



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 06:27 PM GMT

PDB ID : 1T57
Title : Crystal Structure of the Conserved Protein MTH1675 from Methanobacterium thermoautotrophicum
Authors : Kim, Y.; Joachimiak, A.; Saridakis, V.; Xu, X.; Arrowsmith, C.H.; Christendat, D.; Edwards, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2004-05-03
Resolution : 2.30 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 ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
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) : rb-20026982

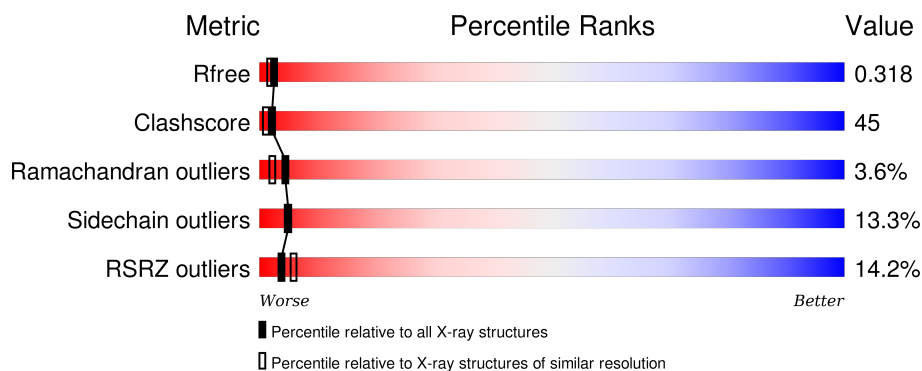
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	3852 (2.30-2.30)
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 $\leq 5\%$. 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	206	
1	B	206	
1	C	206	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	B	303	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4441 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 Conserved Protein MTH1675.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	186	Total	C	N	O	S	Se	0	0	0
			1406	879	247	271	2	7			
1	B	186	Total	C	N	O	S	Se	0	0	0
			1406	879	247	271	2	7			
1	C	186	Total	C	N	O	S	Se	0	0	0
			1406	879	247	271	2	7			

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MSE	-	CLONING ARTIFACT	UNP O27711
A	-18	GLY	-	CLONING ARTIFACT	UNP O27711
A	-17	SER	-	CLONING ARTIFACT	UNP O27711
A	-16	SER	-	CLONING ARTIFACT	UNP O27711
A	-15	HIS	-	CLONING ARTIFACT	UNP O27711
A	-14	HIS	-	CLONING ARTIFACT	UNP O27711
A	-13	HIS	-	CLONING ARTIFACT	UNP O27711
A	-12	HIS	-	CLONING ARTIFACT	UNP O27711
A	-11	HIS	-	CLONING ARTIFACT	UNP O27711
A	-10	HIS	-	CLONING ARTIFACT	UNP O27711
A	-9	SER	-	CLONING ARTIFACT	UNP O27711
A	-8	SER	-	CLONING ARTIFACT	UNP O27711
A	-7	GLY	-	CLONING ARTIFACT	UNP O27711
A	-6	LEU	-	CLONING ARTIFACT	UNP O27711
A	-5	VAL	-	CLONING ARTIFACT	UNP O27711
A	-4	PRO	-	CLONING ARTIFACT	UNP O27711
A	-3	ARG	-	CLONING ARTIFACT	UNP O27711
A	-2	GLY	-	CLONING ARTIFACT	UNP O27711
A	-1	SER	-	CLONING ARTIFACT	UNP O27711
A	0	HIS	-	CLONING ARTIFACT	UNP O27711
A	1	MSE	MET	MODIFIED RESIDUE	UNP O27711
A	51	MSE	MET	MODIFIED RESIDUE	UNP O27711
A	115	MSE	MET	MODIFIED RESIDUE	UNP O27711

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	121	MSE	MET	MODIFIED RESIDUE	UNP O27711
A	135	MSE	MET	MODIFIED RESIDUE	UNP O27711
A	169	MSE	MET	MODIFIED RESIDUE	UNP O27711
A	183	MSE	MET	MODIFIED RESIDUE	UNP O27711
B	-19	MSE	-	CLONING ARTIFACT	UNP O27711
B	-18	GLY	-	CLONING ARTIFACT	UNP O27711
B	-17	SER	-	CLONING ARTIFACT	UNP O27711
B	-16	SER	-	CLONING ARTIFACT	UNP O27711
B	-15	HIS	-	CLONING ARTIFACT	UNP O27711
B	-14	HIS	-	CLONING ARTIFACT	UNP O27711
B	-13	HIS	-	CLONING ARTIFACT	UNP O27711
B	-12	HIS	-	CLONING ARTIFACT	UNP O27711
B	-11	HIS	-	CLONING ARTIFACT	UNP O27711
B	-10	HIS	-	CLONING ARTIFACT	UNP O27711
B	-9	SER	-	CLONING ARTIFACT	UNP O27711
B	-8	SER	-	CLONING ARTIFACT	UNP O27711
B	-7	GLY	-	CLONING ARTIFACT	UNP O27711
B	-6	LEU	-	CLONING ARTIFACT	UNP O27711
B	-5	VAL	-	CLONING ARTIFACT	UNP O27711
B	-4	PRO	-	CLONING ARTIFACT	UNP O27711
B	-3	ARG	-	CLONING ARTIFACT	UNP O27711
B	-2	GLY	-	CLONING ARTIFACT	UNP O27711
B	-1	SER	-	CLONING ARTIFACT	UNP O27711
B	0	HIS	-	CLONING ARTIFACT	UNP O27711
B	1	MSE	MET	MODIFIED RESIDUE	UNP O27711
B	51	MSE	MET	MODIFIED RESIDUE	UNP O27711
B	115	MSE	MET	MODIFIED RESIDUE	UNP O27711
B	121	MSE	MET	MODIFIED RESIDUE	UNP O27711
B	135	MSE	MET	MODIFIED RESIDUE	UNP O27711
B	169	MSE	MET	MODIFIED RESIDUE	UNP O27711
B	183	MSE	MET	MODIFIED RESIDUE	UNP O27711
C	-19	MSE	-	CLONING ARTIFACT	UNP O27711
C	-18	GLY	-	CLONING ARTIFACT	UNP O27711
C	-17	SER	-	CLONING ARTIFACT	UNP O27711
C	-16	SER	-	CLONING ARTIFACT	UNP O27711
C	-15	HIS	-	CLONING ARTIFACT	UNP O27711
C	-14	HIS	-	CLONING ARTIFACT	UNP O27711
C	-13	HIS	-	CLONING ARTIFACT	UNP O27711
C	-12	HIS	-	CLONING ARTIFACT	UNP O27711
C	-11	HIS	-	CLONING ARTIFACT	UNP O27711
C	-10	HIS	-	CLONING ARTIFACT	UNP O27711
C	-9	SER	-	CLONING ARTIFACT	UNP O27711

Continued on next page...

