Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:19 AM GMT

PDB ID	:	2Q62
Title	:	Crystal Structure of ArsH from Sinorhizobium meliloti
Authors	:	Ye, J.; Yang, H.; Bhattacharjee, H.; Rosen, B.P.
Deposited on	:	2007-06-04
Resolution	:	1.80 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

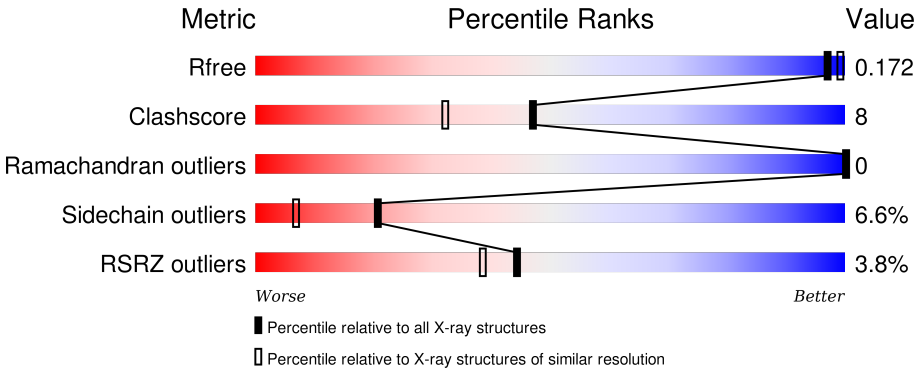
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 1.80 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}	91344	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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 <=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	247	9% 70% 16% • 11%
1	B	247	2% 74% 14% • 10%
1	C	247	2% 77% 10% •• 11%
1	D	247	% 83% 9% • • 5%
1	E	247	2% 72% 14% •• 11%

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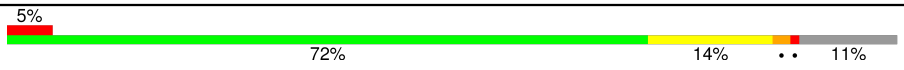
Mol	Chain	Length	Quality of chain
1	F	247	
1	G	247	
1	H	247	

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	2001	-	-	-	X
2	SO4	B	2002	-	-	-	X
2	SO4	C	2003	-	-	-	X
2	SO4	D	2004	-	-	-	X
2	SO4	F	2006	-	-	-	X
2	SO4	G	2007	-	-	-	X
2	SO4	H	2008	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15789 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 arsH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	0	0
			1745	1103	313	320	9			
1	B	222	Total	C	N	O	S	0	0	0
			1756	1109	315	323	9			
1	C	221	Total	C	N	O	S	0	0	0
			1746	1103	312	322	9			
1	D	235	Total	C	N	O	S	0	0	0
			1862	1175	336	342	9			
1	E	221	Total	C	N	O	S	0	0	0
			1746	1103	312	322	9			
1	F	219	Total	C	N	O	S	0	0	0
			1735	1097	310	319	9			
1	G	219	Total	C	N	O	S	0	0	0
			1736	1098	312	317	9			
1	H	221	Total	C	N	O	S	0	0	0
			1746	1103	312	322	9			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	242	HIS	-	EXPRESSION TAG	UNP Q92R45
A	243	HIS	-	EXPRESSION TAG	UNP Q92R45
A	244	HIS	-	EXPRESSION TAG	UNP Q92R45
A	245	HIS	-	EXPRESSION TAG	UNP Q92R45
A	246	HIS	-	EXPRESSION TAG	UNP Q92R45
A	247	HIS	-	EXPRESSION TAG	UNP Q92R45
B	242	HIS	-	EXPRESSION TAG	UNP Q92R45
B	243	HIS	-	EXPRESSION TAG	UNP Q92R45
B	244	HIS	-	EXPRESSION TAG	UNP Q92R45
B	245	HIS	-	EXPRESSION TAG	UNP Q92R45
B	246	HIS	-	EXPRESSION TAG	UNP Q92R45
B	247	HIS	-	EXPRESSION TAG	UNP Q92R45
C	242	HIS	-	EXPRESSION TAG	UNP Q92R45

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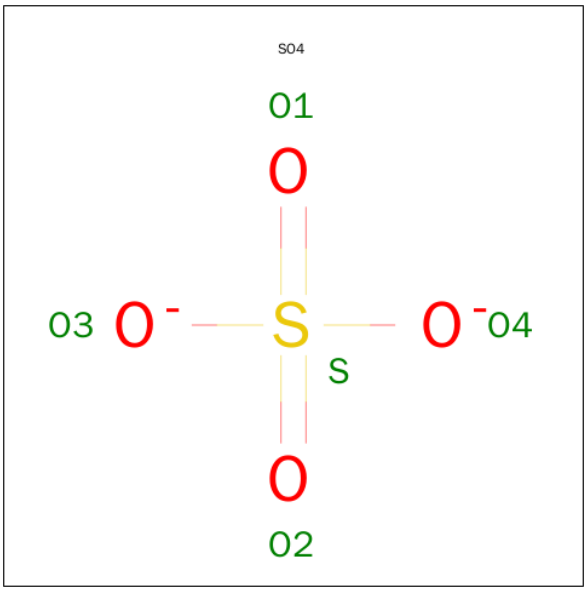
Chain	Residue	Modelled	Actual	Comment	Reference
C	243	HIS	-	EXPRESSION TAG	UNP Q92R45
C	244	HIS	-	EXPRESSION TAG	UNP Q92R45
C	245	HIS	-	EXPRESSION TAG	UNP Q92R45
C	246	HIS	-	EXPRESSION TAG	UNP Q92R45
C	247	HIS	-	EXPRESSION TAG	UNP Q92R45
D	242	HIS	-	EXPRESSION TAG	UNP Q92R45
D	243	HIS	-	EXPRESSION TAG	UNP Q92R45
D	244	HIS	-	EXPRESSION TAG	UNP Q92R45
D	245	HIS	-	EXPRESSION TAG	UNP Q92R45
D	246	HIS	-	EXPRESSION TAG	UNP Q92R45
D	247	HIS	-	EXPRESSION TAG	UNP Q92R45
E	242	HIS	-	EXPRESSION TAG	UNP Q92R45
E	243	HIS	-	EXPRESSION TAG	UNP Q92R45
E	244	HIS	-	EXPRESSION TAG	UNP Q92R45
E	245	HIS	-	EXPRESSION TAG	UNP Q92R45
E	246	HIS	-	EXPRESSION TAG	UNP Q92R45
E	247	HIS	-	EXPRESSION TAG	UNP Q92R45
F	242	HIS	-	EXPRESSION TAG	UNP Q92R45
F	243	HIS	-	EXPRESSION TAG	UNP Q92R45
F	244	HIS	-	EXPRESSION TAG	UNP Q92R45
F	245	HIS	-	EXPRESSION TAG	UNP Q92R45
F	246	HIS	-	EXPRESSION TAG	UNP Q92R45
F	247	HIS	-	EXPRESSION TAG	UNP Q92R45
G	242	HIS	-	EXPRESSION TAG	UNP Q92R45
G	243	HIS	-	EXPRESSION TAG	UNP Q92R45
G	244	HIS	-	EXPRESSION TAG	UNP Q92R45
G	245	HIS	-	EXPRESSION TAG	UNP Q92R45
G	246	HIS	-	EXPRESSION TAG	UNP Q92R45
G	247	HIS	-	EXPRESSION TAG	UNP Q92R45
H	242	HIS	-	EXPRESSION TAG	UNP Q92R45
H	243	HIS	-	EXPRESSION TAG	UNP Q92R45
H	244	HIS	-	EXPRESSION TAG	UNP Q92R45
H	245	HIS	-	EXPRESSION TAG	UNP Q92R45
H	246	HIS	-	EXPRESSION TAG	UNP Q92R45
H	247	HIS	-	EXPRESSION TAG	UNP Q92R45

