Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:43 PM GMT

PDB ID	:	1YDG
Title	:	Crystal Structure of Trp repressor binding protein WrbA
Authors	:	Gorman, J.; Shapiro, L.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on	:	2004-12-23
Resolution	:	2.00 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:

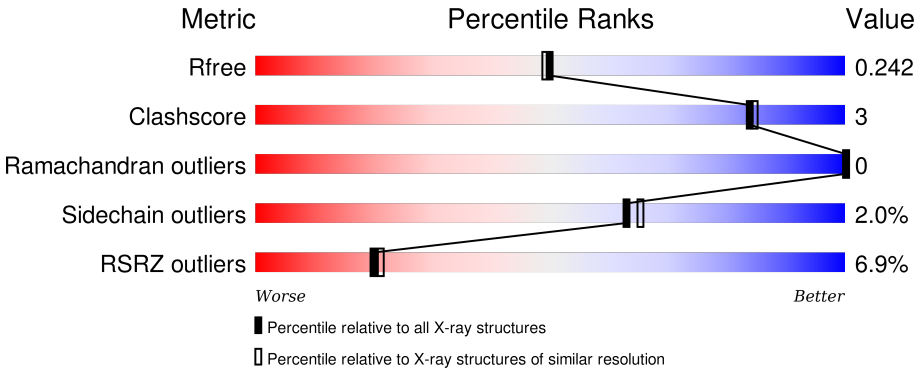
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	211	92% · 5%
1	B	211	8% 90% 6% ·
1	C	211	92% · ·
1	D	211	7% 84% 11% ·
1	E	211	8% 91% 6% ·

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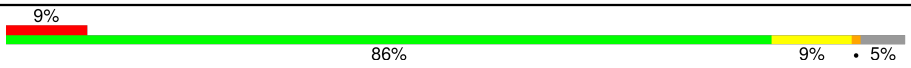
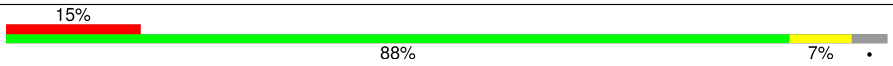
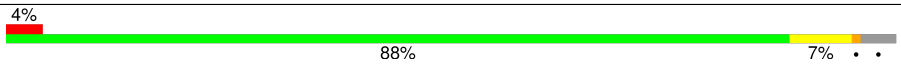
Mol	Chain	Length	Quality of chain
1	F	211	
1	G	211	
1	H	211	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13399 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 trp repressor binding protein WrbA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	201	Total	C	N	O	S	0	0	0
			1500	938	261	295	6			
1	B	202	Total	C	N	O	S	0	0	0
			1507	942	262	297	6			
1	C	202	Total	C	N	O	S	0	0	0
			1507	942	262	297	6			
1	D	202	Total	C	N	O	S	0	0	0
			1507	942	262	297	6			
1	E	204	Total	C	N	O	S	0	0	0
			1521	951	264	300	6			
1	F	201	Total	C	N	O	S	0	0	0
			1500	938	261	295	6			
1	G	202	Total	C	N	O	S	0	0	0
			1507	942	262	297	6			
1	H	202	Total	C	N	O	S	0	0	0
			1507	942	262	297	6			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	cloning artifact	UNP Q9RYU4
A	0	SER	-	cloning artifact	UNP Q9RYU4
A	1	LEU	-	cloning artifact	UNP Q9RYU4
A	200	GLU	-	cloning artifact	UNP Q9RYU4
A	202	GLY	-	cloning artifact	UNP Q9RYU4
A	203	SER	-	cloning artifact	UNP Q9RYU4
A	204	HIS	-	EXPRESSION TAG	UNP Q9RYU4
A	205	HIS	-	EXPRESSION TAG	UNP Q9RYU4
A	206	HIS	-	EXPRESSION TAG	UNP Q9RYU4
A	207	HIS	-	EXPRESSION TAG	UNP Q9RYU4
A	208	HIS	-	EXPRESSION TAG	UNP Q9RYU4
A	209	HIS	-	EXPRESSION TAG	UNP Q9RYU4
B	-1	MET	-	cloning artifact	UNP Q9RYU4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	cloning artifact	UNP Q9RYU4
B	1	LEU	-	cloning artifact	UNP Q9RYU4
B	200	GLU	-	cloning artifact	UNP Q9RYU4
B	202	GLY	-	cloning artifact	UNP Q9RYU4
B	203	SER	-	cloning artifact	UNP Q9RYU4
B	204	HIS	-	EXPRESSION TAG	UNP Q9RYU4
B	205	HIS	-	EXPRESSION TAG	UNP Q9RYU4
B	206	HIS	-	EXPRESSION TAG	UNP Q9RYU4
B	207	HIS	-	EXPRESSION TAG	UNP Q9RYU4
B	208	HIS	-	EXPRESSION TAG	UNP Q9RYU4
B	209	HIS	-	EXPRESSION TAG	UNP Q9RYU4
C	-1	MET	-	cloning artifact	UNP Q9RYU4
C	0	SER	-	cloning artifact	UNP Q9RYU4
C	1	LEU	-	cloning artifact	UNP Q9RYU4
C	200	GLU	-	cloning artifact	UNP Q9RYU4
C	202	GLY	-	cloning artifact	UNP Q9RYU4
C	203	SER	-	cloning artifact	UNP Q9RYU4
C	204	HIS	-	EXPRESSION TAG	UNP Q9RYU4
C	205	HIS	-	EXPRESSION TAG	UNP Q9RYU4
C	206	HIS	-	EXPRESSION TAG	UNP Q9RYU4
C	207	HIS	-	EXPRESSION TAG	UNP Q9RYU4
C	208	HIS	-	EXPRESSION TAG	UNP Q9RYU4
C	209	HIS	-	EXPRESSION TAG	UNP Q9RYU4
D	-1	MET	-	cloning artifact	UNP Q9RYU4
D	0	SER	-	cloning artifact	UNP Q9RYU4
D	1	LEU	-	cloning artifact	UNP Q9RYU4
D	200	GLU	-	cloning artifact	UNP Q9RYU4
D	202	GLY	-	cloning artifact	UNP Q9RYU4
D	203	SER	-	cloning artifact	UNP Q9RYU4
D	204	HIS	-	EXPRESSION TAG	UNP Q9RYU4
D	205	HIS	-	EXPRESSION TAG	UNP Q9RYU4
D	206	HIS	-	EXPRESSION TAG	UNP Q9RYU4
D	207	HIS	-	EXPRESSION TAG	UNP Q9RYU4
D	208	HIS	-	EXPRESSION TAG	UNP Q9RYU4
D	209	HIS	-	EXPRESSION TAG	UNP Q9RYU4
E	-1	MET	-	cloning artifact	UNP Q9RYU4
E	0	SER	-	cloning artifact	UNP Q9RYU4
E	1	LEU	-	cloning artifact	UNP Q9RYU4
E	200	GLU	-	cloning artifact	UNP Q9RYU4
E	202	GLY	-	cloning artifact	UNP Q9RYU4
E	203	SER	-	cloning artifact	UNP Q9RYU4
E	204	HIS	-	EXPRESSION TAG	UNP Q9RYU4

