



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 2, 2017 – 03:54 PM EDT

PDB ID : 2DG2
Title : Crystal Structure of Mouse Apolipoprotein A-I Binding Protein
Authors : Shumilin, I.A.; Jha, K.N.; Zheng, H.; Chruszcz, M.; Cymborowski, M.; Herr, J.C.; Minor, W.
Deposited on : unknown
Resolution : 2.45 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20030345

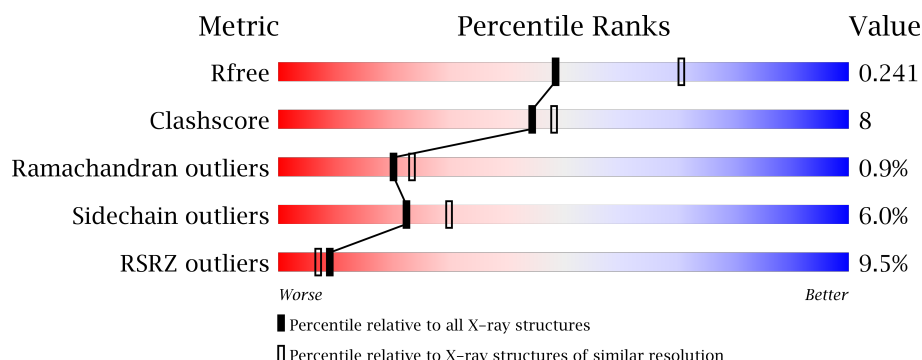
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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}	100719	1119 (2.48-2.44)
Clashscore	112137	1193 (2.48-2.44)
Ramachandran outliers	110173	1185 (2.48-2.44)
Sidechain outliers	110143	1185 (2.48-2.44)
RSRZ outliers	101464	1126 (2.48-2.44)

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	265	<div> <div>8%</div> <div> <div></div> <div>73%</div> <div>12%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	265	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>11%</div> <div>•</div> <div>12%</div> </div> </div>
1	C	265	<div> <div>9%</div> <div> <div></div> <div>72%</div> <div>13%</div> <div>•</div> <div>12%</div> </div> </div>
1	D	265	<div> <div>9%</div> <div> <div></div> <div>74%</div> <div>12%</div> <div>•</div> <div>12%</div> </div> </div>
1	E	265	<div> <div>8%</div> <div> <div></div> <div>72%</div> <div>12%</div> <div>•</div> <div>12%</div> </div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	265	

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	1001	-	-	-	X
2	SO4	B	1003	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11077 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 Apolipoprotein A-I binding protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	233	Total	C	N	O	S	Se	0	0	0
			1805	1168	290	336	5	6			
1	B	233	Total	C	N	O	S	Se	0	0	0
			1805	1168	290	336	5	6			
1	C	233	Total	C	N	O	S	Se	0	0	0
			1805	1168	290	336	5	6			
1	D	233	Total	C	N	O	S	Se	0	0	0
			1805	1168	290	336	5	6			
1	E	233	Total	C	N	O	S	Se	0	0	0
			1805	1168	290	336	5	6			
1	F	233	Total	C	N	O	S	Se	0	0	0
			1805	1168	290	336	5	6			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	INITIATING METHIONINE	GB 37231544
A	22	MSE	MET	MODIFIED RESIDUE	GB 37231544
A	54	MSE	MET	MODIFIED RESIDUE	GB 37231544
A	74	MSE	MET	MODIFIED RESIDUE	GB 37231544
A	131	MSE	MET	MODIFIED RESIDUE	GB 37231544
A	139	MSE	MET	MODIFIED RESIDUE	GB 37231544
A	144	MSE	MET	MODIFIED RESIDUE	GB 37231544
A	145	MSE	MET	MODIFIED RESIDUE	GB 37231544
A	259	HIS	-	EXPRESSION TAG	GB 37231544
A	260	HIS	-	EXPRESSION TAG	GB 37231544
A	261	HIS	-	EXPRESSION TAG	GB 37231544
A	262	HIS	-	EXPRESSION TAG	GB 37231544
A	263	HIS	-	EXPRESSION TAG	GB 37231544
A	264	HIS	-	EXPRESSION TAG	GB 37231544
B	0	MET	-	INITIATING METHIONINE	GB 37231544
B	22	MSE	MET	MODIFIED RESIDUE	GB 37231544
B	54	MSE	MET	MODIFIED RESIDUE	GB 37231544