- 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	D	1	Total O S 5 4 1	0	0
2	F	1	Total O S 5 4 1	0	0
2	G	1	Total O S 5 4 1	0	0
2	H	1	Total O S 5 4 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	172	Total O 172 172	0	0
3	B	188	Total O 188 188	0	0
3	C	245	Total O 245 245	0	0
3	D	256	Total O 256 256	0	0
3	E	232	Total O 232 232	0	0

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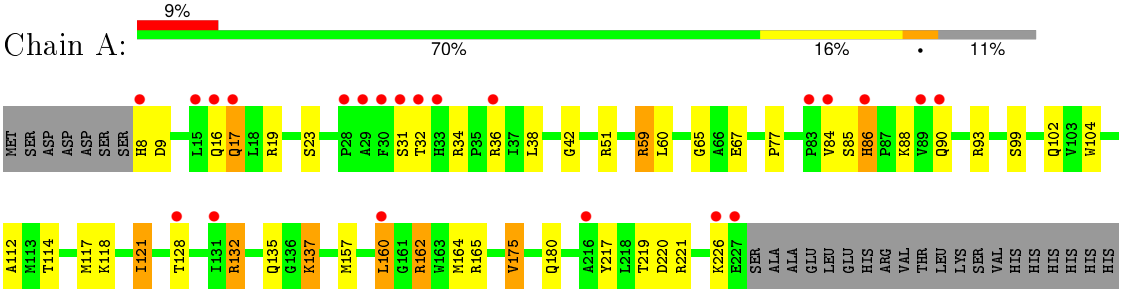
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	207	Total O 207 207	0	0
3	G	184	Total O 184 184	0	0
3	H	198	Total O 198 198	0	0

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 errors 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.

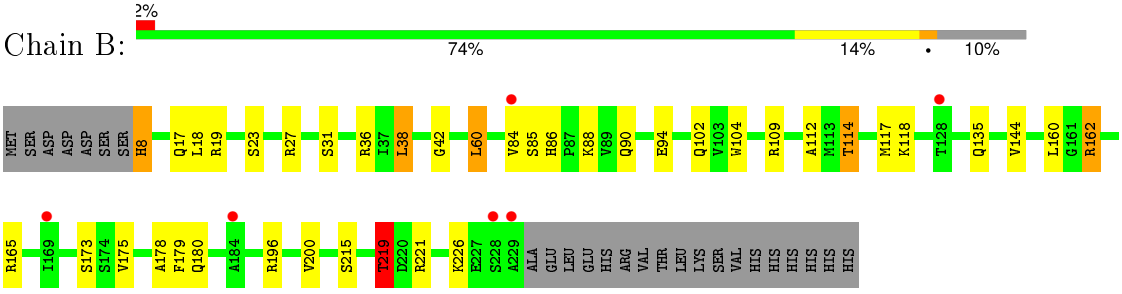
- Molecule 1: arsH

Chain A:



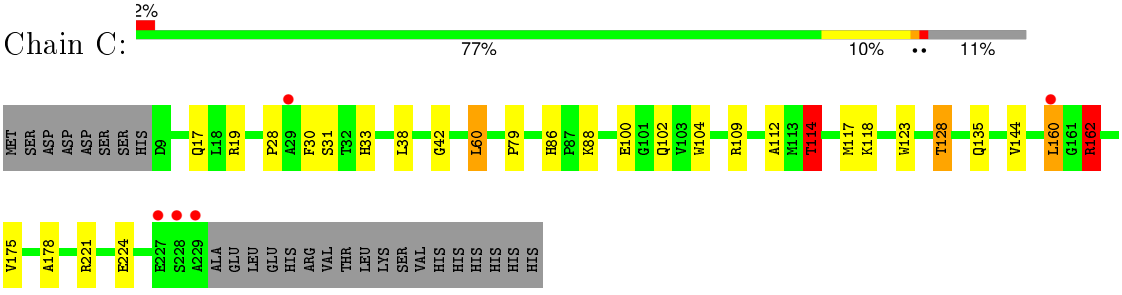
- Molecule 1: arsH

Chain B:



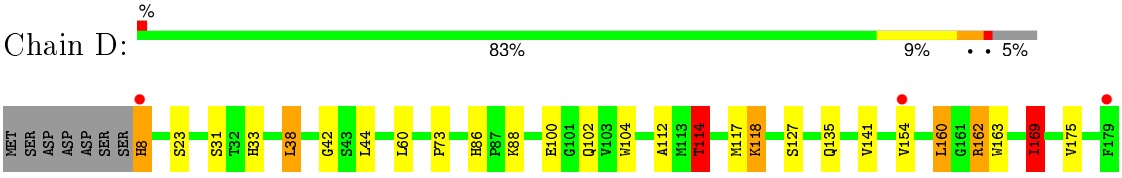
- Molecule 1: arsH

Chain C:



