Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:36 PM GMT

PDB ID	:	1L3I
Title	:	MT0146, THE PRECORRIN-6Y METHYLTRANSFERASE (CBIT) HOMOLOG FROM M. THERMOAUTOTROPHICUM, ADOHCY BINARY COMPLEX
Authors	:	Keller, J.P.; Smith, P.M.; Benach, J.; Christendat, D.; deTitta, G.; Hunt, J.F.
Deposited on	:	2002-02-27
Resolution	:	1.95 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

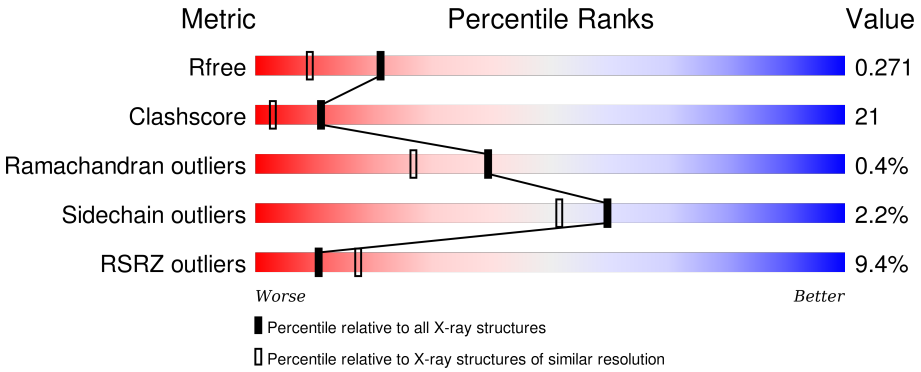
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.95 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	6% 75% 20%
1	B	192	9% 72% 22%
1	C	192	8% 67% 28%
1	D	192	7% 69% 27%
1	E	192	7% 76% 20%

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Mol	Chain	Length	Quality of chain
1	F	192	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9235 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			

There are 48 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
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

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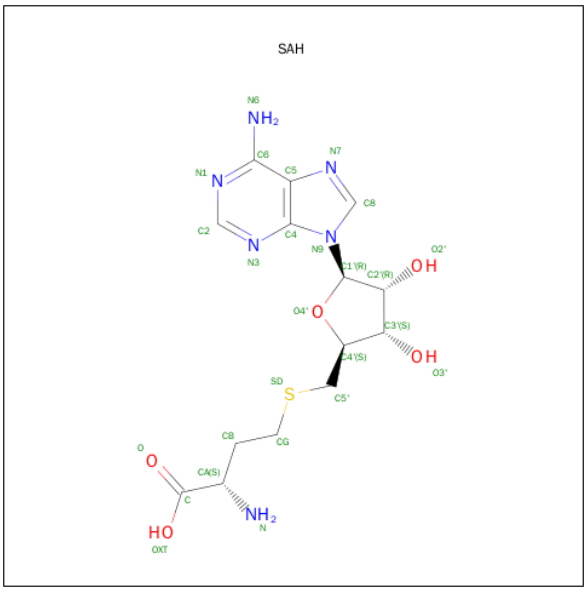
Chain	Residue	Modelled	Actual	Comment	Reference
C	19	MSE	MET	MODIFIED RESIDUE	UNP O26249
C	26	MSE	MET	MODIFIED RESIDUE	UNP O26249
C	73	MSE	MET	MODIFIED RESIDUE	UNP O26249
C	87	MSE	MET	MODIFIED RESIDUE	UNP O26249
C	144	MSE	MET	MODIFIED RESIDUE	UNP O26249
C	172	MSE	MET	MODIFIED RESIDUE	UNP O26249
C	173	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

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O S 26 14 6 5 1	0	0
2	B	1	Total C N O S 26 14 6 5 1	0	0
2	C	1	Total C N O S 26 14 6 5 1	0	0
2	D	1	Total C N O S 26 14 6 5 1	0	0
2	E	1	Total C N O S 26 14 6 5 1	0	0
2	F	1	Total C N O S 26 14 6 5 1	0	0

- Molecule 3 is water.

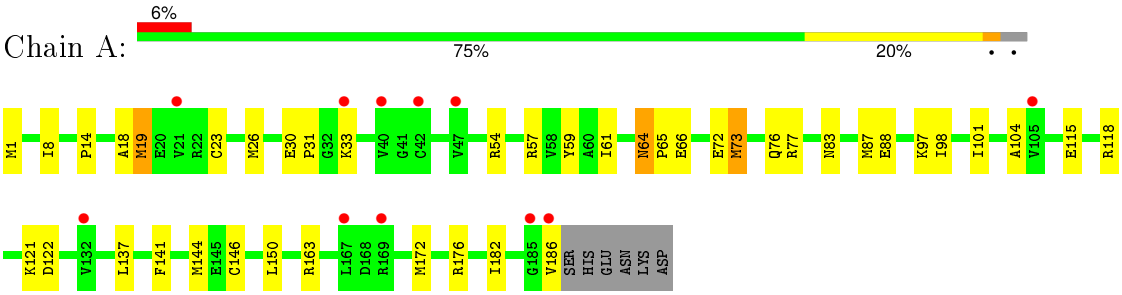
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	133	Total O 133 133	0	0
3	B	117	Total O 117 117	0	0
3	C	144	Total O 144 144	0	0
3	D	134	Total O 134 134	0	0
3	E	103	Total O 103 103	0	0
3	F	96	Total O 96 96	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

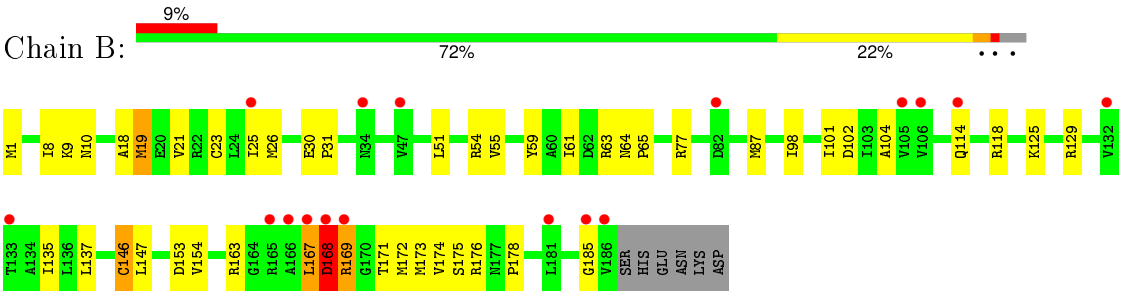
- Molecule 1: Precorrin-6y methyltransferase/putative decarboxylase

Chain A:



