Full wwPDB X-ray Structure Validation Report (i)

Dec 13, 2023 – 05:40 pm GMT

PDB ID	:	4BHD
Title	:	Methanococcus jannaschii serine hydroxymethyl-transferase, apo form
Authors	:	Saccoccia, F.; Angelucci, F.; Ilari, A.
Deposited on	:	2013-04-02
Resolution	:	2.83 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:

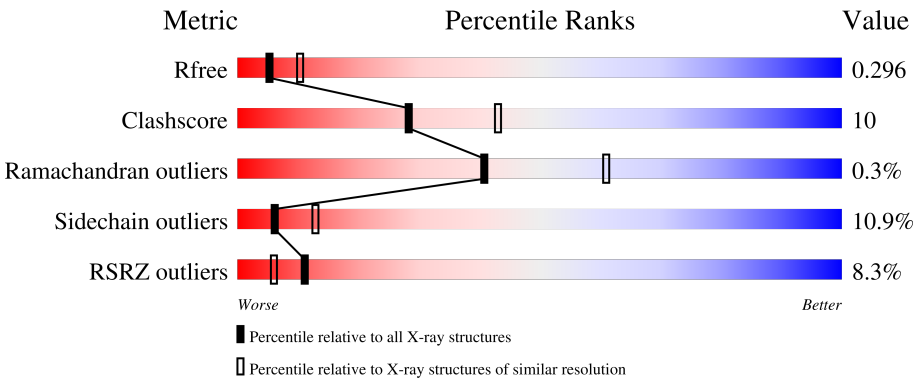
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.83 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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% 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	428	4% 75% 20% • •
1	B	428	11% 69% 21% • 8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6412 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.

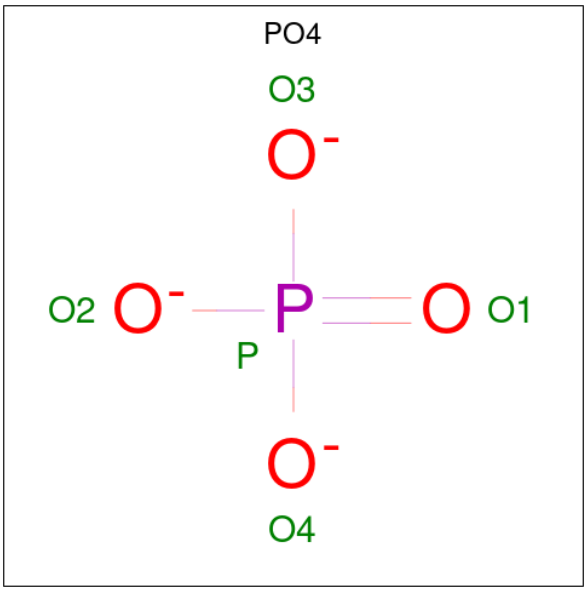
- Molecule 1 is a protein called SERINE HYDROXYMETHYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	415	3269	2085	546	622	16	0	0	0
1	B	395	3122	1991	516	598	17	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	MET	-	expression tag	UNP Q58992
B	2	MET	-	expression tag	UNP Q58992

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	B	1	5	4	1	0	0

- Molecule 3 is water.

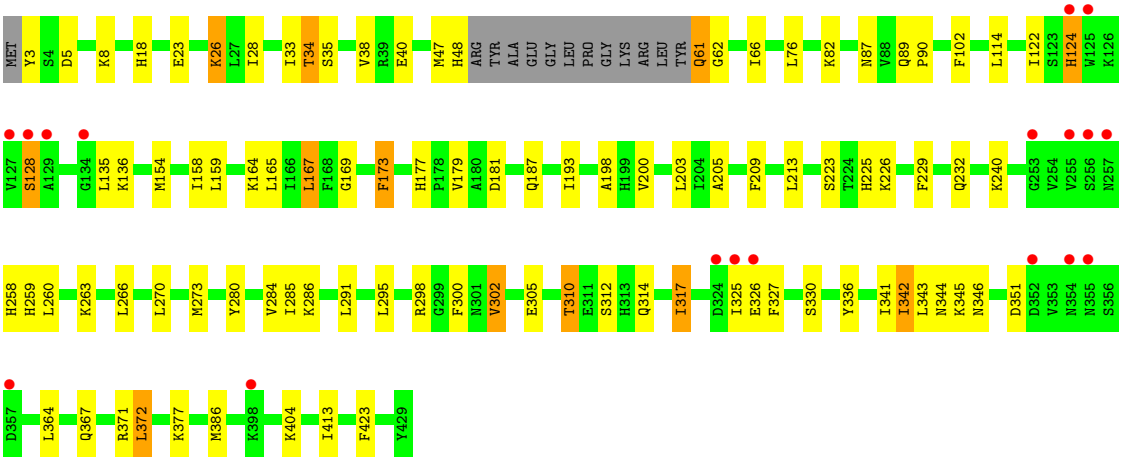
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	13	13	13	0	0
			Total	O		
3	B	3	3	3	0	0