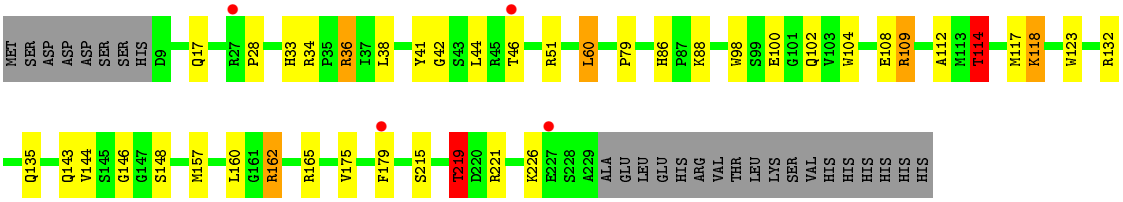
- Molecule 1: arsH

Chain D:



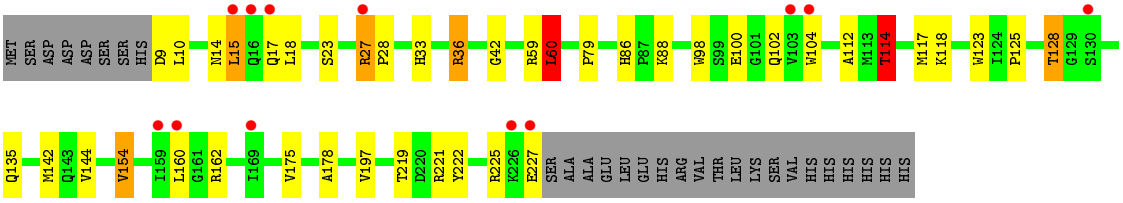
• Molecule 1: arsH

Chain E:



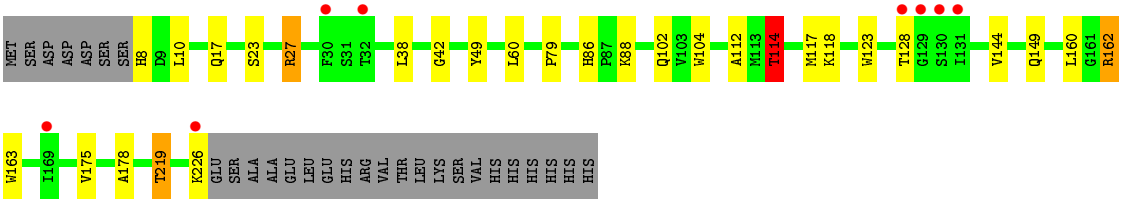
• Molecule 1: arsH

Chain F:



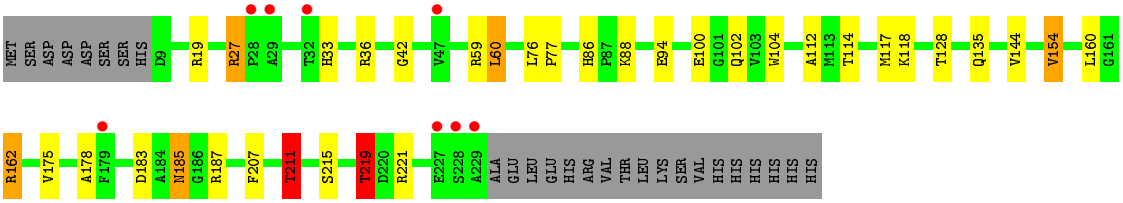
• Molecule 1: arsH

Chain G:



• Molecule 1: arsH

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α, β, γ	158.53Å 158.53Å 87.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.63 – 1.80 39.63 – 1.80	Depositor EDS
% Data completeness (in resolution range)	91.9 (39.63-1.80) 91.9 (39.63-1.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.173 , 0.212 0.174 , 0.172	Depositor DCC
R_{free} test set	9330 reflections (5.30%)	DCC
Wilson B-factor (Å^2)	22.2	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 37.4	EDS
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 185278 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	15789	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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 20.12 % 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 9.3261e-03.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.06	9/1784 (0.5%)	0.99	10/2416 (0.4%)
1	B	0.70	1/1795 (0.1%)	0.79	3/2431 (0.1%)
1	C	0.77	0/1784	0.84	5/2416 (0.2%)
1	D	0.70	0/1903	0.77	4/2577 (0.2%)
1	E	0.73	0/1784	0.87	10/2416 (0.4%)
1	F	0.67	0/1773	0.78	4/2401 (0.2%)
1	G	0.63	0/1775	0.74	2/2404 (0.1%)
1	H	0.69	0/1784	0.81	5/2416 (0.2%)
All	All	0.76	10/14382 (0.1%)	0.82	43/19477 (0.2%)

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	A	1	0
1	C	1	0
1	E	1	0
1	H	1	0
All	All	4	0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	GLU	CD-OE1	9.76	1.36	1.25
1	A	67	GLU	CD-OE2	7.71	1.34	1.25
1	A	32	THR	C-N	7.55	1.51	1.34
1	A	32	THR	C-O	7.46	1.37	1.23
1	A	86	HIS	CG-ND1	6.85	1.53	1.38
1	A	137	LYS	CD-CE	6.28	1.67	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	31	SER	CB-OG	6.03	1.50	1.42
1	B	85	SER	C-O	5.47	1.33	1.23
1	A	90	GLN	C-O	-5.32	1.13	1.23
1	A	137	LYS	CE-NZ	5.10	1.61	1.49