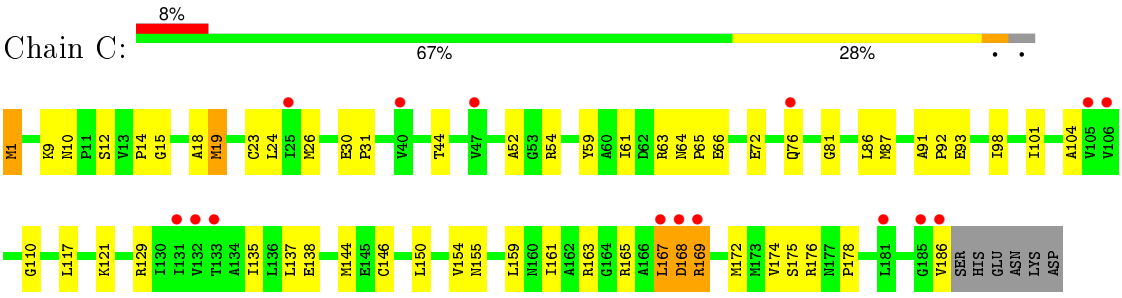
- Molecule 1: Precorrin-6y methyltransferase/putative decarboxylase

Chain B:



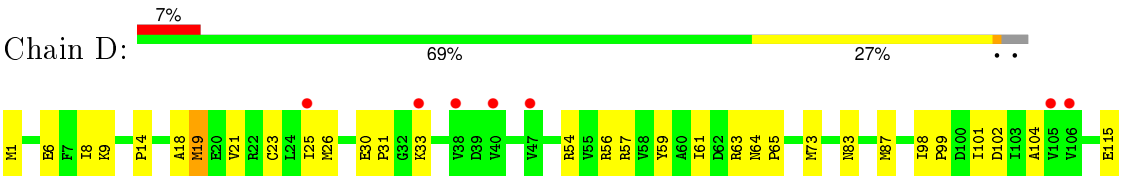
- Molecule 1: Precorrin-6y methyltransferase/putative decarboxylase

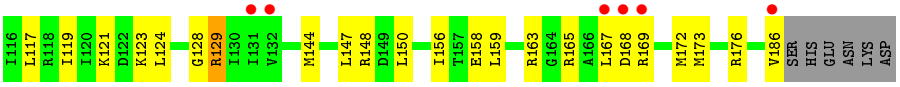
Chain C:



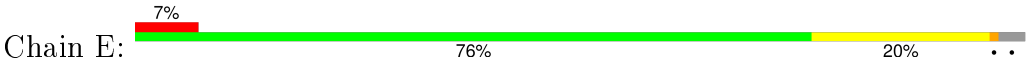
- Molecule 1: Precorrin-6y methyltransferase/putative decarboxylase

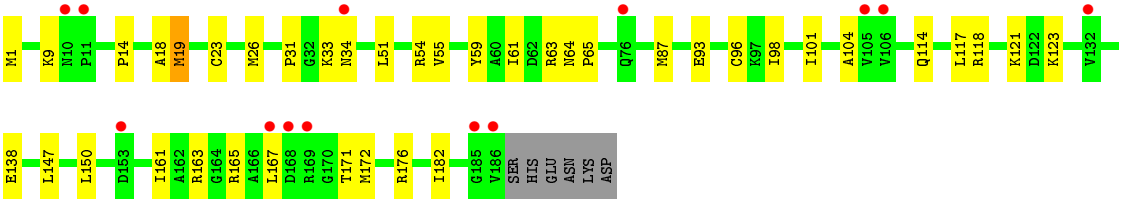
Chain D:



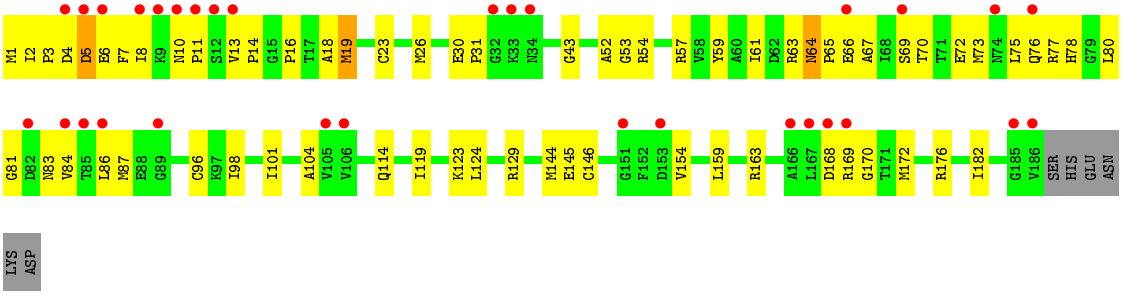


• Molecule 1: Precorrin-6y methyltransferase/putative decarboxylase





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



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	141.10Å 59.40Å 165.90Å 90.00° 109.90° 90.00°	Depositor
Resolution (Å)	26.17 – 1.95 26.17 – 1.95	Depositor EDS
% Data completeness (in resolution range)	(Not available) (26.17-1.95) 87.2 (26.17-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 1.95Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.212 , 0.257 0.227 , 0.271	Depositor DCC
R_{free} test set	4160 reflections (5.04%)	DCC
Wilson B-factor (Å^2)	34.7	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 52.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 91884 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	9235	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.19% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: SAH

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	0.49	0/1400	0.72	1/1882 (0.1%)
1	B	0.48	0/1400	0.74	0/1882
1	C	0.49	0/1400	0.71	0/1882
1	D	0.48	0/1400	0.71	0/1882
1	E	0.48	0/1400	0.70	0/1882
1	F	0.47	0/1400	0.72	0/1882
All	All	0.48	0/8400	0.72	1/11292 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	122	ASP	CB-CG-OD1	5.62	123.36	118.30

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	1435	55	0
1	B	1392	0	1435	58	0
1	C	1392	0	1435	75	0
1	D	1392	0	1435	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1392	0	1435	51	0
1	F	1392	0	1435	75	0
2	A	26	0	19	1	0
2	B	26	0	19	0	0
2	C	26	0	19	2	0
2	D	26	0	19	2	0
2	E	26	0	19	2	0
2	F	26	0	19	3	0
3	A	133	0	0	13	0
3	B	117	0	0	13	0
3	C	144	0	0	19	0
3	D	134	0	0	16	0
3	E	103	0	0	12	0
3	F	96	0	0	21	0
All	All	9235	0	8724	358	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 21.