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 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.

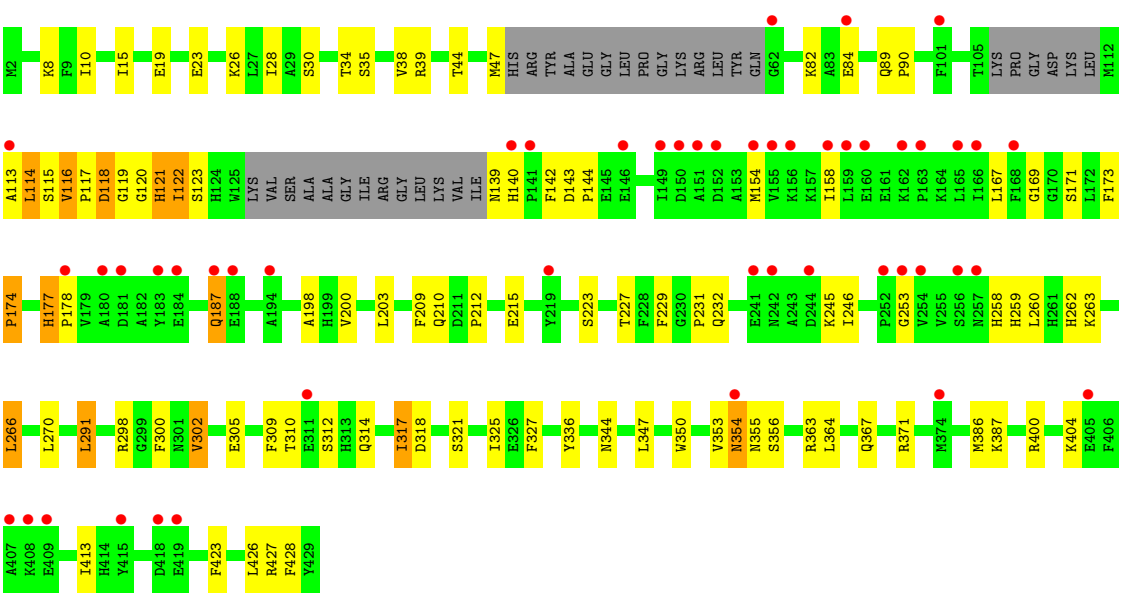
• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

Chain A: 4% 75% 20%



• Molecule 1: SERINE HYDROXYMETHYLTRANSFERASE

Chain B: 11% 69% 21% 8%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.59Å 110.16Å 110.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.83 49.45 – 2.82	Depositor EDS
% Data completeness (in resolution range)	97.9 (50.00-2.83) 97.9 (49.45-2.82)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.97 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.242 , 0.298 0.243 , 0.296	Depositor DCC
R_{free} test set	1293 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	70.5	Xtriage
Anisotropy	0.480	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 73.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -h,l,k	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6412	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.35	0/3341	0.56	3/4505 (0.1%)
1	B	0.36	0/3190	0.55	3/4300 (0.1%)
All	All	0.36	0/6531	0.56	6/8805 (0.1%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	128	SER	N-CA-C	10.54	139.45	111.00
1	B	121	HIS	N-CA-C	8.01	132.62	111.00
1	B	121	HIS	CB-CA-C	-6.17	98.06	110.40
1	B	253	GLY	N-CA-C	-5.53	99.27	113.10
1	A	226	LYS	N-CA-C	5.41	125.59	111.00
1	A	128	SER	CB-CA-C	-5.23	100.16	110.10

There are no chirality outliers.

