



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 10:03 am BST

PDB ID : 2HRT
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 : 2006-07-20
Resolution : 3.00 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

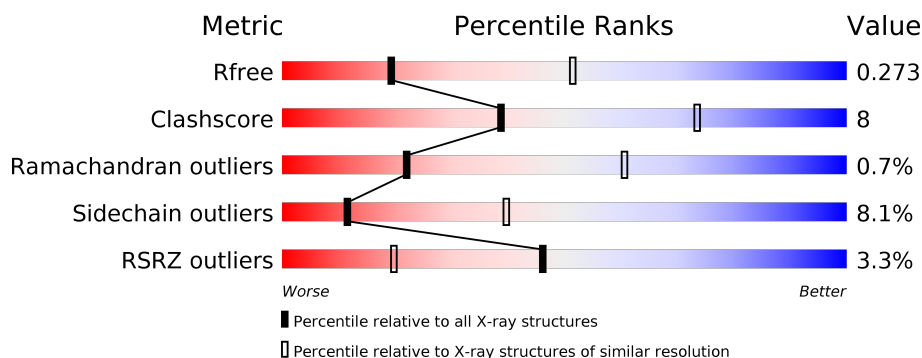
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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>3%</div> <div> <div></div> <div>76%</div> <div>19%</div> <div>• •</div> </div> </div>
1	B	1057	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>• •</div> </div> </div>
1	C	1057	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>21%</div> <div>• •</div> </div> </div>
1	D	1057	<div> <div>6%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>• •</div> </div> </div>
1	E	1057	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>• •</div> </div> </div>
1	F	1057	<div> <div>3%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 47098 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	1032	Total	C	N	O	S	0	0	0
			7841	5047	1294	1457	43			
1	C	1032	Total	C	N	O	S	0	0	0
			7841	5047	1294	1457	43			
1	D	1032	Total	C	N	O	S	0	0	0
			7841	5047	1294	1457	43			
1	E	1032	Total	C	N	O	S	0	0	0
			7841	5047	1294	1457	43			
1	F	1032	Total	C	N	O	S	0	0	0
			7841	5047	1294	1457	43			

There are 48 discrepancies between the modelled and reference sequences:

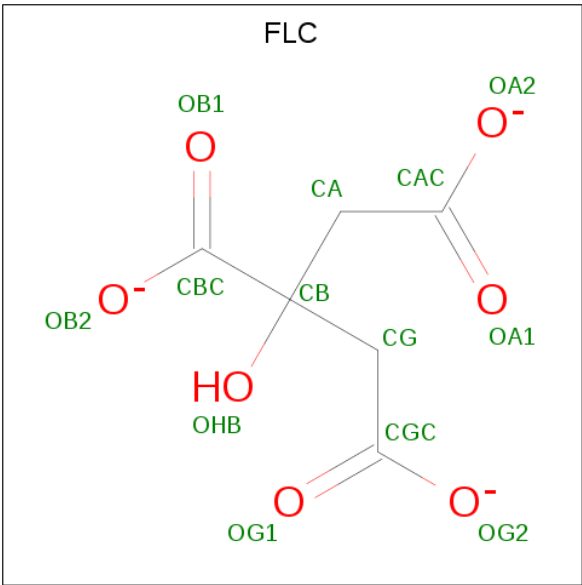
Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	LEU	-	CLONING ARTIFACT	UNP P31224
A	1051	GLU	-	CLONING ARTIFACT	UNP P31224
A	1052	HIS	-	EXPRESSION TAG	UNP P31224
A	1053	HIS	-	EXPRESSION TAG	UNP P31224
A	1054	HIS	-	EXPRESSION TAG	UNP P31224
A	1055	HIS	-	EXPRESSION TAG	UNP P31224
A	1056	HIS	-	EXPRESSION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

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

- Molecule 2 is CITRATE ANION (three-letter code: FLC) (formula: C₆H₅O₇).

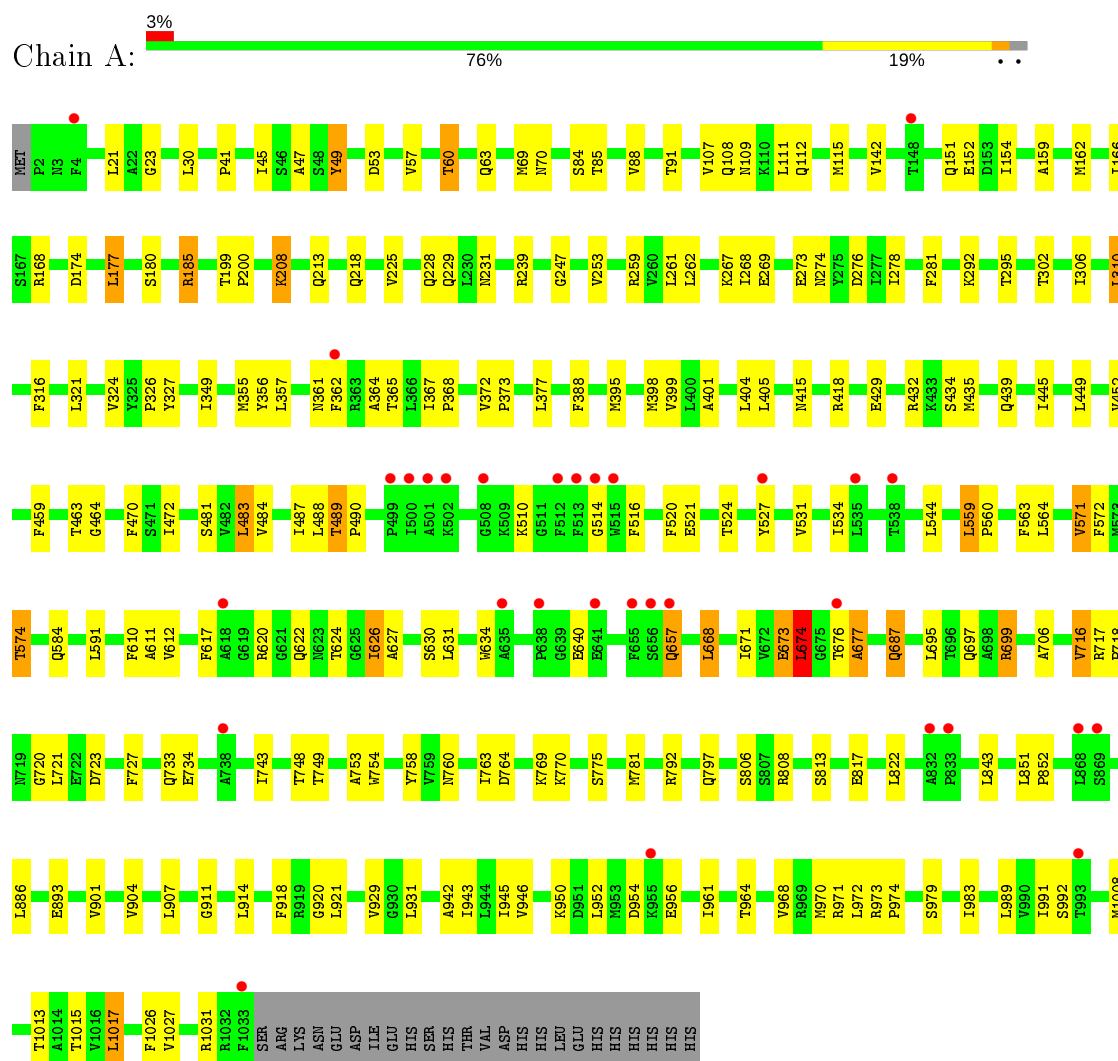


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	6	7		
2	B	1	Total	C	O	0	0
			13	6	7		
2	D	1	Total	C	O	0	0
			13	6	7		
2	E	1	Total	C	O	0	0
			13	6	7		

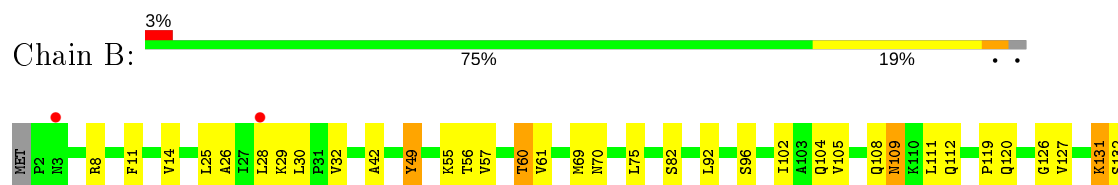
3 Residue-property plots

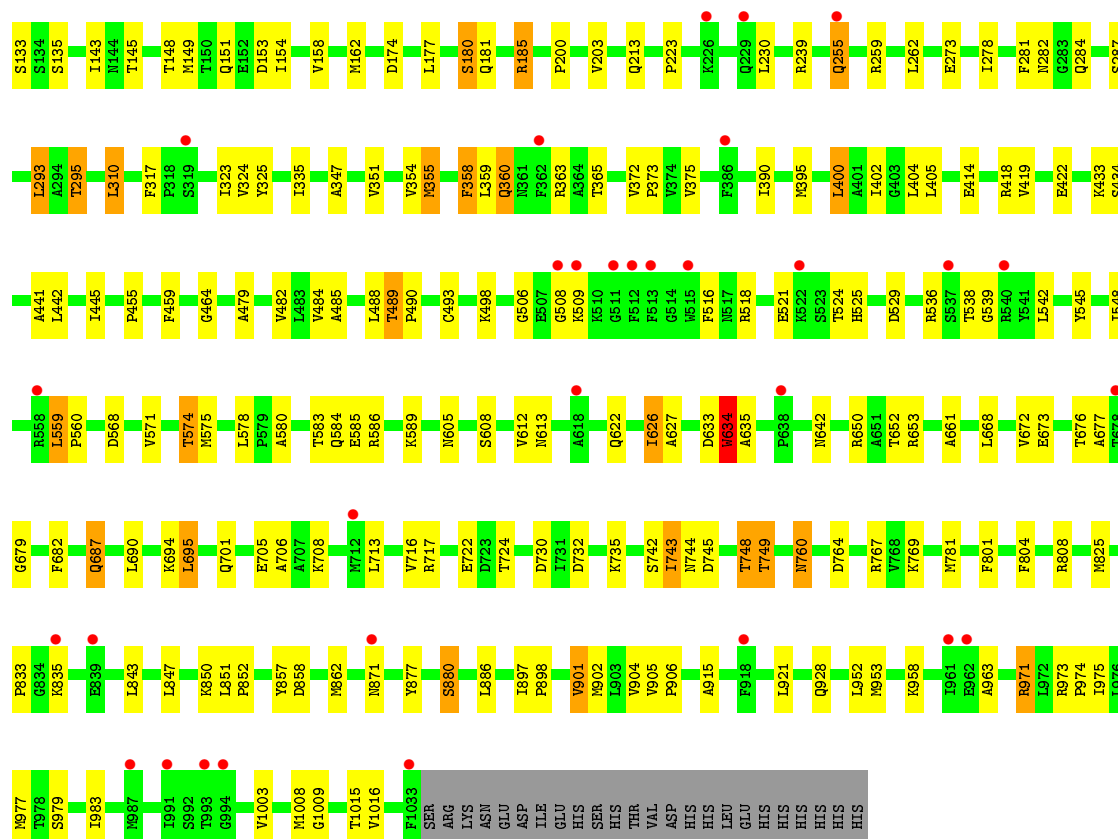
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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

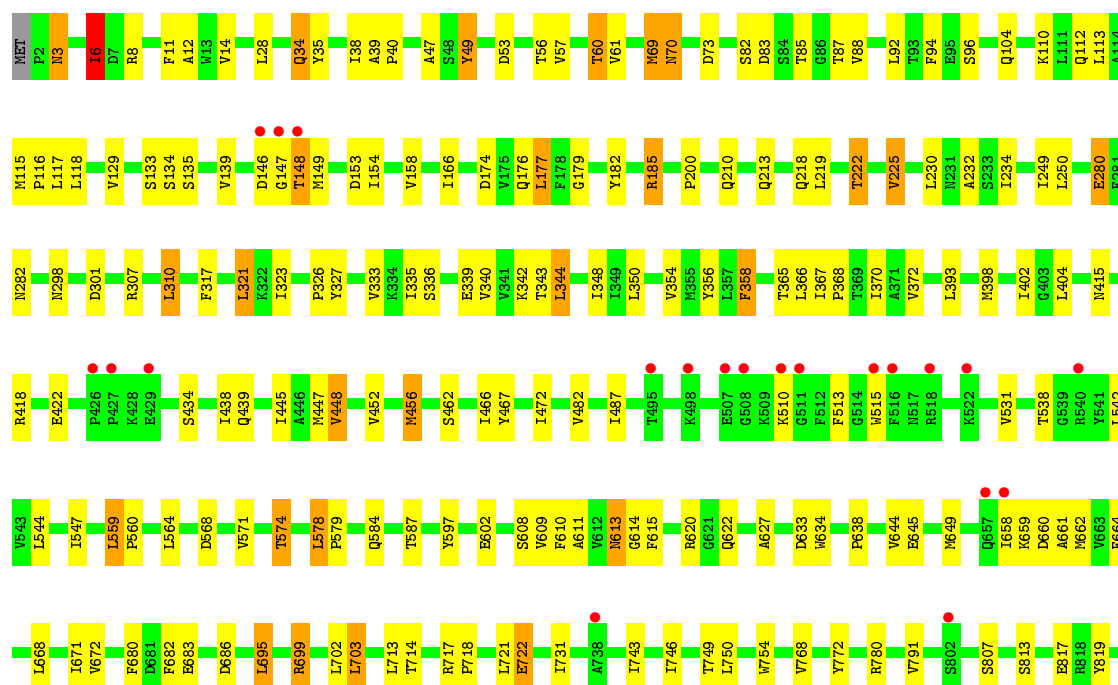
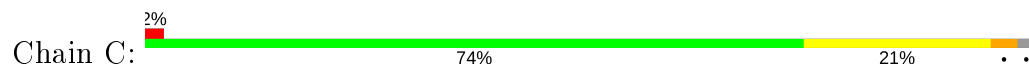


