Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 04:09 am BST

PDB ID	:	3KZ9
Title	:	Crystal structure of the master transcriptional regulator, SmcR, in Vibrio vulnificus provides insight into its DNA recognition mechanism
Authors	:	Kim, M.H.; Kim, Y.; Choi, W.-C.; Hwang, J.
Deposited on	:	2009-12-08
Resolution	:	2.10 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:

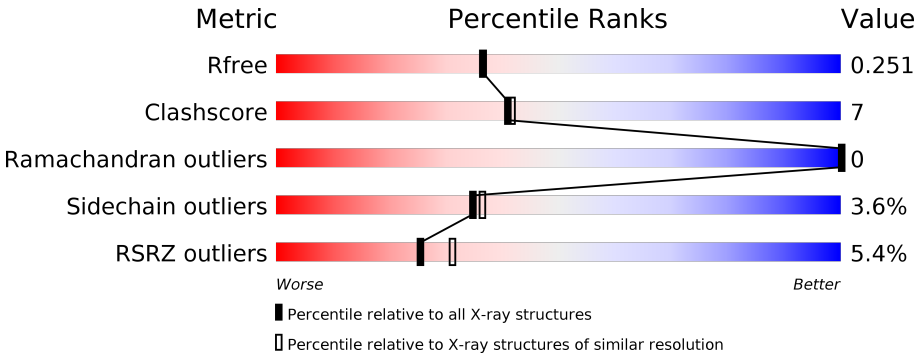
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	206	9% 83% 14%
1	B	206	4% 82% 16%
1	C	206	2% 85% 12%
1	D	206	6% 83% 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7188 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.

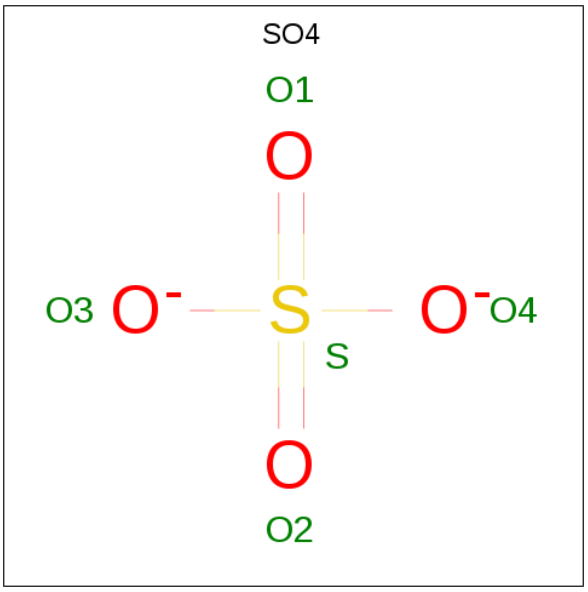
- Molecule 1 is a protein called SmcR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	Se	0	2	0
			1654	1044	296	305	4	5			
1	B	203	Total	C	N	O	S	Se	0	5	0
			1693	1068	306	309	3	7			
1	C	203	Total	C	N	O	S	Se	0	4	0
			1685	1062	303	311	4	5			
1	D	199	Total	C	N	O	S	Se	0	7	0
			1673	1055	300	310	3	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	ALA	-	CLONING ARTIFACT	UNP Q9L8G8
B	0	ALA	-	CLONING ARTIFACT	UNP Q9L8G8
C	0	ALA	-	CLONING ARTIFACT	UNP Q9L8G8
D	0	ALA	-	CLONING ARTIFACT	UNP Q9L8G8

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

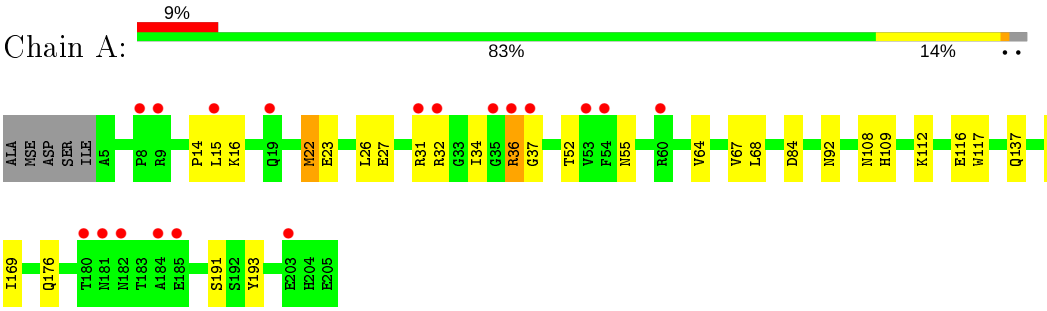
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	79	Total O 79 79	0	0
3	B	126	Total O 126 126	0	0
3	C	149	Total O 149 149	0	0
3	D	99	Total O 99 99	0	0

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.