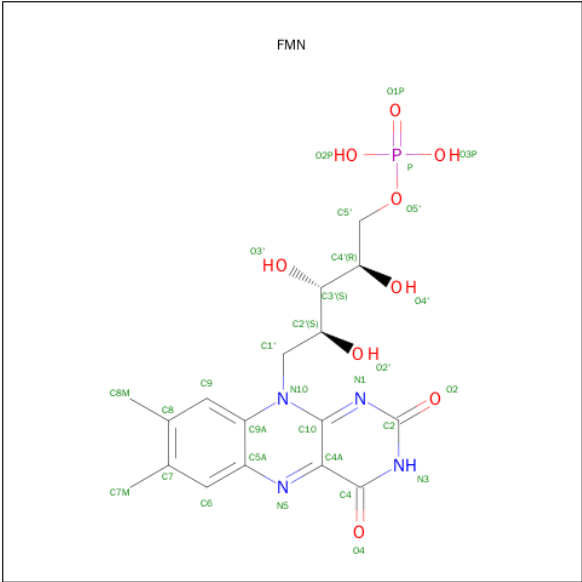
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	SER	-	CLONING ARTIFACT	UNP O27711
C	-7	GLY	-	CLONING ARTIFACT	UNP O27711
C	-6	LEU	-	CLONING ARTIFACT	UNP O27711
C	-5	VAL	-	CLONING ARTIFACT	UNP O27711
C	-4	PRO	-	CLONING ARTIFACT	UNP O27711
C	-3	ARG	-	CLONING ARTIFACT	UNP O27711
C	-2	GLY	-	CLONING ARTIFACT	UNP O27711
C	-1	SER	-	CLONING ARTIFACT	UNP O27711
C	0	HIS	-	CLONING ARTIFACT	UNP O27711
C	1	MSE	MET	MOFIFIED RESIDUE	UNP O27711
C	51	MSE	MET	MOFIFIED RESIDUE	UNP O27711
C	115	MSE	MET	MOFIFIED RESIDUE	UNP O27711
C	121	MSE	MET	MOFIFIED RESIDUE	UNP O27711
C	135	MSE	MET	MOFIFIED RESIDUE	UNP O27711
C	169	MSE	MET	MOFIFIED RESIDUE	UNP O27711
C	183	MSE	MET	MOFIFIED RESIDUE	UNP O27711

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Mg 2 2	0	0
2	A	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C₁₇H₂₁N₄O₉P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	64	Total	O	0	0
			64	64		
4	B	46	Total	O	0	0
			46	46		
4	C	16	Total	O	0	0
			16	16		

F173		
D174		
L175		
R176		
I177		
H178		
E179		
V180		
I181		
A182		
M183		
P184		
R185		
P186		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.98 Å 69.40 Å 90.95 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.92 – 2.30 45.14 – 2.30	Depositor EDS
% Data completeness (in resolution range)	83.9 (32.92-2.30) 84.0 (45.14-2.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.66 (at 2.29 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.252 , 0.318 0.253 , 0.318	Depositor DCC
R_{free} test set	2475 reflections (9.88%)	DCC
Wilson B-factor (Å ²)	38.8	Xtriage
Anisotropy	0.402	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 62.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 29083 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4441	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, MG

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	0.53	0/1420	0.76	1/1908 (0.1%)
1	B	0.51	0/1420	0.76	0/1908
1	C	0.49	0/1420	0.86	1/1908 (0.1%)
All	All	0.51	0/4260	0.79	2/5724 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	12	GLY	N-CA-C	7.18	131.05	113.10
1	A	107	GLY	N-CA-C	6.30	128.84	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1406	0	1408	71	0
1	B	1406	0	1408	111	0
1	C	1406	0	1408	224	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	31	0	19	4	0
3	B	31	0	19	2	0
3	C	31	0	19	6	0
4	A	64	0	0	4	0
4	B	46	0	0	6	0
4	C	16	0	0	3	0
All	All	4441	0	4281	384	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 45.

