



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 08:48 pm BST

PDB ID : 3BJB
Title : Crystal structure of a TetR transcriptional regulator from *Rhodococcus* sp. RHA1
Authors : Tan, K.; Evdokimova, E.; Kudritska, M.; Savchenko, A.; Edwards, A.M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2007-12-03
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

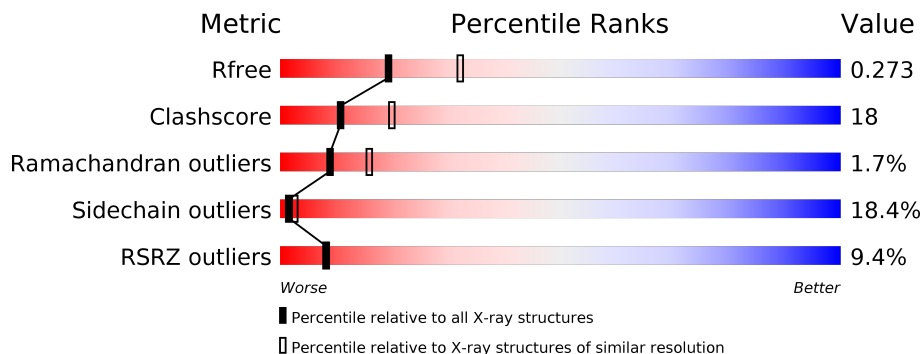
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	207	10% (Poor fit) 54% (0 outliers), 28% (1 outlier), 15% (2+ outliers)
1	B	207	12% (Poor fit) 56% (0 outliers), 27% (1 outlier), 12% (2+ outliers)
1	C	207	% (Poor fit) 57% (0 outliers), 22% (1 outlier), 14% (2+ outliers)
1	D	207	7% (Poor fit) 48% (0 outliers), 28% (1 outlier), 7% (2 outliers), 16% (2+ outliers)
1	E	207	10% (Poor fit) 52% (0 outliers), 27% (1 outlier), 8% (2 outliers), 12% (2+ outliers)
1	F	207	7% (Poor fit) 54% (0 outliers), 29% (1 outlier), 6% (2 outliers), 12% (2+ outliers)

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	SO4	A	306	-	-	-	X
2	SO4	A	321	-	-	X	-
2	SO4	C	301	-	-	X	-
2	SO4	C	309	-	-	X	-
2	SO4	F	313	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8429 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 Probable transcriptional regulator, TetR family protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	175	1356	845	251	252	2	6	0	0	0
1	B	183	1418	887	261	262	2	6	0	0	0
1	C	177	1370	860	255	247	2	6	0	0	0
1	D	174	1348	845	248	247	2	6	0	0	0
1	E	182	1408	879	260	261	2	6	0	0	0
1	F	182	1406	878	260	260	2	6	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

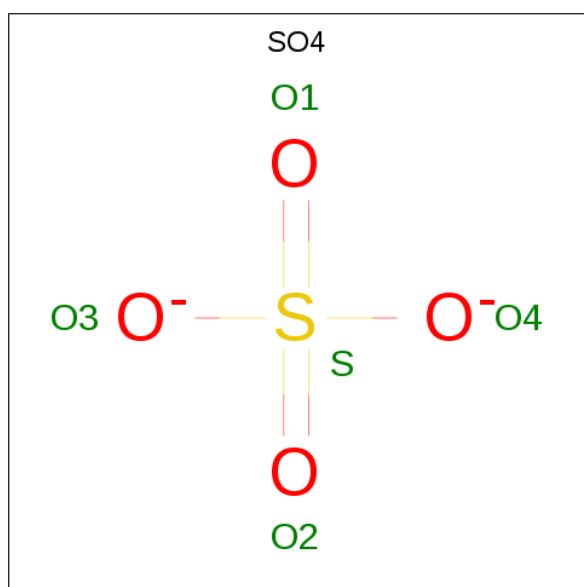
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	EXPRESSION TAG	UNP Q0S4E5
A	0	HIS	-	EXPRESSION TAG	UNP Q0S4E5
A	1	VAL	-	EXPRESSION TAG	UNP Q0S4E5
A	204	GLY	-	EXPRESSION TAG	UNP Q0S4E5
A	205	SER	-	EXPRESSION TAG	UNP Q0S4E5
B	-1	GLY	-	EXPRESSION TAG	UNP Q0S4E5
B	0	HIS	-	EXPRESSION TAG	UNP Q0S4E5
B	1	VAL	-	EXPRESSION TAG	UNP Q0S4E5
B	204	GLY	-	EXPRESSION TAG	UNP Q0S4E5
B	205	SER	-	EXPRESSION TAG	UNP Q0S4E5
C	-1	GLY	-	EXPRESSION TAG	UNP Q0S4E5
C	0	HIS	-	EXPRESSION TAG	UNP Q0S4E5
C	1	VAL	-	EXPRESSION TAG	UNP Q0S4E5
C	204	GLY	-	EXPRESSION TAG	UNP Q0S4E5
C	205	SER	-	EXPRESSION TAG	UNP Q0S4E5
D	-1	GLY	-	EXPRESSION TAG	UNP Q0S4E5
D	0	HIS	-	EXPRESSION TAG	UNP Q0S4E5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	VAL	-	EXPRESSION TAG	UNP Q0S4E5
D	204	GLY	-	EXPRESSION TAG	UNP Q0S4E5
D	205	SER	-	EXPRESSION TAG	UNP Q0S4E5
E	-1	GLY	-	EXPRESSION TAG	UNP Q0S4E5
E	0	HIS	-	EXPRESSION TAG	UNP Q0S4E5
E	1	VAL	-	EXPRESSION TAG	UNP Q0S4E5
E	204	GLY	-	EXPRESSION TAG	UNP Q0S4E5
E	205	SER	-	EXPRESSION TAG	UNP Q0S4E5
F	-1	GLY	-	EXPRESSION TAG	UNP Q0S4E5
F	0	HIS	-	EXPRESSION TAG	UNP Q0S4E5
F	1	VAL	-	EXPRESSION TAG	UNP Q0S4E5
F	204	GLY	-	EXPRESSION TAG	UNP Q0S4E5
F	205	SER	-	EXPRESSION TAG	UNP Q0S4E5

- Molecule 2 is SULFATE ION (three-letter code: SO₄) (formula: O₄S).



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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	O	0	0
			2	2		
3	B	2	Total	O	0	0
			2	2		
3	C	7	Total	O	0	0
			7	7		

Continued on next page...

