Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 01:38 AM EDT

PDB ID	:	3FRM
Title	:	The crystal structure of a functionally unknown conserved protein from Staphylococcus epidermidis ATCC 12228.
Authors	:	Tan, K.; Sather, A.; Clancy, S.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2009-01-08
Resolution	:	2.32 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:

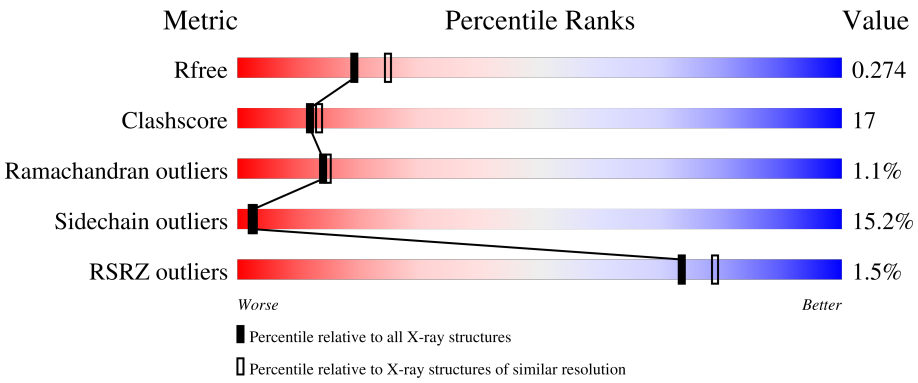
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.32 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	5974 (2.34-2.30)
Clashscore	141614	6604 (2.34-2.30)
Ramachandran outliers	138981	6523 (2.34-2.30)
Sidechain outliers	138945	6523 (2.34-2.30)
RSRZ outliers	127900	5855 (2.34-2.30)

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 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	254	65% 26% 8% •
1	B	254	68% 24% 7% •
1	C	254	2% 61% 30% 9%
1	D	254	72% 22% 6%
1	E	254	2% 67% 26% 5% ••

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	254	4% 60% 28% 11%

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
3	SO4	D	253	-	-	X	-
3	SO4	E	253	-	-	X	-
4	MES	E	255	-	-	X	-
4	MES	F	253	-	-	X	-
4	MES	F	254	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12801 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 uncharacterized conserved protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	Se			
1	A	252	2059	1324	341	386	8	0	0	0
1	B	252	2073	1333	345	387	8	0	2	0
1	C	254	2073	1331	344	390	8	0	0	0
1	D	253	2083	1338	346	391	8	0	3	0
1	E	252	2059	1324	341	386	8	0	0	0
1	F	252	2059	1324	341	386	8	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8CRE9
A	-1	ASN	-	expression tag	UNP Q8CRE9
A	0	ALA	-	expression tag	UNP Q8CRE9
B	-2	SER	-	expression tag	UNP Q8CRE9
B	-1	ASN	-	expression tag	UNP Q8CRE9
B	0	ALA	-	expression tag	UNP Q8CRE9
C	-2	SER	-	expression tag	UNP Q8CRE9
C	-1	ASN	-	expression tag	UNP Q8CRE9
C	0	ALA	-	expression tag	UNP Q8CRE9
D	-2	SER	-	expression tag	UNP Q8CRE9
D	-1	ASN	-	expression tag	UNP Q8CRE9
D	0	ALA	-	expression tag	UNP Q8CRE9
E	-2	SER	-	expression tag	UNP Q8CRE9
E	-1	ASN	-	expression tag	UNP Q8CRE9
E	0	ALA	-	expression tag	UNP Q8CRE9
F	-2	SER	-	expression tag	UNP Q8CRE9
F	-1	ASN	-	expression tag	UNP Q8CRE9

Continued on next page...

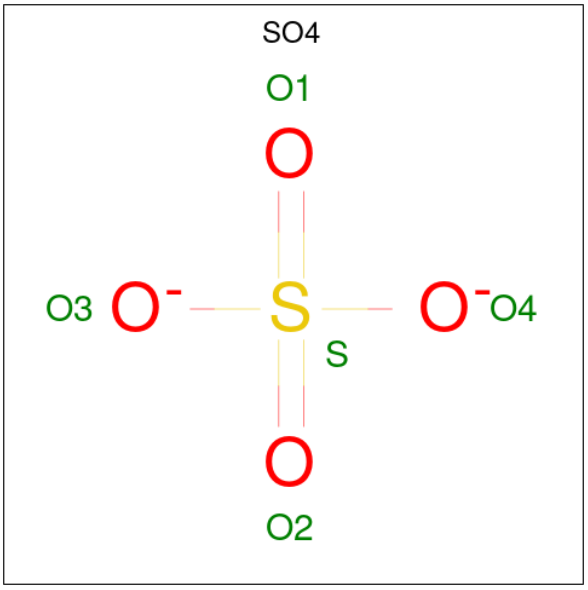
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	expression tag	UNP Q8CRE9

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
2	A	1	1	1	0	0
2	B	1	1	1	0	0
2	C	1	1	1	0	0
2	D	1	1	1	0	0
2	E	1	1	1	0	0
2	F	1	1	1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



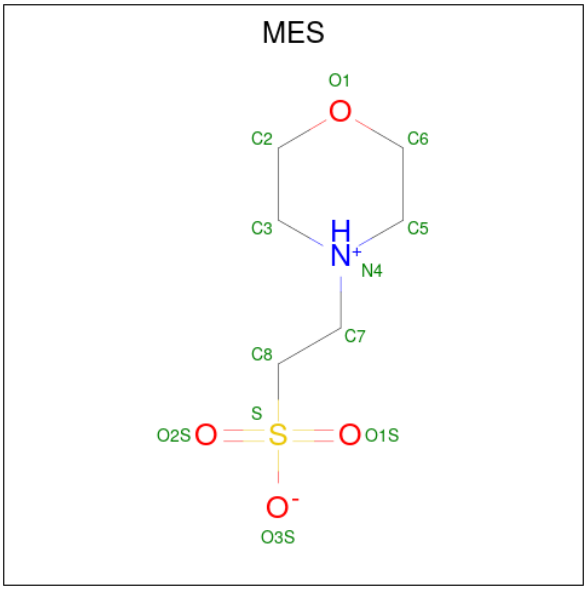
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0
3	B	1	5	4	1	0	0
3	B	1	5	4	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
3	C	1	5	4	1		0	0
			Total	O	S			
3	C	1	5	4	1		0	0
			Total	O	S			
3	D	1	5	4	1		0	0
			Total	O	S			
3	E	1	5	4	1		0	0
			Total	O	S			
3	E	1	5	4	1		0	0

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	E	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
4	F	1	12	6	1	4	1	0	0
			Total	C	N	O	S		
4	F	1	12	6	1	4	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	53	53	53	0	0

Continued on next page...

Continued from previous page...

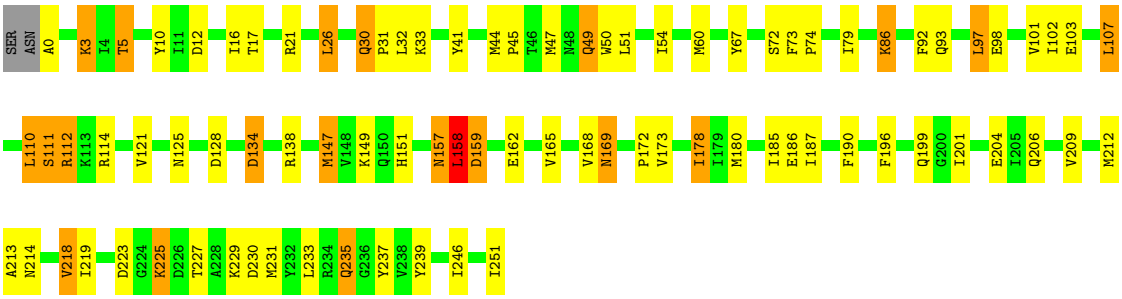
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	B	43	43	43	0	0
			Total	O		
5	C	53	53	53	0	0
			Total	O		
5	D	60	60	60	0	0
			Total	O		
5	E	40	40	40	0	0
			Total	O		
5	F	64	64	64	0	0

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.