All (384) 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:C:48:LEU:HD22	1:C:56:ILE:HD11	1.21	1.20
1:C:120:ARG:HG2	1:C:127:LYS:HG2	1.31	1.10
1:C:26:ARG:HH12	1:C:30:LEU:HD23	1.09	1.07
1:A:131:GLU:HG2	1:A:135:MSE:HE2	1.09	1.04
1:B:131:GLU:HG2	1:B:135:MSE:HE2	1.32	1.03
1:A:132:ILE:HA	1:A:135:MSE:HE3	1.42	1.02
1:B:180:VAL:HG11	1:B:183:MSE:HE3	1.42	1.01
1:A:180:VAL:HG11	1:A:183:MSE:HE2	1.48	0.95
1:C:34:ASN:C	1:C:35:PHE:HD1	1.69	0.95
1:C:26:ARG:NH1	1:C:30:LEU:HD23	1.81	0.95
1:C:130:VAL:O	1:C:134:ILE:HG13	1.66	0.94
1:C:131:GLU:HG2	1:C:135:MSE:HE2	1.48	0.93
1:B:180:VAL:HG11	1:B:183:MSE:CE	1.99	0.93
1:B:78:ARG:O	1:B:82:LEU:HD23	1.70	0.92
1:B:110:THR:HG22	1:B:113:GLU:OE1	1.70	0.91
1:C:56:ILE:CB	1:C:86:VAL:HG11	2.01	0.91
1:C:63:ALA:HB2	1:C:71:LEU:HG	1.52	0.91
1:A:73:LEU:HD11	1:A:78:ARG:HB2	1.54	0.90
1:C:15:ASN:O	1:C:19:VAL:HG23	1.70	0.90
1:C:55:ASN:HD22	1:C:55:ASN:C	1.76	0.89
1:C:26:ARG:HH12	1:C:30:LEU:CD2	1.86	0.89
1:C:19:VAL:HG12	1:C:23:VAL:HG11	1.56	0.87
1:C:19:VAL:HG21	1:C:159:ASP:HA	1.57	0.87
1:C:48:LEU:HD22	1:C:56:ILE:CD1	2.03	0.86
1:C:8:PHE:CE2	1:C:15:ASN:HB3	2.11	0.85
1:C:37:VAL:HG22	1:C:38:ALA:H	1.41	0.85
1:C:19:VAL:HG11	1:C:158:ALA:O	1.77	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ASN:HA	4:B:304:HOH:O	1.78	0.83
1:C:164:LEU:HB3	1:C:177:ILE:HA	1.59	0.83
1:C:56:ILE:HB	1:C:86:VAL:HG11	1.59	0.83
1:B:135:MSE:HE1	3:B:201:FMN:HM73	1.59	0.83
1:C:5:ILE:HG12	1:C:6:CYS:N	1.91	0.83
1:C:19:VAL:O	1:C:23:VAL:HG13	1.78	0.82
1:C:120:ARG:CG	1:C:127:LYS:HG2	2.10	0.82
1:A:132:ILE:CA	1:A:135:MSE:HE3	2.10	0.82
1:A:131:GLU:HG2	1:A:135:MSE:CE	2.02	0.81
1:B:37:VAL:HG13	1:B:151:ILE:HB	1.61	0.81
1:C:20:LEU:HA	1:C:23:VAL:HG22	1.61	0.80
1:C:2:GLU:O	1:C:3:LYS:HD2	1.80	0.80
1:C:48:LEU:CD2	1:C:56:ILE:HD11	2.09	0.80
1:C:57:VAL:HG11	4:C:305:HOH:O	1.81	0.79
1:C:6:CYS:SG	1:C:22:LEU:HD11	2.22	0.79
1:B:131:GLU:CG	1:B:135:MSE:HE2	2.14	0.78
1:C:39:SER:OG	1:C:44:THR:HB	1.83	0.78
1:C:115:MSE:O	1:C:118:THR:HG22	1.83	0.78
1:C:164:LEU:HD13	1:C:166:PRO:HG3	1.66	0.77
1:C:56:ILE:CG2	1:C:86:VAL:HG11	2.15	0.77
1:A:17:GLU:O	1:A:21:GLU:HG3	1.84	0.77
1:C:58:SER:HB3	1:C:81:LEU:HD21	1.66	0.77
1:C:83:GLU:C	1:C:85:GLY:H	1.89	0.75
1:A:73:LEU:CD1	1:A:78:ARG:HB2	2.16	0.75
1:C:115:MSE:HA	1:C:118:THR:HG22	1.69	0.75
1:C:34:ASN:C	1:C:35:PHE:CD1	2.59	0.74
1:C:83:GLU:O	1:C:85:GLY:N	2.19	0.74
1:A:112:VAL:HG11	4:A:352:HOH:O	1.87	0.74
1:C:19:VAL:HG12	1:C:23:VAL:CG1	2.16	0.74
1:A:121:MSE:CE	1:B:119:LEU:HD21	2.17	0.74
1:C:37:VAL:HG23	1:C:151:ILE:HG13	1.69	0.73
1:C:172:VAL:HG13	1:C:173:PHE:H	1.54	0.73
1:C:118:THR:HG23	1:C:119:LEU:H	1.53	0.73
1:C:129:CYS:O	1:C:133:ALA:HB2	1.87	0.73
1:C:44:THR:HG21	1:C:158:ALA:HB2	1.71	0.73
1:B:1:MSE:HE3	1:B:3:LYS:NZ	2.05	0.72
1:C:35:PHE:HD1	1:C:35:PHE:N	1.87	0.72
1:C:8:PHE:CZ	1:C:19:VAL:HG22	2.25	0.72
1:C:43:GLU:O	1:C:46:LEU:N	2.21	0.72
1:C:37:VAL:HG22	1:C:38:ALA:N	2.04	0.72
1:A:40:VAL:HG23	3:A:200:FMN:H5'2	1.72	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:MSE:HE1	1:B:119:LEU:HD21	1.73	0.71
1:C:38:ALA:HB2	1:C:132:ILE:HD13	1.72	0.71
1:C:109:VAL:HG23	1:C:113:GLU:HB2	1.72	0.71
1:C:20:LEU:O	1:C:23:VAL:HG22	1.91	0.70
1:C:81:LEU:HD23	1:C:88:VAL:HG22	1.74	0.70
1:C:35:PHE:CD1	1:C:35:PHE:N	2.60	0.70
1:C:56:ILE:HG22	1:C:86:VAL:HG11	1.72	0.70
1:B:110:THR:HG22	1:B:113:GLU:HG3	1.74	0.69
1:C:20:LEU:CA	1:C:23:VAL:HG22	2.22	0.69
4:A:362:HOH:O	1:B:183:MSE:SE	2.61	0.69
1:C:162:LEU:HD23	1:C:177:ILE:HD12	1.73	0.69
1:B:78:ARG:HG3	1:B:88:VAL:HG11	1.75	0.68
1:C:115:MSE:O	1:C:118:THR:CG2	2.40	0.68
1:A:37:VAL:HG21	1:A:48:LEU:HD22	1.75	0.68
1:B:20:LEU:HB3	1:B:51:MSE:HE1	1.74	0.68
1:C:5:ILE:HG12	1:C:6:CYS:H	1.56	0.68
1:C:56:ILE:O	1:C:86:VAL:CG1	2.42	0.67
1:A:128:VAL:O	1:A:132:ILE:HG12	1.93	0.67
1:C:26:ARG:HG2	1:C:181:ILE:HG12	1.76	0.67
1:B:103:SER:O	4:B:304:HOH:O	2.12	0.67
1:A:19:VAL:O	1:A:23:VAL:HG13	1.95	0.67
1:B:130:VAL:O	1:B:134:ILE:HG13	1.95	0.66
1:B:74:GLU:C	1:B:76:GLU:H	1.96	0.66
1:C:20:LEU:HA	1:C:23:VAL:CG2	2.25	0.66
1:B:122:VAL:HG21	1:B:126:PHE:CD1	2.31	0.66
1:C:120:ARG:HG2	1:C:127:LYS:CG	2.18	0.65
1:C:141:LEU:HB3	4:C:305:HOH:O	1.96	0.65
1:C:19:VAL:C	1:C:23:VAL:HG13	2.17	0.64