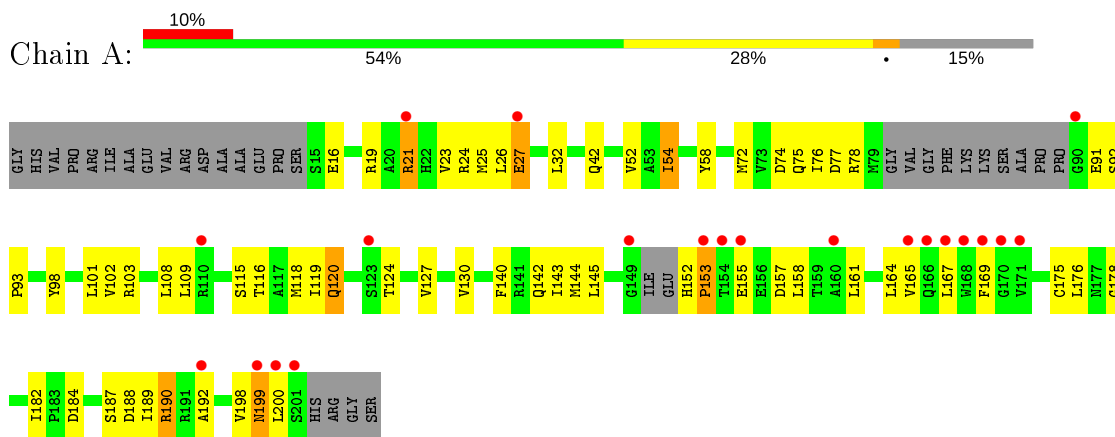
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total O 1 1	0	0
3	E	4	Total O 4 4	0	0
3	F	2	Total O 2 2	0	0

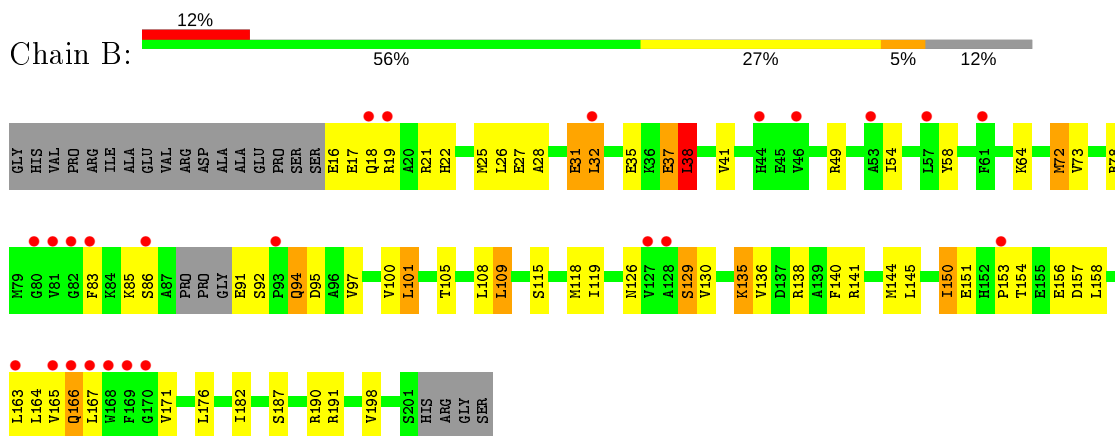
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

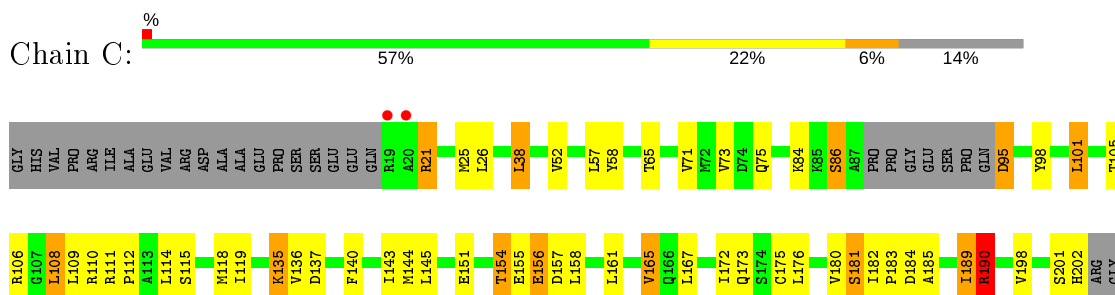
- Molecule 1: Probable transcriptional regulator, TetR family protein



- Molecule 1: Probable transcriptional regulator, TetR family protein



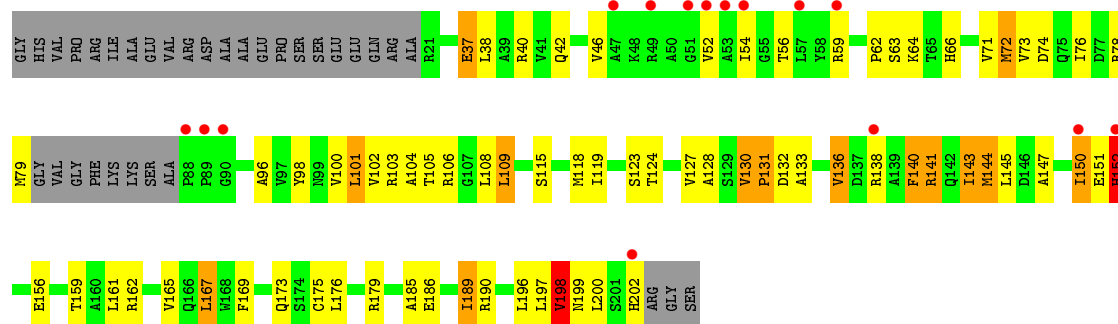
- Molecule 1: Probable transcriptional regulator, TetR family protein



SER

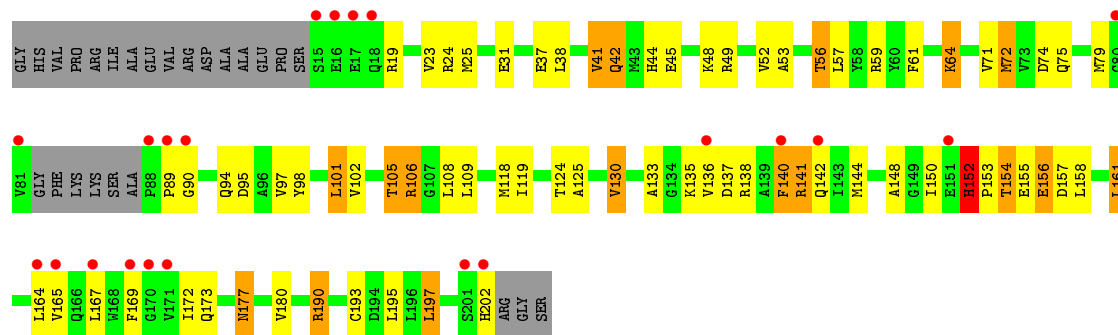
- Molecule 1: Probable transcriptional regulator, TetR family protein

Chain D: 



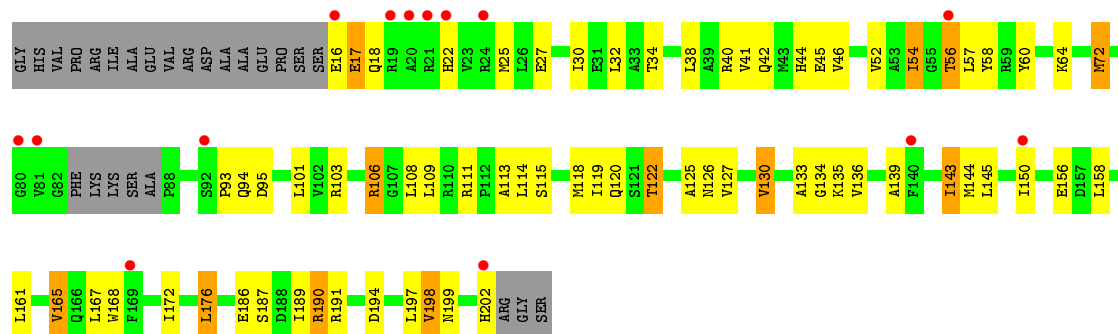
- Molecule 1: Probable transcriptional regulator, TetR family protein