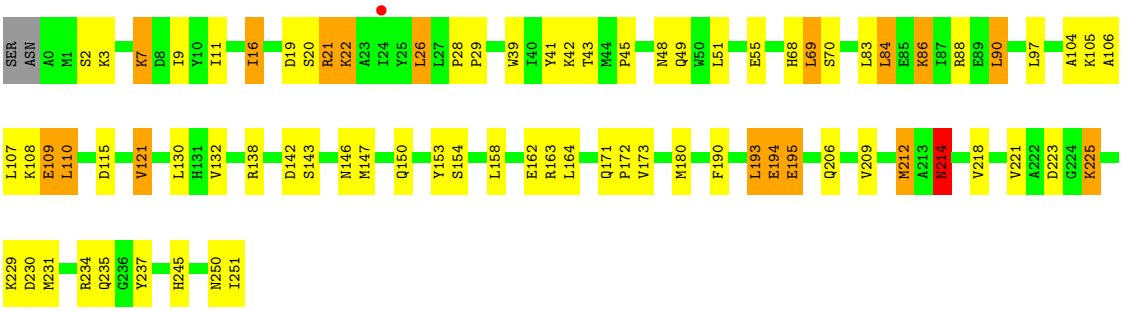
• Molecule 1: uncharacterized conserved protein

Chain A:



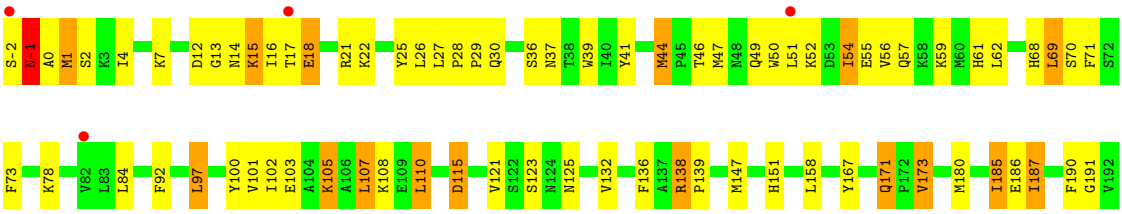
• Molecule 1: uncharacterized conserved protein

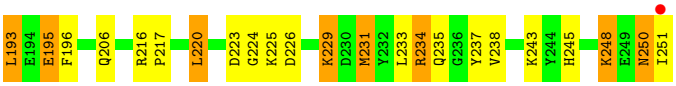
Chain B:



• Molecule 1: uncharacterized conserved protein

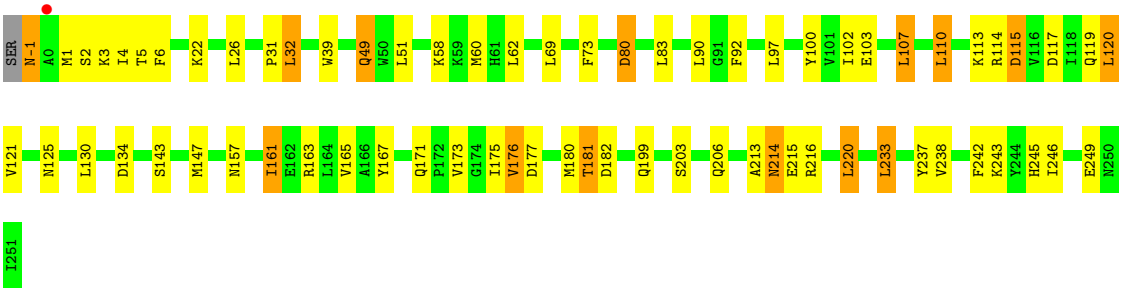
Chain C:





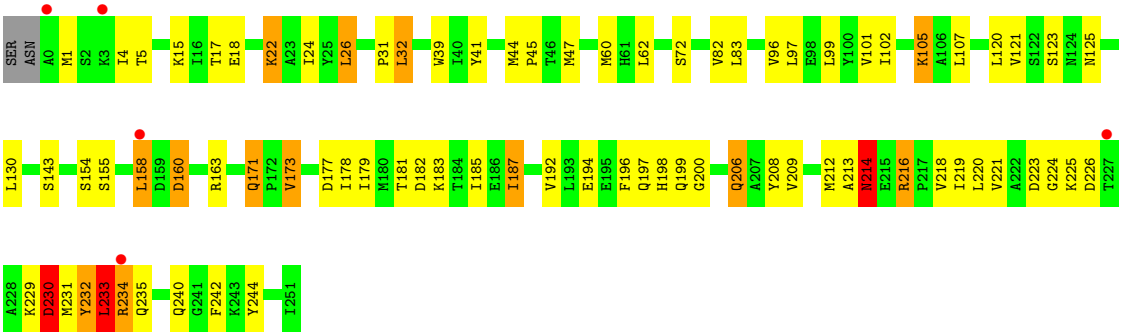
• Molecule 1: uncharacterized conserved protein

Chain D:



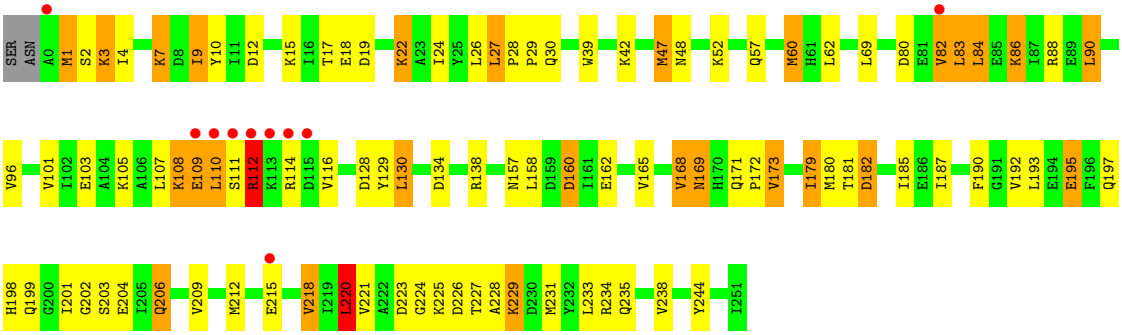
• Molecule 1: uncharacterized conserved protein

Chain E:



• Molecule 1: uncharacterized conserved protein

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	63.71Å 126.55Å 112.81Å 90.00° 94.52° 90.00°	Depositor
Resolution (Å)	41.45 – 2.32 41.43 – 2.32	Depositor EDS
% Data completeness (in resolution range)	99.0 (41.45-2.32) 99.0 (41.43-2.32)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.32Å)	Xtriage
Refinement program	REFMAC 5.5.0054	Depositor
R, R_{free}	0.197 , 0.263 0.207 , 0.274	Depositor DCC
R_{free} test set	3823 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	36.8	Xtriage
Anisotropy	0.716	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 47.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12801	wwPDB-VP
Average B, all atoms (Å^2)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, SO4, MES

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	0.92	1/2095 (0.0%)	0.94	2/2816 (0.1%)
1	B	0.90	0/2115	0.91	3/2842 (0.1%)
1	C	0.80	0/2109	0.89	1/2835 (0.0%)
1	D	0.92	3/2128 (0.1%)	0.93	3/2861 (0.1%)
1	E	0.90	0/2095	0.94	3/2816 (0.1%)
1	F	0.86	0/2095	0.87	2/2816 (0.1%)
All	All	0.88	4/12637 (0.0%)	0.91	14/16986 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	92	PHE	CE1-CZ	5.06	1.47	1.37
1	D	249	GLU	CD-OE2	5.05	1.31	1.25
1	D	6	PHE	CE1-CZ	5.02	1.46	1.37
1	A	72	SER	CB-OG	-5.00	1.35	1.42

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	142	ASP	CB-CG-OD1	-5.88	113.01	118.30
1	F	220	LEU	CA-CB-CG	5.68	128.36	115.30
1	B	84	LEU	CA-CB-CG	5.67	128.34	115.30
1	D	39	TRP	CA-CB-CG	5.55	124.24	113.70
1	B	138	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	138	ARG	NE-CZ-NH2	-5.37	117.62	120.30
1	D	176	VAL	CB-CA-C	-5.34	101.25	111.40
1	A	159	ASP	CB-CG-OD1	5.29	123.06	118.30
1	E	233	LEU	CA-CB-CG	-5.22	103.30	115.30
1	D	120	LEU	CA-CB-CG	5.15	127.15	115.30
1	F	179	ILE	CG1-CB-CG2	5.11	122.63	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	158	LEU	CA-CB-CG	5.08	126.98	115.30
1	C	97	LEU	CA-CB-CG	5.06	126.93	115.30
1	E	220	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2059	0	2054	59	0
1	B	2073	0	2075	49	0
1	C	2073	0	2065	76	0
1	D	2083	0	2080	52	0
1	E	2059	0	2054	97	0
1	F	2059	0	2054	91	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	5	0	0	2	0
3	E	10	0	0	3	0
4	E	12	0	12	22	0
4	F	24	0	24	27	0
5	A	53	0	0	3	0
5	B	43	0	0	1	0
5	C	53	0	0	1	0
5	D	60	0	0	3	0
5	E	40	0	0	7	0
5	F	64	0	0	5	0
All	All	12801	0	12418	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 17.