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	3269	0	3214	50	0
1	B	3122	0	3044	77	0
2	B	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	13	0	0	0	0
3	B	3	0	0	0	0
All	All	6412	0	6258	124	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 10.

All (124) 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:A:61:GLN:C	1:A:61:GLN:HE21	1.47	1.16
1:B:116:VAL:HG12	1:B:117:PRO:N	1.70	1.07
1:B:115:SER:OG	1:B:117:PRO:HD2	1.57	1.03
1:B:118:ASP:OD2	1:B:142:PHE:CD2	2.19	0.95
1:B:122:ILE:HG12	1:B:122:ILE:O	1.62	0.95
1:B:116:VAL:CG1	1:B:117:PRO:N	2.30	0.94
1:B:116:VAL:N	1:B:117:PRO:CD	2.30	0.94
1:B:115:SER:C	1:B:117:PRO:HD2	1.86	0.94
1:B:115:SER:CB	1:B:117:PRO:HD2	1.99	0.93
1:A:169:GLY:H	1:A:177:HIS:HD2	1.17	0.90
1:B:118:ASP:OD2	1:B:142:PHE:CG	2.28	0.86
1:A:61:GLN:C	1:A:61:GLN:NE2	2.30	0.85
1:A:169:GLY:H	1:A:177:HIS:CD2	1.95	0.84
1:A:66:ILE:HG23	1:A:260:LEU:HG	1.63	0.80
1:B:115:SER:OG	1:B:118:ASP:HB2	1.81	0.80
1:A:223:SER:OG	1:A:225:HIS:CD2	2.35	0.80
1:B:115:SER:OG	1:B:117:PRO:CD	2.30	0.78
1:B:116:VAL:N	1:B:117:PRO:HD2	1.98	0.78
1:B:203:LEU:HG	1:B:227:THR:HG21	1.68	0.75
1:A:23:GLU:HB2	1:A:404:LYS:HB2	1.70	0.74
1:B:231:PRO:HB2	1:B:262:HIS:HD2	1.54	0.72
1:A:47:MET:HE2	1:B:34:THR:HB	1.74	0.70
1:B:115:SER:OG	1:B:117:PRO:HG2	1.96	0.65
1:B:116:VAL:N	1:B:117:PRO:HD3	2.12	0.65
1:A:61:GLN:NE2	1:A:61:GLN:O	2.30	0.65
1:A:223:SER:OG	1:A:225:HIS:NE2	2.31	0.63
1:B:353:VAL:O	1:B:355:ASN:N	2.31	0.63
1:B:116:VAL:O	1:B:120:GLY:N	2.30	0.63
1:A:200:VAL:HG11	1:A:209:PHE:CD2	2.34	0.62
1:A:310:THR:HG22	1:A:312:SER:H	1.65	0.62
1:B:291:LEU:HD11	1:B:364:LEU:HD23	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:ILE:O	1:B:19:GLU:HG2	2.00	0.62
1:A:200:VAL:HG12	1:A:200:VAL:O	1.99	0.61
1:B:115:SER:HG	1:B:117:PRO:HG2	1.65	0.61
1:B:116:VAL:HG12	1:B:117:PRO:CD	2.29	0.61
1:A:310:THR:HG21	1:A:314:GLN:O	2.00	0.61
1:B:122:ILE:O	1:B:122:ILE:CG1	2.44	0.61
1:B:89:GLN:N	1:B:90:PRO:HD2	2.16	0.60
1:B:115:SER:CB	1:B:117:PRO:CD	2.76	0.60
