



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:19 AM GMT

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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

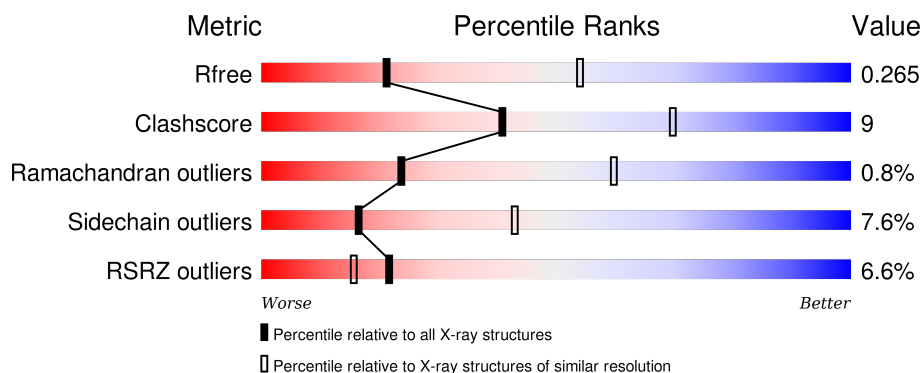
1 Overall quality at a glance

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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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. 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>74%</div> <div>21%</div> <div>..</div> </div>
1	B	1057	<div> <div>7%</div> <div>77%</div> <div>20%</div> <div>..</div> </div>
1	C	1057	<div> <div>6%</div> <div>73%</div> <div>22%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FLC	B	1058	-	-	-	X

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:

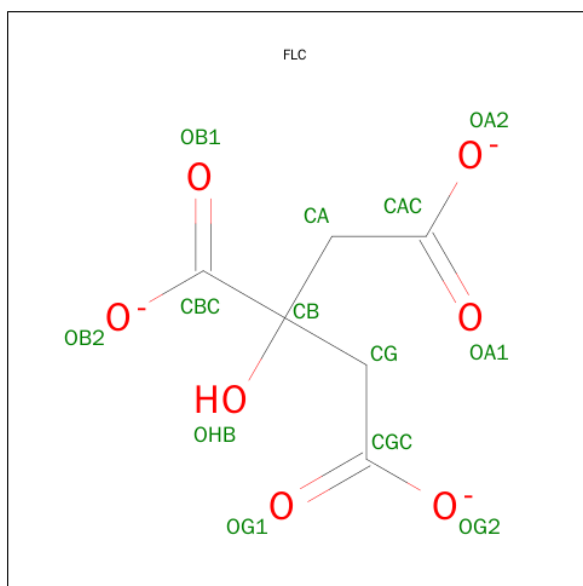
Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	LEU	-	CLONING ARTIFACT	UNP P31224
A	1051	GLU	-	CLONING ARTIFACT	UNP P31224
A	1052	HIS	-	EXPRESSION TAG	UNP P31224
A	1053	HIS	-	EXPRESSION TAG	UNP P31224
A	1054	HIS	-	EXPRESSION TAG	UNP P31224
A	1055	HIS	-	EXPRESSION TAG	UNP P31224
A	1056	HIS	-	EXPRESSION 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: $C_6H_5O_7$).

