Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 02:14 PM EDT

PDB ID	:	1L3B
Title	:	MT0146, THE PRECORRIN-6Y METHYLTRANSFERASE (CBIT) HOMOLOG FROM M. THERMOAUTOTROPHICUM, C2 SPACEGROUP W/ LONG CELL
Authors	:	Keller, J.P.; Smith, P.M.; Benach, J.; Christendat, D.; deTitta, G.; Hunt, J.F.
Deposited on	:	2002-02-26
Resolution	:	2.65 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 (i) 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 (i)) were used in the production of this report:

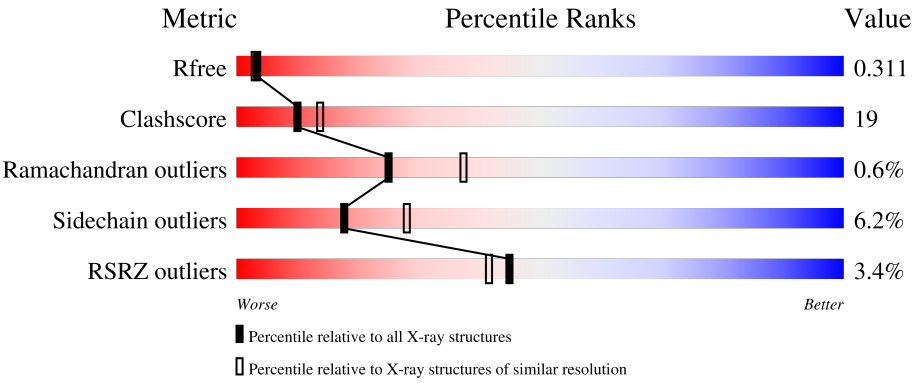
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 <=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	192	64% 31%
1	B	192	69% 28%
1	C	192	59% 33% 5%
1	D	192	56% 38%
1	E	192	63% 32%

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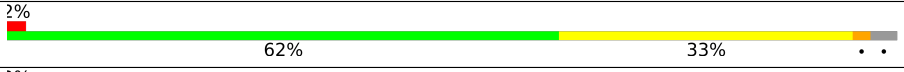
Mol	Chain	Length	Quality of chain
1	F	192	
1	G	192	
1	H	192	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 11205 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 Precorrin-6y methyltransferase/putative decarboxylase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	Se	0	0	0
			1392	868	244	267	5	8			
1	B	186	Total	C	N	O	S	Se	0	0	0
			1392	868	244	267	5	8			
1	C	186	Total	C	N	O	S	Se	0	0	0
			1392	868	244	267	5	8			
1	D	186	Total	C	N	O	S	Se	0	0	0
			1392	868	244	267	5	8			
1	E	186	Total	C	N	O	S	Se	0	0	0
			1392	868	244	267	5	8			
1	F	186	Total	C	N	O	S	Se	0	0	0
			1392	868	244	267	5	8			
1	G	186	Total	C	N	O	S	Se	0	0	0
			1392	868	244	267	5	8			
1	H	186	Total	C	N	O	S	Se	0	0	0
			1392	868	244	267	5	8			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP O26249
A	19	MSE	MET	modified residue	UNP O26249
A	26	MSE	MET	modified residue	UNP O26249
A	73	MSE	MET	modified residue	UNP O26249
A	87	MSE	MET	modified residue	UNP O26249
A	144	MSE	MET	modified residue	UNP O26249
A	172	MSE	MET	modified residue	UNP O26249
A	173	MSE	MET	modified residue	UNP O26249
B	1	MSE	MET	modified residue	UNP O26249
B	19	MSE	MET	modified residue	UNP O26249
B	26	MSE	MET	modified residue	UNP O26249
B	73	MSE	MET	modified residue	UNP O26249
B	87	MSE	MET	modified residue	UNP O26249

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Chain	Residue	Modelled	Actual	Comment	Reference
B	144	MSE	MET	modified residue	UNP O26249
B	172	MSE	MET	modified residue	UNP O26249
B	173	MSE	MET	modified residue	UNP O26249
C	1	MSE	MET	modified residue	UNP O26249
C	19	MSE	MET	modified residue	UNP O26249
C	26	MSE	MET	modified residue	UNP O26249
C	73	MSE	MET	modified residue	UNP O26249
C	87	MSE	MET	modified residue	UNP O26249
C	144	MSE	MET	modified residue	UNP O26249
C	172	MSE	MET	modified residue	UNP O26249
C	173	MSE	MET	modified residue	UNP O26249
D	1	MSE	MET	modified residue	UNP O26249
D	19	MSE	MET	modified residue	UNP O26249
D	26	MSE	MET	modified residue	UNP O26249
D	73	MSE	MET	modified residue	UNP O26249
D	87	MSE	MET	modified residue	UNP O26249
D	144	MSE	MET	modified residue	UNP O26249
D	172	MSE	MET	modified residue	UNP O26249
D	173	MSE	MET	modified residue	UNP O26249
E	1	MSE	MET	modified residue	UNP O26249
E	19	MSE	MET	modified residue	UNP O26249
E	26	MSE	MET	modified residue	UNP O26249
E	73	MSE	MET	modified residue	UNP O26249
E	87	MSE	MET	modified residue	UNP O26249
E	144	MSE	MET	modified residue	UNP O26249
E	172	MSE	MET	modified residue	UNP O26249
E	173	MSE	MET	modified residue	UNP O26249
F	1	MSE	MET	modified residue	UNP O26249
F	19	MSE	MET	modified residue	UNP O26249
F	26	MSE	MET	modified residue	UNP O26249
F	73	MSE	MET	modified residue	UNP O26249
F	87	MSE	MET	modified residue	UNP O26249
F	144	MSE	MET	modified residue	UNP O26249
F	172	MSE	MET	modified residue	UNP O26249
F	173	MSE	MET	modified residue	UNP O26249
G	1	MSE	MET	modified residue	UNP O26249
G	19	MSE	MET	modified residue	UNP O26249
G	26	MSE	MET	modified residue	UNP O26249
G	73	MSE	MET	modified residue	UNP O26249
G	87	MSE	MET	modified residue	UNP O26249
G	144	MSE	MET	modified residue	UNP O26249
G	172	MSE	MET	modified residue	UNP O26249

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Chain	Residue	Modelled	Actual	Comment	Reference
G	173	MSE	MET	modified residue	UNP O26249
H	1	MSE	MET	modified residue	UNP O26249
H	19	MSE	MET	modified residue	UNP O26249
H	26	MSE	MET	modified residue	UNP O26249
H	73	MSE	MET	modified residue	UNP O26249
H	87	MSE	MET	modified residue	UNP O26249
H	144	MSE	MET	modified residue	UNP O26249
H	172	MSE	MET	modified residue	UNP O26249
H	173	MSE	MET	modified residue	UNP O26249

- Molecule 2 is water.

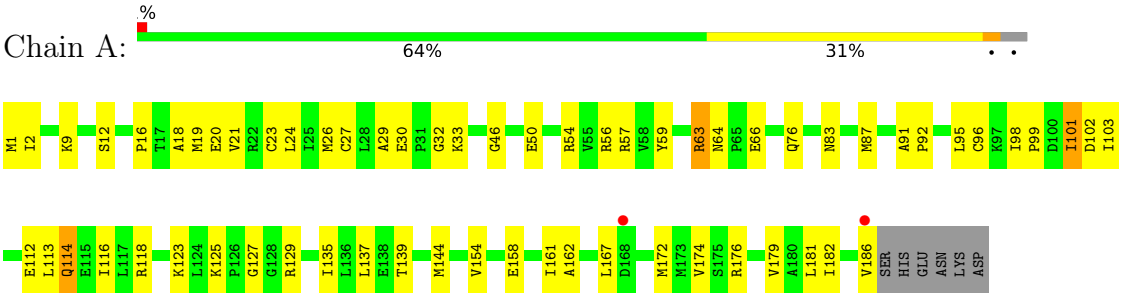
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	12	Total O 12 12	0	0
2	B	12	Total O 12 12	0	0
2	C	7	Total O 7 7	0	0
2	D	7	Total O 7 7	0	0
2	E	9	Total O 9 9	0	0
2	F	7	Total O 7 7	0	0
2	G	7	Total O 7 7	0	0
2	H	8	Total O 8 8	0	0

3 Residue-property plots (i)

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.