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:C:30:GLN:NE2	1:C:151:HIS:HB2	1.57	1.18
1:E:26:LEU:HD21	1:E:60:MSE:HE2	1.26	1.14
1:E:233:LEU:HD12	1:E:233:LEU:N	1.64	1.08
1:E:233:LEU:H	1:E:233:LEU:CD1	1.62	1.05
1:F:197:GLN:O	4:F:254:MES:H81	1.58	1.01
1:D:26:LEU:HD11	1:D:60:MSE:HE2	1.44	1.00
1:E:216:ARG:HH21	1:E:216:ARG:HG3	1.29	0.98
1:F:192:VAL:CG2	4:F:254:MES:H51	1.94	0.96
1:E:233:LEU:HD12	1:E:233:LEU:H	0.80	0.94
1:F:192:VAL:CG1	4:F:254:MES:H51	1.98	0.92
3:E:253:SO4:O2	4:E:255:MES:H32	1.68	0.92
1:F:198:HIS:ND1	4:F:253:MES:H32	1.85	0.91
1:D:102:ILE:HD13	1:D:107:LEU:HD13	1.54	0.89
1:D:100:TYR:HB2	1:D:220:LEU:HD21	1.56	0.88
1:E:182:ASP:O	1:E:216:ARG:HD3	1.73	0.87
1:E:26:LEU:CD2	1:E:60:MSE:HE2	2.04	0.87
1:E:214:ASN:HB3	5:E:289:HOH:O	1.74	0.86
1:C:102:ILE:HD13	1:C:107:LEU:HD13	1.54	0.86
1:C:223:ASP:OD2	1:C:225:LYS:HG2	1.75	0.85
1:E:185:ILE:HD11	1:E:213:ALA:HA	1.59	0.85
1:F:234:ARG:HH22	4:F:253:MES:H52	1.40	0.84
1:F:192:VAL:HG13	4:F:254:MES:C5	2.07	0.84
1:A:107:LEU:HG	1:A:206:GLN:HG3	1.60	0.83
1:F:192:VAL:HG22	4:F:254:MES:H51	1.58	0.83
1:B:121:VAL:HG13	1:B:163:ARG:HB2	1.59	0.82
1:A:26:LEU:HD21	1:A:60:MSE:HE2	1.62	0.82
1:C:30:GLN:HE21	1:C:151:HIS:HB2	1.39	0.81
1:D:26:LEU:HD11	1:D:60:MSE:CE	2.11	0.81
1:D:180:MSE:HE3	1:D:216:ARG:HH12	1.45	0.80
3:E:253:SO4:O2	4:E:255:MES:C3	2.30	0.80
1:F:192:VAL:HG13	4:F:254:MES:H51	1.63	0.79
1:A:209:VAL:HA	1:A:212:MSE:HE2	1.64	0.79
1:D:157[B]:ASN:HD22	1:D:157[B]:ASN:H	1.31	0.78
1:E:15:LYS:HD3	1:E:18:GLU:HG3	1.63	0.78
1:E:231:MSE:HB2	4:E:255:MES:C6	2.13	0.78
1:C:100:TYR:HB2	1:C:220:LEU:CD2	2.14	0.78
1:D:181:THR:HG22	1:D:182:ASP:H	1.48	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:254:MES:H62	5:F:300:HOH:O	1.84	0.77
1:C:-1:ASN:HD22	1:C:0:ALA:H	1.33	0.77
1:F:47:MSE:HE2	1:F:86:LYS:HB2	1.65	0.77
1:E:231:MSE:SE	4:E:255:MES:H62	2.35	0.76
1:F:192:VAL:CG1	4:F:254:MES:C5	2.63	0.76
1:F:198:HIS:ND1	4:F:253:MES:C3	2.47	0.76
1:A:158:LEU:H	1:A:158:LEU:HD12	1.49	0.76
1:D:119:GLN:HG2	5:D:307:HOH:O	1.87	0.74
1:E:233:LEU:HA	5:E:263:HOH:O	1.87	0.73
1:F:187:ILE:HD11	1:F:209:VAL:HG11	1.69	0.72
1:D:100:TYR:HB2	1:D:220:LEU:CD2	2.18	0.72
1:C:92:PHE:CE1	1:C:248:LYS:HB2	2.25	0.72
1:B:164:LEU:HD11	1:B:212:MSE:HE1	1.72	0.72
1:E:231:MSE:CB	4:E:255:MES:C6	2.68	0.71
1:F:197:GLN:O	4:F:254:MES:C8	2.38	0.71
1:E:5:THR:HB	5:E:277:HOH:O	1.91	0.71
1:D:157[B]:ASN:H	1:D:157[B]:ASN:ND2	1.86	0.71
1:F:160:ASP:N	1:F:160:ASP:OD2	2.22	0.71
1:F:198:HIS:CE1	4:F:253:MES:H21	2.26	0.70
1:C:100:TYR:HB2	1:C:220:LEU:HD21	1.73	0.70
1:B:55:GLU:OE1	1:B:55:GLU:HA	1.91	0.70
1:F:107:LEU:HD12	1:F:218:VAL:HG11	1.74	0.69
1:F:27:LEU:HD13	1:F:30:GLN:HB2	1.75	0.69
1:E:206:GLN:NE2	1:E:235:GLN:OE1	2.26	0.69
1:C:97:LEU:HD12	1:C:245:HIS:CD2	2.28	0.69
1:B:9:ILE:HD12	1:B:221:VAL:HG23	1.75	0.68
1:E:26:LEU:HD21	1:E:60:MSE:CE	2.15	0.68
1:F:1:MSE:SE	1:F:101:VAL:HG12	2.43	0.68
1:C:223:ASP:CG	1:C:224:GLY:H	1.97	0.68
1:C:69:LEU:HD22	1:C:251:ILE:HG21	1.76	0.68
1:E:229:LYS:HA	1:E:232:TYR:CD2	2.29	0.68
1:E:231:MSE:CB	4:E:255:MES:H62	2.24	0.68
1:C:54:ILE:HG13	1:C:55:GLU:N	2.08	0.68
1:A:102:ILE:HD13	1:A:107:LEU:HD13	1.76	0.67
1:C:1:MSE:HG2	1:C:101:VAL:CG1	2.25	0.67
1:F:192:VAL:CG2	1:F:197:GLN:HG2	2.25	0.67
1:E:32:LEU:HD12	1:E:32:LEU:H	1.57	0.66
1:A:185:ILE:HG23	1:A:218:VAL:HB	1.77	0.66
1:B:97:LEU:HD13	1:B:245:HIS:CE1	2.31	0.66
1:E:185:ILE:CD1	1:E:213:ALA:HA	2.25	0.66
1:E:231:MSE:O	1:E:233:LEU:N	2.29	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:231:MSE:O	1:E:234:ARG:N	2.29	0.65
1:B:230:ASP:OD2	1:B:234[B]:ARG:NH1	2.25	0.65
1:C:30:GLN:NE2	1:C:151:HIS:CB	2.49	0.65
1:E:198:HIS:HD2	4:E:255:MES:C3	2.09	0.65
1:B:121:VAL:CG1	1:B:163:ARG:HB2	2.26	0.64
1:A:178:ILE:HG22	1:A:187:ILE:HG22	1.79	0.64
1:E:233:LEU:CA	5:E:263:HOH:O	2.45	0.64
1:C:180:MSE:CE	1:C:216:ARG:HH12	2.10	0.64
4:F:253:MES:H51	4:F:254:MES:O2S	1.97	0.64
1:E:216:ARG:HG3	1:E:216:ARG:NH2	2.07	0.64
1:F:215:GLU:O	1:F:215:GLU:HG3	1.97	0.64
1:A:26:LEU:CD2	1:A:60:MSE:HE2	2.26	0.64
1:C:30:GLN:HE21	1:C:151:HIS:CB	2.09	0.64
1:F:112:ARG:HA	1:F:204:GLU:OE2	1.99	0.63
1:C:231:MSE:HA	1:C:234:ARG:HG2	1.79	0.63
1:C:190:PHE:C	1:C:190:PHE:CD2	2.71	0.63
1:E:47:MSE:HE1	1:E:82:VAL:HG22	1.80	0.63
1:A:157:ASN:HB2	1:A:158:LEU:HD12	1.81	0.63
1:E:231:MSE:HB2	4:E:255:MES:H61	1.79	0.63
1:E:47:MSE:HE2	1:E:83:LEU:HA	1.81	0.62
1:A:110:LEU:HD21	1:A:235:GLN:HG2	1.81	0.62
1:C:1:MSE:HG2	1:C:101:VAL:HG11	1.79	0.62
1:B:234[B]:ARG:HH21	1:B:234[B]:ARG:HG3	1.64	0.62
1:D:220:LEU:CD2	1:D:220:LEU:N	2.62	0.62
1:A:26:LEU:HD21	1:A:60:MSE:CE	2.28	0.62
1:E:198:HIS:CD2	4:E:255:MES:H21	2.34	0.61
1:E:102:ILE:HG21	1:E:107:LEU:HD13	1.82	0.61
1:A:0:ALA:HA	1:A:3:LYS:HD2	1.82	0.61
1:C:30:GLN:HE22	1:C:151:HIS:HB2	1.57	0.61