All (358) 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:F:1:MSE:HG3	1:F:19:MSE:HE3	1.21	1.15
1:D:1:MSE:HG3	1:D:19:MSE:HE3	1.29	1.15
1:E:1:MSE:HG3	1:E:19:MSE:HE3	1.35	1.09
1:B:1:MSE:HG3	1:B:19:MSE:HE3	1.33	1.06
1:A:1:MSE:HG3	1:A:19:MSE:HE3	1.04	1.03
1:D:163:ARG:CZ	1:D:176:ARG:HH21	1.80	0.95
1:A:163:ARG:CZ	1:A:176:ARG:HH21	1.80	0.94
1:A:1:MSE:HG3	1:A:19:MSE:CE	1.97	0.94
1:E:163:ARG:CZ	1:E:176:ARG:HH21	1.80	0.94
1:B:19:MSE:HE2	1:B:23:CYS:HB2	1.50	0.93
1:B:163:ARG:CZ	1:B:176:ARG:HH21	1.80	0.93
1:F:19:MSE:HE2	1:F:23:CYS:HB2	1.51	0.93
1:D:19:MSE:HE2	1:D:23:CYS:HB2	1.50	0.92
1:A:19:MSE:HE2	1:A:23:CYS:HB2	1.49	0.92
1:F:163:ARG:CZ	1:F:176:ARG:HH21	1.81	0.92
1:E:19:MSE:HE2	1:E:23:CYS:HB2	1.52	0.91
1:C:163:ARG:CZ	1:C:176:ARG:HH21	1.82	0.90
1:A:146:CYS:HB3	3:A:903:HOH:O	1.72	0.89
1:B:19:MSE:CE	1:B:23:CYS:HB2	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ALA:HB1	1:C:176:ARG:HH11	1.41	0.86
1:E:19:MSE:CE	1:E:23:CYS:HB2	2.06	0.86
1:C:19:MSE:HE2	1:C:23:CYS:HB2	1.55	0.86
1:F:19:MSE:CE	1:F:23:CYS:HB2	2.06	0.85
1:C:19:MSE:CE	1:C:23:CYS:HB2	2.06	0.85
1:A:19:MSE:CE	1:A:23:CYS:HB2	2.06	0.85
1:A:18:ALA:HB1	1:A:176:ARG:HH11	1.39	0.85
1:D:19:MSE:CE	1:D:23:CYS:HB2	2.07	0.84
1:C:138:GLU:HB3	3:C:917:HOH:O	1.78	0.83
1:B:18:ALA:HB1	1:B:176:ARG:HH11	1.43	0.82
1:F:18:ALA:HB1	1:F:176:ARG:HH11	1.45	0.82
1:D:18:ALA:HB1	1:D:176:ARG:HH11	1.43	0.81
1:D:59:TYR:HB3	1:D:87:MSE:HE2	1.63	0.81
1:A:1:MSE:CG	1:A:19:MSE:HE3	2.00	0.81
1:E:18:ALA:HB1	1:E:176:ARG:HH11	1.45	0.81
1:D:8:ILE:HD12	3:D:901:HOH:O	1.81	0.80
1:F:124:LEU:HD11	3:F:877:HOH:O	1.80	0.80
1:F:1:MSE:CG	1:F:19:MSE:HE3	2.09	0.80
1:C:54:ARG:HD3	3:C:863:HOH:O	1.81	0.80
1:A:59:TYR:HB3	1:A:87:MSE:HE2	1.62	0.80
1:F:1:MSE:HG3	1:F:19:MSE:CE	2.07	0.79
1:C:59:TYR:HB3	1:C:87:MSE:HE2	1.64	0.79
1:C:76:GLN:HB3	3:C:845:HOH:O	1.84	0.78
1:B:59:TYR:HB3	1:B:87:MSE:HE2	1.65	0.78
1:E:59:TYR:HB3	1:E:87:MSE:HE2	1.64	0.78
1:C:9:LYS:HG2	3:C:912:HOH:O	1.84	0.77
1:F:59:TYR:HB3	1:F:87:MSE:HE2	1.67	0.77
1:F:75:LEU:HD22	3:F:871:HOH:O	1.85	0.76
1:D:8:ILE:HG23	3:D:901:HOH:O	1.85	0.75
1:A:144:MSE:HE2	1:C:137:LEU:HD23	1.68	0.75
1:F:10:ASN:ND2	1:F:11:PRO:HD2	2.02	0.74
1:C:52:ALA:HB1	3:C:891:HOH:O	1.87	0.73
1:A:1:MSE:HE2	1:A:54:ARG:HH22	1.53	0.73
1:D:1:MSE:CG	1:D:19:MSE:HE3	2.15	0.73
1:F:26:MSE:HE3	1:F:31:PRO:HG2	1.70	0.72
1:D:1:MSE:HG3	1:D:19:MSE:CE	2.15	0.71
1:C:93:GLU:HB2	3:C:926:HOH:O	1.89	0.71
1:B:26:MSE:CE	1:B:54:ARG:HD2	2.20	0.71
1:A:66:GLU:HG3	3:A:892:HOH:O	1.89	0.71
1:E:114:GLN:HB2	3:E:814:HOH:O	1.91	0.71
1:F:14:PRO:HG2	2:F:806:SAH:SD	2.30	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ALA:HB1	1:A:176:ARG:NH1	2.05	0.70
1:C:26:MSE:CE	1:C:54:ARG:HD2	2.21	0.70
1:D:59:TYR:HB3	1:D:87:MSE:CE	2.22	0.70
1:A:18:ALA:CB	1:A:176:ARG:HH11	2.04	0.70
1:D:156:ILE:HG12	3:D:907:HOH:O	1.92	0.70
1:C:14:PRO:HG2	2:C:803:SAH:SD	2.31	0.70
1:F:101:ILE:HD12	1:F:104:ALA:HB2	1.74	0.69
1:C:59:TYR:HB3	1:C:87:MSE:CE	2.21	0.69
1:B:77:ARG:HD2	3:B:916:HOH:O	1.91	0.69
1:C:26:MSE:HE3	1:C:54:ARG:HD2	1.75	0.69
1:A:59:TYR:HB3	1:A:87:MSE:CE	2.22	0.69
1:A:101:ILE:HD12	1:A:104:ALA:HB2	1.75	0.69
1:D:14:PRO:HG2	2:D:804:SAH:SD	2.33	0.68
1:F:26:MSE:CE	1:F:54:ARG:HD2	2.23	0.68
1:A:8:ILE:HG13	1:A:73:MSE:HE1	1.75	0.68
1:D:33:LYS:HE2	3:D:911:HOH:O	1.92	0.68
1:A:26:MSE:HE3	1:A:31:PRO:HG2	1.76	0.68
1:C:18:ALA:HB1	1:C:176:ARG:NH1	2.07	0.68
1:B:18:ALA:CB	1:B:176:ARG:HH11	2.07	0.68
1:C:18:ALA:CB	1:C:176:ARG:HH11	2.06	0.68
1:E:101:ILE:HD12	1:E:104:ALA:HB2	1.75	0.68
1:E:59:TYR:HB3	1:E:87:MSE:CE	2.24	0.68
1:B:178:PRO:HD3	1:C:175:SER:HB3	1.75	0.68
1:E:14:PRO:HG2	2:E:805:SAH:SD	2.33	0.68
1:A:26:MSE:CE	1:A:54:ARG:HD2	2.24	0.68
1:B:18:ALA:HB1	1:B:176:ARG:NH1	2.08	0.68
1:B:26:MSE:HE3	1:B:54:ARG:HD2	1.75	0.67
1:A:1:MSE:CE	1:A:54:ARG:HH22	2.07	0.67
3:C:867:HOH:O	1:D:30:GLU:HG2	1.95	0.67
1:D:18:ALA:CB	1:D:176:ARG:HH11	2.08	0.67
1:B:153:ASP:HB2	3:B:911:HOH:O	1.94	0.67