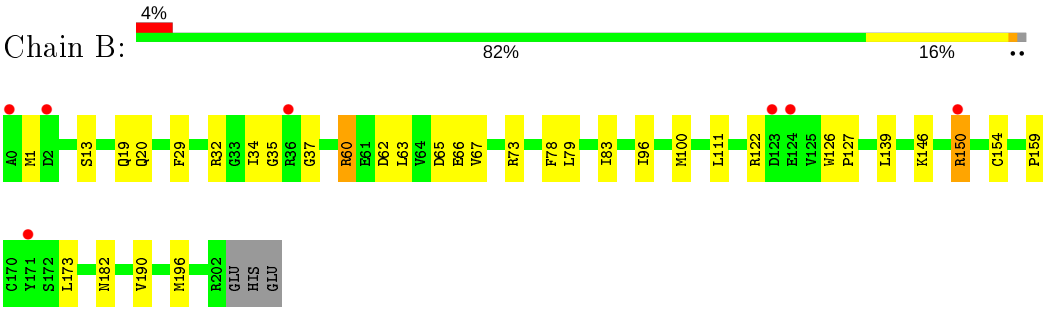
- Molecule 1: SmcR

Chain A:



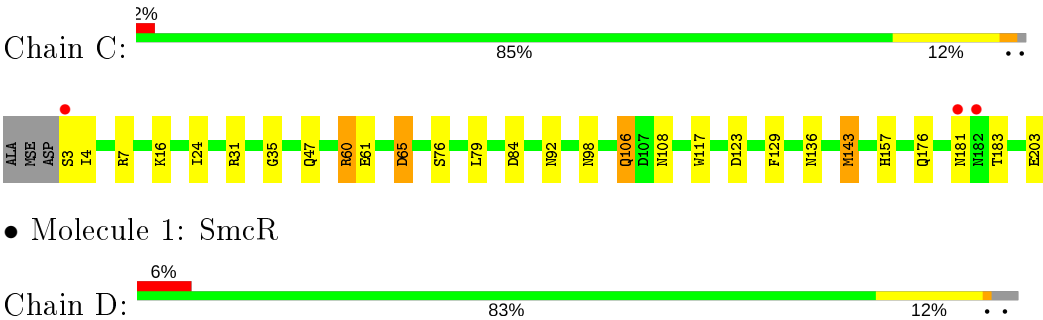
- Molecule 1: SmcR

Chain B:



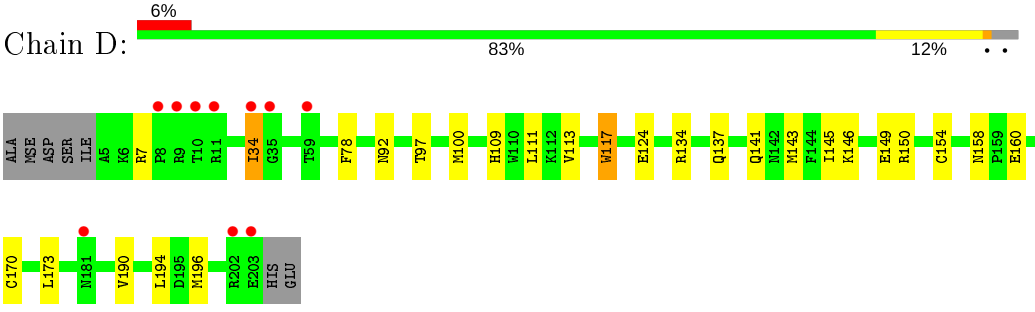
- Molecule 1: SmcR

Chain C:



- Molecule 1: SmcR

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.49Å 99.03Å 129.06Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.92 – 2.10 29.92 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.2 (29.92-2.10) 99.2 (29.92-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.22 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.251 0.199 , 0.251	Depositor DCC
R_{free} test set	2979 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7188	wwPDB-VP
Average B, all atoms (Å^2)	35.0	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 27.91 % 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 2.0213e-03. 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: 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	0.57	0/1683	0.63	0/2273
1	B	0.64	0/1720	0.69	0/2320
1	C	0.69	0/1714	0.67	0/2314
1	D	0.63	0/1701	0.63	0/2299
All	All	0.63	0/6818	0.65	0/9206

There are no bond length outliers.