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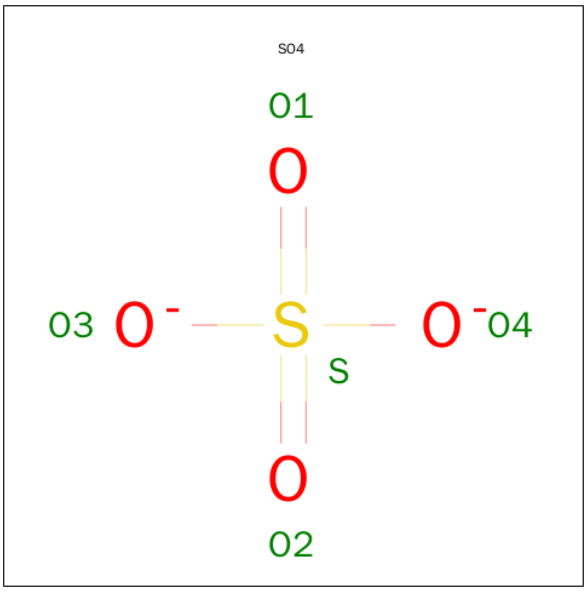
Chain	Residue	Modelled	Actual	Comment	Reference
E	205	HIS	-	EXPRESSION TAG	UNP Q9RYU4
E	206	HIS	-	EXPRESSION TAG	UNP Q9RYU4
E	207	HIS	-	EXPRESSION TAG	UNP Q9RYU4
E	208	HIS	-	EXPRESSION TAG	UNP Q9RYU4
E	209	HIS	-	EXPRESSION TAG	UNP Q9RYU4
F	-1	MET	-	cloning artifact	UNP Q9RYU4
F	0	SER	-	cloning artifact	UNP Q9RYU4
F	1	LEU	-	cloning artifact	UNP Q9RYU4
F	200	GLU	-	cloning artifact	UNP Q9RYU4
F	202	GLY	-	cloning artifact	UNP Q9RYU4
F	203	SER	-	cloning artifact	UNP Q9RYU4
F	204	HIS	-	EXPRESSION TAG	UNP Q9RYU4
F	205	HIS	-	EXPRESSION TAG	UNP Q9RYU4
F	206	HIS	-	EXPRESSION TAG	UNP Q9RYU4
F	207	HIS	-	EXPRESSION TAG	UNP Q9RYU4
F	208	HIS	-	EXPRESSION TAG	UNP Q9RYU4
F	209	HIS	-	EXPRESSION TAG	UNP Q9RYU4
G	-1	MET	-	cloning artifact	UNP Q9RYU4
G	0	SER	-	cloning artifact	UNP Q9RYU4
G	1	LEU	-	cloning artifact	UNP Q9RYU4
G	200	GLU	-	cloning artifact	UNP Q9RYU4
G	202	GLY	-	cloning artifact	UNP Q9RYU4
G	203	SER	-	cloning artifact	UNP Q9RYU4
G	204	HIS	-	EXPRESSION TAG	UNP Q9RYU4
G	205	HIS	-	EXPRESSION TAG	UNP Q9RYU4
G	206	HIS	-	EXPRESSION TAG	UNP Q9RYU4
G	207	HIS	-	EXPRESSION TAG	UNP Q9RYU4
G	208	HIS	-	EXPRESSION TAG	UNP Q9RYU4
G	209	HIS	-	EXPRESSION TAG	UNP Q9RYU4
H	-1	MET	-	cloning artifact	UNP Q9RYU4
H	0	SER	-	cloning artifact	UNP Q9RYU4
H	1	LEU	-	cloning artifact	UNP Q9RYU4
H	200	GLU	-	cloning artifact	UNP Q9RYU4
H	202	GLY	-	cloning artifact	UNP Q9RYU4
H	203	SER	-	cloning artifact	UNP Q9RYU4
H	204	HIS	-	EXPRESSION TAG	UNP Q9RYU4
H	205	HIS	-	EXPRESSION TAG	UNP Q9RYU4
H	206	HIS	-	EXPRESSION TAG	UNP Q9RYU4
H	207	HIS	-	EXPRESSION TAG	UNP Q9RYU4
H	208	HIS	-	EXPRESSION TAG	UNP Q9RYU4
H	209	HIS	-	EXPRESSION TAG	UNP Q9RYU4