1:C:164:LEU:HD13	1:C:166:PRO:CG	2.27	0.64
1:C:55:ASN:ND2	1:C:55:ASN:C	2.49	0.64
1:C:79:ASP:OD1	1:C:80:ALA:N	2.30	0.64
1:B:101:GLY:HA3	1:C:172:VAL:HG12	1.78	0.64
1:B:19:VAL:O	1:B:23:VAL:HG23	1.97	0.64
1:B:110:THR:OG1	1:B:111:PRO:HD2	1.98	0.64
1:C:153:GLY:HA3	1:C:158:ALA:HA	1.79	0.63
1:C:49:SER:HA	1:C:56:ILE:HD12	1.79	0.63
1:C:8:PHE:HE2	1:C:15:ASN:HB3	1.60	0.63
1:B:1:MSE:HE3	1:B:3:LYS:HZ1	1.64	0.63
1:C:17:GLU:HG3	1:C:47:ARG:HH12	1.63	0.63
1:C:93:HIS:HB3	1:C:131:GLU:OE2	1.98	0.63
1:B:93:HIS:HB3	1:B:131:GLU:OE1	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ILE:HA	1:B:135:MSE:HE3	1.80	0.63
1:C:172:VAL:HG13	1:C:173:PHE:N	2.13	0.63
1:B:71:LEU:HD23	1:B:72:GLU:N	2.15	0.62
1:C:18:ARG:HD3	1:C:18:ARG:O	2.00	0.62
1:C:37:VAL:HG23	1:C:151:ILE:CG1	2.29	0.62
1:C:164:LEU:O	1:C:166:PRO:HD3	2.00	0.61
1:C:2:GLU:HG3	1:C:3:LYS:N	2.14	0.61
1:C:110:THR:HG23	1:C:113:GLU:OE2	2.00	0.61
1:C:6:CYS:SG	1:C:22:LEU:CD1	2.89	0.61
1:B:151:ILE:N	1:B:151:ILE:HD12	2.16	0.61
1:C:56:ILE:HG22	1:C:86:VAL:CG1	2.30	0.60
1:B:110:THR:HG22	1:B:113:GLU:CG	2.31	0.60
1:C:16:THR:O	1:C:20:LEU:N	2.33	0.60
1:C:64:GLY:HA2	1:C:67:GLU:O	2.02	0.60
1:B:139:ALA:CB	1:B:141:LEU:HD23	2.31	0.60
1:C:175:LEU:C	1:C:175:LEU:HD23	2.22	0.60
1:B:74:GLU:C	1:B:76:GLU:N	2.55	0.60
1:B:139:ALA:O	1:B:141:LEU:HD22	2.01	0.59
1:C:55:ASN:HD21	1:C:57:VAL:HG12	1.67	0.59
1:C:43:GLU:HG3	1:C:44:THR:N	2.16	0.59
1:A:48:LEU:O	1:A:52:VAL:HG22	2.03	0.59
1:B:139:ALA:HB3	1:B:141:LEU:HD23	1.84	0.59
1:B:146:GLU:HA	4:B:315:HOH:O	2.03	0.59
1:A:36:VAL:HA	1:A:57:VAL:HG13	1.83	0.59
1:C:32:ILE:HG22	1:C:33:ARG:N	2.18	0.59
1:C:74:GLU:O	1:C:78:ARG:N	2.34	0.58
1:B:9:GLU:HG3	1:B:10:GLU:HG2	1.84	0.58
1:C:83:GLU:C	1:C:85:GLY:N	2.51	0.58
1:C:17:GLU:HG3	1:C:47:ARG:NH1	2.18	0.58
1:C:56:ILE:O	1:C:86:VAL:HG13	2.02	0.58
1:C:168:HIS:O	1:C:172:VAL:HA	2.03	0.58
1:A:93:HIS:CD2	3:A:200:FMN:HM72	2.39	0.58
1:C:157:GLY:O	3:C:202:FMN:O4'	2.21	0.58
1:C:5:ILE:CG1	1:C:6:CYS:N	2.63	0.58
1:C:81:LEU:HD23	1:C:88:VAL:CG2	2.34	0.58
1:C:132:ILE:N	1:C:135:MSE:HE3	2.19	0.58
1:B:132:ILE:CA	1:B:135:MSE:HE3	2.34	0.57
1:C:122:VAL:HB	1:C:126:PHE:CD2	2.39	0.57
1:C:5:ILE:CG1	1:C:6:CYS:H	2.16	0.57
1:C:115:MSE:O	1:C:116:ALA:C	2.41	0.57
1:C:121:MSE:SE	4:C:319:HOH:O	2.71	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:HIS:CD2	1:B:65:PHE:HD1	2.23	0.57
1:B:76:GLU:HB2	4:B:337:HOH:O	2.04	0.57
1:C:118:THR:O	1:C:121:MSE:HG3	2.04	0.57
1:A:37:VAL:HG21	1:A:48:LEU:CD2	2.35	0.57
1:B:43:GLU:O	1:B:47:ARG:HG3	2.05	0.57
1:B:110:THR:CG2	1:B:113:GLU:HG3	2.36	0.56
1:C:115:MSE:HA	1:C:118:THR:CG2	2.35	0.56
1:A:165:THR:OG1	1:A:178:HIS:HE1	1.89	0.56
1:B:26:ARG:HG3	1:B:30:LEU:HD12	1.86	0.56
1:A:34:ASN:O	1:A:148:VAL:HG13	2.06	0.56
1:C:98:VAL:O	1:C:101:GLY:N	2.38	0.56
1:C:123:SER:OG	1:C:126:PHE:HB2	2.06	0.56
1:B:148:VAL:HG12	1:B:149:ILE:N	2.20	0.56
1:C:21:GLU:O	1:C:25:GLU:HG3	2.05	0.56
1:C:20:LEU:C	1:C:23:VAL:HG22	2.25	0.56
1:C:180:VAL:HG21	1:C:183:MSE:CE	2.37	0.55
1:B:93:HIS:CD2	1:B:93:HIS:H	2.24	0.55
1:A:135:MSE:HE1	3:A:200:FMN:HM73	1.88	0.55
1:C:115:MSE:CA	1:C:118:THR:HG22	2.37	0.55
1:B:154:THR:O	1:B:155:ALA:HB3	2.06	0.55
1:A:179:GLU:HG2	1:B:7:TYR:CE1	2.42	0.55
1:A:164:LEU:HD12	1:A:164:LEU:C	2.27	0.55
1:B:49:SER:HA	1:B:56:ILE:CD1	2.37	0.55
1:C:26:ARG:CZ	1:C:30:LEU:HD23	2.36	0.55
1:C:93:HIS:CE1	3:C:202:FMN:HM72	2.42	0.55
1:B:110:THR:HG22	1:B:113:GLU:CD	2.28	0.54
1:A:115:MSE:HG2	1:B:118:THR:OG1	2.08	0.54
1:A:80:ALA:O	1:A:84:ARG:HG2	2.08	0.54
1:C:132:ILE:CA	1:C:135:MSE:HE3	2.38	0.53
1:C:124:GLN:O	1:C:127:LYS:HG3	2.09	0.53
1:B:37:VAL:CG1	1:B:151:ILE:HB	2.36	0.53
1:B:180:VAL:HG11	1:B:183:MSE:HE2	1.89	0.53
1:A:131:GLU:O	1:A:135:MSE:HG3	2.09	0.53
1:B:132:ILE:N	1:B:135:MSE:HE3	2.24	0.53
1:C:16:THR:O	1:C:20:LEU:HB2	2.08	0.53
1:C:180:VAL:HG21	1:C:183:MSE:HE3	1.91	0.53
1:B:98:VAL:O	1:B:101:GLY:N	2.41	0.53
1:B:168:HIS:CD2	1:C:64:GLY:HA3	2.42	0.53
1:C:131:GLU:HG2	1:C:135:MSE:CE	2.31	0.53
1:C:5:ILE:HD12	1:C:180:VAL:CG1	2.39	0.53
1:C:23:VAL:O	1:C:27:ALA:HB2	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:LEU:O	1:C:49:SER:OG	2.27	0.52
1:C:154:THR:HG23	1:C:159:ASP:OD1	2.09	0.52