1:F:199:GLN:HB2	1:F:201:ILE:CD1	2.30	0.61
1:E:47:MSE:HE3	1:E:82:VAL:HG13	1.83	0.60
1:A:101:VAL:HG23	1:A:219:ILE:HG22	1.83	0.60
1:B:214:ASN:C	1:B:214:ASN:HD22	2.03	0.60
4:F:254:MES:H31	5:F:292:HOH:O	2.00	0.60
1:A:92:PHE:CD1	1:A:246:ILE:HD12	2.36	0.60
1:E:181:THR:HG22	1:E:183:LYS:H	1.67	0.60
1:F:185:ILE:HD11	1:F:209:VAL:CG1	2.32	0.60
1:C:28:PRO:HD2	1:C:29:PRO:HD2	1.84	0.60
1:D:180:MSE:HE3	1:D:216:ARG:NH1	2.15	0.60
1:D:121:VAL:HA	1:D:125:ASN:HD22	1.67	0.60
1:E:1:MSE:HA	1:E:4:ILE:HD12	1.83	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:TYR:CE2	1:C:71:PHE:HD1	2.20	0.60
1:D:161:ILE:HD12	1:D:177:ASP:HB3	1.84	0.60
1:C:115:ASP:OD2	1:C:115:ASP:N	2.35	0.59
1:C:223:ASP:CG	1:C:224:GLY:N	2.56	0.59
1:C:136:PHE:O	1:C:139:PRO:HD2	2.03	0.59
1:B:130:LEU:HD13	1:B:153:TYR:CE1	2.38	0.59
1:F:190:PHE:HZ	1:F:202:GLY:HA2	1.68	0.59
1:F:108:LYS:O	1:F:110:LEU:N	2.36	0.58
1:A:86:LYS:HE3	1:A:86:LYS:HA	1.84	0.58
1:D:213:ALA:O	1:D:214:ASN:HB2	2.01	0.58
1:D:220:LEU:O	1:D:220:LEU:HD23	2.02	0.58
1:F:1:MSE:HA	1:F:4:ILE:HD12	1.84	0.58
1:B:231:MSE:HE3	1:B:235:GLN:OE1	2.04	0.58
1:E:17:THR:HG22	1:E:24:ILE:HB	1.86	0.58
1:F:198:HIS:CE1	4:F:253:MES:C2	2.87	0.58
1:B:234[B]:ARG:HG3	1:B:234[B]:ARG:NH2	2.19	0.58
1:D:103:GLU:OE2	1:D:103:GLU:HA	2.04	0.58
1:E:26:LEU:CD2	1:E:60:MSE:CE	2.77	0.58
1:C:12:ASP:O	1:C:36:SER:HB3	2.04	0.57
1:F:28:PRO:N	1:F:29:PRO:HD2	2.19	0.57
1:A:158:LEU:HD12	1:A:158:LEU:N	2.18	0.57
1:D:220:LEU:N	1:D:220:LEU:HD22	2.20	0.57
1:A:49:GLN:HG3	5:A:288:HOH:O	2.03	0.57
1:F:192:VAL:CB	4:F:254:MES:H51	2.34	0.57
1:C:-1:ASN:HD22	1:C:0:ALA:N	2.02	0.57
1:E:234:ARG:HD2	4:E:255:MES:H52	1.85	0.56
1:B:107:LEU:HD22	1:B:206:GLN:HG3	1.87	0.56
1:A:121:VAL:HG12	1:A:165:VAL:HG23	1.88	0.56
1:A:157:ASN:O	1:A:159:ASP:N	2.38	0.56
1:E:231:MSE:O	1:E:234:ARG:HB2	2.05	0.56
1:A:134:ASP:OD2	1:A:149:LYS:HD2	2.05	0.56
1:E:198:HIS:HD2	4:E:255:MES:H31	1.70	0.56
1:C:1:MSE:HG3	1:C:103:GLU:HG3	1.88	0.56
1:F:202:GLY:O	1:F:206:GLN:HG2	2.06	0.56
1:D:49:GLN:HG2	5:D:310:HOH:O	2.07	0.55
1:F:195:GLU:N	1:F:195:GLU:OE1	2.39	0.55
1:E:231:MSE:CB	4:E:255:MES:H61	2.34	0.55
1:B:69:LEU:HD22	1:B:251:ILE:HG21	1.87	0.55
1:A:157:ASN:O	1:A:158:LEU:C	2.44	0.55
1:B:9:ILE:CD1	1:B:221:VAL:HG23	2.37	0.55
1:D:-1:ASN:HD22	1:D:2:SER:H	1.55	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:113:LYS:O	1:D:115:ASP:N	2.39	0.55
1:E:231:MSE:HB3	4:E:255:MES:H62	1.89	0.55
1:B:109:GLU:HB3	5:B:281:HOH:O	2.06	0.54
1:A:44:MSE:HE1	1:A:79:ILE:HG12	1.88	0.54
1:C:12:ASP:O	1:C:36:SER:CB	2.55	0.54
1:F:198:HIS:CE1	4:F:253:MES:C3	2.90	0.54
1:B:209:VAL:HA	1:B:212:MSE:HE3	1.88	0.54
1:F:15:LYS:HD2	1:F:18:GLU:OE1	2.07	0.54
1:E:231:MSE:O	1:E:232:TYR:C	2.46	0.54
1:F:223:ASP:O	1:F:226:ASP:HB2	2.08	0.54
1:C:250:ASN:HD22	1:C:250:ASN:H	1.55	0.54
1:B:22:LYS:HD3	1:B:39:TRP:CZ3	2.42	0.53
1:F:129:TYR:HD2	1:F:130:LEU:HD13	1.72	0.53
1:F:84:LEU:HD13	1:F:88:ARG:HH22	1.73	0.53
1:E:198:HIS:CD2	4:E:255:MES:H31	2.44	0.53
1:A:30:GLN:OE1	1:A:151:HIS:ND1	2.41	0.53
1:A:98:GLU:OE2	1:A:229:LYS:HE3	2.08	0.53
1:A:186:GLU:HA	1:A:219:ILE:O	2.08	0.53
1:B:130:LEU:CD1	1:B:153:TYR:CE1	2.91	0.52
1:D:97:LEU:HD13	1:D:245:HIS:CD2	2.44	0.52
1:F:181:THR:HG22	1:F:182:ASP:H	1.74	0.52
1:D:1:MSE:HA	1:D:4:ILE:CD1	2.40	0.52
1:B:146:ASN:O	1:B:150:GLN:HG3	2.10	0.52
1:E:32:LEU:HD12	1:E:32:LEU:N	2.25	0.52
1:A:73:PHE:HB3	1:A:74:PRO:CD	2.39	0.52
1:C:39:TRP:CD1	1:C:57:GLN:NE2	2.77	0.52
1:C:44:MSE:HE1	1:C:78:LYS:O	2.09	0.52
1:C:185:ILE:HD12	1:C:186:GLU:N	2.24	0.52
1:F:231:MSE:HE3	1:F:235:GLN:NE2	2.25	0.52
1:E:234:ARG:CD	4:E:255:MES:H52	2.39	0.52
1:F:157:ASN:HB3	5:F:304:HOH:O	2.09	0.52
1:C:13:GLY:HA2	1:C:27:LEU:HD13	1.91	0.52
1:C:180:MSE:CE	1:C:216:ARG:NH1	2.72	0.52
1:F:114:ARG:NH1	1:F:116:VAL:O	2.42	0.52
1:F:198:HIS:CE1	4:F:253:MES:H32	2.44	0.52
1:E:198:HIS:HD2	4:E:255:MES:H21	1.74	0.52
1:D:220:LEU:CD2	1:D:220:LEU:H	2.21	0.51
1:F:138:ARG:N	5:F:268:HOH:O	2.30	0.51
1:A:26:LEU:CD2	1:A:60:MSE:CE	2.86	0.51
1:C:27:LEU:HD23	1:C:30:GLN:HB2	1.91	0.51
1:B:209:VAL:HA	1:B:212:MSE:CE	2.41	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:250:ASN:HD21	1:E:199:GLN:HE22	1.58	0.51
1:D:5:THR:HB	5:D:280:HOH:O	2.09	0.51
1:E:206:GLN:NE2	1:E:235:GLN:CD	2.63	0.51
1:C:97:LEU:HD12	1:C:245:HIS:HD2	1.73	0.51
1:C:220:LEU:HD23	1:C:220:LEU:O	2.10	0.51
1:C:41:TYR:CE2	1:C:71:PHE:CD1	2.98	0.51
1:D:97:LEU:O	1:D:242:PHE:HA	2.11	0.51
1:C:30:GLN:HE21	1:C:151:HIS:CG	2.29	0.51
1:D:-1:ASN:ND2	1:D:1:MSE:H	2.07	0.51
1:D:180:MSE:HE3	1:D:216:ARG:HH22	1.76	0.51
1:F:171:GLN:HE21	1:F:172:PRO:HD2	1.76	0.51
1:F:192:VAL:HG21	4:F:254:MES:H51	1.90	0.50
1:A:168:VAL:HG12	1:A:169:ASN:ND2	2.26	0.50
1:A:199:GLN:OE1	1:B:88:ARG:NH2	2.44	0.50
1:E:234:ARG:HD2	4:E:255:MES:C5	2.41	0.50
1:F:185:ILE:HD11	1:F:209:VAL:HG13	1.93	0.50