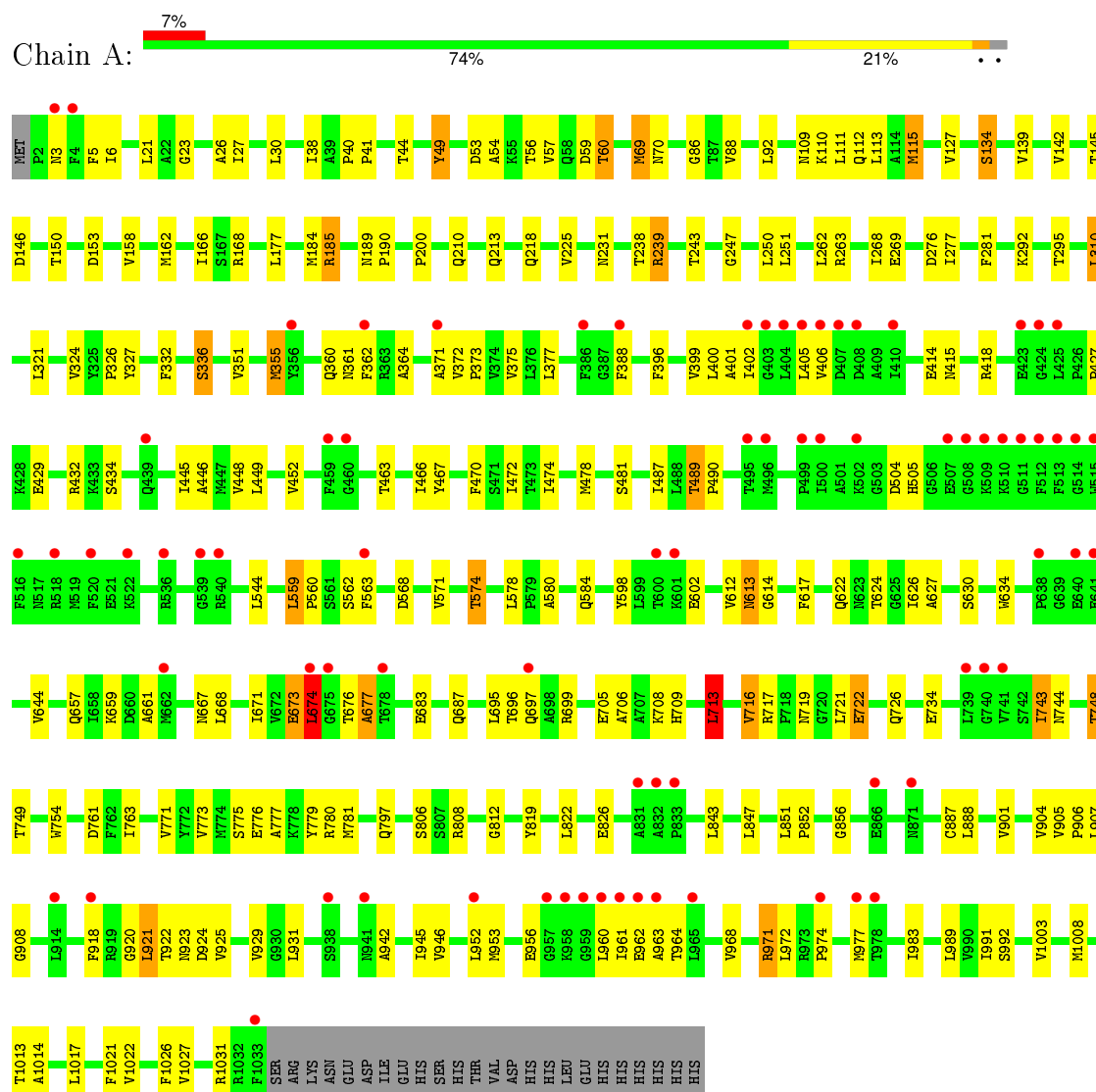


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			13	6	7		
2	A	1	Total	C	O	0	0
			13	6	7		

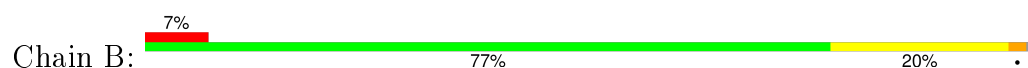
3 Residue-property plots

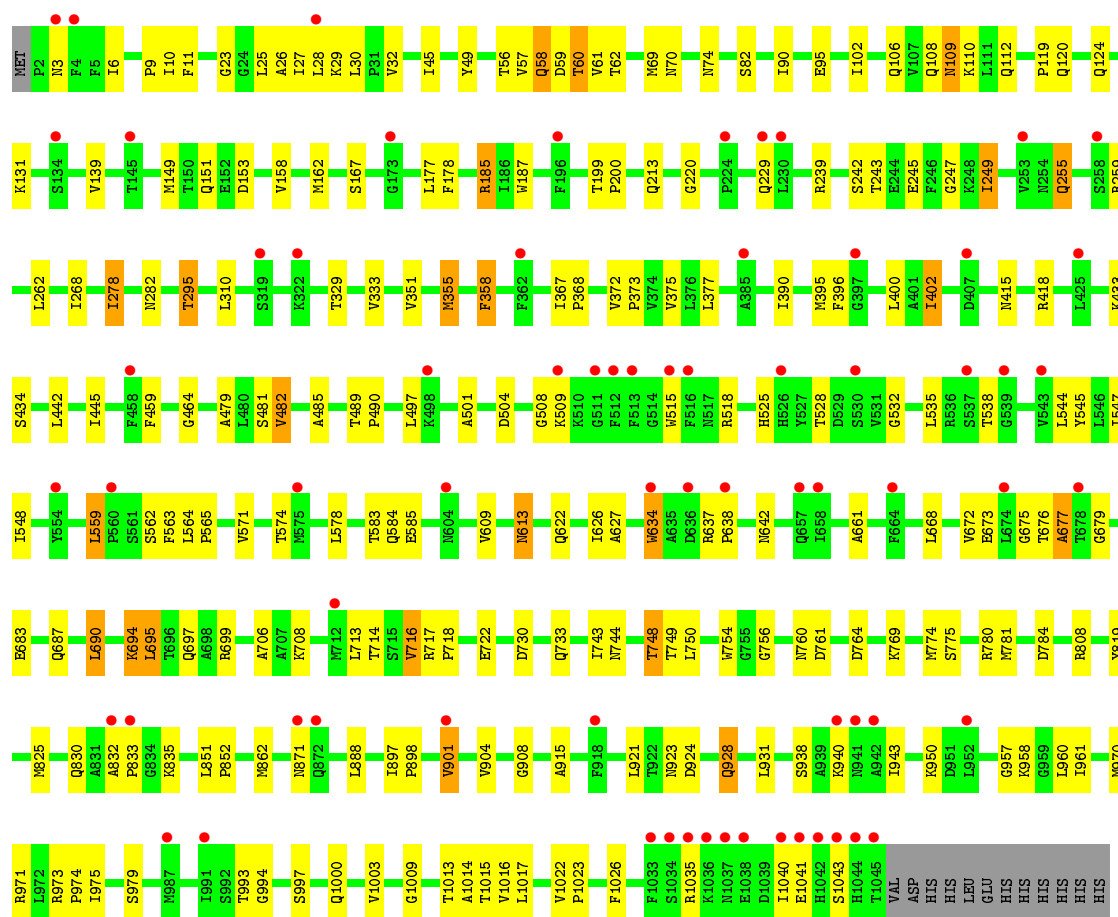
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Acriflavine resistance protein B