1:C:111:PRO:O	1:C:114:ILE:N	2.37	0.52
1:C:15:ASN:C	1:C:19:VAL:HG23	2.30	0.52
1:B:74:GLU:O	1:B:76:GLU:N	2.42	0.52
1:C:75:ASP:HA	1:C:78:ARG:HB3	1.90	0.52
1:B:62:HIS:NE2	1:B:65:PHE:HD1	2.07	0.52
1:C:163:VAL:HB	1:C:179:GLU:HB2	1.92	0.52
1:A:109:VAL:HG13	1:C:106:PHE:CG	2.45	0.52
1:C:135:MSE:HE1	3:C:202:FMN:HM73	1.92	0.52
1:A:93:HIS:NE2	3:A:200:FMN:HM72	2.24	0.52
1:C:165:THR:O	1:C:166:PRO:O	2.27	0.52
1:C:125:GLY:H	1:C:154:THR:HG22	1.73	0.52
1:B:71:LEU:HD22	1:B:73:LEU:H	1.75	0.51
1:C:128:VAL:O	1:C:132:ILE:HG12	2.10	0.51
1:B:100:ARG:O	1:B:104:ASN:ND2	2.43	0.51
1:B:118:THR:O	1:B:121:MSE:HB2	2.09	0.51
1:C:50:GLU:HG3	1:C:51:MSE:HE3	1.93	0.51
1:C:26:ARG:HH22	1:C:30:LEU:HD23	1.76	0.51
1:A:153:GLY:HA2	1:A:159:ASP:OD2	2.11	0.51
1:B:144:VAL:HG12	1:B:144:VAL:O	2.10	0.51
1:C:19:VAL:O	1:C:23:VAL:N	2.29	0.51
1:A:109:VAL:CG1	1:C:106:PHE:CG	2.94	0.51
1:C:43:GLU:O	1:C:46:LEU:HB3	2.11	0.51
1:C:56:ILE:CG2	1:C:57:VAL:N	2.74	0.51
1:C:73:LEU:HD23	1:C:78:ARG:HB2	1.93	0.51
1:C:132:ILE:HA	1:C:135:MSE:HE3	1.92	0.50
1:C:175:LEU:HD23	1:C:176:ARG:N	2.26	0.50
1:B:125:GLY:HA2	1:B:128:VAL:CG1	2.41	0.50
1:C:164:LEU:C	1:C:166:PRO:HD3	2.32	0.50
1:A:177:ILE:HB	1:B:122:VAL:HA	1.94	0.50
1:C:132:ILE:HA	1:C:135:MSE:HG3	1.94	0.50
1:A:169:MSE:HG3	1:A:170:ASN:N	2.27	0.50
1:C:56:ILE:C	1:C:86:VAL:CG1	2.80	0.50
1:C:18:ARG:HD3	1:C:18:ARG:C	2.30	0.50
1:B:109:VAL:HG12	1:B:113:GLU:HB2	1.92	0.49
1:B:19:VAL:HG21	1:B:159:ASP:HA	1.94	0.49
1:B:77:ALA:C	1:B:79:ASP:N	2.65	0.49
1:C:72:GLU:O	1:C:74:GLU:N	2.45	0.49
1:B:34:ASN:O	1:B:148:VAL:HG13	2.12	0.49
1:B:185:ARG:HB3	1:B:186:PRO:HD3	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:VAL:HG12	3:C:202:FMN:C5'	2.42	0.49
1:C:40:VAL:O	1:C:40:VAL:HG22	2.13	0.49
1:C:118:THR:HG23	1:C:119:LEU:N	2.25	0.49
1:B:105:ARG:HH11	1:B:105:ARG:HG3	1.76	0.49
1:C:32:ILE:HG22	1:C:34:ASN:H	1.77	0.49
1:C:75:ASP:O	1:C:79:ASP:HB3	2.12	0.49
1:C:26:ARG:NH1	1:C:26:ARG:HG3	2.28	0.49
1:A:12:GLY:HA3	4:A:350:HOH:O	2.12	0.49
1:C:20:LEU:CD1	1:C:47:ARG:HD2	2.43	0.48
1:C:26:ARG:NH2	1:C:30:LEU:HD23	2.28	0.48
1:B:95:LEU:HB2	1:B:131:GLU:HG3	1.94	0.48
1:C:138:ASP:OD1	1:C:169:MSE:HG2	2.12	0.48
1:A:128:VAL:HG22	1:A:152:GLY:HA3	1.94	0.48
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.69	0.48
1:A:60:THR:OG1	1:A:61:HIS:N	2.47	0.48
1:B:40:VAL:HA	1:B:60:THR:OG1	2.14	0.48
1:B:20:LEU:CB	1:B:51:MSE:HE1	2.44	0.48
1:B:79:ASP:HA	1:B:82:LEU:HB2	1.94	0.47
1:B:140:GLY:HA3	1:C:71:LEU:CD1	2.44	0.47
1:A:75:ASP:O	1:A:79:ASP:OD1	2.32	0.47
1:C:19:VAL:CG1	1:C:158:ALA:O	2.57	0.47
1:A:171:SER:O	1:A:174:ASP:HB2	2.14	0.47
1:C:26:ARG:HH11	1:C:26:ARG:HG3	1.79	0.47
1:C:37:VAL:CG2	1:C:151:ILE:HG13	2.42	0.47
1:C:8:PHE:HZ	1:C:19:VAL:HG22	1.74	0.47
1:B:10:GLU:HA	1:B:10:GLU:OE2	2.14	0.47
1:C:8:PHE:HB2	1:C:184:PRO:HA	1.97	0.47
1:B:1:MSE:HE3	1:B:3:LYS:HZ3	1.79	0.47
1:C:16:THR:O	1:C:20:LEU:CB	2.63	0.47
1:B:75:ASP:HB3	4:B:333:HOH:O	2.14	0.47
1:B:77:ALA:C	1:B:79:ASP:H	2.17	0.47
1:B:126:PHE:O	1:B:130:VAL:HG23	2.15	0.47
1:C:111:PRO:O	1:C:114:ILE:HB	2.14	0.47
1:C:163:VAL:HG12	1:C:178:HIS:HB2	1.96	0.47
1:A:46:LEU:HD21	1:A:81:LEU:HD12	1.96	0.47
1:B:20:LEU:HB3	1:B:51:MSE:CE	2.42	0.47
1:B:93:HIS:N	1:B:93:HIS:CD2	2.80	0.47
1:A:172:VAL:HG23	1:A:173:PHE:N	2.29	0.47
1:C:19:VAL:CG1	1:C:23:VAL:CG1	2.91	0.47
1:C:32:ILE:CG2	1:C:33:ARG:N	2.78	0.47
1:B:149:ILE:HA	1:B:162:LEU:O	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ARG:O	1:C:105:ARG:HD3	2.15	0.46
1:C:123:SER:O	1:C:126:PHE:N	2.42	0.46
1:A:142:ILE:HB	1:A:143:PRO:HD2	1.96	0.46
1:B:138:ASP:OD1	1:B:169:MSE:HB3	2.14	0.46
1:B:137:ALA:O	1:B:168:HIS:HE1	1.98	0.46
1:B:131:GLU:O	1:B:135:MSE:HG3	2.14	0.46
1:C:115:MSE:C	1:C:118:THR:HG22	2.36	0.46
1:B:62:HIS:HE2	1:B:65:PHE:HD1	1.62	0.46
1:A:185:ARG:HG2	4:A:311:HOH:O	2.16	0.46
1:C:161:ALA:O	1:C:162:LEU:HD12	2.15	0.46
1:C:75:ASP:OD2	1:C:78:ARG:HD3	2.15	0.46
1:B:169:MSE:SE	1:C:92:SER:HB3	2.66	0.46
1:C:142:ILE:HA	1:C:143:PRO:HD3	1.73	0.46
1:A:62:HIS:HD2	1:A:63:ALA:O	1.98	0.46
1:B:92:SER:HB3	1:C:138:ASP:OD1	2.16	0.46
1:C:89:TYR:CE1	1:C:139:ALA:HB2	2.51	0.46
1:B:63:ALA:HB2	1:C:140:GLY:N	2.31	0.46
1:C:150:ALA:O	1:C:162:LEU:N	2.49	0.46
1:A:43:GLU:O	1:A:46:LEU:HB2	2.16	0.46
