



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:35 AM UTC

PDB ID : 2GIF / pdb_00002gif
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

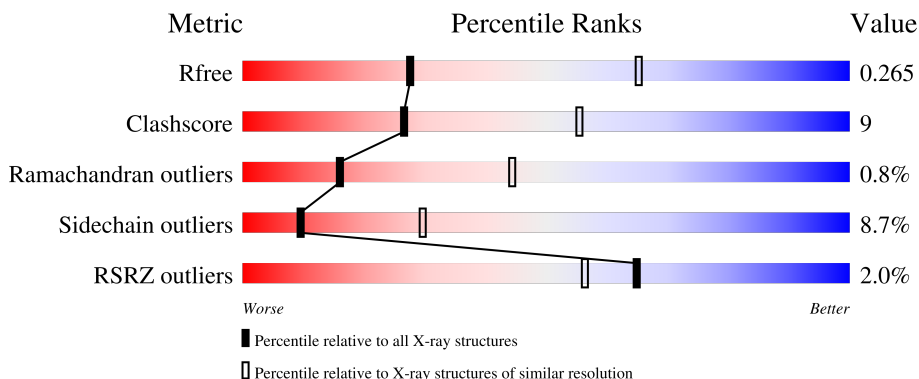
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

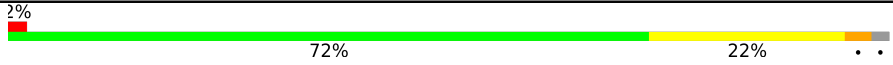
The reported resolution of this entry is 2.90 Å.

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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1057	
1	B	1057	
1	C	1057	

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:

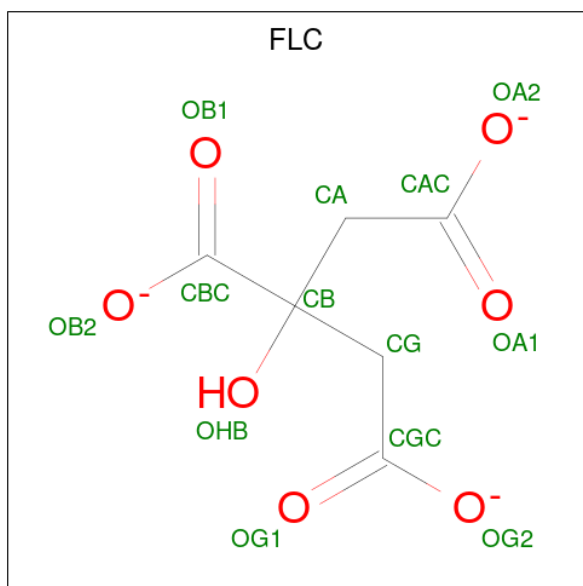
Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	LEU	-	cloning artifact	UNP P31224
A	1051	GLU	-	cloning artifact	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
A	1054	HIS	-	expression tag	UNP P31224
A	1055	HIS	-	expression tag	UNP P31224
A	1056	HIS	-	expression 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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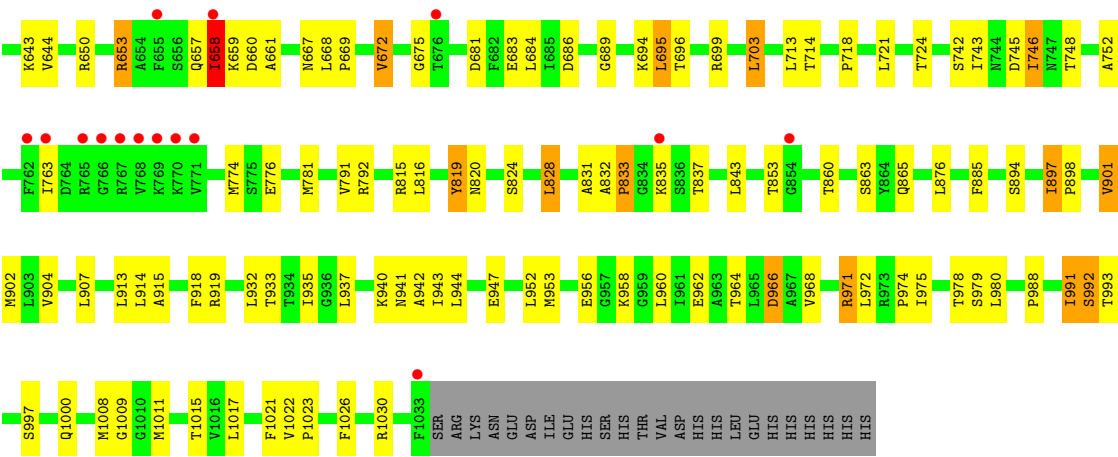
Chain	Residue	Modelled	Actual	Comment	Reference
C	1057	HIS	-	expression tag	UNP P31224