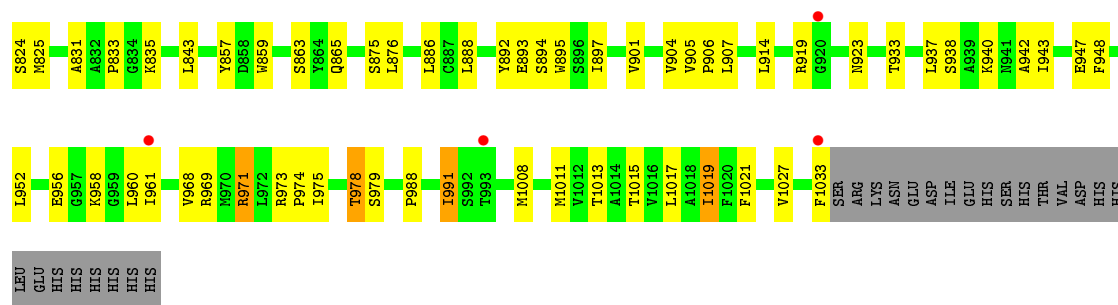
- Molecule 1: Acriflavine resistance protein B



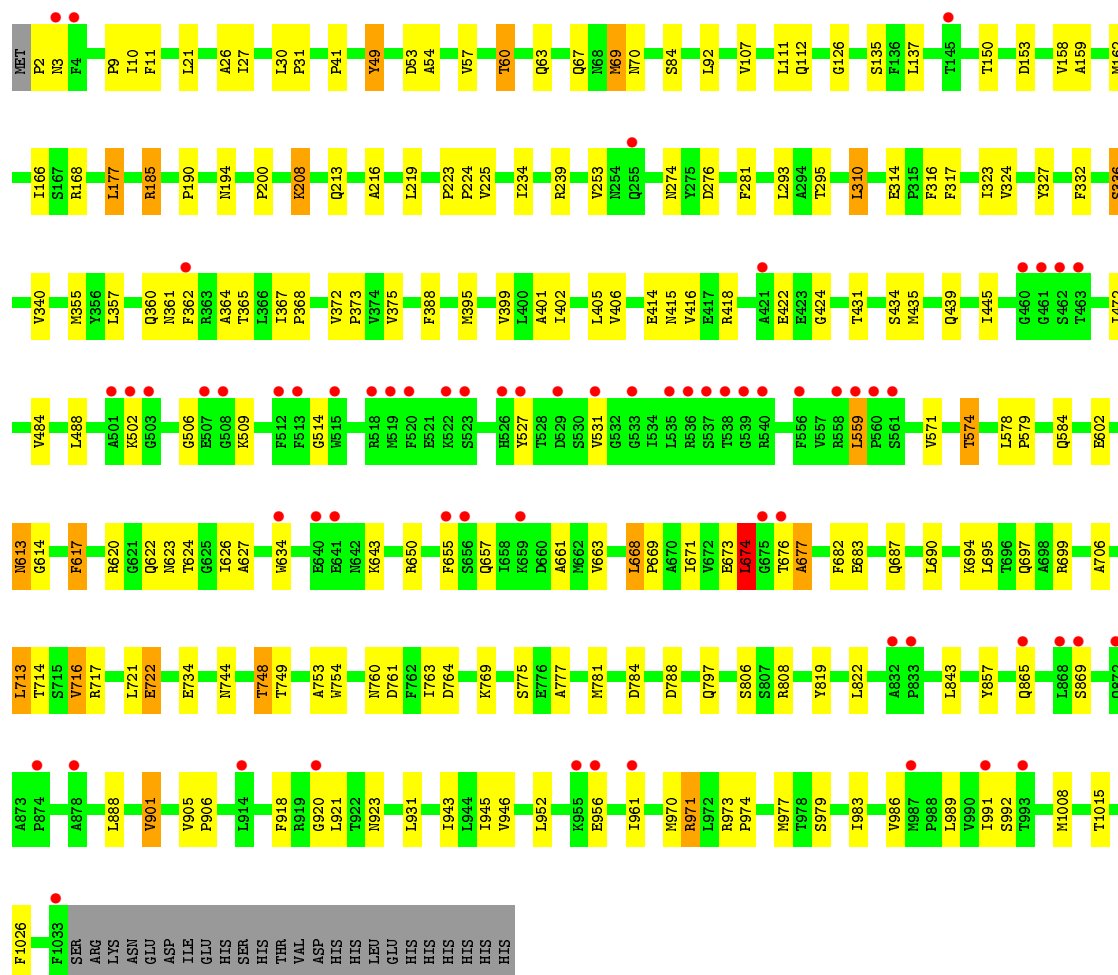
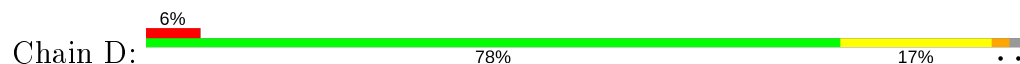


• Molecule 1: Acriflavine resistance protein B

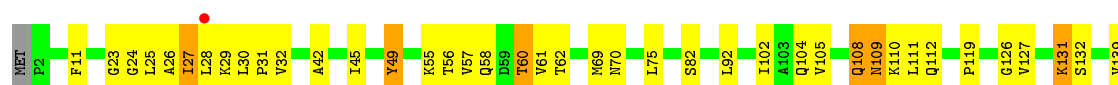
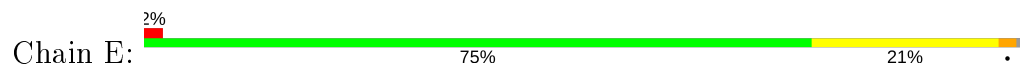


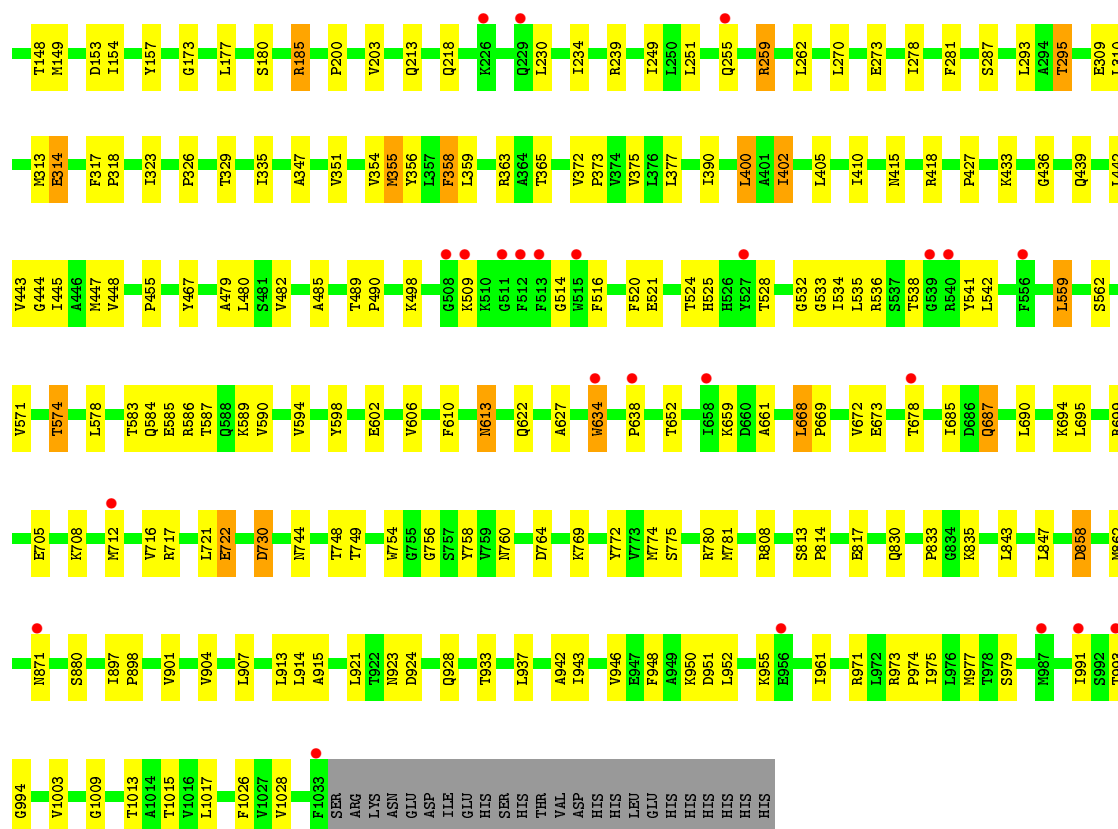


• Molecule 1: Acriflavine resistance protein B

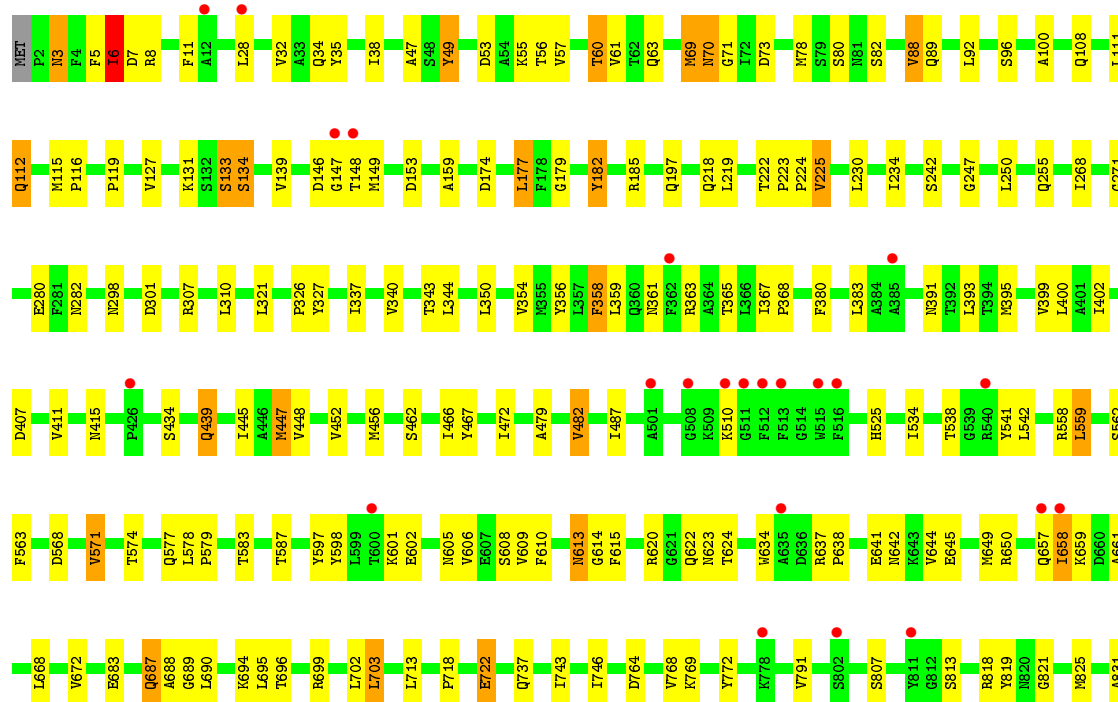
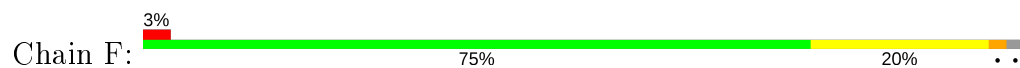


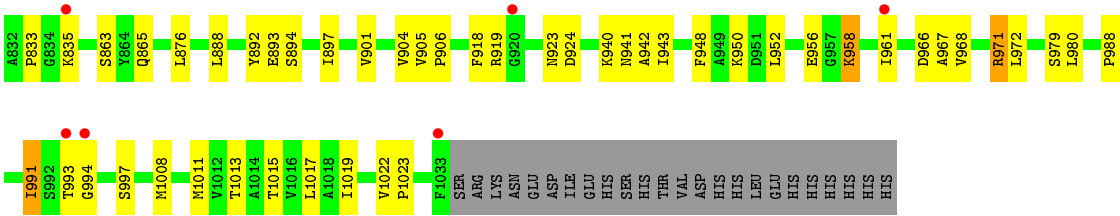
• Molecule 1: Acriflavine resistance protein B





• Molecule 1: Acriflavine resistance protein B





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	127.33Å 134.87Å 140.84Å 103.90° 94.64° 90.11°	Depositor
Resolution (Å)	29.80 – 3.00 29.80 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.80-3.00) 99.9 (29.80-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.231 , 0.274 0.232 , 0.273	Depositor DCC
R_{free} test set	9081 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	70.1	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 73.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	47098	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.55% 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	0.36	0/7991	0.52	1/10852 (0.0%)
1	B	0.37	0/7991	0.53	1/10852 (0.0%)
1	C	0.36	0/7991	0.54	1/10852 (0.0%)
1	D	0.36	0/7991	0.52	0/10852
1	E	0.37	0/7991	0.54	1/10852 (0.0%)
1	F	0.36	0/7991	0.53	0/10852
All	All	0.36	0/47946	0.53	4/65112 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	293	LEU	CA-CB-CG	6.21	129.58	115.30
1	E	293	LEU	CA-CB-CG	5.66	128.32	115.30
1	C	344	LEU	CA-CB-CG	5.21	127.28	115.30
1	A	321	LEU	CA-CB-CG	5.12	127.06	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	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	7841	0	7990	121	0
1	C	7841	0	7990	137	0
1	D	7841	0	7990	115	0
1	E	7841	0	7990	130	0
1	F	7841	0	7990	134	0
2	A	13	0	5	0	0
2	B	13	0	5	2	0
2	D	13	0	5	1	0
2	E	13	0	5	3	0
All	All	47098	0	47960	716	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 8.