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	74	MSE	MET	MODIFIED RESIDUE	GB 37231544
B	131	MSE	MET	MODIFIED RESIDUE	GB 37231544
B	139	MSE	MET	MODIFIED RESIDUE	GB 37231544
B	144	MSE	MET	MODIFIED RESIDUE	GB 37231544
B	145	MSE	MET	MODIFIED RESIDUE	GB 37231544
B	259	HIS	-	EXPRESSION TAG	GB 37231544
B	260	HIS	-	EXPRESSION TAG	GB 37231544
B	261	HIS	-	EXPRESSION TAG	GB 37231544
B	262	HIS	-	EXPRESSION TAG	GB 37231544
B	263	HIS	-	EXPRESSION TAG	GB 37231544
B	264	HIS	-	EXPRESSION TAG	GB 37231544
C	0	MET	-	INITIATING METHIONINE	GB 37231544
C	22	MSE	MET	MODIFIED RESIDUE	GB 37231544
C	54	MSE	MET	MODIFIED RESIDUE	GB 37231544
C	74	MSE	MET	MODIFIED RESIDUE	GB 37231544
C	131	MSE	MET	MODIFIED RESIDUE	GB 37231544
C	139	MSE	MET	MODIFIED RESIDUE	GB 37231544
C	144	MSE	MET	MODIFIED RESIDUE	GB 37231544
C	145	MSE	MET	MODIFIED RESIDUE	GB 37231544
C	259	HIS	-	EXPRESSION TAG	GB 37231544
C	260	HIS	-	EXPRESSION TAG	GB 37231544
C	261	HIS	-	EXPRESSION TAG	GB 37231544
C	262	HIS	-	EXPRESSION TAG	GB 37231544
C	263	HIS	-	EXPRESSION TAG	GB 37231544
C	264	HIS	-	EXPRESSION TAG	GB 37231544
D	0	MET	-	INITIATING METHIONINE	GB 37231544
D	22	MSE	MET	MODIFIED RESIDUE	GB 37231544
D	54	MSE	MET	MODIFIED RESIDUE	GB 37231544
D	74	MSE	MET	MODIFIED RESIDUE	GB 37231544
D	131	MSE	MET	MODIFIED RESIDUE	GB 37231544
D	139	MSE	MET	MODIFIED RESIDUE	GB 37231544
D	144	MSE	MET	MODIFIED RESIDUE	GB 37231544
D	145	MSE	MET	MODIFIED RESIDUE	GB 37231544
D	259	HIS	-	EXPRESSION TAG	GB 37231544
D	260	HIS	-	EXPRESSION TAG	GB 37231544
D	261	HIS	-	EXPRESSION TAG	GB 37231544
D	262	HIS	-	EXPRESSION TAG	GB 37231544
D	263	HIS	-	EXPRESSION TAG	GB 37231544
D	264	HIS	-	EXPRESSION TAG	GB 37231544
E	0	MET	-	INITIATING METHIONINE	GB 37231544
E	22	MSE	MET	MODIFIED RESIDUE	GB 37231544
E	54	MSE	MET	MODIFIED RESIDUE	GB 37231544

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	74	MSE	MET	MODIFIED RESIDUE	GB 37231544
E	131	MSE	MET	MODIFIED RESIDUE	GB 37231544
E	139	MSE	MET	MODIFIED RESIDUE	GB 37231544
E	144	MSE	MET	MODIFIED RESIDUE	GB 37231544
E	145	MSE	MET	MODIFIED RESIDUE	GB 37231544
E	259	HIS	-	EXPRESSION TAG	GB 37231544
E	260	HIS	-	EXPRESSION TAG	GB 37231544
E	261	HIS	-	EXPRESSION TAG	GB 37231544
E	262	HIS	-	EXPRESSION TAG	GB 37231544
E	263	HIS	-	EXPRESSION TAG	GB 37231544
E	264	HIS	-	EXPRESSION TAG	GB 37231544
F	0	MET	-	INITIATING METHIONINE	GB 37231544
F	22	MSE	MET	MODIFIED RESIDUE	GB 37231544
F	54	MSE	MET	MODIFIED RESIDUE	GB 37231544
F	74	MSE	MET	MODIFIED RESIDUE	GB 37231544
F	131	MSE	MET	MODIFIED RESIDUE	GB 37231544
F	139	MSE	MET	MODIFIED RESIDUE	GB 37231544
F	144	MSE	MET	MODIFIED RESIDUE	GB 37231544
F	145	MSE	MET	MODIFIED RESIDUE	GB 37231544
F	259	HIS	-	EXPRESSION TAG	GB 37231544
F	260	HIS	-	EXPRESSION TAG	GB 37231544
F	261	HIS	-	EXPRESSION TAG	GB 37231544
F	262	HIS	-	EXPRESSION TAG	GB 37231544
F	263	HIS	-	EXPRESSION TAG	GB 37231544
F	264	HIS	-	EXPRESSION TAG	GB 37231544

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



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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0

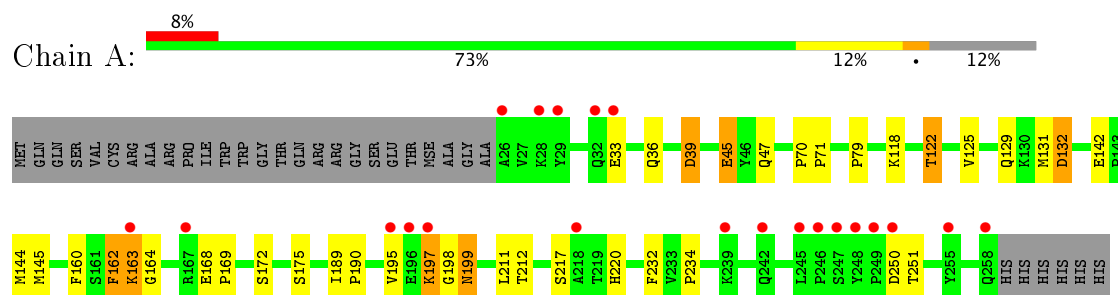
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	44	Total O 44 44	0	0
4	B	41	Total O 41 41	0	0
4	C	41	Total O 41 41	0	0
4	D	26	Total O 26 26	0	0
4	E	30	Total O 30 30	0	0
4	F	29	Total O 29 29	0	0