- Molecule 2 is CITRATE ANION (CCD ID: 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		





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 29.51 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.51-2.90) 99.7 (29.51-2.90)	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 (4.99%)	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)	0.29 , 78.8	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	0.93	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

5.1 Standard geometry

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	0.50	0/7991	0.88	5/10852 (0.0%)
1	B	0.50	3/8094 (0.0%)	0.84	1/10990 (0.0%)
1	C	0.49	3/7991 (0.0%)	0.85	2/10852 (0.0%)
All	All	0.49	6/24076 (0.0%)	0.86	8/32694 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	897	ILE	CA-CB	5.99	1.57	1.54
1	C	820	ASN	C-N	5.80	1.42	1.33
1	B	454	VAL	CA-CB	5.71	1.56	1.54
1	B	678	THR	CA-CB	5.16	1.59	1.52
1	B	905	VAL	CA-CB	5.06	1.56	1.54
1	C	819	TYR	C-N	5.03	1.41	1.33

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426	PRO	CA-C-N	6.78	128.32	119.84
1	A	426	PRO	C-N-CA	6.78	128.32	119.84
1	C	819	TYR	O-C-N	-6.15	116.02	123.27
1	A	972	LEU	N-CA-C	-5.66	106.42	113.55
1	B	659	LYS	N-CA-C	5.57	119.05	110.42
1	C	7	ASP	N-CA-C	-5.54	106.73	112.93
1	A	288	GLY	N-CA-C	5.50	118.78	110.75
1	A	662	MET	N-CA-C	5.29	117.97	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7841	0	7990	168	0
1	B	7942	0	8080	135	0
1	C	7841	0	7990	167	0
2	A	13	0	5	0	0
2	B	13	0	5	0	0
All	All	23650	0	24070	443	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 (443) 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:239:ARG:HG3	1:A:239:ARG:HH11	1.24	1.03
1:B:185:ARG:HG3	1:B:185:ARG:HH11	1.24	1.00
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: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:A:781:MET:HE2	1:C:225:VAL:H	1.40	0.84
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:B:185:ARG:HH22	1:B:774:MET:HE3	1.51	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:HB3	1:C:971:ARG:NH1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:634:TRP:CD1	1:C:634:TRP:H	2.06	0.72
1:A:781:MET:CE	1:C:225:VAL:H	2.03	0.72
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:HG3	1:B:185:ARG:NH1	2.00	0.70
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:A:355:MET:HE3	1:A:355:MET:HA	1.76	0.67
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:B:158:VAL:HA	1:B:162:MET:HE3	1.76	0.66
1:A:225:VAL:H	1:B:781:MET:HE2	1.58	0.66
1:C:578:LEU:HB3	1:C:579:PRO:HD2	1.77	0.65
1:A:573:MET:HE3	1:A:626:ILE:HD11	1.79	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:573:MET:HE2	1:B:626:ILE:HG12	1.79	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: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:650:ARG:HA	1:C:653:ARG:HB2	1.82	0.61
1:C:907:LEU:HD21	1:C:1021:PHE:HB2	1.83	0.61
1:A:781:MET:HE3	1:C:228:GLN:OE1	2.01	0.61
1:C:681:ASP:OD1	1:C:860:THR:HG23	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:158:VAL:HG22	1:A:162:MET:HE2	1.83	0.60
1:A:470:PHE:CD2	1:A:929:VAL:HG11	2.37	0.60
1:C:185:ARG:HH22	1:C:774:MET:HE2	1.68	0.59
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
1:A:414:GLU:HG3	1:A:977:MET:HE1	1.83	0.59
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: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:634:TRP:H	1:A:634:TRP:CD1	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:158:VAL:HA	1:C:162:MET:HE3	1.88	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:A:578:LEU:HD22	1:A:661:ALA:HB3	1.87	0.56