1:D:18:ALA:HB1	1:D:176:ARG:NH1	2.09	0.67
1:E:26:MSE:HE3	1:E:31:PRO:HG2	1.76	0.67
1:E:26:MSE:HE3	1:E:54:ARG:HD2	1.77	0.67
1:E:26:MSE:CE	1:E:54:ARG:HD2	2.25	0.67
1:D:26:MSE:HE3	1:D:54:ARG:HD2	1.76	0.67
1:D:26:MSE:CE	1:D:54:ARG:HD2	2.24	0.66
1:C:101:ILE:HD12	1:C:104:ALA:HB2	1.78	0.66
1:F:8:ILE:HG13	1:F:77:ARG:NH1	2.10	0.66
1:B:59:TYR:HB3	1:B:87:MSE:CE	2.25	0.66
1:F:18:ALA:HB1	1:F:176:ARG:NH1	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:18:ALA:CB	1:F:176:ARG:HH11	2.09	0.65
1:F:86:LEU:HD13	3:F:878:HOH:O	1.95	0.65
1:B:26:MSE:HE3	1:B:31:PRO:HG2	1.77	0.65
1:A:73:MSE:HE3	1:E:96:CYS:SG	2.37	0.65
1:F:59:TYR:HB3	1:F:87:MSE:CE	2.25	0.65
1:E:64:ASN:HD22	1:E:65:PRO:HD2	1.62	0.65
1:B:101:ILE:HD12	1:B:104:ALA:HB2	1.79	0.64
1:B:64:ASN:HD22	1:B:65:PRO:HD2	1.61	0.64
1:D:26:MSE:HE3	1:D:31:PRO:HG2	1.78	0.64
1:D:101:ILE:HD12	1:D:104:ALA:HB2	1.79	0.64
1:A:115:GLU:HB2	3:A:887:HOH:O	1.98	0.64
1:A:137:LEU:HD23	1:C:144:MSE:HE2	1.80	0.64
1:C:26:MSE:HE3	1:C:31:PRO:HG2	1.80	0.64
1:C:165:ARG:NH1	1:C:174:VAL:HG21	2.13	0.63
1:F:26:MSE:HE3	1:F:54:ARG:HD2	1.80	0.63
1:F:176:ARG:HG2	3:F:873:HOH:O	1.97	0.63
1:E:18:ALA:HB1	1:E:176:ARG:NH1	2.12	0.63
1:F:13:VAL:HG22	3:F:867:HOH:O	1.99	0.63
1:F:64:ASN:HD22	1:F:65:PRO:HD2	1.63	0.63
1:E:18:ALA:CB	1:E:176:ARG:HH11	2.10	0.63
3:A:896:HOH:O	1:B:30:GLU:HG2	1.98	0.62
1:C:44:THR:HG21	3:C:912:HOH:O	2.00	0.62
1:F:86:LEU:HD22	3:F:878:HOH:O	1.98	0.62
1:E:171:THR:HG21	1:F:144:MSE:HE1	1.80	0.62
1:A:33:LYS:HG3	3:A:934:HOH:O	1.98	0.62
1:F:84:VAL:HG21	3:F:871:HOH:O	1.99	0.62
1:A:87:MSE:HE1	1:A:98:ILE:HG21	1.82	0.62
1:B:9:LYS:HD2	3:B:892:HOH:O	2.00	0.61
1:F:87:MSE:HE1	1:F:98:ILE:HG21	1.80	0.61
1:D:102:ASP:HB3	3:D:871:HOH:O	2.00	0.61
1:C:81:GLY:N	3:C:891:HOH:O	2.33	0.61
1:C:161:ILE:HG12	1:D:159:LEU:CD2	2.31	0.60
1:F:69:SER:O	1:F:72:GLU:HG2	2.01	0.60
1:A:26:MSE:HE3	1:A:54:ARG:HD2	1.82	0.60
1:E:165:ARG:HD3	3:E:862:HOH:O	2.01	0.60
1:C:168:ASP:O	1:C:169:ARG:HG3	2.01	0.60
1:B:87:MSE:HE1	1:B:98:ILE:HG21	1.83	0.60
1:E:61:ILE:HG12	1:E:87:MSE:HE3	1.84	0.59
1:D:87:MSE:HE1	1:D:98:ILE:HG21	1.84	0.59
1:F:146:CYS:HB2	3:F:874:HOH:O	2.03	0.59
1:B:135:ILE:HD12	1:C:172:MSE:CE	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:LYS:HD2	1:D:150:LEU:HB3	1.83	0.59
1:F:8:ILE:HG13	1:F:77:ARG:HH11	1.67	0.59
1:C:87:MSE:HE1	1:C:98:ILE:HG21	1.86	0.58
1:B:135:ILE:HD12	1:C:172:MSE:HE2	1.85	0.58
1:E:61:ILE:CG1	1:E:87:MSE:HE3	2.32	0.58
1:A:72:GLU:HG3	3:E:906:HOH:O	2.03	0.58
1:A:14:PRO:HG2	2:A:801:SAH:SD	2.43	0.58
1:E:167:LEU:HD22	1:E:172:MSE:HE3	1.86	0.58
1:A:18:ALA:CB	1:A:176:ARG:NH1	2.66	0.58
1:C:1:MSE:N	3:C:867:HOH:O	2.36	0.58
1:B:8:ILE:HD11	3:B:916:HOH:O	2.04	0.58
1:F:67:ALA:HB2	3:F:867:HOH:O	2.03	0.57
1:B:185:GLY:HA3	3:B:914:HOH:O	2.03	0.57
1:B:174:VAL:N	3:B:813:HOH:O	2.36	0.57
1:E:9:LYS:HD3	3:E:882:HOH:O	2.05	0.57
1:B:61:ILE:CG1	1:B:87:MSE:HE3	2.35	0.57
1:C:1:MSE:HG2	1:C:19:MSE:HE3	1.85	0.57
1:D:8:ILE:HG21	1:D:73:MSE:SE	2.55	0.57
1:A:76:GLN:HE22	1:E:96:CYS:HB3	1.69	0.57
1:A:64:ASN:HD22	1:A:65:PRO:HD2	1.70	0.56
1:B:1:MSE:HA	3:B:831:HOH:O	2.03	0.56
1:C:30:GLU:HG2	3:D:872:HOH:O	2.06	0.56
1:E:176:ARG:HG3	3:E:810:HOH:O	2.04	0.56
1:A:65:PRO:HD2	3:A:891:HOH:O	2.05	0.56
1:C:72:GLU:HG2	1:C:86:LEU:CD1	2.35	0.56
1:F:81:GLY:HA2	3:F:871:HOH:O	2.05	0.56
1:D:129:ARG:HG2	1:D:186:VAL:HG22	1.87	0.56
1:A:8:ILE:HG13	1:A:73:MSE:CE	2.36	0.56
1:F:61:ILE:HG12	1:F:87:MSE:HE3	1.87	0.56
1:F:10:ASN:HD22	1:F:11:PRO:HD2	1.69	0.56
1:C:186:VAL:HG13	3:C:862:HOH:O	2.05	0.56
1:C:186:VAL:HG23	3:C:847:HOH:O	2.06	0.56
1:F:168:ASP:C	1:F:170:GLY:H	2.08	0.56
1:F:61:ILE:CG1	1:F:87:MSE:HE3	2.36	0.55
1:F:163:ARG:CZ	1:F:176:ARG:NH2	2.63	0.55
1:B:61:ILE:HG12	1:B:87:MSE:HE3	1.88	0.55
1:C:18:ALA:CB	1:C:176:ARG:NH1	2.69	0.55
1:A:30:GLU:HG2	3:B:885:HOH:O	2.07	0.55
1:E:87:MSE:HE1	1:E:98:ILE:HG21	1.87	0.55
1:C:110:GLY:HA3	3:C:934:HOH:O	2.06	0.55