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	93	ARG	CA-C-O	9.46	139.96	120.10
1	A	93	ARG	O-C-N	-9.36	107.72	122.70
1	F	154	VAL	CG1-CB-CG2	7.93	123.59	110.90
1	E	109	ARG	NE-CZ-NH2	7.89	124.24	120.30
1	A	59	ARG	NE-CZ-NH1	-7.30	116.65	120.30
1	E	36	ARG	NE-CZ-NH2	7.13	123.87	120.30
1	A	93	ARG	NE-CZ-NH1	-6.96	116.82	120.30
1	C	60	LEU	CB-CG-CD1	6.95	122.81	111.00
1	H	154	VAL	CG1-CB-CG2	6.91	121.96	110.90
1	A	93	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	D	38	LEU	CB-CG-CD2	6.50	122.05	111.00
1	C	175	VAL	CG1-CB-CG2	6.47	121.25	110.90
1	A	157	MET	CG-SD-CE	-6.37	90.01	100.20
1	G	114	THR	OG1-CB-CG2	6.26	124.40	110.00
1	C	114	THR	OG1-CB-CG2	6.24	124.36	110.00
1	D	114	THR	N-CA-CB	-6.13	98.66	110.30
1	A	93	ARG	NH1-CZ-NH2	5.96	125.95	119.40
1	E	36	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	E	114	THR	OG1-CB-CG2	5.87	123.50	110.00
1	H	211	THR	N-CA-CB	-5.87	99.15	110.30
1	H	154	VAL	CA-CB-CG1	5.82	119.64	110.90
1	B	38	LEU	CB-CG-CD2	5.79	120.84	111.00
1	D	169	ILE	CG1-CB-CG2	5.77	124.10	111.40
1	E	109	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	B	60	LEU	CA-CB-CG	5.62	128.22	115.30
1	F	114	THR	N-CA-CB	-5.59	99.68	110.30
1	A	175	VAL	CG1-CB-CG2	5.54	119.77	110.90
1	G	114	THR	N-CA-CB	-5.53	99.80	110.30
1	F	114	THR	OG1-CB-CG2	5.51	122.67	110.00
1	C	160	LEU	CB-CG-CD2	5.43	120.23	111.00
1	H	219	THR	OG1-CB-CG2	5.42	122.47	110.00
1	F	60	LEU	CB-CG-CD1	5.42	120.21	111.00
1	A	59	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	D	160	LEU	CB-CG-CD2	5.27	119.96	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	114	THR	N-CA-CB	-5.26	100.30	110.30
1	E	219	THR	N-CA-CB	-5.24	100.35	110.30
1	B	219	THR	N-CA-CB	-5.22	100.37	110.30
1	H	211	THR	OG1-CB-CG2	5.13	121.81	110.00
1	E	60	LEU	CB-CG-CD1	5.13	119.72	111.00
1	A	51	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	E	114	THR	CA-CB-CG2	5.08	119.52	112.40
1	E	157	MET	CG-SD-CE	-5.04	92.13	100.20
1	C	162	ARG	NE-CZ-NH1	5.01	122.81	120.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	114	THR	CB
1	C	114	THR	CB
1	E	114	THR	CB
1	H	114	THR	CB

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1745	0	1754	29	0
1	B	1756	0	1764	28	0
1	C	1746	0	1757	25	0
1	D	1862	0	1873	26	0
1	E	1746	0	1757	34	0
1	F	1735	0	1747	35	0
1	G	1736	0	1748	29	0
1	H	1746	0	1757	27	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	F	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	5	0	0	0	0
2	H	5	0	0	0	0
3	A	172	0	0	3	0
3	B	188	0	0	2	0
3	C	245	0	0	3	0
3	D	256	0	0	3	0
3	E	232	0	0	2	0
3	F	207	0	0	1	0
3	G	184	0	0	0	0
3	H	198	0	0	5	0
All	All	15789	0	14157	213	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 8.

