HB1	1:C:833:PRO:HD2	1.80	0.63
1:B:278:ILE:HG13	1:B:613:ASN:HB3	1.81	0.63
1:A:184:MET:HB3	1:A:771:VAL:HG13	1.80	0.63
1:A:743:ILE:H	1:A:743:ILE:HD12	1.64	0.63
1:A:574:THR:HG23	1:A:627:ALA:HB3	1.81	0.63
1:B:151:GLN:HE22	1:B:278:ILE:HA	1.63	0.63
1:A:218:GLN:HE21	1:A:231:ASN:HD21	1.48	0.62
1:C:941:ASN:HD21	1:C:1015:THR:HG22	1.64	0.62
1:C:907:LEU:HD21	1:C:1021:PHE:HB2	1.83	0.61
1:C:650:ARG:HA	1:C:653:ARG:HB2	1.82	0.61
1:C:681:ASP:OD1	1:C:860:THR:HG23	2.00	0.61
1:B:764:ASP:HB3	1:B:769:LYS:HD2	1.82	0.61
1:A:239:ARG:HG3	1:A:239:ARG:NH1	2.00	0.61
1:A:696:THR:HG23	1:A:699:ARG:HH12	1.64	0.61
1:A:111:LEU:CD1	1:A:115:MET:HG2	2.30	0.60
1:A:763:ILE:HD11	1:B:59:ASP:HB3	1.82	0.60
1:C:355:MET:SD	1:C:368:PRO:HB2	2.41	0.60
1:B:775:SER:HB3	1:B:780:ARG:HD3	1.82	0.60
1:A:613:ASN:HD22	1:A:614:GLY:N	1.99	0.60
1:A:470:PHE:CD2	1:A:929:VAL:HG11	2.37	0.60
1:C:659:LYS:HG3	1:C:661:ALA:H	1.67	0.59
1:B:901:VAL:HG21	1:B:943:ILE:HG13	1.84	0.59
1:B:1013:THR:O	1:B:1017:LEU:HB2	2.03	0.59
1:A:713:LEU:HD21	1:A:843:LEU:HD12	1.84	0.59
1:A:158:VAL:HA	1:A:162:MET:HG3	1.83	0.59
1:A:705:GLU:HB3	1:A:847:LEU:HD22	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:TYR:HA	1:C:365:THR:HG21	1.84	0.59
1:B:418:ARG:HD2	1:B:970:MET:HB2	1.84	0.58
1:A:57:VAL:HG21	1:A:86:GLY:HA2	1.85	0.58
1:C:577:GLN:HG3	1:C:624:THR:HG22	1.83	0.58
1:A:110:LYS:HA	1:A:113:LEU:HD12	1.84	0.58
1:C:1026:PHE:O	1:C:1030:ARG:HB2	2.02	0.58
1:A:414:GLU:HG3	1:A:977:MET:HE1	1.85	0.58
1:B:200:PRO:HD2	1:B:749:THR:HG22	1.85	0.58
1:A:463:THR:HG23	1:A:467:TYR:CE1	2.38	0.58
1:C:683:GLU:HG2	1:C:819:TYR:CG	2.39	0.58
1:A:705:GLU:HA	1:A:708:LYS:HD3	1.86	0.58
1:A:921:LEU:HD13	1:A:922:THR:H	1.68	0.58
1:C:135:SER:OG	1:C:672:VAL:HG12	2.04	0.58
1:C:952:LEU:HD13	1:C:966:ASP:HB3	1.86	0.57
1:B:897:ILE:N	1:B:898:PRO:HD2	2.19	0.57
1:A:687:GLN:HG3	1:A:822:LEU:HD13	1.86	0.57
1:B:26:ALA:O	1:B:30:LEU:HB2	2.04	0.57
1:C:5:PHE:HD2	1:C:6:ILE:HG12	1.69	0.57
1:A:372:VAL:HB	1:A:373:PRO:CD	2.33	0.57
1:C:35:TYR:HB3	1:C:38:ILE:HD12	1.85	0.57
1:A:449:LEU:O	1:A:452:VAL:HG22	2.05	0.56
1:A:946:VAL:HG13	1:A:1026:PHE:CE1	2.40	0.56
1:C:979:SER:HB3	1:C:1015:THR:HG21	1.87	0.56
1:A:945:ILE:HG12	1:A:971:ARG:NH2	2.20	0.56
1:B:415:ASN:HD22	1:B:434:SER:HB2	1.70	0.56
1:C:343:THR:HG23	1:C:988:PRO:HB2	1.87	0.56
1:C:158:VAL:HG22	1:C:162:MET:HE3	1.88	0.56
1:A:578:LEU:HD22	1:A:661:ALA:HB3	1.87	0.56
1:C:703:LEU:HD11	1:C:718:PRO:HD3	1.88	0.56
1:B:756:GLY:HA2	1:B:774:MET:HG3	1.88	0.56
1:A:109:ASN:ND2	1:C:129:VAL:HG23	2.21	0.55
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.87	0.55
1:A:158:VAL:HG22	1:A:162:MET:HE2	1.88	0.55
1:C:56:THR:O	1:C:60:THR:HB	2.05	0.55
1:C:398:MET:HG2	1:C:473:THR:HG21	1.88	0.55
1:A:983:ILE:HG23	1:A:1008:MET:HG3	1.87	0.55
1:A:111:LEU:HD13	1:A:115:MET:HG2	1.89	0.55
1:B:249:ILE:HD13	1:B:262:LEU:HB2	1.89	0.55
1:C:166:ILE:HD11	1:C:310:LEU:HD13	1.88	0.55
1:C:70:ASN:HD22	1:C:70:ASN:H	1.55	0.55
1:A:213:GLN:HB3	1:B:56:THR:HG23	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:MET:HB2	1:B:153:ASP:HB2	1.88	0.54
1:A:612:VAL:HB	1:A:626:ILE:HG22	1.90	0.54
1:B:23:GLY:HA3	1:B:377:LEU:O	2.08	0.54
1:A:57:VAL:CG2	1:A:86:GLY:HA2	2.38	0.54
1:A:399:VAL:HG11	1:A:989:LEU:HD11	1.90	0.54
1:A:907:LEU:HG	1:A:1017:LEU:HD23	1.90	0.53