1:A:613:ASN:HD22	1:A:613:ASN:C	2.14	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:225:VAL:HG22	1:B:781:MET:HE2	1.88	0.55
1:A:375:VAL:HG11	1:A:405:LEU:HD22	1.87	0.55
1:C:56:THR:O	1:C:60:THR:HB	2.05	0.55
1:A:987:MET:SD	1:A:1008:MET:HE1	2.46	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
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:A:726:GLN:CD	1:A:812:GLY:HA3	2.33	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:184:MET:HE3	1:A:184:MET:HA	1.90	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:HB3	1:A:971:ARG:NH1	2.22	0.53
1:A:781:MET:HE2	1:C:225:VAL:HG13	1.91	0.53
1:C:573:MET:HE1	1:C:617:PHE:HE2	1.72	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:945:ILE:HG12	1:A:971:ARG:HH21	1.73	0.53
1:B:108:GLN:CD	1:C:112:GLN:HB3	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:953:MET:HE1	1:C:1026:PHE:HE2	1.75	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:504:ASP:O	1:A:505:HIS:HB2	2.09	0.51
1:A:225:VAL:H	1:B:781:MET:CE	2.23	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:C:462:SER:HB3	1:C:865:GLN:CD	2.35	0.51
1:C:937:LEU:HD22	1:C:1011:MET:HE2	1.91	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:76:MET:HE3	1:A:95:GLU:HA	1.92	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:568:ASP:CG	1:A:644:VAL:HG23	2.36	0.50
1:A:109:ASN:HD21	1:C:129:VAL:HG23	1.74	0.50
1:A:429:GLU:CD	1:A:429:GLU:H	2.19	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: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:6:ILE:HD12	1:C:487:ILE:HG23	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:991:ILE:HD13	1:C:991:ILE:C	2.37	0.49
1:B:844:MET:HE2	1:B:844:MET:HA	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:676:THR:O	1:A:677:ALA:C	2.56	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: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: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:B:295:THR:HG23	1:C:73:ASP:OD1	2.13	0.48
1:C:149:MET:HB2	1:C:153:ASP:HB3	1.94	0.48
1:A:69:MET:HG3	1:A:92:LEU:HD21	1.94	0.48
1:A:706:ALA:HB1	1:A:716:VAL:HG21	1.96	0.48
1:A:415:ASN:HA	1:A:418:ARG:NH1	2.29	0.48
1:C:380:PHE:CE1	1:C:398:MET:HE1	2.48	0.48
1:A:781:MET:HE1	1:C:224:PRO:HB2	1.96	0.48
1:B:908:GLY:HA2	1:B:1014:ALA:HB2	1.94	0.48
1:B:185:ARG:NH1	1:B:185:ARG:CG	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
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:184:MET:HA	1:C:184:MET:HE3	1.95	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:A:53:ASP:O	1:A:54:ALA:C	2.58	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:501:ALA:O	1:B:504:ASP:HB2	2.15	0.47
1:B:578:LEU:HD13	1:B:661:ALA:HB2	1.96	0.47
1:B:973:ARG:HB3	1:B:974:PRO:HD3	1.96	0.47
1:A:401:ALA:O	1:A:405:LEU:HG	2.15	0.47
1:B:224:PRO:HA	1:C:781:MET:HE1	1.97	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: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:38:ILE:HD11	1:A:466:ILE:HD11	1.95	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:282:ASN:HD21	1:C:609:VAL:H	1.63	0.46
1:A:781:MET:HE1	1:C:224:PRO:CB	2.45	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: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: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:HD12	1:C:743:ILE:H	1.80	0.46
1:A:489:THR:N	1:A:490:PRO:HD2	2.30	0.46
