



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:07 PM UTC

PDB ID : 2HRT / pdb_00002hrt
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 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

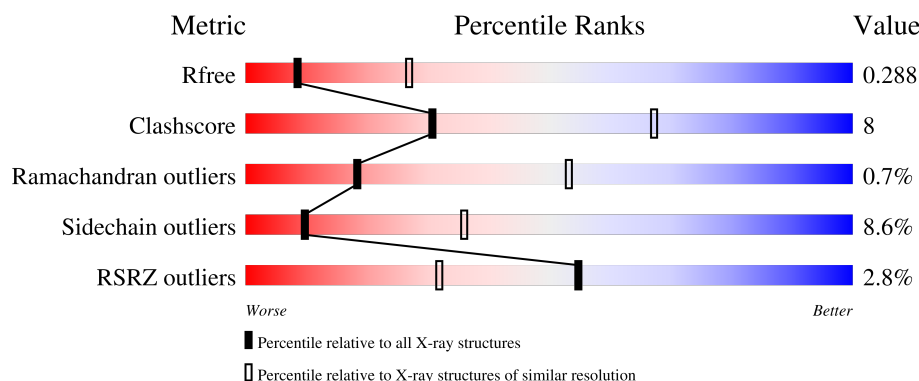
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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	2% 75% 20% ..
1	B	1057	3% 74% 21% ..
1	C	1057	3% 72% 22% ..
1	D	1057	2% 77% 19% ..
1	E	1057	2% 73% 22% ..

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Mol	Chain	Length	Quality of chain
1	F	1057	3% 73% 21% ••

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:

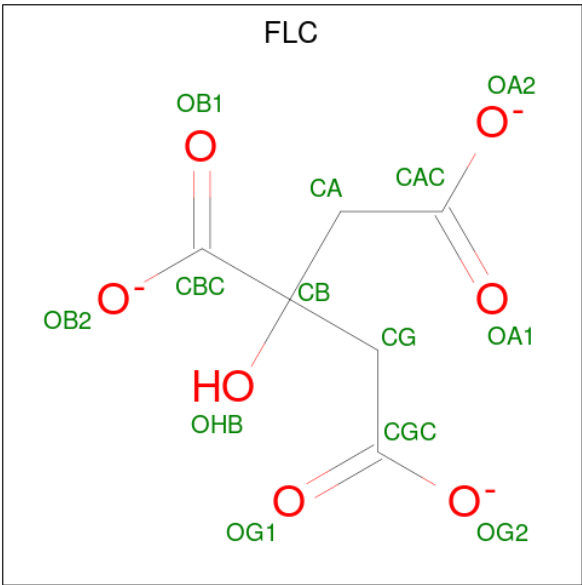
Chain	Residue	Modelled	Actual	Comment	Reference
A	1050	LEU	-	cloning artifact	UNP P31224
A	1051	GLU	-	cloning artifact	UNP P31224
A	1052	HIS	-	expression tag	UNP P31224
A	1053	HIS	-	expression tag	UNP P31224
A	1054	HIS	-	expression tag	UNP P31224
A	1055	HIS	-	expression tag	UNP P31224
A	1056	HIS	-	expression 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 (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		
2	D	1	Total	C	O	0	0
			13	6	7		
2	E	1	Total	C	O	0	0
			13	6	7		

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

Chain A:

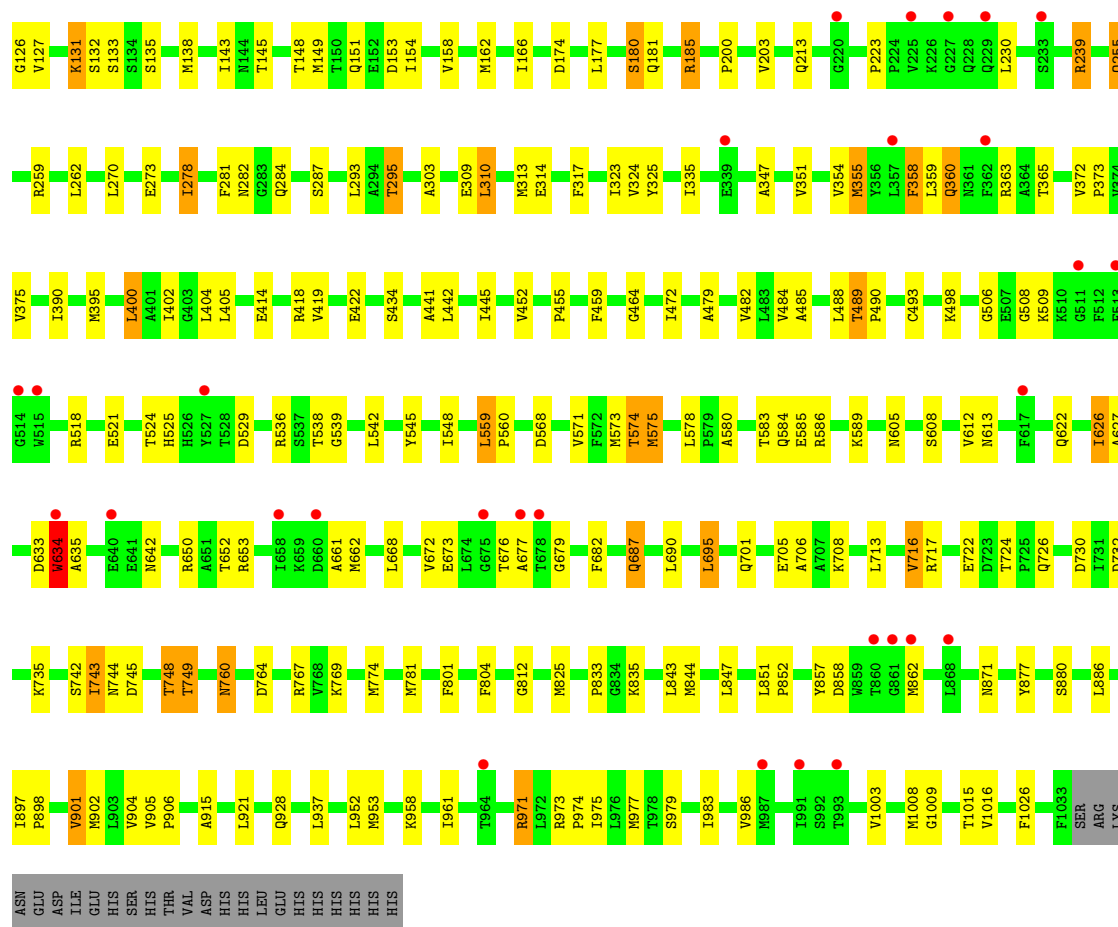
2%

75%

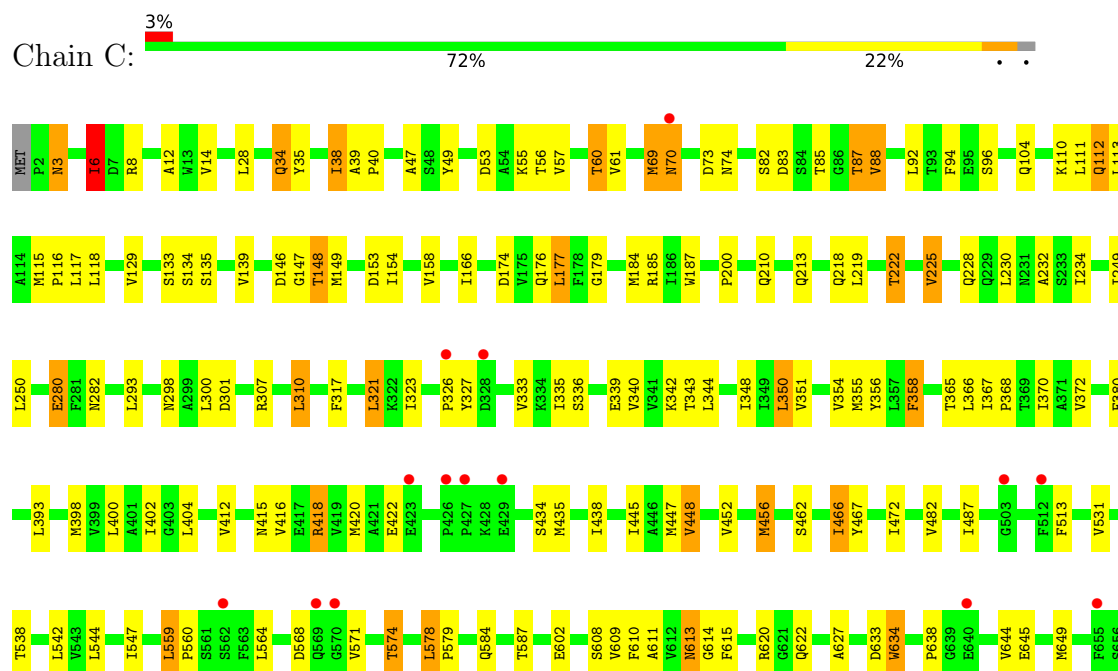
20%

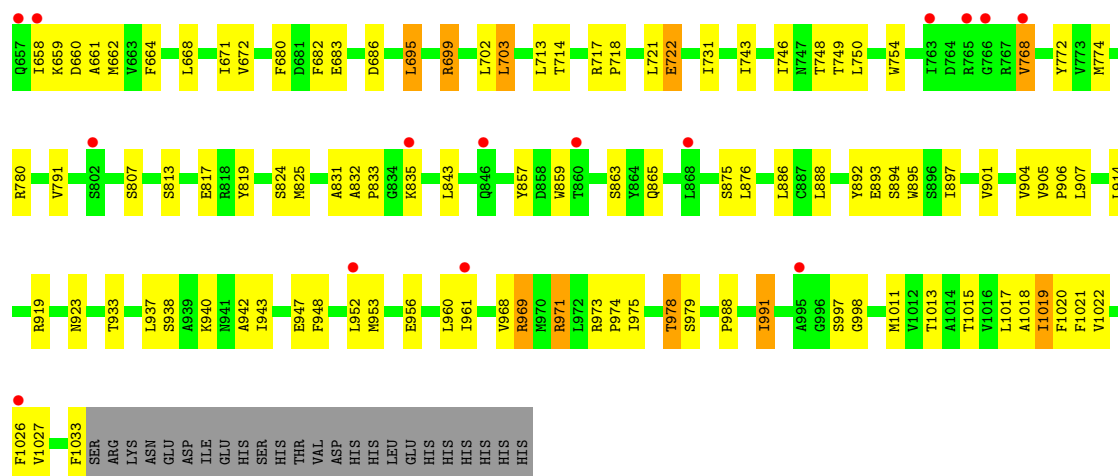
Chain B:

Amino Acid	Percentage
MET	0%
P2	0%
R8	0%
V14	0%
L25	0%
A26	0%
I27	0%
L28	0%
K29	0%
L30	0%
P31	0%
V32	0%
A39	3%
A42	0%
Y49	0%
K55	0%
T56	0%
V57	0%
T60	0%
V61	0%
M69	0%
N70	0%
L75	0%
M76	0%
S82	0%
L92	0%
E95	0%
S96	0%
I102	0%
A103	0%
Q104	0%
V105	0%
Q108	0%
M109	0%
K110	0%
L111	0%
Q112	0%
M115	0%
P119	0%
Q120	0%
Q123	0%

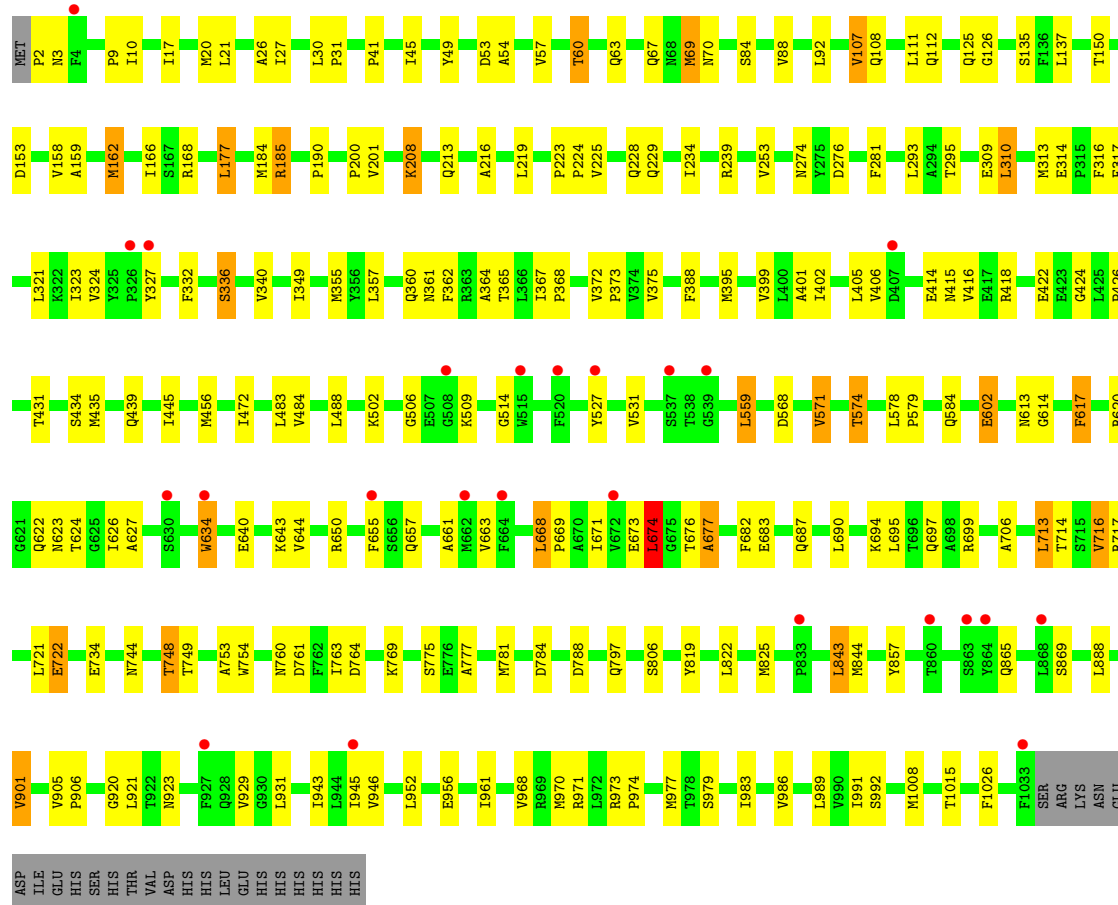
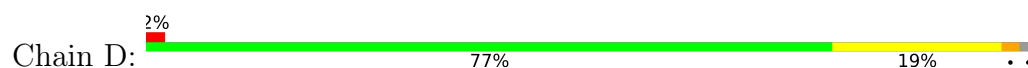