1:A:50:TRP:CZ2	1:A:54:ILE:HD11	2.47	0.50
1:C:223:ASP:OD2	1:C:224:GLY:N	2.45	0.50
1:E:198:HIS:HD2	4:E:255:MES:C2	2.24	0.50
1:C:195:GLU:O	1:C:195:GLU:HG2	2.11	0.50
1:E:178:ILE:HG23	1:E:185:ILE:CG2	2.42	0.50
1:E:208:TYR:HE2	1:E:212:MSE:HE3	1.75	0.50
1:E:213:ALA:O	1:E:214:ASN:HB2	2.11	0.50
1:E:231:MSE:C	1:E:233:LEU:N	2.65	0.50
1:A:50:TRP:CH2	1:A:54:ILE:HD11	2.47	0.49
1:B:223:ASP:OD1	1:B:225:LYS:HG3	2.11	0.49
1:A:16:ILE:HG13	1:A:26:LEU:HD22	1.92	0.49
1:E:229:LYS:O	1:E:232:TYR:N	2.40	0.49
1:E:231:MSE:HB3	4:E:255:MES:C6	2.40	0.49
1:E:206:GLN:NE2	1:E:235:GLN:NE2	2.60	0.49
1:E:230:ASP:O	1:E:233:LEU:CD1	2.60	0.49
1:E:234:ARG:HD2	4:E:255:MES:H61	1.94	0.49
1:F:112:ARG:HB2	1:F:112:ARG:CZ	2.42	0.49
1:B:19:ASP:OD2	1:B:21:ARG:N	2.40	0.49
1:D:206:GLN:NE2	1:D:237:TYR:OH	2.46	0.49
1:F:96:VAL:HG22	1:F:244:TYR:CE1	2.48	0.49
1:B:41:TYR:CZ	1:B:45:PRO:HG3	2.48	0.49
1:C:46:THR:H	1:C:49:GLN:HE21	1.61	0.49
1:C:190:PHE:CZ	1:C:231:MSE:HE1	2.48	0.49
1:E:163:ARG:HG2	1:E:177:ASP:OD2	2.12	0.49
1:F:231:MSE:HE3	1:F:235:GLN:HE22	1.78	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ILE:HG21	1:B:26:LEU:HB2	1.94	0.49
1:D:215:GLU:HA	1:D:215:GLU:OE1	2.13	0.49
1:F:107:LEU:HD12	1:F:218:VAL:CG1	2.43	0.49
1:F:192:VAL:HG22	4:F:254:MES:C5	2.38	0.48
1:F:197:GLN:HA	4:F:254:MES:H72	1.95	0.48
1:E:230:ASP:O	1:E:233:LEU:HD13	2.13	0.48
1:F:168:VAL:O	1:F:169:ASN:HB2	2.12	0.48
1:E:96:VAL:HG22	1:E:244:TYR:CE1	2.49	0.48
1:B:190:PHE:C	1:B:190:PHE:CD2	2.86	0.48
1:E:187:ILE:HD11	1:E:209:VAL:HG11	1.95	0.48
1:C:185:ILE:HD12	1:C:185:ILE:C	2.33	0.48
1:D:220:LEU:HD23	1:D:220:LEU:C	2.34	0.48
1:E:223:ASP:OD1	1:E:224:GLY:N	2.46	0.48
1:E:231:MSE:HE3	1:E:235:GLN:NE2	2.29	0.48
1:B:28:PRO:HD2	1:B:29:PRO:HD3	1.96	0.47
1:E:41:TYR:CZ	1:E:45:PRO:HG3	2.49	0.47
1:E:200:GLY:N	4:E:255:MES:O2S	2.44	0.47
1:A:185:ILE:HG21	1:A:213:ALA:HB2	1.96	0.47
1:C:223:ASP:O	1:C:229:LYS:HE2	2.14	0.47
1:F:17:THR:CG2	1:F:24:ILE:HD12	2.44	0.47
1:F:105:LYS:O	1:F:109:GLU:HB2	2.14	0.47
1:B:132:VAL:HG13	1:B:193:LEU:HD13	1.97	0.47
1:B:195:GLU:H	1:B:195:GLU:CD	2.15	0.47
1:E:233:LEU:HB3	5:E:263:HOH:O	2.13	0.47
1:A:5:THR:HB	5:A:269:HOH:O	2.14	0.47
1:A:32:LEU:HD21	5:E:279:HOH:O	2.13	0.47
1:C:15:LYS:HD2	1:C:18:GLU:HG3	1.97	0.47
1:D:161:ILE:CD1	1:D:177:ASP:HB3	2.45	0.47
1:E:206:GLN:HE22	1:E:235:GLN:CD	2.18	0.47
1:F:10:TYR:CZ	1:F:12:ASP:HB3	2.49	0.47
1:F:128:ASP:HB3	1:F:172:PRO:HB3	1.96	0.47
1:C:1:MSE:HG2	1:C:101:VAL:HG12	1.96	0.47
1:E:206:GLN:HE22	1:E:235:GLN:NE2	2.13	0.47
1:A:229:LYS:NZ	5:A:270:HOH:O	2.48	0.47
1:C:28:PRO:CD	1:C:29:PRO:HD2	2.44	0.47
1:D:-1:ASN:O	1:D:3:LYS:HG3	2.15	0.47
1:F:84:LEU:HD13	1:F:88:ARG:NH2	2.29	0.47
1:A:114:ARG:HD2	1:A:204:GLU:HG2	1.96	0.46
1:A:121:VAL:HA	1:A:125:ASN:OD1	2.15	0.46
1:D:73:PHE:O	1:D:243:LYS:HG2	2.15	0.46
1:C:132:VAL:HG13	1:C:193:LEU:HD13	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:165:VAL:HG23	1:D:175:ILE:HG22	1.97	0.46
1:B:206:GLN:NE2	1:B:237:TYR:OH	2.49	0.46
1:E:105:LYS:HD3	1:E:105:LYS:N	2.30	0.46
1:B:104:ALA:O	1:B:108:LYS:HD3	2.15	0.46
1:C:61:HIS:CE1	1:C:68:HIS:CE1	3.03	0.46
1:C:167:TYR:HA	1:C:171:GLN:O	2.15	0.46
1:D:120:LEU:O	1:D:125:ASN:ND2	2.47	0.46
1:C:52:LYS:O	1:C:56:VAL:HG23	2.16	0.46
1:E:223:ASP:HB3	1:E:226:ASP:HB2	1.97	0.46
1:F:47:MSE:HE3	1:F:82:VAL:HG22	1.98	0.46
1:F:10:TYR:OH	1:F:12:ASP:HB3	2.15	0.46
1:A:98:GLU:HG2	1:A:239:TYR:HE1	1.80	0.46
1:F:234:ARG:NH2	4:F:253:MES:H52	2.21	0.46
1:C:2:SER:HB2	5:C:279:HOH:O	2.16	0.46
1:A:47:MSE:SE	1:A:86:LYS:HD2	2.67	0.45
1:F:224:GLY:O	1:F:229:LYS:HE3	2.17	0.45
1:A:97:LEU:HD12	1:A:223:ASP:HB3	1.98	0.45
1:A:190:PHE:C	1:A:190:PHE:CD2	2.89	0.45
1:B:234[B]:ARG:HH21	1:B:234[B]:ARG:CG	2.29	0.45
1:F:192:VAL:HG23	1:F:197:GLN:HG2	1.98	0.45
1:F:201:ILE:N	1:F:201:ILE:HD12	2.32	0.45
1:A:31:PRO:HG2	1:A:32:LEU:HD22	1.98	0.45
1:B:171:GLN:HA	1:B:172:PRO:HD3	1.68	0.45
1:E:173:VAL:CG2	1:E:196:PHE:CG	3.00	0.45
1:E:231:MSE:HG2	1:E:232:TYR:N	2.30	0.45
1:F:107:LEU:HD22	1:F:206:GLN:HB3	1.98	0.45
1:A:10:TYR:HE2	1:A:12:ASP:HB2	1.81	0.45
1:D:117:ASP:C	1:D:117:ASP:OD1	2.56	0.45
1:D:180:MSE:CE	1:D:216:ARG:HH22	2.30	0.45
1:F:28:PRO:CD	1:F:29:PRO:HD2	2.47	0.45
1:C:50:TRP:O	1:C:54:ILE:HG23	2.17	0.44
1:E:229:LYS:O	1:E:230:ASP:C	2.55	0.44
1:B:162:GLU:HG2	1:B:180:MSE:HE2	1.99	0.44
1:C:41:TYR:HE2	1:C:71:PHE:CD1	2.36	0.44
1:A:111:SER:O	1:A:112:ARG:HD3	2.18	0.44
1:C:173:VAL:HG22	1:C:196:PHE:CD2	2.53	0.44
1:F:193:LEU:O	1:F:197:GLN:HG3	2.17	0.44
1:E:96:VAL:O	1:E:224:GLY:N	2.46	0.44
1:C:121:VAL:HA	1:C:125:ASN:OD1	2.18	0.44
1:F:209:VAL:HA	1:F:212:MSE:HG2	1.99	0.44
1:A:206:GLN:NE2	1:A:237:TYR:OH	2.51	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ALA:O	1:A:214:ASN:HB2	2.17	0.44
1:B:163:ARG:HG3	1:B:163:ARG:HH11	1.82	0.44
1:E:160:ASP:OD1	1:E:160:ASP:N	2.50	0.44