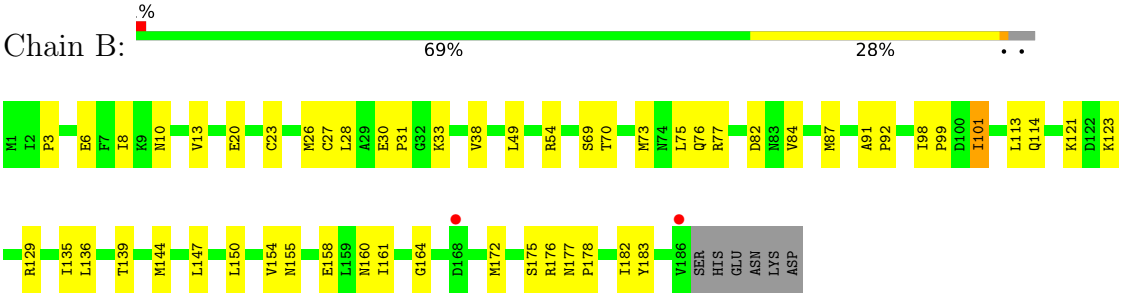
• Molecule 1: Precorrin-6y methyltransferase/putative decarboxylase

Chain A:



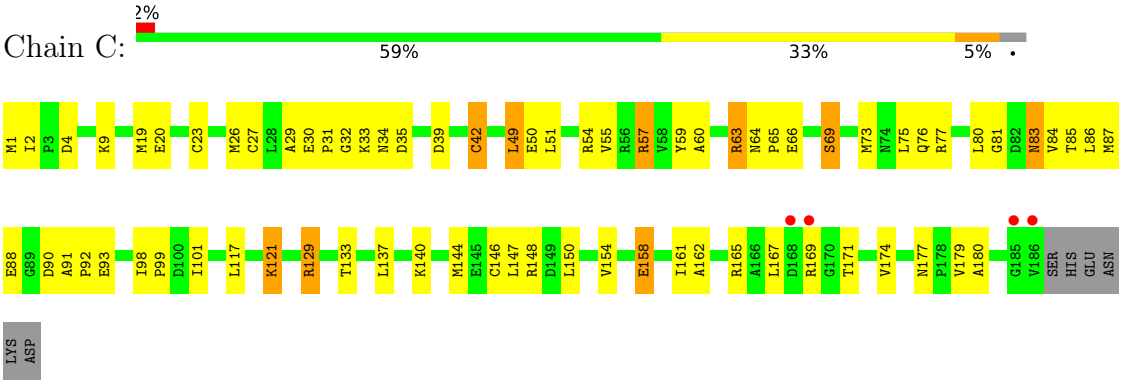
• Molecule 1: Precorrin-6y methyltransferase/putative decarboxylase

Chain B:



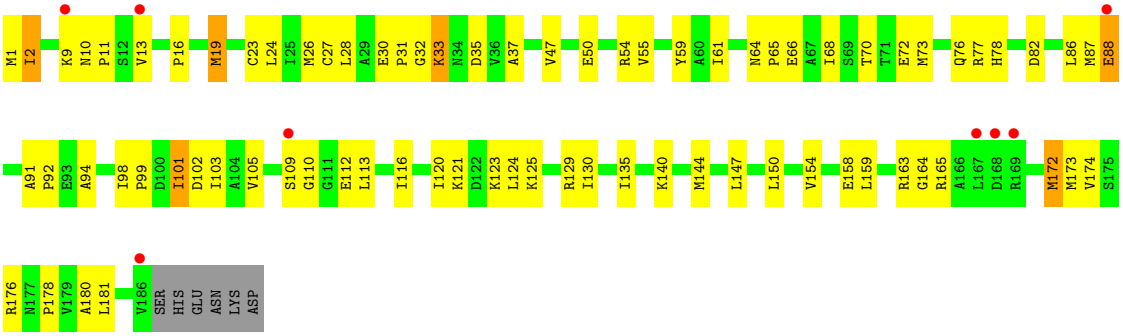
• Molecule 1: Precorrin-6y methyltransferase/putative decarboxylase

Chain C:

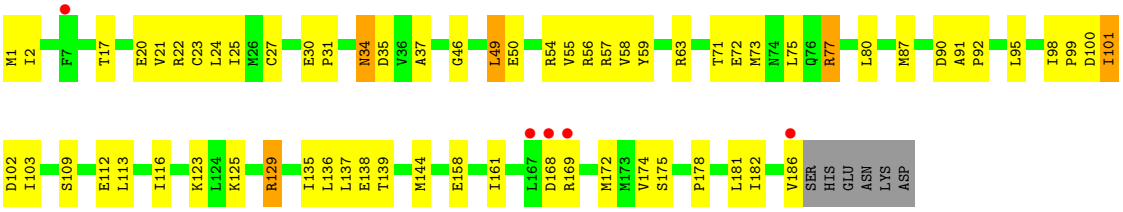


• Molecule 1: Precorrin-6y methyltransferase/putative decarboxylase

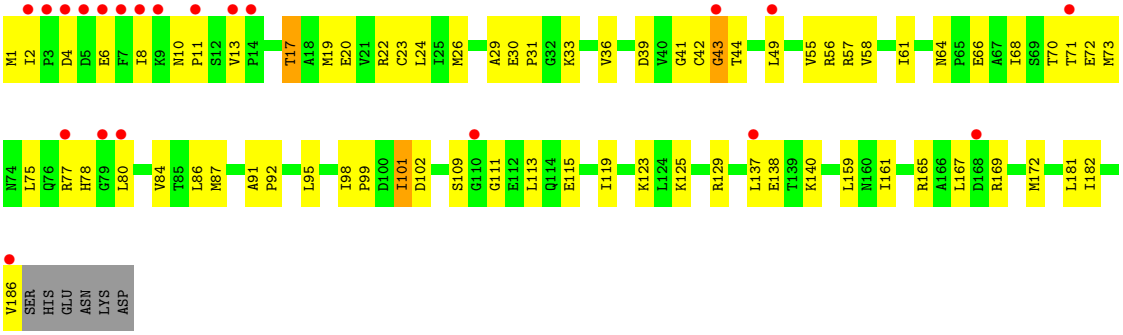
Chain D:



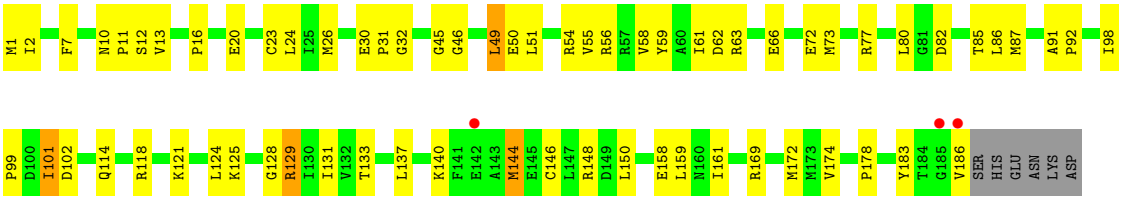
• Molecule 1: Precorrin-6y methyltransferase/putative decarboxylase