- Molecule 1: Acriflavine resistance protein B

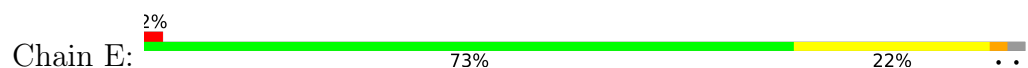


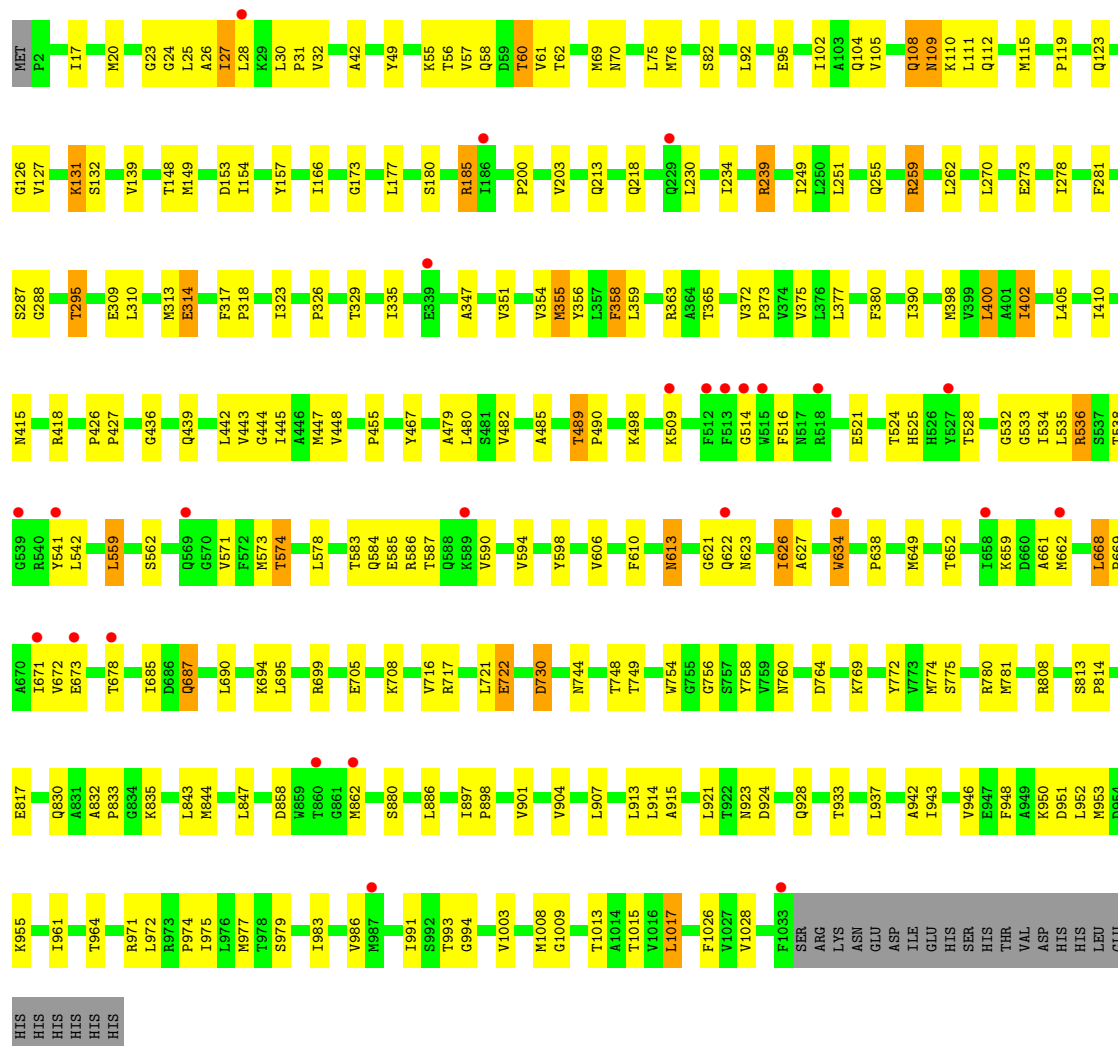


• Molecule 1: Acriflavine resistance protein B

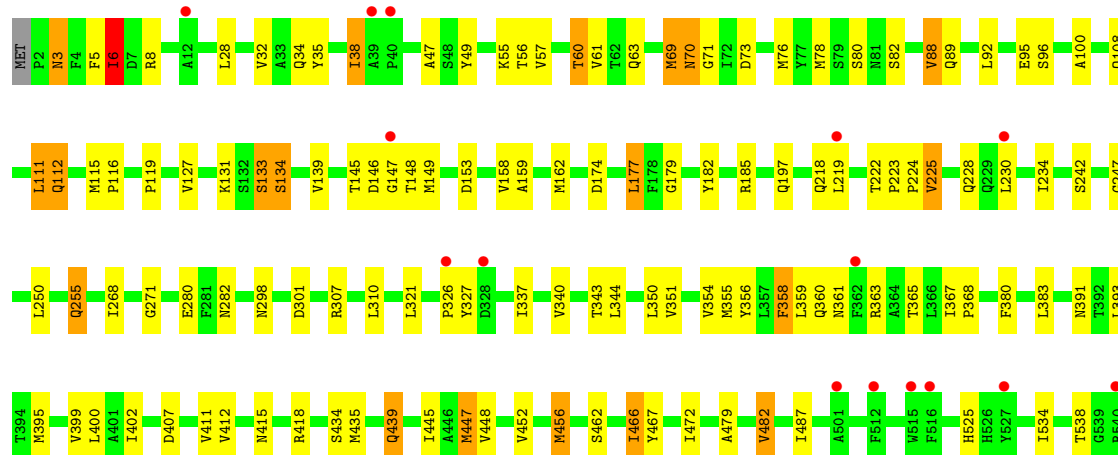
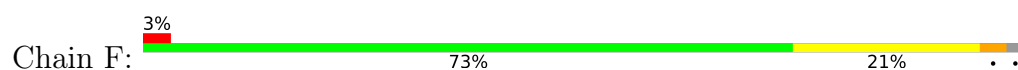


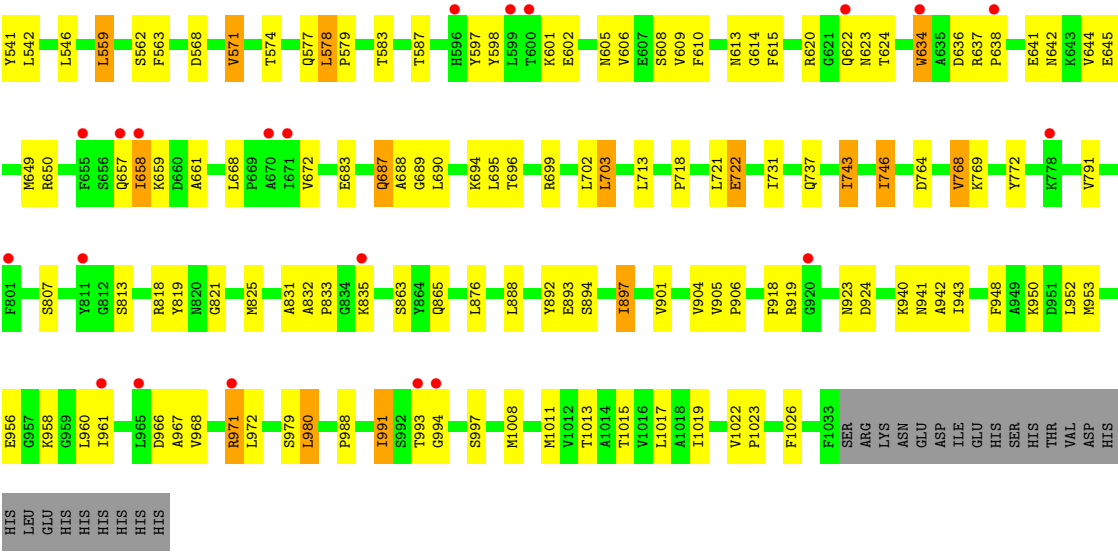
• Molecule 1: Acriflavine resistance protein B





• 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) 99.8 (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 (Not available) , 0.288	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)	0.29 , 65.3	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	0.89	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

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	0.48	0/7991	0.85	1/10852 (0.0%)
1	B	0.49	0/7991	0.85	0/10852
1	C	0.48	1/7991 (0.0%)	0.86	3/10852 (0.0%)
1	D	0.48	0/7991	0.85	2/10852 (0.0%)
1	E	0.49	0/7991	0.87	5/10852 (0.0%)
1	F	0.48	1/7991 (0.0%)	0.85	2/10852 (0.0%)
All	All	0.49	2/47946 (0.0%)	0.86	13/65112 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	897	ILE	CA-CB	6.08	1.57	1.54
1	C	1022	VAL	CA-CB	5.04	1.56	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	426	PRO	CA-C-N	6.85	128.41	119.84
1	E	426	PRO	C-N-CA	6.85	128.41	119.84
1	E	832	ALA	CA-C-N	6.28	127.68	119.84
1	E	832	ALA	C-N-CA	6.28	127.68	119.84
1	F	832	ALA	CA-C-N	5.79	127.08	119.84
1	F	832	ALA	C-N-CA	5.79	127.08	119.84
1	E	288	GLY	N-CA-C	5.69	118.83	110.80
1	D	426	PRO	CA-C-N	5.64	126.89	119.84
1	D	426	PRO	C-N-CA	5.64	126.89	119.84
1	C	74	ASN	N-CA-C	5.59	119.28	111.90
1	C	832	ALA	CA-C-N	5.40	126.59	119.84
1	C	832	ALA	C-N-CA	5.40	126.59	119.84
1	A	125	GLN	N-CA-C	-5.40	106.74	113.38