1:E:121:VAL:HA	1:E:125:ASN:OD1	2.18	0.44
1:E:229:LYS:HA	1:E:232:TYR:HD2	1.82	0.44
1:E:173:VAL:HG21	1:E:196:PHE:CD1	2.53	0.43
1:E:231:MSE:HE3	1:E:235:GLN:CD	2.38	0.43
1:D:167:TYR:HA	1:D:171:GLN:O	2.18	0.43
1:C:25:TYR:O	1:C:37:ASN:HA	2.18	0.43
1:A:93:GLN:O	1:A:246:ILE:HA	2.19	0.43
1:D:1:MSE:HA	1:D:4:ILE:HD12	2.01	0.43
1:F:10:TYR:CD2	1:F:179:ILE:HD12	2.54	0.43
1:E:231:MSE:HB2	1:E:234:ARG:HD2	2.01	0.43
1:F:82:VAL:CG1	1:F:83:LEU:N	2.82	0.43
1:A:157:ASN:HB2	1:A:158:LEU:H	1.51	0.43
1:D:107:LEU:HG	1:D:206:GLN:HG3	2.00	0.43
1:E:233:LEU:N	1:E:233:LEU:CD1	2.32	0.43
3:E:253:SO4:O2	4:E:255:MES:N4	2.51	0.43
1:A:180:MSE:HG2	1:A:185:ILE:HD12	2.01	0.43
1:C:180:MSE:HE2	1:C:216:ARG:HH12	1.80	0.43
1:F:90:LEU:HD12	1:F:90:LEU:HA	1.87	0.43
1:B:97:LEU:HG	1:B:221:VAL:HG11	2.01	0.43
1:C:78:LYS:NZ	3:D:253:SO4:O1	2.52	0.43
1:D:31:PRO:HG2	1:D:32:LEU:HD13	2.00	0.43
1:E:31:PRO:HD2	1:E:32:LEU:HD12	2.00	0.43
1:B:16:ILE:CG2	1:B:26:LEU:HB2	2.49	0.42
1:F:1:MSE:SE	1:F:101:VAL:CG1	3.16	0.42
4:F:254:MES:H82	4:F:254:MES:H32	1.06	0.42
1:A:231:MSE:O	1:A:235:GLN:HB2	2.19	0.42
1:D:161:ILE:HD11	1:D:163:ARG:CZ	2.49	0.42
1:E:22:LYS:HD2	1:E:39:TRP:CZ3	2.54	0.42
1:A:0:ALA:O	1:A:3:LYS:HG2	2.18	0.42
1:A:67:TYR:O	1:A:251:ILE:HG13	2.20	0.42
1:D:-1:ASN:ND2	1:D:1:MSE:N	2.68	0.42
1:F:7:LYS:HB2	1:F:7:LYS:HE2	1.25	0.42
1:C:100:TYR:HB2	1:C:220:LEU:HD23	2.00	0.42
1:D:203:SER:HB2	3:D:253:SO4:O3	2.19	0.42
1:E:60:MSE:HE3	5:F:312:HOH:O	2.18	0.42
1:E:101:VAL:HG12	1:E:219:ILE:HG22	2.00	0.42
1:F:22:LYS:HD2	1:F:39:TRP:CZ3	2.55	0.42
1:D:80:ASP:N	1:D:80:ASP:OD2	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:LYS:HB2	1:E:15:LYS:HE3	1.87	0.42
1:E:105:LYS:CD	1:E:105:LYS:H	2.33	0.42
1:E:194:GLU:HA	1:E:197:GLN:HG3	2.01	0.42
1:C:187:ILE:HD13	1:C:187:ILE:HG21	1.83	0.42
1:E:44:MSE:HE3	1:E:45:PRO:O	2.19	0.42
1:F:234:ARG:HH12	4:F:253:MES:H81	1.85	0.42
1:A:196:PHE:HB3	1:A:201:ILE:HD12	2.01	0.42
1:B:194:GLU:HG2	1:B:195:GLU:N	2.34	0.42
1:C:4:ILE:HD11	1:C:217:PRO:HG2	2.01	0.42
1:E:240:GLN:HG3	1:E:240:GLN:O	2.19	0.42
1:F:187:ILE:HB	1:F:220:LEU:HB3	2.02	0.42
1:C:107:LEU:O	1:C:110:LEU:HB2	2.19	0.42
1:E:82:VAL:HG13	1:E:83:LEU:N	2.34	0.42
1:F:28:PRO:HD2	1:F:29:PRO:HD2	2.01	0.42
1:B:107:LEU:HD12	1:B:218:VAL:HG21	2.02	0.42
1:C:27:LEU:HG	1:C:29:PRO:HG2	2.02	0.42
1:D:233:LEU:HD12	1:D:233:LEU:HA	1.86	0.42
1:A:33:LYS:HA	1:A:147:MSE:HE1	2.02	0.42
1:B:214:ASN:C	1:B:214:ASN:ND2	2.72	0.42
1:E:171:GLN:HG3	5:E:265:HOH:O	2.19	0.42
1:F:57:GLN:OE1	1:F:69:LEU:HA	2.20	0.42
1:F:19:ASP:OD1	1:F:22:LYS:NZ	2.53	0.41
1:F:192:VAL:HG13	4:F:254:MES:H52	1.95	0.41
1:B:22:LYS:HD3	1:B:39:TRP:CE3	2.55	0.41
1:D:-1:ASN:HD21	1:D:1:MSE:H	1.67	0.41
1:A:41:TYR:CZ	1:A:45:PRO:HG3	2.56	0.41
1:F:199:GLN:HB2	1:F:201:ILE:HD13	1.99	0.41
1:C:4:ILE:HD11	1:C:217:PRO:CG	2.50	0.41
1:E:242:PHE:CD1	1:E:242:PHE:C	2.94	0.41
1:C:105:LYS:H	1:C:105:LYS:HG2	1.71	0.41
1:F:180:MSE:HG2	1:F:185:ILE:CG2	2.50	0.41
1:A:158:LEU:N	1:A:158:LEU:CD1	2.83	0.41
1:A:128:ASP:HB3	1:A:172:PRO:HB3	2.01	0.41
1:B:107:LEU:HD22	1:B:206:GLN:CG	2.51	0.41
1:C:138:ARG:N	1:C:139:PRO:CD	2.84	0.41
1:F:9:ILE:HG21	1:F:221:VAL:HG13	2.02	0.41
1:B:7:LYS:HE3	1:B:7:LYS:HB2	1.87	0.41
1:C:73:PHE:O	1:C:243:LYS:HG3	2.21	0.41
1:E:231:MSE:CG	1:E:232:TYR:N	2.84	0.41
1:C:47:MSE:HE3	1:C:47:MSE:HB3	2.01	0.41
1:C:206:GLN:NE2	1:C:237:TYR:OH	2.54	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:231:MSE:SE	1:C:235:GLN:HE22	2.54	0.41
1:E:82:VAL:CG1	1:E:83:LEU:N	2.84	0.41
1:F:201:ILE:HD12	1:F:201:ILE:H	1.86	0.41
1:A:225:LYS:HE3	1:A:225:LYS:HB3	1.93	0.40
1:B:106:ALA:O	1:B:110:LEU:HD13	2.21	0.40
1:C:226:ASP:O	1:C:229:LYS:HG3	2.21	0.40
1:F:84:LEU:HD23	1:F:84:LEU:HA	1.87	0.40
1:B:68:HIS:HD2	1:B:70:SER:HB2	1.86	0.40
1:B:86:LYS:HE2	1:B:90:LEU:HD22	2.03	0.40
1:B:97:LEU:HG	1:B:221:VAL:CG1	2.51	0.40
1:F:107:LEU:HD23	1:F:107:LEU:HA	1.91	0.40
1:D:110:LEU:HD23	1:D:206:GLN:HB3	2.03	0.40
1:F:1:MSE:HE3	1:F:1:MSE:HB3	1.84	0.40
1:F:129:TYR:CD2	1:F:129:TYR:C	2.94	0.40
1:F:173:VAL:HA	1:F:193:LEU:HD12	2.02	0.40
1:C:190:PHE:CD2	1:C:191:GLY:N	2.89	0.40
1:C:250:ASN:O	1:C:251:ILE:HG12	2.21	0.40
1:D:220:LEU:HD22	1:D:220:LEU:H	1.83	0.40
1:F:57:GLN:HA	1:F:60:MSE:HE2	2.03	0.40
1:F:171:GLN:NE2	1:F:172:PRO:HD2	2.36	0.40
1:F:192:VAL:CG1	4:F:254:MES:H52	2.47	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	250/254 (98%)	238 (95%)	10 (4%)	2 (1%)	19 23
1	B	252/254 (99%)	240 (95%)	11 (4%)	1 (0%)	34 41
1	C	252/254 (99%)	234 (93%)	17 (7%)	1 (0%)	34 41
1	D	254/254 (100%)	241 (95%)	11 (4%)	2 (1%)	19 23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	250/254 (98%)	231 (92%)	16 (6%)	3 (1%)	13	13
1	F	250/254 (98%)	232 (93%)	11 (4%)	7 (3%)	5	3
All	All	1508/1524 (99%)	1416 (94%)	76 (5%)	16 (1%)	14	15