Chain E: 



- Molecule 1: Probable transcriptional regulator, TetR family protein

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	93.77Å 93.77Å 314.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.46 – 2.50 32.46 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.1 (32.46-2.50) 98.1 (32.46-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 2.51Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.232 , 0.278 0.228 , 0.273	Depositor DCC
R_{free} test set	2468 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	58.5	Xtrriage
Anisotropy	0.081	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 66.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8429	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

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

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	0.69	0/1366	0.83	0/1836
1	B	0.74	0/1430	0.86	1/1922 (0.1%)
1	C	0.92	0/1382	0.94	3/1857 (0.2%)
1	D	0.81	1/1362 (0.1%)	0.88	0/1835
1	E	0.80	0/1422	0.93	1/1915 (0.1%)
1	F	0.77	0/1420	0.85	0/1912
All	All	0.79	1/8382 (0.0%)	0.88	5/11277 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	175	CYS	CB-SG	-10.42	1.64	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	190	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	C	95	ASP	CB-CG-OD1	-5.76	113.12	118.30
1	B	38	LEU	CA-CB-CG	5.64	128.28	115.30
1	E	167	LEU	CB-CG-CD2	-5.35	101.91	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	38	LEU	CB-CG-CD2	5.32	120.04	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	152	HIS	Peptide
1	E	152	HIS	Peptide

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	1356	0	1384	49	0
1	B	1418	0	1454	41	0
1	C	1370	0	1415	58	0
1	D	1348	0	1381	52	0
1	E	1408	0	1436	74	0
1	F	1406	0	1434	43	0
2	A	20	0	0	2	0
2	B	20	0	0	0	0
2	C	30	0	0	9	0
2	E	15	0	0	0	0
2	F	20	0	0	3	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	7	0	0	1	0
3	D	1	0	0	0	0
3	E	4	0	0	0	0
3	F	2	0	0	0	0
All	All	8429	0	8504	309	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 18.