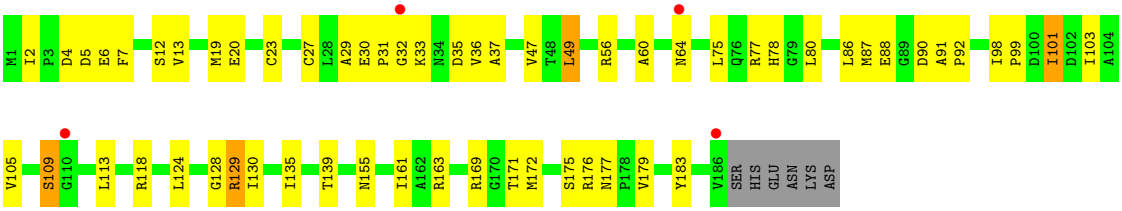
• Molecule 1: Precorrin-6y methyltransferase/putative decarboxylase



• Molecule 1: Precorrin-6y methyltransferase/putative decarboxylase



• Molecule 1: Precorrin-6y methyltransferase/putative decarboxylase


M1 I2 P3 D4 D5 E6 F7 S12 V13 M19 E20 C23 C27 L28 A29 E30 P31 G32 K33 N34 D35 V36 A37 V47 T48 L49 R56 A60 N64 L75 Q76 R77 H78 G79 L80 L86 M87 E88 G89 D90 A91 P92 I98 P99 D100 I101 D102 I103 A104
V105 S109 G110 L113 R118 L124 G128 R129 I130 I135 T139 N155 I161 A162 R163 R169 G170 T171 M172 S175 R176 N177 P178 V179 Y183 V185 SER HIS GLU ASN LYS ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	141.30Å 59.20Å 192.20Å 90.00° 108.60° 90.00°	Depositor
Resolution (Å)	36.65 – 2.65 39.19 – 2.65	Depositor EDS
% Data completeness (in resolution range)	(Not available) (36.65-2.65) 96.1 (39.19-2.65)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.69 (at 2.65Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.246 , 0.286 0.257 , 0.311	Depositor DCC
R_{free} test set	2260 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å^2)	35.8	Xtriage
Anisotropy	0.546	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11205	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.32 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5526e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.46	0/1400	0.70	0/1882
1	B	0.43	0/1400	0.70	0/1882
1	C	0.42	0/1400	0.70	0/1882
1	D	0.40	0/1400	0.68	0/1882
1	E	0.40	0/1400	0.71	0/1882
1	F	0.42	0/1400	0.66	0/1882
1	G	0.43	0/1400	0.71	0/1882
1	H	0.45	0/1400	0.73	0/1882
All	All	0.43	0/11200	0.70	0/15056

There are no bond length outliers.

There are no bond angle outliers.

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	1392	0	1436	51	0
1	B	1392	0	1437	42	0
1	C	1392	0	1437	67	0
1	D	1392	0	1436	61	0
1	E	1392	0	1437	64	0
1	F	1392	0	1437	69	0
1	G	1392	0	1437	52	0
1	H	1392	0	1437	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	12	0	0	3	0
2	B	12	0	0	0	0
2	C	7	0	0	1	0
2	D	7	0	0	1	0
2	E	9	0	0	2	0
2	F	7	0	0	2	0
2	G	7	0	0	2	0
2	H	8	0	0	2	0
All	All	11205	0	11494	429	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 19.