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total O S 5 4 1	0	0
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
2	G	1	Total O S 5 4 1	0	0
2	H	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	225	Total O 225 225	0	0
3	B	198	Total O 198 198	0	0

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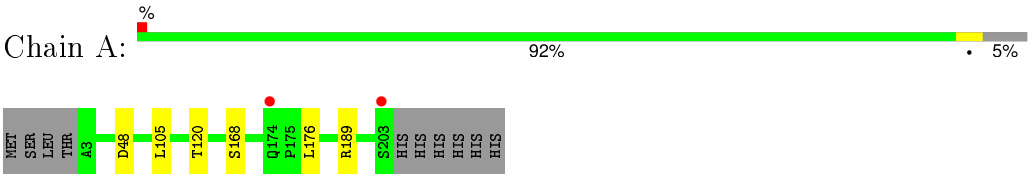
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	156	Total O 156 156	0	0
3	D	195	Total O 195 195	0	0
3	E	97	Total O 97 97	0	0
3	F	143	Total O 143 143	0	0
3	G	82	Total O 82 82	0	0
3	H	197	Total O 197 197	0	0

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.

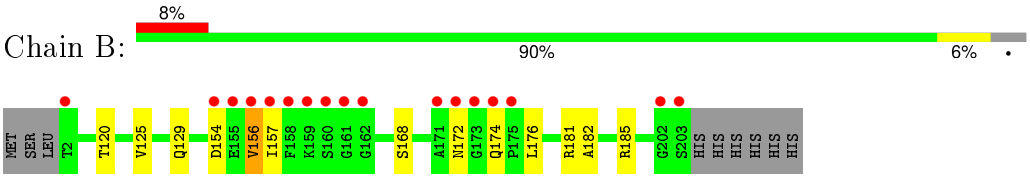
- Molecule 1: trp repressor binding protein WrbA

Chain A:



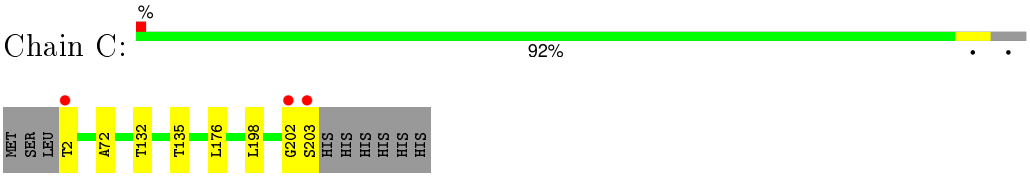
- Molecule 1: trp repressor binding protein WrbA

Chain B:



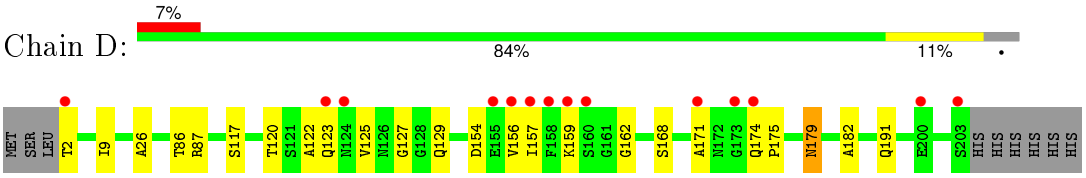
- Molecule 1: trp repressor binding protein WrbA

Chain C:



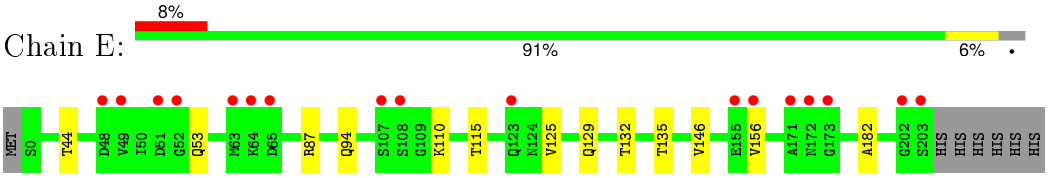
- Molecule 1: trp repressor binding protein WrbA

Chain D:



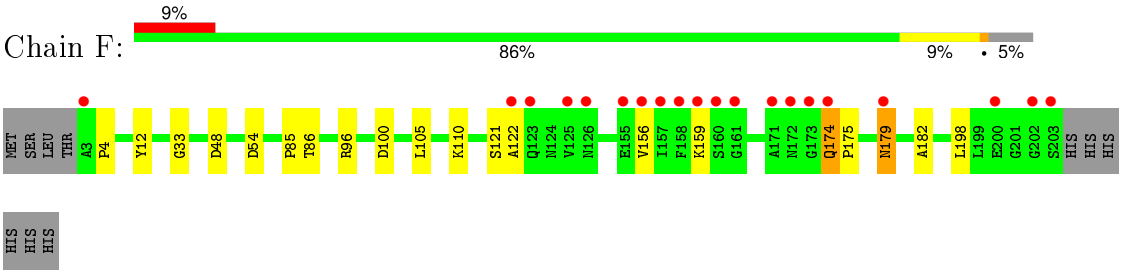
- Molecule 1: trp repressor binding protein WrbA

Chain E:



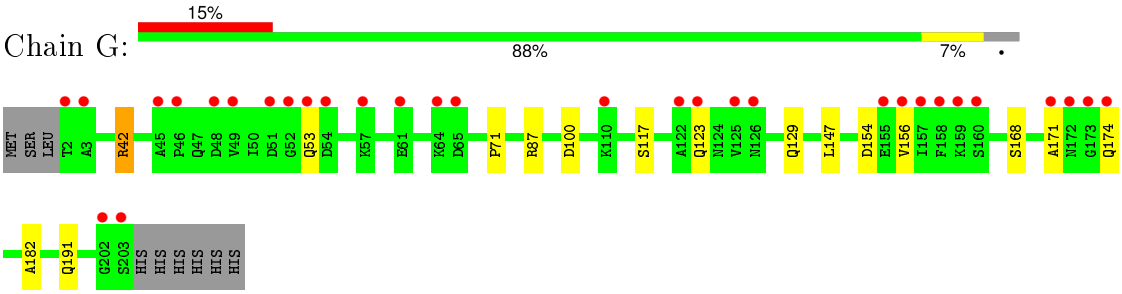
- Molecule 1: trp repressor binding protein WrbA

Chain F:



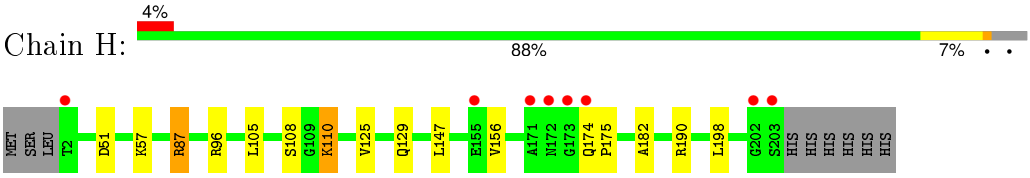
• Molecule 1: trp repressor binding protein WrbA

Chain G:



• Molecule 1: trp repressor binding protein WrbA

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	121.61Å 121.61Å 207.93Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.98 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.9 (20.00-2.00) 96.9 (19.98-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.49 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.186 , 0.236 0.196 , 0.242	Depositor DCC
R_{free} test set	5845 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	20.2	Xtriage
Anisotropy	0.134	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 53.6	EDS
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	1 of 116507 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	13399	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% of the height of the origin peak. No significant pseudotranslation is detected.*

[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	0.56	0/1529	0.66	1/2077 (0.0%)
1	B	0.55	0/1536	0.65	0/2087
1	C	0.52	0/1536	0.62	0/2087
1	D	0.55	0/1536	0.65	0/2087
1	E	0.48	0/1550	0.56	0/2106
1	F	0.48	0/1529	0.59	0/2077
1	G	0.48	0/1536	0.56	0/2087
1	H	0.54	0/1536	0.64	0/2087
All	All	0.52	0/12288	0.62	1/16695 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	189	ARG	NE-CZ-NH1	5.02	122.81	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	1500	0	1470	2	0
1	B	1507	0	1477	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1507	0	1477	5	0
1	D	1507	0	1477	18	0
1	E	1521	0	1496	10	0
1	F	1500	0	1470	12	0
1	G	1507	0	1477	11	0
1	H	1507	0	1477	12	1
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	10	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	10	0	0	0	0
3	A	225	0	0	1	0
3	B	198	0	0	2	0
3	C	156	0	0	2	0
3	D	195	0	0	3	0
3	E	97	0	0	2	0
3	F	143	0	0	1	0
3	G	82	0	0	3	0
3	H	197	0	0	4	0
All	All	13399	0	11821	72	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 3.