1:E:54:ARG:NE	3:E:896:HOH:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:18:ALA:CB	1:D:176:ARG:NH1	2.70	0.55
1:D:61:ILE:CG1	1:D:87:MSE:HE3	2.37	0.54
1:A:163:ARG:CZ	1:A:176:ARG:NH2	2.62	0.54
1:C:163:ARG:CZ	1:C:176:ARG:NH2	2.64	0.54
1:B:1:MSE:N	3:B:885:HOH:O	2.41	0.54
1:E:176:ARG:HG2	3:E:866:HOH:O	2.08	0.54
1:B:18:ALA:CB	1:B:176:ARG:NH1	2.69	0.54
1:A:73:MSE:HG3	1:E:93:GLU:HA	1.89	0.54
1:E:1:MSE:HG3	1:E:19:MSE:CE	2.23	0.54
1:A:61:ILE:CG1	1:A:87:MSE:HE3	2.38	0.54
1:E:33:LYS:HE2	3:E:908:HOH:O	2.08	0.53
1:B:172:MSE:HE2	1:C:135:ILE:HD12	1.89	0.53
1:E:163:ARG:CZ	1:E:176:ARG:NH2	2.63	0.53
1:A:121:LYS:HD2	1:A:150:LEU:HB3	1.90	0.53
1:E:1:MSE:CG	1:E:19:MSE:HE3	2.25	0.53
1:A:141:PHE:HB2	3:A:855:HOH:O	2.08	0.53
1:D:63:ARG:HG3	2:D:804:SAH:C2	2.39	0.53
1:C:1:MSE:HG2	1:C:19:MSE:HG2	1.89	0.53
1:C:19:MSE:HE1	1:C:23:CYS:HB2	1.90	0.53
1:C:63:ARG:HG3	2:C:803:SAH:C2	2.38	0.53
1:F:18:ALA:CB	1:F:176:ARG:NH1	2.72	0.53
1:F:4:ASP:HB2	1:F:16:PRO:HG2	1.91	0.52
1:B:1:MSE:CG	1:B:19:MSE:HE3	2.23	0.52
1:F:70:THR:HA	1:F:73:MSE:HE3	1.92	0.52
1:C:61:ILE:CG1	1:C:87:MSE:HE3	2.40	0.52
1:F:4:ASP:HA	1:F:7:PHE:HD1	1.74	0.52
1:D:57:ARG:HD3	1:D:83:ASN:O	2.09	0.52
1:C:92:PRO:HD2	3:C:812:HOH:O	2.09	0.52
1:F:145:GLU:HB3	3:F:842:HOH:O	2.09	0.52
1:C:167:LEU:O	1:C:169:ARG:N	2.44	0.51
1:E:19:MSE:HE1	1:E:23:CYS:HB2	1.91	0.51
1:A:61:ILE:HG12	1:A:87:MSE:HE3	1.92	0.51
1:B:147:LEU:HB2	1:B:154:VAL:HG11	1.92	0.51
1:A:1:MSE:HE2	1:A:54:ARG:NH2	2.25	0.51
1:A:76:GLN:NE2	1:E:96:CYS:HB3	2.25	0.51
1:C:1:MSE:HB3	3:C:816:HOH:O	2.11	0.51
1:B:19:MSE:HE1	1:B:23:CYS:HB2	1.92	0.50
1:A:144:MSE:HE2	1:C:137:LEU:CD2	2.38	0.50
1:D:61:ILE:HG12	1:D:87:MSE:HE3	1.93	0.50
1:D:163:ARG:CZ	1:D:176:ARG:NH2	2.62	0.50
1:F:145:GLU:HB2	3:F:864:HOH:O	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:SER:HB3	1:C:178:PRO:HD3	1.94	0.49
1:E:18:ALA:CB	1:E:176:ARG:NH1	2.73	0.49
1:F:43:GLY:HA3	2:F:806:SAH:HB1	1.95	0.49
1:F:101:ILE:HG13	1:F:124:LEU:HD12	1.95	0.49
1:E:34:ASN:HB3	3:E:842:HOH:O	2.13	0.49
1:F:76:GLN:HA	1:F:76:GLN:OE1	2.12	0.49
1:C:167:LEU:HD13	1:C:172:MSE:SE	2.63	0.49
1:C:1:MSE:CE	1:C:54:ARG:HH22	2.26	0.48
1:C:129:ARG:HG2	1:C:186:VAL:HG22	1.95	0.48
1:F:80:LEU:HD13	3:F:899:HOH:O	2.13	0.48
1:E:121:LYS:HD2	1:E:150:LEU:HB3	1.96	0.48
1:C:146:CYS:HB2	3:C:913:HOH:O	2.13	0.48
1:D:165:ARG:HD3	3:D:917:HOH:O	2.12	0.48
1:C:72:GLU:CG	1:C:86:LEU:HD13	2.44	0.47
1:D:119:ILE:O	1:D:123:LYS:HG3	2.14	0.47
1:D:169:ARG:HG2	1:D:169:ARG:O	2.15	0.47
1:C:9:LYS:HE3	1:C:15:GLY:O	2.14	0.47
1:E:138:GLU:HB3	3:E:880:HOH:O	2.13	0.47
1:B:63:ARG:NH1	3:B:896:HOH:O	2.48	0.47
1:F:19:MSE:HE1	1:F:23:CYS:HB2	1.94	0.46
1:F:163:ARG:NH2	1:F:176:ARG:HH21	2.11	0.46
1:F:75:LEU:HA	1:F:75:LEU:HD23	1.75	0.46
1:F:168:ASP:O	1:F:169:ARG:HB2	2.14	0.46
1:E:98:ILE:HG13	1:E:123:LYS:HE2	1.98	0.46
1:D:117:LEU:HD22	1:D:147:LEU:HD21	1.98	0.46
1:A:1:MSE:N	3:A:896:HOH:O	2.48	0.46
1:E:161:ILE:HG12	1:F:159:LEU:CD2	2.46	0.46
1:F:96:CYS:HA	3:F:837:HOH:O	2.15	0.46
1:F:53:GLY:N	3:F:899:HOH:O	2.48	0.46
1:C:10:ASN:ND2	1:C:66:GLU:HB3	2.31	0.46
1:B:26:MSE:CE	1:B:31:PRO:HG2	2.45	0.46
1:E:63:ARG:HG3	2:E:805:SAH:C2	2.46	0.46
1:D:168:ASP:O	1:D:169:ARG:HB3	2.14	0.46
1:F:63:ARG:HG3	2:F:806:SAH:C2	2.45	0.45
1:A:57:ARG:HD3	1:A:83:ASN:O	2.16	0.45
1:A:88:GLU:HB2	3:A:929:HOH:O	2.15	0.45
1:E:163:ARG:NH2	1:E:176:ARG:HH21	2.13	0.45
1:D:6:GLU:HA	3:D:925:HOH:O	2.16	0.45
1:C:61:ILE:HG12	1:C:87:MSE:HE3	1.98	0.45
1:F:66:GLU:O	1:F:69:SER:HB3	2.16	0.45
1:D:99:PRO:HG3	3:D:851:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ASP:O	1:B:169:ARG:CB	2.65	0.45
1:F:57:ARG:HD3	1:F:83:ASN:O	2.17	0.45
1:F:54:ARG:NE	3:F:879:HOH:O	2.50	0.45
1:F:3:PRO:C	1:F:5:ASP:H	2.21	0.44
1:B:163:ARG:N	3:B:813:HOH:O	2.51	0.44
1:F:26:MSE:CE	1:F:31:PRO:HG2	2.42	0.44
1:D:172:MSE:HB2	1:D:172:MSE:HE3	1.78	0.44
3:A:860:HOH:O	1:D:172:MSE:HE1	2.16	0.44
1:F:6:GLU:HB3	1:F:78:HIS:CE1	2.53	0.44
1:B:167:LEU:HD12	1:B:167:LEU:HA	1.87	0.44