1:B:115:SER:C	1:B:117:PRO:CD	2.63	0.60
1:B:347:LEU:HD21	1:B:356:SER:OG	2.01	0.60
1:A:291:LEU:HD11	1:A:364:LEU:HD23	1.84	0.59
1:B:118:ASP:OD2	1:B:142:PHE:CB	2.50	0.59
1:A:35:SER:HA	1:A:413:ILE:HD13	1.86	0.58
1:B:115:SER:OG	1:B:117:PRO:CG	2.51	0.58
1:A:258:HIS:HB3	1:A:260:LEU:HD23	1.84	0.57
1:B:115:SER:CA	1:B:117:PRO:HD2	2.36	0.56
1:A:325:ILE:HG22	1:A:327:PHE:H	1.69	0.56
1:A:179:VAL:HG13	1:A:193:ILE:HD11	1.88	0.56
1:B:325:ILE:HG22	1:B:327:PHE:H	1.69	0.56
1:B:34:THR:HG23	1:B:38:VAL:HB	1.87	0.55
1:B:34:THR:HG22	1:B:39:ARG:HG3	1.89	0.55
1:A:61:GLN:HE21	1:A:62:GLY:N	2.04	0.54
1:B:35:SER:HA	1:B:413:ILE:HD13	1.89	0.54
1:A:200:VAL:O	1:A:200:VAL:CG1	2.56	0.53
1:B:266:LEU:HD22	1:B:270:LEU:HD23	1.91	0.52
1:B:118:ASP:OD2	1:B:142:PHE:HB3	2.09	0.52
1:B:200:VAL:HG11	1:B:209:PHE:CD2	2.45	0.52
1:A:205:ALA:HB3	1:A:273:MET:HE2	1.92	0.51
1:B:298:ARG:HG2	1:B:387:LYS:HD2	1.91	0.51
1:A:124:HIS:CD2	1:A:167:LEU:HD13	2.46	0.51
1:A:26:LYS:HZ2	1:A:423:PHE:HZ	1.56	0.50
1:B:140:HIS:HE1	1:B:167:LEU:O	1.94	0.50
1:A:122:ILE:HG22	1:A:128:SER:HB2	1.94	0.50
1:B:344:ASN:HD21	1:B:363:ARG:HH21	1.60	0.50
1:A:205:ALA:CB	1:A:273:MET:HE2	2.42	0.50
1:A:34:THR:HG23	1:A:38:VAL:HB	1.94	0.49
1:A:26:LYS:HA	1:A:342:ILE:HG23	1.94	0.49
1:A:285:ILE:HG13	1:A:286:LYS:N	2.27	0.49
1:B:259:HIS:NE2	1:B:263:LYS:HG3	2.28	0.49
1:B:300:PHE:HB3	1:B:317:ILE:HD13	1.94	0.49
1:B:117:PRO:CD	1:B:118:ASP:H	2.25	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:PRO:HB2	1:B:262:HIS:CD2	2.42	0.48
1:A:343:LEU:HD22	1:A:364:LEU:HD11	1.96	0.48
1:A:89:GLN:N	1:A:90:PRO:CD	2.77	0.48
1:A:154:MET:O	1:A:158:ILE:HG12	2.14	0.48
1:B:26:LYS:HE3	1:B:423:PHE:HZ	1.79	0.48
1:A:302:VAL:HA	1:A:317:ILE:HA	1.95	0.47
1:A:48:HIS:C	1:A:258:HIS:HB2	2.33	0.47
1:B:302:VAL:HA	1:B:317:ILE:HA	1.96	0.47
1:A:40:GLU:HB2	1:B:428:PHE:HB2	1.97	0.47
1:A:200:VAL:HG13	1:A:203:LEU:HD12	1.97	0.47
1:B:173:PHE:H	1:B:314:GLN:HE22	1.63	0.47
1:A:173:PHE:H	1:A:314:GLN:HE22	1.62	0.46