All (309) 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:25:MSE:CE	1:C:57:LEU:HA	1.71	1.19
1:F:42:GLN:HB2	1:F:45:GLU:HG3	1.27	1.16
1:D:71:VAL:HG12	1:D:118:MSE:CE	1.76	1.14
1:A:72:MSE:HA	1:A:118:MSE:CE	1.78	1.12
1:C:25:MSE:HE2	1:C:57:LEU:HD12	1.22	1.12
1:E:75:GLN:HG3	1:E:118:MSE:HE1	1.33	1.10
1:E:72:MSE:HA	1:E:118:MSE:HE2	1.33	1.09
1:E:25:MSE:HE3	1:E:57:LEU:HD12	1.36	1.08
1:E:25:MSE:CE	1:E:57:LEU:HD12	1.87	1.03
1:C:25:MSE:HE1	1:C:57:LEU:HA	1.03	1.03
1:B:150:ILE:HD11	1:B:153:PRO:HA	1.41	1.01
1:E:71:VAL:CG1	1:E:118:MSE:HE3	1.90	1.00
1:E:71:VAL:HG12	1:E:118:MSE:HE3	1.02	0.99
1:A:72:MSE:CA	1:A:118:MSE:HE3	1.91	0.99
1:E:25:MSE:CE	1:E:57:LEU:HA	1.94	0.98
1:E:71:VAL:HG12	1:E:118:MSE:CE	1.92	0.98
1:C:25:MSE:HE2	1:C:57:LEU:CD1	1.94	0.97
1:C:95:ASP:HB2	2:C:316:SO4:O3	1.63	0.96
1:A:72:MSE:HA	1:A:118:MSE:HE3	0.99	0.95
1:F:113:ALA:N	2:F:313:SO4:O1	2.02	0.92
1:D:71:VAL:HG12	1:D:118:MSE:HE2	1.51	0.91
1:D:141:ARG:HG3	1:D:141:ARG:HH21	1.35	0.90
1:E:25:MSE:HE3	1:E:57:LEU:HA	1.52	0.90
1:E:72:MSE:CA	1:E:118:MSE:HE2	2.02	0.90
1:C:144:MSE:HE2	1:C:144:MSE:HA	1.54	0.89
1:E:177:ASN:HB2	1:F:126:ASN:HA	1.54	0.89
1:D:71:VAL:HG12	1:D:118:MSE:HE3	1.53	0.88
1:E:101:LEU:O	1:E:105:THR:HG22	1.75	0.86
1:F:34:THR:HG22	1:F:114:LEU:HB2	1.58	0.86
1:E:75:GLN:CG	1:E:118:MSE:HE1	2.05	0.84
1:C:180:VAL:HG22	1:C:184:ASP:HB2	1.57	0.84
1:D:145:LEU:HD13	1:D:150:ILE:HD12	1.58	0.84
1:A:42:GLN:NE2	2:C:309:SO4:S	2.52	0.82
1:E:141:ARG:HA	1:E:144:MSE:HE3	1.62	0.81
1:F:93:PRO:HG2	1:F:202:HIS:HB3	1.62	0.81
1:D:73:VAL:HG23	1:D:136:VAL:HG12	1.63	0.80
1:F:22:HIS:HA	1:F:25:MSE:HE2	1.64	0.80
1:C:109:LEU:HD11	1:C:175:CYS:HB3	1.64	0.79
1:E:144:MSE:HE1	1:E:165:VAL:CG1	2.12	0.79
1:F:30:ILE:O	1:F:34:THR:HG23	1.83	0.79
1:E:75:GLN:HG3	1:E:118:MSE:CE	2.14	0.77
1:E:72:MSE:CG	1:E:118:MSE:HB3	2.14	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ILE:HD11	1:B:153:PRO:CA	2.14	0.76
1:E:140:PHE:HD2	1:E:144:MSE:HE2	1.51	0.76
1:E:25:MSE:HE1	1:E:57:LEU:HA	1.67	0.75
1:E:25:MSE:HE3	1:E:57:LEU:CD1	2.13	0.75
1:C:25:MSE:HE1	1:C:57:LEU:CA	1.99	0.75
1:E:72:MSE:HG3	1:E:118:MSE:HB3	1.69	0.75
1:C:71:VAL:HG12	1:C:118:MSE:HE2	1.69	0.73
1:E:25:MSE:HE2	1:E:57:LEU:HD12	1.71	0.73
1:D:54:ILE:HD12	1:D:54:ILE:H	1.53	0.72
1:B:101:LEU:HD13	1:B:144:MSE:HE3	1.71	0.72
1:B:97:VAL:CG1	1:B:144:MSE:HE2	2.19	0.72
1:B:97:VAL:HG13	1:B:144:MSE:HE2	1.70	0.72
1:A:72:MSE:HE3	1:A:118:MSE:CE	2.20	0.71
1:D:106:ARG:HD3	1:D:186:GLU:OE2	1.90	0.71
1:E:144:MSE:HE1	1:E:165:VAL:HG12	1.71	0.71
1:A:152:HIS:O	1:A:152:HIS:CG	2.44	0.71
1:B:38:LEU:HD22	1:B:64:LYS:HE3	1.73	0.71
1:C:25:MSE:CE	1:C:57:LEU:CA	2.61	0.70
1:C:75:GLN:HG3	1:C:118:MSE:CE	2.22	0.69
1:A:199:ASN:H	1:A:199:ASN:HD22	1.40	0.69
1:E:119:ILE:CG2	1:E:173:GLN:HG3	2.22	0.69
1:C:25:MSE:CE	1:C:57:LEU:HD12	2.12	0.69
1:C:71:VAL:CG1	1:C:118:MSE:HE2	2.22	0.69
1:F:103:ARG:HD2	2:F:303:SO4:O2	1.92	0.69
1:D:71:VAL:CG1	1:D:118:MSE:HE3	2.23	0.68
1:E:153:PRO:HB2	1:E:158:LEU:CD1	2.23	0.68
1:B:135:LYS:HG2	1:B:138:ARG:HH21	1.57	0.68
1:C:111:ARG:HD2	3:C:407:HOH:O	1.93	0.68
1:D:144:MSE:HG2	1:D:161:LEU:HD22	1.76	0.67
1:A:115:SER:O	1:A:119:ILE:HD12	1.95	0.66
1:B:32:LEU:HD11	1:B:49:ARG:HG3	1.78	0.66
1:D:98:TYR:CZ	1:D:102:VAL:HG21	2.31	0.65
1:E:72:MSE:HA	1:E:118:MSE:CE	2.19	0.65
1:E:31:GLU:OE2	1:E:49:ARG:NH1	2.27	0.65
1:C:154:THR:HG22	1:C:157:ASP:H	1.62	0.65
1:E:153:PRO:HB2	1:E:158:LEU:HD11	1.78	0.65
1:E:19:ARG:O	1:E:23:VAL:HG23	1.97	0.64
1:B:73:VAL:HG23	1:B:136:VAL:HG12	1.79	0.64
1:C:75:GLN:HG3	1:C:118:MSE:HE1	1.78	0.64
1:A:199:ASN:HD22	1:A:199:ASN:N	1.95	0.64
1:D:100:VAL:HG21	1:D:147:ALA:CB	2.28	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:141:ARG:HG3	1:D:141:ARG:NH2	2.12	0.64
1:F:17:GLU:HG3	1:F:18:GLN:H	1.62	0.64
1:E:25:MSE:HE3	1:E:57:LEU:CA	2.26	0.63
1:C:137:ASP:OD2	1:D:179:ARG:HD2	1.99	0.63
1:B:101:LEU:CD1	1:B:144:MSE:HE3	2.29	0.63
1:C:181:SER:OG	1:C:183:PRO:HD2	1.98	0.63
1:B:18:GLN:O	1:B:22:HIS:HB2	1.99	0.62
1:E:136:VAL:HG23	1:E:137:ASP:H	1.64	0.62
1:B:167:LEU:O	1:B:171:VAL:HG23	1.99	0.62
1:B:73:VAL:CG2	1:B:136:VAL:HG12	2.28	0.62
1:A:42:GLN:NE2	2:C:309:SO4:O1	2.32	0.62
1:F:42:GLN:HG2	1:F:45:GLU:OE1	2.00	0.62
1:C:154:THR:HG23	1:C:156:GLU:H	1.65	0.62
1:E:136:VAL:HG23	1:E:137:ASP:N	2.14	0.62
1:F:32:LEU:CD1	1:F:46:VAL:HA	2.30	0.62
1:D:159:THR:HA	1:D:162:ARG:NH1	2.15	0.61
1:A:25:MSE:HE2	1:A:52:VAL:HG21	1.81	0.61
1:E:72:MSE:N	1:E:118:MSE:HE2	2.16	0.61
1:D:100:VAL:HG21	1:D:147:ALA:HB2	1.81	0.61
1:C:101:LEU:HB3	1:C:189:ILE:CD1	2.30	0.61
1:E:25:MSE:HE2	1:E:61:PHE:CD2	2.35	0.61
1:C:105:THR:O	1:C:109:LEU:HD23	2.01	0.60
1:E:144:MSE:HE1	1:E:165:VAL:HG11	1.84	0.60