All (716) 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:225:VAL:H	1:B:781:MET:HE2	1.06	1.18
1:A:781:MET:HE2	1:C:225:VAL:H	1.24	1.02
1:D:781:MET:HE2	1:F:225:VAL:H	1.28	0.98
1:D:112:GLN:HG3	1:E:112:GLN:HE21	1.28	0.97
1:E:185:ARG:HG3	1:E:185:ARG:HH11	1.30	0.94
1:E:55:LYS:HE2	2:E:1058:FLC:HA1	1.49	0.93
1:C:456:MET:HG3	1:C:467:TYR:HB3	1.52	0.91
1:A:239:ARG:HH11	1:A:239:ARG:HG3	1.36	0.88
1:A:971:ARG:HB3	1:A:971:ARG:CZ	2.02	0.87
1:D:213:GLN:HG2	1:D:239:ARG:HG2	1.56	0.87
1:B:185:ARG:HH11	1:B:185:ARG:HG3	1.40	0.86
1:A:213:GLN:HG2	1:A:239:ARG:HG2	1.57	0.86
1:A:225:VAL:N	1:B:781:MET:HE2	1.89	0.85
1:F:35:TYR:HB3	1:F:38:ILE:HD12	1.57	0.85
1:C:344:LEU:HD22	1:C:402:ILE:HD11	1.60	0.84
1:D:584:GLN:H	1:D:622:GLN:HE21	1.26	0.84
1:B:55:LYS:HE2	2:B:1058:FLC:HA1	1.60	0.83
1:B:32:VAL:HG12	1:B:390:ILE:HB	1.59	0.83
1:B:109:ASN:HA	1:B:112:GLN:HB2	1.60	0.82
1:B:145:THR:HG22	1:B:284:GLN:HE22	1.42	0.82
1:F:415:ASN:HD22	1:F:434:SER:HB2	1.45	0.82
1:D:225:VAL:H	1:E:781:MET:HE1	1.44	0.81
1:E:56:THR:O	1:E:60:THR:HB	1.79	0.80
1:A:781:MET:HE2	1:C:225:VAL:N	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:605:ASN:HD21	1:B:642:ASN:HD22	1.30	0.79
1:F:356:TYR:HA	1:F:365:THR:HG21	1.65	0.79
1:E:979:SER:OG	1:E:1015:THR:HG21	1.85	0.77
1:F:578:LEU:HG	1:F:587:THR:HG22	1.66	0.77
1:E:467:TYR:OH	1:E:928:GLN:NE2	2.17	0.77
1:C:56:THR:O	1:C:60:THR:HB	1.85	0.76
1:B:200:PRO:HD2	1:B:749:THR:HG22	1.68	0.76
1:F:343:THR:HG23	1:F:988:PRO:HB2	1.67	0.76
1:C:578:LEU:HG	1:C:587:THR:HG22	1.66	0.76
1:F:979:SER:HB3	1:F:1015:THR:HG21	1.69	0.74
1:D:239:ARG:HG3	1:D:239:ARG:HH11	1.52	0.74
1:A:415:ASN:HD22	1:A:434:SER:HB2	1.52	0.74
1:C:979:SER:HB3	1:C:1015:THR:HG21	1.67	0.74
1:C:578:LEU:HB3	1:C:579:PRO:HD2	1.69	0.74
1:B:56:THR:O	1:B:60:THR:HB	1.88	0.73
1:C:1011:MET:O	1:C:1015:THR:HG23	1.86	0.73
1:E:109:ASN:HA	1:E:112:GLN:HB2	1.67	0.73
1:C:356:TYR:HA	1:C:365:THR:HG21	1.69	0.73
1:E:32:VAL:HG12	1:E:390:ILE:HB	1.70	0.73
1:E:971:ARG:O	1:E:975:ILE:HG12	1.90	0.72
1:D:200:PRO:HD2	1:D:749:THR:HG22	1.71	0.72
1:F:56:THR:O	1:F:60:THR:HB	1.90	0.72
1:F:605:ASN:HD21	1:F:642:ASN:HD22	1.37	0.71
1:E:185:ARG:NH1	1:E:185:ARG:HG3	2.06	0.71
1:A:907:LEU:HG	1:A:1017:LEU:HD23	1.73	0.70
1:F:971:ARG:HB3	1:F:971:ARG:CZ	2.20	0.70
1:D:112:GLN:HG3	1:E:112:GLN:NE2	2.04	0.70
1:F:32:VAL:HG12	1:F:337:ILE:HD13	1.71	0.70
1:D:971:ARG:HB3	1:D:971:ARG:CZ	2.20	0.70
1:B:143:ILE:HG21	1:B:281:PHE:HB3	1.71	0.69
1:F:60:THR:HG22	1:F:61:VAL:HG23	1.75	0.69
1:F:904:VAL:HG21	1:F:942:ALA:HB2	1.73	0.69
1:B:584:GLN:H	1:B:622:GLN:HE21	1.37	0.69
1:D:781:MET:HE2	1:F:225:VAL:N	2.05	0.69
1:F:578:LEU:HB3	1:F:579:PRO:HD2	1.73	0.69
1:B:979:SER:OG	1:B:1015:THR:HG21	1.93	0.69
1:A:112:GLN:HG3	1:B:112:GLN:HE21	1.57	0.69
1:E:60:THR:HG22	1:E:61:VAL:HG23	1.74	0.68
1:F:605:ASN:HD21	1:F:642:ASN:ND2	1.92	0.68
1:F:78:MET:HG3	1:F:92:LEU:HD13	1.75	0.68
1:F:456:MET:HG3	1:F:467:TYR:HB3	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:GLY:HA3	1:C:116:PRO:HB3	1.76	0.67
1:C:638:PRO:HG3	1:E:314:GLU:HG3	1.77	0.67
1:B:354:VAL:O	1:B:358:PHE:HB2	1.94	0.67
1:C:904:VAL:HG21	1:C:942:ALA:HB2	1.77	0.66
1:A:112:GLN:HG3	1:B:112:GLN:NE2	2.10	0.66
1:A:41:PRO:HB3	1:A:295:THR:HG21	1.78	0.66
1:E:583:THR:HB	1:E:586:ARG:HG3	1.76	0.66
1:C:683:GLU:HG2	1:C:819:TYR:CG	2.31	0.65
1:D:41:PRO:HB3	1:D:295:THR:HG21	1.77	0.65
1:F:699:ARG:NH2	1:F:722:GLU:OE1	2.29	0.65
1:A:945:ILE:HG12	1:A:971:ARG:HH21	1.61	0.65
1:A:971:ARG:NH1	1:A:971:ARG:HB3	2.10	0.65
1:E:149:MET:HB2	1:E:153:ASP:HB2	1.78	0.65
1:A:372:VAL:HB	1:A:373:PRO:HD3	1.79	0.64
1:A:401:ALA:O	1:A:405:LEU:HG	1.97	0.64
1:C:343:THR:HG23	1:C:988:PRO:HB2	1.79	0.64
1:B:55:LYS:CE	2:B:1058:FLC:HA1	2.27	0.64
1:D:158:VAL:HA	1:D:162:MET:HG3	1.80	0.64
1:C:659:LYS:HG3	1:C:661:ALA:H	1.62	0.64
1:C:699:ARG:NH2	1:C:722:GLU:OE1	2.30	0.64
1:C:282:ASN:ND2	1:C:609:VAL:H	1.95	0.64
1:F:941:ASN:HD21	1:F:1015:THR:HG22	1.62	0.64
1:F:247:GLY:HA2	1:F:268:ILE:HD13	1.80	0.64
1:E:993:THR:HG22	1:E:994:GLY:H	1.62	0.63
1:A:973:ARG:HB3	1:A:974:PRO:HD3	1.79	0.63
1:D:764:ASP:HB3	1:D:769:LYS:HD2	1.80	0.63
1:F:897:ILE:O	1:F:901:VAL:HG12	1.98	0.63
1:B:539:GLY:HA2	1:B:542:LEU:HD12	1.81	0.63
1:B:971:ARG:O	1:B:975:ILE:HG12	1.98	0.63
1:D:713:LEU:HD21	1:D:843:LEU:HD12	1.80	0.63
1:D:734:GLU:HG2	1:F:250:LEU:HD22	1.81	0.63
1:E:278:ILE:HG13	1:E:613:ASN:HB3	1.81	0.63
1:A:459:PHE:HB3	1:A:464:GLY:HA2	1.81	0.62
1:B:485:ALA:HA	1:B:489:THR:OG1	2.00	0.62
1:C:538:THR:HG22	1:C:542:LEU:HB2	1.81	0.62
1:B:701:GLN:NE2	1:B:852:PRO:HD3	2.14	0.62
1:C:971:ARG:HB3	1:C:971:ARG:CZ	2.30	0.62
1:B:239:ARG:NH2	1:C:49:TYR:OH	2.33	0.62
1:C:200:PRO:HD2	1:C:749:THR:HG22	1.82	0.62
1:C:578:LEU:HG	1:C:587:THR:CG2	2.29	0.62
1:C:686:ASP:HB2	1:C:695:LEU:HG	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:ALA:HB3	1:F:88:VAL:HG13	1.81	0.61
1:E:259:ARG:H	1:E:259:ARG:HD3	1.64	0.61
1:E:613:ASN:HD22	1:E:613:ASN:C	2.04	0.61
1:A:239:ARG:HG3	1:A:239:ARG:NH1	2.06	0.61
1:A:1013:THR:O	1:A:1017:LEU:HB2	2.00	0.61
1:D:973:ARG:HB3	1:D:974:PRO:HD3	1.81	0.61
1:C:282:ASN:HD21	1:C:608:SER:HA	1.65	0.60
1:F:1011:MET:O	1:F:1015:THR:HG23	2.01	0.60
1:A:274:ASN:ND2	1:A:276:ASP:HB2	2.16	0.60
1:D:225:VAL:N	1:E:781:MET:HE1	2.16	0.60
1:B:149:MET:HB2	1:B:153:ASP:HB2	1.83	0.60
1:D:274:ASN:HD21	1:D:620:ARG:HH21	1.48	0.60
1:B:363:ARG:HD2	1:B:498:LYS:HB2	1.83	0.59
1:F:892:TYR:O	1:F:894:SER:N	2.31	0.59
1:E:578:LEU:HD23	1:E:587:THR:HG23	1.84	0.59
1:A:399:VAL:HG11	1:A:989:LEU:HD11	1.85	0.59
1:F:901:VAL:HG23	1:F:942:ALA:HB3	1.84	0.59
1:D:372:VAL:HB	1:D:373:PRO:HD3	1.83	0.59
1:E:574:THR:HG23	1:E:627:ALA:HB3	1.85	0.59
1:F:952:LEU:HD23	1:F:956:GLU:HG3	1.84	0.59
1:A:49:TYR:HE1	1:A:60:THR:HG21	1.67	0.59
1:B:583:THR:HB	1:B:586:ARG:HG3	1.83	0.59
1:F:598:TYR:HB3	1:F:606:VAL:HG21	1.84	0.59
1:B:57:VAL:HG23	1:B:82:SER:HB3	1.84	0.58
1:A:435:MET:O	1:A:439:GLN:HB2	2.02	0.58
1:B:441:ALA:O	1:B:445:ILE:HG23	2.03	0.58
1:D:946:VAL:HG13	1:D:1026:PHE:CE1	2.39	0.58
1:E:584:GLN:H	1:E:622:GLN:HE21	1.49	0.58
1:C:298:ASN:HB3	1:C:301:ASP:HB2	1.86	0.58
1:B:508:GLY:HA2	1:B:518:ARG:HH21	1.69	0.58
1:E:400:LEU:O	1:E:933:THR:HG21	2.04	0.58
1:C:943:ILE:O	1:C:947:GLU:HB3	2.03	0.58
1:A:218:GLN:HE21	1:A:231:ASN:HD21	1.52	0.57
1:C:971:ARG:NH1	1:C:971:ARG:HB3	2.20	0.57
1:E:951:ASP:O	1:E:955:LYS:HB3	2.04	0.57
1:B:60:THR:HG22	1:B:61:VAL:HG23	1.86	0.57
1:C:166:ILE:HD11	1:C:310:LEU:HD13	1.87	0.57
1:C:703:LEU:HD11	1:C:718:PRO:HD3	1.85	0.57
1:E:445:ILE:HG22	1:E:943:ILE:HD13	1.86	0.57
1:E:239:ARG:NH2	1:F:49:TYR:OH	2.38	0.57
1:E:347:ALA:O	1:E:351:VAL:HG23	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:PRO:HD2	1:A:749:THR:HG22	1.86	0.57
1:A:945:ILE:HA	1:A:971:ARG:NH2	2.19	0.57
1:C:615:PHE:HD2	1:C:620:ARG:HH12	1.52	0.57
1:F:1013:THR:O	1:F:1017:LEU:HB2	2.05	0.57
1:F:703:LEU:HD11	1:F:718:PRO:HD3	1.87	0.57
1:C:139:VAL:O	1:C:326:PRO:HD2	2.05	0.56
1:F:380:PHE:HA	1:F:383:LEU:HD12	1.86	0.56
1:A:45:ILE:HD11	1:A:69:MET:CE	2.35	0.56
1:D:112:GLN:CG	1:E:112:GLN:HE21	2.11	0.56
1:F:659:LYS:HG3	1:F:661:ALA:H	1.69	0.56
1:B:706:ALA:HB1	1:B:716:VAL:HG11	1.87	0.56
1:D:574:THR:HG23	1:D:627:ALA:HB3	1.87	0.56
1:E:149:MET:HB2	1:E:153:ASP:CB	2.35	0.56
1:E:699:ARG:NH2	1:E:722:GLU:OE1	2.37	0.56
1:C:69:MET:HG3	1:C:92:LEU:HD11	1.88	0.56
1:C:991:ILE:O	1:C:991:ILE:HG23	2.06	0.56
1:E:442:LEU:O	1:E:445:ILE:HG13	2.05	0.56
1:D:213:GLN:HB3	1:E:56:THR:HG23	1.88	0.56
1:E:126:GLY:HA2	1:F:116:PRO:HB3	1.87	0.56
1:D:401:ALA:O	1:D:405:LEU:HG	2.05	0.56
1:D:945:ILE:HG12	1:D:971:ARG:NH2	2.21	0.56
1:B:744:ASN:O	1:B:748:THR:HG23	2.06	0.56
1:D:367:ILE:HB	1:D:368:PRO:HD3	1.88	0.56
1:F:818:ARG:NH2	1:F:821:GLY:O	2.39	0.56
1:A:218:GLN:NE2	1:A:231:ASN:HD21	2.03	0.56
1:C:1013:THR:O	1:C:1017:LEU:HB2	2.06	0.56
1:B:901:VAL:O	1:B:904:VAL:HG23	2.05	0.55
1:C:434:SER:O	1:C:438:ILE:HG12	2.06	0.55
1:A:961:ILE:HD12	1:A:961:ILE:H	1.72	0.55
1:B:583:THR:HG22	1:B:585:GLU:H	1.72	0.55
1:F:743:ILE:H	1:F:743:ILE:HD12	1.70	0.55
1:E:400:LEU:HD13	1:E:1003:VAL:HG13	1.88	0.55
1:A:239:ARG:HB2	1:A:763:ILE:HD12	1.88	0.55
1:D:415:ASN:HD22	1:D:434:SER:HB2	1.72	0.55
1:D:744:ASN:O	1:D:748:THR:HG23	2.06	0.55
1:A:946:VAL:HG13	1:A:1026:PHE:CE1	2.41	0.55
1:A:449:LEU:O	1:A:452:VAL:HG22	2.07	0.55
1:A:968:VAL:O	1:A:972:LEU:HB2	2.06	0.55
1:B:695:LEU:HD13	1:B:825:MET:HG3	1.89	0.55
1:D:414:GLU:HG3	1:D:977:MET:HE1	1.88	0.55
1:D:578:LEU:HB2	1:D:623:ASN:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:952:LEU:HB3	1:F:958:LYS:HD3	1.88	0.55
1:C:282:ASN:HD21	1:C:609:VAL:H	1.55	0.55
1:F:69:MET:HG3	1:F:92:LEU:HD11	1.89	0.54
1:C:35:TYR:HB3	1:C:38:ILE:HD12	1.89	0.54
1:E:436:GLY:HA2	1:E:439:GLN:HE21	1.72	0.54
1:A:111:LEU:HD13	1:A:115:MET:HG2	1.89	0.54
1:D:316:PHE:CD1	1:E:687:GLN:HG2	2.42	0.54
1:B:801:PHE:HA	1:B:804:PHE:CZ	2.42	0.54
1:A:109:ASN:HD21	1:C:129:VAL:H	1.55	0.54
1:F:32:VAL:CG1	1:F:337:ILE:HD13	2.37	0.54
1:F:683:GLU:HG2	1:F:819:TYR:CG	2.43	0.54
1:A:764:ASP:HB3	1:A:769:LYS:HD2	1.89	0.54
1:D:687:GLN:HG3	1:D:822:LEU:HD13	1.90	0.54
1:B:742:SER:HB3	1:B:745:ASP:HB2	1.90	0.54
1:F:361:ASN:O	1:F:365:THR:HG23	2.08	0.54
1:A:734:GLU:HG2	1:C:250:LEU:HD22	1.89	0.54
1:D:527:TYR:O	1:D:531:VAL:HG23	2.08	0.54
1:D:388:PHE:CZ	1:D:472:ILE:HG21	2.43	0.54
1:E:590:VAL:O	1:E:594:VAL:HG23	2.08	0.54
1:E:26:ALA:O	1:E:30:LEU:HB2	2.08	0.53
1:A:247:GLY:HA2	1:A:268:ILE:HD13	1.90	0.53
1:C:6:ILE:HD12	1:C:487:ILE:HG23	1.91	0.53
1:F:70:ASN:HD22	1:F:70:ASN:H	1.57	0.53
1:B:108:GLN:CD	1:C:112:GLN:HB3	2.29	0.53
1:E:203:VAL:HG13	1:E:262:LEU:HD11	1.90	0.53
1:B:455:PRO:HG2	1:B:880:SER:OG	2.09	0.53
1:F:746:ILE:HG22	1:F:791:VAL:HG11	1.89	0.53
1:A:559:LEU:HD23	1:A:560:PRO:HD2	1.90	0.53
1:B:521:GLU:HA	1:B:524:THR:HG22	1.91	0.53
1:A:85:THR:HG21	1:A:620:ARG:O	2.09	0.53
1:B:317:PHE:CE2	1:B:323:ILE:HD13	2.44	0.53
1:B:60:THR:CG2	1:B:119:PRO:HG3	2.38	0.53
1:D:971:ARG:NH1	1:D:971:ARG:HB3	2.24	0.53
1:D:509:LYS:H	1:D:514:GLY:HA3	1.74	0.52
1:C:831:ALA:HB3	1:C:835:LYS:HG3	1.90	0.52
1:A:706:ALA:HB1	1:A:716:VAL:HG21	1.91	0.52
1:C:952:LEU:HA	1:C:956:GLU:HB2	1.91	0.52
1:D:418:ARG:HH21	1:D:970:MET:HG3	1.73	0.52
1:D:399:VAL:HG11	1:D:989:LEU:HD11	1.92	0.52
1:E:372:VAL:HG23	1:E:373:PRO:HD3	1.90	0.52
1:A:361:ASN:HB3	1:A:364:ALA:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ASP:O	1:A:57:VAL:HG23	2.10	0.52
1:C:892:TYR:O	1:C:894:SER:N	2.42	0.52
1:E:295:THR:HG23	1:F:73:ASP:OD1	2.10	0.52
1:F:894:SER:CB	1:F:897:ILE:HG12	2.40	0.52
1:A:159:ALA:HB2	1:A:177:LEU:HD11	1.90	0.52
1:A:657:GLN:HA	1:A:657:GLN:HE21	1.74	0.52
1:B:185:ARG:HG3	1:B:185:ARG:NH1	2.13	0.52
1:A:687:GLN:HG3	1:A:822:LEU:HD13	1.92	0.52
1:B:897:ILE:N	1:B:898:PRO:HD2	2.25	0.52
1:F:350:LEU:O	1:F:354:VAL:HG23	2.10	0.52
1:F:971:ARG:HB3	1:F:971:ARG:NH1	2.25	0.52