1:A:971:ARG:NH1	1:A:971:ARG:HB3	2.22	0.53
1:B:242:SER:HB2	1:B:245:GLU:H	1.74	0.53
1:C:144:ASN:HB3	1:C:148:THR:HG23	1.90	0.53
1:B:699:ARG:HE	1:B:718:PRO:HB3	1.74	0.53
1:A:504:ASP:O	1:A:505:HIS:HB2	2.09	0.53
1:A:945:ILE:HG12	1:A:971:ARG:HH21	1.73	0.53
1:A:281:PHE:CZ	1:A:324:VAL:HG21	2.45	0.52
1:A:466:ILE:HG13	1:A:563:PHE:HZ	1.74	0.52
1:B:102:ILE:O	1:B:106:GLN:HG3	2.10	0.52
1:C:408:ASP:O	1:C:412:VAL:HG23	2.09	0.52
1:A:332:PHE:O	1:A:336:SER:HB3	2.08	0.52
1:A:150:THR:O	1:A:153:ASP:HB2	2.07	0.52
1:B:637:ARG:HB3	1:B:642:ASN:HB3	1.92	0.52
1:A:327:TYR:CE1	1:A:571:VAL:HG13	2.45	0.52
1:C:944:LEU:HD13	1:C:975:ILE:HG12	1.92	0.52
1:A:38:ILE:HD11	1:A:466:ILE:CD1	2.40	0.52
1:A:683:GLU:HG2	1:A:819:TYR:CG	2.45	0.52
1:B:957:GLY:O	1:B:1043:SER:HA	2.10	0.52
1:B:676:THR:OG1	1:B:679:GLY:HA3	2.10	0.52
1:B:832:ALA:HB1	1:B:833:PRO:HD2	1.91	0.52
1:B:372:VAL:CG2	1:B:373:PRO:HD3	2.39	0.52
1:C:578:LEU:HD22	1:C:661:ALA:CB	2.40	0.52
1:A:613:ASN:C	1:A:613:ASN:HD22	2.14	0.51
1:C:82:SER:O	1:C:815:ARG:HA	2.10	0.51
1:A:448:VAL:HG22	1:A:887:CYS:HB3	1.93	0.51
1:A:584:GLN:H	1:A:622:GLN:HE21	1.58	0.51
1:A:744:ASN:O	1:A:748:THR:HG23	2.11	0.51
1:A:38:ILE:CD1	1:A:466:ILE:HD11	2.40	0.51
1:A:699:ARG:NH2	1:A:722:GLU:OE1	2.44	0.51
1:A:574:THR:HG21	1:A:598:TYR:HE2	1.76	0.50
1:A:109:ASN:HD21	1:C:129:VAL:HG23	1.74	0.50
1:B:706:ALA:HB1	1:B:716:VAL:HG11	1.94	0.50
1:C:282:ASN:ND2	1:C:609:VAL:H	2.09	0.50
1:C:971:ARG:HH21	1:C:975:ILE:HD11	1.76	0.50
1:A:225:VAL:N	1:B:781:MET:HE2	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1011:MET:O	1:C:1015:THR:HG23	2.11	0.50
1:B:239:ARG:HD3	1:B:761:ASP:O	2.12	0.50
1:B:928:GLN:HA	1:B:931:LEU:HD12	1.93	0.50
1:A:372:VAL:HG22	1:A:406:VAL:HG22	1.94	0.50
1:A:414:GLU:HG3	1:A:977:MET:CE	2.41	0.50
1:C:6:ILE:HG21	1:C:487:ILE:HG23	1.94	0.50
1:A:754:TRP:HZ3	1:C:219:LEU:HD23	1.77	0.50
1:C:418:ARG:O	1:C:422:GLU:HB2	2.11	0.50
1:C:6:ILE:HD12	1:C:487:ILE:HG23	1.94	0.50
1:A:168:ARG:CG	1:B:69:MET:O	2.57	0.49
1:C:6:ILE:HD12	1:C:487:ILE:HG12	1.93	0.49
1:C:669:PRO:HG2	1:C:672:VAL:HA	1.94	0.49
1:B:993:THR:HG22	1:B:994:GLY:N	2.27	0.49
1:C:901:VAL:HG23	1:C:942:ALA:HB3	1.93	0.49
1:B:442:LEU:O	1:B:445:ILE:HG13	2.12	0.49
1:C:274:ASN:HD22	1:C:276:ASP:HB2	1.78	0.49
1:A:112:GLN:HG3	1:B:112:GLN:NE2	2.28	0.49
1:A:415:ASN:HD22	1:A:434:SER:HB2	1.77	0.49
1:B:58:GLN:HA	1:B:62:THR:HB	1.94	0.49
1:C:247:GLY:HA2	1:C:268:ILE:HD13	1.95	0.49
1:A:726:GLN:CD	1:A:812:GLY:HA3	2.33	0.49
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.94	0.49
1:C:108:GLN:HB2	1:C:129:VAL:HG21	1.95	0.49
1:B:950:LYS:HE2	1:B:1026:PHE:HZ	1.78	0.49
1:B:247:GLY:HA2	1:B:268:ILE:CD1	2.43	0.49
1:B:979:SER:OG	1:B:1015:THR:HG21	2.12	0.49
1:A:562:SER:HB2	1:A:924:ASP:HB3	1.95	0.48
1:B:45:ILE:HB	1:B:90:ILE:HB	1.94	0.48
1:C:149:MET:HB2	1:C:153:ASP:HB3	1.94	0.48
1:B:295:THR:HG23	1:C:73:ASP:OD1	2.13	0.48
1:A:706:ALA:HB1	1:A:716:VAL:HG21	1.96	0.48
1:A:69:MET:HG3	1:A:92:LEU:HD21	1.94	0.48
1:A:415:ASN:HA	1:A:418:ARG:NH1	2.29	0.48
1:A:953:MET:HE1	1:A:960:LEU:HD12	1.95	0.48
1:B:908:GLY:HA2	1:B:1014:ALA:HB2	1.94	0.48
1:B:108:GLN:CD	1:C:112:GLN:HB3	2.34	0.48
1:B:185:ARG:CG	1:B:185:ARG:NH1	2.73	0.48
1:C:193:LEU:HG	1:C:265:VAL:HB	1.94	0.48
1:C:952:LEU:O	1:C:956:GLU:HB2	2.13	0.48
1:C:962:GLU:O	1:C:966:ASP:HB2	2.14	0.48