1:B:150:ILE:CD1	1:B:153:PRO:HA	2.26	0.60
1:A:74:ASP:O	1:A:78:ARG:HD2	2.02	0.60
1:A:91:GLU:HG3	1:A:92:SER:H	1.65	0.60
1:A:72:MSE:HE3	1:A:118:MSE:HE1	1.84	0.59
1:D:98:TYR:CE1	1:D:190:ARG:HB2	2.36	0.59
1:C:73:VAL:HG11	1:C:135:LYS:HD3	1.83	0.59
1:C:65:THR:N	2:C:309:SO4:O4	2.22	0.59
1:F:22:HIS:HA	1:F:25:MSE:CE	2.31	0.59
1:A:167:LEU:HD23	1:A:192:ALA:HB1	1.83	0.59
1:A:72:MSE:HE3	1:A:118:MSE:HE2	1.85	0.59
1:A:93:PRO:HB2	1:A:200:LEU:HD22	1.84	0.58
1:C:201:SER:O	1:C:202:HIS:HB2	2.02	0.58
1:C:101:LEU:HB3	1:C:189:ILE:HD12	1.84	0.58
1:A:21:ARG:HH11	1:A:21:ARG:HG2	1.68	0.58
1:B:105:THR:HG22	1:B:109:LEU:HD22	1.86	0.58
1:A:23:VAL:O	1:A:27:GLU:HG2	2.04	0.58
1:F:118:MSE:O	1:F:122:THR:HG23	2.04	0.57
1:E:154:THR:HG22	1:E:157:ASP:OD2	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:150:ILE:HG23	1:E:152:HIS:CD2	2.39	0.57
1:F:118:MSE:O	1:F:122:THR:CG2	2.53	0.57
1:B:135:LYS:HG2	1:B:138:ARG:NH2	2.20	0.57
1:A:75:GLN:HB2	1:A:118:MSE:HE1	1.86	0.57
1:C:75:GLN:HG3	1:C:118:MSE:SE	2.55	0.57
1:E:150:ILE:HG23	1:E:152:HIS:HD2	1.69	0.57
1:E:140:PHE:CD2	1:E:144:MSE:HE2	2.36	0.57
1:E:25:MSE:HE2	1:E:61:PHE:HD2	1.70	0.56
1:E:72:MSE:HG2	1:E:118:MSE:HB3	1.88	0.56
1:E:119:ILE:HG21	1:E:173:GLN:HG3	1.87	0.56
1:F:130:VAL:HG23	1:F:130:VAL:O	2.04	0.56
1:A:24:ARG:NH2	2:A:321:SO4:S	2.79	0.56
1:D:145:LEU:O	1:D:150:ILE:HG22	2.05	0.56
1:A:21:ARG:HH11	1:A:21:ARG:CG	2.18	0.56
1:B:58:TYR:HB3	1:D:128:ALA:HB3	1.88	0.56
1:C:115:SER:O	1:C:119:ILE:HG12	2.05	0.56
1:F:190:ARG:NH2	1:F:194:ASP:OD1	2.39	0.55
1:F:168:TRP:HD1	1:F:189:ILE:HG12	1.72	0.55
1:D:100:VAL:HG11	1:D:143:ILE:HD12	1.89	0.55
1:C:144:MSE:HA	1:C:144:MSE:CE	2.33	0.55
1:F:41:VAL:O	1:F:64:LYS:HE2	2.06	0.55
1:E:119:ILE:HG22	1:E:173:GLN:HG3	1.86	0.55
1:F:167:LEU:O	1:F:167:LEU:HD12	2.07	0.55
1:D:42:GLN:O	1:D:46:VAL:HG23	2.07	0.54
1:C:21:ARG:NH1	2:C:307:SO4:O1	2.40	0.54
1:C:109:LEU:HD11	1:C:175:CYS:CB	2.34	0.54
1:F:54:ILE:HD12	1:F:58:TYR:CE1	2.43	0.54
1:A:98:TYR:CZ	1:A:102:VAL:HG21	2.42	0.54
1:C:25:MSE:HE3	1:C:52:VAL:HG21	1.89	0.53
1:A:140:PHE:HE2	1:A:169:PHE:CZ	2.26	0.53
1:E:133:ALA:O	1:E:136:VAL:HG22	2.08	0.53
1:A:42:GLN:NE2	2:C:309:SO4:O2	2.42	0.53
1:E:161:LEU:O	1:E:165:VAL:HG13	2.09	0.53
1:B:126:ASN:HB3	1:B:129:SER:OG	2.08	0.53
1:A:21:ARG:O	1:A:25:MSE:HG3	2.09	0.53
1:B:28:ALA:HB1	1:B:49:ARG:HB2	1.91	0.53
1:A:24:ARG:NH2	2:A:321:SO4:O1	2.42	0.53
1:B:83:PHE:CZ	1:B:100:VAL:HG12	2.44	0.53
1:D:79:MSE:HE1	1:D:104:ALA:HB2	1.91	0.53
1:B:58:TYR:HB3	1:D:128:ALA:CB	2.39	0.53
1:A:54:ILE:HD11	1:A:58:TYR:HE1	1.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:SER:OG	1:D:66:HIS:ND1	2.37	0.52
1:D:130:VAL:HG22	1:D:130:VAL:O	2.08	0.52
1:C:75:GLN:CG	1:C:118:MSE:HE1	2.40	0.52
1:E:75:GLN:CB	1:E:118:MSE:HE1	2.40	0.52
1:F:94:GLN:HG3	1:F:197:LEU:HB2	1.91	0.52
1:E:53:ALA:HB3	1:E:56:THR:CG2	2.40	0.52
1:B:92:SER:H	1:B:95:ASP:HB3	1.74	0.52
1:D:144:MSE:CG	1:D:161:LEU:HD22	2.39	0.51
1:F:143:ILE:HG22	1:F:144:MSE:HE3	1.92	0.51
1:F:130:VAL:CG2	1:F:130:VAL:O	2.58	0.51
1:D:123:SER:HB3	1:D:169:PHE:HE2	1.76	0.51
1:E:153:PRO:HB2	1:E:158:LEU:HD12	1.93	0.50
1:A:76:ILE:O	1:A:78:ARG:N	2.44	0.50
1:F:103:ARG:HG3	1:F:103:ARG:HH21	1.77	0.50
1:D:96:ALA:O	1:D:100:VAL:HG23	2.12	0.50
1:B:166:GLN:HA	1:B:166:GLN:NE2	2.27	0.49
1:D:100:VAL:CG1	1:D:143:ILE:HD12	2.43	0.49
1:D:150:ILE:C	1:D:151:GLU:HG2	2.32	0.49
1:E:95:ASP:OD2	1:E:190:ARG:NH1	2.45	0.49
1:E:98:TYR:CZ	1:E:102:VAL:CG2	2.96	0.49
1:A:140:PHE:CE2	1:A:169:PHE:CZ	3.01	0.49
1:A:25:MSE:HE2	1:A:52:VAL:HG11	1.95	0.49
1:B:144:MSE:HE1	1:B:164:LEU:HD23	1.95	0.49
1:C:25:MSE:CE	1:C:57:LEU:CD1	2.79	0.49
1:B:17:GLU:C	1:B:19:ARG:H	2.15	0.48
1:D:167:LEU:HD23	1:D:196:LEU:HD11	1.95	0.48
1:A:152:HIS:N	1:A:153:PRO:HA	2.28	0.48
1:E:101:LEU:O	1:E:105:THR:CG2	2.53	0.48
1:C:180:VAL:CG2	1:C:184:ASP:HB2	2.36	0.48
1:F:54:ILE:HD12	1:F:58:TYR:CD1	2.48	0.48
1:C:75:GLN:CG	1:C:118:MSE:CE	2.90	0.48
1:A:188:ASP:HB3	1:B:163:LEU:HD21	1.96	0.48
1:C:106:ARG:O	1:C:110:ARG:HG3	2.14	0.48
1:A:54:ILE:HD12	1:C:58:TYR:CD1	2.48	0.48
1:F:198:VAL:HG23	1:F:199:ASN:ND2	2.28	0.48
1:A:72:MSE:CE	1:A:118:MSE:HE2	2.43	0.48
1:E:42:GLN:HB2	1:E:45:GLU:HG3	1.96	0.48
1:E:154:THR:OG1	1:E:155:GLU:N	2.47	0.47
1:A:21:ARG:NH1	1:A:21:ARG:HG2	2.28	0.47
1:D:37:GLU:OE2	1:D:40:ARG:HG3	2.15	0.47
1:D:130:VAL:HA	1:D:131:PRO:HD2	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ARG:HH21	1:A:190:ARG:HB2	1.80	0.47
1:A:144:MSE:HA	1:A:144:MSE:HE2	1.97	0.46
1:E:124:THR:HG22	1:F:120:GLN:HG3	1.98	0.46
1:B:92:SER:H	1:B:95:ASP:CB	2.29	0.46
1:F:143:ILE:HG22	1:F:144:MSE:CE	2.46	0.46
1:D:130:VAL:CG2	1:D:130:VAL:O	2.63	0.46