1:A:1027:VAL:O	1:A:1031:ARG:HG3	2.16	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:34:GLN:HB2	1:C:333:VAL:HG22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:TRP:HB3	1:C:776:GLU:HG2	1.97	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: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: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:282:ASN:ND2	1:B:609:VAL:H	2.15	0.44
1:B:416:VAL:HG12	1:B:420:MET:HE2	2.00	0.44
1:C:69:MET:HG3	1:C:92:LEU:HD11	1.99	0.44
1:C:404:LEU:HD21	1:C:449:LEU:HD22	2.00	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
1:A:277:ILE:HA	1:A:613:ASN:O	2.18	0.44
1:A:893:GLU:CD	1:C:8:ARG:HB3	2.43	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:964:THR:HG22	1:A:1026:PHE:CD2	2.53	0.44
1:B:402:ILE:H	1:B:402:ILE:HG13	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:142:VAL:HG21	1:A:162:MET:HE1	1.99	0.43
1:A:239:ARG:HD2	1:A:761:ASP:O	2.18	0.43
1:C:572:PHE:HE2	1:C:631:LEU:HD21	1.82	0.43
1:C:941:ASN:ND2	1:C:1015:THR:HG22	2.32	0.43
1:A:904:VAL:HG22	1:A:1022:VAL:HG22	1.99	0.43
1:A:69:MET:HE1	1:A:107:VAL:HG13	2.00	0.43
1:B:115:MET:HE3	1:B:123:GLN:HG2	1.99	0.43
1:A:239:ARG:NH1	1:A:239:ARG:CG	2.73	0.43
1:A:695:LEU:HD13	1:A:825:MET:HE3	2.00	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:239:ARG:HB2	1:C:763:ILE:HD12	2.00	0.43
1:C:885:PHE:HD1	1:C:902:MET:HG3	1.82	0.43
1:A:274:ASN:OD1	1:A:274:ASN:C	2.61	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:OD2	1:C:660:ASP:N	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
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:B:986:VAL:HG12	1:B:1008:MET:HE3	2.01	0.42
1:C:968:VAL:O	1:C:972:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:5:PHE:CD2	1:C:6:ILE:HG12	2.52	0.42
1:C:222:THR:HA	1:C:224:PRO:HD3	2.02	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:B:1015:THR:C	1:B:1017:LEU:H	2.28	0.42
1:C:115:MET:HB2	1:C:116:PRO:HD3	2.02	0.42
1:C:659:LYS:HD3	1:C:659:LYS:HA	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:59:ASP:O	1:C:239:ARG:NH1	2.53	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:B:151:GLN:NE2	1:B:278:ILE:HA	2.32	0.41
1:C:669:PRO:HG3	1:C:675:GLY:C	2.45	0.41
1:A:925:VAL:O	1:A:929:VAL:HG23	2.20	0.41
1:A:984:LEU:HD22	1:A:987:MET:HE2	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:49:TYR:HE1	1:C:60:THR:HG21	1.85	0.41
1:C:456:MET:HG3	1:C:467:TYR:CB	2.35	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:102:ILE:HD13	1:C:102:ILE:HA	1.96	0.41
1:C:937:LEU:HD13	1:C:1011:MET:HB2	2.01	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:309:GLU:HG3	1:A:313:MET:HE3	2.02	0.41
1:A:56:THR:HG23	1:C:213:GLN:HB3	2.03	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:B:74:ASN:HB3	1:B:95:GLU:HG2	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:C:454:VAL:HB	1:C:455:PRO:HD3	2.03	0.41
1:C:595:THR:C	1:C:597:TYR:H	2.29	0.41
1:C:907:LEU:HD23	1:C:1017:LEU:HB3	2.02	0.41
1:A:5:PHE:CE1	1:A:487:ILE:HG12	2.56	0.41
1:A:228:GLN:OE1	1:B:781:MET:HE3	2.20	0.41
1:A:579:PRO:O	1:A:580:ALA:C	2.63	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:HE21	1:B:255:GLN:HB2	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
1:B:76:MET:HE3	1:B:95:GLU:HA	2.02	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:82:SER:HB2	1:C:816:LEU:HB2	2.04	0.40
1:C:278:ILE:HG13	1:C:613:ASN:HB3	2.03	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%)	12	39
1	B	1042/1057 (99%)	984 (94%)	50 (5%)	8 (1%)	16	44
1	C	1030/1057 (97%)	965 (94%)	58 (6%)	7 (1%)	18	48
All	All	3102/3171 (98%)	2912 (94%)	165 (5%)	25 (1%)	16	44