1:A:73:MSE:HE2	1:A:77:ARG:HD3	1.99	0.44
1:F:144:MSE:SE	1:F:154:VAL:HG12	2.68	0.44
1:B:137:LEU:HD23	1:D:144:MSE:HE2	1.99	0.44
1:D:64:ASN:HD22	1:D:65:PRO:HD2	1.83	0.44
1:B:163:ARG:CZ	1:B:176:ARG:NH2	2.63	0.44
1:C:1:MSE:CG	1:C:19:MSE:HE3	2.48	0.44
1:A:172:MSE:HB2	1:A:172:MSE:HE3	1.94	0.44
1:B:21:VAL:O	1:B:25:ILE:HG13	2.18	0.44
1:A:26:MSE:CE	1:A:31:PRO:HG2	2.46	0.43
1:D:56:ARG:O	1:D:83:ASN:HB2	2.18	0.43
1:D:167:LEU:HD22	1:D:172:MSE:SE	2.68	0.43
1:A:163:ARG:NH2	1:A:176:ARG:HH21	2.12	0.43
1:C:19:MSE:O	1:C:19:MSE:HE2	2.18	0.43
1:D:158:GLU:HB2	3:D:907:HOH:O	2.18	0.43
1:F:72:GLU:O	1:F:76:GLN:HG2	2.18	0.43
1:C:12:SER:HB2	3:C:875:HOH:O	2.18	0.43
1:F:182:ILE:HD12	1:F:182:ILE:N	2.34	0.43
1:F:2:ILE:HG13	3:F:869:HOH:O	2.18	0.43
1:D:148:ARG:NH2	3:D:935:HOH:O	2.52	0.43
1:C:26:MSE:CE	1:C:31:PRO:HG2	2.48	0.43
1:B:114:GLN:HG3	1:B:146:CYS:SG	2.58	0.43
1:B:102:ASP:OD1	1:B:125:LYS:HD2	2.18	0.43
1:C:24:LEU:HD23	1:C:159:LEU:HD11	2.01	0.43
1:F:78:HIS:O	1:F:80:LEU:HG	2.18	0.43
1:B:1:MSE:HG3	1:B:19:MSE:CE	2.24	0.43
1:D:129:ARG:NH2	3:D:871:HOH:O	2.47	0.43
1:C:91:ALA:HB3	1:C:92:PRO:HD3	2.01	0.43
1:D:19:MSE:HE1	1:D:23:CYS:HB2	1.96	0.42
1:F:4:ASP:HA	1:F:7:PHE:CD1	2.52	0.42
1:C:64:ASN:HD22	1:C:65:PRO:HD2	1.82	0.42
1:B:9:LYS:HG2	1:B:10:ASN:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:129:ARG:CG	1:C:186:VAL:HG22	2.49	0.42
1:D:64:ASN:HA	1:D:65:PRO:HD2	1.96	0.42
1:D:165:ARG:NH2	3:D:884:HOH:O	2.40	0.42
1:C:163:ARG:NH2	1:C:176:ARG:HH21	2.14	0.42
1:F:52:ALA:HB3	3:F:899:HOH:O	2.19	0.42
1:F:80:LEU:HA	3:F:838:HOH:O	2.19	0.42
1:D:26:MSE:CE	1:D:31:PRO:HG2	2.47	0.42
1:D:9:LYS:HD3	3:D:905:HOH:O	2.19	0.42
1:B:118:ARG:NH1	3:B:884:HOH:O	2.53	0.42
1:E:1:MSE:HB3	1:E:1:MSE:HE3	1.95	0.42
1:C:63:ARG:NH1	3:C:934:HOH:O	2.53	0.42
1:C:72:GLU:CG	1:C:86:LEU:CD1	2.98	0.42
1:F:4:ASP:HB2	1:F:16:PRO:CG	2.49	0.42
1:B:19:MSE:HE2	1:B:19:MSE:O	2.20	0.42
1:D:1:MSE:HB3	1:D:1:MSE:HE3	1.96	0.41
1:F:30:GLU:N	1:F:31:PRO:HD3	2.35	0.41
1:B:168:ASP:O	1:B:169:ARG:HG2	2.19	0.41
1:A:118:ARG:NH1	3:A:906:HOH:O	2.51	0.41
1:F:119:ILE:O	1:F:123:LYS:HG3	2.20	0.41
1:B:51:LEU:O	1:B:55:VAL:HG22	2.20	0.41
1:E:51:LEU:O	1:E:55:VAL:HG22	2.21	0.41
1:B:173:MSE:HE3	3:B:813:HOH:O	2.19	0.41
3:A:805:HOH:O	1:D:173:MSE:HB2	2.21	0.41
1:D:115:GLU:HB2	3:D:888:HOH:O	2.20	0.41
1:C:121:LYS:HD2	1:C:150:LEU:HB3	2.03	0.41
1:E:19:MSE:O	1:E:19:MSE:HE2	2.20	0.41
1:C:168:ASP:O	1:C:169:ARG:CG	2.68	0.41
1:F:114:GLN:HB2	3:F:891:HOH:O	2.20	0.41
1:E:182:ILE:HD12	1:E:182:ILE:N	2.36	0.41
1:A:97:LYS:NZ	3:A:877:HOH:O	2.54	0.41
1:E:114:GLN:HG2	1:E:118:ARG:CZ	2.50	0.41
1:C:30:GLU:OE1	1:C:186:VAL:HG21	2.20	0.41
1:B:168:ASP:O	1:B:169:ARG:CG	2.69	0.41
1:B:168:ASP:OD1	1:B:168:ASP:N	2.53	0.41
1:A:1:MSE:CE	1:A:54:ARG:NH2	2.81	0.41
1:D:163:ARG:NH2	1:D:176:ARG:HH21	2.13	0.41
1:E:123:LYS:HE3	3:E:888:HOH:O	2.20	0.41
1:A:144:MSE:HE1	1:B:171:THR:HG21	2.03	0.41
1:D:56:ARG:NH1	3:D:850:HOH:O	2.54	0.41
1:B:147:LEU:HB2	1:B:154:VAL:CG1	2.50	0.41
1:A:182:ILE:N	1:A:182:ILE:HD12	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:LEU:HD22	1:E:147:LEU:HD21	2.02	0.41
1:F:1:MSE:N	3:F:898:HOH:O	2.54	0.40
1:E:33:LYS:HG2	3:E:908:HOH:O	2.20	0.40
1:C:117:LEU:HD23	1:C:117:LEU:HA	1.95	0.40
1:D:21:VAL:O	1:D:25:ILE:HG13	2.20	0.40
1:C:63:ARG:CZ	3:C:934:HOH:O	2.69	0.40
1:C:72:GLU:HG2	1:C:86:LEU:HD11	2.04	0.40
1:B:30:GLU:N	1:B:31:PRO:HD3	2.37	0.40
1:B:64:ASN:HD22	1:B:65:PRO:CD	2.31	0.40
1:D:124:LEU:HD11	1:D:128:GLY:HA3	2.03	0.40
1:C:154:VAL:HG12	1:C:155:ASN:N	2.36	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%)	177 (96%)	7 (4%)	0	100 100
1	B	184/192 (96%)	176 (96%)	6 (3%)	2 (1%)	17 6
1	C	184/192 (96%)	178 (97%)	4 (2%)	2 (1%)	17 6
1	D	184/192 (96%)	179 (97%)	5 (3%)	0	100 100
1	E	184/192 (96%)	180 (98%)	4 (2%)	0	100 100
1	F	184/192 (96%)	179 (97%)	5 (3%)	0	100 100
All	All	1104/1152 (96%)	1069 (97%)	31 (3%)	4 (0%)	39 27

