Full wwPDB X-ray Structure Validation Report (i)

Nov 25, 2024 – 06:25 PM EST

PDB ID	:	3K6A
Title	:	Crystal structure of molybdenum cofactor biosynthesis protein mog from shewanella oneidensis
Authors	:	Chang, C.; Bigelow, L.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on	:	2009-10-08
Resolution	:	1.89 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:

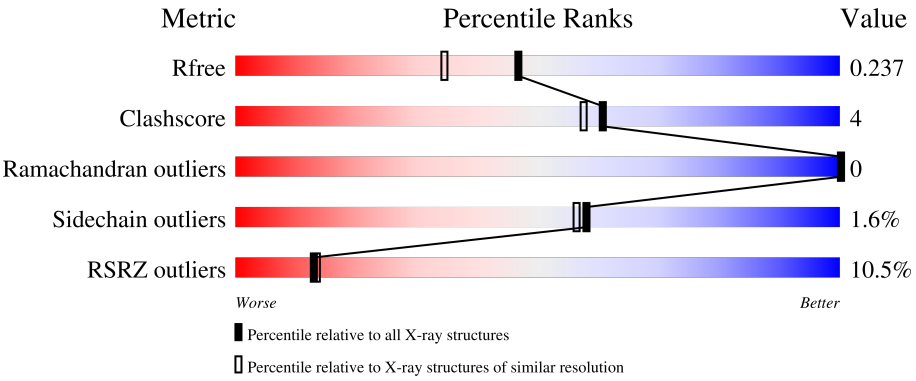
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.89 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}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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%

Mol	Chain	Length	Quality of chain
1	A	180	6% 92% 5%
1	B	180	4% 87% 8%
1	C	180	3% 88% 7%
1	D	180	4% 88% 6%
1	E	180	% 90% 5%
1	F	180	40% 81% 13% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 8852 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 Molybdenum cofactor biosynthesis protein Mog.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	176	Total	C	N	O	S	Se	0	1	0
			1340	846	218	265	6	5			
1	B	172	Total	C	N	O	S	Se	0	1	0
			1319	834	214	259	6	6			
1	C	173	Total	C	N	O	S	Se	0	4	0
			1353	853	221	267	6	6			
1	D	172	Total	C	N	O	S	Se	0	3	0
			1336	843	216	265	6	6			
1	E	171	Total	C	N	O	S	Se	0	2	0
			1318	832	214	259	7	6			
1	F	170	Total	C	N	O	S	Se	0	0	0
			1290	816	210	253	6	5			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q8EKM7
A	-1	ASN	-	expression tag	UNP Q8EKM7
A	0	ALA	-	expression tag	UNP Q8EKM7
B	-2	SER	-	expression tag	UNP Q8EKM7
B	-1	ASN	-	expression tag	UNP Q8EKM7
B	0	ALA	-	expression tag	UNP Q8EKM7
C	-2	SER	-	expression tag	UNP Q8EKM7
C	-1	ASN	-	expression tag	UNP Q8EKM7
C	0	ALA	-	expression tag	UNP Q8EKM7
D	-2	SER	-	expression tag	UNP Q8EKM7
D	-1	ASN	-	expression tag	UNP Q8EKM7
D	0	ALA	-	expression tag	UNP Q8EKM7
E	-2	SER	-	expression tag	UNP Q8EKM7
E	-1	ASN	-	expression tag	UNP Q8EKM7
E	0	ALA	-	expression tag	UNP Q8EKM7
F	-2	SER	-	expression tag	UNP Q8EKM7
F	-1	ASN	-	expression tag	UNP Q8EKM7

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	expression tag	UNP Q8EKM7

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

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

- Molecule 3 is water.