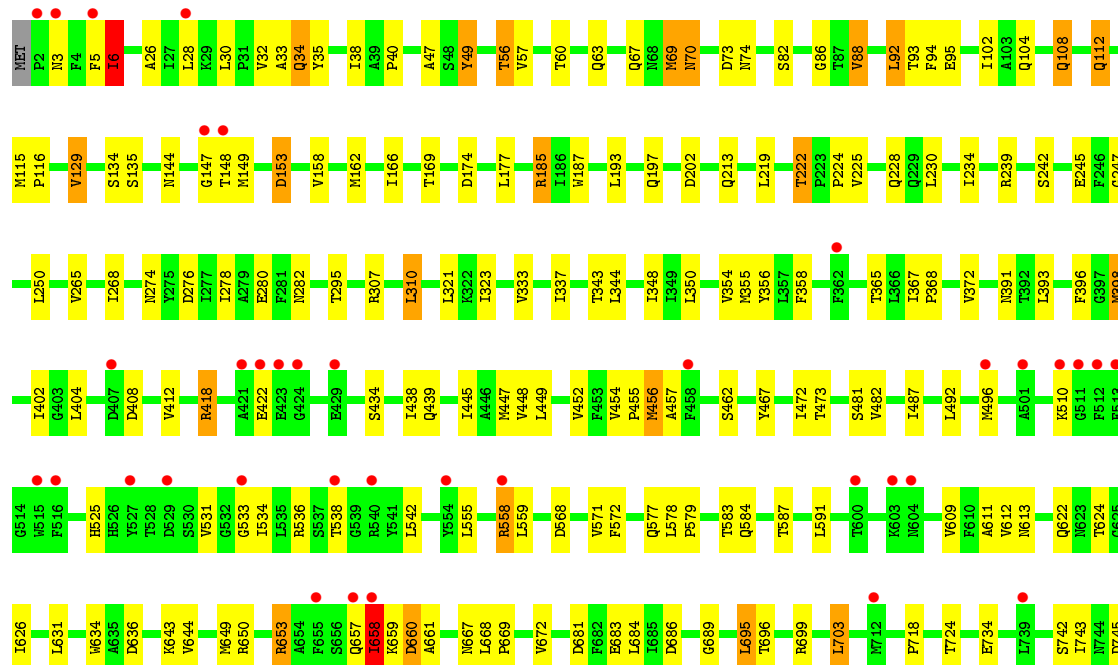


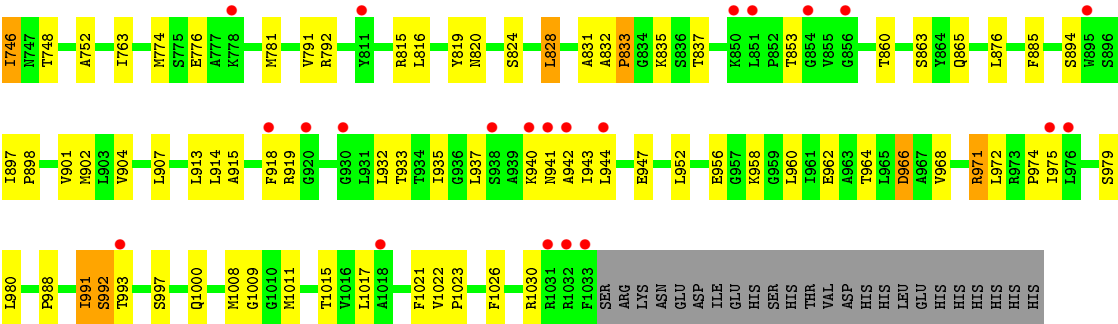
- Molecule 1: Acriflavine resistance protein B