All (72) 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:D:123:GLN:NE2	1:D:171:ALA:O	2.25	0.70
1:H:129:GLN:C	3:H:1453:HOH:O	2.30	0.70
1:D:159:LYS:HB3	1:D:179:ASN:HD21	1.58	0.67
1:E:129:GLN:C	3:E:1378:HOH:O	2.37	0.63
1:G:154:ASP:HB3	1:G:156:VAL:HG12	1.82	0.62
1:B:125:VAL:HG11	1:D:125:VAL:HG11	1.81	0.61
1:H:57:LYS:NZ	3:H:1479:HOH:O	2.31	0.61
1:E:87:ARG:HG2	1:G:100:ASP:OD1	2.02	0.59
1:F:48:ASP:HB2	3:F:1448:HOH:O	2.02	0.59
1:G:123:GLN:HA	1:G:171:ALA:O	2.04	0.58
1:E:125:VAL:HG11	1:H:125:VAL:HG11	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:VAL:HG21	1:E:182:ALA:HB1	1.86	0.57
1:F:100:ASP:OD1	1:H:87:ARG:HG2	2.05	0.56
1:F:156:VAL:HG21	1:F:182:ALA:HB3	1.88	0.55
1:D:86:THR:HG21	1:D:122:ALA:HB2	1.89	0.54
1:G:42:ARG:HD3	3:G:1329:HOH:O	2.08	0.54
1:D:159:LYS:HB3	1:D:179:ASN:ND2	2.23	0.53
1:D:129:GLN:HG3	3:D:1457:HOH:O	2.09	0.53
1:D:156:VAL:HG21	1:D:182:ALA:C	2.29	0.53
1:H:174:GLN:HG3	1:H:175:PRO:HD2	1.91	0.52
1:H:190:ARG:HD2	3:H:1446:HOH:O	2.08	0.52
1:D:154:ASP:HB3	1:D:156:VAL:HG12	1.92	0.52
1:D:86:THR:CG2	1:D:122:ALA:HB2	2.41	0.51
1:F:96:ARG:HG3	1:H:96:ARG:HG3	1.92	0.51
1:C:2:THR:N	3:C:1447:HOH:O	2.43	0.51
1:D:157:ILE:HG22	1:D:162:GLY:HA2	1.93	0.51
1:G:117:SER:OG	1:G:191:GLN:NE2	2.44	0.50
1:H:156:VAL:HG21	1:H:182:ALA:CB	2.42	0.49
1:F:156:VAL:HG21	1:F:182:ALA:CB	2.42	0.49
1:E:156:VAL:HG21	1:E:182:ALA:CB	2.42	0.49
1:B:156:VAL:HG21	1:B:182:ALA:CB	2.42	0.49
1:C:132:THR:O	1:C:135:THR:HG22	2.12	0.48
1:H:125:VAL:HG23	3:H:1382:HOH:O	2.12	0.48
1:D:174:GLN:HG3	1:D:175:PRO:HD2	1.96	0.48
1:B:157:ILE:N	1:B:157:ILE:HD13	2.28	0.48
1:D:127:GLY:N	3:D:1457:HOH:O	2.46	0.48
1:C:202:GLY:O	1:C:203:SER:CB	2.62	0.47
1:D:129:GLN:NE2	1:D:168:SER:HB2	2.29	0.47
1:E:44:THR:OG1	1:E:94:GLN:HG3	2.13	0.47
1:G:71:PRO:HD3	3:G:1330:HOH:O	2.14	0.46
1:D:129:GLN:NE2	3:D:1450:HOH:O	2.47	0.46
1:F:86:THR:HG22	1:F:122:ALA:HB2	1.98	0.45
1:F:12:TYR:O	1:F:85:PRO:HD3	2.16	0.45
1:D:156:VAL:HG21	1:D:182:ALA:CB	2.47	0.44
1:C:72:ALA:HB1	1:F:54:ASP:HA	1.99	0.44
1:B:154:ASP:O	1:B:157:ILE:HG12	2.17	0.44
1:F:159:LYS:HB2	1:F:179:ASN:HD21	1.83	0.44
1:E:115:THR:HA	1:E:146:VAL:O	2.18	0.43
1:B:129:GLN:NE2	3:B:1382:HOH:O	2.51	0.43
1:G:53:GLN:NE2	3:G:1377:HOH:O	2.51	0.43
1:H:156:VAL:HG21	1:H:182:ALA:HB1	2.00	0.43
1:G:147:LEU:HD12	1:H:147:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:SER:OG	1:D:191:GLN:NE2	2.51	0.42
1:A:120:THR:O	1:A:168:SER:HA	2.18	0.42
1:F:4:PRO:HB3	1:F:33:GLY:O	2.19	0.42
1:A:48:ASP:HB3	3:A:1527:HOH:O	2.17	0.42
1:F:174:GLN:HE21	1:F:174:GLN:HA	1.83	0.42
1:B:181:ARG:O	1:B:185:ARG:HG3	2.20	0.42
1:H:108:SER:HB3	1:H:110:LYS:HE3	2.02	0.41
1:F:174:GLN:HG3	1:F:175:PRO:HD2	2.01	0.41
1:B:176:LEU:HB2	1:B:181:ARG:NH2	2.36	0.41
1:E:129:GLN:HG2	3:E:1402:HOH:O	2.19	0.41
1:D:120:THR:O	1:D:168:SER:HA	2.20	0.41
1:B:157:ILE:HD12	3:B:1319:HOH:O	2.20	0.41
1:B:120:THR:O	1:B:168:SER:HA	2.21	0.41
1:G:156:VAL:HG21	1:G:182:ALA:CB	2.51	0.41
1:C:135:THR:CG2	3:C:1373:HOH:O	2.67	0.41
1:G:129:GLN:HE21	1:G:168:SER:HB2	1.85	0.41
1:E:125:VAL:HA	1:E:129:GLN:OE1	2.21	0.40
1:G:156:VAL:HG21	1:G:182:ALA:HB1	2.02	0.40
1:E:132:THR:O	1:E:135:THR:HG22	2.21	0.40
1:D:9:ILE:CD1	1:D:26:ALA:HA	2.51	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:H:51:ASP:OD2	1:H:51:ASP:OD2[6_555]	2.08	0.12