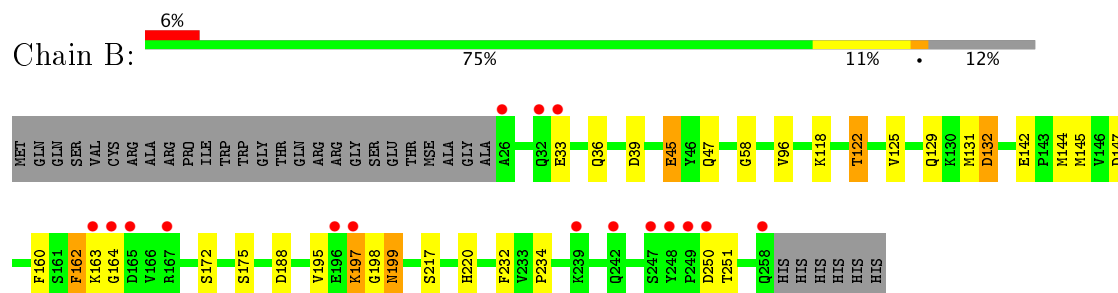
3 Residue-property plots [i](#)

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.

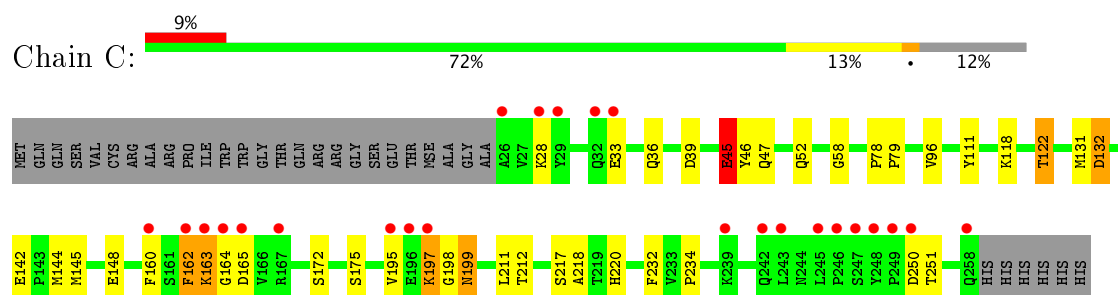
- Molecule 1: Apolipoprotein A-I binding protein



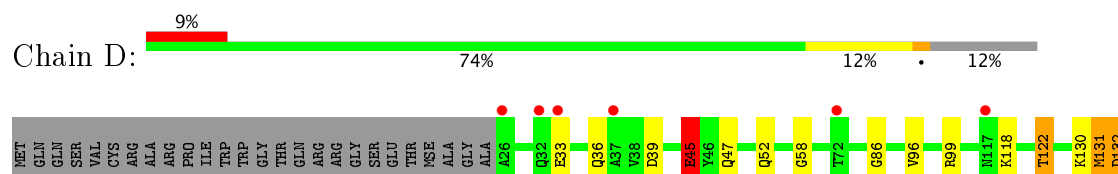
- Molecule 1: Apolipoprotein A-I binding protein

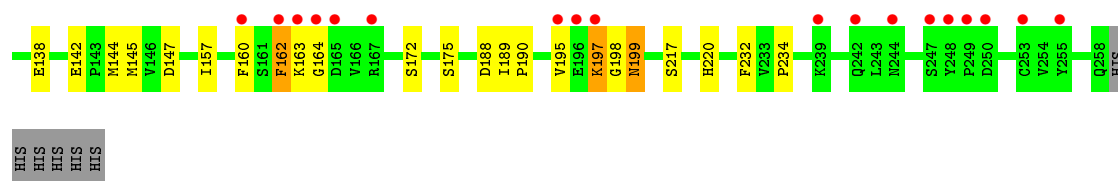


- Molecule 1: Apolipoprotein A-I binding protein

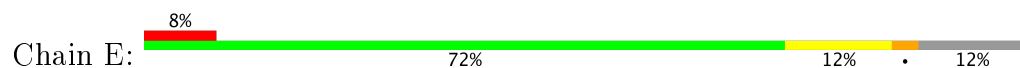


- Molecule 1: Apolipoprotein A-I binding protein

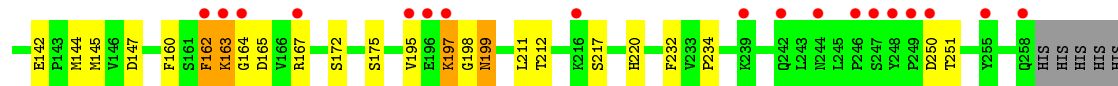
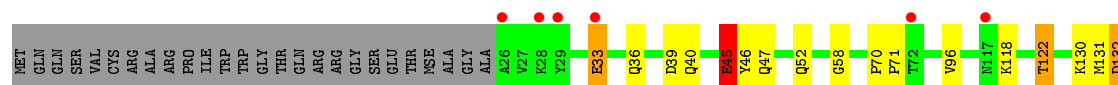