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	144	0
1	B	7841	0	7990	133	0
1	C	7841	0	7990	151	0
1	D	7841	0	7990	128	0
1	E	7841	0	7990	144	0
1	F	7841	0	7990	145	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	786	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 (786) 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:D:112:GLN:HG3	1:E:112:GLN:HE21	1.28	0.97
1:E:185:ARG:HH11	1:E:185:ARG:HG3	1.30	0.94
1:E:55:LYS:HE2	2:E:1058:FLC:HA1	1.49	0.93
1:A:225:VAL:H	1:B:781:MET:HE2	1.34	0.92
1:C:456:MET:HG3	1:C:467:TYR:HB3	1.52	0.91
1:A:239:ARG:HG3	1:A:239:ARG:HH11	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:HG3	1:B:185:ARG:HH11	1.40	0.86
1:A:213:GLN:HG2	1:A:239:ARG:HG2	1.57	0.86
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:56:THR:O	1:E:60:THR:HB	1.79	0.80
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:A:781:MET:HE2	1:C:225:VAL:H	1.51	0.75
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:578:LEU:HB3	1:C:579:PRO:HD2	1.69	0.74
1:C:979:SER:HB3	1:C:1015:THR:HG21	1.67	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:A:69:MET:HE1	1:A:107:VAL:HG13	1.71	0.72
1:D:781:MET:HE2	1:F:225:VAL:H	1.55	0.72
1:D:200:PRO:HD2	1:D:749:THR:HG22	1.71	0.72
1:A:309:GLU:HG3	1:A:313:MET:HE3	1.71	0.72
1:F:56:THR:O	1:F:60:THR:HB	1.90	0.72
1:E:573:MET:HE2	1:E:626:ILE:HG12	1.73	0.71
1:F:605:ASN:HD21	1:F:642:ASN:HD22	1.37	0.71
1:E:185:ARG:HG3	1:E:185:ARG:NH1	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:CZ	1:D:971:ARG:HB3	2.20	0.70
1:B:143:ILE:HG21	1:B:281:PHE:HB3	1.71	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:225:VAL:H	1:B:781:MET:CE	2.03	0.69
1:B:584:GLN:H	1:B:622:GLN:HE21	1.37	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:634:TRP:H	1:F:634:TRP:CD1	2.10	0.68
1:F:78:MET:HG3	1:F:92:LEU:HD13	1.75	0.68
1:F:605:ASN:HD21	1:F:642:ASN:ND2	1.92	0.68
1:F:456:MET:HG3	1:F:467:TYR:HB3	1.77	0.67
1:A:844:MET:HA	1:A:844:MET:HE2	1.75	0.67
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:HB3	1:A:971:ARG:NH1	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:E:613:ASN:C	1:E:613:ASN:HD22	2.04	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:634:TRP:CD1	1:C:634:TRP:H	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:CZ	1:C:971:ARG:HB3	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
1:D:225:VAL:H	1:E:781:MET:HE2	1.65	0.61
1:F:47:ALA:HB3	1:F:88:VAL:HG13	1.81	0.61
1:E:259:ARG:HD3	1:E:259:ARG:H	1.64	0.61
1:A:239:ARG:HG3	1:A:239:ARG:NH1	2.06	0.61
1:B:76:MET:HE3	1:B:95:GLU:HA	1.82	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:A:781:MET:HE3	1:C:228:GLN:OE1	2.01	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: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:D:355:MET:HA	1:D:355:MET:HE3	1.84	0.60
1:B:363:ARG:HD2	1:B:498:LYS:HB2	1.83	0.59
1:F:76:MET:HE3	1:F:95:GLU:HA	1.82	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:D:225:VAL:HG22	1:E:781:MET:HE2	1.84	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:108:GLN:CD	1:C:112:GLN:HB3	2.29	0.58
1:B:573:MET:HE2	1:B:626:ILE:HG12	1.85	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:HB3	1:C:971:ARG:NH1	2.20	0.57
1:E:76:MET:HE3	1:E:95:GLU:HA	1.85	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:239:ARG:NH2	1:F:49:TYR:OH	2.38	0.57
1:E:445:ILE:HG22	1:E:943:ILE:HD13	1.86	0.57
1:B:185:ARG:HH22	1:B:774:MET:HE3	1.69	0.57
1:D:456:MET:HE1	1:D:929:VAL:HG13	1.84	0.57
1:E:347:ALA:O	1:E:351:VAL:HG23	2.04	0.57
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:703:LEU:HD11	1:F:718:PRO:HD3	1.87	0.57
1:F:1013:THR:O	1:F:1017:LEU:HB2	2.05	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:E:108:GLN:CD	1:F:112:GLN:HB3	2.30	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:HG23	1:C:991:ILE:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:442:LEU:O	1:E:445:ILE:HG13	2.05	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:HD12	1:F:743:ILE:H	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:449:LEU:O	1:A:452:VAL:HG22	2.07	0.55
1:A:946:VAL:HG13	1:A:1026:PHE:CE1	2.41	0.55
1:A:968:VAL:O	1:A:972:LEU:HB2	2.06	0.55
1:B:158:VAL:HA	1:B:162:MET:HE3	1.89	0.55
1:C:184:MET:HA	1:C:184:MET:HE3	1.88	0.55
1:E:115:MET:HE3	1:E:123:GLN:HG2	1.89	0.55
1:A:634:TRP:CD1	1:A:634:TRP:H	2.24	0.55
1:D:781:MET:HE2	1:F:225:VAL:HG13	1.88	0.55
1:B:695:LEU:HD13	1:B:825:MET:HG3	1.89	0.55
1:D:578:LEU:HB2	1:D:623:ASN:HB2	1.89	0.55
1:F:952:LEU:HB3	1:F:958:LYS:HD3	1.88	0.55
1:A:781:MET:CE	1:C:225:VAL:H	2.18	0.55
1:C:282:ASN:HD21	1:C:609:VAL:H	1.55	0.55
1:A:228:GLN:OE1	1:B:781:MET:HE3	2.07	0.54
1:F:69:MET:HG3	1:F:92:LEU:HD11	1.89	0.54
1:F:412:VAL:HG13	1:F:435:MET:HE1	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:A:109:ASN:HD21	1:C:129:VAL:H	1.55	0.54
1:B:801:PHE:HA	1:B:804:PHE:CZ	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:844:MET:HE2	1:D:844:MET:HA	1.90	0.54
1:A:355:MET:HE3	1:A:355:MET:HA	1.89	0.54
1:D:388:PHE:CZ	1:D:472:ILE:HG21	2.43	0.54
1:D:781:MET:HE3	1:F:228:GLN:OE1	2.07	0.54
1:E:590:VAL:O	1:E:594:VAL:HG23	2.08	0.54
1:F:351:VAL:HG12	1:F:355:MET:HE2	1.90	0.53
1:B:138:MET:HE1	1:B:303:ALA:HA	1.89	0.53
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: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:E:309:GLU:HG3	1:E:313:MET:HE3	1.90	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:HB3	1:D:971:ARG:NH1	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:399:VAL:HG11	1:D:989:LEU:HD11	1.92	0.52
1:D:418:ARG:HH21	1:D:970:MET:HG3	1.73	0.52
1:E:372:VAL:HG23	1:E:373:PRO:HD3	1.90	0.52
1:A:974:PRO:HA	1:A:977:MET:HE3	1.91	0.52
1:A:53:ASP:O	1:A:57:VAL:HG23	2.10	0.52
1:A:361:ASN:HB3	1:A:364:ALA:HB3	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE21	1:A:657:GLN:HA	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:57:VAL:HG23	1:E:82:SER:HB3	1.90	0.52
1:E:542:LEU:HD21	1:E:1028:VAL:HG21	1.91	0.52
1:F:356:TYR:C	1:F:358:PHE:H	2.17	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: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:228:GLN:OE1	1:E:781:MET:HE3	2.09	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:180:SER:HB3	1:B:273:GLU:HB2	1.92	0.51
1:B:203:VAL:HG13	1:B:262:LEU:HD11	1.93	0.51
1:D:239:ARG:HD2	1:D:761:ASP:O	2.10	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:309:GLU:HG3	1:B:313:MET:HE3	1.93	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:950:LYS:HD2	1:A:954:ASP:OD2	2.11	0.50
1:A:952:LEU:HD23	1:A:956:GLU:HG3	1.93	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:112:GLN:CG	1:B:112:GLN:HE21	2.25	0.50
1:A:699:ARG:HE	1:A:718:PRO:HB3	1.76	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:C:568:ASP:CG	1:C:644:VAL:HG23	2.36	0.50
1:E:17:ILE:HA	1:E:20:MET:HE3	1.92	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:350:LEU:O	1:C:354:VAL:HG23	2.12	0.49
1:C:907:LEU:HD21	1:C:1021:PHE:HB2	1.93	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:158:VAL:HG22	1:A:162:MET:HE2	1.93	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:C:356:TYR:C	1:C:358:PHE:H	2.20	0.49
1:C:412:VAL:HG13	1:C:435:MET:HE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:LYS:HE2	2:E:1058:FLC:CA	2.34	0.49
1:C:892:TYR:C	1:C:894:SER:H	2.20	0.49
1:C:953:MET:HE1	1:C:1026:PHE:HE2	1.77	0.49
1:E:154:ILE:HG22	1:E:287:SER:HB3	1.95	0.49
1:F:953:MET:HE2	1:F:960:LEU:HA	1.95	0.49
1:E:356:TYR:C	1:E:358:PHE:H	2.21	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
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:75:LEU:HD11	1:B:92:LEU:HB3	1.95	0.49
1:B:154:ILE:HG22	1:B:287:SER:HB3	1.95	0.49
1:E:444:GLY:O	1:E:448:VAL:HG23	2.13	0.49
1:E:953:MET:HE1	1:E:1026:PHE:HE2	1.78	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:D:45:ILE:HD11	1:D:69:MET:HE2	1.96	0.48
1:F:888:LEU:HD21	1:F:943:ILE:HD11	1.94	0.48
1:A:754:TRP:CE3	1:C:234:ILE:HD11	2.49	0.48
1:B:743:ILE:H	1:B:743:ILE:HD12	1.76	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:69:MET:HE1	1:D:107:VAL:HG13	1.94	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:A:953:MET:HE1	1:A:1026:PHE:HE2	1.78	0.48
1:C:574:THR:HG23	1:C:627:ALA:HB3	1.95	0.48
1:D:185:ARG:HA	1:D:185:ARG:HD2	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: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:E:1013:THR:O	1:E:1017:LEU:HB2	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:781:MET:CE	1:F:225:VAL:H	2.24	0.48
1:E:662:MET:HE3	1:E:662:MET:HA	1.94	0.48
1:E:185:ARG:HH11	1:E:185:ARG:CG	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:B:844:MET:HE2	1:B:844:MET:HA	1.95	0.47
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:A:456:MET:HE1	1:A:929:VAL:HG13	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:C:416:VAL:HG12	1:C:420:MET:HE2	1.95	0.47
1:F:159:ALA:HB2	1:F:177:LEU:HD11	1.95	0.47
1:A:676:THR:O	1:A:677:ALA:C	2.56	0.47
1:A:781:MET:HE2	1:C:225:VAL:HG13	1.96	0.47