1:C:89:TYR:CD2	1:C:90:ALA:N	2.84	0.46
1:C:40:VAL:HA	1:C:60:THR:OG1	2.16	0.45
1:B:172:VAL:HG21	1:C:98:VAL:HG13	1.98	0.45
1:A:131:GLU:CG	1:A:135:MSE:HE2	2.05	0.45
1:C:55:ASN:HD21	1:C:57:VAL:CG1	2.30	0.45
1:B:160:THR:HA	1:B:182:ALA:O	2.16	0.45
1:C:56:ILE:O	1:C:57:VAL:HG12	2.17	0.45
1:C:62:HIS:HB3	1:C:91:GLY:O	2.17	0.45
1:B:36:VAL:HG21	1:B:142:ILE:HD13	1.98	0.45
1:C:19:VAL:HG21	1:C:158:ALA:O	2.17	0.45
1:A:109:VAL:HG11	1:C:106:PHE:CD1	2.51	0.45
1:C:8:PHE:CD1	1:C:8:PHE:N	2.85	0.45
1:B:164:LEU:HD12	1:B:164:LEU:C	2.37	0.45
1:C:55:ASN:ND2	1:C:57:VAL:HG12	2.31	0.44
1:A:179:GLU:HG2	1:B:7:TYR:CZ	2.52	0.44
1:C:185:ARG:O	1:C:186:PRO:O	2.35	0.44
1:A:25:GLU:O	1:A:29:GLN:HG3	2.17	0.44
1:C:151:ILE:HD11	1:C:158:ALA:HB1	1.99	0.44
1:C:47:ARG:O	1:C:51:MSE:HE3	2.17	0.44
1:A:5:ILE:HD11	1:A:183:MSE:HE3	1.99	0.44
1:A:75:ASP:OD1	1:A:75:ASP:N	2.45	0.44
1:C:5:ILE:HD12	1:C:180:VAL:HG13	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:GLY:HA3	1:C:71:LEU:HD11	2.00	0.44
1:C:157:GLY:N	3:C:202:FMN:O4'	2.51	0.44
1:C:6:CYS:C	1:C:7:TYR:CD1	2.91	0.44
1:A:94:ALA:HB2	1:A:135:MSE:HG2	2.00	0.44
1:C:74:GLU:OE2	1:C:74:GLU:HA	2.18	0.44
1:C:40:VAL:HG12	3:C:202:FMN:H5'2	1.99	0.43
1:C:162:LEU:CD2	1:C:177:ILE:HD12	2.47	0.43
1:B:148:VAL:CG1	1:B:149:ILE:N	2.80	0.43
1:C:37:VAL:CG2	1:C:38:ALA:H	2.21	0.43
1:B:39:SER:HA	3:B:201:FMN:H5'1	2.01	0.43
1:C:122:VAL:CB	1:C:126:PHE:CD2	3.02	0.43
1:C:37:VAL:CG2	1:C:38:ALA:N	2.77	0.43
1:C:55:ASN:ND2	1:C:55:ASN:O	2.51	0.43
1:C:127:LYS:HB2	1:C:127:LYS:HE2	1.85	0.43
1:A:46:LEU:CD2	1:A:81:LEU:HD12	2.48	0.43
1:C:36:VAL:HA	1:C:57:VAL:HG22	2.00	0.43
1:C:78:ARG:CZ	1:C:82:LEU:HD11	2.48	0.43
1:B:63:ALA:HB2	1:C:140:GLY:CA	2.48	0.43
1:C:19:VAL:CG2	1:C:159:ASP:HA	2.38	0.43
1:A:149:ILE:HD13	1:A:181:ILE:HD11	2.01	0.43
1:C:172:VAL:O	1:C:174:ASP:N	2.52	0.43
1:A:164:LEU:O	1:A:164:LEU:HD12	2.19	0.43
1:A:52:VAL:HG23	1:A:56:ILE:HD11	2.02	0.42
1:C:48:LEU:HD23	1:C:48:LEU:O	2.19	0.42
1:B:110:THR:OG1	1:B:111:PRO:CD	2.66	0.42
1:B:172:VAL:HG13	1:B:173:PHE:N	2.33	0.42
1:B:63:ALA:HB2	1:C:140:GLY:HA2	2.00	0.42
1:B:98:VAL:O	1:B:99:GLY:C	2.58	0.42
1:A:172:VAL:C	1:A:174:ASP:H	2.22	0.42
1:B:142:ILE:HD12	1:B:166:PRO:HG2	2.01	0.42
1:C:33:ARG:HB3	1:C:33:ARG:HE	1.64	0.42
1:C:105:ARG:C	1:C:105:ARG:HD3	2.40	0.42
1:C:185:ARG:HB3	1:C:186:PRO:HD3	2.01	0.42
1:C:23:VAL:O	1:C:27:ALA:CB	2.67	0.42
1:B:17:GLU:HB2	4:B:334:HOH:O	2.19	0.42
1:C:43:GLU:O	1:C:46:LEU:CB	2.68	0.41
1:B:101:GLY:O	1:B:104:ASN:HB2	2.19	0.41
1:A:16:THR:HG22	1:A:20:LEU:HD12	2.01	0.41
1:A:20:LEU:O	1:A:23:VAL:HG22	2.21	0.41
1:A:47:ARG:HA	1:A:47:ARG:HD3	1.70	0.41
1:B:75:ASP:HA	1:B:78:ARG:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:HIS:CD2	1:C:63:ALA:O	2.73	0.41
1:C:58:SER:CB	1:C:81:LEU:HD21	2.44	0.41
1:A:16:THR:HG22	1:A:20:LEU:CD1	2.50	0.41
1:A:23:VAL:CG2	1:A:24:GLY:N	2.83	0.41
1:B:10:GLU:HA	1:B:11:PRO:HD3	1.92	0.41
1:B:172:VAL:HG11	1:C:98:VAL:HG13	2.02	0.41
1:C:8:PHE:CD2	1:C:15:ASN:HB3	2.53	0.41
1:A:125:GLY:HA2	1:A:128:VAL:HG13	2.02	0.41
1:A:36:VAL:HG13	1:A:36:VAL:O	2.21	0.41
1:B:17:GLU:HG2	1:B:47:ARG:HH22	1.85	0.41
1:C:24:GLY:O	1:C:25:GLU:C	2.59	0.41
1:C:19:VAL:CG1	1:C:23:VAL:HG11	2.39	0.41
1:C:37:VAL:CG2	1:C:151:ILE:CG1	2.98	0.41
1:A:56:ILE:HB	1:A:86:VAL:HG22	2.03	0.41
1:C:120:ARG:HE	1:C:127:LYS:HE3	1.85	0.41
1:B:126:PHE:N	1:B:160:THR:HG21	2.36	0.41
1:A:117:GLU:HB3	1:B:173:PHE:CE1	2.56	0.41
1:C:16:THR:HA	1:C:19:VAL:HB	2.03	0.40
1:C:35:PHE:HE2	1:C:52:VAL:CG1	2.34	0.40
1:A:179:GLU:HA	1:B:7:TYR:CE2	2.56	0.40
1:C:49:SER:HB2	1:C:84:ARG:HG2	2.04	0.40
1:A:5:ILE:HG13	1:A:180:VAL:O	2.22	0.40
1:B:75:ASP:HA	1:B:78:ARG:CB	2.51	0.40
1:C:164:LEU:HD12	1:C:164:LEU:H	1.87	0.40
1:C:142:ILE:O	1:C:142:ILE:HG13	2.19	0.40
1:A:18:ARG:HA	1:A:18:ARG:HD2	1.89	0.40
1:C:36:VAL:O	1:C:151:ILE:HG23	2.21	0.40
1:A:23:VAL:HG23	1:A:24:GLY:N	2.36	0.40
1:A:172:VAL:HG23	1:A:173:PHE:H	1.86	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	184/206 (89%)	173 (94%)	10 (5%)	1 (0%)	34	41
1	B	184/206 (89%)	162 (88%)	19 (10%)	3 (2%)	12	11
1	C	184/206 (89%)	138 (75%)	30 (16%)	16 (9%)	1	0
All	All	552/618 (89%)	473 (86%)	59 (11%)	20 (4%)	4	2