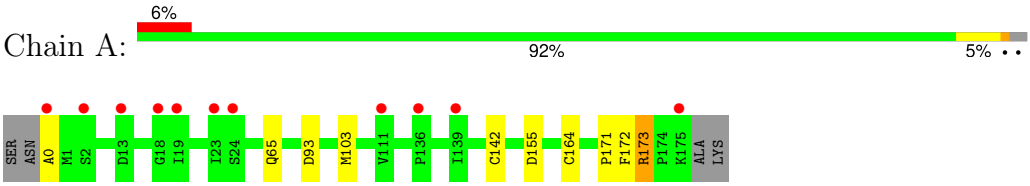
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	172	Total O 172 172	0	0
3	B	157	Total O 157 157	0	0
3	C	173	Total O 173 173	0	0
3	D	149	Total O 149 149	0	0
3	E	159	Total O 159 159	0	0
3	F	83	Total O 83 83	0	0

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. 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. 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.

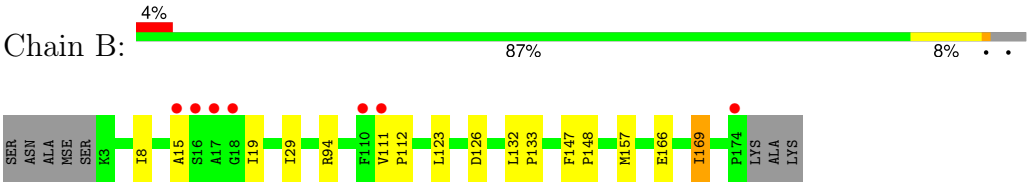
• Molecule 1: Molybdenum cofactor biosynthesis protein Mog

Chain A:



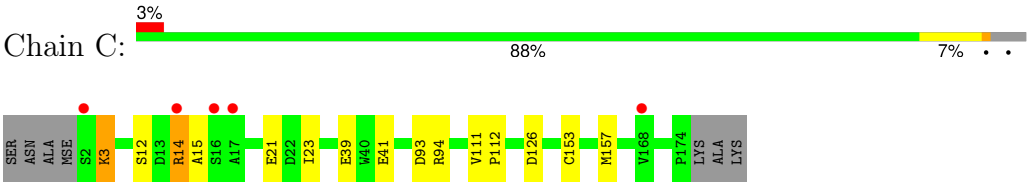
• Molecule 1: Molybdenum cofactor biosynthesis protein Mog

Chain B:



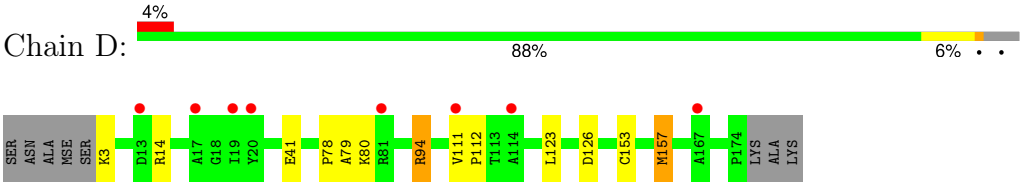
• Molecule 1: Molybdenum cofactor biosynthesis protein Mog

Chain C:



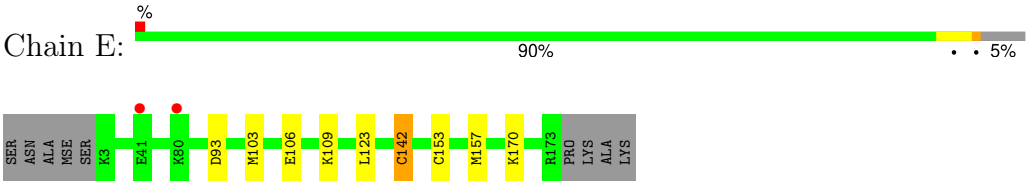
• Molecule 1: Molybdenum cofactor biosynthesis protein Mog

Chain D:



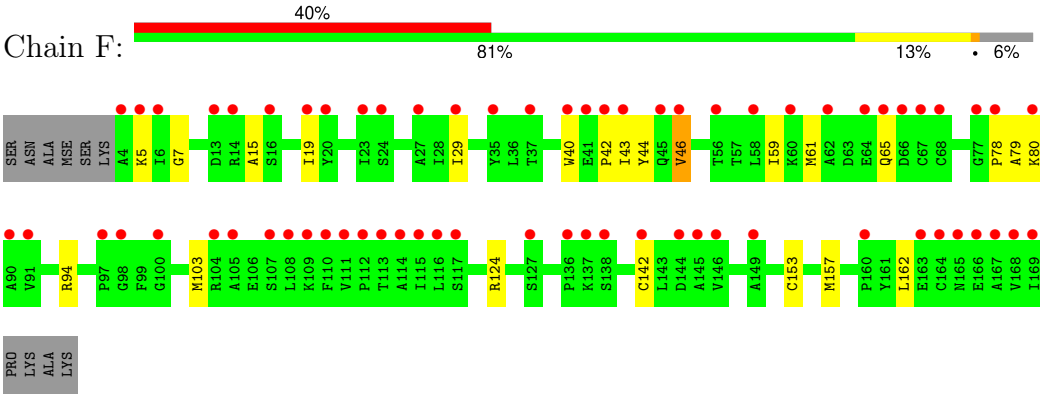
• Molecule 1: Molybdenum cofactor biosynthesis protein Mog

Chain E:



• Molecule 1: Molybdenum cofactor biosynthesis protein Mog

Chain F:


40%
81%
13%
6%
SER ASN ALA MSE SER LYS A4 K5 I6 G7 D13 R14 A15 S16 I19 Y20 I23 S24 A27 I28 I29 Y35 L36 T37 W40 E41 P42 I43 Y44 Q45 V46 T56 T57 L58 I59 K60 M61 A62 D63 E64 Q65 D66 C67 C68 G77 P78 A79 K80 R81 D82 V83
A90 V91 R94 P97 G98 F99 G100 M103 R104 A105 E106 S107 L108 K109 F110 V111 P112 T113 A114 I115 L116 S117 R124 S127 P136 K137 S138 C142 L143 D144 A145 V146 A149 C153 M157 P160 Y161 L162 E163 C164 N165 E166 A167 V168 I169 K170 P171 F172 R173
PRO LYS ALA LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	66.13Å 66.31Å 74.33Å 92.15° 103.64° 119.98°	Depositor
Resolution (Å)	50.00 – 1.89 50.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	96.0 (50.00-1.89) 96.0 (50.00-1.90)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.09 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.177 , 0.216 0.200 , 0.237	Depositor DCC
R_{free} test set	3987 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	22.6	Xtriage
Anisotropy	0.380	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 32.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h-k,k,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8852	wwPDB-VP
Average B, all atoms (Å^2)	16.0	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 65.73 % 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 6.7619e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

5.1 Standard geometry

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

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	0.58	0/1357	0.68	2/1835 (0.1%)
1	B	0.54	0/1337	0.63	0/1808
1	C	0.58	0/1371	0.63	0/1853
1	D	0.57	0/1354	0.63	0/1831
1	E	0.56	2/1335 (0.1%)	0.61	0/1804
1	F	0.48	0/1307	0.60	0/1769
All	All	0.55	2/8061 (0.0%)	0.63	2/10900 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	142[A]	CYS	CB-SG	-5.91	1.72	1.81
1	E	142[B]	CYS	CB-SG	-5.91	1.72	1.81

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	173	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	173	ARG	NE-CZ-NH1	5.58	123.09	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1340	0	1340	7	0
1	B	1319	0	1330	12	0
1	C	1353	0	1354	13	0
1	D	1336	0	1338	18	0
1	E	1318	0	1326	6	0
1	F	1290	0	1295	17	0
2	A	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
3	A	172	0	0	3	0
3	B	157	0	0	0	0
3	C	173	0	0	4	0
3	D	149	0	0	3	0
3	E	159	0	0	1	0
3	F	83	0	0	0	0
All	All	8852	0	7983	66	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 4.