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:380:PHE:CE1	1:C:398:MET:HE1	2.50	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:D:184:MET:HE3	1:D:184:MET:HA	1.97	0.47
1:F:445:ILE:HG23	1:F:940:LYS:HG3	1.97	0.47
1:A:302:THR:O	1:A:306:ILE:HG13	2.14	0.47
1:A:361:ASN:O	1:A:365:THR:HG22	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: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: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: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:D:54:ALA:H	1:D:84:SER:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:309:GLU:HG3	1:D:313:MET:HE3	1.96	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:A:225:VAL:N	1:B:781:MET:HE2	2.16	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:17:ILE:HA	1:D:20:MET:HE3	1.96	0.46
1:D:228:GLN:CD	1:E:781:MET:HE3	2.40	0.46
1:F:6:ILE:C	1:F:8:ARG:H	2.22	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
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:F:953:MET:HE1	1:F:1026:PHE:HE2	1.80	0.46
1:A:893:GLU:CD	1:C:8:ARG:HB3	2.40	0.46
1:B:705:GLU:HB3	1:B:847:LEU:HD22	1.98	0.46
1:D:676:THR:O	1:D:677:ALA:C	2.58	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:D:225:VAL:H	1:E:781:MET:CE	2.29	0.46
1:E:455:PRO:HG2	1:E:880:SER:OG	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:168:ARG:HG2	1:B:69:MET:O	2.16	0.45
1:A:281:PHE:CZ	1:A:324:VAL:HG21	2.51	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:897:ILE:HD11	1:E:950:LYS:HE3	1.98	0.45
1:E:904:VAL:HG21	1:E:942:ALA:HB2	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:575:MET:HE2	1:B:575:MET:HB2	1.87	0.45
1:B:877:TYR:HA	1:B:880:SER:HB2	1.97	0.45
1:E:173:GLY:O	1:F:71:GLY:HA3	2.16	0.45
1:A:267:LYS:NZ	1:A:267:LYS:HB3	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
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:C:402:ILE:C	1:C:404:LEU:H	2.24	0.45
1:D:945:ILE:HG12	1:D:971:ARG:HH21	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:1018:ALA:C	1:C:1020:PHE:H	2.25	0.45
1:F:393:LEU:HD11	1:F:466:ILE:HD13	1.99	0.45
1:F:658:ILE:H	1:F:658:ILE:HG13	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:A:568:ASP:CG	1:A:644:VAL:HG23	2.42	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:414:GLU:HG3	1:D:977:MET:HE1	1.98	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:B:953:MET:HE1	1:B:1026:PHE:HE2	1.82	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:A:781:MET:HE2	1:C:225:VAL:N	2.26	0.44
1:B:442:LEU:O	1:B:445:ILE:HG13	2.17	0.44
1:D:634:TRP:CD1	1:D:634:TRP:H	2.35	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: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:255:GLN:CD	1:F:255:GLN:H	2.26	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:115:MET:HE3	1:B:123:GLN:HG2	1.99	0.44
1:B:732:ASP:HB3	1:B:735:LYS:HB2	1.99	0.44
1:C:139:VAL:HB	1:C:327:TYR:HB3	1.98	0.44
1:F:636:ASP:C	1:F:638:PRO:HD3	2.42	0.44
1:B:181:GLN:HE21	1:B:767:ARG:HH11	1.66	0.44
1:E:621:GLY:C	1:E:623:ASN:H	2.25	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:B:898:PRO:HB2	1:B:902:MET:HE2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:38:ILE:HG23	1:F:462:SER:OG	2.18	0.44
1:F:340:VAL:HG11	1:F:395:MET:HB3	2.00	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: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: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:F:1015:THR:O	1:F:1019:ILE:HG12	2.18	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:B:662:MET:HA	1:B:662:MET:HE3	1.99	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:HD3	1:E:110:LYS:HA	1.81	0.43
1:A:720:GLY:HA3	1:A:817:GLU:OE1	2.18	0.43
1:A:753:ALA:O	1:A:775:SER:HB3	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:6:ILE:HG21	1:F:487:ILE:HG23	2.00	0.43
1:F:133:SER:O	1:F:134:SER:HB2	2.18	0.43
1:A:47:ALA:HB3	1:A:88:VAL:CG1	2.48	0.43
1:C:40:PRO:HB2	1:C:94:PHE:O	2.18	0.43
1:C:154:ILE:O	1:C:158:VAL:HG23	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:LEU:HD13	1:B:661:ALA:HB2	2.00	0.43
1:C:937:LEU:HD22	1:C:1011:MET:HE2	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:A:228:GLN:HB2	1:B:781:MET:HE3	2.01	0.43
1:B:726:GLN:CD	1:B:812:GLY:HA3	2.43	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:355:MET:HE1	1:E:410:ILE:HG23	1.99	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:414:GLU:HG3	1:B:977:MET:HE2	2.01	0.43
1:B:418:ARG:O	1:B:422:GLU:HB2	2.19	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: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:F:894:SER:HB3	1:F:897:ILE:HG12	2.00	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:1022:VAL:N	1:F:1023:PRO:HD2	2.34	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:351:VAL:HG12	1:C:355:MET:HE2	2.01	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:168:ARG:CG	1:E:69:MET:O	2.68	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: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:414:GLU:HG3	1:B:977:MET:CE	2.49	0.42
1:B:1016:VAL:O	1:B:1016:VAL:HG12	2.19	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:E:775:SER:HB3	1:E:780:ARG:HD3	2.01	0.42
1:A:63:GLN:HB3	1:C:768:VAL:HG12	2.02	0.42
1:B:490:PRO:HA	1:B:493:CYS:HB2	2.01	0.42
1:C:213:GLN:HE21	1:C:213:GLN:HB3	1.66	0.42
1:C:979:SER:CB	1:C:1015:THR:HG21	2.43	0.42
1:D:63:GLN:HB3	1:F:768:VAL:HG12	2.02	0.42
1:D:135:SER:HA	1:D:617:PHE:HZ	1.85	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
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:613:ASN:C	1:C:613:ASN:HD22	2.28	0.42
1:C:664:PHE:CD2	1:C:717:ARG:HD2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:699:ARG:HH11	1:C:699:ARG:HB3	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:C:544:LEU:HA	1:C:547:ILE:HD12	2.02	0.42
1:E:946:VAL:HG13	1:E:1026:PHE:HE1	1.85	0.42
1:E:953:MET:HE3	1:E:953:MET:HB2	1.94	0.42
1:F:737:GLN:HE21	1:F:743:ILE:HD11	1.85	0.42
1:A:274:ASN:HD22	1:A:276:ASP:HB2	1.85	0.41
1:B:223:PRO:HD2	1:C:780:ARG:HH22	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:HA	1:C:659:LYS:HD3	1.82	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:E:380:PHE:CE2	1:E:398:MET:HE1	2.55	0.41
1:B:355:MET:HG3	1:B:359:LEU:HD12	2.01	0.41
1:C:83:ASP:HB3	1:C:85:THR:H	1.85	0.41
1:C:185:ARG:HD2	1:C:772:TYR:HB2	2.02	0.41
1:C:1015:THR:O	1:C:1019:ILE:HG12	2.20	0.41
1:D:986:VAL:O	1:D:986:VAL:HG12	2.18	0.41
1:F:578:LEU:HD22	1:F:661:ALA:HB2	2.02	0.41
1:C:187:TRP:HZ3	1:C:774:MET:HE3	1.85	0.41
1:D:668:LEU:HD23	1:D:668:LEU:H	1.84	0.41
1:F:158:VAL:HA	1:F:162:MET:HE3	2.03	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:695:LEU:HB3	1:A:825:MET:HE3	2.01	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:E:559:LEU:HD12	1:E:913:LEU:HD23	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:F:563:PHE:O	1:F:924:ASP:HB2	2.21	0.41
1:E:479:ALA:O	1:E:482:VAL:HG12	2.20	0.41
1:F:327:TYR:CE1	1:F:571:VAL:HG13	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:562:SER:HB2	1:F:924:ASP:HB3	2.02	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:C:326:PRO:HB2	1:C:610:PHE:HB2	2.01	0.41
1:C:559:LEU:HA	1:C:560:PRO:HD2	1.91	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:185:ARG:HD2	1:A:185:ARG:HA	1.58	0.41
1:A:591:LEU:HD22	1:A:611:ALA:HB1	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: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: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:D:431:THR:O	1:D:435:MET:HG2	2.21	0.41
1:E:157:TYR:CZ	1:E:318:PRO:HD3	2.56	0.41
1:E:649:MET:HE3	1:E:649:MET:HA	2.03	0.41
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:80:SER:HA	1:F:89:GLN:O	2.21	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:A:180:SER:HB2	1:A:274:ASN:OD1	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:ASN:CG	1:A:418:ARG:HH12	2.26	0.40
1:B:973:ARG:HB3	1:B:974:PRO:HD3	2.03	0.40
1:D:239:ARG:HG3	1:D:239:ARG:NH1	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:E:621:GLY:C	1:E:623:ASN:N	2.78	0.40
1:A:184:MET:HA	1:A:184:MET:HE3	2.03	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:H	1:A:743:ILE:HD12	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:70:ASN:O	1:C:110:LYS:HE3	2.22	0.40
1:C:578:LEU:HD22	1:C:661:ALA:CB	2.51	0.40
1:C:997:SER:O	1:C:998:GLY:C	2.64	0.40
1:D:375:VAL:HG11	1:D:405:LEU:HD22	2.03	0.40
1:D:568:ASP:CG	1:D:644:VAL:HG23	2.46	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:HE21	1:B:255:GLN:HB2	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:E:983:ILE:HG23	1:E:1008:MET:HE2	2.03	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%)	24	60
1	B	1030/1057 (97%)	969 (94%)	54 (5%)	7 (1%)	18	53
1	C	1030/1057 (97%)	968 (94%)	54 (5%)	8 (1%)	16	50
1	D	1030/1057 (97%)	980 (95%)	43 (4%)	7 (1%)	18	53
1	E	1030/1057 (97%)	966 (94%)	57 (6%)	7 (1%)	18	53
1	F	1030/1057 (97%)	964 (94%)	56 (5%)	10 (1%)	12	45
All	All	6180/6342 (97%)	5825 (94%)	311 (5%)	44 (1%)	18	53