Chain C: 6% 73% 22%





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 (5.26%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 103538 reflections (0.001%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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:781:MET:HE2	1:C:225:VAL:N	1.88	0.87
1:A:213:GLN:HG2	1:A:239:ARG:HG2	1.55	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:HB3	1:C:971:ARG:CZ	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:B:400:LEU:HD13	1:B:1003:VAL:HG13	1.73	0.69
1:A:23:GLY:HA3	1:A:377:LEU:O	1.93	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:HD12	1:A:743:ILE:H	1.64	0.63
1:B:151:GLN:HE22	1:B:278:ILE:HA	1.63	0.63
1:A:574:THR:HG23	1:A:627:ALA:HB3	1.81	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: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:A:111:LEU:CD1	1:A:115:MET:HG2	2.30	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:C:577:GLN:HG3	1:C:624:THR:HG22	1.83	0.58
1:A:57:VAL:HG21	1:A:86:GLY:HA2	1.85	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:B:200:PRO:HD2	1:B:749:THR:HG22	1.85	0.58
1:A:414:GLU:HG3	1:A:977:MET:HE1	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:B:26:ALA:O	1:B:30:LEU:HB2	2.04	0.57
1:A:687:GLN:HG3	1:A:822:LEU:HD13	1.86	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:C:703:LEU:HD11	1:C:718:PRO:HD3	1.88	0.56
1:A:578:LEU:HD22	1:A:661:ALA:HB3	1.87	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:C:166:ILE:HD11	1:C:310:LEU:HD13	1.88	0.55
1:B:249:ILE:HD13	1:B:262:LEU:HB2	1.89	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:C:408:ASP:O	1:C:412:VAL:HG23	2.09	0.52
1:A:466:ILE:HG13	1:A:563:PHE:HZ	1.74	0.52
1:A:281:PHE:CZ	1:A:324:VAL:HG21	2.45	0.52
1:B:102:ILE:O	1:B:106:GLN:HG3	2.10	0.52
1:A:332:PHE:O	1:A:336:SER:HB3	2.08	0.52
1:B:637:ARG:HB3	1:B:642:ASN:HB3	1.92	0.52
1:A:150:THR:O	1:A:153:ASP:HB2	2.07	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:832:ALA:HB1	1:B:833:PRO:HD2	1.91	0.52
1:B:676:THR:OG1	1:B:679:GLY:HA3	2.10	0.52
1:C:578:LEU:HD22	1:C:661:ALA:CB	2.40	0.52
1:B:372:VAL:CG2	1:B:373:PRO:HD3	2.39	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:744:ASN:O	1:A:748:THR:HG23	2.11	0.51
1:A:584:GLN:H	1:A:622:GLN:HE21	1.58	0.51
1:A:699:ARG:NH2	1:A:722:GLU:OE1	2.44	0.51
1:A:38:ILE:CD1	1:A:466:ILE:HD11	2.40	0.51
1:A:574:THR:HG21	1:A:598:TYR:HE2	1.76	0.50
1:C:971:ARG:HH21	1:C:975:ILE:HD11	1.76	0.50
1:A:109:ASN:HD21	1:C:129:VAL:HG23	1.74	0.50
1:C:282:ASN:ND2	1:C:609:VAL:H	2.09	0.50
1:B:706:ALA:HB1	1:B:716:VAL:HG11	1.94	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:C:6:ILE:HD12	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: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:C:901:VAL:HG23	1:C:942:ALA:HB3	1.93	0.49
1:B:993:THR:HG22	1:B:994:GLY:N	2.27	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:C:247:GLY:HA2	1:C:268:ILE:HD13	1.95	0.49
1:B:58:GLN:HA	1:B:62:THR:HB	1.94	0.49
1:A:726:GLN:CD	1:A:812:GLY:HA3	2.33	0.49
1:C:108:GLN:HB2	1:C:129:VAL:HG21	1.95	0.49
1:A:905:VAL:HB	1:A:906:PRO:HD3	1.94	0.49
1:B:979:SER:OG	1:B:1015:THR:HG21	2.12	0.49
1:B:247:GLY:HA2	1:B:268:ILE:CD1	2.43	0.49
1:B:950:LYS:HE2	1:B:1026:PHE:HZ	1.78	0.49
1:A:562:SER:HB2	1:A:924:ASP:HB3	1.95	0.48
1:C:149:MET:HB2	1:C:153:ASP:HB3	1.94	0.48
1:B:45:ILE:HB	1:B:90:ILE:HB	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: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:193:LEU:HG	1:C:265:VAL:HB	1.94	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:B:888:LEU:HB2	1:B:898:PRO:HB3	1.96	0.47