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 [i](#)

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%)	763 (91%)	75 (9%)	9	28
1	B	850/863 (98%)	785 (92%)	65 (8%)	12	36
1	C	838/863 (97%)	759 (91%)	79 (9%)	8	26
All	All	2526/2589 (98%)	2307 (91%)	219 (9%)	9	30

All (219) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	27	ILE
1	A	38	ILE

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Mol	Chain	Res	Type
1	A	44	THR
1	A	60	THR
1	A	67	GLN
1	A	68	ASN
1	A	69	MET
1	A	70	ASN
1	A	88	VAL
1	A	107	VAL
1	A	111	LEU
1	A	118	LEU
1	A	134	SER
1	A	145	THR
1	A	146	ASP
1	A	177	LEU
1	A	185	ARG
1	A	195	LYS
1	A	208	LYS
1	A	239	ARG
1	A	243	THR
1	A	263	ARG
1	A	269	GLU
1	A	273	GLU
1	A	310	LEU
1	A	321	LEU
1	A	336	SER
1	A	349	ILE
1	A	351	VAL
1	A	355	MET
1	A	357	LEU
1	A	362	PHE
1	A	463	THR
1	A	483	LEU
1	A	489	THR
1	A	537	SER
1	A	559	LEU
1	A	571	VAL
1	A	574	THR
1	A	624	THR
1	A	626	ILE
1	A	630	SER
1	A	634	TRP
1	A	657	GLN

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Mol	Chain	Res	Type
1	A	658	ILE
1	A	671	ILE
1	A	673	GLU
1	A	674	LEU
1	A	687	GLN
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
1	A	743	ILE
1	A	748	THR
1	A	773	VAL
1	A	784	ASP
1	A	797	GLN
1	A	806	SER
1	A	808	ARG
1	A	843	LEU
1	A	901	VAL
1	A	907	LEU
1	A	914	LEU
1	A	921	LEU
1	A	931	LEU
1	A	961	ILE
1	A	962	GLU
1	A	969	ARG
1	A	971	ARG
1	A	972	LEU
1	B	3	ASN
1	B	6	ILE
1	B	25	LEU
1	B	27	ILE
1	B	28	LEU
1	B	29	LYS
1	B	58	GLN
1	B	60	THR
1	B	70	ASN
1	B	102	ILE
1	B	109	ASN
1	B	120	GLN

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Mol	Chain	Res	Type
1	B	131	LYS
1	B	166	ILE
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	277	ILE
1	B	278	ILE
1	B	293	LEU
1	B	295	THR
1	B	310	LEU
1	B	335	ILE
1	B	355	MET
1	B	402	ILE
1	B	452	VAL
1	B	472	ILE
1	B	482	VAL
1	B	489	THR
1	B	538	THR
1	B	559	LEU
1	B	571	VAL
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