There are no bond angle outliers.

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	1654	0	1628	22	0
1	B	1693	0	1681	34	0
1	C	1685	0	1660	24	0
1	D	1673	0	1650	22	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	79	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	126	0	0	3	0
3	C	149	0	0	5	0
3	D	99	0	0	3	0
All	All	7188	0	6619	95	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 7.

All (95) 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:B:35:GLY:HA2	1:B:60:ARG:HH22	1.25	1.02
1:C:157:HIS:HB3	1:D:196:MSE:HE2	1.47	0.97
1:D:134:ARG:NH1	1:D:137[B]:GLN:OE1	1.97	0.96
1:B:146:LYS:O	1:B:150:ARG:HD3	1.63	0.96
1:B:1:MSE:HE2	1:B:32:ARG:HD2	1.55	0.89
1:D:158[A]:ASN:OD1	1:D:160:GLU:OE1	1.99	0.81
1:C:84:ASP:H	1:C:92:ASN:HD21	1.29	0.80
1:C:4:ILE:HG13	1:C:31:ARG:HD3	1.67	0.76
1:A:137:GLN:HE21	1:A:141:GLN:HE21	1.35	0.74
1:B:1:MSE:CE	1:B:32:ARG:HD2	2.17	0.73
1:D:92:ASN:ND2	1:D:143:MSE:SE	2.72	0.73
1:A:157:HIS:HB3	1:B:196:MSE:HE2	1.69	0.73
1:C:84:ASP:H	1:C:92:ASN:ND2	1.90	0.69
1:C:76:SER:HB2	1:C:136:ASN:HD21	1.56	0.69
1:A:112:LYS:NZ	1:A:116:GLU:OE2	2.26	0.69
1:B:1:MSE:CE	1:B:32:ARG:CD	2.72	0.66
1:D:34:ILE:HD12	1:D:113:VAL:HG13	1.76	0.66
1:A:27:GLU:HG2	1:A:109:HIS:CE1	2.32	0.65
1:B:1:MSE:HE1	1:B:32:ARG:HD3	1.80	0.62
1:D:78:PHE:CZ	1:D:100[B]:MSE:HG3	2.35	0.62
1:B:83:ILE:HG12	1:B:96:ILE:HD11	1.82	0.61
1:B:1:MSE:HE2	1:B:32:ARG:CD	2.26	0.60
1:B:1:MSE:HE1	1:B:32:ARG:HH11	1.67	0.59
1:B:35:GLY:HA2	1:B:60:ARG:NH2	2.08	0.59
1:B:73[B]:ARG:NH2	3:B:244:HOH:O	2.13	0.59
1:B:1:MSE:CE	1:B:32:ARG:HH11	2.15	0.59
1:B:182:ASN:HD21	1:C:47:GLN:HE22	1.51	0.58
1:B:37:GLY:O	1:B:60:ARG:NH2	2.36	0.58
1:A:169:ILE:HG23	1:A:193:TYR:HD1	1.69	0.57
1:A:22[A]:MSE:HG3	1:A:23:GLU:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22[A]:MSE:HE1	1:A:67:VAL:HA	1.87	0.57
1:C:123:ASP:OD1	3:C:261:HOH:O	2.17	0.57
1:A:112:LYS:O	1:A:116:GLU:HG2	2.05	0.56
1:B:79:LEU:HD22	1:B:83:ILE:HD11	1.86	0.56
1:C:181:ASN:ND2	3:C:264:HOH:O	2.35	0.56
1:D:145:ILE:O	1:D:149:GLU:HG3	2.06	0.56
1:B:1:MSE:HE1	1:B:32:ARG:CD	2.36	0.55
1:B:150:ARG:HG2	3:B:404:HOH:O	2.05	0.55
1:D:97[B]:THR:HG21	1:D:173:LEU:CD1	2.36	0.55
1:C:61:GLU:H	1:C:61:GLU:CD	2.12	0.53
1:D:92:ASN:HD22	1:D:143:MSE:SE	2.39	0.53
1:C:3:SER:HB3	1:C:31:ARG:NH2	2.22	0.53
1:D:100[A]:MSE:HG2	1:D:111:LEU:HD21	1.90	0.53
1:B:150:ARG:CD	1:B:150:ARG:N	2.71	0.52
1:C:157:HIS:CB	1:D:196:MSE:HE2	2.30	0.52
1:A:15:LEU:HD12	1:A:16:LYS:N	2.24	0.52
1:A:34:ILE:HD11	1:A:117:TRP:CE2	2.45	0.52
1:D:92:ASN:HD21	1:D:143:MSE:SE	2.42	0.52
1:D:137[B]:GLN:NE2	3:D:220:HOH:O	2.44	0.51