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	14	GLU
1	C	84	ARG
1	C	166	PRO
1	A	108	GLY
1	B	64	GLY
1	C	73	LEU
1	C	87	ASN
1	C	173	PHE
1	B	68	LYS
1	C	31	GLY
1	C	44	THR
1	C	131	GLU
1	C	81	LEU
1	B	75	ASP
1	C	43	GLU
1	C	111	PRO
1	C	155	ALA
1	C	141	LEU
1	C	172	VAL
1	C	112	VAL

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	148/157 (94%)	133 (90%)	15 (10%)	9	11
1	B	148/157 (94%)	131 (88%)	17 (12%)	7	7

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	148/157 (94%)	121 (82%)	27 (18%)	2	2
All	All	444/471 (94%)	385 (87%)	59 (13%)	5	5

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	17	GLU
1	A	26	ARG
1	A	47	ARG
1	A	59	VAL
1	A	60	THR
1	A	66	ARG
1	A	75	ASP
1	A	79	ASP
1	A	105	ARG
1	A	109	VAL
1	A	112	VAL
1	A	127	LYS
1	A	128	VAL
1	A	149	ILE
1	B	1	MSE
1	B	3	LYS
1	B	9	GLU
1	B	14	GLU
1	B	18	ARG
1	B	33	ARG
1	B	37	VAL
1	B	53	GLU
1	B	83	GLU
1	B	95	LEU
1	B	109	VAL
1	B	111	PRO
1	B	112	VAL
1	B	123	SER
1	B	128	VAL
1	B	169	MSE
1	B	171	SER
1	C	1	MSE
1	C	2	GLU
1	C	18	ARG
1	C	22	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	26	ARG
1	C	30	LEU
1	C	33	ARG
1	C	35	PHE
1	C	36	VAL
1	C	39	SER
1	C	43	GLU
1	C	55	ASN
1	C	56	ILE
1	C	57	VAL
1	C	61	HIS
1	C	66	ARG
1	C	79	ASP
1	C	84	ARG
1	C	105	ARG
1	C	118	THR
1	C	126	PHE
1	C	127	LYS
1	C	145	ASP
1	C	151	ILE
1	C	162	LEU
1	C	164	LEU
1	C	177	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	62	HIS
1	A	104	ASN
1	A	178	HIS
1	B	70	GLN
1	B	104	ASN
1	C	55	ASN
1	C	61	HIS

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 ⓘ

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z > 2$
3	FMN	A	200	-	32,33,33	1.18	3 (9%)	34,50,50	1.98	7 (20%)
3	FMN	B	201	2	32,33,33	2.42	11 (34%)	34,50,50	3.18	11 (32%)
3	FMN	C	202	-	32,33,33	2.43	10 (31%)	34,50,50	3.32	11 (32%)

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
3	FMN	A	200	-	-	0/18/18/18	0/3/3/3
3	FMN	B	201	2	-	0/18/18/18	0/3/3/3
3	FMN	C	202	-	-	0/18/18/18	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	FMN	C4A-N5	-3.24	1.28	1.33
3	C	202	FMN	C4A-N5	-2.90	1.28	1.33
3	B	201	FMN	C1'-N10	-2.30	1.45	1.48
3	C	202	FMN	C8M-C8	-2.17	1.46	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	201	FMN	C8-C7	2.12	1.46	1.41
3	B	201	FMN	C5'-C4'	2.14	1.55	1.51
3	C	202	FMN	C5'-C4'	2.31	1.55	1.51
3	B	201	FMN	C9A-C5A	2.35	1.47	1.42
3	A	200	FMN	C4-N3	2.52	1.37	1.33
3	B	201	FMN	C6-C7	2.60	1.45	1.37
3	C	202	FMN	C6-C7	2.69	1.45	1.37
3	C	202	FMN	C9A-C5A	2.88	1.48	1.42
3	A	200	FMN	C4A-N5	3.10	1.38	1.33
3	A	200	FMN	C1'-N10	3.17	1.51	1.48
3	C	202	FMN	C9-C9A	3.80	1.49	1.40
3	B	201	FMN	C9-C9A	4.00	1.49	1.40
3	C	202	FMN	C5A-N5	4.00	1.41	1.35
3	B	201	FMN	C5A-N5	4.34	1.42	1.35
3	C	202	FMN	C2-N3	4.35	1.47	1.38
3	B	201	FMN	C2-N3	4.63	1.47	1.38
3	C	202	FMN	C4-N3	5.64	1.43	1.33
3	B	201	FMN	C4-N3	5.65	1.43	1.33
3	B	201	FMN	C4A-C10	6.27	1.52	1.40
3	C	202	FMN	C4A-C10	7.22	1.54	1.40