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	199/211 (94%)	198 (100%)	1 (0%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	200/211 (95%)	199 (100%)	1 (0%)	0	100	100
1	C	200/211 (95%)	198 (99%)	2 (1%)	0	100	100
1	D	200/211 (95%)	198 (99%)	2 (1%)	0	100	100
1	E	202/211 (96%)	201 (100%)	1 (0%)	0	100	100
1	F	199/211 (94%)	195 (98%)	4 (2%)	0	100	100
1	G	200/211 (95%)	195 (98%)	5 (2%)	0	100	100
1	H	200/211 (95%)	198 (99%)	2 (1%)	0	100	100
All	All	1600/1688 (95%)	1582 (99%)	18 (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	152/162 (94%)	150 (99%)	2 (1%)	76	79
1	B	153/162 (94%)	150 (98%)	3 (2%)	63	65
1	C	153/162 (94%)	151 (99%)	2 (1%)	76	79
1	D	153/162 (94%)	150 (98%)	3 (2%)	63	65
1	E	155/162 (96%)	153 (99%)	2 (1%)	76	79
1	F	152/162 (94%)	146 (96%)	6 (4%)	39	35
1	G	153/162 (94%)	150 (98%)	3 (2%)	63	65
1	H	153/162 (94%)	149 (97%)	4 (3%)	54	54
All	All	1224/1296 (94%)	1199 (98%)	25 (2%)	63	65

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	LEU
1	A	176	LEU

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Mol	Chain	Res	Type
1	B	156	VAL
1	B	172	ASN
1	B	174	GLN
1	C	176	LEU
1	C	198	LEU
1	D	2	THR
1	D	87	ARG
1	D	179	ASN
1	E	53	GLN
1	E	110	LYS
1	F	105	LEU
1	F	110	LYS
1	F	121	SER
1	F	174	GLN
1	F	179	ASN
1	F	198	LEU
1	G	42	ARG
1	G	87	ARG
1	G	174	GLN
1	H	87	ARG
1	H	105	LEU
1	H	110	LYS
1	H	198	LEU

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

Mol	Chain	Res	Type
1	A	129	GLN
1	A	191	GLN
1	C	129	GLN
1	C	191	GLN
1	D	23	GLN
1	D	124	ASN
1	D	191	GLN
1	E	53	GLN
1	E	129	GLN
1	E	191	GLN
1	F	174	GLN
1	F	191	GLN
1	G	129	GLN
1	G	174	GLN
1	G	191	GLN

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Mol	Chain	Res	Type
1	H	129	GLN
1	H	191	GLN