All (66) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:7:GLY:HA3	1:F:61:MSE:HE2	1.27	1.12
1:D:123:LEU:HD22	1:D:157[A]:MSE:SE	2.09	1.02
1:C:3:LYS:HE3	1:C:41:GLU:HG3	1.46	0.94
1:B:123:LEU:HD22	1:B:157[A]:MSE:SE	2.23	0.89
1:F:7:GLY:CA	1:F:61:MSE:HE2	2.04	0.87
1:F:7:GLY:HA3	1:F:61:MSE:CE	2.07	0.84
1:F:153:CYS:O	1:F:157:MSE:HG2	1.77	0.83
1:E:142[B]:CYS:SG	3:E:278:HOH:O	2.38	0.80
1:C:157[B]:MSE:HA	1:C:157[B]:MSE:HE3	1.65	0.78
1:F:7:GLY:CA	1:F:61:MSE:CE	2.61	0.78
1:D:157[B]:MSE:HE3	1:D:157[B]:MSE:HA	1.67	0.76
1:C:14:ARG:HG2	3:C:355:HOH:O	1.86	0.75
1:F:162:LEU:O	1:F:173:ARG:NH2	2.24	0.70
1:E:123:LEU:HD22	1:E:157[B]:MSE:SE	2.43	0.68
1:C:157[A]:MSE:CE	3:C:276:HOH:O	2.44	0.66
1:B:94:ARG:HH22	1:D:79:ALA:C	2.00	0.65
1:F:5:LYS:HD2	1:F:65:GLN:O	1.97	0.64
1:D:94:ARG:NH2	1:F:80:LYS:HA	2.12	0.63
1:C:157[B]:MSE:HA	1:C:157[B]:MSE:CE	2.27	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103:MSE:SE	1:E:142[A]:CYS:SG	3.08	0.61
1:B:94:ARG:NH2	1:D:80:LYS:HA	2.16	0.61
1:D:123:LEU:CD2	1:D:157[A]:MSE:SE	2.94	0.61
1:A:155:ASP:OD2	1:A:173:ARG:HD3	2.01	0.60
1:A:65:GLN:HG2	3:A:336:HOH:O	2.00	0.59
1:D:126:ASP:HA	1:D:157[B]:MSE:HE2	1.85	0.59
1:C:153:CYS:O	1:C:157[A]:MSE:HG3	2.05	0.56
1:B:94:ARG:NH2	1:D:78:PRO:O	2.39	0.55
1:D:157[B]:MSE:HE3	1:D:157[B]:MSE:CA	2.31	0.55
1:F:103:MSE:SE	1:F:142:CYS:SG	3.15	0.55
1:B:157[B]:MSE:HE3	1:B:157[B]:MSE:HA	1.89	0.54
1:A:172:PHE:CZ	1:C:111:VAL:HG12	2.42	0.54
1:F:43:ILE:HD13	1:F:65:GLN:HB3	1.91	0.53
1:A:164:CYS:SG	1:A:171:PRO:HG3	2.49	0.53
1:D:157[B]:MSE:HA	1:D:157[B]:MSE:CE	2.34	0.52
1:B:15:ALA:HA	1:B:19:ILE:HB	1.91	0.52
1:F:43:ILE:O	1:F:61:MSE:HE3	2.08	0.52
1:C:157[A]:MSE:HE3	3:C:276:HOH:O	2.10	0.49
1:D:14:ARG:NH1	3:D:330:HOH:O	2.45	0.49
1:E:106:GLU:HA	1:E:109:LYS:HE2	1.94	0.49
1:F:44:TYR:CZ	1:F:46:VAL:HG22	2.48	0.49
1:E:153:CYS:O	1:E:157[B]:MSE:HG3	2.15	0.47
1:B:126:ASP:HA	1:B:157[B]:MSE:HE2	1.99	0.45
1:F:59:ILE:HG12	1:F:124:ARG:CZ	2.46	0.45
1:C:3:LYS:HA	3:C:281:HOH:O	2.16	0.45
1:D:94:ARG:HH22	1:F:79:ALA:C	2.20	0.45
1:F:15:ALA:HA	1:F:19:ILE:HG12	1.97	0.45
1:C:111:VAL:HA	1:C:112:PRO:HD3	1.76	0.45
1:C:21[B]:GLU:HG3	1:C:23:ILE:HG23	1.99	0.44
1:D:94:ARG:NH2	1:F:78:PRO:O	2.50	0.44
1:B:8:ILE:HD13	1:B:29:ILE:HG12	2.00	0.43
1:D:3:LYS:HD2	1:D:41:GLU:HG3	1.99	0.43
1:D:94:ARG:NH2	3:D:201:HOH:O	2.40	0.43
1:F:40:TRP:CZ3	1:F:42:PRO:HB3	2.54	0.43
1:C:126:ASP:HA	1:C:157[A]:MSE:HE2	2.00	0.42
1:C:12:SER:HB3	1:C:15:ALA:HB3	2.01	0.42
1:D:153:CYS:O	1:D:157[B]:MSE:HG2	2.19	0.42
1:A:103:MSE:SE	1:A:142:CYS:SG	3.28	0.42
1:B:111:VAL:HA	1:B:112:PRO:HD3	1.84	0.42
1:D:111:VAL:HA	1:D:112:PRO:HD3	1.92	0.42
1:B:132:LEU:HB3	1:B:133:PRO:HD2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:GLU:HA	1:B:169:ILE:O	2.20	0.41
1:E:153:CYS:O	1:E:157[A]:MSE:HG2	2.20	0.41
1:A:65:GLN:NE2	3:A:302:HOH:O	2.53	0.41
1:A:0:ALA:HB2	3:A:232:HOH:O	2.20	0.41
1:D:3:LYS:HA	3:D:310:HOH:O	2.20	0.40
1:B:147:PHE:N	1:B:148:PRO:CD	2.85	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	175/180 (97%)	172 (98%)	3 (2%)	0	100	100
1	B	171/180 (95%)	167 (98%)	4 (2%)	0	100	100
1	C	175/180 (97%)	172 (98%)	3 (2%)	0	100	100
1	D	173/180 (96%)	171 (99%)	2 (1%)	0	100	100
1	E	171/180 (95%)	169 (99%)	2 (1%)	0	100	100
1	F	168/180 (93%)	163 (97%)	5 (3%)	0	100	100
All	All	1033/1080 (96%)	1014 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	147/146 (101%)	146 (99%)	1 (1%)	81 83
1	B	147/146 (101%)	146 (99%)	1 (1%)	81 83
1	C	150/146 (103%)	145 (97%)	5 (3%)	33 26
1	D	149/146 (102%)	146 (98%)	3 (2%)	50 47
1	E	147/146 (101%)	145 (99%)	2 (1%)	62 62
1	F	142/146 (97%)	139 (98%)	3 (2%)	48 45
All	All	882/876 (101%)	867 (98%)	15 (2%)	58 54