1:E:23:GLY:HA3	1:E:377:LEU:O	2.10	0.52
1:F:6:ILE:HD12	1:F:487:ILE:HG23	1.92	0.52
1:C:578:LEU:HD22	1:C:661:ALA:HB2	1.92	0.52
1:E:55:LYS:CE	2:E:1058:FLC:HA1	2.33	0.52
1:E:542:LEU:HD21	1:E:1028:VAL:HG21	1.91	0.52
1:E:57:VAL:HG23	1:E:82:SER:HB3	1.90	0.52
1:F:967:ALA:HB1	1:F:971:ARG:HH12	1.75	0.52
1:A:327:TYR:CE1	1:A:571:VAL:HG13	2.45	0.52
1:F:367:ILE:HB	1:F:368:PRO:HD3	1.92	0.52
1:C:115:MET:HA	1:C:118:LEU:HD12	1.91	0.51
1:E:354:VAL:O	1:E:358:PHE:HB2	2.10	0.51
1:E:108:GLN:CD	1:F:112:GLN:HB3	2.30	0.51
1:F:613:ASN:HD22	1:F:614:GLY:N	2.08	0.51
1:C:974:PRO:O	1:C:978:THR:HB	2.10	0.51
1:F:57:VAL:HG23	1:F:82:SER:HB3	1.93	0.51
1:E:281:PHE:HD1	1:E:610:PHE:HD1	1.58	0.51
1:A:166:ILE:HD12	1:A:306:ILE:HG23	1.92	0.51
1:A:484:VAL:HG13	1:A:488:LEU:HB3	1.93	0.51
1:B:151:GLN:HE22	1:B:278:ILE:HA	1.76	0.51
1:C:218:GLN:HB2	1:C:232:ALA:O	2.10	0.51
1:D:281:PHE:CZ	1:D:324:VAL:HG21	2.46	0.51
1:F:479:ALA:O	1:F:482:VAL:HG23	2.11	0.51
1:A:527:TYR:O	1:A:531:VAL:HG23	2.09	0.51
1:B:701:GLN:HE21	1:B:852:PRO:HD3	1.75	0.51
1:C:336:SER:O	1:C:340:VAL:HG23	2.11	0.51
1:C:952:LEU:HD23	1:C:956:GLU:HG3	1.92	0.51
1:D:69:MET:HG3	1:D:92:LEU:HD21	1.93	0.51
1:B:203:VAL:HG13	1:B:262:LEU:HD11	1.93	0.51
1:B:180:SER:HB3	1:B:273:GLU:HB2	1.92	0.51
1:D:239:ARG:HD2	1:D:761:ASP:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:754:TRP:CE3	1:F:234:ILE:HD11	2.45	0.51
1:F:831:ALA:HB3	1:F:835:LYS:HG3	1.93	0.51
1:A:49:TYR:CE1	1:A:60:THR:HG21	2.45	0.51
1:F:282:ASN:ND2	1:F:609:VAL:H	2.09	0.51
1:F:991:ILE:O	1:F:991:ILE:HG23	2.10	0.51
1:B:282:ASN:HD21	1:B:608:SER:HA	1.75	0.51
1:A:405:LEU:HD22	1:A:481:SER:HB3	1.93	0.51
1:B:278:ILE:HG13	1:B:613:ASN:HB3	1.92	0.51
1:A:952:LEU:HD23	1:A:956:GLU:HG3	1.93	0.50
1:A:950:LYS:HD2	1:A:954:ASP:OD2	2.11	0.50
1:B:281:PHE:CZ	1:B:324:VAL:HG21	2.46	0.50
1:D:602:GLU:OE2	1:D:650:ARG:NH1	2.44	0.50
1:A:463:THR:HG23	1:A:563:PHE:HE1	1.77	0.50
1:C:135:SER:OG	1:C:672:VAL:HG12	2.11	0.50
1:A:699:ARG:HE	1:A:718:PRO:HB3	1.76	0.50
1:A:112:GLN:CG	1:B:112:GLN:HE21	2.25	0.50
1:D:674:LEU:HD11	1:D:865:GLN:HE21	1.76	0.50
1:E:532:GLY:HA2	1:E:535:LEU:HD12	1.93	0.50
1:F:326:PRO:HB2	1:F:610:PHE:HB2	1.94	0.50
1:A:208:LYS:HA	1:A:760:ASN:HD21	1.75	0.50
1:D:905:VAL:HB	1:D:906:PRO:HD3	1.94	0.50
1:E:104:GLN:OE1	1:E:131:LYS:HD3	2.12	0.50
1:D:699:ARG:NH2	1:D:722:GLU:OE1	2.45	0.50
1:C:83:ASP:HB2	1:C:87:THR:H	1.77	0.50
1:C:445:ILE:HG23	1:C:940:LYS:HG3	1.93	0.50
1:E:578:LEU:HD13	1:E:661:ALA:HB2	1.93	0.50
1:A:706:ALA:CB	1:A:716:VAL:HG21	2.42	0.49
1:C:907:LEU:HD21	1:C:1021:PHE:HB2	1.93	0.49
1:C:350:LEU:O	1:C:354:VAL:HG23	2.12	0.49
1:A:470:PHE:CD2	1:A:929:VAL:HG11	2.47	0.49
1:D:445:ILE:HG22	1:D:943:ILE:HG21	1.93	0.49
1:F:177:LEU:HD13	1:F:179:GLY:O	2.11	0.49
1:A:316:PHE:CD1	1:B:687:GLN:HG2	2.47	0.49
1:A:356:TYR:HD1	1:A:365:THR:HG21	1.77	0.49
1:C:34:GLN:HB2	1:C:333:VAL:HG22	1.95	0.49
1:D:361:ASN:HB3	1:D:364:ALA:HB3	1.94	0.49
1:D:506:GLY:HA2	1:D:509:LYS:HD2	1.94	0.49
1:E:55:LYS:HE2	2:E:1058:FLC:CA	2.34	0.49
1:E:154:ILE:HG22	1:E:287:SER:HB3	1.95	0.49
1:A:572:PHE:HE2	1:A:631:LEU:HD21	1.78	0.49
1:C:60:THR:HG22	1:C:61:VAL:HG23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:888:LEU:HD21	1:C:943:ILE:HD11	1.94	0.49
1:F:149:MET:HB2	1:F:153:ASP:HB3	1.94	0.49
1:B:154:ILE:HG22	1:B:287:SER:HB3	1.95	0.49
1:B:75:LEU:HD11	1:B:92:LEU:HB3	1.95	0.49
1:E:444:GLY:O	1:E:448:VAL:HG23	2.13	0.49
1:A:754:TRP:CZ3	1:C:219:LEU:HD23	2.48	0.48
1:D:310:LEU:HG	1:D:323:ILE:HD13	1.94	0.48
1:E:415:ASN:OD1	1:E:418:ARG:NH1	2.46	0.48
1:C:971:ARG:HG2	1:C:974:PRO:HG3	1.94	0.48
1:F:888:LEU:HD21	1:F:943:ILE:HD11	1.94	0.48
1:B:743:ILE:H	1:B:743:ILE:HD12	1.76	0.48
1:A:754:TRP:CE3	1:C:234:ILE:HD11	2.49	0.48
1:E:705:GLU:HB3	1:E:847:LEU:HD22	1.96	0.48
1:F:578:LEU:HG	1:F:587:THR:CG2	2.41	0.48
1:F:587:THR:HG21	1:F:623:ASN:HA	1.95	0.48
1:F:905:VAL:HB	1:F:906:PRO:HD3	1.95	0.48
1:F:968:VAL:O	1:F:972:LEU:HB2	2.14	0.48
1:C:905:VAL:HB	1:C:906:PRO:HD3	1.95	0.48
1:D:674:LEU:HD21	1:D:865:GLN:HG2	1.95	0.48
1:F:979:SER:CB	1:F:1015:THR:HG21	2.40	0.48
1:C:574:THR:HG23	1:C:627:ALA:HB3	1.95	0.48
1:D:185:ARG:HD2	1:D:185:ARG:HA	1.62	0.48
1:A:668:LEU:HD23	1:A:668:LEU:H	1.79	0.48
1:B:574:THR:HG23	1:B:627:ALA:HB3	1.94	0.48
1:E:1013:THR:O	1:E:1017:LEU:HB2	2.14	0.48
1:E:534:ILE:HB	1:E:541:TYR:CE1	2.49	0.48
1:E:764:ASP:HB3	1:E:769:LYS:HD2	1.95	0.48
1:F:115:MET:HB2	1:F:116:PRO:HD3	1.95	0.48
1:F:185:ARG:HD2	1:F:772:TYR:HB2	1.94	0.48
1:C:317:PHE:CD2	1:C:321:LEU:HB3	2.49	0.48
1:D:683:GLU:HG2	1:D:819:TYR:CG	2.49	0.48
1:E:185:ARG:CG	1:E:185:ARG:HH11	2.13	0.48
1:E:249:ILE:HD11	1:E:262:LEU:HD22	1.95	0.48
1:C:210:GLN:HB2	1:C:249:ILE:HD13	1.96	0.48
1:E:111:LEU:HD21	1:E:127:VAL:HG11	1.96	0.48
1:C:971:ARG:HH21	1:C:975:ILE:HD11	1.78	0.47
1:F:100:ALA:HB1	1:F:131:LYS:HG2	1.96	0.47
1:D:952:LEU:HD23	1:D:956:GLU:HG3	1.96	0.47
1:E:443:VAL:O	1:E:447:MET:HG2	2.14	0.47
1:B:952:LEU:O	1:B:958:LYS:HB2	2.14	0.47
1:F:159:ALA:HB2	1:F:177:LEU:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:126:GLY:CA	1:F:116:PRO:HB3	2.45	0.47
1:E:218:GLN:HA	1:E:234:ILE:HG13	1.96	0.47
1:A:259:ARG:NH1	1:A:261:LEU:HD21	2.29	0.47
1:A:983:ILE:HG23	1:A:1008:MET:HG3	1.95	0.47
1:B:612:VAL:HB	1:B:626:ILE:HG22	1.96	0.47
1:C:438:ILE:HG22	1:C:948:PHE:HZ	1.79	0.47
1:D:9:PRO:HG2	1:D:10:ILE:HD12	1.96	0.47
1:F:445:ILE:HG23	1:F:940:LYS:HG3	1.97	0.47
1:A:361:ASN:O	1:A:365:THR:HG22	2.14	0.47
1:B:390:ILE:HG23	1:B:395:MET:SD	2.55	0.47
1:C:746:ILE:HG22	1:C:791:VAL:HG21	1.97	0.47
1:D:579:PRO:HD3	1:D:661:ALA:HB2	1.97	0.47
1:E:180:SER:HB3	1:E:273:GLU:HB2	1.96	0.47
1:F:356:TYR:C	1:F:358:PHE:H	2.17	0.47
1:A:302:THR:O	1:A:306:ILE:HG13	2.14	0.47
1:A:445:ILE:HG22	1:A:943:ILE:HG21	1.97	0.47
1:B:111:LEU:HD21	1:B:127:VAL:HG11	1.96	0.47
1:C:971:ARG:NH2	1:C:975:ILE:HD11	2.29	0.47
1:D:159:ALA:HB2	1:D:177:LEU:HD11	1.96	0.47
1:D:559:LEU:HD13	1:D:923:ASN:HB2	1.96	0.47
1:D:54:ALA:H	1:D:84:SER:HB3	1.79	0.47
1:E:251:LEU:HD11	1:E:262:LEU:HA	1.97	0.47
1:A:166:ILE:HD11	1:A:310:LEU:HD13	1.97	0.47
1:B:764:ASP:HB3	1:B:769:LYS:HD2	1.96	0.47
1:C:658:ILE:O	1:C:659:LYS:HB2	2.15	0.47
1:D:53:ASP:O	1:D:57:VAL:HG23	2.15	0.47
1:D:613:ASN:HD22	1:D:614:GLY:N	2.13	0.47
1:D:655:PHE:HB3	1:D:663:VAL:HB	1.97	0.47
1:B:310:LEU:HD23	1:B:325:TYR:OH	2.14	0.46
1:D:239:ARG:HB2	1:D:763:ILE:HD12	1.96	0.46
1:E:49:TYR:HE1	1:E:60:THR:HG21	1.79	0.46
1:F:534:ILE:HG22	1:F:541:TYR:CZ	2.51	0.46
1:B:484:VAL:HG13	1:B:488:LEU:HB3	1.97	0.46
1:C:895:TRP:HB3	1:C:1033:PHE:CE1	2.49	0.46
1:D:777:ALA:O	1:D:781:MET:HG2	2.16	0.46
1:E:590:VAL:HG13	1:E:659:LYS:HE2	1.97	0.46
1:F:359:LEU:HB2	1:F:365:THR:HG22	1.96	0.46
1:F:538:THR:HG22	1:F:542:LEU:HB2	1.96	0.46
1:F:587:THR:CG2	1:F:623:ASN:HA	2.46	0.46
1:A:1027:VAL:O	1:A:1031:ARG:HG3	2.15	0.46
1:B:568:ASP:O	1:B:634:TRP:HZ3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:904:VAL:HG21	1:A:942:ALA:HB2	1.98	0.46
1:C:366:LEU:O	1:C:370:ILE:HG13	2.15	0.46
1:E:756:GLY:HA2	1:E:774:MET:HG3	1.96	0.46
1:B:705:GLU:HB3	1:B:847:LEU:HD22	1.98	0.46
1:E:372:VAL:CG2	1:E:373:PRO:HD3	2.45	0.46
1:E:562:SER:HB3	1:E:924:ASP:HB3	1.97	0.46
1:A:276:ASP:OD1	1:C:222:THR:HG21	2.16	0.46
1:A:388:PHE:CZ	1:A:472:ILE:HG21	2.50	0.46
1:A:851:LEU:HB3	1:A:852:PRO:HD2	1.97	0.46
1:F:687:GLN:HG3	1:F:688:ALA:N	2.31	0.46
1:B:580:ALA:HB1	1:B:724:THR:HG22	1.97	0.46
1:E:455:PRO:HG2	1:E:880:SER:OG	2.16	0.46
1:F:47:ALA:HB3	1:F:88:VAL:CG1	2.45	0.46
1:A:112:GLN:OE1	1:B:112:GLN:HG2	2.16	0.46
1:B:905:VAL:HB	1:B:906:PRO:HD3	1.98	0.46
1:D:219:LEU:HD23	1:E:754:TRP:CZ3	2.51	0.46
1:C:568:ASP:CG	1:C:644:VAL:HG23	2.36	0.46
1:E:58:GLN:HA	1:E:62:THR:HB	1.97	0.46
1:E:75:LEU:HD11	1:E:92:LEU:HB3	1.98	0.46
1:D:332:PHE:O	1:D:336:SER:HB3	2.16	0.45
1:F:407:ASP:O	1:F:411:VAL:HG23	2.15	0.45
1:A:281:PHE:CZ	1:A:324:VAL:HG21	2.51	0.45
1:A:168:ARG:HG2	1:B:69:MET:O	2.16	0.45
1:B:898:PRO:HB2	1:B:902:MET:HE2	1.99	0.45
1:C:393:LEU:HD11	1:C:466:ILE:HD13	1.98	0.45
1:D:414:GLU:HG3	1:D:977:MET:CE	2.46	0.45
1:E:904:VAL:HG21	1:E:942:ALA:HB2	1.98	0.45
1:E:897:ILE:HD11	1:E:950:LYS:HE3	1.98	0.45
1:F:399:VAL:HA	1:F:402:ILE:HD12	1.97	0.45
1:A:459:PHE:CB	1:A:464:GLY:HA2	2.47	0.45
1:B:877:TYR:HA	1:B:880:SER:HB2	1.97	0.45
1:E:309:GLU:HG3	1:E:313:MET:HE3	1.98	0.45
1:E:173:GLY:O	1:F:71:GLY:HA3	2.16	0.45
1:A:267:LYS:HB3	1:A:267:LYS:NZ	2.31	0.45
1:B:400:LEU:HD13	1:B:1003:VAL:HG13	1.98	0.45
1:D:682:PHE:CZ	1:D:857:TYR:HB2	2.52	0.45
1:B:295:THR:HG23	1:C:73:ASP:OD1	2.17	0.45
1:D:690:LEU:HB3	1:D:694:LYS:HD3	1.99	0.45
1:E:485:ALA:HA	1:E:489:THR:OG1	2.17	0.45
1:F:615:PHE:HD2	1:F:620:ARG:HH12	1.65	0.45
1:F:690:LEU:O	1:F:694:LYS:HD3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:ILE:O	1:B:105:VAL:HG12	2.17	0.45
1:C:817:GLU:HB2	1:C:824:SER:O	2.16	0.45
1:E:363:ARG:HD2	1:E:498:LYS:HB2	1.97	0.45
1:F:354:VAL:HG11	1:F:980:LEU:HB3	1.97	0.45
1:F:583:THR:HA	1:F:622:GLN:HE21	1.81	0.45
1:F:764:ASP:HB3	1:F:769:LYS:HD2	1.99	0.45
1:C:149:MET:HB2	1:C:153:ASP:HB3	1.98	0.45
1:D:30:LEU:HD12	1:D:31:PRO:HD2	1.99	0.45
1:E:974:PRO:HA	1:E:977:MET:HB2	1.99	0.45
1:A:23:GLY:HA3	1:A:377:LEU:HB3	1.99	0.45
1:A:574:THR:HG23	1:A:627:ALA:HB3	1.98	0.45
1:B:104:GLN:OE1	1:B:131:LYS:HD3	2.16	0.45
1:D:945:ILE:HG12	1:D:971:ARG:HH21	1.80	0.45
1:E:30:LEU:HD12	1:E:31:PRO:HD2	1.99	0.45
1:A:418:ARG:HE	1:A:970:MET:HB2	1.81	0.45
1:C:335:ILE:O	1:C:339:GLU:HG2	2.16	0.45
1:F:393:LEU:HD11	1:F:466:ILE:HD13	1.99	0.45
1:F:658:ILE:HG13	1:F:658:ILE:H	1.58	0.45
1:A:262:LEU:HG	1:A:268:ILE:HD11	1.97	0.45
1:A:367:ILE:HB	1:A:368:PRO:HD3	1.98	0.45
1:B:60:THR:HG23	1:B:119:PRO:HG3	1.99	0.45
1:C:615:PHE:HD2	1:C:620:ARG:NH1	2.15	0.45
1:C:699:ARG:HD3	1:C:825:MET:SD	2.57	0.45
1:D:166:ILE:HD11	1:D:310:LEU:HD13	1.99	0.45
1:D:706:ALA:HB1	1:D:716:VAL:HG21	1.98	0.45
1:E:309:GLU:HG3	1:E:313:MET:CE	2.47	0.45
1:F:218:GLN:HA	1:F:234:ILE:HG13	1.99	0.45
1:A:673:GLU:O	1:A:674:LEU:HB2	2.17	0.44
1:C:218:GLN:HA	1:C:234:ILE:HG13	1.99	0.44
1:C:559:LEU:HD13	1:C:923:ASN:HB2	2.00	0.44
1:B:442:LEU:O	1:B:445:ILE:HG13	2.17	0.44
1:C:356:TYR:C	1:C:358:PHE:H	2.20	0.44
1:D:979:SER:HB2	1:D:1015:THR:HG21	1.99	0.44
1:E:948:PHE:O	1:E:952:LEU:HG	2.17	0.44
1:C:892:TYR:C	1:C:894:SER:H	2.20	0.44
1:D:418:ARG:O	1:D:422:GLU:N	2.50	0.44
1:D:888:LEU:HD13	1:D:901:VAL:HG13	1.99	0.44
1:E:907:LEU:HD23	1:E:1017:LEU:HB3	1.98	0.44
1:F:696:THR:HG23	1:F:699:ARG:HH12	1.82	0.44
1:A:326:PRO:HB2	1:A:610:PHE:HB2	1.99	0.44
1:B:732:ASP:HB3	1:B:735:LYS:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:VAL:HB	1:C:327:TYR:HB3	1.98	0.44
1:E:356:TYR:C	1:E:358:PHE:H	2.21	0.44
1:B:181:GLN:HE21	1:B:767:ARG:HH11	1.66	0.44
1:F:5:PHE:HD2	1:F:6:ILE:HG12	1.82	0.44
1:B:650:ARG:HA	1:B:653:ARG:HB3	2.00	0.44
1:C:280:GLU:HB3	1:C:611:ALA:HB3	1.99	0.44