All (213) 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:H:211:THR:HG23	3:H:2200:HOH:O	1.59	1.02
1:E:42:GLY:O	1:E:114:THR:HG21	1.67	0.95
1:B:42:GLY:O	1:B:114:THR:HG21	1.70	0.91
1:C:42:GLY:O	1:C:114:THR:HG21	1.71	0.90
1:A:114:THR:HG23	1:A:117:MET:H	1.37	0.89
1:D:42:GLY:O	1:D:114:THR:HG21	1.76	0.86
1:F:42:GLY:O	1:F:114:THR:HG21	1.74	0.85
1:H:114:THR:HG23	1:H:117:MET:H	1.44	0.83
1:G:42:GLY:O	1:G:114:THR:HG21	1.78	0.83
1:F:59:ARG:HE	1:G:8:HIS:CD2	1.97	0.82
1:A:42:GLY:O	1:A:114:THR:HG21	1.79	0.81
1:H:42:GLY:O	1:H:114:THR:HG21	1.82	0.80
1:D:102:GLN:HE21	1:D:104:TRP:HE1	1.30	0.79
1:E:108:GLU:HG3	1:E:143:GLN:NE2	1.97	0.79
1:E:17:GLN:HG2	1:E:226:LYS:HA	1.66	0.78
1:A:118:LYS:HE3	1:B:112:ALA:HB3	1.66	0.77
1:B:114:THR:HG22	1:B:117:MET:H	1.50	0.76
1:H:144:VAL:HG22	1:H:178:ALA:HB2	1.68	0.75
1:C:102:GLN:HE21	1:C:104:TRP:HE1	1.34	0.75
1:B:114:THR:CG2	1:B:117:MET:H	2.00	0.74
1:D:114:THR:HG22	1:D:117:MET:H	1.54	0.71
1:A:102:GLN:HE21	1:A:104:TRP:HE1	1.39	0.70
1:E:102:GLN:HE21	1:E:104:TRP:HE1	1.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:VAL:HG22	1:B:178:ALA:CB	2.22	0.70
1:C:224:GLU:OE1	3:C:2237:HOH:O	2.10	0.70
1:H:102:GLN:HE21	1:H:104:TRP:HE1	1.38	0.69
1:F:102:GLN:HE21	1:F:104:TRP:HE1	1.39	0.69
1:D:211:THR:HG23	3:D:2257:HOH:O	1.91	0.69
1:B:102:GLN:HE21	1:B:104:TRP:HE1	1.39	0.69
1:E:33:HIS:HE1	1:E:100:GLU:OE1	1.75	0.68
1:F:33:HIS:HE1	1:F:100:GLU:OE1	1.75	0.68
1:C:33:HIS:HE1	1:C:100:GLU:OE1	1.76	0.68
1:D:141:VAL:HG23	1:D:154:VAL:CG2	2.24	0.68
1:G:102:GLN:HE21	1:G:104:TRP:HE1	1.41	0.67
1:H:144:VAL:HG22	1:H:178:ALA:CB	2.24	0.67
1:B:219:THR:HG21	3:B:2185:HOH:O	1.94	0.67
1:C:86:HIS:CD2	1:C:88:LYS:H	2.11	0.67
1:F:144:VAL:HG22	1:F:178:ALA:HB2	1.77	0.67
1:G:86:HIS:HD2	1:G:88:LYS:H	1.41	0.66
1:C:118:LYS:HE3	1:D:112:ALA:HB3	1.77	0.66
1:D:207:PHE:O	1:D:211:THR:HB	1.95	0.66
1:C:128:THR:HG21	3:C:2091:HOH:O	1.94	0.66
1:D:33:HIS:HE1	1:D:100:GLU:OE1	1.80	0.65
1:D:102:GLN:NE2	1:D:104:TRP:HE1	1.94	0.65
1:C:86:HIS:HD2	1:C:88:LYS:H	1.42	0.65
1:H:33:HIS:HD2	3:H:2203:HOH:O	1.79	0.64
1:F:28:PRO:O	1:G:27:ARG:NH2	2.29	0.64
1:A:59:ARG:HD3	1:D:8:HIS:CG	2.33	0.64
1:C:114:THR:HG23	1:C:117:MET:H	1.61	0.64
1:D:114:THR:CG2	1:D:117:MET:H	2.11	0.63
1:G:86:HIS:CD2	1:G:88:LYS:H	2.16	0.63
1:H:86:HIS:HD2	1:H:88:LYS:H	1.45	0.63
1:D:141:VAL:HG23	1:D:154:VAL:HG23	1.80	0.63
1:H:86:HIS:CD2	1:H:88:LYS:H	2.17	0.63
1:C:144:VAL:CG2	1:C:178:ALA:HB2	2.29	0.63
1:G:118:LYS:HE3	1:H:112:ALA:HB3	1.80	0.63
1:E:86:HIS:CD2	1:E:88:LYS:H	2.18	0.61
1:F:102:GLN:NE2	1:F:104:TRP:HE1	1.98	0.61
1:E:118:LYS:HE3	1:F:112:ALA:HB3	1.83	0.61
1:B:102:GLN:NE2	1:B:104:TRP:HE1	2.00	0.60
1:F:27:ARG:HH11	1:G:27:ARG:HD2	1.65	0.60
1:B:144:VAL:HG22	1:B:178:ALA:HB2	1.83	0.60
1:D:135:GLN:HE22	1:D:221:ARG:HH12	1.49	0.60
1:H:185:ASN:ND2	1:H:187:ARG:H	1.99	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ILE:HD11	1:A:164:MET:SD	2.42	0.59
1:A:121:ILE:HD11	1:A:164:MET:CG	2.32	0.59
1:A:59:ARG:HH21	1:D:8:HIS:CE1	2.21	0.59
1:A:121:ILE:CD1	1:A:164:MET:HG3	2.33	0.59
1:C:102:GLN:NE2	1:C:104:TRP:HE1	1.99	0.59
1:C:135:GLN:HE22	1:C:221:ARG:HH12	1.50	0.59
1:E:41:TYR:CZ	1:E:51:ARG:HD3	2.39	0.58
1:C:31:SER:HB3	1:C:33:HIS:CD2	2.38	0.58
1:E:114:THR:HG22	1:E:117:MET:HB2	1.84	0.58
1:F:27:ARG:NH1	1:G:27:ARG:HD2	2.19	0.58
1:A:102:GLN:NE2	1:A:104:TRP:HE1	2.02	0.57
1:H:207:PHE:O	1:H:211:THR:HB	2.05	0.57
1:F:114:THR:CG2	1:F:117:MET:H	2.16	0.57
1:D:86:HIS:HD2	1:D:88:LYS:H	1.53	0.57
1:F:128:THR:HB	3:F:2193:HOH:O	2.04	0.56
1:H:102:GLN:NE2	1:H:104:TRP:HE1	2.03	0.56
1:H:219:THR:HG21	3:H:2199:HOH:O	2.04	0.56
1:H:33:HIS:HE1	1:H:100:GLU:OE1	1.90	0.55
1:E:114:THR:CG2	1:E:117:MET:H	2.19	0.55
1:A:99:SER:O	1:A:137:LYS:HE2	2.07	0.55
1:F:114:THR:HG22	1:F:117:MET:H	1.72	0.54
1:F:27:ARG:O	1:F:27:ARG:HG3	2.06	0.54
1:B:135:GLN:HE22	1:B:221:ARG:HH22	1.55	0.54
1:B:162:ARG:C	1:B:162:ARG:HD3	2.28	0.54
1:G:102:GLN:NE2	1:G:104:TRP:HE1	2.05	0.54
1:H:59:ARG:NH2	3:H:2031:HOH:O	2.36	0.54
1:F:86:HIS:HD2	1:F:88:LYS:H	1.55	0.54
1:B:17:GLN:HG3	1:B:226:LYS:HA	1.88	0.54
1:G:114:THR:CG2	1:G:117:MET:H	2.20	0.54
1:B:144:VAL:CG2	1:B:178:ALA:CB	2.85	0.54
1:C:114:THR:CG2	1:C:117:MET:H	2.22	0.53
1:E:86:HIS:HD2	1:E:88:LYS:H	1.55	0.53
1:A:77:PRO:HD3	1:A:86:HIS:CD2	2.44	0.53
1:B:27:ARG:NH2	1:C:28:PRO:O	2.40	0.53
1:A:59:ARG:NH1	3:A:2163:HOH:O	2.41	0.53
1:F:86:HIS:CD2	1:F:88:LYS:H	2.27	0.53
1:A:217:TYR:O	1:A:220:ASP:HB3	2.09	0.53
1:B:215:SER:O	1:B:219:THR:HB	2.09	0.53
1:E:148:SER:HB2	1:G:149:GLN:HE22	1.74	0.53
1:E:17:GLN:HG2	1:E:226:LYS:CA	2.37	0.53
1:F:144:VAL:HG22	1:F:178:ALA:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:HIS:CD2	1:D:88:LYS:H	2.27	0.52
1:F:125:PRO:HG2	1:F:128:THR:HG22	1.91	0.52
1:G:114:THR:HG23	1:G:117:MET:H	1.75	0.52
1:A:162:ARG:C	1:A:162:ARG:HD3	2.30	0.52
1:D:135:GLN:NE2	1:D:221:ARG:HH12	2.07	0.52
1:E:102:GLN:NE2	1:E:104:TRP:HE1	2.05	0.52
1:E:135:GLN:HE22	1:E:221:ARG:HH12	1.56	0.52
1:G:112:ALA:HB3	1:H:118:LYS:HE3	1.92	0.51
1:H:135:GLN:HE22	1:H:221:ARG:HH12	1.56	0.51
1:F:135:GLN:HE22	1:F:221:ARG:HH12	1.56	0.51
1:F:9:ASP:OD2	1:F:10:LEU:N	2.43	0.51