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	201	FMN	N3-C2-N1	-6.00	117.58	127.69
3	C	202	FMN	N3-C2-N1	-5.98	117.63	127.69
3	C	202	FMN	C4A-C4-N3	-5.65	116.13	123.52
3	A	200	FMN	O4'-C4'-C5'	-5.47	98.17	110.09
3	B	201	FMN	C4A-C4-N3	-5.31	116.58	123.52
3	A	200	FMN	C4A-C4-N3	-4.59	117.52	123.52
3	B	201	FMN	C7M-C7-C6	-4.18	108.53	120.33
3	C	202	FMN	C7M-C7-C6	-4.10	108.74	120.33
3	B	201	FMN	C9A-C5A-N5	-3.39	116.66	122.18
3	C	202	FMN	C9A-C5A-N5	-2.99	117.31	122.18
3	A	200	FMN	N3-C2-N1	-2.67	123.20	127.69
3	C	202	FMN	O3'-C3'-C4'	-2.23	102.95	108.73
3	A	200	FMN	O4'-C4'-C3'	-2.10	103.54	108.96
3	B	201	FMN	O3'-C3'-C4'	-2.01	103.51	108.73
3	A	200	FMN	O2P-P-O5'	2.19	113.13	106.72
3	C	202	FMN	C6-C5A-N5	3.09	122.76	118.92
3	C	202	FMN	C4A-N5-C5A	3.18	120.47	116.72
3	A	200	FMN	C1'-N10-C9A	3.36	122.73	118.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	201	FMN	C4A-N5-C5A	3.53	120.88	116.72
3	B	201	FMN	C6-C5A-N5	3.58	123.38	118.92
3	C	202	FMN	C7M-C7-C8	4.70	130.84	120.73
3	B	201	FMN	C7M-C7-C8	4.95	131.38	120.73
3	A	200	FMN	C4-N3-C2	5.63	119.86	115.16
3	C	202	FMN	C4-N3-C2	7.02	121.01	115.16
3	B	201	FMN	C5A-C9A-N10	7.56	123.24	117.58
3	B	201	FMN	C4-N3-C2	7.68	121.56	115.16
3	B	201	FMN	C1'-N10-C9A	7.87	127.95	118.83
3	C	202	FMN	C5A-C9A-N10	8.63	124.05	117.58
3	C	202	FMN	C1'-N10-C9A	9.32	129.64	118.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	200	FMN	4	0
3	B	201	FMN	2	0
3	C	202	FMN	6	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	179/206 (86%)	0.15	1 (0%)	90 93	18, 38, 78, 106	0
1	B	179/206 (86%)	0.33	6 (3%)	49 58	26, 46, 92, 117	0
1	C	179/206 (86%)	1.89	69 (38%)	0 0	33, 83, 122, 146	0
All	All	537/618 (86%)	0.79	76 (14%)	4 6	18, 54, 109, 146	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	143	PRO	8.8
1	C	144	VAL	7.2
1	C	82	LEU	6.3
1	C	181	ILE	6.1
1	C	56	ILE	6.0
1	C	81	LEU	5.8
1	C	52	VAL	5.6
1	C	156	TRP	5.6
1	C	79	ASP	4.5
1	C	168	HIS	4.3
1	C	155	ALA	4.2
1	C	7	TYR	4.1
1	C	28	ASP	4.1
1	C	54	GLY	4.0
1	C	84	ARG	3.8
1	C	142	ILE	3.8
1	C	86	VAL	3.7
1	C	20	LEU	3.7
1	C	182	ALA	3.6
1	C	8	PHE	3.4
1	C	49	SER	3.4
1	C	32	ILE	3.4
1	C	167	ALA	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	53	GLU	3.3
1	B	70	GLN	3.3
1	C	5	ILE	3.2
1	C	65	PHE	3.2
1	C	180	VAL	3.2
1	C	77	ALA	3.1
1	C	11	PRO	3.1
1	C	161	ALA	3.1
1	C	122	VAL	3.0
1	C	50	GLU	3.0
1	C	185	ARG	3.0
1	C	148	VAL	3.0
1	A	28	ASP	2.9
1	C	80	ALA	2.9
1	C	37	VAL	2.9
1	C	88	VAL	2.9
1	C	13	LYS	2.9
1	C	178	HIS	2.9
1	C	176	ARG	2.9
1	B	76	GLU	2.8
1	B	79	ASP	2.8
1	C	73	LEU	2.8
1	C	16	THR	2.8
1	C	162	LEU	2.8
1	C	55	ASN	2.8
1	C	163	VAL	2.8
1	C	41	SER	2.8
1	C	145	ASP	2.7
1	C	40	VAL	2.7
1	C	33	ARG	2.7
1	B	74	GLU	2.6
1	C	43	GLU	2.6
1	C	66	ARG	2.6
1	C	71	LEU	2.6
1	C	4	LYS	2.5
1	C	136	ALA	2.4
1	C	46	LEU	2.4
1	C	119	LEU	2.4
1	C	177	ILE	2.4
1	C	61	HIS	2.4
1	C	67	GLU	2.3
1	C	57	VAL	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	78	ARG	2.2
1	B	78	ARG	2.2
1	C	127	LYS	2.2
1	C	139	ALA	2.2
1	C	160	THR	2.2
1	C	18	ARG	2.2
1	B	69	GLY	2.2
1	C	150	ALA	2.2
1	C	58	SER	2.1
1	C	118	THR	2.1
1	C	184	PRO	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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	MG	B	303	1/1	0.88	0.45	16.79	71,71,71,71	0
3	FMN	A	200	31/31	0.95	0.15	0.41	29,39,54,58	0
3	FMN	B	201	31/31	0.95	0.16	-0.18	23,48,71,76	0
3	FMN	C	202	31/31	0.78	0.22	-0.26	84,102,105,108	0
2	MG	A	302	1/1	0.92	0.08	-2.01	46,46,46,46	0
2	MG	C	304	1/1	0.74	0.12	-2.46	75,75,75,75	0
2	MG	B	301	1/1	0.94	0.21	-	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.