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	LEU
1	D	114	ARG
1	F	109	GLU
1	A	157	ASN
1	F	112	ARG
1	D	214	ASN
1	E	214	ASN
1	F	228	ALA
1	B	214	ASN
1	C	-1	ASN
1	E	230	ASP
1	E	232	TYR
1	F	111	SER
1	F	3	LYS
1	F	108	LYS
1	F	173	VAL

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	225/219 (103%)	197 (88%)	28 (12%)	4	4
1	B	227/219 (104%)	191 (84%)	36 (16%)	2	2
1	C	227/219 (104%)	184 (81%)	43 (19%)	1	1
1	D	229/219 (105%)	203 (89%)	26 (11%)	5	6
1	E	225/219 (103%)	195 (87%)	30 (13%)	4	4

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	225/219 (103%)	183 (81%)	42 (19%)	1 1
All	All	1358/1314 (103%)	1153 (85%)	205 (15%)	3 2

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	5	THR
1	A	17	THR
1	A	21	ARG
1	A	26	LEU
1	A	30	GLN
1	A	49	GLN
1	A	51	LEU
1	A	86	LYS
1	A	97	LEU
1	A	103	GLU
1	A	107	LEU
1	A	110	LEU
1	A	111	SER
1	A	112	ARG
1	A	134	ASP
1	A	147	MSE
1	A	158	LEU
1	A	162	GLU
1	A	169	ASN
1	A	173	VAL
1	A	178	ILE
1	A	218	VAL
1	A	225	LYS
1	A	227	THR
1	A	230	ASP
1	A	233	LEU
1	A	235	GLN
1	B	2	SER
1	B	3	LYS
1	B	7	LYS
1	B	11	ILE
1	B	16	ILE
1	B	20	SER
1	B	21	ARG
1	B	22	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	26	LEU
1	B	42	LYS
1	B	43	THR
1	B	48	ASN
1	B	49	GLN
1	B	51	LEU
1	B	69	LEU
1	B	83	LEU
1	B	84	LEU
1	B	86	LYS
1	B	90	LEU
1	B	105	LYS
1	B	109	GLU
1	B	110	LEU
1	B	115	ASP
1	B	121	VAL
1	B	143	SER
1	B	147	MSE
1	B	154	SER
1	B	158	LEU
1	B	173	VAL
1	B	193	LEU
1	B	194	GLU
1	B	195	GLU
1	B	212	MSE
1	B	214	ASN
1	B	225	LYS
1	B	229	LYS
1	C	-2	SER
1	C	-1	ASN
1	C	1	MSE
1	C	7	LYS
1	C	14	ASN
1	C	15	LYS
1	C	16	ILE
1	C	17	THR
1	C	18	GLU
1	C	21	ARG
1	C	22	LYS
1	C	26	LEU
1	C	44	MSE
1	C	51	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	54	ILE
1	C	59	LYS
1	C	62	LEU
1	C	69	LEU
1	C	70	SER
1	C	84	LEU
1	C	105	LYS
1	C	107	LEU
1	C	108	LYS
1	C	110	LEU
1	C	115	ASP
1	C	123	SER
1	C	138	ARG
1	C	147	MSE
1	C	158	LEU
1	C	171	GLN
1	C	173	VAL
1	C	185	ILE
1	C	187	ILE
1	C	193	LEU
1	C	195	GLU
1	C	220	LEU
1	C	229	LYS
1	C	231	MSE
1	C	233	LEU
1	C	234	ARG
1	C	238	VAL
1	C	248	LYS
1	C	250	ASN
1	D	-1	ASN
1	D	22	LYS
1	D	32	LEU
1	D	49	GLN
1	D	51	LEU
1	D	58	LYS
1	D	62	LEU
1	D	69	LEU
1	D	80	ASP
1	D	83	LEU
1	D	90	LEU
1	D	107	LEU
1	D	110	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	115	ASP
1	D	130	LEU
1	D	134	ASP
1	D	143	SER
1	D	147	MSE
1	D	161	ILE
1	D	173	VAL
1	D	176	VAL
1	D	181	THR
1	D	199	GLN
1	D	220	LEU
1	D	233	LEU
1	D	238	VAL
1	E	22	LYS
1	E	26	LEU
1	E	32	LEU
1	E	62	LEU
1	E	72	SER
1	E	97	LEU
1	E	99	LEU
1	E	105	LYS
1	E	120	LEU
1	E	123	SER
1	E	130	LEU
1	E	143	SER
1	E	154	SER
1	E	155	SER
1	E	158	LEU
1	E	160	ASP
1	E	171	GLN
1	E	173	VAL
1	E	179	ILE
1	E	187	ILE
1	E	192	VAL
1	E	206	GLN
1	E	214	ASN
1	E	216	ARG
1	E	218	VAL
1	E	221	VAL
1	E	225	LYS
1	E	230	ASP
1	E	233	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	234	ARG
1	F	1	MSE
1	F	2	SER
1	F	3	LYS
1	F	7	LYS
1	F	9	ILE
1	F	22	LYS
1	F	26	LEU
1	F	27	LEU
1	F	42	LYS
1	F	47	MSE
1	F	48	ASN
1	F	52	LYS
1	F	60	MSE
1	F	62	LEU
1	F	80	ASP
1	F	82	VAL
1	F	83	LEU
1	F	84	LEU
1	F	86	LYS
1	F	90	LEU
1	F	103	GLU
1	F	110	LEU
1	F	112	ARG
1	F	130	LEU
1	F	134	ASP
1	F	158	LEU
1	F	160	ASP
1	F	162	GLU
1	F	165	VAL
1	F	168	VAL
1	F	169	ASN
1	F	182	ASP
1	F	195	GLU
1	F	203	SER
1	F	206	GLN
1	F	218	VAL
1	F	220	LEU
1	F	225	LYS
1	F	227	THR
1	F	229	LYS
1	F	233	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	238	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	49	GLN
1	A	169	ASN
1	A	171	GLN
1	A	206	GLN
1	B	30	GLN
1	B	49	GLN
1	B	150	GLN
1	B	151	HIS
1	B	206	GLN
1	B	214	ASN
1	B	245	HIS
1	C	-1	ASN
1	C	30	GLN
1	C	48	ASN
1	C	49	GLN
1	C	206	GLN
1	C	245	HIS
1	C	250	ASN
1	D	-1	ASN
1	D	14	ASN
1	D	49	GLN
1	D	119	GLN
1	D	125	ASN
1	D	206	GLN
1	E	14	ASN
1	E	48	ASN
1	E	63	ASN
1	E	157	ASN
1	E	198	HIS
1	E	199	GLN
1	E	206	GLN
1	E	235	GLN
1	E	250	ASN
1	F	171	GLN
1	F	235	GLN