1:C:682:PHE:CZ	1:C:857:TYR:HB2	2.52	0.44
1:D:484:VAL:HG13	1:D:488:LEU:HB3	1.99	0.44
1:E:744:ASN:O	1:E:748:THR:HG23	2.17	0.44
1:E:946:VAL:HG13	1:E:1026:PHE:CE1	2.51	0.44
1:F:340:VAL:HG11	1:F:395:MET:HB3	2.00	0.44
1:F:38:ILE:HG23	1:F:462:SER:OG	2.18	0.44
1:F:568:ASP:OD1	1:F:644:VAL:HG23	2.18	0.44
1:A:489:THR:N	1:A:490:PRO:HD2	2.32	0.44
1:A:531:VAL:O	1:A:534:ILE:HG13	2.17	0.44
1:B:14:VAL:HG13	1:C:886:LEU:HD12	1.98	0.44
1:A:676:THR:O	1:A:677:ALA:C	2.56	0.44
1:C:367:ILE:HB	1:C:368:PRO:HD3	2.00	0.44
1:C:447:MET:HG3	1:C:448:VAL:N	2.33	0.44
1:D:216:ALA:HB3	1:D:234:ILE:O	2.18	0.44
1:A:510:LYS:H	1:A:514:GLY:HA3	1.83	0.44
1:B:760:ASN:HD22	1:B:760:ASN:HA	1.56	0.44
1:C:3:ASN:OD1	1:C:3:ASN:N	2.51	0.44
1:D:327:TYR:CE1	1:D:571:VAL:HG13	2.53	0.44
1:E:102:ILE:O	1:E:105:VAL:HG12	2.18	0.44
1:F:1015:THR:O	1:F:1019:ILE:HG12	2.18	0.44
1:F:3:ASN:HD21	1:F:439:GLN:HG3	1.83	0.44
1:F:60:THR:HG23	1:F:119:PRO:HG2	2.00	0.44
1:A:228:GLN:HB2	1:B:781:MET:CE	2.48	0.43
1:A:521:GLU:HA	1:A:524:THR:HG22	2.00	0.43
1:A:971:ARG:CG	1:A:974:PRO:HG2	2.48	0.43
1:C:6:ILE:HG22	1:C:12:ALA:HB2	2.00	0.43
1:D:137:LEU:HD13	1:D:293:LEU:HG	2.00	0.43
1:E:110:LYS:HA	1:E:110:LYS:HD3	1.81	0.43
1:A:753:ALA:O	1:A:775:SER:HB3	2.18	0.43
1:A:720:GLY:HA3	1:A:817:GLU:OE1	2.18	0.43
1:A:979:SER:HB2	1:A:1015:THR:HG21	2.00	0.43
1:B:633:ASP:O	1:B:635:ALA:N	2.52	0.43
1:E:355:MET:HG3	1:E:359:LEU:HD12	1.99	0.43
1:F:133:SER:O	1:F:134:SER:HB2	2.18	0.43
1:F:6:ILE:HG21	1:F:487:ILE:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ALA:HB3	1:A:88:VAL:CG1	2.48	0.43
1:C:154:ILE:O	1:C:158:VAL:HG23	2.17	0.43
1:C:398:MET:HB3	1:C:398:MET:HE3	1.79	0.43
1:C:40:PRO:HB2	1:C:94:PHE:O	2.18	0.43
1:E:489:THR:N	1:E:490:PRO:HD2	2.34	0.43
1:A:758:TYR:CE1	1:A:770:LYS:HD3	2.53	0.43
1:B:578:LEU:HD13	1:B:661:ALA:HB2	2.00	0.43
1:D:63:GLN:O	1:D:67:GLN:HG3	2.18	0.43
1:E:375:VAL:HG11	1:E:405:LEU:HD22	2.00	0.43
1:C:53:ASP:O	1:C:57:VAL:HG22	2.18	0.43
1:D:208:LYS:HA	1:D:760:ASN:HD21	1.84	0.43
1:D:276:ASP:OD1	1:F:222:THR:HG21	2.18	0.43
1:A:395:MET:O	1:A:398:MET:HB2	2.19	0.43
1:B:479:ALA:O	1:B:482:VAL:HG12	2.17	0.43
1:B:983:ILE:HG23	1:B:1008:MET:HG3	2.00	0.43
1:E:24:GLY:O	1:E:27:ILE:HG22	2.17	0.43
1:E:583:THR:HG22	1:E:585:GLU:H	1.82	0.43
1:C:531:VAL:HG21	1:C:968:VAL:HG11	2.00	0.43
1:E:598:TYR:HB3	1:E:606:VAL:HG11	2.01	0.43
1:A:727:PHE:HB2	1:C:219:LEU:HD11	2.01	0.43
1:B:418:ARG:O	1:B:422:GLU:HB2	2.19	0.43
1:B:414:GLU:HG3	1:B:977:MET:HE2	2.01	0.43
1:C:57:VAL:HG23	1:C:82:SER:HB3	2.01	0.43
2:D:1058:FLC:OG2	2:D:1058:FLC:HA2	2.17	0.43
1:E:355:MET:HG2	1:E:365:THR:HA	2.01	0.43
1:E:730:ASP:OD1	1:E:808:ARG:NH2	2.48	0.43
1:E:758:TYR:HB2	1:E:772:TYR:CE1	2.53	0.43
1:A:851:LEU:HB3	1:A:852:PRO:CD	2.48	0.43
1:B:676:THR:OG1	1:B:679:GLY:HA3	2.19	0.43
1:D:26:ALA:O	1:D:30:LEU:HB2	2.18	0.43
1:E:139:VAL:O	1:E:326:PRO:HD2	2.19	0.43
1:B:851:LEU:HB3	1:B:852:PRO:CD	2.49	0.43
1:C:418:ARG:O	1:C:422:GLU:HB2	2.19	0.43
1:E:355:MET:HE1	1:E:410:ILE:HG23	2.00	0.43
1:E:42:ALA:HB3	1:E:132:SER:HB3	2.01	0.43
1:A:483:LEU:HD13	1:A:487:ILE:HD12	2.00	0.42
1:C:47:ALA:HB3	1:C:88:VAL:HG13	2.00	0.42
1:C:680:PHE:HB2	1:C:859:TRP:CZ3	2.53	0.42
1:D:223:PRO:HA	1:D:224:PRO:HD3	1.84	0.42
1:D:676:THR:O	1:D:677:ALA:C	2.58	0.42
1:F:894:SER:HB3	1:F:897:ILE:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:200:PRO:HD2	1:E:749:THR:HG22	2.00	0.42
1:B:181:GLN:HE21	1:B:767:ARG:NH1	2.17	0.42
1:C:146:ASP:O	1:C:148:THR:N	2.53	0.42
1:E:897:ILE:N	1:E:898:PRO:HD2	2.33	0.42
1:F:1022:VAL:N	1:F:1023:PRO:HD2	2.34	0.42
1:F:182:TYR:HA	1:F:271:GLY:O	2.18	0.42
1:F:559:LEU:HD13	1:F:923:ASN:HB2	1.99	0.42
1:F:699:ARG:HD3	1:F:825:MET:SD	2.59	0.42
1:A:326:PRO:CB	1:A:610:PHE:HB2	2.50	0.42
1:A:584:GLN:H	1:A:622:GLN:HE21	1.66	0.42
1:C:584:GLN:H	1:C:622:GLN:HE21	1.67	0.42
1:C:904:VAL:HG12	1:C:938:SER:HB2	2.00	0.42
1:D:706:ALA:CB	1:D:716:VAL:HG21	2.50	0.42
1:E:60:THR:HG23	1:E:119:PRO:HG3	2.01	0.42
1:D:168:ARG:CG	1:E:69:MET:O	2.68	0.42
1:C:177:LEU:HD13	1:C:179:GLY:O	2.19	0.42
1:D:150:THR:O	1:D:153:ASP:HB2	2.19	0.42
1:D:435:MET:O	1:D:439:GLN:HB2	2.19	0.42
1:F:139:VAL:O	1:F:326:PRO:HD2	2.20	0.42
1:F:447:MET:HG3	1:F:448:VAL:N	2.34	0.42
1:F:615:PHE:HD2	1:F:620:ARG:NH1	2.18	0.42
1:A:151:GLN:HA	1:A:154:ILE:HD12	2.01	0.42
1:A:886:LEU:HB3	1:C:14:VAL:HG13	2.01	0.42
1:E:445:ILE:HG22	1:E:943:ILE:CD1	2.49	0.42
1:A:259:ARG:HH12	1:A:261:LEU:HD21	1.84	0.42
1:B:1016:VAL:O	1:B:1016:VAL:HG12	2.19	0.42
1:B:414:GLU:HG3	1:B:977:MET:CE	2.49	0.42
1:C:6:ILE:HG21	1:C:487:ILE:HG23	2.00	0.42
1:D:49:TYR:HE1	1:D:60:THR:HG21	1.83	0.42
1:D:961:ILE:H	1:D:961:ILE:HD12	1.85	0.42
1:D:986:VAL:O	1:D:986:VAL:HG12	2.18	0.42
1:E:775:SER:HB3	1:E:780:ARG:HD3	2.01	0.42
1:B:490:PRO:HA	1:B:493:CYS:HB2	2.01	0.42
1:C:979:SER:CB	1:C:1015:THR:HG21	2.43	0.42
1:C:213:GLN:HE21	1:C:213:GLN:HB3	1.66	0.42
1:A:63:GLN:HB3	1:C:768:VAL:HG12	2.02	0.42
1:A:893:GLU:CD	1:C:8:ARG:HB3	2.40	0.42
1:D:135:SER:HA	1:D:617:PHE:HZ	1.85	0.42
1:D:63:GLN:HB3	1:F:768:VAL:HG12	2.02	0.42
1:E:402:ILE:H	1:E:402:ILE:HG13	1.56	0.42
1:F:577:GLN:HG3	1:F:624:THR:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ASP:HB3	1:A:292:LYS:HB2	2.02	0.42
1:A:273:GLU:OE2	1:A:770:LYS:HE2	2.20	0.42
1:B:459:PHE:O	1:B:464:GLY:HA3	2.19	0.42
1:C:664:PHE:CD2	1:C:717:ARG:HD2	2.55	0.42
1:C:699:ARG:HB3	1:C:699:ARG:HH11	1.84	0.42
1:D:314:GLU:HA	1:D:317:PHE:CE2	2.55	0.42
1:E:49:TYR:CE1	1:E:60:THR:HG21	2.54	0.42
1:E:559:LEU:HD13	1:E:923:ASN:HB2	2.02	0.42
1:F:363:ARG:H	1:F:363:ARG:HG2	1.69	0.42
1:F:391:ASN:O	1:F:395:MET:HG2	2.20	0.42
1:F:6:ILE:C	1:F:8:ARG:H	2.22	0.42
1:A:228:GLN:HB2	1:B:781:MET:HE1	2.01	0.42
1:C:544:LEU:HA	1:C:547:ILE:HD12	2.02	0.42
1:D:69:MET:HE1	1:D:107:VAL:HG13	2.01	0.42
1:E:946:VAL:HG13	1:E:1026:PHE:HE1	1.85	0.42
1:F:737:GLN:HE21	1:F:743:ILE:HD11	1.85	0.42
1:A:142:VAL:HG21	1:A:162:MET:HE1	2.01	0.41
1:A:274:ASN:HD22	1:A:276:ASP:HB2	1.85	0.41
1:B:419:VAL:HG21	1:B:434:SER:HB3	2.02	0.41
1:B:973:ARG:HB3	1:B:974:PRO:CD	2.50	0.41
1:C:659:LYS:HD3	1:C:659:LYS:HA	1.82	0.41
1:B:223:PRO:HD2	1:C:780:ARG:HH22	1.85	0.41
1:D:63:GLN:HB3	1:F:768:VAL:CG1	2.50	0.41
1:B:26:ALA:O	1:B:30:LEU:HB2	2.20	0.41
1:B:347:ALA:O	1:B:351:VAL:HG23	2.21	0.41
1:D:340:VAL:HG11	1:D:395:MET:HB3	2.02	0.41
1:B:355:MET:HG3	1:B:359:LEU:HD12	2.01	0.41
1:C:1015:THR:O	1:C:1019:ILE:HG12	2.20	0.41
1:C:185:ARG:HD2	1:C:772:TYR:HB2	2.02	0.41
1:C:83:ASP:HB3	1:C:85:THR:H	1.85	0.41
1:F:578:LEU:HD22	1:F:661:ALA:HB2	2.02	0.41
1:D:668:LEU:HD23	1:D:668:LEU:H	1.84	0.41
1:F:223:PRO:HA	1:F:224:PRO:HD3	1.90	0.41
1:F:948:PHE:CD1	1:F:971:ARG:HD3	2.56	0.41
1:A:733:GLN:HE22	1:A:743:ILE:HG21	1.85	0.41
1:B:49:TYR:HE1	1:B:60:THR:HG21	1.85	0.41
1:C:462:SER:H	1:C:865:GLN:NE2	2.19	0.41
1:D:69:MET:HE3	1:D:107:VAL:HG22	2.02	0.41
1:E:668:LEU:HA	1:E:669:PRO:HD3	1.95	0.41
1:E:685:ILE:HD11	1:E:858:ASP:HB2	2.01	0.41
1:E:559:LEU:HD12	1:E:913:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:563:PHE:O	1:F:924:ASP:HB2	2.21	0.41
1:A:69:MET:CE	1:A:107:VAL:HG13	2.51	0.41
1:E:479:ALA:O	1:E:482:VAL:HG12	2.20	0.41
1:F:562:SER:HB2	1:F:924:ASP:HB3	2.02	0.41
1:F:327:TYR:CE1	1:F:571:VAL:HG13	2.55	0.41
1:A:911:GLY:HA3	1:A:1013:THR:OG1	2.20	0.41
1:B:355:MET:HG2	1:B:365:THR:HA	2.01	0.41
1:B:953:MET:HE2	1:B:963:ALA:HB3	2.03	0.41
1:C:402:ILE:C	1:C:404:LEU:H	2.24	0.41
1:C:559:LEU:HA	1:C:560:PRO:HD2	1.91	0.41
1:C:326:PRO:HB2	1:C:610:PHE:HB2	2.01	0.41
1:E:317:PHE:CE2	1:E:323:ILE:HD13	2.56	0.41
1:E:813:SER:HA	1:E:814:PRO:HD3	1.93	0.41
1:F:149:MET:HB2	1:F:153:ASP:CB	2.51	0.41
1:F:994:GLY:O	1:F:997:SER:HB3	2.20	0.41
1:A:199:THR:HG21	1:A:792:ARG:H	1.85	0.41
1:B:545:TYR:HA	1:B:548:ILE:HD12	2.03	0.41
1:C:176:GLN:HE22	1:C:620:ARG:HH22	1.69	0.41
1:C:933:THR:O	1:C:937:LEU:HG	2.20	0.41
1:D:361:ASN:O	1:D:365:THR:HG22	2.21	0.41
1:D:753:ALA:O	1:D:775:SER:HB3	2.20	0.41
1:A:591:LEU:HD22	1:A:611:ALA:HB1	2.02	0.41
1:B:158:VAL:HA	1:B:162:MET:HE3	2.02	0.41
1:B:682:PHE:CZ	1:B:857:TYR:HB2	2.55	0.41
1:B:915:ALA:HB2	1:B:1009:GLY:HA3	2.02	0.41
1:C:39:ALA:HB2	1:C:671:ILE:CG2	2.51	0.41
1:A:185:ARG:HD2	1:A:185:ARG:HA	1.58	0.41
1:C:960:LEU:HD11	1:C:1027:VAL:HA	2.02	0.41
1:D:416:VAL:HG22	1:D:434:SER:OG	2.20	0.41
1:D:683:GLU:O	1:D:857:TYR:HA	2.20	0.41
1:D:983:ILE:HG23	1:D:1008:MET:HG3	2.01	0.41
1:A:516:PHE:O	1:A:520:PHE:HD1	2.04	0.41
1:A:612:VAL:HB	1:A:626:ILE:HG22	2.03	0.41
1:B:372:VAL:CG2	1:B:373:PRO:HD3	2.50	0.41
1:B:489:THR:N	1:B:490:PRO:HD2	2.35	0.41
1:C:348:ILE:HG12	1:C:372:VAL:HG11	2.03	0.41
1:D:431:THR:O	1:D:435:MET:HG2	2.21	0.41
1:D:49:TYR:CE1	1:D:60:THR:HG21	2.56	0.41
1:D:190:PRO:HB2	1:D:788:ASP:O	2.21	0.41
1:E:157:TYR:CZ	1:E:318:PRO:HD3	2.56	0.41
1:E:45:ILE:HD11	1:E:69:MET:HE2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:756:GLY:CA	1:E:774:MET:HG3	2.51	0.41
1:E:907:LEU:HG	1:E:1017:LEU:HD23	2.02	0.41
1:F:462:SER:H	1:F:865:GLN:NE2	2.19	0.41
1:F:597:TYR:CE1	1:F:601:LYS:HD2	2.56	0.41
1:F:637:ARG:N	1:F:638:PRO:HD3	2.36	0.41
1:F:80:SER:HA	1:F:89:GLN:O	2.21	0.41
1:A:180:SER:HB2	1:A:274:ASN:OD1	2.21	0.40
1:B:973:ARG:HB3	1:B:974:PRO:HD3	2.03	0.40
1:D:239:ARG:NH1	1:D:239:ARG:HG3	2.26	0.40
1:E:521:GLU:HA	1:E:524:THR:HG22	2.02	0.40
1:F:111:LEU:HD21	1:F:127:VAL:HG11	2.03	0.40
1:B:375:VAL:HG11	1:B:405:LEU:HD22	2.03	0.40
1:C:310:LEU:HG	1:C:323:ILE:HD13	2.03	0.40
1:D:2:PRO:HB2	1:D:3:ASN:H	1.64	0.40
1:B:559:LEU:HD23	1:B:560:PRO:HD2	2.02	0.40
1:C:613:ASN:HD22	1:C:614:GLY:N	2.17	0.40
1:C:750:LEU:HD12	1:C:754:TRP:CD1	2.56	0.40
1:D:402:ILE:O	1:D:406:VAL:HG23	2.21	0.40
1:D:668:LEU:HA	1:D:669:PRO:HD3	1.96	0.40
1:E:533:GLY:O	1:E:536:ARG:HG3	2.22	0.40
1:A:743:ILE:HD12	1:A:743:ILE:H	1.87	0.40
1:B:42:ALA:O	1:B:132:SER:HB3	2.21	0.40
1:B:506:GLY:HA2	1:B:509:LYS:HD2	2.04	0.40
1:B:745:ASP:O	1:B:749:THR:OG1	2.28	0.40
1:C:578:LEU:HD22	1:C:661:ALA:CB	2.51	0.40
1:C:70:ASN:O	1:C:110:LYS:HE3	2.22	0.40
1:D:375:VAL:HG11	1:D:405:LEU:HD22	2.03	0.40
1:E:678:THR:O	1:E:830:GLN:HB2	2.22	0.40
1:F:641:GLU:HB2	1:F:650:ARG:HH22	1.87	0.40
1:B:255:GLN:HB2	1:B:255:GLN:HE21	1.67	0.40
1:B:584:GLN:N	1:B:622:GLN:HB3	2.37	0.40
1:C:897:ILE:HD13	1:C:897:ILE:HA	1.91	0.40
1:D:424:GLY:HA3	1:D:502:LYS:HB3	2.03	0.40
1:E:915:ALA:HB2	1:E:1009:GLY:HA3	2.04	0.40
1:F:282:ASN:HD21	1:F:608:SER:HA	1.85	0.40
1:F:298:ASN:HB3	1:F:301:ASP:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1030/1057 (97%)	978 (95%)	47 (5%)	5 (0%)	29	68
1	B	1030/1057 (97%)	969 (94%)	54 (5%)	7 (1%)	22	60
1	C	1030/1057 (97%)	968 (94%)	54 (5%)	8 (1%)	19	57
1	D	1030/1057 (97%)	980 (95%)	43 (4%)	7 (1%)	22	60
1	E	1030/1057 (97%)	966 (94%)	57 (6%)	7 (1%)	22	60
1	F	1030/1057 (97%)	964 (94%)	56 (5%)	10 (1%)	15	53
All	All	6180/6342 (97%)	5825 (94%)	311 (5%)	44 (1%)	22	60