1:A:705:GLU:O	1:A:709:HIS:HD2	1.97	0.47
1:A:402:ILE:O	1:A:406:VAL:HG23	2.14	0.47
1:A:142:VAL:HG21	1:A:162:MET:CE	2.44	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:367:ILE:HB	1:B:368:PRO:HD3	1.97	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:B:578:LEU:HD13	1:B:661:ALA:HB2	1.96	0.47
1:A:968:VAL:O	1:A:972:LEU:HB2	2.14	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:C:462:SER:HB3	1:C:865:GLN:CD	2.35	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:696:THR:HG23	1:C:699:ARG:NH1	2.24	0.46
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:B:532:GLY:HA2	1:B:535:LEU:HD12	1.97	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:A:210:GLN:NE2	1:A:250:LEU:O	2.41	0.46
1:C:63:GLN:O	1:C:67:GLN:HG3	2.15	0.46
1:C:904:VAL:HA	1:C:907:LEU:HD13	1.96	0.46
1:B:525:HIS:HA	1:B:528:THR:HG22	1.97	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:C:568:ASP:HB2	1:C:643:LYS:HD2	1.98	0.46
1:B:973:ARG:HB3	1:B:974:PRO:CD	2.46	0.46
1:A:904:VAL:HG21	1:A:942:ALA:CB	2.46	0.46
1:B:683:GLU:HG2	1:B:819:TYR:CG	2.51	0.46
1:B:960:LEU:HB2	1:B:1040:ILE:HG22	1.97	0.46
1:B:756:GLY:CA	1:B:774:MET:HG3	2.45	0.46
1:A:568:ASP:CG	1:A:644:VAL:HG23	2.36	0.46
1:C:743:ILE:H	1:C:743:ILE:HD12	1.80	0.46
1:A:429:GLU:CD	1:A:429:GLU:H	2.19	0.46
1:A:888:LEU:HD13	1:A:901:VAL:HG13	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:242:SER:HB2	1:C:245:GLU:H	1.81	0.46
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:971:ARG:HG2	1:C:974:PRO:CG	2.45	0.45
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:187:TRP:HB3	1:C:776:GLU:HG2	1.97	0.45
1:C:960:LEU:O	1:C:964:THR:HG23	2.16	0.45
1:C:555:LEU:HB3	1:C:913:LEU:HB3	1.98	0.45
1:B:351:VAL:O	1:B:355:MET:HB2	2.16	0.45
1:C:612:VAL:HB	1:C:626:ILE:HG22	1.98	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:B:675:GLY:HA3	1:B:862:MET:HG3	1.97	0.45
1:C:933:THR:O	1:C:937:LEU:HG	2.17	0.45
1:A:41:PRO:HB3	1:A:295:THR:HG21	1.98	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:A:400:LEU:HD11	1:A:1003:VAL:HG13	1.99	0.45
1:B:744:ASN:O	1:B:748:THR:HG23	2.16	0.45
1:C:991:ILE:HD13	1:C:991:ILE:C	2.37	0.45
1:C:583:THR:HA	1:C:622:GLN:HE21	1.82	0.45
1:B:60:THR:CG2	1:B:119:PRO:HG3	2.47	0.45
1:C:242:SER:HB2	1:C:245:GLU:HG3	1.99	0.45
1:B:562:SER:HB3	1:B:924:ASP:HB3	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:C:456:MET:CG	1:C:467:TYR:HB3	2.34	0.45
1:B:375:VAL:HG11	1:B:481:SER:HB3	1.99	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:690:LEU:HB2	1:B:694:LYS:HB3	1.98	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:C:404:LEU:HD21	1:C:449:LEU:HD22	2.00	0.44
1:B:158:VAL:HG22	1:B:162:MET:HE3	2.00	0.44
1:C:69:MET:HG3	1:C:92:LEU:HD11	1.99	0.44
1:B:282:ASN:ND2	1:B:609:VAL:H	2.15	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:C:587:THR:OG1	1:C:613:ASN:ND2	2.44	0.44
1:B:139:VAL:HG13	1:B:178:PHE:CE1	2.49	0.44
1:A:277:ILE:HA	1:A:613:ASN:O	2.18	0.44
1:C:531:VAL:O	1:C:534:ILE:HG13	2.17	0.44
1:A:213:GLN:HE22	1:A:238:THR:HG22	1.81	0.44
1:C:578:LEU:HD22	1:C:661:ALA:HB1	2.00	0.44
1:A:110:LYS:O	1:A:113:LEU:HB2	2.18	0.44
1:C:348:ILE:HG12	1:C:372:VAL:HG11	1.99	0.44
1:A:964:THR:HG22	1:A:1026:PHE:CD2	2.53	0.44
1:C:746:ILE:HG22	1:C:791:VAL:HG21	2.00	0.44
1:C:33:ALA:O	1:C:391:ASN:HA	2.18	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:545:TYR:HA	1:B:548:ILE:HD12	1.99	0.44