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	169	ARG

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Mol	Chain	Res	Type
1	C	168	ASP
1	C	169	ARG
1	B	168	ASP

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%)	148 (97%)	4 (3%)	54	43
1	B	152/150 (101%)	147 (97%)	5 (3%)	45	32
1	C	152/150 (101%)	149 (98%)	3 (2%)	63	55
1	D	152/150 (101%)	150 (99%)	2 (1%)	76	72
1	E	152/150 (101%)	151 (99%)	1 (1%)	88	88
1	F	152/150 (101%)	147 (97%)	5 (3%)	45	32
All	All	912/900 (101%)	892 (98%)	20 (2%)	60	51

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	MSE
1	A	64	ASN
1	A	73	MSE
1	A	186	VAL
1	B	19	MSE
1	B	129	ARG
1	B	146	CYS
1	B	167	LEU
1	B	168	ASP
1	C	1	MSE
1	C	19	MSE
1	C	167	LEU
1	D	19	MSE
1	D	129	ARG
1	E	19	MSE

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Mol	Chain	Res	Type
1	F	5	ASP
1	F	19	MSE
1	F	64	ASN
1	F	129	ARG
1	F	172	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	76	GLN
1	B	64	ASN
1	C	64	ASN
1	D	64	ASN
1	E	64	ASN
1	F	64	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

6 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	SAH	A	801	-	20,28,28	1.12	2 (10%)	19,40,40	2.04	4 (21%)
2	SAH	B	802	-	20,28,28	1.16	3 (15%)	19,40,40	1.71	4 (21%)
2	SAH	C	803	-	20,28,28	1.25	3 (15%)	19,40,40	2.00	4 (21%)
2	SAH	D	804	-	20,28,28	1.18	2 (10%)	19,40,40	2.00	5 (26%)
2	SAH	E	805	-	20,28,28	1.15	2 (10%)	19,40,40	1.95	4 (21%)
2	SAH	F	806	-	20,28,28	1.36	2 (10%)	19,40,40	1.95	4 (21%)