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	674	LEU
1	B	634	TRP
1	D	677	ALA
1	F	134	SER
1	F	657	GLN
1	A	992	SER
1	C	147	GLY
1	C	893	GLU
1	D	920	GLY
1	D	991	ILE
1	D	992	SER
1	E	509	LYS
1	E	634	TRP
1	F	133	SER
1	F	147	GLY
1	F	893	GLU
1	A	677	ALA
1	B	536	ARG
1	D	360	GLN
1	D	674	LEU

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Mol	Chain	Res	Type
1	E	833	PRO
1	F	146	ASP
1	B	672	VAL
1	B	833	PRO
1	C	134	SER
1	F	687	GLN
1	B	360	GLN
1	C	833	PRO
1	F	833	PRO
1	A	920	GLY
1	B	133	SER
1	B	677	ALA
1	C	133	SER
1	C	969	ARG
1	E	427	PRO
1	C	6	ILE
1	C	1019	ILE
1	E	672	VAL
1	A	991	ILE
1	E	514	GLY
1	E	638	PRO
1	F	689	GLY
1	D	126	GLY
1	F	6	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%)	775 (92%)	63 (8%)	13	43
1	B	838/863 (97%)	764 (91%)	74 (9%)	10	36
1	C	838/863 (97%)	760 (91%)	78 (9%)	9	33
1	D	838/863 (97%)	788 (94%)	50 (6%)	19	53
1	E	838/863 (97%)	768 (92%)	70 (8%)	11	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	838/863 (97%)	766 (91%)	72 (9%)	10	37
All	All	5028/5178 (97%)	4621 (92%)	407 (8%)	11	40