1:B:402:ILE:HG13	1:B:402:ILE:H	1.60	0.44
1:B:459:PHE:O	1:B:464:GLY:HA3	2.18	0.43
1:A:3:ASN:HA	1:A:6:ILE:HG12	1.99	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: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:239:ARG:HB2	1:C:763:ILE:HD12	2.00	0.43
1:C:396:PHE:CE2	1:C:1000:GLN:HG2	2.54	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:559:LEU:HD23	1:A:560:PRO:HD2	2.00	0.43
1:A:388:PHE:CZ	1:A:472:ILE:HG21	2.54	0.43
1:A:952:LEU:HA	1:A:956:GLU:HB2	2.00	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:C:660:ASP:N	1:C:660:ASP:OD2	2.52	0.43
1:C:907:LEU:HD21	1:C:1021:PHE:CB	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:888:LEU:HD13	1:B:901:VAL:HG13	2.01	0.42
1:A:908:GLY:CA	1:A:1014:ALA:HB2	2.49	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:A:139:VAL:O	1:A:326:PRO:HD2	2.18	0.42
1:C:434:SER:O	1:C:438:ILE:HG12	2.19	0.42
1:B:544:LEU:HA	1:B:547:ILE:HD12	2.02	0.42
1:A:644:VAL:HG12	1:A:667:ASN:HB2	2.00	0.42
1:C:591:LEU:HD22	1:C:611:ALA:HB1	2.00	0.42
1:B:904:VAL:HG12	1:B:938:SER:HB3	2.00	0.42
1:A:185:ARG:HD2	1:A:185:ARG:HA	1.69	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:A:53:ASP:O	1:A:54:ALA:C	2.58	0.42
1:B:851:LEU:HB3	1:B:852:PRO:CD	2.50	0.42
1:B:445:ILE:HG22	1:B:943:ILE:HD13	2.01	0.42
1:C:5:PHE:CD2	1:C:6:ILE:HG12	2.52	0.42
1:A:396:PHE:O	1:A:400:LEU:HD13	2.19	0.42
1:C:222:THR:HA	1:C:224:PRO:HD3	2.02	0.42
1:A:189:ASN:HA	1:A:190:PRO:HD3	1.83	0.42
1:B:915:ALA:HB2	1:B:1009:GLY:HA3	2.01	0.42
1:C:932:LEU:HA	1:C:935:ILE:HD12	2.02	0.42
1:C:897:ILE:O	1:C:901:VAL:HG12	2.20	0.42
1:C:367:ILE:HB	1:C:368:PRO:HD3	2.01	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:659:LYS:HA	1:C:659:LYS:HD3	1.90	0.42
1:B:733:GLN:OE1	1:B:743:ILE:HG12	2.20	0.42
1:B:563:PHE:CE1	1:B:677:ALA:HA	2.55	0.42
1:C:115:MET:HB2	1:C:116:PRO:HD3	2.02	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:B:199:THR:HB	1:B:200:PRO:HD2	2.02	0.42
1:A:59:ASP:O	1:C:239:ARG:NH1	2.53	0.42
1:A:559:LEU:HD13	1:A:923:ASN:HB2	2.02	0.42
1:A:445:ILE:HD12	1:A:446:ALA:N	2.34	0.42
1:A:355:MET:CE	1:A:355:MET:HA	2.50	0.42
1:C:202:ASP:OD1	1:C:792:ARG:NH2	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:B:187:TRP:HA	1:B:774:MET:O	2.21	0.41
1:A:925:VAL:O	1:A:929:VAL:HG23	2.20	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:B:961:ILE:H	1:B:961:ILE:HG13	1.63	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:C:310:LEU:HG	1:C:323:ILE:HD13	2.01	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: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:C:937:LEU:HD13	1:C:1011:MET:HB2	2.01	0.41
1:B:564:LEU:HA	1:B:565:PRO:HD3	1.92	0.41
1:C:102:ILE:HA	1:C:102:ILE:HD13	1.96	0.41
1:C:952:LEU:HD23	1:C:956:GLU:HG3	2.01	0.41
1:C:658:ILE:H	1:C:658:ILE:HG13	1.74	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: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:A:964:THR:HG22	1:A:1026:PHE:HD2	1.85	0.41
1:B:459:PHE:HB2	1:B:464:GLY:HA2	2.03	0.41
1:B:57:VAL:HG23	1:B:82:SER:HB3	2.03	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:B:508:GLY:HA2	1:B:518:ARG:HE	1.86	0.41
1:C:454:VAL:HB	1:C:455:PRO:HD3	2.03	0.41
1:C:456:MET:HG2	1:C:457:ALA:N	2.36	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:B:329:THR:O	1:B:333:VAL:HG23	2.20	0.40
1:C:897:ILE:HB	1:C:898:PRO:HD3	2.03	0.40
1:B:367:ILE:HD11	1:B:497:LEU:HD13	2.02	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