1:C:117:TRP:CD1	1:C:129:PHE:HB2	2.46	0.50
1:C:106:GLN:NE2	1:C:108:ASN:HD21	2.10	0.49
1:B:182:ASN:HD21	1:C:47:GLN:NE2	2.09	0.49
1:D:141:GLN:O	1:D:145:ILE:HG13	2.13	0.49
1:A:22[A]:MSE:SE	1:A:26:LEU:HD13	2.63	0.48
1:A:64:VAL:O	1:A:68:LEU:HB2	2.14	0.48
1:D:190:VAL:O	1:D:194:LEU:HG	2.13	0.48
1:A:176:GLN:HE22	1:B:164:ASN:HB3	1.79	0.47
1:B:62:ASP:O	1:B:66:GLU:HG3	2.14	0.47
1:C:106:GLN:HE21	1:C:108:ASN:HD21	1.61	0.47
1:A:84:ASP:H	1:A:92:ASN:HD21	1.61	0.47
1:B:29:PHE:HE2	1:B:67:VAL:HG21	1.80	0.47
1:C:61:GLU:O	1:C:65:ASP:HB2	2.15	0.46
1:A:14:PRO:HD2	3:A:263:HOH:O	2.15	0.46
1:C:84:ASP:N	1:C:92:ASN:HD21	2.07	0.46
1:D:97[B]:THR:HG21	1:D:173:LEU:HD13	1.97	0.46
1:D:150:ARG:NH1	3:D:277:HOH:O	2.49	0.46
1:B:173:LEU:HD13	1:B:190:VAL:HG22	1.99	0.45
1:D:97[B]:THR:CG2	1:D:173:LEU:HD13	2.47	0.45
1:B:150:ARG:HD3	1:B:150:ARG:N	2.32	0.44
1:B:1:MSE:CE	1:B:32:ARG:NH1	2.80	0.44
1:D:109:HIS:HD2	3:D:414:HOH:O	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:GLN:HE21	1:A:141:GLN:NE2	2.09	0.44
1:D:78:PHE:HZ	1:D:100[B]:MSE:HG3	1.82	0.44
1:A:84:ASP:H	1:A:92:ASN:ND2	2.14	0.44
1:C:7:ARG:HG3	1:C:24:ILE:HD11	1.98	0.44
1:D:100[B]:MSE:SE	1:D:170:CYS:SG	3.27	0.43
1:B:83:ILE:HD12	1:B:139:LEU:HG	2.01	0.42
1:C:4:ILE:CG1	1:C:31:ARG:HD3	2.43	0.42
1:B:126:TRP:N	1:B:127:PRO:CD	2.83	0.42
1:A:36:ARG:O	1:A:37:GLY:C	2.57	0.42
1:A:26:LEU:HD12	1:A:67:VAL:HG13	2.02	0.42
1:B:19[B]:GLN:HG3	1:B:20:GLN:N	2.34	0.42
1:B:78:PHE:CZ	1:B:100[B]:MSE:HG3	2.54	0.41
1:D:34:ILE:HG21	1:D:117:TRP:CZ3	2.55	0.41
1:A:176:GLN:HE22	1:B:164:ASN:CB	2.34	0.41
1:B:34:ILE:HD12	3:B:412:HOH:O	2.20	0.41
1:A:52:THR:O	1:A:55:ASN:HB2	2.21	0.41
1:B:63:LEU:O	1:B:67:VAL:HG23	2.21	0.41
1:C:79:LEU:HA	1:C:79:LEU:HD23	1.95	0.41
1:B:100[A]:MSE:HG2	1:B:111:LEU:HD21	2.02	0.41
1:C:203:GLU:HB3	3:C:320:HOH:O	2.21	0.41
1:A:27:GLU:HG2	1:A:109:HIS:ND1	2.36	0.40
1:C:143:MSE:HB3	3:C:283:HOH:O	2.22	0.40
1:C:35:GLY:CA	1:C:60:ARG:HH22	2.33	0.40
1:C:98:ASN:ND2	3:C:432:HOH:O	2.52	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	201/206 (98%)	195 (97%)	6 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	206/206 (100%)	205 (100%)	1 (0%)	0	100	100
1	C	205/206 (100%)	202 (98%)	3 (2%)	0	100	100
1	D	204/206 (99%)	201 (98%)	3 (2%)	0	100	100
All	All	816/824 (99%)	803 (98%)	13 (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	182/179 (102%)	175 (96%)	7 (4%)	33	34
1	B	186/179 (104%)	179 (96%)	7 (4%)	33	34
1	C	186/179 (104%)	179 (96%)	7 (4%)	33	34
1	D	185/179 (103%)	179 (97%)	6 (3%)	39	41
All	All	739/716 (103%)	712 (96%)	27 (4%)	35	35