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Mol	Chain	Res	Type
1	B	760	ASN
1	B	835	LYS
1	B	843	LEU
1	B	844	MET
1	B	871	ASN
1	B	901	VAL
1	B	921	LEU
1	B	928	GLN
1	B	958	LYS
1	B	961	ILE
1	B	1035	ARG
1	C	6	ILE
1	C	28	LEU
1	C	38	ILE
1	C	55	LYS
1	C	56	THR
1	C	69	MET
1	C	70	ASN
1	C	88	VAL
1	C	93	THR
1	C	104	GLN
1	C	108	GLN
1	C	111	LEU
1	C	112	GLN
1	C	127	VAL
1	C	129	VAL
1	C	148	THR
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	225	VAL
1	C	230	LEU
1	C	280	GLU
1	C	293	LEU
1	C	295	THR
1	C	310	LEU
1	C	321	LEU
1	C	358	PHE

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Mol	Chain	Res	Type
1	C	398	MET
1	C	418	ARG
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	525	HIS
1	C	555	LEU
1	C	558	ARG
1	C	559	LEU
1	C	571	VAL
1	C	578	LEU
1	C	634	TRP
1	C	653	ARG
1	C	658	ILE
1	C	668	LEU
1	C	672	VAL
1	C	694	LYS
1	C	695	LEU
1	C	703	LEU
1	C	713	LEU
1	C	714	THR
1	C	721	LEU
1	C	724	THR
1	C	746	ILE
1	C	748	THR
1	C	828	LEU
1	C	837	THR
1	C	843	LEU
1	C	853	THR
1	C	863	SER
1	C	876	LEU
1	C	901	VAL
1	C	914	LEU
1	C	918	PHE
1	C	919	ARG
1	C	958	LYS
1	C	966	ASP
1	C	971	ARG

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Mol	Chain	Res	Type
1	C	978	THR
1	C	980	LEU
1	C	991	ILE
1	C	992	SER
1	C	993	THR
1	C	1008	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	67	GLN
1	A	74	ASN
1	A	108	GLN
1	A	109	ASN
1	A	124	GLN
1	A	125	GLN
1	A	151	GLN
1	A	161	ASN
1	A	213	GLN
1	A	229	GLN
1	A	231	ASN
1	A	360	GLN
1	A	415	ASN
1	A	439	GLN
1	A	569	GLN
1	A	605	ASN
1	A	613	ASN
1	A	622	GLN
1	A	657	GLN
1	A	667	ASN
1	A	701	GLN
1	A	709	HIS
1	A	830	GLN
1	A	1001	ASN
1	B	67	GLN
1	B	81	ASN
1	B	89	GLN
1	B	109	ASN
1	B	112	GLN
1	B	124	GLN
1	B	125	GLN

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Mol	Chain	Res	Type
1	B	194	ASN
1	B	197	GLN
1	B	213	GLN
1	B	237	GLN
1	B	255	GLN
1	B	282	ASN
1	B	284	GLN
1	B	360	GLN
1	B	415	ASN
1	B	437	GLN
1	B	439	GLN
1	B	525	HIS
1	B	577	GLN
1	B	605	ASN
1	B	613	ASN
1	B	622	GLN
1	B	623	ASN
1	B	701	GLN
1	B	928	GLN
1	B	1001	ASN
1	B	1044	HIS
1	C	63	GLN
1	C	67	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	237	GLN
1	C	274	ASN
1	C	282	ASN
1	C	361	ASN
1	C	569	GLN
1	C	588	GLN
1	C	605	ASN
1	C	613	ASN
1	C	622	GLN
1	C	657	GLN
1	C	667	ASN
1	C	692	HIS
1	C	700	ASN

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Mol	Chain	Res	Type
1	C	726	GLN
1	C	872	GLN
1	C	941	ASN
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 oligosaccharides 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	-	12,12,12	1.09	0	17,17,17	1.21	2 (11%)
2	FLC	B	1058	-	12,12,12	1.03	0	17,17,17	1.33	3 (17%)