1:A:61:GLN:HE21	1:A:61:GLN:CA	2.23	0.46
1:B:210:GLN:HG3	1:B:212:PRO:HD3	1.97	0.46
1:B:266:LEU:HD22	1:B:270:LEU:CD2	2.46	0.46
1:B:200:VAL:HG13	1:B:203:LEU:HD12	1.97	0.46
1:B:120:GLY:O	1:B:121:HIS:HB2	2.16	0.45
1:A:47:MET:SD	1:A:47:MET:N	2.89	0.45
1:A:33:ILE:HG21	1:A:372:LEU:HD13	1.99	0.45
1:B:119:GLY:O	1:B:171:SER:N	2.50	0.45
1:B:23:GLU:HB2	1:B:404:LYS:HB2	1.99	0.44
1:B:89:GLN:N	1:B:90:PRO:CD	2.81	0.44
1:B:198:ALA:HA	1:B:223:SER:H	1.82	0.44
1:A:280:TYR:O	1:A:284:VAL:HG23	2.17	0.44
1:A:173:PHE:H	1:A:314:GLN:NE2	2.15	0.44
1:B:309:PHE:O	1:B:310:THR:HG23	2.18	0.44
1:A:300:PHE:HB3	1:A:317:ILE:HD13	1.99	0.43
1:B:113:ALA:O	1:B:139:ASN:HA	2.18	0.43
1:B:154:MET:O	1:B:158:ILE:HG12	2.18	0.43
1:B:115:SER:HG	1:B:118:ASP:HB2	1.80	0.43
1:A:198:ALA:HA	1:A:223:SER:H	1.83	0.43
1:B:174:PRO:HB3	1:B:310:THR:HG22	2.00	0.43
1:B:318:ASP:OD2	1:B:321:SER:OG	2.37	0.43
1:B:113:ALA:HB2	1:B:167:LEU:HB3	2.00	0.42
1:B:28:ILE:HG22	1:B:30:SER:H	1.84	0.42
1:A:18:HIS:HE1	1:B:44:THR:HB	1.84	0.42
1:B:114:LEU:HD13	1:B:114:LEU:HA	1.65	0.42
1:B:310:THR:HG21	1:B:314:GLN:O	2.18	0.42
1:A:209:PHE:CE1	1:A:312:SER:HB3	2.55	0.42
1:A:295:LEU:HD11	1:A:386:MET:HE3	2.01	0.42
1:B:336:TYR:HE1	1:B:386:MET:HA	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:ALA:HA	1:B:140:HIS:CE1	2.55	0.42
1:A:66:ILE:CG2	1:A:260:LEU:HG	2.41	0.41
1:B:177:HIS:HA	1:B:178:PRO:HD3	1.94	0.41
1:B:259:HIS:HE2	1:B:263:LYS:HG3	1.84	0.41
1:B:209:PHE:CE1	1:B:312:SER:HB3	2.56	0.41
1:B:212:PRO:HA	1:B:215:GLU:HB2	2.02	0.41
1:B:143:ASP:HA	1:B:144:PRO:HD3	1.95	0.41
1:B:169:GLY:HA2	1:B:173:PHE:HE2	1.86	0.41
1:B:187:GLN:H	1:B:187:GLN:NE2	2.19	0.41
1:A:330:SER:HA	1:A:345:LYS:HD3	2.04	0.40
1:A:336:TYR:HB3	1:A:341:ILE:O	2.21	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	411/428 (96%)	384 (93%)	27 (7%)	0	100 100
1	B	387/428 (90%)	347 (90%)	38 (10%)	2 (0%)	29 51
All	All	798/856 (93%)	731 (92%)	65 (8%)	2 (0%)	41 61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	354	ASN
1	B	174	PRO