1:E:162:ARG:HD3	1:E:162:ARG:C	2.31	0.51
1:E:215:SER:O	1:E:219:THR:HB	2.11	0.50
1:C:112:ALA:HB3	1:D:118:LYS:HE3	1.93	0.50
1:G:49:TYR:HB2	1:G:144:VAL:HG11	1.93	0.50
1:E:114:THR:HG23	1:E:117:MET:H	1.76	0.49
1:D:162:ARG:HD3	1:D:162:ARG:C	2.32	0.49
1:B:114:THR:HG22	1:B:117:MET:HB2	1.95	0.49
1:B:196:ARG:O	1:B:200:VAL:HG23	2.12	0.49
1:G:114:THR:HG22	1:G:117:MET:HB2	1.93	0.49
1:F:27:ARG:HH11	1:F:27:ARG:CB	2.24	0.49
1:B:135:GLN:NE2	1:B:165:ARG:HH11	2.11	0.49
1:F:135:GLN:NE2	1:F:221:ARG:HH22	2.11	0.48
1:G:219:THR:O	1:G:219:THR:CG2	2.60	0.48
1:H:162:ARG:C	1:H:162:ARG:HD3	2.33	0.48
1:C:128:THR:HB	3:C:2041:HOH:O	2.12	0.48
1:A:121:ILE:HG12	1:A:160:LEU:HD11	1.96	0.48
1:G:17:GLN:CD	1:G:226:LYS:HB3	2.34	0.48
1:F:142:MET:HE1	1:F:197:VAL:HG13	1.95	0.48
1:D:169:ILE:HD11	1:D:207:PHE:HB2	1.96	0.48
1:B:8:HIS:HA	3:B:2046:HOH:O	2.13	0.48
1:B:144:VAL:CG2	1:B:178:ALA:HB2	2.44	0.48
1:A:112:ALA:HB3	1:B:118:LYS:HE3	1.96	0.48
1:F:114:THR:HG22	1:F:117:MET:HB2	1.96	0.47
1:A:34:ARG:HG2	1:A:65:GLY:O	2.13	0.47
1:A:85:SER:O	1:A:86:HIS:C	2.52	0.47
1:E:28:PRO:O	1:H:27:ARG:NH2	2.38	0.47
1:F:36:ARG:HG2	1:F:98:TRP:CE2	2.50	0.47
1:H:185:ASN:C	1:H:185:ASN:HD22	2.18	0.46
1:A:17:GLN:HG2	1:A:226:LYS:HA	1.97	0.46
1:A:121:ILE:CD1	1:A:164:MET:CG	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:219:THR:O	1:G:219:THR:HG23	2.15	0.46
1:F:17:GLN:O	1:F:225:ARG:HD2	2.16	0.46
1:F:114:THR:HG22	1:F:117:MET:CB	2.45	0.46
1:C:162:ARG:HD3	1:C:162:ARG:C	2.36	0.46
1:F:60:LEU:HD13	1:G:10:LEU:HD22	1.98	0.46
1:B:135:GLN:NE2	1:B:221:ARG:HH12	2.14	0.46
1:F:59:ARG:NE	1:G:8:HIS:CD2	2.77	0.46
1:A:135:GLN:NE2	1:A:221:ARG:HH22	2.14	0.45
1:E:114:THR:HG22	1:E:117:MET:CB	2.45	0.45
1:E:144:VAL:HG23	1:E:175:VAL:HG22	1.98	0.45
1:E:108:GLU:CG	1:E:143:GLN:NE2	2.74	0.45
1:C:86:HIS:HD2	1:C:88:LYS:N	2.12	0.45
1:C:135:GLN:NE2	1:C:221:ARG:HH12	2.13	0.45
1:E:33:HIS:CD2	1:E:33:HIS:H	2.34	0.45
1:D:219:THR:HG21	3:D:2246:HOH:O	2.16	0.45
1:B:90:GLN:O	1:B:94:GLU:HG2	2.17	0.45
1:F:27:ARG:HH11	1:F:27:ARG:HB3	1.82	0.44
1:E:33:HIS:CD2	3:E:468:HOH:O	2.70	0.44
1:G:162:ARG:C	1:G:162:ARG:HD3	2.38	0.44
1:G:86:HIS:HD2	1:G:88:LYS:N	2.12	0.44
1:H:60:LEU:HD22	3:H:2128:HOH:O	2.18	0.44
1:H:185:ASN:HD22	1:H:187:ARG:H	1.64	0.44
1:H:215:SER:O	1:H:219:THR:HB	2.18	0.44
1:G:17:GLN:NE2	1:G:226:LYS:HB3	2.33	0.44
1:A:180:GLN:NE2	3:A:2159:HOH:O	2.50	0.44
1:F:15:LEU:HD22	1:F:18:LEU:HD12	1.98	0.44
1:D:135:GLN:NE2	1:D:221:ARG:HH22	2.16	0.43
1:D:141:VAL:CG2	1:D:154:VAL:HG23	2.47	0.43
1:H:183:ASP:HB2	1:H:185:ASN:ND2	2.33	0.43
1:B:114:THR:HG22	1:B:117:MET:CB	2.49	0.43
1:A:135:GLN:HE22	1:A:221:ARG:HH12	1.66	0.43
1:F:17:GLN:HB2	1:F:222:TYR:CE2	2.53	0.43
1:G:79:PRO:HA	1:G:123:TRP:CE2	2.54	0.43
1:H:135:GLN:NE2	1:H:221:ARG:HH12	2.17	0.42
1:E:135:GLN:NE2	1:E:221:ARG:HH12	2.16	0.42
1:B:86:HIS:HD2	1:B:88:LYS:H	1.67	0.42
1:C:79:PRO:HA	1:C:123:TRP:CE2	2.55	0.42
1:E:146:GLY:O	1:E:179:PHE:HE1	2.03	0.42
1:A:135:GLN:HE21	1:A:165:ARG:HD3	1.83	0.42
1:E:112:ALA:HB3	1:F:118:LYS:HE3	2.01	0.42
1:B:179:PHE:CE2	1:B:180:GLN:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:86:HIS:CD2	1:B:88:LYS:H	2.37	0.42
1:G:162:ARG:HD2	1:G:163:TRP:CE3	2.54	0.42
1:D:169:ILE:HD11	1:D:207:PHE:CB	2.49	0.42
1:E:36:ARG:HG2	1:E:98:TRP:CZ2	2.55	0.42
1:E:34:ARG:HD3	3:E:452:HOH:O	2.19	0.42
1:H:76:LEU:HD12	1:H:77:PRO:HD2	2.02	0.41
1:C:144:VAL:HG23	1:C:178:ALA:HB2	2.00	0.41
1:A:86:HIS:CD2	1:A:88:LYS:H	2.39	0.41
1:F:14:ASN:OD1	1:F:17:GLN:HG2	2.20	0.41
1:A:84:VAL:HG11	3:A:2081:HOH:O	2.20	0.41
1:D:33:HIS:HD2	3:D:2063:HOH:O	2.03	0.41
1:C:135:GLN:NE2	1:C:221:ARG:HH22	2.18	0.41
1:E:148:SER:HB2	1:G:149:GLN:NE2	2.35	0.41
1:E:135:GLN:NE2	1:E:165:ARG:HH11	2.19	0.41
1:G:144:VAL:HG13	1:G:178:ALA:CB	2.51	0.41
1:A:121:ILE:CD1	1:A:164:MET:SD	3.09	0.41
1:C:144:VAL:CG2	1:C:178:ALA:CB	2.97	0.40
1:B:135:GLN:NE2	1:B:221:ARG:HH22	2.19	0.40
1:D:44:LEU:HD21	1:D:73:PRO:HG2	2.02	0.40
1:C:144:VAL:HG22	1:C:178:ALA:HB2	2.03	0.40
1:E:36:ARG:HG2	1:E:98:TRP:CE2	2.57	0.40
1:G:128:THR:O	1:G:128:THR:HG23	2.22	0.40
1:A:132:ARG:HH11	1:A:132:ARG:HG3	1.86	0.40
1:E:44:LEU:HD23	1:E:44:LEU:HA	1.81	0.40
1:E:79:PRO:HA	1:E:123:TRP:CE2	2.57	0.40
1:F:79:PRO:HA	1:F:123:TRP:CZ2	2.56	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	218/247 (88%)	210 (96%)	8 (4%)	0	100	100
1	B	220/247 (89%)	218 (99%)	2 (1%)	0	100	100
1	C	219/247 (89%)	219 (100%)	0	0	100	100
1	D	233/247 (94%)	232 (100%)	1 (0%)	0	100	100
1	E	219/247 (89%)	218 (100%)	1 (0%)	0	100	100
1	F	217/247 (88%)	216 (100%)	1 (0%)	0	100	100
1	G	217/247 (88%)	216 (100%)	1 (0%)	0	100	100
1	H	219/247 (89%)	218 (100%)	1 (0%)	0	100	100
All	All	1762/1976 (89%)	1747 (99%)	15 (1%)	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	191/216 (88%)	175 (92%)	16 (8%)	14	4
1	B	192/216 (89%)	176 (92%)	16 (8%)	14	4
1	C	191/216 (88%)	181 (95%)	10 (5%)	29	12
1	D	204/216 (94%)	189 (93%)	15 (7%)	17	5
1	E	191/216 (88%)	181 (95%)	10 (5%)	29	12
1	F	190/216 (88%)	177 (93%)	13 (7%)	20	6
1	G	190/216 (88%)	181 (95%)	9 (5%)	32	14
1	H	191/216 (88%)	178 (93%)	13 (7%)	20	6
All	All	1540/1728 (89%)	1438 (93%)	102 (7%)	21	7