1:C:746:ILE:HG22	1:C:791:VAL:HG11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:705:GLU:O	1:A:709:HIS:HD2	1.97	0.47
1:B:888:LEU:HB2	1:B:898:PRO:HB3	1.96	0.47
1:A:142:VAL:HG21	1:A:162:MET:CE	2.44	0.47
1:A:402:ILE:O	1:A:406:VAL:HG23	2.14	0.47
1:C:350:LEU:O	1:C:354:VAL:HG23	2.15	0.47
1:C:752:ALA:O	1:C:774:MET:HA	2.15	0.47
1:C:915:ALA:HB2	1:C:1009:GLY:HA3	1.96	0.47
1:B:501:ALA:O	1:B:504:ASP:HB2	2.15	0.47
1:B:973:ARG:HB3	1:B:974:PRO:HD3	1.96	0.47
1:A:968:VAL:O	1:A:972:LEU:HB2	2.14	0.47
1:B:367:ILE:HB	1:B:368:PRO:HD3	1.97	0.47
1:B:578:LEU:HD13	1:B:661:ALA:HB2	1.96	0.47
1:A:401:ALA:O	1:A:405:LEU:HG	2.15	0.47
1:A:251:LEU:HD11	1:A:262:LEU:HA	1.96	0.47
1:A:544:LEU:HD23	1:A:1021:PHE:HZ	1.80	0.47
1:B:559:LEU:HD13	1:B:923:ASN:HB2	1.96	0.47
1:B:714:THR:HG23	1:B:830:GLN:HG3	1.97	0.47
1:C:32:VAL:HG12	1:C:337:ILE:HD13	1.97	0.47
1:C:462:SER:HB3	1:C:865:GLN:CD	2.35	0.47
1:A:134:SER:O	1:A:292:LYS:HE2	2.15	0.46
1:B:1022:VAL:N	1:B:1023:PRO:HD2	2.30	0.46
1:C:696:THR:HG23	1:C:699:ARG:NH1	2.24	0.46
1:B:532:GLY:HA2	1:B:535:LEU:HD12	1.97	0.46
1:A:210:GLN:NE2	1:A:250:LEU:O	2.41	0.46
1:A:38:ILE:HD11	1:A:466:ILE:HD11	1.95	0.46
1:C:282:ASN:HD21	1:C:609:VAL:H	1.63	0.46
1:C:63:GLN:O	1:C:67:GLN:HG3	2.15	0.46
1:A:952:LEU:HD23	1:A:956:GLU:HG3	1.97	0.46
1:B:9:PRO:HG2	1:B:10:ILE:HD12	1.97	0.46
1:B:525:HIS:HA	1:B:528:THR:HG22	1.97	0.46
1:C:568:ASP:HB2	1:C:643:LYS:HD2	1.98	0.46
1:C:904:VAL:HA	1:C:907:LEU:HD13	1.96	0.46
1:A:904:VAL:HG21	1:A:942:ALA:CB	2.46	0.46
1:B:973:ARG:HB3	1:B:974:PRO:CD	2.46	0.46
1:B:960:LEU:HB2	1:B:1040:ILE:HG22	1.97	0.46
1:B:683:GLU:HG2	1:B:819:TYR:CG	2.51	0.46
1:A:429:GLU:CD	1:A:429:GLU:H	2.19	0.46
1:A:568:ASP:CG	1:A:644:VAL:HG23	2.36	0.46
1:A:888:LEU:HD13	1:A:901:VAL:HG13	1.98	0.46
1:B:756:GLY:CA	1:B:774:MET:HG3	2.45	0.46
1:C:743:ILE:H	1:C:743:ILE:HD12	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1027:VAL:O	1:A:1031:ARG:HG3	2.16	0.46
1:A:489:THR:N	1:A:490:PRO:HD2	2.30	0.46
1:C:242:SER:HB2	1:C:245:GLU:H	1.81	0.46
1:A:754:TRP:CE3	1:C:234:ILE:HD11	2.51	0.45
1:C:40:PRO:HB2	1:C:94:PHE:O	2.16	0.45
1:C:971:ARG:HG2	1:C:974:PRO:CG	2.45	0.45
1:B:351:VAL:O	1:B:355:MET:HB2	2.16	0.45
1:C:187:TRP:HB3	1:C:776:GLU:HG2	1.97	0.45
1:C:34:GLN:HB2	1:C:333:VAL:HG22	1.98	0.45
1:C:391:ASN:OD1	1:C:393:LEU:HB2	2.17	0.45
1:C:555:LEU:HB3	1:C:913:LEU:HB3	1.98	0.45
1:C:612:VAL:HB	1:C:626:ILE:HG22	1.98	0.45
1:C:960:LEU:O	1:C:964:THR:HG23	2.16	0.45
1:B:675:GLY:HA3	1:B:862:MET:HG3	1.97	0.45
1:A:41:PRO:HB3	1:A:295:THR:HG21	1.98	0.45
1:C:933:THR:O	1:C:937:LEU:HG	2.17	0.45
1:A:400:LEU:HD11	1:A:1003:VAL:HG13	1.99	0.45
1:B:489:THR:N	1:B:490:PRO:HD2	2.31	0.45
1:C:185:ARG:HD2	1:C:185:ARG:HA	1.75	0.45
1:B:744:ASN:O	1:B:748:THR:HG23	2.16	0.45
1:C:583:THR:HA	1:C:622:GLN:HE21	1.82	0.45
1:C:991:ILE:HD13	1:C:991:ILE:C	2.37	0.45
1:B:60:THR:CG2	1:B:119:PRO:HG3	2.47	0.45
1:B:562:SER:HB3	1:B:924:ASP:HB3	1.99	0.45
1:C:242:SER:HB2	1:C:245:GLU:HG3	1.99	0.45
1:A:781:MET:HE1	1:C:228:GLN:HB2	1.98	0.45
1:C:558:ARG:HH11	1:C:558:ARG:HA	1.81	0.45
1:A:200:PRO:HD2	1:A:749:THR:HG22	1.99	0.45
1:A:775:SER:HB3	1:A:780:ARG:HD3	1.98	0.45
1:B:375:VAL:HG11	1:B:481:SER:HB3	1.99	0.45
1:B:690:LEU:HB2	1:B:694:LYS:HB3	1.98	0.45
1:C:456:MET:CG	1:C:467:TYR:HB3	2.34	0.45