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%)	771 (92%)	67 (8%)	11	38
1	B	838/863 (97%)	761 (91%)	77 (9%)	8	33
1	C	838/863 (97%)	755 (90%)	83 (10%)	7	30
1	D	838/863 (97%)	780 (93%)	58 (7%)	14	45
1	E	838/863 (97%)	767 (92%)	71 (8%)	10	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	838/863 (97%)	760 (91%)	78 (9%)	8	32
All	All	5028/5178 (97%)	4594 (91%)	434 (9%)	10	36

All (434) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	30	LEU
1	A	60	THR
1	A	70	ASN
1	A	84	SER
1	A	88	VAL
1	A	91	THR
1	A	107	VAL
1	A	108	GLN
1	A	152	GLU
1	A	177	LEU
1	A	185	ARG
1	A	197	GLN
1	A	208	LYS
1	A	225	VAL
1	A	229	GLN
1	A	239	ARG
1	A	253	VAL
1	A	269	GLU
1	A	278	ILE
1	A	310	LEU
1	A	330	THR
1	A	337	ILE
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

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Mol	Chain	Res	Type
1	A	574	THR
1	A	624	THR
1	A	626	ILE
1	A	634	TRP
1	A	640	GLU
1	A	657	GLN
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	713	LEU
1	A	716	VAL
1	A	717	ARG
1	A	721	LEU
1	A	748	THR
1	A	797	GLN
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	961	ILE
1	A	964	THR
1	A	986	VAL
1	A	1017	LEU
1	B	8	ARG
1	B	25	LEU
1	B	28	LEU
1	B	29	LYS
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

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Mol	Chain	Res	Type
1	B	148	THR
1	B	166	ILE
1	B	174	ASP
1	B	177	LEU
1	B	180	SER
1	B	185	ARG
1	B	213	GLN
1	B	230	LEU
1	B	239	ARG
1	B	255	GLN
1	B	259	ARG
1	B	270	LEU
1	B	278	ILE
1	B	293	LEU
1	B	295	THR
1	B	310	LEU
1	B	314	GLU
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	452	VAL
1	B	472	ILE
1	B	489	THR
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

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Mol	Chain	Res	Type
1	B	695	LEU
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	743	ILE
1	B	748	THR
1	B	749	THR
1	B	760	ASN
1	B	835	LYS
1	B	843	LEU
1	B	858	ASP
1	B	862	MET
1	B	871	ASN
1	B	886	LEU
1	B	901	VAL
1	B	921	LEU
1	B	928	GLN
1	B	937	LEU
1	B	961	ILE
1	B	971	ARG
1	B	986	VAL
1	C	3	ASN
1	C	6	ILE
1	C	28	LEU
1	C	34	GLN
1	C	38	ILE
1	C	55	LYS
1	C	60	THR
1	C	69	MET
1	C	70	ASN
1	C	87	THR
1	C	88	VAL
1	C	96	SER
1	C	104	GLN
1	C	111	LEU
1	C	112	GLN
1	C	113	LEU
1	C	117	LEU
1	C	148	THR

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Mol	Chain	Res	Type
1	C	174	ASP
1	C	177	LEU
1	C	222	THR
1	C	225	VAL
1	C	230	LEU
1	C	280	GLU
1	C	293	LEU
1	C	300	LEU
1	C	307	ARG
1	C	310	LEU
1	C	321	LEU
1	C	342	LYS
1	C	350	LEU
1	C	358	PHE
1	C	400	LEU
1	C	415	ASN
1	C	418	ARG
1	C	448	VAL
1	C	452	VAL
1	C	456	MET
1	C	466	ILE
1	C	472	ILE
1	C	482	VAL
1	C	513	PHE
1	C	559	LEU
1	C	564	LEU
1	C	571	VAL
1	C	574	THR
1	C	578	LEU
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