All (429) 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:26:MSE:HE2	1:D:50:GLU:HB3	1.39	1.03
1:A:87:MSE:HE1	1:A:98:ILE:HD11	1.42	1.02
1:D:2:ILE:HD12	1:D:2:ILE:H	1.23	1.01
1:D:59:TYR:HB3	1:D:87:MSE:HE1	1.43	0.97
1:A:137:LEU:HD23	1:E:144:MSE:HE2	1.48	0.95
1:H:49:LEU:HD13	1:H:80:LEU:HD12	1.52	0.91
1:C:2:ILE:HD12	1:C:2:ILE:H	1.38	0.89
1:H:91:ALA:HB3	1:H:92:PRO:HD3	1.52	0.89
1:A:23:CYS:HG	1:D:27:CYS:HG	0.89	0.87
1:C:59:TYR:HB3	1:C:87:MSE:HE1	1.56	0.85
1:B:87:MSE:HE1	1:B:98:ILE:HD11	1.57	0.83
1:E:129:ARG:HG2	1:E:186:VAL:HG22	1.58	0.83
1:C:26:MSE:HB3	1:C:54:ARG:HH12	1.44	0.82
1:E:20:GLU:HB2	1:E:161:ILE:HD13	1.61	0.82
1:A:2:ILE:H	1:A:2:ILE:HD12	1.46	0.81
1:E:23:CYS:SG	1:H:27:CYS:HB2	2.21	0.80
1:F:73:MSE:O	1:F:77:ARG:HG2	1.81	0.80
1:G:59:TYR:HD2	1:G:87:MSE:HE1	1.47	0.79
1:C:148:ARG:HD2	2:C:9018:HOH:O	1.83	0.79
1:C:65:PRO:HG3	1:C:88:GLU:OE1	1.82	0.78
1:H:163:ARG:HH21	1:H:176:ARG:HE	1.28	0.78
1:E:2:ILE:HD12	1:E:2:ILE:H	1.48	0.77
1:E:101:ILE:HD13	1:E:101:ILE:H	1.50	0.77
1:G:2:ILE:HD12	1:G:2:ILE:H	1.48	0.76
1:D:102:ASP:OD1	1:D:125:LYS:HD2	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:101:ILE:HD13	1:G:101:ILE:H	1.49	0.76
1:B:144:MSE:HE1	1:C:171:THR:HG21	1.66	0.76
1:D:26:MSE:HE3	1:D:54:ARG:NH2	2.01	0.75
1:B:87:MSE:CE	1:B:98:ILE:HD11	2.16	0.74
1:H:118:ARG:HG2	1:H:118:ARG:HH11	1.51	0.74
1:D:26:MSE:HE3	1:D:54:ARG:CZ	2.17	0.74
1:E:27:CYS:HB2	1:H:23:CYS:SG	2.28	0.73
1:D:10:ASN:OD1	1:D:11:PRO:HD2	1.88	0.73
1:C:167:LEU:HD13	1:C:169:ARG:NH2	2.03	0.73
1:G:146:CYS:O	1:G:150:LEU:HG	1.88	0.73
2:A:9048:HOH:O	1:H:135:ILE:HG23	1.88	0.73
1:G:137:LEU:HD12	2:G:9051:HOH:O	1.88	0.72
1:C:87:MSE:HE1	1:C:98:ILE:HD11	1.71	0.71
1:E:46:GLY:O	1:E:50:GLU:HG2	1.90	0.71
1:H:2:ILE:HD12	1:H:2:ILE:H	1.56	0.71
1:F:167:LEU:HD21	1:F:172:MSE:HE2	1.71	0.71
1:A:59:TYR:HB3	1:A:87:MSE:CE	2.21	0.71
1:F:20:GLU:HB2	1:F:161:ILE:HD13	1.72	0.71
1:A:30:GLU:HG2	2:A:9033:HOH:O	1.91	0.70
1:C:91:ALA:HB3	1:C:92:PRO:HD3	1.74	0.70
1:E:49:LEU:HD22	1:E:75:LEU:HD23	1.73	0.70
1:F:56:ARG:HG2	1:F:56:ARG:HH11	1.56	0.70
1:F:8:ILE:HD12	1:F:70:THR:HG23	1.74	0.70
1:G:91:ALA:HB3	1:G:92:PRO:HD3	1.73	0.70
1:D:2:ILE:H	1:D:2:ILE:CD1	2.00	0.70
1:B:101:ILE:HD13	1:B:101:ILE:H	1.56	0.69
1:H:101:ILE:HD13	1:H:101:ILE:H	1.58	0.68
1:B:87:MSE:SE	1:B:98:ILE:HD11	2.43	0.68
1:G:20:GLU:HB2	1:G:161:ILE:HD13	1.76	0.68
1:G:102:ASP:OD2	1:G:125:LYS:HD2	1.94	0.68
1:A:137:LEU:CD2	1:E:144:MSE:HE2	2.21	0.67
1:A:59:TYR:HB3	1:A:87:MSE:HE1	1.76	0.66
1:F:13:VAL:CG2	1:F:66:GLU:HB2	2.26	0.66
1:A:20:GLU:HB2	1:A:161:ILE:HD13	1.77	0.66
1:F:73:MSE:C	1:F:77:ARG:HG2	2.16	0.66
1:A:101:ILE:HD13	1:A:101:ILE:H	1.61	0.65
1:A:135:ILE:HD11	1:A:179:VAL:HG22	1.76	0.65
1:C:26:MSE:HE3	1:C:54:ARG:NH1	2.11	0.65
1:H:19:MSE:HE2	2:H:9059:HOH:O	1.95	0.65
1:C:90:ASP:HB3	1:C:93:GLU:OE2	1.97	0.65
1:B:98:ILE:HG23	1:B:99:PRO:HD2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:PRO:HG3	1:D:88:GLU:OE2	1.96	0.65
1:H:163:ARG:NH2	1:H:176:ARG:HE	1.95	0.65
1:B:3:PRO:HG2	1:B:6:GLU:HG3	1.80	0.64
1:G:85:THR:HG22	1:G:87:MSE:HE2	1.78	0.64
1:B:20:GLU:HB2	1:B:161:ILE:HD13	1.80	0.64
1:B:175:SER:OG	1:G:178:PRO:HD3	1.98	0.64
1:F:8:ILE:HB	1:F:70:THR:HG23	1.80	0.64
1:D:73:MSE:O	1:D:77:ARG:HG2	1.97	0.63
1:D:101:ILE:HD13	1:D:123:LYS:O	1.98	0.63
1:F:49:LEU:HD21	1:F:78:HIS:CE1	2.33	0.63
1:F:140:LYS:HD3	2:F:9071:HOH:O	1.98	0.62
1:G:124:LEU:HD11	1:G:128:GLY:HA3	1.82	0.62
1:C:26:MSE:HB3	1:C:54:ARG:NH1	2.13	0.62
1:E:73:MSE:O	1:E:77:ARG:HG2	1.98	0.62
1:H:163:ARG:HH21	1:H:176:ARG:NE	1.97	0.62
1:H:118:ARG:HG2	1:H:118:ARG:NH1	2.14	0.62
1:G:45:GLY:O	1:G:49:LEU:HD23	2.00	0.61
1:C:59:TYR:HB3	1:C:87:MSE:CE	2.30	0.61
1:H:20:GLU:HB2	1:H:161:ILE:HD13	1.81	0.61
1:G:10:ASN:HB3	1:G:13:VAL:HB	1.82	0.61
1:D:76:GLN:HA	2:D:9075:HOH:O	2.00	0.60
1:H:36:VAL:HG12	1:H:101:ILE:HG22	1.82	0.60
1:F:102:ASP:OD1	1:F:125:LYS:HD2	2.01	0.60
1:E:31:PRO:HB2	1:E:54:ARG:HD2	1.83	0.60
1:A:112:GLU:O	1:A:116:ILE:HG13	2.01	0.60
1:D:163:ARG:HH12	1:D:176:ARG:HD2	1.67	0.60
1:D:109:SER:HB2	1:D:113:LEU:HB2	1.83	0.59
1:A:114:GLN:HE22	1:A:118:ARG:HH21	1.51	0.58
1:B:27:CYS:HB2	1:C:23:CYS:SG	2.44	0.58
1:A:56:ARG:O	1:A:83:ASN:HB2	2.03	0.58
1:F:13:VAL:HG21	1:F:66:GLU:HB2	1.85	0.58
1:B:91:ALA:HB3	1:B:92:PRO:HD3	1.85	0.58
1:G:10:ASN:OD1	1:G:11:PRO:HD2	2.04	0.58
1:A:29:ALA:HB1	1:A:103:ILE:HD13	1.85	0.57
1:H:163:ARG:HE	1:H:176:ARG:NE	2.01	0.57
1:A:91:ALA:HB3	1:A:92:PRO:HD3	1.86	0.57
1:C:35:ASP:HB2	1:C:55:VAL:HG12	1.86	0.57
1:H:7:PHE:HE2	1:H:49:LEU:HG	1.70	0.57
1:G:129:ARG:HG3	1:G:186:VAL:O	2.05	0.57
1:E:138:GLU:OE1	1:E:138:GLU:N	2.38	0.57
1:F:73:MSE:HG2	1:F:77:ARG:HH21	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:8:ILE:HB	1:F:70:THR:CG2	2.35	0.56
1:F:138:GLU:CD	1:F:138:GLU:H	2.09	0.56
1:D:158:GLU:OE2	1:D:180:ALA:HB2	2.05	0.56
1:F:33:LYS:O	1:F:56:ARG:HB2	2.05	0.56
1:D:163:ARG:NH1	1:D:176:ARG:HD2	2.21	0.56
1:E:20:GLU:CB	1:E:161:ILE:HD13	2.31	0.56
1:E:21:VAL:O	1:E:25:ILE:HG13	2.04	0.56
1:F:91:ALA:HB3	1:F:92:PRO:HD3	1.88	0.56
1:H:30:GLU:N	1:H:31:PRO:HD3	2.20	0.56
1:C:69:SER:HB3	1:C:73:MSE:HE2	1.87	0.55
1:D:9:LYS:HE3	1:D:16:PRO:HD2	1.88	0.55
1:B:28:LEU:O	1:B:30:GLU:HG3	2.07	0.55
1:D:91:ALA:HB3	1:D:92:PRO:HD3	1.88	0.55
1:E:129:ARG:CG	1:E:186:VAL:HG13	2.37	0.55
1:D:1:MSE:HB3	1:D:19:MSE:HE2	1.88	0.55
1:G:7:PHE:CZ	1:G:46:GLY:HA2	2.42	0.55
1:H:13:VAL:HG22	1:H:64:ASN:ND2	2.20	0.55
1:F:36:VAL:N	1:F:102:ASP:OD2	2.39	0.55
1:G:26:MSE:O	1:G:31:PRO:HD3	2.07	0.55
1:D:163:ARG:HH22	1:D:176:ARG:HD2	1.71	0.55
1:F:24:LEU:HD23	1:F:181:LEU:HD12	1.87	0.54
1:G:59:TYR:CD2	1:G:87:MSE:HE1	2.35	0.54
1:H:37:ALA:HB2	1:H:103:ILE:HB	1.89	0.54
1:F:56:ARG:HG2	1:F:56:ARG:NH1	2.21	0.54
1:G:11:PRO:HG2	1:G:12:SER:H	1.72	0.54
1:C:35:ASP:O	1:C:55:VAL:HB	2.07	0.54
1:B:75:LEU:HD11	1:B:84:VAL:HG11	1.89	0.54
1:H:91:ALA:HB3	1:H:92:PRO:CD	2.32	0.54
1:A:63:ARG:CB	1:A:63:ARG:HH11	2.21	0.54
1:C:98:ILE:HG23	1:C:99:PRO:HD2	1.88	0.54
1:F:2:ILE:HD11	1:F:78:HIS:HE1	1.73	0.54
1:E:71:THR:O	1:E:75:LEU:HG	2.07	0.53
1:A:24:LEU:HD23	1:A:181:LEU:HD12	1.89	0.53
1:G:66:GLU:OE2	1:G:66:GLU:HA	2.08	0.53
1:G:118:ARG:HG2	1:G:118:ARG:HH11	1.73	0.53
1:D:163:ARG:NH2	1:D:176:ARG:HD2	2.23	0.53
1:F:101:ILE:HD13	1:F:101:ILE:H	1.73	0.53
1:H:32:GLY:N	1:H:35:ASP:OD2	2.41	0.53
1:H:49:LEU:HD22	1:H:75:LEU:HD23	1.91	0.53