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	348/358 (97%)	304 (87%)	44 (13%)	4 8
1	B	333/358 (93%)	303 (91%)	30 (9%)	9 19
All	All	681/716 (95%)	607 (89%)	74 (11%)	6 13

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	TYR
1	A	5	ASP
1	A	8	LYS
1	A	26	LYS
1	A	28	ILE
1	A	34	THR
1	A	61	GLN
1	A	76	LEU
1	A	82	LYS
1	A	87	ASN
1	A	102	PHE
1	A	114	LEU
1	A	124	HIS
1	A	135	LEU
1	A	136	LYS
1	A	159	LEU
1	A	164	LYS
1	A	165	LEU
1	A	167	LEU
1	A	173	PHE
1	A	181	ASP
1	A	187	GLN
1	A	213	LEU
1	A	229	PHE
1	A	232	GLN
1	A	240	LYS
1	A	259	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	263	LYS
1	A	266	LEU
1	A	270	LEU
1	A	298	ARG
1	A	302	VAL
1	A	305	GLU
1	A	310	THR
1	A	317	ILE
1	A	326	GLU
1	A	342	ILE
1	A	344	ASN
1	A	346	ASN
1	A	351	ASP
1	A	367	GLN
1	A	371	ARG
1	A	372	LEU
1	A	377	LYS
1	B	8	LYS
1	B	10	ILE
1	B	47	MET
1	B	82	LYS
1	B	84	GLU
1	B	114	LEU
1	B	116	VAL
1	B	118	ASP
1	B	122	ILE
1	B	123	SER
1	B	177	HIS
1	B	187	GLN
1	B	229	PHE
1	B	232	GLN
1	B	245	LYS
1	B	246	ILE
1	B	258	HIS
1	B	260	LEU
1	B	266	LEU
1	B	291	LEU
1	B	302	VAL
1	B	305	GLU
1	B	317	ILE
1	B	350	TRP
1	B	354	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	367	GLN
1	B	371	ARG
1	B	400	ARG
1	B	426	LEU
1	B	427	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	61	GLN
1	A	87	ASN
1	A	97	ASN
1	A	140	HIS
1	A	177	HIS
1	A	242	ASN
1	A	259	HIS
1	A	283	GLN
1	A	293	GLN
1	A	306	HIS
1	A	314	GLN
1	A	340	ASN
1	A	346	ASN
1	B	97	ASN
1	B	121	HIS
1	B	140	HIS
1	B	187	GLN
1	B	232	GLN
1	B	262	HIS
1	B	283	GLN
1	B	301	ASN
1	B	314	GLN
1	B	340	ASN
1	B	344	ASN
1	B	367	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	PO4	B	1430	-	4,4,4	0.87	0	6,6,6	0.55	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	415/428 (96%)	0.32	18 (4%)	35	27	44, 66, 104, 130	0
1	B	395/428 (92%)	0.82	49 (12%)	4	2	56, 94, 166, 204	0
All	All	810/856 (94%)	0.57	67 (8%)	11	6	44, 79, 147, 204	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	352	ASP	7.7
1	B	183	TYR	7.2
1	B	162	LYS	5.9
1	B	155	VAL	5.8
1	B	156	LYS	5.7
1	B	113	ALA	5.6
1	B	159	LEU	5.3
1	B	180	ALA	5.3
1	B	163	PRO	5.2
1	B	149	ILE	5.1
1	B	241	GLU	5.1
1	B	151	ALA	5.0
1	B	244	ASP	4.9
1	A	255	VAL	4.7
1	B	165	LEU	4.5
1	B	194	ALA	4.5
1	A	253	GLY	4.5
1	A	355	ASN	4.3
1	B	184	GLU	4.2
1	B	166	ILE	4.2
1	B	158	ILE	4.1
1	A	325	ILE	4.1
1	B	419	GLU	4.0
1	B	146	GLU	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	256	SER	4.0
1	A	124	HIS	4.0
1	A	357	ASP	3.9
1	B	242	ASN	3.9
1	B	219	TYR	3.8
1	B	181	ASP	3.8
1	B	152	ASP	3.7
1	B	254	VAL	3.7
1	B	418	ASP	3.6
1	B	257	ASN	3.4
1	A	134	GLY	3.3
1	A	256	SER	3.1
1	B	252	PRO	3.1
1	B	101	PHE	3.1
1	B	160	GLU	3.1
1	B	253	GLY	3.1
1	B	354	ASN	3.0
1	A	128	SER	3.0
1	A	354	ASN	3.0
1	B	405	GLU	2.9
1	B	408	LYS	2.9
1	B	154	MET	2.9
1	B	187	GLN	2.8
1	A	125	TRP	2.7
1	B	407	ALA	2.7
1	B	141	PRO	2.6
1	B	168	PHE	2.4
1	A	129	ALA	2.4
1	B	62	GLY	2.4
1	A	398	LYS	2.4
1	B	140	HIS	2.4
1	B	374	MET	2.4
1	B	415	TYR	2.3
1	B	150	ASP	2.3
1	A	257	ASN	2.2
1	B	188	GLU	2.2
1	B	409	GLU	2.2
1	B	311	GLU	2.2
1	A	127	VAL	2.1
1	B	178	PRO	2.1
1	A	324	ASP	2.0
1	A	326	GLU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	84	GLU	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PO4	B	1430	5/5	0.92	0.27	54,54,55,55	5

6.5 Other polymers (i)

There are no such residues in this entry.