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	ASP
1	B	169	ILE
1	C	3	LYS
1	C	14	ARG
1	C	39	GLU
1	C	93	ASP
1	C	94	ARG
1	D	94	ARG
1	D	157[A]	MSE
1	D	157[B]	MSE
1	E	93	ASP
1	E	170	LYS
1	F	29	ILE
1	F	46	VAL
1	F	94	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	65	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Warning: The R factor obtained from EDS is 0.2406, which does not match the depositor's R factor of 0.17684. Please interpret the results in this section carefully.

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	170/180 (94%)	0.39	11 (6%) 26 27	6, 12, 20, 42	1 (0%)
1	B	167/180 (92%)	0.37	7 (4%) 41 43	7, 14, 22, 28	0
1	C	168/180 (93%)	0.14	5 (2%) 52 55	5, 13, 21, 27	3 (1%)
1	D	167/180 (92%)	0.58	8 (4%) 36 37	8, 15, 24, 30	2 (1%)
1	E	166/180 (92%)	0.22	2 (1%) 76 78	7, 14, 21, 24	1 (0%)
1	F	165/180 (91%)	1.97	72 (43%) 1 0	12, 19, 26, 31	0
All	All	1003/1080 (92%)	0.61	105 (10%) 13 13	5, 15, 24, 42	7 (0%)