1:B:144:MSE:HE2	1:F:137:LEU:HD22	1.91	0.53
1:C:158:GLU:OE2	1:C:180:ALA:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ALA:HB3	1:D:158:GLU:HB2	1.90	0.52
1:C:2:ILE:H	1:C:2:ILE:CD1	2.14	0.52
1:C:144:MSE:O	1:C:148:ARG:HB2	2.10	0.52
1:D:35:ASP:O	1:D:55:VAL:HB	2.09	0.52
1:C:2:ILE:HD12	1:C:2:ILE:N	2.18	0.52
1:F:165:ARG:CZ	1:F:172:MSE:HE3	2.40	0.52
1:G:140:LYS:O	1:G:144:MSE:HG3	2.10	0.52
1:H:183:TYR:N	1:H:183:TYR:CD2	2.76	0.52
1:B:87:MSE:HE1	1:B:98:ILE:CD1	2.34	0.52
1:C:87:MSE:CE	1:C:98:ILE:HD11	2.37	0.52
1:B:121:LYS:HD2	1:B:150:LEU:HB3	1.92	0.52
1:D:64:ASN:HD21	1:D:66:GLU:HB2	1.74	0.52
1:F:8:ILE:HD12	1:F:70:THR:HA	1.91	0.52
1:F:41:GLY:C	1:F:43:GLY:H	2.13	0.52
1:D:72:GLU:HG3	1:D:76:GLN:HE21	1.75	0.52
1:F:61:ILE:HD11	1:F:98:ILE:HD11	1.92	0.52
1:A:2:ILE:HD12	1:A:2:ILE:N	2.19	0.52
1:G:26:MSE:HE1	1:G:51:LEU:HA	1.90	0.52
1:B:177:ASN:OD1	1:G:174:VAL:HA	2.10	0.52
1:D:163:ARG:HH12	1:D:176:ARG:CD	2.22	0.52
1:A:135:ILE:CD1	1:A:179:VAL:HG22	2.40	0.51
1:G:1:MSE:CE	1:G:54:ARG:NH2	2.73	0.51
1:B:101:ILE:HD13	1:B:101:ILE:N	2.25	0.51
1:D:101:ILE:HD13	1:D:101:ILE:H	1.75	0.51
1:A:87:MSE:CE	1:A:98:ILE:HD11	2.28	0.51
1:C:85:THR:HG22	1:C:87:MSE:HE2	1.93	0.51
1:B:113:LEU:HD22	1:B:139:THR:HG23	1.91	0.51
1:F:73:MSE:HB3	1:F:77:ARG:HE	1.76	0.51
1:A:20:GLU:HB2	1:A:161:ILE:CD1	2.39	0.51
1:B:144:MSE:HE2	1:F:137:LEU:CD2	2.41	0.51
1:A:2:ILE:H	1:A:2:ILE:CD1	2.20	0.51
1:F:26:MSE:HE3	1:F:31:PRO:HG2	1.93	0.51
1:A:174:VAL:HA	1:H:177:ASN:OD1	2.10	0.50
1:F:13:VAL:HG23	1:F:66:GLU:HB2	1.91	0.50
1:F:44:THR:HG22	1:F:70:THR:HG21	1.93	0.50
1:B:8:ILE:HD11	1:B:77:ARG:HG3	1.93	0.50
1:E:59:TYR:CD2	1:E:87:MSE:HE1	2.47	0.50
1:H:78:HIS:O	1:H:80:LEU:HG	2.11	0.50
1:A:1:MSE:HE2	1:A:50:GLU:CD	2.32	0.50
1:C:73:MSE:O	1:C:77:ARG:HG2	2.11	0.50
1:C:87:MSE:SE	1:C:98:ILE:HD11	2.61	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:MSE:HE1	1:H:171:THR:HG21	1.93	0.50
1:H:163:ARG:HE	1:H:176:ARG:HE	1.59	0.50
1:A:23:CYS:CB	1:D:27:CYS:HG	2.24	0.50
1:F:24:LEU:HD22	1:F:159:LEU:HD11	1.94	0.50
1:F:10:ASN:CG	1:F:11:PRO:HD2	2.31	0.50
1:C:30:GLU:N	1:C:31:PRO:HD3	2.27	0.50
1:G:30:GLU:N	1:G:31:PRO:HD3	2.27	0.50
1:F:30:GLU:N	1:F:31:PRO:HD3	2.27	0.50
1:F:95:LEU:HA	1:F:98:ILE:HD12	1.92	0.50
1:G:101:ILE:HD13	1:G:101:ILE:N	2.24	0.50
1:G:73:MSE:O	1:G:77:ARG:HG2	2.11	0.49
1:E:59:TYR:HB3	1:E:87:MSE:HE1	1.94	0.49
1:A:27:CYS:O	1:A:30:GLU:HG3	2.12	0.49
1:G:1:MSE:HE2	1:G:50:GLU:OE1	2.12	0.49
1:E:135:ILE:HG23	2:E:9008:HOH:O	2.11	0.49
1:H:56:ARG:HH11	1:H:56:ARG:HG2	1.77	0.49
1:C:20:GLU:HB2	1:C:161:ILE:HD13	1.95	0.49
1:D:32:GLY:O	1:D:55:VAL:HA	2.11	0.49
1:E:49:LEU:CD2	1:E:75:LEU:HD23	2.42	0.49
1:E:72:GLU:HA	1:E:75:LEU:HD12	1.94	0.49
1:E:91:ALA:HB3	1:E:92:PRO:HD3	1.95	0.49
1:E:129:ARG:HG3	1:E:186:VAL:HG13	1.93	0.49
1:F:30:GLU:OE1	1:F:186:VAL:HG21	2.13	0.49
1:F:2:ILE:HD11	1:F:78:HIS:CE1	2.48	0.49
1:H:98:ILE:HG23	1:H:99:PRO:HD2	1.95	0.49
1:D:10:ASN:HB3	1:D:13:VAL:HB	1.95	0.48
1:D:47:VAL:HG11	1:D:105:VAL:HG11	1.95	0.48
1:F:72:GLU:HB2	1:F:86:LEU:CD1	2.43	0.48
1:E:23:CYS:SG	1:H:27:CYS:CB	2.99	0.48
1:F:109:SER:C	1:F:111:GLY:H	2.17	0.48
1:H:135:ILE:HD11	1:H:179:VAL:HG22	1.95	0.48
1:A:26:MSE:HE3	1:A:54:ARG:HD2	1.95	0.48
1:E:102:ASP:OD1	1:E:125:LYS:HD2	2.13	0.48
1:B:136:LEU:HD11	1:G:169:ARG:HD3	1.94	0.48
1:C:117:LEU:HD22	1:C:147:LEU:HD21	1.96	0.48
1:C:165:ARG:NH2	1:C:174:VAL:HG11	2.28	0.48
1:E:90:ASP:OD1	1:E:92:PRO:HD2	2.13	0.48
1:C:167:LEU:HD13	1:C:169:ARG:CZ	2.44	0.48
1:A:96:CYS:HA	1:A:123:LYS:HE3	1.96	0.48
1:A:102:ASP:OD1	1:A:125:LYS:HD3	2.14	0.48
1:C:121:LYS:O	1:C:121:LYS:HD3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:ASN:CG	1:D:11:PRO:HD2	2.33	0.48
1:A:135:ILE:HG22	1:H:172:MSE:HG3	1.95	0.47
1:B:33:LYS:HD3	1:B:54:ARG:O	2.13	0.47
1:B:30:GLU:N	1:B:31:PRO:HD3	2.28	0.47
1:A:1:MSE:HE2	1:A:50:GLU:OE1	2.15	0.47
1:E:34:ASN:ND2	1:E:34:ASN:H	2.11	0.47
1:E:59:TYR:HB3	1:E:87:MSE:CE	2.44	0.47
1:C:177:ASN:O	1:C:179:VAL:HG23	2.14	0.47
1:D:61:ILE:HD13	1:D:94:ALA:HB3	1.97	0.47
1:E:98:ILE:HG22	1:E:99:PRO:O	2.15	0.47
1:E:182:ILE:HD12	1:E:182:ILE:N	2.29	0.47
1:F:8:ILE:CD1	1:F:70:THR:HG23	2.43	0.47
1:G:98:ILE:HG23	1:G:99:PRO:HD2	1.96	0.47
1:G:49:LEU:HD13	1:G:80:LEU:HD12	1.95	0.47
1:G:121:LYS:HD3	1:G:150:LEU:HB3	1.97	0.47
1:F:182:ILE:N	1:F:182:ILE:HD12	2.30	0.47
1:A:23:CYS:SG	1:D:23:CYS:SG	3.13	0.47
1:F:71:THR:O	1:F:75:LEU:HG	2.15	0.47
1:G:24:LEU:HD23	1:G:159:LEU:HD11	1.97	0.47
1:C:63:ARG:HB3	1:C:63:ARG:HH11	1.80	0.47
1:F:2:ILE:HG23	1:F:6:GLU:OE1	2.15	0.47
1:H:155:ASN:HB3	1:H:183:TYR:CZ	2.50	0.47
1:F:167:LEU:HD11	1:F:172:MSE:HE2	1.97	0.46
1:G:26:MSE:HE3	1:G:54:ARG:HD2	1.97	0.46
1:D:110:GLY:O	1:D:112:GLU:HG3	2.15	0.46
1:E:59:TYR:HD2	1:E:87:MSE:HE1	1.80	0.46
1:G:144:MSE:HB3	1:G:144:MSE:HE3	1.82	0.46
1:D:121:LYS:HD2	1:D:150:LEU:HB3	1.97	0.46
1:H:13:VAL:HG22	1:H:64:ASN:HD21	1.79	0.46
1:A:101:ILE:HD13	1:A:101:ILE:N	2.30	0.46
1:B:98:ILE:HG23	1:B:99:PRO:CD	2.44	0.46
1:B:147:LEU:HB2	1:B:154:VAL:CG1	2.46	0.46
1:C:64:ASN:OD1	1:C:66:GLU:HB2	2.16	0.46
1:E:172:MSE:HE3	1:E:174:VAL:CG2	2.45	0.46
1:H:33:LYS:HD2	2:H:9065:HOH:O	2.15	0.46
1:E:17:THR:O	1:E:22:ARG:NE	2.39	0.46
1:E:56:ARG:HG2	1:E:56:ARG:HH11	1.80	0.46
1:E:63:ARG:CB	1:E:63:ARG:HH11	2.28	0.46
1:A:33:LYS:HA	1:A:54:ARG:O	2.16	0.46
1:F:1:MSE:HB2	1:F:19:MSE:HE2	1.98	0.46
1:A:144:MSE:HG3	1:E:137:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:LEU:HD12	1:B:182:ILE:HG22	1.97	0.45
1:C:26:MSE:HE3	1:C:31:PRO:HG2	1.98	0.45
1:A:57:ARG:NH2	1:A:83:ASN:HA	2.32	0.45
1:F:8:ILE:CG1	1:F:70:THR:HG23	2.46	0.45
1:G:1:MSE:HE3	1:G:54:ARG:NH2	2.30	0.45
1:H:128:GLY:HA2	1:H:129:ARG:HH21	1.82	0.45
1:D:28:LEU:O	1:D:30:GLU:HG3	2.16	0.45
1:D:33:LYS:NZ	1:D:33:LYS:HA	2.32	0.45
1:A:101:ILE:HD13	1:A:123:LYS:O	2.16	0.45
1:F:55:VAL:CG2	1:F:58:VAL:HG23	2.46	0.45
1:H:135:ILE:HG22	1:H:135:ILE:O	2.17	0.45
1:H:163:ARG:HE	1:H:176:ARG:CZ	2.30	0.45
1:B:38:VAL:HG13	1:B:38:VAL:O	2.16	0.45
1:C:51:LEU:O	1:C:55:VAL:HG22	2.16	0.45
1:A:127:GLY:O	1:A:186:VAL:HG13	2.16	0.45
1:B:160:ASN:OD1	1:B:178:PRO:HG3	2.17	0.45
1:E:37:ALA:HB2	1:E:103:ILE:HB	1.99	0.45
1:C:57:ARG:HG2	1:C:57:ARG:HH11	1.82	0.44
1:E:30:GLU:N	1:E:31:PRO:HD3	2.31	0.44
1:A:167:LEU:HD11	1:A:172:MSE:HE2	2.00	0.44
1:B:101:ILE:HD13	1:B:123:LYS:O	2.18	0.44
1:C:146:CYS:O	1:C:150:LEU:HG	2.17	0.44