All (407) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	30	LEU
1	A	49	TYR
1	A	60	THR
1	A	70	ASN
1	A	84	SER
1	A	91	THR
1	A	108	GLN
1	A	152	GLU
1	A	177	LEU
1	A	185	ARG
1	A	208	LYS
1	A	229	GLN
1	A	253	VAL
1	A	269	GLU
1	A	278	ILE
1	A	310	LEU
1	A	349	ILE
1	A	355	MET
1	A	357	LEU
1	A	362	PHE
1	A	404	LEU
1	A	429	GLU
1	A	432	ARG
1	A	483	LEU
1	A	489	THR
1	A	544	LEU
1	A	559	LEU
1	A	564	LEU
1	A	571	VAL
1	A	574	THR
1	A	617	PHE
1	A	624	THR
1	A	626	ILE
1	A	630	SER
1	A	634	TRP

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Mol	Chain	Res	Type
1	A	640	GLU
1	A	657	GLN
1	A	668	LEU
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	699	ARG
1	A	716	VAL
1	A	717	ARG
1	A	721	LEU
1	A	723	ASP
1	A	748	THR
1	A	797	GLN
1	A	806	SER
1	A	808	ARG
1	A	813	SER
1	A	843	LEU
1	A	901	VAL
1	A	914	LEU
1	A	918	PHE
1	A	921	LEU
1	A	931	LEU
1	A	964	THR
1	A	1017	LEU
1	B	8	ARG
1	B	11	PHE
1	B	25	LEU
1	B	28	LEU
1	B	29	LYS
1	B	49	TYR
1	B	60	THR
1	B	70	ASN
1	B	96	SER
1	B	109	ASN
1	B	120	GLN
1	B	131	LYS
1	B	135	SER
1	B	148	THR
1	B	174	ASP

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Mol	Chain	Res	Type
1	B	177	LEU
1	B	180	SER
1	B	185	ARG
1	B	213	GLN
1	B	230	LEU
1	B	255	GLN
1	B	259	ARG
1	B	293	LEU
1	B	295	THR
1	B	310	LEU
1	B	335	ILE
1	B	355	MET
1	B	358	PHE
1	B	360	GLN
1	B	400	LEU
1	B	402	ILE
1	B	404	LEU
1	B	433	LYS
1	B	489	THR
1	B	516	PHE
1	B	525	HIS
1	B	529	ASP
1	B	538	THR
1	B	559	LEU
1	B	571	VAL
1	B	574	THR
1	B	575	MET
1	B	589	LYS
1	B	626	ILE
1	B	634	TRP
1	B	652	THR
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	708	LYS
1	B	713	LEU
1	B	717	ARG
1	B	722	GLU
1	B	730	ASP

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Mol	Chain	Res	Type
1	B	743	ILE
1	B	748	THR
1	B	749	THR
1	B	760	ASN
1	B	808	ARG
1	B	835	LYS
1	B	843	LEU
1	B	850	LYS
1	B	858	ASP
1	B	862	MET
1	B	871	ASN
1	B	880	SER
1	B	886	LEU
1	B	901	VAL
1	B	921	LEU
1	B	928	GLN
1	B	971	ARG
1	C	3	ASN
1	C	6	ILE
1	C	11	PHE
1	C	28	LEU
1	C	34	GLN
1	C	49	TYR
1	C	60	THR
1	C	69	MET
1	C	70	ASN
1	C	96	SER
1	C	104	GLN
1	C	113	LEU
1	C	117	LEU
1	C	148	THR
1	C	174	ASP
1	C	177	LEU
1	C	182	TYR
1	C	185	ARG
1	C	222	THR
1	C	225	VAL
1	C	230	LEU
1	C	280	GLU
1	C	307	ARG
1	C	310	LEU
1	C	321	LEU

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Mol	Chain	Res	Type
1	C	342	LYS
1	C	358	PHE
1	C	415	ASN
1	C	439	GLN
1	C	448	VAL
1	C	452	VAL
1	C	456	MET
1	C	472	ILE
1	C	482	VAL
1	C	510	LYS
1	C	513	PHE
1	C	515	TRP
1	C	559	LEU
1	C	564	LEU
1	C	571	VAL
1	C	574	THR
1	C	578	LEU
1	C	597	TYR
1	C	602	GLU
1	C	613	ASN
1	C	633	ASP
1	C	634	TRP
1	C	645	GLU
1	C	649	MET
1	C	660	ASP
1	C	662	MET
1	C	668	LEU
1	C	695	LEU
1	C	699	ARG
1	C	702	LEU
1	C	703	LEU
1	C	713	LEU
1	C	714	THR
1	C	721	LEU
1	C	722	GLU
1	C	731	ILE
1	C	743	ILE
1	C	807	SER
1	C	813	SER
1	C	843	LEU
1	C	863	SER
1	C	875	SER

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Mol	Chain	Res	Type
1	C	876	LEU
1	C	901	VAL
1	C	914	LEU
1	C	919	ARG
1	C	958	LYS
1	C	961	ILE
1	C	971	ARG
1	C	973	ARG
1	C	978	THR
1	C	991	ILE
1	C	1008	MET
1	D	11	PHE
1	D	21	LEU
1	D	27	ILE
1	D	49	TYR
1	D	60	THR
1	D	69	MET
1	D	70	ASN
1	D	111	LEU
1	D	177	LEU
1	D	185	ARG
1	D	194	ASN
1	D	208	LYS
1	D	253	VAL
1	D	310	LEU
1	D	336	SER
1	D	355	MET
1	D	357	LEU
1	D	362	PHE
1	D	559	LEU
1	D	574	THR
1	D	613	ASN
1	D	617	PHE
1	D	624	THR
1	D	626	ILE
1	D	634	TRP
1	D	643	LYS
1	D	657	GLN
1	D	668	LEU
1	D	671	ILE
1	D	673	GLU
1	D	674	LEU

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Mol	Chain	Res	Type
1	D	695	LEU
1	D	697	GLN
1	D	713	LEU
1	D	714	THR
1	D	716	VAL
1	D	717	ARG
1	D	721	LEU
1	D	722	GLU
1	D	748	THR
1	D	784	ASP
1	D	797	GLN
1	D	806	SER
1	D	808	ARG
1	D	869	SER
1	D	901	VAL
1	D	918	PHE
1	D	921	LEU
1	D	931	LEU
1	D	971	ARG
1	E	11	PHE
1	E	25	LEU
1	E	27	ILE
1	E	28	LEU
1	E	29	LYS
1	E	49	TYR
1	E	60	THR
1	E	70	ASN
1	E	108	GLN
1	E	109	ASN
1	E	131	LYS
1	E	148	THR
1	E	177	LEU
1	E	185	ARG
1	E	213	GLN
1	E	230	LEU
1	E	255	GLN
1	E	259	ARG
1	E	270	LEU
1	E	295	THR
1	E	310	LEU
1	E	314	GLU
1	E	329	THR

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Mol	Chain	Res	Type
1	E	335	ILE
1	E	355	MET
1	E	358	PHE
1	E	400	LEU
1	E	402	ILE
1	E	433	LYS
1	E	480	LEU
1	E	516	PHE
1	E	520	PHE
1	E	525	HIS
1	E	528	THR
1	E	538	THR
1	E	559	LEU
1	E	571	VAL
1	E	574	THR
1	E	589	LYS
1	E	602	GLU
1	E	613	ASN
1	E	634	TRP
1	E	652	THR
1	E	668	LEU
1	E	673	GLU
1	E	687	GLN
1	E	690	LEU
1	E	694	LYS
1	E	695	LEU
1	E	708	LYS
1	E	712	MET
1	E	716	VAL
1	E	717	ARG
1	E	721	LEU
1	E	722	GLU
1	E	730	ASP
1	E	760	ASN
1	E	817	GLU
1	E	835	LYS
1	E	843	LEU
1	E	858	ASP
1	E	862	MET
1	E	871	ASN
1	E	901	VAL
1	E	914	LEU