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	9	ASP

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Mol	Chain	Res	Type
1	A	16	GLN
1	A	17	GLN
1	A	19	ARG
1	A	23	SER
1	A	36	ARG
1	A	38	LEU
1	A	60	LEU
1	A	121	ILE
1	A	128	THR
1	A	132	ARG
1	A	160	LEU
1	A	162	ARG
1	A	175	VAL
1	A	219	THR
1	B	8	HIS
1	B	18	LEU
1	B	19	ARG
1	B	23	SER
1	B	31	SER
1	B	36	ARG
1	B	38	LEU
1	B	60	LEU
1	B	84	VAL
1	B	109	ARG
1	B	114	THR
1	B	160	LEU
1	B	162	ARG
1	B	173	SER
1	B	175	VAL
1	B	219	THR
1	C	17	GLN
1	C	19	ARG
1	C	30	PHE
1	C	38	LEU
1	C	60	LEU
1	C	109	ARG
1	C	114	THR
1	C	128	THR
1	C	160	LEU
1	C	162	ARG
1	D	8	HIS
1	D	23	SER

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Mol	Chain	Res	Type
1	D	31	SER
1	D	38	LEU
1	D	60	LEU
1	D	114	THR
1	D	118	LYS
1	D	127	SER
1	D	160	LEU
1	D	162	ARG
1	D	163	TRP
1	D	169	ILE
1	D	175	VAL
1	D	211	THR
1	D	219	THR
1	E	38	LEU
1	E	46	THR
1	E	60	LEU
1	E	109	ARG
1	E	114	THR
1	E	118	LYS
1	E	132	ARG
1	E	160	LEU
1	E	162	ARG
1	E	219	THR
1	F	15	LEU
1	F	23	SER
1	F	27	ARG
1	F	36	ARG
1	F	60	LEU
1	F	114	THR
1	F	128	THR
1	F	154	VAL
1	F	160	LEU
1	F	162	ARG
1	F	175	VAL
1	F	219	THR
1	F	227	GLU
1	G	23	SER
1	G	27	ARG
1	G	38	LEU
1	G	60	LEU
1	G	114	THR
1	G	160	LEU