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	-	-	4/16/16/16	-
2	FLC	B	1058	-	-	9/16/16/16	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1058	FLC	OB1-CBC-CB	-2.80	116.66	122.09
2	B	1058	FLC	OB1-CBC-CB	-2.68	116.90	122.09
2	B	1058	FLC	OG1-CGC-CG	-2.46	115.99	122.95
2	B	1058	FLC	OB2-CBC-CB	2.14	117.25	113.14
2	A	1058	FLC	OG1-CGC-CG	-2.01	117.25	122.95

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1058	FLC	CA-CB-CBC-OB1
2	B	1058	FLC	CA-CB-CBC-OB2
2	B	1058	FLC	OHB-CB-CBC-OB1
2	B	1058	FLC	OHB-CB-CBC-OB2
2	A	1058	FLC	OHB-CB-CG-CGC
2	A	1058	FLC	CA-CB-CG-CGC
2	A	1058	FLC	CA-CB-CBC-OB2
2	B	1058	FLC	CG-CB-CBC-OB1
2	B	1058	FLC	CG-CB-CBC-OB2
2	B	1058	FLC	CAC-CA-CB-OHB
2	A	1058	FLC	CG-CB-CBC-OB2
2	B	1058	FLC	CB-CG-CGC-OG1
2	B	1058	FLC	CB-CG-CGC-OG2

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%)	0.15	26 (2%) 58 48	59, 73, 83, 88	0
1	B	1044/1057 (98%)	0.02	7 (0%) 84 79	66, 74, 82, 87	0
1	C	1032/1057 (97%)	0.17	28 (2%) 56 47	65, 74, 79, 82	0
All	All	3108/3171 (98%)	0.11	61 (1%) 65 56	59, 73, 81, 88	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	768	VAL	4.2
1	C	766	GLY	4.1
1	A	864	TYR	4.0
1	A	2	PRO	3.8
1	A	860	THR	3.6
1	A	508	GLY	3.6
1	A	515	TRP	3.6
1	C	658	ILE	3.5
1	C	763	ILE	3.5
1	B	871	ASN	3.1
1	C	515	TRP	3.1
1	C	769	LYS	2.9
1	A	640	GLU	2.9
1	C	232	ALA	2.9
1	C	655	PHE	2.9
1	B	440	GLY	2.9
1	C	767	ARG	2.9
1	C	1033	PHE	2.8
1	A	861	GLY	2.7
1	C	762	PHE	2.7
1	A	622	GLN	2.7
1	B	186	ILE	2.7
1	C	59	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	835	LYS	2.6
1	C	421	ALA	2.6
1	A	563	PHE	2.5
1	C	188	MET	2.5
1	A	678	THR	2.5
1	C	771	VAL	2.5
1	A	965	LEU	2.4
1	C	854	GLY	2.4
1	A	513	PHE	2.4
1	C	329	THR	2.4
1	A	613	ASN	2.3
1	C	604	ASN	2.3
1	B	181	GLN	2.3
1	A	658	ILE	2.3
1	C	233	SER	2.3
1	A	675	GLY	2.3
1	C	234	ILE	2.2
1	A	971	ARG	2.2
1	C	765	ARG	2.2
1	B	658	ILE	2.2
1	A	821	GLY	2.2
1	A	84	SER	2.2
1	C	81	ASN	2.1
1	A	617	PHE	2.1
1	C	462	SER	2.1
1	C	231	ASN	2.1
1	C	676	THR	2.1
1	A	641	GLU	2.1
1	C	770	LYS	2.1
1	B	515	TRP	2.1
1	A	677	ALA	2.1
1	A	638	PRO	2.1
1	A	995	ALA	2.1
1	A	443	VAL	2.0
1	A	40	PRO	2.0
1	A	112	GLN	2.0
1	C	228	GLN	2.0
1	B	516	PHE	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FLC	A	1058	13/13	0.71	0.14	64,65,66,67	0
2	FLC	B	1058	13/13	0.85	0.24	48,51,52,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.