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)

Of 17 ligands modelled in this entry, 6 are monoatomic - leaving 11 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	SO4	B	254	-	4,4,4	0.30	0	6,6,6	0.57	0
3	SO4	B	253	-	4,4,4	0.20	0	6,6,6	0.49	0
3	SO4	E	253	-	4,4,4	0.26	0	6,6,6	0.23	0
4	MES	E	255	-	12,12,12	2.81	1 (8%)	15,16,16	2.78	10 (66%)
4	MES	F	254	-	12,12,12	2.16	3 (25%)	15,16,16	3.77	11 (73%)
3	SO4	A	253	-	4,4,4	0.23	0	6,6,6	0.52	0
3	SO4	D	253	-	4,4,4	0.24	0	6,6,6	0.29	0
3	SO4	C	253	-	4,4,4	0.36	0	6,6,6	0.60	0
3	SO4	E	254	-	4,4,4	0.56	0	6,6,6	0.38	0
3	SO4	C	254	-	4,4,4	0.32	0	6,6,6	0.28	0
4	MES	F	253	-	12,12,12	2.08	1 (8%)	15,16,16	2.80	8 (53%)

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
4	MES	E	255	-	-	1/6/14/14	0/1/1/1
4	MES	F	254	-	-	2/6/14/14	0/1/1/1
4	MES	F	253	-	-	2/6/14/14	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	255	MES	C8-S	-9.27	1.64	1.77
4	F	254	MES	C8-S	-6.52	1.68	1.77
4	F	253	MES	C8-S	-6.34	1.68	1.77
4	F	254	MES	O2S-S	2.56	1.52	1.45
4	F	254	MES	O1S-S	2.16	1.51	1.45

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	254	MES	O1S-S-C8	9.23	120.67	106.73
4	F	253	MES	C5-N4-C3	6.87	123.65	108.84
4	E	255	MES	C5-N4-C3	5.69	121.10	108.84
4	F	254	MES	C6-C5-N4	5.22	118.05	110.12
4	F	254	MES	C5-N4-C3	4.70	118.97	108.84
4	F	254	MES	C8-C7-N4	-4.48	95.41	112.36
4	F	253	MES	C7-N4-C5	4.43	123.03	111.24
4	E	255	MES	O2S-S-C8	3.84	112.53	106.73
4	F	253	MES	O2S-S-C8	3.70	112.33	106.73
4	E	255	MES	C8-C7-N4	-3.60	98.73	112.36
4	F	254	MES	C7-N4-C5	3.58	120.78	111.24
4	E	255	MES	O1S-S-C8	3.40	111.86	106.73
4	F	254	MES	C7-N4-C3	3.36	120.19	111.24
4	E	255	MES	C7-N4-C5	3.28	119.97	111.24
4	F	254	MES	C2-C3-N4	-3.12	105.37	110.12
4	E	255	MES	C7-N4-C3	2.89	118.93	111.24
4	F	254	MES	O3S-S-O1S	-2.65	104.77	111.40
4	F	253	MES	O1-C6-C5	-2.60	106.18	111.77
4	F	253	MES	O1-C2-C3	-2.59	106.19	111.77
4	E	255	MES	C2-C3-N4	-2.50	106.31	110.12
4	E	255	MES	O1-C2-C3	-2.43	106.54	111.77
4	F	253	MES	O2S-S-O1S	-2.31	106.33	113.82
4	F	254	MES	O3S-S-O2S	-2.30	105.64	111.40
4	F	254	MES	O2S-S-C8	-2.30	103.26	106.73
4	E	255	MES	O2S-S-O1S	-2.23	106.56	113.82
4	E	255	MES	C6-C5-N4	-2.21	106.77	110.12
4	F	254	MES	O1-C2-C3	-2.20	107.03	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	253	MES	C6-C5-N4	-2.19	106.80	110.12
4	F	253	MES	C8-C7-N4	-2.16	104.18	112.36

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	254	MES	C8-C7-N4-C3
4	E	255	MES	C8-C7-N4-C5
4	F	253	MES	C8-C7-N4-C3
4	F	254	MES	N4-C7-C8-S
4	F	253	MES	C8-C7-N4-C5

There are no ring outliers.

5 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	253	SO4	3	0
4	E	255	MES	22	0
4	F	254	MES	18	0
3	D	253	SO4	2	0
4	F	253	MES	10	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	244/254 (96%)	0.01	0	100	100	13, 21, 34, 47	0
1	B	244/254 (96%)	-0.03	1 (0%)	92	95	10, 20, 31, 46	0
1	C	246/254 (96%)	0.17	5 (2%)	65	72	7, 23, 38, 57	0
1	D	245/254 (96%)	0.02	1 (0%)	92	95	12, 21, 35, 47	0
1	E	244/254 (96%)	0.06	5 (2%)	65	72	10, 20, 39, 49	0
1	F	244/254 (96%)	0.20	10 (4%)	37	44	5, 18, 34, 42	0
All	All	1467/1524 (96%)	0.07	22 (1%)	73	79	5, 21, 36, 57	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	112	ARG	5.7
1	C	251	ILE	5.2
1	F	0	ALA	5.1
1	F	113	LYS	4.6
1	F	114	ARG	4.2
1	D	0	ALA	3.8
1	F	110	LEU	3.7
1	F	111	SER	3.2
1	F	82	VAL	3.2
1	F	115	ASP	3.1
1	F	109	GLU	2.9
1	E	234	ARG	2.6
1	E	158	LEU	2.5
1	E	227	THR	2.4
1	E	3	LYS	2.4
1	C	-2	SER	2.2
1	E	0	ALA	2.2
1	C	51	LEU	2.1
1	C	82	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	17	THR	2.1
1	B	24	ILE	2.1
1	F	215	GLU	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 (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MES	F	253	12/12	0.80	0.21	39,41,44,44	12
4	MES	F	254	12/12	0.82	0.19	31,35,38,39	12
3	SO4	B	254	5/5	0.83	0.27	63,64,66,67	5
3	SO4	E	254	5/5	0.85	0.25	49,53,53,54	5
2	NA	D	252	1/1	0.86	0.20	37,37,37,37	0
3	SO4	C	254	5/5	0.89	0.17	64,65,67,68	5
4	MES	E	255	12/12	0.89	0.18	31,38,41,41	12
2	NA	A	252	1/1	0.91	0.10	37,37,37,37	0
2	NA	C	252	1/1	0.95	0.18	24,24,24,24	0
2	NA	B	252	1/1	0.95	0.24	28,28,28,28	0
2	NA	E	252	1/1	0.95	0.11	41,41,41,41	0
2	NA	F	252	1/1	0.96	0.16	30,30,30,30	0
3	SO4	C	253	5/5	0.97	0.10	43,47,50,50	0
3	SO4	E	253	5/5	0.97	0.11	57,57,59,59	5
3	SO4	D	253	5/5	0.99	0.13	51,52,53,55	0
3	SO4	B	253	5/5	0.99	0.12	41,43,45,46	0
3	SO4	A	253	5/5	0.99	0.12	50,51,53,57	0

6.5 Other polymers (i)

There are no such residues in this entry.