1:H:124:LEU:HD22	1:H:130:ILE:HD11	2.00	0.44
1:D:124:LEU:HD22	1:D:130:ILE:HD11	1.99	0.44
1:G:148:ARG:HH11	1:G:148:ARG:HG3	1.83	0.44
1:H:47:VAL:HG11	1:H:105:VAL:HG11	1.98	0.44
1:A:179:VAL:HG21	2:A:9036:HOH:O	2.17	0.44
1:C:26:MSE:HG3	1:C:50:GLU:HB3	2.00	0.44
1:E:100:ASP:O	1:E:125:LYS:HE3	2.18	0.44
1:C:121:LYS:HG3	1:C:150:LEU:HB3	1.98	0.44
1:E:63:ARG:HD2	2:E:9004:HOH:O	2.17	0.44
1:E:109:SER:HB3	1:E:113:LEU:HB2	1.98	0.44
1:B:182:ILE:HD12	1:B:182:ILE:N	2.33	0.44
1:C:49:LEU:HD13	1:C:80:LEU:HD12	2.00	0.44
1:D:37:ALA:CB	1:D:103:ILE:HB	2.48	0.44
1:D:70:THR:HA	1:D:73:MSE:HE2	1.99	0.44
1:D:165:ARG:CZ	1:D:174:VAL:HG21	2.48	0.44
1:F:115:GLU:O	1:F:119:ILE:HG13	2.17	0.44
1:G:131:ILE:N	1:G:131:ILE:HD12	2.33	0.44
1:A:182:ILE:N	1:A:182:ILE:HD12	2.33	0.44
1:D:178:PRO:HD3	1:E:175:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:29:ALA:O	1:F:129:ARG:HD2	2.18	0.44
1:H:4:ASP:O	1:H:6:GLU:N	2.51	0.44
1:B:27:CYS:SG	1:C:1:MSE:HB3	2.57	0.44
1:F:87:MSE:HE1	1:F:98:ILE:HG12	1.99	0.44
1:A:64:ASN:HD21	1:A:66:GLU:HB2	1.83	0.43
1:F:95:LEU:O	1:F:123:LYS:HE2	2.18	0.43
1:C:57:ARG:HD3	1:D:78:HIS:O	2.17	0.43
1:E:101:ILE:HD13	1:E:101:ILE:N	2.24	0.43
1:F:61:ILE:HD11	1:F:98:ILE:CD1	2.47	0.43
1:A:18:ALA:HB3	1:A:21:VAL:HG23	2.00	0.43
1:C:29:ALA:O	1:C:129:ARG:HD2	2.18	0.43
1:C:32:GLY:C	1:C:34:ASN:H	2.22	0.43
1:C:57:ARG:HE	1:C:83:ASN:HA	1.83	0.43
1:D:61:ILE:HD13	1:D:94:ALA:CB	2.48	0.43
1:G:26:MSE:HB3	1:G:54:ARG:NH1	2.33	0.43
1:B:23:CYS:HG	1:C:23:CYS:HG	1.63	0.43
1:E:75:LEU:HB3	1:E:80:LEU:O	2.17	0.43
1:E:98:ILE:HG23	1:E:99:PRO:HD2	2.01	0.43
1:H:113:LEU:HD22	1:H:139:THR:HG23	2.00	0.43
1:E:31:PRO:HA	1:E:103:ILE:HD11	2.01	0.43
1:F:77:ARG:HD3	2:F:9047:HOH:O	2.19	0.43
1:F:8:ILE:CB	1:F:70:THR:HG23	2.48	0.43
1:F:10:ASN:ND2	1:F:11:PRO:HD2	2.34	0.43
1:F:64:ASN:OD1	1:F:66:GLU:HG2	2.19	0.43
1:H:60:ALA:HB3	1:H:86:LEU:HD23	2.01	0.43
1:H:56:ARG:HG2	1:H:56:ARG:NH1	2.34	0.43
1:A:98:ILE:HG22	1:A:99:PRO:O	2.19	0.42
1:B:8:ILE:HD11	1:B:77:ARG:NE	2.34	0.42
1:B:26:MSE:CE	1:B:31:PRO:HG2	2.48	0.42
1:E:24:LEU:HD23	1:E:181:LEU:HD12	2.01	0.42
1:F:10:ASN:HB3	1:F:13:VAL:HB	2.01	0.42
1:F:55:VAL:HG21	1:F:58:VAL:HG23	1.99	0.42
1:A:98:ILE:HG23	1:A:99:PRO:HD2	2.00	0.42
1:D:116:ILE:O	1:D:120:ILE:HG13	2.19	0.42
1:E:112:GLU:O	1:E:116:ILE:HG13	2.18	0.42
1:F:17:THR:HB	1:F:22:ARG:CG	2.49	0.42
1:G:98:ILE:HG22	1:G:99:PRO:O	2.19	0.42
1:F:73:MSE:HB3	1:F:77:ARG:NE	2.34	0.42
1:G:16:PRO:HA	2:G:9057:HOH:O	2.19	0.42
1:C:39:ASP:OD2	1:C:42:CYS:HA	2.20	0.42
1:G:183:TYR:N	1:G:183:TYR:CD2	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:121:LYS:CD	1:G:150:LEU:HB3	2.49	0.42
1:D:147:LEU:HB2	1:D:154:VAL:HG11	2.01	0.42
1:C:49:LEU:HD22	1:C:75:LEU:HD23	2.00	0.42
1:E:95:LEU:HA	1:E:98:ILE:HD12	2.02	0.42
1:A:32:GLY:HA3	1:C:76:GLN:HE22	1.85	0.42
1:C:93:GLU:CD	1:C:93:GLU:H	2.23	0.42
1:C:117:LEU:HD13	1:C:147:LEU:HG	2.02	0.42
1:D:37:ALA:HB2	1:D:103:ILE:HB	2.01	0.42
1:E:49:LEU:CD1	1:E:80:LEU:HD13	2.49	0.42
1:C:147:LEU:HB2	1:C:154:VAL:CG1	2.50	0.42
1:D:159:LEU:HD23	1:D:159:LEU:HA	1.86	0.42
1:E:49:LEU:HD11	1:E:80:LEU:HD13	2.02	0.42
1:D:163:ARG:CZ	1:D:176:ARG:HD2	2.50	0.42
1:H:90:ASP:OD2	1:H:92:PRO:HD2	2.20	0.41
1:B:164:GLY:HA2	1:B:172:MSE:O	2.20	0.41
1:G:61:ILE:HG22	1:G:62:ASP:N	2.34	0.41
1:C:98:ILE:HG22	1:C:99:PRO:O	2.19	0.41
1:F:24:LEU:CD2	1:F:159:LEU:HD11	2.50	0.41
1:F:119:ILE:O	1:F:123:LYS:HG3	2.20	0.41
1:G:32:GLY:O	1:G:55:VAL:HA	2.20	0.41
1:A:95:LEU:HD11	1:A:116:ILE:HG23	2.03	0.41
1:C:26:MSE:HE1	1:C:51:LEU:HA	2.02	0.41
1:C:69:SER:HB3	1:C:73:MSE:CE	2.48	0.41
1:G:86:LEU:H	1:G:86:LEU:HD12	1.84	0.41
1:B:26:MSE:HE3	1:B:31:PRO:HG2	2.02	0.41
1:C:59:TYR:CD2	1:C:87:MSE:HE1	2.55	0.41
1:D:135:ILE:HD13	1:D:135:ILE:HA	1.79	0.41
1:E:1:MSE:HE2	1:E:50:GLU:OE1	2.21	0.41
1:E:59:TYR:HD2	1:E:87:MSE:CE	2.33	0.41
1:G:10:ASN:OD1	1:G:11:PRO:CD	2.67	0.41
1:H:101:ILE:HD13	1:H:101:ILE:N	2.29	0.41
1:D:24:LEU:HD23	1:D:181:LEU:HD12	2.03	0.41
1:D:121:LYS:O	1:D:121:LYS:HG2	2.20	0.41
1:E:56:ARG:HG2	1:E:56:ARG:NH1	2.35	0.41
1:G:56:ARG:HG2	1:G:56:ARG:HH11	1.86	0.41
1:A:161:ILE:HG22	1:A:162:ALA:N	2.35	0.41
1:E:20:GLU:HB2	1:E:161:ILE:CD1	2.39	0.41
1:E:35:ASP:O	1:E:55:VAL:HB	2.20	0.41
1:E:57:ARG:CG	1:E:58:VAL:N	2.84	0.41
1:E:63:ARG:HH11	1:E:63:ARG:HB2	1.85	0.41
1:E:169:ARG:H	1:E:169:ARG:HG3	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:23:CYS:HG	1:G:23:CYS:HG	1.63	0.41
1:H:7:PHE:CE2	1:H:49:LEU:HG	2.52	0.41
1:B:155:ASN:HB2	1:B:183:TYR:CZ	2.56	0.41
1:E:136:LEU:HB2	1:E:139:THR:OG1	2.21	0.41
1:B:10:ASN:HB3	1:B:13:VAL:HB	2.02	0.41
1:C:32:GLY:O	1:C:34:ASN:N	2.54	0.41
1:C:59:TYR:HD2	1:C:87:MSE:HE1	1.85	0.41
1:E:98:ILE:O	1:E:123:LYS:NZ	2.53	0.41
1:H:29:ALA:O	1:H:129:ARG:HD2	2.21	0.41
1:B:70:THR:HA	1:B:73:MSE:HE3	2.02	0.41
1:C:147:LEU:HB2	1:C:154:VAL:HG11	2.03	0.41
1:D:33:LYS:HA	1:D:33:LYS:HZ3	1.85	0.41
1:F:64:ASN:O	1:F:68:ILE:HG12	2.21	0.41
1:H:135:ILE:O	1:H:135:ILE:CG2	2.69	0.41
1:C:81:GLY:C	1:C:83:ASN:H	2.25	0.40
1:C:83:ASN:OD1	1:C:84:VAL:HG23	2.21	0.40
1:A:113:LEU:HD22	1:A:139:THR:HG23	2.03	0.40
1:B:135:ILE:HG22	1:G:172:MSE:HG3	2.03	0.40
1:D:68:ILE:HG23	1:D:86:LEU:HD22	2.03	0.40
1:D:140:LYS:O	1:D:144:MSE:HG2	2.21	0.40
1:F:75:LEU:HD11	1:F:84:VAL:HG11	2.04	0.40
1:F:109:SER:OG	1:F:113:LEU:HB2	2.20	0.40
1:D:98:ILE:HG23	1:D:99:PRO:HD2	2.03	0.40
1:G:55:VAL:CG2	1:G:58:VAL:HG22	2.51	0.40
1:C:137:LEU:HD12	1:C:140:LYS:NZ	2.36	0.40
1:D:64:ASN:ND2	1:D:66:GLU:HB2	2.36	0.40
1:D:164:GLY:HA2	1:D:172:MSE:O	2.20	0.40
1:D:173:MSE:O	1:E:178:PRO:HD2	2.21	0.40
1:F:73:MSE:CB	1:F:77:ARG:HE	2.33	0.40
1:F:98:ILE:HA	1:F:99:PRO:HD3	1.91	0.40
1:H:91:ALA:CB	1:H:92:PRO:HD3	2.36	0.40
1:B:98:ILE:HG22	1:B:99:PRO:O	2.21	0.40
1:C:60:ALA:HB3	1:C:86:LEU:HD23	2.03	0.40
1:C:161:ILE:HG22	1:C:162:ALA:N	2.37	0.40
1:C:165:ARG:CZ	1:C:174:VAL:HG21	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	184/192 (96%)	175 (95%)	8 (4%)	1 (0%)	29	43
1	B	184/192 (96%)	171 (93%)	13 (7%)	0	100	100
1	C	184/192 (96%)	172 (94%)	9 (5%)	3 (2%)	9	14
1	D	184/192 (96%)	168 (91%)	15 (8%)	1 (0%)	29	43
1	E	184/192 (96%)	173 (94%)	11 (6%)	0	100	100
1	F	184/192 (96%)	168 (91%)	14 (8%)	2 (1%)	14	21
1	G	184/192 (96%)	175 (95%)	9 (5%)	0	100	100
1	H	184/192 (96%)	176 (96%)	6 (3%)	2 (1%)	14	21
All	All	1472/1536 (96%)	1378 (94%)	85 (6%)	9 (1%)	25	37