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

10 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	1302	-	4,4,4	0.48	0	6,6,6	0.21	0
2	SO4	B	1303	-	4,4,4	0.34	0	6,6,6	0.32	0
2	SO4	C	1304	-	4,4,4	0.37	0	6,6,6	0.37	0
2	SO4	D	1305	-	4,4,4	0.29	0	6,6,6	0.23	0
2	SO4	D	1310	-	4,4,4	0.23	0	6,6,6	0.15	0
2	SO4	E	1306	-	4,4,4	0.21	0	6,6,6	0.36	0
2	SO4	F	1307	-	4,4,4	0.37	0	6,6,6	0.21	0
2	SO4	G	1308	-	4,4,4	0.12	0	6,6,6	0.40	0
2	SO4	H	1301	-	4,4,4	0.41	0	6,6,6	0.52	0
2	SO4	H	1309	-	4,4,4	0.27	0	6,6,6	0.21	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	1302	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1303	-	-	0/0/0/0	0/0/0/0
2	SO4	C	1304	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1305	-	-	0/0/0/0	0/0/0/0
2	SO4	D	1310	-	-	0/0/0/0	0/0/0/0
2	SO4	E	1306	-	-	0/0/0/0	0/0/0/0
2	SO4	F	1307	-	-	0/0/0/0	0/0/0/0
2	SO4	G	1308	-	-	0/0/0/0	0/0/0/0
2	SO4	H	1301	-	-	0/0/0/0	0/0/0/0
2	SO4	H	1309	-	-	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 (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, 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	201/211 (95%)	-0.46	2 (0%) 84 84	10, 15, 27, 39	0
1	B	202/211 (95%)	0.00	17 (8%) 14 14	10, 18, 44, 53	0
1	C	202/211 (95%)	-0.25	3 (1%) 76 77	11, 19, 35, 42	0
1	D	202/211 (95%)	-0.07	14 (6%) 20 21	11, 17, 38, 47	0
1	E	204/211 (96%)	0.22	17 (8%) 14 15	21, 31, 47, 57	0
1	F	201/211 (95%)	0.17	20 (9%) 9 10	17, 28, 48, 53	0
1	G	202/211 (95%)	0.52	31 (15%) 3 3	19, 33, 54, 60	0
1	H	202/211 (95%)	-0.29	8 (3%) 42 44	14, 19, 38, 46	0
All	All	1616/1688 (95%)	-0.02	112 (6%) 20 21	10, 23, 45, 60	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	156	VAL	9.3
1	B	2	THR	7.4
1	F	202	GLY	7.3
1	E	203	SER	7.3
1	D	203	SER	7.1
1	B	174	GLN	7.1
1	B	173	GLY	7.0
1	C	2	THR	6.2
1	B	160	SER	5.8
1	A	203	SER	5.7
1	F	174	GLN	5.7
1	F	122	ALA	5.3
1	G	173	GLY	5.2
1	G	2	THR	5.1
1	G	156	VAL	5.1
1	B	159	LYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	F	159	LYS	4.9
1	F	203	SER	4.9
1	B	161	GLY	4.9
1	G	171	ALA	4.9
1	E	51	ASP	4.7
1	G	172	ASN	4.7
1	E	48	ASP	4.6
1	G	52	GLY	4.6
1	F	3	ALA	4.5
1	B	157	ILE	4.4
1	C	203	SER	4.4
1	B	203	SER	4.3
1	D	156	VAL	4.3
1	H	173	GLY	4.3
1	G	49	VAL	4.1
1	G	123	GLN	4.1
1	D	173	GLY	4.0
1	G	203	SER	4.0
1	H	174	GLN	3.9
1	G	48	ASP	3.9
1	G	160	SER	3.9
1	H	203	SER	3.8
1	D	157	ILE	3.8
1	D	158	PHE	3.7
1	E	202	GLY	3.5
1	G	64	LYS	3.5
1	G	61	GLU	3.5
1	G	122	ALA	3.5
1	G	46	PRO	3.5
1	E	155	GLU	3.4
1	G	158	PHE	3.4
1	E	173	GLY	3.4
1	G	174	GLN	3.3
1	F	158	PHE	3.3
1	G	159	LYS	3.2
1	F	157	ILE	3.2
1	F	155	GLU	3.2
1	B	172	ASN	3.2
1	G	202	GLY	3.2
1	E	108	SER	3.1
1	G	125	VAL	3.1
1	D	159	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	125	VAL	3.1
1	F	156	VAL	3.1
1	G	155	GLU	3.1
1	E	172	ASN	3.0
1	B	171	ALA	3.0
1	D	171	ALA	3.0
1	E	171	ALA	3.0
1	G	54	ASP	2.8
1	G	3	ALA	2.8
1	G	65	ASP	2.8
1	F	173	GLY	2.8
1	H	202	GLY	2.7
1	B	155	GLU	2.6
1	B	202	GLY	2.6
1	D	123	GLN	2.6
1	D	2	THR	2.6
1	D	160	SER	2.6
1	G	157	ILE	2.5
1	E	107	SER	2.5
1	H	155	GLU	2.5
1	A	174	GLN	2.5
1	H	172	ASN	2.5
1	F	200	GLU	2.5
1	E	123	GLN	2.5
1	F	126	ASN	2.5
1	F	161	GLY	2.5
1	B	175	PRO	2.5
1	G	51	ASP	2.5
1	F	179	ASN	2.4
1	B	162	GLY	2.4
1	D	174	GLN	2.4
1	E	52	GLY	2.4
1	E	65	ASP	2.4
1	H	2	THR	2.4
1	D	155	GLU	2.4
1	F	172	ASN	2.3
1	G	53	GLN	2.3
1	H	171	ALA	2.3
1	F	123	GLN	2.3
1	F	171	ALA	2.3
1	G	45	ALA	2.3
1	G	57	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	110	LYS	2.2
1	B	154	ASP	2.2
1	E	49	VAL	2.2
1	D	200	GLU	2.1
1	C	202	GLY	2.1
1	E	63	MET	2.1
1	E	64	LYS	2.1
1	D	124	ASN	2.1
1	G	126	ASN	2.1
1	B	158	PHE	2.0
1	E	156	VAL	2.0
1	F	160	SER	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	H	1309	5/5	0.94	0.12	0.11	69,69,70,70	0
2	SO4	F	1307	5/5	0.99	0.06	-0.73	16,18,19,20	0
2	SO4	B	1303	5/5	0.99	0.07	-0.80	14,15,15,17	0
2	SO4	G	1308	5/5	0.98	0.07	-0.80	29,30,32,32	0
2	SO4	E	1306	5/5	0.97	0.07	-0.99	29,31,32,33	0
2	SO4	H	1301	5/5	0.99	0.05	-1.12	15,17,18,18	0
2	SO4	D	1305	5/5	1.00	0.04	-1.28	14,16,18,18	0
2	SO4	A	1302	5/5	1.00	0.05	-1.56	12,12,15,16	0
2	SO4	C	1304	5/5	0.99	0.07	-2.05	18,20,21,24	0
2	SO4	D	1310	5/5	0.94	0.17	-	72,72,73,73	0

6.5 Other polymers (i)

There are no such residues in this entry.