- Molecule 1: Apolipoprotein A-I binding protein



- Molecule 1: Apolipoprotein A-I binding protein



HIS

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	104.86Å 125.75Å 163.62Å 90.00° 106.56° 90.00°	Depositor
Resolution (Å)	80.00 – 2.45 38.69 – 2.44	Depositor EDS
% Data completeness (in resolution range)	98.3 (80.00-2.45) 97.8 (38.69-2.44)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.206 , 0.228 0.220 , 0.241	Depositor DCC
R_{free} test set	3692 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11077	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 84.37 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.6955e-07. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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, CL

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	0.99	0/1850	0.84	1/2510 (0.0%)
1	B	0.98	0/1850	0.84	2/2510 (0.1%)
1	C	1.02	1/1850 (0.1%)	0.84	1/2510 (0.0%)
1	D	1.02	2/1850 (0.1%)	0.86	2/2510 (0.1%)
1	E	1.01	1/1850 (0.1%)	0.84	1/2510 (0.0%)
1	F	1.00	2/1850 (0.1%)	0.84	2/2510 (0.1%)
All	All	1.00	6/11100 (0.1%)	0.84	9/15060 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	40	GLN	CD-OE1	5.25	1.35	1.24
1	D	138	GLU	CG-CD	5.24	1.59	1.51
1	D	52	GLN	CD-OE1	5.23	1.35	1.24
1	E	97	CYS	CB-SG	-5.23	1.73	1.81
1	C	52	GLN	CD-OE1	5.12	1.35	1.24
1	F	52	GLN	CD-OE1	5.01	1.34	1.24

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	147	ASP	CB-CG-OD1	6.42	124.08	118.30
1	B	147	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	B	147	ASP	CB-CG-OD1	6.02	123.72	118.30
1	D	147	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	F	147	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	163	LYS	N-CA-C	5.11	124.79	111.00
1	E	163	LYS	N-CA-C	5.08	124.71	111.00
1	F	163	LYS	N-CA-C	5.05	124.64	111.00
1	C	163	LYS	N-CA-C	5.03	124.58	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1805	0	1790	30	0
1	B	1805	0	1790	23	0
1	C	1805	0	1790	32	0
1	D	1805	0	1790	24	0
1	E	1805	0	1790	33	0
1	F	1805	0	1790	26	1
2	A	5	0	0	1	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	1	0
4	A	44	0	0	13	0
4	B	41	0	0	9	0
4	C	41	0	0	12	0
4	D	26	0	0	6	0
4	E	30	0	0	16	0
4	F	29	0	0	5	1
All	All	11077	0	10740	162	1

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 8.