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Mol	Chain	Res	Type
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	748	THR
1	C	768	VAL
1	C	807	SER
1	C	813	SER
1	C	843	LEU
1	C	863	SER
1	C	875	SER
1	C	876	LEU
1	C	901	VAL
1	C	914	LEU
1	C	919	ARG
1	C	961	ILE
1	C	969	ARG
1	C	971	ARG
1	C	973	ARG
1	C	978	THR
1	C	991	ILE
1	D	21	LEU
1	D	27	ILE
1	D	60	THR
1	D	69	MET
1	D	70	ASN
1	D	88	VAL
1	D	107	VAL
1	D	108	GLN
1	D	111	LEU
1	D	125	GLN
1	D	162	MET
1	D	177	LEU
1	D	185	ARG
1	D	201	VAL
1	D	208	LYS
1	D	229	GLN
1	D	253	VAL
1	D	310	LEU
1	D	321	LEU

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Mol	Chain	Res	Type
1	D	336	SER
1	D	349	ILE
1	D	357	LEU
1	D	362	PHE
1	D	483	LEU
1	D	559	LEU
1	D	571	VAL
1	D	574	THR
1	D	602	GLU
1	D	617	PHE
1	D	624	THR
1	D	626	ILE
1	D	634	TRP
1	D	640	GLU
1	D	643	LYS
1	D	657	GLN
1	D	668	LEU
1	D	671	ILE
1	D	673	GLU
1	D	674	LEU
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	825	MET
1	D	843	LEU
1	D	869	SER
1	D	901	VAL
1	D	921	LEU
1	D	931	LEU
1	D	968	VAL
1	E	25	LEU
1	E	27	ILE
1	E	28	LEU

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Mol	Chain	Res	Type
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	166	ILE
1	E	177	LEU
1	E	185	ARG
1	E	213	GLN
1	E	230	LEU
1	E	239	ARG
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
1	E	335	ILE
1	E	355	MET
1	E	358	PHE
1	E	400	LEU
1	E	402	ILE
1	E	480	LEU
1	E	489	THR
1	E	516	PHE
1	E	525	HIS
1	E	528	THR
1	E	536	ARG
1	E	538	THR
1	E	559	LEU
1	E	571	VAL
1	E	574	THR
1	E	613	ASN
1	E	626	ILE
1	E	634	TRP
1	E	652	THR
1	E	668	LEU
1	E	671	ILE
1	E	673	GLU
1	E	687	GLN

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Mol	Chain	Res	Type
1	E	690	LEU
1	E	694	LYS
1	E	695	LEU
1	E	708	LYS
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	844	MET
1	E	862	MET
1	E	886	LEU
1	E	901	VAL
1	E	914	LEU
1	E	921	LEU
1	E	937	LEU
1	E	961	ILE
1	E	964	THR
1	E	972	LEU
1	E	986	VAL
1	E	991	ILE
1	E	1017	LEU
1	F	3	ASN
1	F	6	ILE
1	F	28	LEU
1	F	34	GLN
1	F	38	ILE
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	111	LEU
1	F	112	GLN
1	F	145	THR

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Mol	Chain	Res	Type
1	F	148	THR
1	F	174	ASP
1	F	177	LEU
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	360	GLN
1	F	400	LEU
1	F	418	ARG
1	F	439	GLN
1	F	447	MET
1	F	452	VAL
1	F	456	MET
1	F	466	ILE
1	F	472	ILE
1	F	482	VAL
1	F	525	HIS
1	F	546	LEU
1	F	559	LEU
1	F	571	VAL
1	F	574	THR
1	F	578	LEU
1	F	602	GLU
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

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Mol	Chain	Res	Type
1	F	721	LEU
1	F	722	GLU
1	F	731	ILE
1	F	743	ILE
1	F	746	ILE
1	F	768	VAL
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	961	ILE
1	F	966	ASP
1	F	971	ARG
1	F	980	LEU
1	F	991	ILE
1	F	993	THR
1	F	1008	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (150) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	67	GLN
1	A	68	ASN
1	A	108	GLN
1	A	109	ASN
1	A	124	GLN
1	A	125	GLN
1	A	161	ASN
1	A	194	ASN
1	A	197	GLN
1	A	229	GLN
1	A	231	ASN
1	A	274	ASN
1	A	360	GLN
1	A	439	GLN
1	A	569	GLN
1	A	605	ASN
1	A	613	ASN

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Mol	Chain	Res	Type
1	A	622	GLN
1	A	657	GLN
1	A	667	ASN
1	A	701	GLN
1	A	928	GLN
1	B	3	ASN
1	B	34	GLN
1	B	67	GLN
1	B	74	ASN
1	B	81	ASN
1	B	109	ASN
1	B	112	GLN
1	B	125	GLN
1	B	181	GLN
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	439	GLN
1	B	469	GLN
1	B	588	GLN
1	B	605	ASN
1	B	613	ASN
1	B	622	GLN
1	B	642	ASN
1	B	657	GLN
1	B	760	ASN
1	B	928	GLN
1	C	58	GLN
1	C	63	GLN
1	C	70	ASN
1	C	124	GLN
1	C	176	GLN
1	C	189	ASN
1	C	213	GLN
1	C	282	ASN
1	C	284	GLN
1	C	360	GLN
1	C	361	ASN
1	C	569	GLN

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Mol	Chain	Res	Type
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	865	GLN
1	C	1001	ASN
1	D	34	GLN
1	D	67	GLN
1	D	68	ASN
1	D	109	ASN
1	D	124	GLN
1	D	161	ASN
1	D	194	ASN
1	D	218	GLN
1	D	229	GLN
1	D	231	ASN
1	D	254	ASN
1	D	274	ASN
1	D	439	GLN
1	D	517	ASN
1	D	525	HIS
1	D	569	GLN
1	D	605	ASN
1	D	613	ASN
1	D	622	GLN
1	D	657	GLN
1	D	701	GLN
1	D	865	GLN
1	D	928	GLN
1	E	67	GLN
1	E	74	ASN
1	E	89	GLN
1	E	109	ASN
1	E	112	GLN
1	E	120	GLN
1	E	213	GLN
1	E	218	GLN
1	E	231	ASN
1	E	282	ASN
1	E	284	GLN

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Mol	Chain	Res	Type
1	E	361	ASN
1	E	439	GLN
1	E	469	GLN
1	E	588	GLN
1	E	605	ASN
1	E	613	ASN
1	E	622	GLN
1	E	657	GLN
1	E	701	GLN
1	E	726	GLN
1	E	846	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	124	GLN
1	F	151	GLN
1	F	161	ASN
1	F	189	ASN
1	F	197	GLN
1	F	213	GLN
1	F	218	GLN
1	F	237	GLN
1	F	282	ASN
1	F	360	GLN
1	F	415	ASN
1	F	439	GLN
1	F	569	GLN
1	F	577	GLN
1	F	604	ASN
1	F	605	ASN
1	F	613	ASN
1	F	622	GLN
1	F	642	ASN
1	F	667	ASN
1	F	692	HIS
1	F	697	GLN
1	F	701	GLN
1	F	719	ASN

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Mol	Chain	Res	Type
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 oligosaccharides 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	B	1058	-	12,12,12	1.14	1 (8%)	17,17,17	1.32	3 (17%)
2	FLC	A	1058	-	12,12,12	1.20	1 (8%)	17,17,17	1.40	2 (11%)
2	FLC	D	1058	-	12,12,12	1.16	1 (8%)	17,17,17	1.41	2 (11%)
2	FLC	E	1058	-	12,12,12	1.33	1 (8%)	17,17,17	1.28	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	B	1058	-	-	10/16/16/16	-
2	FLC	A	1058	-	-	2/16/16/16	-
2	FLC	D	1058	-	-	4/16/16/16	-
2	FLC	E	1058	-	-	3/16/16/16	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1058	FLC	CB-CBC	-3.14	1.50	1.53
2	A	1058	FLC	CB-CBC	-2.36	1.51	1.53
2	B	1058	FLC	CB-CBC	-2.24	1.51	1.53
2	D	1058	FLC	CB-CBC	-2.07	1.51	1.53