1:F:115:SER:O	1:F:119:ILE:HG12	2.16	0.46
1:C:110:ARG:C	1:C:112:PRO:HD3	2.36	0.46
1:A:19:ARG:O	1:A:23:VAL:HG23	2.16	0.46
1:D:185:ALA:O	1:D:189:ILE:HG23	2.15	0.46
1:C:98:TYR:CE1	1:C:190:ARG:HB2	2.50	0.46
1:E:75:GLN:HB2	1:E:118:MSE:HE1	1.98	0.45
1:A:72:MSE:SE	1:A:118:MSE:HE2	2.66	0.45
1:D:76:ILE:O	1:D:79:MSE:HG2	2.17	0.45
1:E:25:MSE:HE3	1:E:57:LEU:CB	2.45	0.45
1:F:134:GLY:O	1:F:136:VAL:N	2.49	0.45
1:C:143:ILE:HG13	1:C:144:MSE:N	2.32	0.45
1:E:41:VAL:HG22	1:E:64:LYS:HD2	1.99	0.45
1:B:16:GLU:HB2	1:B:19:ARG:HG3	1.98	0.45
1:B:21:ARG:HG2	1:B:25:MSE:HE2	1.98	0.45
1:C:109:LEU:CD1	1:C:175:CYS:SG	3.05	0.45
1:E:156:GLU:O	1:E:156:GLU:HG3	2.13	0.45
1:B:105:THR:HG22	1:B:109:LEU:CD2	2.47	0.44
1:C:161:LEU:O	1:C:165:VAL:HG13	2.17	0.44
1:A:109:LEU:HD13	1:A:182:ILE:HG13	1.99	0.44
1:D:62:PRO:O	1:D:63:SER:HB3	2.17	0.44
1:C:144:MSE:HB3	1:C:161:LEU:HD22	1.98	0.44
1:C:101:LEU:HD12	1:C:101:LEU:HA	1.81	0.44
1:F:161:LEU:O	1:F:165:VAL:HG13	2.18	0.44
1:C:114:LEU:HD11	1:C:118:MSE:HE3	2.00	0.44
1:D:37:GLU:HG3	1:D:37:GLU:H	1.68	0.44
1:C:182:ILE:HB	1:C:183:PRO:HD3	2.00	0.44
1:B:154:THR:O	1:B:157:ASP:HB2	2.18	0.44
1:D:72:MSE:HE3	1:D:118:MSE:SE	2.68	0.44
1:D:145:LEU:HB3	1:D:150:ILE:HB	1.99	0.44
1:C:172:ILE:HG22	1:C:173:GLN:N	2.32	0.43
1:B:115:SER:O	1:B:119:ILE:HG12	2.18	0.43
1:F:32:LEU:HD13	1:F:46:VAL:HG22	2.00	0.43
1:A:184:ASP:O	1:A:187:SER:HB2	2.18	0.43
1:E:109:LEU:HA	1:E:109:LEU:HD23	1.80	0.43
1:F:115:SER:HA	1:F:118:MSE:HE2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:MSE:HE2	1:E:119:ILE:HA	2.00	0.43
1:A:140:PHE:HE2	1:A:169:PHE:HZ	1.67	0.43
2:C:301:SO4:S	1:E:48:LYS:HE2	2.59	0.43
1:D:197:LEU:HB3	1:D:200:LEU:HD22	2.00	0.43
1:E:97:VAL:HG23	1:E:148:ALA:HB2	2.00	0.43
1:D:199:ASN:OD1	1:F:44:HIS:HB3	2.18	0.42
1:E:44:HIS:CE1	1:E:45:GLU:HG2	2.53	0.42
1:E:98:TYR:CZ	1:E:102:VAL:HG21	2.54	0.42
1:C:106:ARG:HG2	1:C:110:ARG:HH21	1.84	0.42
1:D:144:MSE:CE	1:D:144:MSE:HA	2.50	0.42
1:D:150:ILE:O	1:D:151:GLU:HG2	2.20	0.42
1:D:197:LEU:O	1:D:198:VAL:C	2.57	0.42
1:C:154:THR:CG2	1:C:156:GLU:H	2.30	0.42
1:B:28:ALA:HA	1:B:31:GLU:HG3	2.02	0.42
1:D:140:PHE:O	1:D:144:MSE:HB2	2.19	0.42
1:E:105:THR:HB	1:E:172:ILE:HD11	2.00	0.42
1:E:193:CYS:O	1:E:197:LEU:HB2	2.19	0.42
1:C:106:ARG:CG	1:C:110:ARG:HH21	2.33	0.42
1:D:200:LEU:HD12	1:D:200:LEU:HA	1.80	0.42
1:F:72:MSE:HB2	1:F:118:MSE:HB3	2.02	0.42
1:C:119:ILE:HG21	1:C:173:GLN:HG3	2.01	0.42
1:E:125:ALA:HB1	1:E:130:VAL:HG13	2.00	0.42
1:A:127:VAL:CG1	1:A:127:VAL:O	2.68	0.42
1:B:31:GLU:O	1:B:35:GLU:HG3	2.19	0.41
1:D:119:ILE:HG21	1:D:173:GLN:HG2	2.02	0.41
1:B:72:MSE:HE3	1:B:118:MSE:SE	2.70	0.41
1:C:185:ALA:O	1:C:189:ILE:HG23	2.20	0.41
1:F:125:ALA:HB1	1:F:130:VAL:CG2	2.50	0.41
1:F:113:ALA:CA	2:F:313:SO4:O1	2.68	0.41
1:B:28:ALA:HB1	1:B:49:ARG:CB	2.50	0.41
1:E:136:VAL:CG2	1:E:137:ASP:N	2.83	0.41
1:A:116:THR:O	1:A:120:GLN:HB2	2.19	0.41
1:B:54:ILE:HG13	1:B:58:TYR:CD1	2.56	0.41
1:C:108:LEU:HD12	1:C:108:LEU:HA	1.70	0.41
1:C:86:SER:OG	1:C:151:GLU:HG2	2.21	0.41
1:E:102:VAL:O	1:E:106:ARG:HG2	2.20	0.41
1:B:94:GLN:CD	1:B:94:GLN:H	2.23	0.41
1:A:153:PRO:HB2	1:A:157:ASP:OD2	2.21	0.41
1:A:164:LEU:O	1:A:164:LEU:HG	2.21	0.41
1:C:84:LYS:HA	2:C:315:SO4:O3	2.20	0.41
1:E:72:MSE:HE1	1:E:169:PHE:CE2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:130:VAL:HG22	1:E:130:VAL:O	2.21	0.41
1:C:154:THR:HG23	1:C:155:GLU:N	2.36	0.41
1:D:59:ARG:NH2	1:D:59:ARG:O	2.53	0.41
1:A:144:MSE:HB3	1:A:161:LEU:HD22	2.03	0.41
1:B:167:LEU:HD12	1:B:167:LEU:O	2.21	0.41
1:F:95:ASP:OD2	1:F:190:ARG:NH1	2.52	0.41
1:B:37:GLU:O	1:B:41:VAL:HG23	2.21	0.41
1:F:56:THR:O	1:F:60:TYR:HD2	2.04	0.41
1:C:109:LEU:HD11	1:C:175:CYS:SG	2.61	0.40
2:C:301:SO4:O4	1:E:48:LYS:HE2	2.22	0.40
1:D:105:THR:HG22	1:D:109:LEU:HD22	2.02	0.40
1:E:24:ARG:NH2	1:E:49:ARG:O	2.54	0.40
1:A:76:ILE:C	1:A:78:ARG:H	2.25	0.40
1:D:101:LEU:HB3	1:D:189:ILE:CD1	2.51	0.40
1:F:106:ARG:HD3	1:F:186:GLU:OE2	2.22	0.40
1:F:130:VAL:CG2	1:F:133:ALA:HB2	2.51	0.40
1:D:131:PRO:O	1:D:133:ALA:N	2.54	0.40
1:E:141:ARG:HG3	1:E:142:GLN:N	2.36	0.40
1:F:125:ALA:HB1	1:F:130:VAL:HG22	2.04	0.40
1:F:172:ILE:HG22	1:F:176:LEU:HD22	2.03	0.40
1:B:73:VAL:HG22	1:B:136:VAL:HG12	2.02	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	169/207 (82%)	155 (92%)	11 (6%)	3 (2%)	8	14
1	B	179/207 (86%)	168 (94%)	7 (4%)	4 (2%)	6	10
1	C	173/207 (84%)	171 (99%)	2 (1%)	0	100	100
1	D	170/207 (82%)	160 (94%)	6 (4%)	4 (2%)	6	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	178/207 (86%)	167 (94%)	7 (4%)	4 (2%)	6	10
1	F	178/207 (86%)	167 (94%)	8 (4%)	3 (2%)	9	16
All	All	1047/1242 (84%)	988 (94%)	41 (4%)	18 (2%)	9	16