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Mol	Chain	Res	Type
1	G	162	ARG
1	G	175	VAL
1	G	219	THR
1	H	19	ARG
1	H	27	ARG
1	H	36	ARG
1	H	60	LEU
1	H	94	GLU
1	H	128	THR
1	H	154	VAL
1	H	160	LEU
1	H	162	ARG
1	H	175	VAL
1	H	185	ASN
1	H	211	THR
1	H	219	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	33	HIS
1	A	86	HIS
1	A	102	GLN
1	A	135	GLN
1	A	155	ASN
1	B	17	GLN
1	B	33	HIS
1	B	86	HIS
1	B	90	GLN
1	B	102	GLN
1	B	135	GLN
1	B	155	ASN
1	B	180	GLN
1	C	17	GLN
1	C	33	HIS
1	C	86	HIS
1	C	102	GLN
1	C	135	GLN
1	C	155	ASN
1	D	17	GLN
1	D	33	HIS

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Mol	Chain	Res	Type
1	D	86	HIS
1	D	102	GLN
1	D	135	GLN
1	D	155	ASN
1	E	33	HIS
1	E	86	HIS
1	E	102	GLN
1	E	135	GLN
1	E	155	ASN
1	E	180	GLN
1	F	16	GLN
1	F	33	HIS
1	F	86	HIS
1	F	102	GLN
1	F	135	GLN
1	F	155	ASN
1	G	8	HIS
1	G	33	HIS
1	G	86	HIS
1	G	102	GLN
1	G	120	GLN
1	G	149	GLN
1	G	155	ASN
1	G	180	GLN
1	H	33	HIS
1	H	86	HIS
1	H	90	GLN
1	H	102	GLN
1	H	135	GLN
1	H	155	ASN
1	H	185	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 (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

7 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	A	2001	-	4,4,4	0.54	0	6,6,6	0.78	0
2	SO4	B	2002	-	4,4,4	0.40	0	6,6,6	0.21	0
2	SO4	C	2003	-	4,4,4	0.23	0	6,6,6	0.32	0
2	SO4	D	2004	-	4,4,4	0.21	0	6,6,6	0.12	0
2	SO4	F	2006	-	4,4,4	0.26	0	6,6,6	0.32	0
2	SO4	G	2007	-	4,4,4	0.26	0	6,6,6	0.39	0
2	SO4	H	2008	-	4,4,4	0.19	0	6,6,6	0.40	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	2001	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2002	-	-	0/0/0/0	0/0/0/0
2	SO4	C	2003	-	-	0/0/0/0	0/0/0/0
2	SO4	D	2004	-	-	0/0/0/0	0/0/0/0
2	SO4	F	2006	-	-	0/0/0/0	0/0/0/0
2	SO4	G	2007	-	-	0/0/0/0	0/0/0/0
2	SO4	H	2008	-	-	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.

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	220/247 (89%)	0.57	22 (10%) 9 7	16, 23, 33, 40	0
1	B	222/247 (89%)	0.21	6 (2%) 58 53	16, 21, 29, 38	0
1	C	221/247 (89%)	0.26	5 (2%) 64 59	16, 20, 32, 41	0
1	D	235/247 (95%)	0.22	3 (1%) 79 76	16, 20, 31, 45	0
1	E	221/247 (89%)	0.33	4 (1%) 71 67	16, 20, 32, 40	0
1	F	219/247 (88%)	0.29	12 (5%) 29 23	16, 21, 31, 43	0
1	G	219/247 (88%)	0.24	8 (3%) 45 39	16, 20, 30, 36	0
1	H	221/247 (89%)	0.19	8 (3%) 46 40	16, 21, 30, 40	0
All	All	1778/1976 (89%)	0.29	68 (3%) 44 38	16, 21, 31, 45	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	8	HIS	7.3
1	A	29	ALA	6.7
1	H	228	SER	5.0
1	A	227	GLU	4.6
1	B	84	VAL	4.3
1	F	227	GLU	4.2
1	A	128	THR	4.2
1	A	30	PHE	4.2
1	A	32	THR	4.1
1	G	32	THR	4.0
1	A	84	VAL	3.8
1	G	30	PHE	3.7
1	H	227	GLU	3.7
1	F	226	LYS	3.7
1	A	226	LYS	3.6
1	F	17	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	16	GLN	3.6
1	G	129	GLY	3.5
1	G	128	THR	3.5
1	F	27	ARG	3.4
1	A	17	GLN	3.2
1	H	32	THR	3.2
1	G	130	SER	3.2
1	H	229	ALA	3.1
1	E	179	PHE	3.0
1	A	31	SER	2.9
1	F	16	GLN	2.9
1	B	128	THR	2.8
1	G	131	ILE	2.8
1	F	159	ILE	2.8
1	H	29	ALA	2.8
1	G	226	LYS	2.7
1	E	46	THR	2.7
1	A	33	HIS	2.7
1	C	229	ALA	2.7
1	A	8	HIS	2.6
1	B	228	SER	2.6
1	A	15	LEU	2.6
1	H	28	PRO	2.6
1	A	86	HIS	2.6
1	B	184	ALA	2.5
1	A	36	ARG	2.4
1	C	160	LEU	2.4
1	F	160	LEU	2.4
1	H	179	PHE	2.4
1	A	216	ALA	2.4
1	C	227	GLU	2.3
1	A	28	PRO	2.3
1	F	15	LEU	2.3
1	C	29	ALA	2.3
1	D	179	PHE	2.3
1	A	89	VAL	2.2
1	F	104	TRP	2.2
1	B	229	ALA	2.2
1	A	131	ILE	2.2
1	A	83	PRO	2.2
1	F	169	ILE	2.2
1	A	160	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	228	SER	2.2
1	G	169	ILE	2.1
1	D	154	VAL	2.1
1	H	47	VAL	2.1
1	E	227	GLU	2.1
1	A	90	GLN	2.1
1	E	27	ARG	2.1
1	F	103	VAL	2.1
1	F	130	SER	2.0
1	B	169	ILE	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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	D	2004	5/5	0.97	0.23	5.72	15,22,23,23	0
2	SO4	G	2007	5/5	0.98	0.22	4.60	23,25,29,31	0
2	SO4	H	2008	5/5	0.97	0.29	4.55	29,30,34,35	0
2	SO4	C	2003	5/5	0.99	0.23	4.00	16,17,18,19	0
2	SO4	A	2001	5/5	0.98	0.21	3.58	19,20,24,24	0
2	SO4	F	2006	5/5	0.98	0.23	3.32	21,21,24,26	0
2	SO4	B	2002	5/5	0.98	0.18	3.00	20,22,25,25	0

6.5 Other polymers (i)

There are no such residues in this entry.