All (162) 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:E:144:MSE:SE	1:E:144:MSE:CE	2.16	1.42
1:C:144:MSE:SE	1:C:144:MSE:CE	2.19	1.40
1:A:144:MSE:SE	1:A:144:MSE:CE	2.18	1.40
1:F:144:MSE:SE	1:F:144:MSE:CE	2.20	1.39
1:B:144:MSE:CE	1:B:144:MSE:SE	2.21	1.38
1:D:144:MSE:SE	1:D:144:MSE:CE	2.22	1.37
1:E:132:ASP:HB3	4:E:1029:HOH:O	1.25	1.31
1:C:144:MSE:HE3	4:C:1030:HOH:O	1.27	1.31
1:B:132:ASP:HB3	4:B:1006:HOH:O	1.26	1.26
1:A:132:ASP:HB3	4:A:1011:HOH:O	1.14	1.25
1:D:132:ASP:HB3	4:D:1031:HOH:O	1.43	1.17
1:A:47:GLN:HG3	4:A:1018:HOH:O	1.53	1.07
1:A:39:ASP:HB3	4:A:1031:HOH:O	1.60	1.00
1:B:162:PHE:HD1	4:B:1042:HOH:O	1.42	1.00
1:E:148:GLU:HG3	4:E:1031:HOH:O	1.67	0.94
1:F:165:ASP:HA	4:F:1041:HOH:O	1.69	0.90
1:E:131:MSE:SE	4:E:1014:HOH:O	2.40	0.88
1:D:131:MSE:SE	4:D:1017:HOH:O	2.44	0.85
1:E:144:MSE:HE3	4:E:1031:HOH:O	1.76	0.85
1:B:162:PHE:CD1	4:B:1042:HOH:O	2.23	0.80
1:C:162:PHE:CE2	4:C:1047:HOH:O	2.35	0.80
1:E:74:MSE:SE	4:E:1028:HOH:O	2.48	0.80
1:A:162:PHE:HB3	4:A:1008:HOH:O	1.82	0.79
1:C:162:PHE:HB3	4:C:1011:HOH:O	1.85	0.76
1:F:162:PHE:HB3	4:F:1032:HOH:O	1.88	0.73
1:E:118:LYS:O	1:E:122:THR:HG23	1.89	0.72
1:D:118:LYS:O	1:D:122:THR:HG23	1.91	0.71
1:F:118:LYS:O	1:F:122:THR:HG23	1.92	0.68
1:C:165:ASP:HA	4:C:1022:HOH:O	1.93	0.68
1:A:232:PHE:O	1:A:234:PRO:HD3	1.94	0.68
1:E:160:PHE:O	1:E:195:VAL:HG21	1.93	0.67
1:D:232:PHE:O	1:D:234:PRO:HD3	1.94	0.67
1:A:168:GLU:HB3	4:A:1022:HOH:O	1.96	0.66
1:D:160:PHE:O	1:D:195:VAL:HG21	1.95	0.66
1:B:232:PHE:O	1:B:234:PRO:HD3	1.95	0.66
1:F:232:PHE:O	1:F:234:PRO:HD3	1.95	0.66
1:B:118:LYS:O	1:B:122:THR:HG23	1.96	0.65
1:E:232:PHE:O	1:E:234:PRO:HD3	1.97	0.65
1:C:160:PHE:O	1:C:195:VAL:HG21	1.97	0.65
1:B:160:PHE:O	1:B:195:VAL:HG21	1.96	0.65
1:C:118:LYS:O	1:C:122:THR:HG23	1.95	0.64
1:E:131:MSE:HA	4:E:1023:HOH:O	1.97	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:PHE:O	1:A:195:VAL:HG21	1.98	0.64
1:C:232:PHE:O	1:C:234:PRO:HD3	1.98	0.63
1:D:163:LYS:H	1:D:164:GLY:HA2	1.64	0.63
1:F:160:PHE:O	1:F:195:VAL:HG21	1.97	0.63
1:E:131:MSE:CG	4:E:1014:HOH:O	2.46	0.62
1:D:132:ASP:CB	4:D:1031:HOH:O	2.19	0.62
1:A:118:LYS:O	1:A:122:THR:HG23	2.00	0.61
1:B:188:ASP:OD2	4:B:1035:HOH:O	2.16	0.61
1:F:163:LYS:H	1:F:164:GLY:HA2	1.65	0.61
1:B:163:LYS:H	1:B:164:GLY:HA2	1.64	0.61
1:C:163:LYS:H	1:C:164:GLY:HA2	1.65	0.60
1:B:163:LYS:N	1:B:164:GLY:HA2	2.17	0.60
1:D:131:MSE:CG	4:D:1017:HOH:O	2.50	0.60
1:B:160:PHE:HD1	4:B:1035:HOH:O	1.85	0.60
1:C:162:PHE:HD1	4:C:1046:HOH:O	1.84	0.59
1:D:163:LYS:N	1:D:164:GLY:HA2	2.17	0.59
1:E:163:LYS:H	1:E:164:GLY:HA2	1.66	0.59
1:E:163:LYS:N	1:E:164:GLY:HA2	2.18	0.59
1:F:163:LYS:N	1:F:164:GLY:HA2	2.17	0.58
1:A:163:LYS:N	1:A:164:GLY:HA2	2.18	0.58
1:C:163:LYS:N	1:C:164:GLY:HA2	2.17	0.58
1:A:163:LYS:H	1:A:164:GLY:HA2	1.68	0.58
1:A:144:MSE:HB2	4:A:1006:HOH:O	2.04	0.57
4:C:1034:HOH:O	1:D:47:GLN:HG3	2.06	0.54
1:C:132:ASP:HB2	4:C:1038:HOH:O	2.08	0.53
1:E:132:ASP:CB	4:E:1029:HOH:O	2.10	0.53
1:E:162:PHE:HD1	4:E:1021:HOH:O	1.92	0.53
1:E:127:GLN:NE2	4:E:1039:HOH:O	2.30	0.52
1:F:162:PHE:HD1	4:F:1018:HOH:O	1.92	0.52
1:F:167:ARG:HA	3:F:1012:CL:CL	2.47	0.51
1:E:162:PHE:HB3	4:E:1021:HOH:O	2.11	0.50
1:A:79:PRO:HB3	4:A:1039:HOH:O	2.12	0.49
1:A:160:PHE:HD1	4:A:1035:HOH:O	1.94	0.49
1:A:198:GLY:O	1:A:199:ASN:HB2	2.13	0.49
1:B:198:GLY:O	1:B:199:ASN:HB2	2.12	0.49
1:A:132:ASP:HB2	4:A:1032:HOH:O	2.13	0.48
1:E:142:GLU:H	1:E:145:MSE:HE3	1.78	0.48
1:C:45:GLU:HG3	1:F:45:GLU:HA	1.95	0.48
1:F:45:GLU:O	1:F:47:GLN:HG2	2.13	0.48
1:A:142:GLU:HB2	1:A:145:MSE:CE	2.44	0.48