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	132	ASP
1	E	135	LYS
1	F	17	GLU
1	A	77	ASP
1	A	178	GLY
1	D	198	VAL
1	E	90	GLY
1	F	135	LYS
1	A	153	PRO
1	B	37	GLU
1	B	86	SER
1	D	131	PRO
1	B	135	LYS
1	E	152	HIS
1	F	139	ALA
1	B	141	ARG
1	D	152	HIS
1	E	89	PRO

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	145/163 (89%)	121 (83%)	24 (17%)	2	4
1	B	151/163 (93%)	122 (81%)	29 (19%)	1	2
1	C	145/163 (89%)	125 (86%)	20 (14%)	3	6
1	D	145/163 (89%)	114 (79%)	31 (21%)	1	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	151/163 (93%)	120 (80%)	31 (20%)	1	2
1	F	150/163 (92%)	122 (81%)	28 (19%)	1	2
All	All	887/978 (91%)	724 (82%)	163 (18%)	1	2

All (163) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	GLU
1	A	21	ARG
1	A	26	LEU
1	A	27	GLU
1	A	32	LEU
1	A	54	ILE
1	A	101	LEU
1	A	103	ARG
1	A	108	LEU
1	A	120	GLN
1	A	124	THR
1	A	130	VAL
1	A	142	GLN
1	A	143	ILE
1	A	145	LEU
1	A	155	GLU
1	A	158	LEU
1	A	165	VAL
1	A	175	CYS
1	A	176	LEU
1	A	189	ILE
1	A	190	ARG
1	A	198	VAL
1	A	199	ASN
1	B	26	LEU
1	B	27	GLU
1	B	31	GLU
1	B	32	LEU
1	B	38	LEU
1	B	72	MSE
1	B	78	ARG
1	B	85	LYS
1	B	91	GLU
1	B	94	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	101	LEU
1	B	108	LEU
1	B	109	LEU
1	B	129	SER
1	B	130	VAL
1	B	140	PHE
1	B	145	LEU
1	B	150	ILE
1	B	151	GLU
1	B	156	GLU
1	B	158	LEU
1	B	165	VAL
1	B	166	GLN
1	B	176	LEU
1	B	182	ILE
1	B	187	SER
1	B	190	ARG
1	B	191	ARG
1	B	198	VAL
1	C	21	ARG
1	C	26	LEU
1	C	38	LEU
1	C	86	SER
1	C	101	LEU
1	C	108	LEU
1	C	135	LYS
1	C	136	VAL
1	C	140	PHE
1	C	145	LEU
1	C	154	THR
1	C	156	GLU
1	C	158	LEU
1	C	165	VAL
1	C	167	LEU
1	C	176	LEU
1	C	181	SER
1	C	189	ILE
1	C	190	ARG
1	C	198	VAL
1	D	37	GLU
1	D	38	LEU
1	D	52	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	56	THR
1	D	64	LYS
1	D	72	MSE
1	D	74	ASP
1	D	78	ARG
1	D	101	LEU
1	D	103	ARG
1	D	108	LEU
1	D	109	LEU
1	D	115	SER
1	D	124	THR
1	D	127	VAL
1	D	130	VAL
1	D	136	VAL
1	D	138	ARG
1	D	140	PHE
1	D	141	ARG
1	D	143	ILE
1	D	144	MSE
1	D	150	ILE
1	D	152	HIS
1	D	156	GLU
1	D	165	VAL
1	D	167	LEU
1	D	176	LEU
1	D	189	ILE
1	D	198	VAL
1	D	202	HIS
1	E	37	GLU
1	E	38	LEU
1	E	41	VAL
1	E	42	GLN
1	E	52	VAL
1	E	56	THR
1	E	59	ARG
1	E	64	LYS
1	E	72	MSE
1	E	74	ASP
1	E	79	MSE
1	E	94	GLN
1	E	101	LEU
1	E	105	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	106	ARG
1	E	108	LEU
1	E	130	VAL
1	E	138	ARG
1	E	140	PHE
1	E	141	ARG
1	E	152	HIS
1	E	154	THR
1	E	156	GLU
1	E	161	LEU
1	E	164	LEU
1	E	177	ASN
1	E	180	VAL
1	E	190	ARG
1	E	195	LEU
1	E	197	LEU
1	E	202	HIS
1	F	16	GLU
1	F	27	GLU
1	F	38	LEU
1	F	40	ARG
1	F	52	VAL
1	F	54	ILE
1	F	56	THR
1	F	57	LEU
1	F	72	MSE
1	F	101	LEU
1	F	106	ARG
1	F	108	LEU
1	F	109	LEU
1	F	111	ARG
1	F	122	THR
1	F	127	VAL
1	F	130	VAL
1	F	143	ILE
1	F	145	LEU
1	F	150	ILE
1	F	156	GLU
1	F	158	LEU
1	F	165	VAL
1	F	176	LEU
1	F	187	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	190	ARG
1	F	191	ARG
1	F	198	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	75	GLN
1	A	99	ASN
1	A	199	ASN
1	B	42	GLN
1	B	44	HIS
1	B	99	ASN
1	B	142	GLN
1	C	166	GLN
1	D	75	GLN
1	D	202	HIS
1	E	18	GLN
1	E	152	HIS
1	E	173	GLN
1	E	177	ASN
1	E	202	HIS
1	F	199	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry

21 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	SO4	C	316	-	4,4,4	0.30	0	6,6,6	0.39	0
2	SO4	A	319	-	4,4,4	0.22	0	6,6,6	0.55	0
2	SO4	B	308	-	4,4,4	0.16	0	6,6,6	0.81	0
2	SO4	C	301	-	4,4,4	0.33	0	6,6,6	0.67	0
2	SO4	A	306	-	4,4,4	0.11	0	6,6,6	0.12	0
2	SO4	C	318	-	4,4,4	0.19	0	6,6,6	0.36	0
2	SO4	C	315	-	4,4,4	0.14	0	6,6,6	0.34	0
2	SO4	F	313	-	4,4,4	0.19	0	6,6,6	0.32	0
2	SO4	C	309	-	4,4,4	0.24	0	6,6,6	0.37	0
2	SO4	B	312	-	4,4,4	0.18	0	6,6,6	0.25	0
2	SO4	F	304	-	4,4,4	0.14	0	6,6,6	0.34	0
2	SO4	F	303	-	4,4,4	0.14	0	6,6,6	0.33	0
2	SO4	B	314	-	4,4,4	0.08	0	6,6,6	0.31	0
2	SO4	A	320	-	4,4,4	0.08	0	6,6,6	0.24	0
2	SO4	E	302	-	4,4,4	0.12	0	6,6,6	0.22	0
2	SO4	B	311	-	4,4,4	0.15	0	6,6,6	0.18	0
2	SO4	F	310	-	4,4,4	0.13	0	6,6,6	0.16	0
2	SO4	C	307	-	4,4,4	0.09	0	6,6,6	0.34	0
2	SO4	E	317	-	4,4,4	0.18	0	6,6,6	0.23	0
2	SO4	A	321	-	4,4,4	0.19	0	6,6,6	0.19	0
2	SO4	E	305	-	4,4,4	0.14	0	6,6,6	0.26	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	316	SO4	1	0
2	C	301	SO4	2	0
2	C	315	SO4	1	0
2	F	313	SO4	2	0
2	C	309	SO4	4	0
2	F	303	SO4	1	0
2	C	307	SO4	1	0
2	A	321	SO4	2	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	169/207 (81%)	0.88	21 (12%) 4 3	53, 66, 80, 88	0
1	B	177/207 (85%)	0.88	24 (13%) 3 2	51, 64, 82, 97	0
1	C	171/207 (82%)	0.24	2 (1%) 79 80	53, 65, 77, 96	0
1	D	168/207 (81%)	0.72	15 (8%) 9 9	46, 64, 78, 93	0
1	E	176/207 (85%)	1.00	21 (11%) 4 4	50, 63, 83, 118	0
1	F	176/207 (85%)	0.57	14 (7%) 12 12	50, 65, 84, 106	0
All	All	1037/1242 (83%)	0.72	97 (9%) 8 8	46, 65, 82, 118	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	81	VAL	13.2
1	A	201	SER	7.1
1	D	88	PRO	6.5
1	E	89	PRO	6.1
1	E	80	GLY	5.8
1	D	52	VAL	5.5
1	E	202	HIS	5.2
1	F	81	VAL	4.9
1	B	18	GLN	4.8
1	D	51	GLY	4.7
1	A	153	PRO	4.7
1	A	90	GLY	4.7
1	B	127	VAL	4.6
1	D	53	ALA	4.5
1	E	90	GLY	4.3
1	D	150	ILE	4.3
1	F	56	THR	4.3
1	E	17	GLU	4.3
1	D	47	ALA	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	89	PRO	4.0
1	B	19	ARG	3.9
1	E	16	GLU	3.9
1	B	128	ALA	3.9
1	D	152	HIS	3.8
1	E	18	GLN	3.8
1	B	170	GLY	3.7
1	F	202	HIS	3.7
1	B	169	PHE	3.6
1	F	140	PHE	3.5
1	A	200	LEU	3.5
1	A	167	LEU	3.5
1	E	136	VAL	3.4
1	B	86	SER	3.4
1	D	90	GLY	3.4
1	F	21	ARG	3.2
1	F	24	ARG	3.2
1	A	192	ALA	3.2
1	C	20	ALA	3.2
1	D	59	ARG	3.2
1	B	82	GLY	3.1
1	A	155	GLU	3.1
1	A	21	ARG	3.0
1	F	20	ALA	3.0
1	B	168	TRP	3.0
1	E	151	GLU	2.8
1	E	167	LEU	2.8
1	A	199	ASN	2.8
1	A	149	GLY	2.8
1	B	80	GLY	2.8
1	F	169	PHE	2.8
1	A	170	GLY	2.7
1	B	165	VAL	2.7
1	E	171	VAL	2.7
1	E	201	SER	2.7
1	A	168	TRP	2.7
1	B	81	VAL	2.7
1	D	202	HIS	2.6
1	D	54	ILE	2.6
1	F	92	SER	2.6
1	B	44	HIS	2.6
1	A	154	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	166	GLN	2.5
1	A	123	SER	2.5
1	D	57	LEU	2.5
1	A	166	GLN	2.5
1	D	49	ARG	2.4
1	F	19	ARG	2.4
1	A	169	PHE	2.4
1	B	57	LEU	2.4
1	B	167	LEU	2.4
1	E	165	VAL	2.4
1	B	83	PHE	2.4
1	F	80	GLY	2.3
1	E	88	PRO	2.3
1	E	142	GLN	2.3
1	F	150	ILE	2.3
1	A	171	VAL	2.3
1	C	19	ARG	2.3
1	A	165	VAL	2.3
1	D	138	ARG	2.2
1	A	110	ARG	2.2
1	B	93	PRO	2.2
1	E	15	SER	2.2
1	E	169	PHE	2.2
1	E	164	LEU	2.2
1	A	27	GLU	2.1
1	A	160	ALA	2.1
1	B	53	ALA	2.1
1	B	163	LEU	2.1
1	E	170	GLY	2.1
1	F	16	GLU	2.1
1	B	32	LEU	2.1
1	F	22	HIS	2.1
1	E	140	PHE	2.1
1	B	46	VAL	2.0
1	B	61	PHE	2.0
1	B	153	PRO	2.0

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

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. 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
2	SO4	A	306	5/5	0.55	0.47	102,102,102,102	5
2	SO4	B	312	5/5	0.69	0.25	95,95,95,96	5
2	SO4	C	318	5/5	0.76	0.30	71,72,72,73	5
2	SO4	A	321	5/5	0.80	0.29	91,91,91,92	5
2	SO4	F	310	5/5	0.82	0.30	97,97,98,98	5
2	SO4	B	314	5/5	0.82	0.34	83,83,83,83	5
2	SO4	E	317	5/5	0.83	0.25	84,84,85,85	5
2	SO4	F	313	5/5	0.83	0.47	73,73,73,74	5
2	SO4	E	305	5/5	0.83	0.36	83,84,85,85	5
2	SO4	A	319	5/5	0.85	0.40	68,69,69,70	5
2	SO4	B	311	5/5	0.87	0.28	89,89,90,90	5
2	SO4	C	316	5/5	0.88	0.23	78,78,79,80	5
2	SO4	C	309	5/5	0.88	0.25	74,75,75,75	5
2	SO4	C	315	5/5	0.89	0.17	83,84,84,84	5
2	SO4	E	302	5/5	0.90	0.27	86,86,87,87	5
2	SO4	F	303	5/5	0.90	0.19	89,89,90,90	5
2	SO4	A	320	5/5	0.91	0.25	72,72,73,73	5
2	SO4	B	308	5/5	0.92	0.14	73,74,74,74	5
2	SO4	F	304	5/5	0.94	0.30	80,80,80,81	5
2	SO4	C	307	5/5	0.96	0.27	75,76,76,76	5
2	SO4	C	301	5/5	0.97	0.31	73,73,74,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.