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22[A]	MSE
1	A	22[B]	MSE
1	A	31	ARG
1	A	32	ARG
1	A	36	ARG
1	A	108	ASN
1	A	191	SER
1	B	13	SER
1	B	60	ARG
1	B	65	ASP
1	B	122	ARG
1	B	150	ARG
1	B	154	CYS

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Mol	Chain	Res	Type
1	B	159	PRO
1	C	16	LYS
1	C	60	ARG
1	C	65	ASP
1	C	106	GLN
1	C	143	MSE
1	C	176	GLN
1	C	183	THR
1	D	7	ARG
1	D	34	ILE
1	D	117	TRP
1	D	124	GLU
1	D	146	LYS
1	D	154	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	141	GLN
1	A	176	GLN
1	B	47	GLN
1	B	106	GLN
1	B	136	ASN
1	B	142	ASN
1	B	178	ASN
1	C	47	GLN
1	C	92	ASN
1	C	98	ASN
1	C	106	GLN
1	C	136	ASN
1	C	167	HIS
1	C	178	ASN
1	C	181	ASN
1	D	47	GLN
1	D	82	ASN
1	D	106	GLN
1	D	108	ASN
1	D	141	GLN
1	D	142	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

6 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	D	207	-	4,4,4	0.15	0	6,6,6	0.25	0
2	SO4	C	206	-	4,4,4	0.13	0	6,6,6	0.10	0
2	SO4	D	206	-	4,4,4	0.14	0	6,6,6	0.12	0
2	SO4	B	206	-	4,4,4	0.22	0	6,6,6	0.53	0
2	SO4	C	207	-	4,4,4	0.11	0	6,6,6	0.20	0
2	SO4	A	206	-	4,4,4	0.15	0	6,6,6	0.07	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.

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

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	197/206 (95%)	0.53	18 (9%)	9	12	26, 38, 56, 64	0
1	B	198/206 (96%)	0.14	8 (4%)	38	44	23, 31, 49, 57	0
1	C	199/206 (96%)	0.05	4 (2%)	65	69	20, 28, 45, 57	0
1	D	195/206 (94%)	0.25	13 (6%)	17	22	23, 35, 54, 61	0
All	All	789/824 (95%)	0.24	43 (5%)	25	31	20, 33, 52, 64	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	LEU	5.0
1	A	37	GLY	5.0
1	A	181	ASN	4.9
1	A	35	GLY	4.2
1	B	2	ASP	4.2
1	C	181	ASN	4.1
1	A	184	ALA	3.7
1	A	182	ASN	3.6
1	A	31	ARG	3.5
1	A	203	GLU	3.3
1	A	19	GLN	3.3
1	B	123	ASP	3.3
1	A	180	THR	3.3
1	D	9	ARG	3.2
1	A	185	GLU	3.0
1	C	204	HIS	2.9
1	A	32	ARG	2.8
1	D	165	LEU	2.6
1	D	202	ARG	2.6
1	B	124	GLU	2.5
1	D	34	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	8	PRO	2.5
1	B	150	ARG	2.4
1	D	10	THR	2.4
1	C	3	SER	2.4
1	B	0	ALA	2.4
1	A	54	PHE	2.3
1	A	53	VAL	2.3
1	A	36	ARG	2.3
1	D	59	THR	2.3
1	C	182	ASN	2.3
1	D	166	PHE	2.3
1	B	36	ARG	2.2
1	D	8	PRO	2.2
1	A	9	ARG	2.2
1	D	203	GLU	2.1
1	D	11	ARG	2.1
1	A	60	ARG	2.1
1	D	35	GLY	2.1
1	D	181	ASN	2.1
1	B	169	ILE	2.1
1	D	169	ILE	2.0
1	B	171	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	SO4	D	206	5/5	0.58	0.29	125,125,125,125	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SO4	C	207	5/5	0.79	0.32	90,91,92,93	0
2	SO4	A	206	5/5	0.81	0.27	112,112,112,113	0
2	SO4	C	206	5/5	0.82	0.18	97,97,97,98	0
2	SO4	D	207	5/5	0.82	0.26	82,83,84,84	0
2	SO4	B	206	5/5	0.99	0.06	39,39,40,40	0

6.5 Other polymers (i)

There are no such residues in this entry.