1:B:142:GLU:HB2	1:B:145:MSE:CE	2.44	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:45:GLU:O	1:C:47:GLN:HG2	2.14	0.48
1:C:46:TYR:CE2	1:D:130:LYS:HB3	2.48	0.47
1:D:142:GLU:H	1:D:145:MSE:HE3	1.80	0.47
1:D:197:LYS:O	1:D:220:HIS:CE1	2.68	0.46
1:F:197:LYS:O	1:F:220:HIS:CE1	2.68	0.46
1:E:138:GLU:HB2	4:E:1026:HOH:O	2.14	0.46
1:E:142:GLU:HB2	1:E:145:MSE:CE	2.46	0.46
1:F:164:GLY:N	4:F:1041:HOH:O	2.49	0.46
1:A:142:GLU:HB2	1:A:145:MSE:HE3	1.96	0.46
1:E:198:GLY:O	1:E:199:ASN:HB2	2.15	0.46
1:C:197:LYS:O	1:C:220:HIS:CE1	2.68	0.46
1:E:45:GLU:O	1:E:47:GLN:HG2	2.16	0.46
1:A:79:PRO:CB	4:A:1039:HOH:O	2.63	0.46
1:D:142:GLU:HB2	1:D:145:MSE:CE	2.46	0.45
1:A:189:ILE:HA	1:A:190:PRO:HD3	1.85	0.45
1:B:162:PHE:HB3	4:B:1042:HOH:O	2.17	0.45
1:F:142:GLU:HB2	1:F:145:MSE:CE	2.47	0.45
1:C:142:GLU:H	1:C:145:MSE:HE3	1.81	0.45
1:C:28:LYS:C	4:C:1032:HOH:O	2.54	0.45
1:B:197:LYS:O	1:B:220:HIS:CE1	2.69	0.45
1:D:188:ASP:OD2	4:D:1014:HOH:O	2.21	0.45
1:A:197:LYS:O	1:A:220:HIS:CE1	2.69	0.45
1:F:198:GLY:O	1:F:199:ASN:HB2	2.16	0.45
1:E:250:ASP:CG	1:E:251:THR:H	2.21	0.44
1:E:197:LYS:O	1:E:220:HIS:CE1	2.70	0.44
1:C:45:GLU:HA	1:F:45:GLU:HG3	1.99	0.44
1:F:211:LEU:O	1:F:212:THR:HB	2.17	0.44
1:F:250:ASP:CG	1:F:251:THR:H	2.20	0.44
1:A:132:ASP:CB	4:A:1032:HOH:O	2.65	0.44
1:A:169:PRO:HB2	4:A:1026:HOH:O	2.18	0.44
1:A:250:ASP:CG	1:A:251:THR:H	2.19	0.44
1:D:198:GLY:O	1:D:199:ASN:HB2	2.17	0.44
1:E:116:PRO:N	4:E:1018:HOH:O	2.51	0.44
1:C:142:GLU:HB2	1:C:145:MSE:HE3	2.00	0.44
1:C:250:ASP:CG	1:C:251:THR:H	2.21	0.44
1:C:198:GLY:O	1:C:199:ASN:HB2	2.18	0.44
1:A:142:GLU:H	1:A:145:MSE:HE3	1.83	0.43
1:B:250:ASP:CG	1:B:251:THR:H	2.22	0.43
1:D:189:ILE:HA	1:D:190:PRO:HD3	1.87	0.43
1:B:144:MSE:HB2	4:B:1007:HOH:O	2.17	0.43
1:E:130:LYS:HB3	1:F:46:TYR:CE2	2.53	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:GLU:HB2	1:B:145:MSE:HE3	2.00	0.43
1:E:142:GLU:HB2	1:E:145:MSE:HE3	2.00	0.43
1:A:162:PHE:CD2	2:A:1001:SO4:O2	2.72	0.43
1:B:47:GLN:HG3	4:B:1019:HOH:O	2.18	0.43
1:B:142:GLU:H	1:B:145:MSE:HE3	1.84	0.43
1:D:58:GLY:HA3	1:D:96:VAL:CG1	2.49	0.42
1:E:125:VAL:HG12	1:E:129:GLN:OE1	2.18	0.42
1:F:142:GLU:H	1:F:145:MSE:HE3	1.84	0.42
1:A:162:PHE:HD1	4:A:1008:HOH:O	2.02	0.42
1:A:70:PRO:HA	1:A:71:PRO:HD3	1.93	0.42
1:E:188:ASP:OD2	4:E:1030:HOH:O	2.22	0.42
1:C:144:MSE:HB2	4:C:1012:HOH:O	2.20	0.42
1:F:33:GLU:HA	4:F:1020:HOH:O	2.19	0.42
1:F:70:PRO:HA	1:F:71:PRO:HD3	1.93	0.42
1:C:45:GLU:HG3	1:F:45:GLU:HG3	2.02	0.42
1:C:142:GLU:HB2	1:C:145:MSE:CE	2.49	0.42
1:C:111:TYR:OH	4:C:1026:HOH:O	2.22	0.41
1:F:58:GLY:HA3	1:F:96:VAL:CG1	2.50	0.41
1:A:125:VAL:HG12	1:A:129:GLN:NE2	2.36	0.41
1:E:131:MSE:HG3	4:E:1014:HOH:O	2.16	0.41
1:D:45:GLU:O	1:D:47:GLN:HG2	2.20	0.41
1:C:148:GLU:HG3	4:C:1030:HOH:O	2.19	0.41
1:C:78:PRO:HA	1:C:79:PRO:HD3	1.96	0.41
1:B:132:ASP:CB	4:B:1025:HOH:O	2.69	0.41
1:E:46:TYR:CE2	1:F:130:LYS:HB3	2.55	0.41
1:D:86:GLY:HA3	1:D:157:ILE:O	2.21	0.41
1:E:189:ILE:HA	1:E:190:PRO:HD3	1.89	0.41
1:D:99:ARG:HG2	1:D:99:ARG:HH11	1.85	0.41
1:C:144:MSE:CE	4:C:1030:HOH:O	2.15	0.40
1:C:211:LEU:O	1:C:212:THR:HB	2.21	0.40
1:B:58:GLY:HA3	1:B:96:VAL:CG1	2.51	0.40
1:C:197:LYS:O	1:C:220:HIS:ND1	2.54	0.40
1:A:211:LEU:O	1:A:212:THR:HB	2.22	0.40
1:B:125:VAL:HG12	1:B:129:GLN:NE2	2.36	0.40
1:C:58:GLY:HA3	1:C:96:VAL:CG1	2.52	0.40
1:D:142:GLU:HB2	1:D:145:MSE:HE3	2.03	0.40
1:D:162:PHE:HB3	4:D:1032:HOH:O	2.21	0.40
1:E:144:MSE:HB2	4:E:1016:HOH:O	2.20	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:132:ASP:CB	4:F:1014:HOH:O[2_555]	2.16	0.04