1:B:415:ASN:ND2	1:B:434:SER:HB2	2.32	0.44
1:B:997:SER:HA	1:B:1000:GLN:HB2	1.99	0.44
1:B:158:VAL:HG22	1:B:162:MET:HE3	2.00	0.44
1:B:282:ASN:ND2	1:B:609:VAL:H	2.15	0.44
1:C:404:LEU:HD21	1:C:449:LEU:HD22	2.00	0.44
1:C:69:MET:HG3	1:C:92:LEU:HD11	1.99	0.44
1:A:676:THR:O	1:A:677:ALA:C	2.56	0.44
1:C:492:LEU:O	1:C:496:MET:HG2	2.17	0.44
1:C:1022:VAL:N	1:C:1023:PRO:HD2	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:ILE:HA	1:A:613:ASN:O	2.18	0.44
1:B:139:VAL:HG13	1:B:178:PHE:CE1	2.49	0.44
1:C:531:VAL:O	1:C:534:ILE:HG13	2.17	0.44
1:C:587:THR:OG1	1:C:613:ASN:ND2	2.44	0.44
1:A:110:LYS:O	1:A:113:LEU:HB2	2.18	0.44
1:A:213:GLN:HE22	1:A:238:THR:HG22	1.81	0.44
1:C:348:ILE:HG12	1:C:372:VAL:HG11	1.99	0.44
1:C:578:LEU:HD22	1:C:661:ALA:HB1	2.00	0.44
1:A:964:THR:HG22	1:A:1026:PHE:CD2	2.53	0.44
1:A:40:PRO:HA	1:A:41:PRO:HD2	1.82	0.44
1:A:719:ASN:HB3	1:A:826:GLU:HB3	2.00	0.44
1:B:402:ILE:HG13	1:B:402:ILE:H	1.60	0.44
1:B:545:TYR:HA	1:B:548:ILE:HD12	1.99	0.44
1:C:33:ALA:O	1:C:391:ASN:HA	2.18	0.44
1:C:746:ILE:HG22	1:C:791:VAL:HG21	2.00	0.44
1:A:3:ASN:HA	1:A:6:ILE:HG12	1.99	0.43
1:B:459:PHE:O	1:B:464:GLY:HA3	2.18	0.43
1:C:742:SER:HB3	1:C:745:ASP:HB2	1.99	0.43
1:A:239:ARG:HD2	1:A:761:ASP:O	2.18	0.43
1:C:941:ASN:ND2	1:C:1015:THR:HG22	2.32	0.43
1:C:398:MET:HB3	1:C:398:MET:HE3	1.86	0.43
1:C:572:PHE:HE2	1:C:631:LEU:HD21	1.82	0.43
1:A:904:VAL:HG22	1:A:1022:VAL:HG22	1.99	0.43
1:A:239:ARG:CG	1:A:239:ARG:NH1	2.73	0.43
1:B:220:GLY:HA2	1:C:781:MET:SD	2.58	0.43
1:A:351:VAL:HG21	1:A:406:VAL:HG21	1.99	0.43
1:C:239:ARG:HB2	1:C:763:ILE:HD12	2.00	0.43
1:C:26:ALA:O	1:C:30:LEU:HB2	2.19	0.43
1:C:885:PHE:HD1	1:C:902:MET:HG3	1.82	0.43
1:C:396:PHE:CE2	1:C:1000:GLN:HG2	2.54	0.43
1:A:388:PHE:CZ	1:A:472:ILE:HG21	2.54	0.43
1:A:559:LEU:HD23	1:A:560:PRO:HD2	2.00	0.43
1:B:185:ARG:HG2	1:B:187:TRP:CZ2	2.53	0.43
1:C:686:ASP:HB2	1:C:695:LEU:HG	2.01	0.43
1:A:166:ILE:HD11	1:A:310:LEU:HD13	2.00	0.43
1:A:361:ASN:HB3	1:A:364:ALA:HB3	2.01	0.43
1:A:952:LEU:HA	1:A:956:GLU:HB2	2.00	0.43
1:C:660:ASP:N	1:C:660:ASP:OD2	2.52	0.43
1:A:371:ALA:O	1:A:375:VAL:HG23	2.19	0.43
1:B:750:LEU:HD12	1:B:754:TRP:CD1	2.54	0.43
1:C:907:LEU:HD21	1:C:1021:PHE:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:GLY:CA	1:A:1014:ALA:HB2	2.49	0.42
1:B:888:LEU:HD13	1:B:901:VAL:HG13	2.01	0.42
1:A:139:VAL:O	1:A:326:PRO:HD2	2.18	0.42
1:A:777:ALA:O	1:A:781:MET:HG2	2.19	0.42
1:C:968:VAL:O	1:C:972:LEU:HB2	2.19	0.42
1:B:544:LEU:HA	1:B:547:ILE:HD12	2.02	0.42
1:C:434:SER:O	1:C:438:ILE:HG12	2.19	0.42
1:A:185:ARG:HD2	1:A:185:ARG:HA	1.69	0.42
1:A:644:VAL:HG12	1:A:667:ASN:HB2	2.00	0.42
1:B:904:VAL:HG12	1:B:938:SER:HB3	2.00	0.42
1:C:591:LEU:HD22	1:C:611:ALA:HB1	2.00	0.42
1:A:53:ASP:O	1:A:54:ALA:C	2.58	0.42
1:A:644:VAL:CG1	1:A:667:ASN:HB2	2.50	0.42
1:B:574:THR:HG23	1:B:627:ALA:HB3	1.99	0.42
1:B:851:LEU:HB3	1:B:852:PRO:CD	2.50	0.42
1:A:189:ASN:HA	1:A:190:PRO:HD3	1.83	0.42
1:A:396:PHE:O	1:A:400:LEU:HD13	2.19	0.42
1:B:445:ILE:HG22	1:B:943:ILE:HD13	2.01	0.42
1:B:915:ALA:HB2	1:B:1009:GLY:HA3	2.01	0.42
1:C:222:THR:HA	1:C:224:PRO:HD3	2.02	0.42
1:C:5:PHE:CD2	1:C:6:ILE:HG12	2.52	0.42
1:C:932:LEU:HA	1:C:935:ILE:HD12	2.02	0.42
1:A:115:MET:SD	1:A:127:VAL:HG21	2.59	0.42
1:A:687:GLN:OE1	1:A:856:GLY:HA3	2.20	0.42
1:B:110:LYS:HD3	1:B:110:LYS:HA	1.93	0.42