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	31	PRO
1	F	43	GLY
1	H	5	ASP
1	H	109	SER
1	F	42	CYS
1	C	33	LYS
1	C	42	CYS
1	C	83	ASN
1	A	46	GLY

5.3.2 Protein sidechains (i)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	152/150 (101%)	140 (92%)	12 (8%)	12	19
1	B	152/150 (101%)	143 (94%)	9 (6%)	19	30
1	C	152/150 (101%)	139 (91%)	13 (9%)	10	15
1	D	152/150 (101%)	144 (95%)	8 (5%)	22	35
1	E	152/150 (101%)	145 (95%)	7 (5%)	27	41
1	F	152/150 (101%)	145 (95%)	7 (5%)	27	41
1	G	152/150 (101%)	142 (93%)	10 (7%)	16	25
1	H	152/150 (101%)	142 (93%)	10 (7%)	16	25
All	All	1216/1200 (101%)	1140 (94%)	76 (6%)	18	28

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	12	SER
1	A	16	PRO
1	A	19	MSE
1	A	63	ARG
1	A	76	GLN
1	A	101	ILE
1	A	114	GLN
1	A	129	ARG
1	A	154	VAL
1	A	158	GLU
1	A	176	ARG
1	B	49	LEU
1	B	69	SER
1	B	76	GLN
1	B	82	ASP
1	B	101	ILE
1	B	114	GLN
1	B	129	ARG
1	B	158	GLU
1	B	176	ARG
1	C	4	ASP
1	C	9	LYS
1	C	19	MSE
1	C	27	CYS