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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:681:ASP:HB2	1:C:828:LEU:HD22	2.03	0.40
1:C:187:TRP:HA	1:C:774:MET:O	2.21	0.40
1:C:584:GLN:HB2	1:C:622:GLN:HG2	2.02	0.40
1:C:992:SER:HB3	1:C:997:SER:HB2	2.02	0.40
1:C:533:GLY:HA2	1:C:536:ARG:HG3	2.03	0.40
1:C:278:ILE:HG13	1:C:613:ASN:HB3	2.03	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:C:82:SER:HB2	1:C:816:LEU:HB2	2.04	0.40
1:B:479:ALA:O	1:B:482:VAL:HG12	2.22	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%)	19	54
1	B	1042/1057 (99%)	984 (94%)	50 (5%)	8 (1%)	24	60
1	C	1030/1057 (97%)	965 (94%)	58 (6%)	7 (1%)	26	63
All	All	3102/3171 (98%)	2912 (94%)	165 (5%)	25 (1%)	24	60

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%)	20	49
1	B	850/863 (98%)	787 (93%)	63 (7%)	17	44
1	C	838/863 (97%)	766 (91%)	72 (9%)	13	36
All	All	2526/2589 (98%)	2334 (92%)	192 (8%)	16	43

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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	0.55	0	3,17,17	0.72	0
2	FLC	B	1058	-	3,12,12	0.37	0	3,17,17	1.72	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	-	-	0/6/16/16	0/0/0/0
2	FLC	B	1058	-	-	0/6/16/16	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	B	1058	FLC	CB-CA-CAC	-2.78	110.51	114.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1032/1057 (97%)	0.28	78 (7%) 17 11	59, 73, 83, 88	0
1	B	1044/1057 (98%)	0.32	69 (6%) 22 16	66, 74, 82, 87	0
1	C	1032/1057 (97%)	0.25	59 (5%) 27 21	65, 74, 79, 82	0
All	All	3108/3171 (98%)	0.28	206 (6%) 22 16	59, 73, 81, 88	0

All (206) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	513	PHE	8.0
1	C	511	GLY	7.8
1	C	512	PHE	6.8
1	C	604	ASN	6.5
1	A	515	TRP	6.3
1	A	1033	PHE	6.0
1	C	658	ILE	5.9
1	B	1034	SER	5.8
1	B	1045	THR	5.8
1	A	511	GLY	5.8
1	C	510	LYS	5.8
1	A	508	GLY	5.6
1	A	512	PHE	5.6
1	C	918	PHE	5.4
1	B	871	ASN	5.3
1	B	918	PHE	5.3
1	C	540	ARG	5.3
1	C	516	PHE	5.3
1	B	513	PHE	5.3
1	B	1037	ASN	5.3
1	A	978	THR	5.2
1	B	512	PHE	5.2
1	B	511	GLY	5.1