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	231/265 (87%)	214 (93%)	15 (6%)	2 (1%)	20	23
1	B	231/265 (87%)	214 (93%)	15 (6%)	2 (1%)	20	23
1	C	231/265 (87%)	210 (91%)	18 (8%)	3 (1%)	14	13
1	D	231/265 (87%)	212 (92%)	17 (7%)	2 (1%)	20	23
1	E	231/265 (87%)	210 (91%)	19 (8%)	2 (1%)	20	23
1	F	231/265 (87%)	209 (90%)	20 (9%)	2 (1%)	20	23
All	All	1386/1590 (87%)	1269 (92%)	104 (8%)	13 (1%)	20	23

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	B	45	GLU
1	C	45	GLU
1	D	45	GLU
1	E	45	GLU
1	F	45	GLU
1	C	218	ALA
1	A	199	ASN
1	B	199	ASN
1	E	199	ASN
1	F	199	ASN
1	C	199	ASN
1	D	199	ASN

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	199/220 (90%)	187 (94%)	12 (6%)	22	30
1	B	199/220 (90%)	187 (94%)	12 (6%)	22	30
1	C	199/220 (90%)	187 (94%)	12 (6%)	22	30
1	D	199/220 (90%)	187 (94%)	12 (6%)	22	30
1	E	199/220 (90%)	187 (94%)	12 (6%)	22	30
1	F	199/220 (90%)	187 (94%)	12 (6%)	22	30
All	All	1194/1320 (90%)	1122 (94%)	72 (6%)	22	30

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLU
1	A	36	GLN
1	A	39	ASP
1	A	45	GLU
1	A	122	THR
1	A	131	MSE
1	A	132	ASP
1	A	162	PHE
1	A	172	SER
1	A	175	SER
1	A	197	LYS
1	A	217	SER
1	B	33	GLU
1	B	36	GLN
1	B	39	ASP
1	B	45	GLU
1	B	122	THR
1	B	131	MSE
1	B	132	ASP
1	B	162	PHE
1	B	172	SER
1	B	175	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	197	LYS
1	B	217	SER
1	C	33	GLU
1	C	36	GLN
1	C	39	ASP
1	C	45	GLU
1	C	122	THR
1	C	131	MSE
1	C	132	ASP
1	C	162	PHE
1	C	172	SER
1	C	175	SER
1	C	197	LYS
1	C	217	SER
1	D	33	GLU
1	D	36	GLN
1	D	39	ASP
1	D	45	GLU
1	D	122	THR
1	D	131	MSE
1	D	132	ASP
1	D	162	PHE
1	D	172	SER
1	D	175	SER
1	D	197	LYS
1	D	217	SER
1	E	33	GLU
1	E	36	GLN
1	E	39	ASP
1	E	45	GLU
1	E	122	THR
1	E	131	MSE
1	E	132	ASP
1	E	162	PHE
1	E	172	SER
1	E	175	SER
1	E	197	LYS
1	E	217	SER
1	F	33	GLU
1	F	36	GLN
1	F	39	ASP
1	F	45	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	122	THR
1	F	131	MSE
1	F	132	ASP
1	F	162	PHE
1	F	172	SER
1	F	175	SER
1	F	197	LYS
1	F	217	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	GLN
1	B	32	GLN
1	D	107	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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
2	SO4	A	1001	-	4,4,4	0.09	0	6,6,6	0.30	0
2	SO4	B	1003	-	4,4,4	0.12	0	6,6,6	0.20	0
2	SO4	C	1005	-	4,4,4	0.20	0	6,6,6	0.20	0
2	SO4	D	1007	-	4,4,4	0.14	0	6,6,6	0.22	0
2	SO4	E	1009	-	4,4,4	0.14	0	6,6,6	0.27	0
2	SO4	F	1011	-	4,4,4	0.13	0	6,6,6	0.24	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	A	1001	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1003	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1005	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1007	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1009	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1011	-	-	0/0/0/0	0/0/0/0

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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	SO4	1	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	227/265 (85%)	0.20	21 (9%) 9 7	18, 39, 70, 79	0
1	B	227/265 (85%)	0.24	16 (7%) 17 15	18, 39, 70, 79	0
1	C	227/265 (85%)	0.32	24 (10%) 7 5	18, 39, 70, 79	0
1	D	227/265 (85%)	0.36	24 (10%) 7 5	18, 39, 70, 79	0
1	E	227/265 (85%)	0.41	21 (9%) 9 7	18, 39, 70, 80	0
1	F	227/265 (85%)	0.34	24 (10%) 7 5	18, 39, 70, 79	0
All	All	1362/1590 (85%)	0.31	130 (9%) 9 7	18, 39, 71, 80	0