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Mol	Chain	Res	Type
1	C	49	LEU
1	C	57	ARG
1	C	63	ARG
1	C	69	SER
1	C	101	ILE
1	C	121	LYS
1	C	129	ARG
1	C	133	THR
1	C	158	GLU
1	D	2	ILE
1	D	19	MSE
1	D	33	LYS
1	D	82	ASP
1	D	88	GLU
1	D	101	ILE
1	D	129	ARG
1	D	172	MSE
1	E	34	ASN
1	E	49	LEU
1	E	77	ARG
1	E	101	ILE
1	E	129	ARG
1	E	158	GLU
1	E	168	ASP
1	F	4	ASP
1	F	17	THR
1	F	39	ASP
1	F	57	ARG
1	F	80	LEU
1	F	101	ILE
1	F	169	ARG
1	G	49	LEU
1	G	63	ARG
1	G	72	GLU
1	G	82	ASP
1	G	101	ILE
1	G	114	GLN
1	G	129	ARG
1	G	133	THR
1	G	144	MSE
1	G	158	GLU
1	H	12	SER

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Mol	Chain	Res	Type
1	H	49	LEU
1	H	77	ARG
1	H	87	MSE
1	H	88	GLU
1	H	101	ILE
1	H	109	SER
1	H	129	ARG
1	H	169	ARG
1	H	175	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	76	GLN
1	C	76	GLN
1	D	64	ASN
1	D	76	GLN
1	E	34	ASN
1	E	114	GLN
1	F	76	GLN
1	F	78	HIS
1	G	78	HIS
1	H	78	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 95^{th} 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	178/192 (92%)	0.03	2 (1%) 80 79	14, 33, 47, 58	0
1	B	178/192 (92%)	-0.09	2 (1%) 80 79	13, 32, 49, 57	0
1	C	178/192 (92%)	0.12	4 (2%) 62 57	14, 32, 56, 63	0
1	D	178/192 (92%)	0.36	8 (4%) 33 30	13, 39, 62, 69	0
1	E	178/192 (92%)	0.18	5 (2%) 53 49	15, 34, 59, 66	0
1	F	178/192 (92%)	0.66	21 (11%) 4 3	14, 43, 84, 93	0
1	G	178/192 (92%)	0.02	3 (1%) 70 67	13, 32, 51, 58	0
1	H	178/192 (92%)	0.10	4 (2%) 62 57	9, 31, 48, 57	0
All	All	1424/1536 (92%)	0.17	49 (3%) 45 41	9, 34, 60, 93	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	186	VAL	8.1
1	F	7	PHE	7.3
1	F	13	VAL	5.9
1	G	186	VAL	4.7
1	B	186	VAL	4.6
1	H	186	VAL	4.6
1	F	8	ILE	4.5
1	C	168	ASP	4.3
1	F	3	PRO	4.0
1	F	5	ASP	3.9
1	F	6	GLU	3.9
1	E	168	ASP	3.9
1	E	186	VAL	3.9
1	F	14	PRO	3.8
1	F	2	ILE	3.7
1	D	9	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	11	PRO	3.7
1	D	186	VAL	3.6
1	F	43	GLY	3.6
1	E	167	LEU	3.4
1	D	13	VAL	3.3
1	F	9	LYS	3.3
1	A	186	VAL	3.3
1	F	186	VAL	3.0
1	F	110	GLY	3.0
1	D	169	ARG	3.0
1	E	169	ARG	2.9
1	F	168	ASP	2.8
1	D	88	GLU	2.7
1	E	7	PHE	2.6
1	H	32	GLY	2.5
1	F	80	LEU	2.5
1	G	185	GLY	2.5
1	F	77	ARG	2.5
1	F	71	THR	2.4
1	G	142	GLU	2.4
1	D	168	ASP	2.4
1	B	168	ASP	2.3
1	C	169	ARG	2.3
1	F	49	LEU	2.2
1	F	4	ASP	2.2
1	F	137	LEU	2.2
1	C	185	GLY	2.2
1	H	64	ASN	2.1
1	F	79	GLY	2.1
1	H	110	GLY	2.1
1	D	167	LEU	2.1
1	A	168	ASP	2.1
1	D	109	SER	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 monosaccharides in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.