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Mol	Chain	Res	Type	RSRZ
1	B	832	ALA	4.9
1	A	965	LEU	4.8
1	C	421	ALA	4.8
1	B	509	LYS	4.7
1	A	510	LYS	4.7
1	A	404	LEU	4.6
1	B	516	PHE	4.5
1	B	543	VAL	4.5
1	C	515	TRP	4.4
1	C	657	GLN	4.3
1	A	362	PHE	4.2
1	C	854	GLY	4.2
1	B	1033	PHE	4.2
1	A	974	PRO	3.9
1	C	993	THR	3.9
1	B	1044	HIS	3.9
1	B	658	ILE	3.8
1	B	425	LEU	3.8
1	B	229	GLN	3.7
1	C	941	ASN	3.7
1	B	515	TRP	3.6
1	A	507	GLU	3.6
1	C	600	THR	3.6
1	A	407	ASP	3.6
1	C	501	ALA	3.6
1	A	403	GLY	3.6
1	C	1033	PHE	3.6
1	A	741	VAL	3.5
1	B	134	SER	3.5
1	C	655	PHE	3.5
1	B	362	PHE	3.5
1	B	833	PRO	3.4
1	A	675	GLY	3.4
1	A	833	PRO	3.4
1	B	1038	GLU	3.4
1	B	537	SER	3.4
1	A	959	GLY	3.4
1	A	914	LEU	3.3
1	C	850	LYS	3.3
1	A	388	PHE	3.3
1	B	1036	LYS	3.2
1	C	975	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	712	MET	3.2
1	C	538	THR	3.2
1	A	958	LYS	3.2
1	A	460	GLY	3.2
1	C	429	GLU	3.2
1	A	674	LEU	3.2
1	A	539	GLY	3.2
1	C	603	LYS	3.2
1	A	495	THR	3.1
1	B	678	THR	3.1
1	B	1043	SER	3.1
1	A	977	MET	3.1
1	A	962	GLU	3.1
1	A	601	LYS	3.1
1	A	963	ALA	3.1
1	A	640	GLU	3.1
1	C	422	GLU	3.1
1	B	458	PHE	3.1
1	A	536	ARG	3.0
1	A	941	ASN	3.0
1	B	407	ASP	3.0
1	C	423	GLU	3.0
1	A	516	PHE	3.0
1	A	641	GLU	2.9
1	B	941	ASN	2.9
1	B	987	MET	2.9
1	C	527	TYR	2.9
1	C	2	PRO	2.9
1	B	575	MET	2.9
1	C	5	PHE	2.9
1	C	895	TRP	2.9
1	A	866	GLU	2.9
1	B	991	ILE	2.9
1	C	942	ALA	2.9
1	B	253	VAL	2.8
1	B	638	PRO	2.8
1	A	408	ASP	2.8
1	A	386	PHE	2.8
1	A	496	MET	2.8
1	B	526	HIS	2.8
1	C	558	ARG	2.8
1	B	1035	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	405	LEU	2.7
1	B	28	LEU	2.7
1	B	1040	ILE	2.7
1	B	224	PRO	2.7
1	A	514	GLY	2.7
1	C	28	LEU	2.7
1	A	499	PRO	2.7
1	A	406	VAL	2.7
1	A	600	THR	2.7
1	A	871	ASN	2.7
1	B	901	VAL	2.7
1	A	662	MET	2.7
1	A	938	SER	2.6
1	C	778	LYS	2.6
1	A	502	LYS	2.6
1	B	942	ALA	2.6
1	A	740	GLY	2.6
1	B	145	THR	2.6
1	A	697	GLN	2.6
1	B	3	ASN	2.6
1	B	385	ALA	2.6
1	C	513	PHE	2.5
1	A	424	GLY	2.5
1	B	1042	HIS	2.5
1	B	657	GLN	2.5
1	C	712	MET	2.5
1	A	509	LYS	2.5
1	B	322	LYS	2.5
1	C	944	LEU	2.5
1	C	458	PHE	2.5
1	C	554	TYR	2.5
1	B	498	LYS	2.5
1	B	634	TRP	2.5
1	A	638	PRO	2.5
1	B	604	ASN	2.5
1	B	664	PHE	2.5
1	C	424	GLY	2.5
1	A	961	ILE	2.5
1	C	148	THR	2.4
1	A	371	ALA	2.4
1	B	530	SER	2.4
1	B	872	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	940	LYS	2.4
1	A	540	ARG	2.4
1	A	459	PHE	2.4
1	B	1041	GLU	2.4
1	A	518	ARG	2.4
1	A	410	ILE	2.4
1	A	563	PHE	2.4
1	A	402	ILE	2.4
1	A	423	GLU	2.4
1	B	554	TYR	2.4
1	C	811	TYR	2.3
1	C	147	GLY	2.3
1	A	356	TYR	2.3
1	A	500	ILE	2.3
1	C	407	ASP	2.3
1	A	831	ALA	2.3
1	A	439	GLN	2.3
1	C	940	LYS	2.3
1	B	196	PHE	2.3
1	A	918	PHE	2.3
1	C	362	PHE	2.3
1	B	539	GLY	2.3
1	B	560	PRO	2.3
1	C	920	GLY	2.2
1	C	1018	ALA	2.2
1	C	1032	ARG	2.2
1	B	636	ASP	2.2
1	C	1031	ARG	2.2
1	C	930	GLY	2.2
1	A	520	PHE	2.2
1	A	960	LEU	2.2
1	A	957	GLY	2.2
1	B	258	SER	2.2
1	B	319	SER	2.2
1	A	952	LEU	2.2
1	A	739	LEU	2.1
1	A	3	ASN	2.1
1	A	832	ALA	2.1
1	C	529	ASP	2.1
1	C	856	GLY	2.1
1	C	739	LEU	2.1
1	C	496	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	522	LYS	2.1
1	A	678	THR	2.1
1	B	397	GLY	2.1
1	C	3	ASN	2.1
1	C	938	SER	2.1
1	B	952	LEU	2.1
1	B	4	PHE	2.1
1	C	851	LEU	2.1
1	B	674	LEU	2.0
1	C	976	LEU	2.0
1	A	425	LEU	2.0
1	B	230	LEU	2.0
1	B	173	GLY	2.0
1	C	533	GLY	2.0
1	A	4	PHE	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. 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	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	FLC	B	1058	13/13	0.94	0.26	2.47	48,51,52,53	0
2	FLC	A	1058	13/13	0.88	0.29	1.86	64,65,66,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.