1:C:367:ILE:HB	1:C:368:PRO:HD3	2.01	0.42
1:C:897:ILE:O	1:C:901:VAL:HG12	2.20	0.42
1:B:563:PHE:CE1	1:B:677:ALA:HA	2.55	0.42
1:B:733:GLN:OE1	1:B:743:ILE:HG12	2.20	0.42
1:C:115:MET:HB2	1:C:116:PRO:HD3	2.02	0.42
1:C:659:LYS:HA	1:C:659:LYS:HD3	1.90	0.42
1:C:943:ILE:O	1:C:947:GLU:HB3	2.19	0.42
1:A:239:ARG:HB2	1:A:763:ILE:HD12	2.01	0.42
1:B:390:ILE:HG23	1:B:395:MET:SD	2.59	0.42
1:C:404:LEU:HG	1:C:449:LEU:HD13	2.01	0.42
1:A:355:MET:CE	1:A:355:MET:HA	2.50	0.42
1:A:445:ILE:HD12	1:A:446:ALA:N	2.34	0.42
1:A:559:LEU:HD13	1:A:923:ASN:HB2	2.02	0.42
1:B:199:THR:HB	1:B:200:PRO:HD2	2.02	0.42
1:C:202:ASP:OD1	1:C:792:ARG:NH2	2.53	0.42
1:A:59:ASP:O	1:C:239:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:GLN:NE2	1:B:278:ILE:HA	2.32	0.41
1:A:925:VAL:O	1:A:929:VAL:HG23	2.20	0.41
1:B:187:TRP:HA	1:B:774:MET:O	2.21	0.41
1:B:961:ILE:H	1:B:961:ILE:HG13	1.63	0.41
1:C:344:LEU:HD22	1:C:402:ILE:HD11	2.01	0.41
1:C:538:THR:HG22	1:C:542:LEU:HB2	2.02	0.41
1:C:644:VAL:HG11	1:C:667:ASN:ND2	2.35	0.41
1:A:974:PRO:HA	1:A:977:MET:HB2	2.02	0.41
1:B:249:ILE:CD1	1:B:262:LEU:HB2	2.50	0.41
1:C:247:GLY:HA2	1:C:268:ILE:CD1	2.49	0.41
1:C:310:LEU:HG	1:C:323:ILE:HD13	2.01	0.41
1:C:456:MET:HG3	1:C:467:TYR:CB	2.35	0.41
1:C:49:TYR:HE1	1:C:60:THR:HG21	1.85	0.41
1:B:368:PRO:O	1:B:372:VAL:HG22	2.20	0.41
1:B:564:LEU:HA	1:B:565:PRO:HD3	1.92	0.41
1:C:937:LEU:HD13	1:C:1011:MET:HB2	2.01	0.41
1:C:102:ILE:HA	1:C:102:ILE:HD13	1.96	0.41
1:C:658:ILE:H	1:C:658:ILE:HG13	1.74	0.41
1:C:952:LEU:HD23	1:C:956:GLU:HG3	2.01	0.41
1:B:247:GLY:HA2	1:B:268:ILE:HD12	2.03	0.41
1:C:684:LEU:O	1:C:824:SER:HA	2.20	0.41
1:A:953:MET:HE2	1:A:963:ALA:HB3	2.02	0.41
1:A:964:THR:HG22	1:A:1026:PHE:HD2	1.85	0.41
1:B:57:VAL:HG23	1:B:82:SER:HB3	2.03	0.41
1:C:907:LEU:HD23	1:C:1017:LEU:HB3	2.02	0.41
1:B:445:ILE:HG21	1:B:940:LYS:HD2	2.02	0.41
1:B:459:PHE:HB2	1:B:464:GLY:HA2	2.03	0.41
1:B:508:GLY:HA2	1:B:518:ARG:HE	1.86	0.41
1:B:74:ASN:HB3	1:B:95:GLU:HG2	2.02	0.41
1:A:56:THR:HG23	1:C:213:GLN:HB3	2.03	0.41
1:C:454:VAL:HB	1:C:455:PRO:HD3	2.03	0.41
1:A:5:PHE:CE1	1:A:487:ILE:HG12	2.56	0.41
1:A:851:LEU:HB3	1:A:852:PRO:HD2	2.03	0.41
1:C:456:MET:HG2	1:C:457:ALA:N	2.36	0.41
1:B:329:THR:O	1:B:333:VAL:HG23	2.20	0.40
1:A:405:LEU:HD22	1:A:481:SER:HB3	2.04	0.40
1:A:474:ILE:O	1:A:478:MET:HB2	2.21	0.40
1:A:776:GLU:HB3	1:A:779:TYR:HD1	1.86	0.40
1:B:255:GLN:HB2	1:B:255:GLN:HE21	1.68	0.40
1:B:367:ILE:HD11	1:B:497:LEU:HD13	2.02	0.40
1:C:897:ILE:HB	1:C:898:PRO:HD3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:583:THR:HG22	1:B:584:GLN:N	2.37	0.40
1:C:187:TRP:HA	1:C:774:MET:O	2.21	0.40
1:C:533:GLY:HA2	1:C:536:ARG:HG3	2.03	0.40
1:C:584:GLN:HB2	1:C:622:GLN:HG2	2.02	0.40
1:C:681:ASP:HB2	1:C:828:LEU:HD22	2.03	0.40
1:C:992:SER:HB3	1:C:997:SER:HB2	2.02	0.40
1:A:218:GLN:NE2	1:A:231:ASN:HD21	2.16	0.40
1:B:149:MET:HB2	1:B:153:ASP:CB	2.51	0.40
1:B:479:ALA:O	1:B:482:VAL:HG12	2.22	0.40
1:C:278:ILE:HG13	1:C:613:ASN:HB3	2.03	0.40
1:C:82:SER:HB2	1:C:816:LEU:HB2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1030/1057 (97%)	963 (94%)	57 (6%)	10 (1%)	15	45
1	B	1042/1057 (99%)	984 (94%)	50 (5%)	8 (1%)	19	51
1	C	1030/1057 (97%)	965 (94%)	58 (6%)	7 (1%)	22	54
All	All	3102/3171 (98%)	2912 (94%)	165 (5%)	25 (1%)	19	51