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	SAH	A	801	-	-	0/7/31/31	0/3/3/3
2	SAH	B	802	-	-	0/7/31/31	0/3/3/3
2	SAH	C	803	-	-	0/7/31/31	0/3/3/3
2	SAH	D	804	-	-	0/7/31/31	0/3/3/3
2	SAH	E	805	-	-	0/7/31/31	0/3/3/3
2	SAH	F	806	-	-	0/7/31/31	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	SAH	C8-N7	-2.80	1.29	1.34
2	F	806	SAH	C8-N7	-2.67	1.29	1.34
2	D	804	SAH	C8-N7	-2.41	1.30	1.34
2	A	801	SAH	C8-N7	-2.24	1.30	1.34
2	C	803	SAH	C8-N7	-2.20	1.30	1.34
2	E	805	SAH	C8-N7	-2.20	1.30	1.34
2	C	803	SAH	O3'-C3'	2.01	1.47	1.43
2	B	802	SAH	O3'-C3'	2.03	1.47	1.43
2	A	801	SAH	C3'-C4'	3.07	1.61	1.53
2	B	802	SAH	C3'-C4'	3.15	1.61	1.53
2	E	805	SAH	C3'-C4'	3.29	1.61	1.53
2	D	804	SAH	C3'-C4'	3.47	1.62	1.53
2	C	803	SAH	C3'-C4'	3.90	1.63	1.53
2	F	806	SAH	C3'-C4'	4.09	1.64	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	SAH	C4'-O4'-C1'	-5.90	103.23	109.72
2	E	805	SAH	C4'-O4'-C1'	-5.87	103.27	109.72
2	C	803	SAH	C4'-O4'-C1'	-5.76	103.39	109.72
2	D	804	SAH	C4'-O4'-C1'	-5.53	103.64	109.72
2	F	806	SAH	C4'-O4'-C1'	-5.00	104.23	109.72
2	B	802	SAH	C4'-O4'-C1'	-4.94	104.29	109.72
2	C	803	SAH	O4'-C1'-N9	-3.37	101.04	108.10
2	F	806	SAH	O4'-C1'-N9	-3.31	101.17	108.10
2	D	804	SAH	O4'-C1'-N9	-3.15	101.50	108.10
2	A	801	SAH	O4'-C1'-N9	-2.99	101.83	108.10
2	B	802	SAH	O4'-C1'-N9	-2.77	102.30	108.10
2	E	805	SAH	O4'-C1'-N9	-2.69	102.47	108.10
2	B	802	SAH	O3'-C3'-C4'	2.03	117.15	111.05
2	D	804	SAH	O2'-C2'-C3'	2.08	118.58	111.83
2	F	806	SAH	O3'-C3'-C4'	2.28	117.90	111.05
2	C	803	SAH	O3'-C3'-C4'	2.39	118.21	111.05
2	A	801	SAH	O3'-C3'-C4'	2.40	118.25	111.05
2	D	804	SAH	C4-C5-N7	2.44	111.72	109.48
2	E	805	SAH	O3'-C3'-C4'	2.59	118.81	111.05
2	B	802	SAH	C2'-C1'-N9	2.70	118.42	114.29
2	E	805	SAH	C2'-C1'-N9	3.16	119.13	114.29
2	C	803	SAH	C2'-C1'-N9	3.35	119.42	114.29
2	D	804	SAH	C2'-C1'-N9	3.54	119.71	114.29
2	A	801	SAH	C2'-C1'-N9	3.57	119.75	114.29
2	F	806	SAH	C2'-C1'-N9	3.85	120.18	114.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	SAH	1	0
2	C	803	SAH	2	0
2	D	804	SAH	2	0
2	E	805	SAH	2	0
2	F	806	SAH	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	0.40	11 (6%)	24	34	22, 36, 57, 89	0
1	B	178/192 (92%)	0.47	17 (9%)	10	16	21, 36, 62, 85	0
1	C	178/192 (92%)	0.63	15 (8%)	14	22	23, 37, 65, 93	0
1	D	178/192 (92%)	0.41	13 (7%)	18	28	21, 36, 56, 78	0
1	E	178/192 (92%)	0.57	13 (7%)	18	28	25, 39, 64, 102	0
1	F	178/192 (92%)	0.94	31 (17%)	2	3	26, 43, 79, 103	0
All	All	1068/1152 (92%)	0.57	100 (9%)	11	17	21, 38, 65, 103	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	186	VAL	9.7
1	F	186	VAL	9.7
1	C	186	VAL	9.0
1	C	168	ASP	8.6
1	A	186	VAL	8.2
1	B	186	VAL	7.6
1	C	185	GLY	7.0
1	D	167	LEU	6.9
1	A	185	GLY	6.8
1	F	185	GLY	6.7
1	F	76	GLN	5.4
1	B	185	GLY	5.1
1	C	167	LEU	5.0
1	B	167	LEU	5.0
1	E	169	ARG	4.9
1	E	168	ASP	4.7
1	E	185	GLY	4.7
1	F	11	PRO	4.5
1	E	167	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	168	ASP	4.4
1	F	33	LYS	4.3
1	F	6	GLU	3.8
1	E	105	VAL	3.8
1	C	169	ARG	3.6
1	E	106	VAL	3.5
1	D	169	ARG	3.5
1	C	105	VAL	3.4
1	F	169	ARG	3.4
1	A	105	VAL	3.4
1	A	33	LYS	3.3
1	F	168	ASP	3.3
1	A	40	VAL	3.3
1	F	8	ILE	3.3
1	E	11	PRO	3.2
1	F	5	ASP	3.2
1	F	106	VAL	3.2
1	F	34	ASN	3.2
1	C	106	VAL	3.1
1	F	10	ASN	3.1
1	F	12	SER	3.0
1	B	166	ALA	3.0
1	D	105	VAL	3.0
1	F	167	LEU	2.9
1	D	168	ASP	2.9
1	F	4	ASP	2.8
1	F	9	LYS	2.8
1	A	169	ARG	2.8
1	B	169	ARG	2.8
1	C	47	VAL	2.7
1	B	105	VAL	2.7
1	B	34	ASN	2.6
1	E	34	ASN	2.6
1	B	106	VAL	2.6
1	F	32	GLY	2.6
1	D	33	LYS	2.6
1	F	82	ASP	2.6
1	F	151	GLY	2.6
1	B	47	VAL	2.6
1	D	40	VAL	2.6
1	D	106	VAL	2.6
1	D	132	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	132	VAL	2.6
1	C	133	THR	2.6
1	F	105	VAL	2.5
1	C	25	ILE	2.5
1	F	86	LEU	2.5
1	D	186	VAL	2.5
1	F	89	GLY	2.4
1	F	74	ASN	2.4
1	D	131	ILE	2.4
1	F	84	VAL	2.4
1	B	165	ARG	2.4
1	A	132	VAL	2.4
1	B	133	THR	2.4
1	D	25	ILE	2.3
1	B	181	LEU	2.3
1	A	47	VAL	2.3
1	D	38	VAL	2.3
1	C	131	ILE	2.3
1	C	132	VAL	2.3
1	F	69	SER	2.3
1	C	40	VAL	2.3
1	A	167	LEU	2.2
1	C	76	GLN	2.2
1	E	10	ASN	2.2
1	C	181	LEU	2.2
1	D	47	VAL	2.2
1	F	166	ALA	2.2
1	B	114	GLN	2.1
1	A	42	CYS	2.1
1	F	153	ASP	2.1
1	E	76	GLN	2.1
1	F	85	THR	2.1
1	B	25	ILE	2.1
1	F	66	GLU	2.1
1	E	153	ASP	2.1
1	B	132	VAL	2.1
1	A	21	VAL	2.0
1	F	13	VAL	2.0
1	B	82	ASP	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SAH	D	804	26/26	0.94	0.10	-0.55	21,28,33,33	0
2	SAH	E	805	26/26	0.94	0.10	-0.55	30,37,40,45	0
2	SAH	B	802	26/26	0.94	0.10	-0.71	18,24,29,32	0
2	SAH	F	806	26/26	0.92	0.10	-0.74	39,47,51,56	0
2	SAH	A	801	26/26	0.96	0.10	-0.76	22,27,32,35	0
2	SAH	C	803	26/26	0.95	0.09	-0.92	21,31,34,35	0

6.5 Other polymers (i)

There are no such residues in this entry.