All (105) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	41	GLU	7.1
1	B	15	ALA	7.0
1	F	62	ALA	6.8
1	F	113	THR	5.5
1	F	66	ASP	5.1
1	B	17	ALA	5.1
1	F	111	VAL	4.7
1	F	116	LEU	4.4
1	A	175	LYS	4.4
1	F	67	CYS	4.4
1	F	115	ILE	4.3
1	B	111	VAL	4.3
1	A	2	SER	4.3
1	F	138	SER	4.0
1	F	145	ALA	4.0
1	D	20	TYR	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	19	ILE	4.0
1	F	107	SER	3.9
1	F	40	TRP	3.9
1	F	169	ILE	3.8
1	A	0	ALA	3.7
1	F	64	GLU	3.7
1	F	165	ASN	3.7
1	F	68	CYS	3.6
1	F	108	LEU	3.6
1	F	4	ALA	3.5
1	F	105	ALA	3.5
1	A	19	ILE	3.4
1	F	23	ILE	3.4
1	F	149	ALA	3.4
1	F	35	TYR	3.3
1	F	24	SER	3.3
1	F	91	VAL	3.3
1	F	43	ILE	3.3
1	C	2	SER	3.2
1	F	46	VAL	3.1
1	F	80	LYS	3.1
1	F	65	GLN	3.1
1	F	81	ARG	3.1
1	F	110	PHE	3.1
1	B	174	PRO	3.0
1	F	45	GLN	3.0
1	B	16	SER	3.0
1	F	172	PHE	2.9
1	F	98	GLY	2.9
1	C	14	ARG	2.9
1	F	58	LEU	2.8
1	F	77	GLY	2.8
1	A	139	ILE	2.8
1	F	112	PRO	2.8
1	F	37	THR	2.7
1	D	111	VAL	2.7
1	F	136	PRO	2.6
1	F	104	ARG	2.6
1	B	110	PHE	2.6
1	A	23	ILE	2.6
1	D	81	ARG	2.6
1	F	90	ALA	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	168	VAL	2.6
1	F	27	ALA	2.6
1	F	109	LYS	2.5
1	F	42	PRO	2.5
1	A	24	SER	2.5
1	D	13	ASP	2.5
1	F	82	ASP	2.5
1	F	166	GLU	2.5
1	F	83	VAL	2.5
1	A	136	PRO	2.4
1	F	146	VAL	2.4
1	B	18	GLY	2.4
1	F	29	ILE	2.4
1	F	60	LYS	2.4
1	A	18	GLY	2.4
1	F	20	TYR	2.4
1	D	19	ILE	2.4
1	F	164	CYS	2.4
1	F	14	ARG	2.3
1	C	17	ALA	2.3
1	F	13	ASP	2.3
1	F	100	GLY	2.3
1	F	16	SER	2.3
1	F	117	SER	2.3
1	F	163	GLU	2.3
1	F	78	PRO	2.2
1	F	171	PRO	2.2
1	F	167	ALA	2.2
1	F	160	PRO	2.2
1	F	142	CYS	2.2
1	D	17	ALA	2.2
1	F	6	ILE	2.2
1	F	137	LYS	2.1
1	A	111	VAL	2.1
1	C	168	VAL	2.1
1	F	97	PRO	2.1
1	F	56	THR	2.1
1	F	127	SER	2.1
1	D	114	ALA	2.1
1	F	114	ALA	2.1
1	E	80	LYS	2.1
1	F	5	LYS	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	13	ASP	2.0
1	E	41	GLU	2.0
1	C	16	SER	2.0
1	F	144	ASP	2.0
1	D	167	ALA	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NA	D	178	1/1	0.82	0.12	48,48,48,48	0
2	NA	E	178	1/1	0.89	0.11	37,37,37,37	0
2	NA	A	178	1/1	0.91	0.08	25,25,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.