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	115	MET
1	A	674	LEU
1	A	677	ALA
1	A	992	SER
1	B	634	TRP
1	A	580	ALA

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Mol	Chain	Res	Type
1	C	147	GLY
1	B	358	PHE
1	B	1041	GLU
1	C	658	ILE
1	A	276	ASP
1	A	360	GLN
1	B	509	LYS
1	B	672	VAL
1	B	677	ALA
1	B	1016	VAL
1	C	134	SER
1	C	657	GLN
1	C	6	ILE
1	A	427	PRO
1	B	638	PRO
1	C	689	GLY
1	C	833	PRO
1	A	920	GLY
1	A	991	ILE

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	838/863 (97%)	781 (93%)	57 (7%)	16	42
1	B	850/863 (98%)	787 (93%)	63 (7%)	13	38
1	C	838/863 (97%)	766 (91%)	72 (9%)	10	30
All	All	2526/2589 (98%)	2334 (92%)	192 (8%)	13	36

All (192) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	27	ILE
1	A	44	THR

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Mol	Chain	Res	Type
1	A	49	TYR
1	A	60	THR
1	A	69	MET
1	A	70	ASN
1	A	88	VAL
1	A	134	SER
1	A	145	THR
1	A	146	ASP
1	A	177	LEU
1	A	185	ARG
1	A	239	ARG
1	A	243	THR
1	A	263	ARG
1	A	269	GLU
1	A	310	LEU
1	A	321	LEU
1	A	336	SER
1	A	355	MET
1	A	362	PHE
1	A	432	ARG
1	A	489	THR
1	A	559	LEU
1	A	574	THR
1	A	602	GLU
1	A	613	ASN
1	A	617	PHE
1	A	624	THR
1	A	630	SER
1	A	634	TRP
1	A	657	GLN
1	A	659	LYS
1	A	668	LEU
1	A	671	ILE
1	A	673	GLU
1	A	674	LEU
1	A	695	LEU
1	A	697	GLN
1	A	713	LEU
1	A	716	VAL
1	A	717	ARG
1	A	721	LEU
1	A	722	GLU

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Mol	Chain	Res	Type
1	A	743	ILE
1	A	748	THR
1	A	773	VAL
1	A	797	GLN
1	A	806	SER
1	A	808	ARG
1	A	918	PHE
1	A	921	LEU
1	A	931	LEU
1	A	961	ILE
1	A	962	GLU
1	A	971	ARG
1	B	3	ASN
1	B	6	ILE
1	B	11	PHE
1	B	25	LEU
1	B	27	ILE
1	B	28	LEU
1	B	29	LYS
1	B	49	TYR
1	B	58	GLN
1	B	60	THR
1	B	70	ASN
1	B	109	ASN
1	B	120	GLN
1	B	124	GLN
1	B	131	LYS
1	B	167	SER
1	B	177	LEU
1	B	185	ARG
1	B	213	GLN
1	B	229	GLN
1	B	243	THR
1	B	249	ILE
1	B	255	GLN
1	B	259	ARG
1	B	278	ILE
1	B	295	THR
1	B	310	LEU
1	B	355	MET
1	B	358	PHE
1	B	402	ILE

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Mol	Chain	Res	Type
1	B	433	LYS
1	B	482	VAL
1	B	515	TRP
1	B	538	THR
1	B	559	LEU
1	B	571	VAL
1	B	613	ASN
1	B	626	ILE
1	B	634	TRP
1	B	668	LEU
1	B	673	GLU
1	B	687	GLN
1	B	690	LEU
1	B	694	LYS
1	B	695	LEU
1	B	697	GLN
1	B	708	LYS
1	B	713	LEU
1	B	716	VAL
1	B	717	ARG
1	B	722	GLU
1	B	730	ASP
1	B	748	THR
1	B	760	ASN
1	B	784	ASP
1	B	808	ARG
1	B	835	LYS
1	B	871	ASN
1	B	901	VAL
1	B	921	LEU
1	B	928	GLN
1	B	958	LYS
1	B	1035	ARG
1	C	3	ASN
1	C	6	ILE
1	C	28	LEU
1	C	34	GLN
1	C	49	TYR
1	C	56	THR
1	C	69	MET
1	C	70	ASN
1	C	88	VAL