All (130) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	163	LYS	5.9
1	C	163	LYS	5.8
1	D	163	LYS	5.6
1	E	117	ASN	5.5
1	D	249	PRO	5.5
1	E	163	LYS	5.4
1	B	163	LYS	5.4
1	C	249	PRO	5.2
1	D	247	SER	4.7
1	F	197	LYS	4.5
1	E	197	LYS	4.4
1	D	164	GLY	4.4
1	A	197	LYS	4.4
1	F	26	ALA	4.2
1	B	249	PRO	4.2
1	E	249	PRO	4.0
1	F	247	SER	3.9
1	F	196	GLU	3.9
1	E	195	VAL	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	165	ASP	3.8
1	C	248	TYR	3.8
1	D	196	GLU	3.8
1	A	247	SER	3.6
1	F	258	GLN	3.6
1	C	195	VAL	3.6
1	A	196	GLU	3.6
1	A	26	ALA	3.6
1	E	164	GLY	3.6
1	F	195	VAL	3.5
1	C	250	ASP	3.5
1	B	239	LYS	3.5
1	C	197	LYS	3.5
1	C	164	GLY	3.5
1	C	28	LYS	3.4
1	D	160	PHE	3.4
1	F	255	TYR	3.4
1	A	163	LYS	3.4
1	D	250	ASP	3.4
1	F	242	GLN	3.4
1	D	165	ASP	3.3
1	E	26	ALA	3.3
1	F	29	TYR	3.3
1	D	72	THR	3.3
1	E	196	GLU	3.3
1	D	37	ALA	3.2
1	D	117	ASN	3.2
1	D	33	GLU	3.2
1	E	162	PHE	3.2
1	E	165	ASP	3.2
1	C	33	GLU	3.2
1	B	247	SER	3.1
1	D	197	LYS	3.1
1	F	28	LYS	3.1
1	F	249	PRO	3.1
1	B	250	ASP	3.1
1	F	248	TYR	3.1
1	A	249	PRO	3.1
1	B	164	GLY	3.1
1	F	239	LYS	3.1
1	B	165	ASP	3.1
1	C	196	GLU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	195	VAL	3.0
1	B	242	GLN	3.0
1	A	242	GLN	3.0
1	E	239	LYS	3.0
1	C	239	LYS	3.0
1	F	117	ASN	2.9
1	F	250	ASP	2.9
1	C	247	SER	2.9
1	D	239	LYS	2.9
1	D	26	ALA	2.9
1	E	242	GLN	2.9
1	E	250	ASP	2.8
1	C	26	ALA	2.8
1	A	258	GLN	2.8
1	C	32	GLN	2.8
1	C	245	LEU	2.8
1	B	258	GLN	2.8
1	F	33	GLU	2.8
1	C	242	GLN	2.8
1	D	32	GLN	2.7
1	B	167	ARG	2.7
1	E	33	GLU	2.7
1	C	243	LEU	2.7
1	D	167	ARG	2.7
1	A	33	GLU	2.6
1	A	245	LEU	2.5
1	C	160	PHE	2.5
1	D	242	GLN	2.5
1	E	167	ARG	2.5
1	E	253	CYS	2.5
1	E	32	GLN	2.4
1	C	162	PHE	2.4
1	F	72	THR	2.4
1	A	250	ASP	2.4
1	F	167	ARG	2.4
1	B	32	GLN	2.4
1	B	33	GLU	2.4
1	D	255	TYR	2.4
1	E	248	TYR	2.4
1	B	26	ALA	2.4
1	C	258	GLN	2.3
1	F	216	LYS	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	246	PRO	2.3
1	C	167	ARG	2.3
1	D	244	ASN	2.3
1	F	244	ASN	2.3
1	D	162	PHE	2.3
1	C	29	TYR	2.3
1	F	162	PHE	2.3
1	D	248	TYR	2.3
1	A	246	PRO	2.2
1	A	255	TYR	2.2
1	A	195	VAL	2.2
1	A	32	GLN	2.2
1	A	29	TYR	2.1
1	A	218	ALA	2.1
1	C	246	PRO	2.1
1	D	253	CYS	2.1
1	B	196	GLU	2.1
1	B	248	TYR	2.1
1	E	241	TYR	2.1
1	E	244	ASN	2.1
1	A	239	LYS	2.1
1	A	248	TYR	2.1
1	B	197	LYS	2.1
1	E	97	CYS	2.1
1	F	164	GLY	2.1
1	A	28	LYS	2.1
1	A	167	ARG	2.1

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(\AA^2)	Q<0.9
2	SO4	A	1001	5/5	0.73	0.23	2.78	114,124,126,127	0
2	SO4	B	1003	5/5	0.77	0.24	2.06	113,120,122,124	0
2	SO4	F	1011	5/5	0.70	0.21	1.12	130,134,137,139	0
2	SO4	D	1007	5/5	0.71	0.19	0.20	128,129,132,133	0
2	SO4	C	1005	5/5	0.84	0.15	-0.30	127,127,133,133	0
2	SO4	E	1009	5/5	0.75	0.16	-0.38	122,129,129,132	0
3	CL	E	1010	1/1	0.76	0.64	-	100,100,100,100	0
3	CL	A	1002	1/1	0.59	0.45	-	101,101,101,101	0
3	CL	B	1004	1/1	0.70	0.37	-	89,89,89,89	0
3	CL	C	1006	1/1	0.83	0.44	-	89,89,89,89	0
3	CL	F	1012	1/1	0.85	0.68	-	81,81,81,81	0
3	CL	D	1008	1/1	0.51	0.58	-	96,96,96,96	0

6.5 Other polymers [i](#)

There are no such residues in this entry.