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Mol	Chain	Res	Type
1	E	921	LEU
1	E	937	LEU
1	E	961	ILE
1	E	973	ARG
1	E	991	ILE
1	F	3	ASN
1	F	6	ILE
1	F	7	ASP
1	F	11	PHE
1	F	28	LEU
1	F	34	GLN
1	F	49	TYR
1	F	53	ASP
1	F	55	LYS
1	F	60	THR
1	F	63	GLN
1	F	69	MET
1	F	70	ASN
1	F	88	VAL
1	F	96	SER
1	F	108	GLN
1	F	112	GLN
1	F	148	THR
1	F	174	ASP
1	F	177	LEU
1	F	182	TYR
1	F	197	GLN
1	F	219	LEU
1	F	225	VAL
1	F	230	LEU
1	F	242	SER
1	F	255	GLN
1	F	280	GLU
1	F	307	ARG
1	F	310	LEU
1	F	321	LEU
1	F	344	LEU
1	F	358	PHE
1	F	400	LEU
1	F	439	GLN
1	F	447	MET
1	F	452	VAL

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Mol	Chain	Res	Type
1	F	472	ILE
1	F	482	VAL
1	F	510	LYS
1	F	525	HIS
1	F	558	ARG
1	F	559	LEU
1	F	571	VAL
1	F	574	THR
1	F	602	GLU
1	F	613	ASN
1	F	634	TRP
1	F	645	GLU
1	F	649	MET
1	F	658	ILE
1	F	668	LEU
1	F	672	VAL
1	F	695	LEU
1	F	702	LEU
1	F	703	LEU
1	F	713	LEU
1	F	722	GLU
1	F	807	SER
1	F	813	SER
1	F	863	SER
1	F	876	LEU
1	F	918	PHE
1	F	919	ARG
1	F	950	LYS
1	F	958	LYS
1	F	961	ILE
1	F	966	ASP
1	F	971	ARG
1	F	991	ILE
1	F	993	THR
1	F	1008	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	67	GLN
1	A	70	ASN

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Mol	Chain	Res	Type
1	A	109	ASN
1	A	124	GLN
1	A	125	GLN
1	A	194	ASN
1	A	197	GLN
1	A	218	GLN
1	A	229	GLN
1	A	274	ASN
1	A	360	GLN
1	A	569	GLN
1	A	592	ASN
1	A	605	ASN
1	A	613	ASN
1	A	622	GLN
1	A	642	ASN
1	A	657	GLN
1	A	667	ASN
1	A	701	GLN
1	A	928	GLN
1	A	1001	ASN
1	B	34	GLN
1	B	67	GLN
1	B	74	ASN
1	B	109	ASN
1	B	112	GLN
1	B	125	GLN
1	B	181	GLN
1	B	194	ASN
1	B	213	GLN
1	B	237	GLN
1	B	255	GLN
1	B	282	ASN
1	B	284	GLN
1	B	361	ASN
1	B	577	GLN
1	B	605	ASN
1	B	613	ASN
1	B	622	GLN
1	B	701	GLN
1	B	760	ASN
1	B	928	GLN
1	B	1001	ASN

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Mol	Chain	Res	Type
1	C	58	GLN
1	C	70	ASN
1	C	89	GLN
1	C	124	GLN
1	C	176	GLN
1	C	213	GLN
1	C	231	ASN
1	C	282	ASN
1	C	569	GLN
1	C	605	ASN
1	C	613	ASN
1	C	622	GLN
1	C	667	ASN
1	C	697	GLN
1	C	701	GLN
1	C	726	GLN
1	C	846	GLN
1	C	865	GLN
1	D	34	GLN
1	D	67	GLN
1	D	70	ASN
1	D	108	GLN
1	D	112	GLN
1	D	124	GLN
1	D	194	ASN
1	D	218	GLN
1	D	229	GLN
1	D	231	ASN
1	D	517	ASN
1	D	569	GLN
1	D	605	ASN
1	D	613	ASN
1	D	622	GLN
1	D	642	ASN
1	D	657	GLN
1	D	667	ASN
1	D	701	GLN
1	D	865	GLN
1	D	928	GLN
1	E	67	GLN
1	E	89	GLN
1	E	109	ASN

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Mol	Chain	Res	Type
1	E	112	GLN
1	E	125	GLN
1	E	194	ASN
1	E	213	GLN
1	E	282	ASN
1	E	284	GLN
1	E	439	GLN
1	E	577	GLN
1	E	605	ASN
1	E	613	ASN
1	E	622	GLN
1	E	657	GLN
1	E	701	GLN
1	E	928	GLN
1	F	3	ASN
1	F	58	GLN
1	F	70	ASN
1	F	81	ASN
1	F	104	GLN
1	F	108	GLN
1	F	112	GLN
1	F	124	GLN
1	F	161	ASN
1	F	197	GLN
1	F	213	GLN
1	F	218	GLN
1	F	274	ASN
1	F	282	ASN
1	F	415	ASN
1	F	569	GLN
1	F	605	ASN
1	F	613	ASN
1	F	622	GLN
1	F	667	ASN
1	F	697	GLN
1	F	737	GLN
1	F	846	GLN
1	F	865	GLN
1	F	941	ASN
1	F	1000	GLN
1	F	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 ⓘ

4 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	E	1058	-	3,12,12	1.13	0	3,17,17	1.85	1 (33%)
2	FLC	D	1058	-	3,12,12	0.72	0	3,17,17	0.53	0
2	FLC	A	1058	-	3,12,12	0.71	0	3,17,17	1.03	0
2	FLC	B	1058	-	3,12,12	0.89	0	3,17,17	1.35	0

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	E	1058	-	-	1/6/16/16	-
2	FLC	D	1058	-	-	4/6/16/16	-
2	FLC	A	1058	-	-	3/6/16/16	-
2	FLC	B	1058	-	-	3/6/16/16	-

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	E	1058	FLC	CB-CG-CGC	-2.26	111.36	114.98

There are no chirality outliers.

All (11) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1058	FLC	3	0
2	D	1058	FLC	1	0
2	B	1058	FLC	2	0

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%)	-0.14	31 (3%)	50	22	42, 52, 59, 71	0
1	B	1032/1057 (97%)	-0.11	33 (3%)	47	20	38, 50, 57, 63	0
1	C	1032/1057 (97%)	-0.15	25 (2%)	59	30	41, 52, 58, 61	0
1	D	1032/1057 (97%)	-0.01	64 (6%)	20	7	42, 53, 62, 70	0
1	E	1032/1057 (97%)	-0.14	25 (2%)	59	30	37, 51, 57, 61	0
1	F	1032/1057 (97%)	-0.13	29 (2%)	53	25	42, 51, 57, 63	0
All	All	6192/6342 (97%)	-0.11	207 (3%)	46	20	37, 51, 58, 71	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	657	GLN	7.2
1	A	514	GLY	7.1
1	C	657	GLN	6.9
1	E	513	PHE	6.3
1	F	511	GLY	6.2
1	E	1033	PHE	5.7
1	B	229	GLN	5.4
1	F	510	LYS	5.1
1	B	255	GLN	5.1
1	B	511	GLY	5.0
1	D	539	GLY	4.9
1	D	1033	PHE	4.9
1	F	658	ILE	4.9
1	A	656	SER	4.7
1	B	993	THR	4.6
1	B	540	ARG	4.5
1	A	638	PRO	4.4
1	A	513	PHE	4.3
1	F	540	ARG	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	513	PHE	4.2
1	D	508	GLY	4.2
1	D	462	SER	4.1
1	E	511	GLY	4.1
1	A	738	ALA	4.1
1	C	993	THR	4.0
1	D	526	HIS	4.0
1	B	871	ASN	3.9
1	A	515	TRP	3.8
1	B	515	TRP	3.8
1	A	501	ALA	3.8
1	E	638	PRO	3.8
1	B	512	PHE	3.7
1	E	229	GLN	3.7
1	D	961	ILE	3.7
1	E	678	THR	3.7
1	D	513	PHE	3.7
1	C	508	GLY	3.7
1	A	502	LYS	3.7
1	D	833	PRO	3.7
1	D	501	ALA	3.7
1	F	835	LYS	3.6
1	F	920	GLY	3.6
1	D	3	ASN	3.6
1	D	523	SER	3.6
1	A	635	ALA	3.6
1	C	522	LYS	3.6
1	D	461	GLY	3.6
1	C	511	GLY	3.5
1	A	1033	PHE	3.5
1	F	515	TRP	3.5
1	D	518	ARG	3.5
1	B	362	PHE	3.4
1	D	560	PRO	3.4
1	E	956	GLU	3.4
1	D	655	PHE	3.4
1	E	508	GLY	3.4
1	E	28	LEU	3.4
1	B	991	ILE	3.4
1	D	955	LYS	3.3
1	E	539	GLY	3.3
1	E	540	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	558	ARG	3.3
1	D	533	GLY	3.3
1	C	658	ILE	3.3
1	C	961	ILE	3.3
1	E	509	LYS	3.2
1	A	512	PHE	3.2
1	B	509	LYS	3.2
1	F	811	TYR	3.2
1	C	147	GLY	3.1
1	C	738	ALA	3.1
1	A	868	LEU	3.1
1	E	512	PHE	3.1
1	B	28	LEU	3.1
1	E	991	ILE	3.1
1	F	961	ILE	3.1
1	D	527	TYR	3.1
1	D	538	THR	3.1
1	E	515	TRP	3.0
1	E	871	ASN	3.0
1	E	993	THR	2.9
1	F	148	THR	2.9
1	A	508	GLY	2.9
1	F	501	ALA	2.9
1	C	507	GLU	2.9
1	C	920	GLY	2.9
1	F	993	THR	2.9
1	C	426	PRO	2.9
1	C	1033	PHE	2.9
1	C	515	TRP	2.9
1	B	961	ILE	2.9
1	F	426	PRO	2.8
1	C	510	LYS	2.8
1	D	993	THR	2.8
1	B	678	THR	2.8
1	D	463	THR	2.8
1	D	556	PHE	2.8
1	B	522	LYS	2.8
1	D	537	SER	2.8
1	C	802	SER	2.8
1	D	515	TRP	2.7
1	A	676	THR	2.7
1	B	987	MET	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	4	PHE	2.7
1	D	641	GLU	2.7
1	D	520	PHE	2.7
1	D	558	ARG	2.7
1	E	987	MET	2.7
1	D	874	PRO	2.7
1	F	512	PHE	2.7
1	F	778	LYS	2.7
1	D	640	GLU	2.7
1	D	362	PHE	2.6
1	A	833	PRO	2.6
1	B	918	PHE	2.6
1	D	659	LYS	2.6
1	F	516	PHE	2.6
1	F	147	GLY	2.6
1	F	12	ALA	2.6
1	F	362	PHE	2.6
1	E	658	ILE	2.6
1	D	512	PHE	2.6
1	F	802	SER	2.6
1	D	460	GLY	2.6
1	C	518	ARG	2.5
1	D	865	GLN	2.5
1	D	535	LEU	2.5
1	D	519	MET	2.5
1	A	499	PRO	2.5
1	D	920	GLY	2.5
1	B	994	GLY	2.5
1	B	319	SER	2.5
1	E	255	GLN	2.5
1	F	994	GLY	2.4
1	A	618	ALA	2.4
1	B	618	ALA	2.4
1	B	1033	PHE	2.4
1	C	540	ARG	2.4
1	B	962	GLU	2.4
1	D	914	LEU	2.4
1	C	429	GLU	2.4
1	D	868	LEU	2.4
1	E	712	MET	2.4
1	D	540	ARG	2.4
1	C	495	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	634	TRP	2.4
1	A	869	SER	2.4
1	A	500	ILE	2.4
1	B	638	PRO	2.4
1	A	641	GLU	2.3
1	D	531	VAL	2.3
1	A	4	PHE	2.3
1	C	427	PRO	2.3
1	D	145	THR	2.3
1	D	675	GLY	2.3
1	B	712	MET	2.3
1	A	993	THR	2.3
1	C	516	PHE	2.3
1	D	502	LYS	2.3
1	A	657	GLN	2.3
1	D	559	LEU	2.3
1	B	226	LYS	2.3
1	D	656	SER	2.3
1	E	556	PHE	2.3
1	D	255	GLN	2.2
1	D	991	ILE	2.2
1	D	522	LYS	2.2
1	A	538	THR	2.2
1	C	146	ASP	2.2
1	A	148	THR	2.2
1	D	869	SER	2.2
1	D	507	GLU	2.2
1	D	536	ARG	2.2
1	A	832	ALA	2.2
1	D	529	ASP	2.2
1	E	634	TRP	2.2
1	F	635	ALA	2.2
1	D	503	GLY	2.2
1	D	987	MET	2.1
1	A	362	PHE	2.1
1	A	955	LYS	2.1
1	B	835	LYS	2.1
1	F	513	PHE	2.1
1	D	832	ALA	2.1
1	D	872	GLN	2.1
1	A	535	LEU	2.1
1	D	421	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	878	ALA	2.1
1	D	676	THR	2.1
1	A	655	PHE	2.1
1	B	3	ASN	2.1
1	C	148	THR	2.1
1	B	839	GLU	2.1
1	B	537	SER	2.1
1	F	508	GLY	2.1
1	D	956	GLU	2.1
1	B	508	GLY	2.1
1	C	498	LYS	2.1
1	A	527	TYR	2.1
1	F	385	ALA	2.1
1	F	1033	PHE	2.0
1	D	561	SER	2.0
1	F	28	LEU	2.0
1	B	386	PHE	2.0
1	E	527	TYR	2.0
1	E	226	LYS	2.0
1	F	600	THR	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	0.94	0.21	39,41,41,41	0
2	FLC	D	1058	13/13	0.95	0.29	42,44,45,46	0
2	FLC	E	1058	13/13	0.95	0.26	31,35,36,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	FLC	B	1058	13/13	0.96	0.26	30,32,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.