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Mol	Chain	Res	Type
1	C	93	THR
1	C	104	GLN
1	C	108	GLN
1	C	112	GLN
1	C	129	VAL
1	C	153	ASP
1	C	169	THR
1	C	174	ASP
1	C	177	LEU
1	C	185	ARG
1	C	197	GLN
1	C	222	THR
1	C	230	LEU
1	C	280	GLU
1	C	295	THR
1	C	307	ARG
1	C	310	LEU
1	C	321	LEU
1	C	358	PHE
1	C	398	MET
1	C	418	ARG
1	C	439	GLN
1	C	447	MET
1	C	448	VAL
1	C	452	VAL
1	C	456	MET
1	C	472	ILE
1	C	481	SER
1	C	482	VAL
1	C	510	LYS
1	C	525	HIS
1	C	558	ARG
1	C	559	LEU
1	C	571	VAL
1	C	634	TRP
1	C	636	ASP
1	C	649	MET
1	C	653	ARG
1	C	658	ILE
1	C	660	ASP
1	C	668	LEU
1	C	695	LEU

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Mol	Chain	Res	Type
1	C	703	LEU
1	C	724	THR
1	C	734	GLU
1	C	746	ILE
1	C	748	THR
1	C	828	LEU
1	C	837	THR
1	C	853	THR
1	C	863	SER
1	C	876	LEU
1	C	914	LEU
1	C	918	PHE
1	C	919	ARG
1	C	958	LYS
1	C	966	ASP
1	C	971	ARG
1	C	980	LEU
1	C	991	ILE
1	C	992	SER
1	C	993	THR
1	C	1008	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	67	GLN
1	A	74	ASN
1	A	109	ASN
1	A	124	GLN
1	A	151	GLN
1	A	213	GLN
1	A	218	GLN
1	A	229	GLN
1	A	415	ASN
1	A	569	GLN
1	A	605	ASN
1	A	613	ASN
1	A	622	GLN
1	A	642	ASN
1	A	657	GLN
1	A	667	ASN

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Mol	Chain	Res	Type
1	A	701	GLN
1	A	709	HIS
1	A	830	GLN
1	A	1001	ASN
1	B	34	GLN
1	B	67	GLN
1	B	89	GLN
1	B	109	ASN
1	B	112	GLN
1	B	124	GLN
1	B	125	GLN
1	B	194	ASN
1	B	197	GLN
1	B	213	GLN
1	B	255	GLN
1	B	282	ASN
1	B	284	GLN
1	B	439	GLN
1	B	569	GLN
1	B	605	ASN
1	B	613	ASN
1	B	622	GLN
1	B	701	GLN
1	B	709	HIS
1	B	928	GLN
1	B	1001	ASN
1	C	58	GLN
1	C	70	ASN
1	C	104	GLN
1	C	108	GLN
1	C	120	GLN
1	C	124	GLN
1	C	151	GLN
1	C	161	ASN
1	C	231	ASN
1	C	274	ASN
1	C	282	ASN
1	C	361	ASN
1	C	415	ASN
1	C	569	GLN
1	C	588	GLN
1	C	605	ASN

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Mol	Chain	Res	Type
1	C	613	ASN
1	C	622	GLN
1	C	667	ASN
1	C	726	GLN
1	C	865	GLN
1	C	872	GLN
1	C	1001	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	FLC	A	1058	-	3,12,12	0.59	0	3,17,17	0.70	0
2	FLC	B	1058	-	3,12,12	0.50	0	3,17,17	1.75	1 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FLC	A	1058	-	-	2/6/16/16	-
2	FLC	B	1058	-	-	2/6/16/16	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1058	FLC	CB-CA-CAC	-2.80	110.51	114.98

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1058	FLC	OHB-CB-CG-CGC
2	A	1058	FLC	CA-CB-CG-CGC
2	B	1058	FLC	CAC-CA-CB-CBC
2	B	1058	FLC	CAC-CA-CB-OHB

There are no ring outliers.

No monomer is involved in short contacts.

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	1032/1057 (97%)	0.26	77 (7%) 14 11	59, 73, 83, 88	0
1	B	1044/1057 (98%)	0.30	70 (6%) 17 13	66, 74, 82, 87	0
1	C	1032/1057 (97%)	0.24	58 (5%) 24 20	65, 74, 79, 82	0
All	All	3108/3171 (98%)	0.27	205 (6%) 18 14	59, 73, 81, 88	0