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1058	FLC	OB2-CBC-CB	3.74	120.32	113.14
2	A	1058	FLC	OB2-CBC-CB	3.39	119.65	113.14
2	B	1058	FLC	OB2-CBC-CB	2.87	118.64	113.14
2	A	1058	FLC	OB1-CBC-CB	-2.82	116.62	122.09
2	D	1058	FLC	OB1-CBC-CB	-2.82	116.64	122.09
2	E	1058	FLC	OB2-CBC-CB	2.58	118.09	113.14
2	B	1058	FLC	OG2-CGC-CG	2.18	121.25	114.35
2	E	1058	FLC	OG1-CGC-CG	-2.13	116.93	122.95
2	B	1058	FLC	OG1-CGC-CG	-2.11	116.96	122.95
2	E	1058	FLC	OB1-CBC-CB	-2.10	118.02	122.09

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1058	FLC	CA-CB-CBC-OB2
2	B	1058	FLC	OHB-CB-CBC-OB2
2	B	1058	FLC	CAC-CA-CB-CBC
2	B	1058	FLC	CAC-CA-CB-OHB
2	D	1058	FLC	CAC-CA-CB-CBC
2	D	1058	FLC	CAC-CA-CB-OHB
2	B	1058	FLC	CAC-CA-CB-CG
2	D	1058	FLC	CAC-CA-CB-CG

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

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1058	FLC	2	0
2	D	1058	FLC	1	0
2	E	1058	FLC	3	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%)	0.19	26 (2%)	58	35	42, 52, 59, 71	0
1	B	1032/1057 (97%)	0.20	30 (2%)	53	31	38, 50, 57, 63	0
1	C	1032/1057 (97%)	0.32	29 (2%)	55	32	41, 52, 58, 61	0
1	D	1032/1057 (97%)	0.19	24 (2%)	61	38	42, 53, 62, 70	0
1	E	1032/1057 (97%)	0.18	26 (2%)	58	35	37, 51, 57, 61	0
1	F	1032/1057 (97%)	0.29	36 (3%)	47	27	42, 51, 57, 63	0
All	All	6192/6342 (97%)	0.23	171 (2%)	55	32	37, 51, 58, 71	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	657	GLN	5.2
1	B	229	GLN	4.6
1	F	657	GLN	4.4
1	A	508	GLY	4.4
1	B	860	THR	4.3
1	F	658	ILE	4.2
1	E	987	MET	4.1
1	F	596	HIS	4.1
1	F	12	ALA	4.0
1	A	515	TRP	3.9
1	C	766	GLY	3.9
1	F	920	GLY	3.8
1	A	514	GLY	3.8
1	E	658	ILE	3.7
1	E	860	THR	3.7
1	B	362	PHE	3.7
1	D	630	SER	3.6
1	E	515	TRP	3.6
1	C	658	ILE	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	862	MET	3.5
1	B	515	TRP	3.5
1	B	993	THR	3.4
1	F	622	GLN	3.3
1	D	508	GLY	3.3
1	A	656	SER	3.3
1	C	763	ILE	3.3
1	C	429	GLU	3.2
1	D	539	GLY	3.2
1	D	326	PRO	3.2
1	F	655	PHE	3.2
1	A	860	THR	3.1
1	B	357	LEU	3.1
1	E	186	ILE	3.1
1	B	233	SER	3.0
1	C	995	ALA	3.0
1	A	513	PHE	3.0
1	F	501	ALA	3.0
1	C	860	THR	3.0
1	D	655	PHE	3.0
1	C	802	SER	3.0
1	D	860	THR	3.0
1	A	864	TYR	3.0
1	A	671	ILE	2.9
1	E	513	PHE	2.9
1	A	738	ALA	2.9
1	C	503	GLY	2.9
1	E	512	PHE	2.9
1	B	220	GLY	2.9
1	C	569	GLN	2.8
1	E	634	TRP	2.8
1	C	427	PRO	2.8
1	F	671	ILE	2.8
1	F	801	PHE	2.8
1	A	4	PHE	2.8
1	B	513	PHE	2.8
1	C	961	ILE	2.8
1	D	945	ILE	2.7
1	D	4	PHE	2.7
1	E	539	GLY	2.7
1	F	527	TYR	2.7
1	F	638	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	835	LYS	2.7
1	B	987	MET	2.7
1	E	527	TYR	2.7
1	C	768	VAL	2.6
1	C	328	ASP	2.6
1	B	861	GLY	2.6
1	A	655	PHE	2.6
1	D	868	LEU	2.6
1	B	511	GLY	2.6
1	B	862	MET	2.6
1	F	599	LEU	2.6
1	D	634	TRP	2.5
1	D	527	TYR	2.5
1	D	864	TYR	2.5
1	A	618	ALA	2.5
1	A	670	ALA	2.5
1	F	670	ALA	2.5
1	E	339	GLU	2.5
1	E	671	ILE	2.5
1	F	515	TRP	2.5
1	B	527	TYR	2.5
1	C	326	PRO	2.5
1	F	326	PRO	2.5
1	B	868	LEU	2.5
1	F	230	LEU	2.5
1	C	423	GLU	2.5
1	C	1026	PHE	2.4
1	E	1033	PHE	2.4
1	B	227	GLY	2.4
1	F	362	PHE	2.4
1	A	822	LEU	2.4
1	C	426	PRO	2.4
1	F	147	GLY	2.4
1	C	512	PHE	2.4
1	F	512	PHE	2.4
1	D	833	PRO	2.4
1	A	861	GLY	2.4
1	B	39	ALA	2.4
1	B	678	THR	2.4
1	F	600	THR	2.4
1	E	229	GLN	2.4
1	B	677	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	846	GLN	2.3
1	B	339	GLU	2.3
1	C	562	SER	2.3
1	F	778	LYS	2.3
1	F	516	PHE	2.3
1	F	328	ASP	2.3
1	D	672	VAL	2.3
1	B	658	ILE	2.3
1	A	527	TYR	2.3
1	B	660	ASP	2.3
1	A	994	GLY	2.3
1	E	514	GLY	2.3
1	D	863	SER	2.3
1	C	835	LYS	2.3
1	A	531	VAL	2.3
1	E	662	MET	2.2
1	D	515	TRP	2.2
1	C	570	GLY	2.2
1	F	40	PRO	2.2
1	F	994	GLY	2.2
1	A	1033	PHE	2.2
1	F	39	ALA	2.2
1	D	537	SER	2.2
1	D	662	MET	2.2
1	D	407	ASP	2.2
1	C	765	ARG	2.2
1	D	327	TYR	2.2
1	A	662	MET	2.2
1	D	664	PHE	2.2
1	F	993	THR	2.1
1	C	640	GLU	2.1
1	F	971	ARG	2.1
1	C	70	ASN	2.1
1	E	622	GLN	2.1
1	B	675	GLY	2.1
1	A	672	VAL	2.1
1	B	225	VAL	2.1
1	B	634	TRP	2.1
1	C	868	LEU	2.1
1	E	518	ARG	2.1
1	A	638	PRO	2.1
1	E	673	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	520	PHE	2.1
1	E	589	LYS	2.1
1	E	678	THR	2.1
1	E	569	GLN	2.1
1	A	691	GLY	2.1
1	D	1033	PHE	2.1
1	F	540	ARG	2.1
1	F	634	TRP	2.1
1	B	514	GLY	2.1
1	B	617	PHE	2.1
1	C	655	PHE	2.1
1	E	509	LYS	2.0
1	F	961	ILE	2.0
1	F	811	TYR	2.0
1	A	147	GLY	2.0
1	A	520	PHE	2.0
1	E	28	LEU	2.0
1	F	965	LEU	2.0
1	B	991	ILE	2.0
1	A	661	ALA	2.0
1	B	964	THR	2.0
1	E	541	TYR	2.0
1	D	927	PHE	2.0
1	B	640	GLU	2.0
1	C	952	LEU	2.0
1	F	219	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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	0.87	0.20	39,41,41,41	0
2	FLC	D	1058	13/13	0.87	0.21	42,44,45,46	0
2	FLC	B	1058	13/13	0.89	0.23	30,32,33,33	0
2	FLC	E	1058	13/13	0.90	0.22	31,35,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.