All (205) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	513	PHE	7.8
1	C	511	GLY	7.6
1	C	512	PHE	6.6
1	C	604	ASN	6.4
1	A	515	TRP	6.1
1	A	1033	PHE	6.0
1	B	1045	THR	5.9
1	C	658	ILE	5.8
1	A	508	GLY	5.7
1	C	510	LYS	5.7
1	B	1034	SER	5.6
1	A	511	GLY	5.6
1	C	540	ARG	5.5
1	C	918	PHE	5.4
1	B	918	PHE	5.4
1	A	512	PHE	5.4
1	C	516	PHE	5.3
1	B	871	ASN	5.2
1	B	513	PHE	5.2
1	A	978	THR	5.1
1	B	511	GLY	5.1
1	B	512	PHE	5.1
1	B	1037	ASN	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	832	ALA	5.0
1	C	421	ALA	4.9
1	A	965	LEU	4.8
1	A	510	LYS	4.6
1	B	509	LYS	4.6
1	A	404	LEU	4.5
1	B	543	VAL	4.5
1	B	516	PHE	4.4
1	C	515	TRP	4.2
1	B	1033	PHE	4.1
1	C	657	GLN	4.1
1	C	854	GLY	4.1
1	A	362	PHE	4.0
1	B	1044	HIS	3.9
1	A	974	PRO	3.8
1	B	425	LEU	3.7
1	C	993	THR	3.7
1	B	658	ILE	3.7
1	B	515	TRP	3.6
1	C	501	ALA	3.6
1	B	229	GLN	3.6
1	A	403	GLY	3.6
1	A	741	VAL	3.6
1	C	941	ASN	3.6
1	C	1033	PHE	3.5
1	A	507	GLU	3.5
1	C	600	THR	3.5
1	A	407	ASP	3.5
1	B	134	SER	3.4
1	A	675	GLY	3.4
1	B	362	PHE	3.4
1	C	655	PHE	3.4
1	B	537	SER	3.4
1	A	959	GLY	3.4
1	A	914	LEU	3.3
1	B	833	PRO	3.3
1	A	833	PRO	3.3
1	A	388	PHE	3.2
1	B	1038	GLU	3.2
1	C	975	ILE	3.2
1	A	674	LEU	3.2
1	A	958	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	1036	LYS	3.2
1	C	850	LYS	3.2
1	B	712	MET	3.2
1	A	601	LYS	3.1
1	A	963	ALA	3.1
1	C	538	THR	3.1
1	C	603	LYS	3.1
1	A	536	ARG	3.1
1	A	539	GLY	3.1
1	B	1043	SER	3.1
1	C	429	GLU	3.1
1	B	678	THR	3.1
1	C	422	GLU	3.1
1	A	977	MET	3.0
1	A	495	THR	3.0
1	A	460	GLY	3.0
1	B	458	PHE	3.0
1	A	962	GLU	3.0
1	A	516	PHE	2.9
1	B	526	HIS	2.9
1	A	640	GLU	2.9
1	C	423	GLU	2.9
1	C	558	ARG	2.9
1	C	942	ALA	2.9
1	A	641	GLU	2.9
1	A	941	ASN	2.9
1	B	407	ASP	2.9
1	C	5	PHE	2.9
1	C	2	PRO	2.8
1	B	1035	ARG	2.8
1	C	527	TYR	2.8
1	B	987	MET	2.8
1	B	941	ASN	2.8
1	C	895	TRP	2.8
1	B	575	MET	2.8
1	A	866	GLU	2.7
1	B	253	VAL	2.7
1	A	496	MET	2.7
1	A	514	GLY	2.7
1	A	405	LEU	2.7
1	C	28	LEU	2.7
1	A	386	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	991	ILE	2.7
1	B	638	PRO	2.7
1	A	406	VAL	2.7
1	A	408	ASP	2.7
1	B	28	LEU	2.7
1	B	1040	ILE	2.7
1	A	499	PRO	2.7
1	A	740	GLY	2.6
1	A	871	ASN	2.6
1	B	901	VAL	2.6
1	B	145	THR	2.6
1	A	600	THR	2.6
1	A	662	MET	2.6
1	A	938	SER	2.6
1	B	942	ALA	2.6
1	A	502	LYS	2.6
1	B	385	ALA	2.6
1	B	224	PRO	2.6
1	A	424	GLY	2.5
1	C	778	LYS	2.5
1	C	513	PHE	2.5
1	B	1042	HIS	2.5
1	A	697	GLN	2.5
1	B	3	ASN	2.5
1	C	424	GLY	2.5
1	A	518	ARG	2.5
1	A	371	ALA	2.5
1	C	944	LEU	2.5
1	B	604	ASN	2.4
1	B	322	LYS	2.4
1	A	509	LYS	2.4
1	B	498	LYS	2.4
1	B	530	SER	2.4
1	C	458	PHE	2.4
1	C	554	TYR	2.4
1	B	664	PHE	2.4
1	A	540	ARG	2.4
1	B	657	GLN	2.4
1	B	634	TRP	2.4
1	A	961	ILE	2.4
1	A	563	PHE	2.3
1	A	638	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	1031	ARG	2.3
1	C	147	GLY	2.3
1	B	554	TYR	2.3
1	C	712	MET	2.3
1	C	1032	ARG	2.3
1	A	410	ILE	2.3
1	B	940	LYS	2.3
1	C	148	THR	2.3
1	B	872	GLN	2.3
1	A	423	GLU	2.3
1	B	1041	GLU	2.3
1	A	402	ILE	2.3
1	A	500	ILE	2.3
1	C	811	TYR	2.3
1	C	1018	ALA	2.2
1	A	459	PHE	2.2
1	B	196	PHE	2.2
1	A	356	TYR	2.2
1	C	930	GLY	2.2
1	A	831	ALA	2.2
1	C	362	PHE	2.2
1	A	957	GLY	2.2
1	A	960	LEU	2.2
1	A	918	PHE	2.2
1	A	3	ASN	2.2
1	B	230	LEU	2.2
1	C	407	ASP	2.2
1	A	439	GLN	2.2
1	C	940	LYS	2.2
1	A	739	LEU	2.1
1	A	952	LEU	2.1
1	B	560	PRO	2.1
1	B	539	GLY	2.1
1	B	258	SER	2.1
1	C	920	GLY	2.1
1	A	520	PHE	2.1
1	B	319	SER	2.1
1	C	739	LEU	2.1
1	C	938	SER	2.1
1	B	4	PHE	2.1
1	C	533	GLY	2.0
1	C	856	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	636	ASP	2.0
1	C	518	ARG	2.0
1	A	522	LYS	2.0
1	B	397	GLY	2.0
1	A	4	PHE	2.0
1	C	851	LEU	2.0
1	C	529	ASP	2.0
1	A	794	ALA	2.0
1	A	832	ALA	2.0
1	B	173	GLY	2.0
1	B	263	ARG	2.0
1	B	952	LEU	2.0
1	C	976	LEU	2.0
1	B	674	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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(\AA^2)	Q<0.9
2	FLC	A	1058	13/13	0.88	0.29	64,65,66,67	0
2	FLC	B	1058	13/13	0.94	0.26	48,51,52,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.