



# Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 11:48 am BST

PDB ID : 5XNF  
Title : Crystal structure of the branched-chain polyamine synthase (BpsA) from *Thermococcus kodakarensis*  
Authors : Mizohata, E.; Tse, K.M.; Fujita, J.; Inoue, T.  
Deposited on : 2017-05-22  
Resolution : 1.90 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](mailto: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

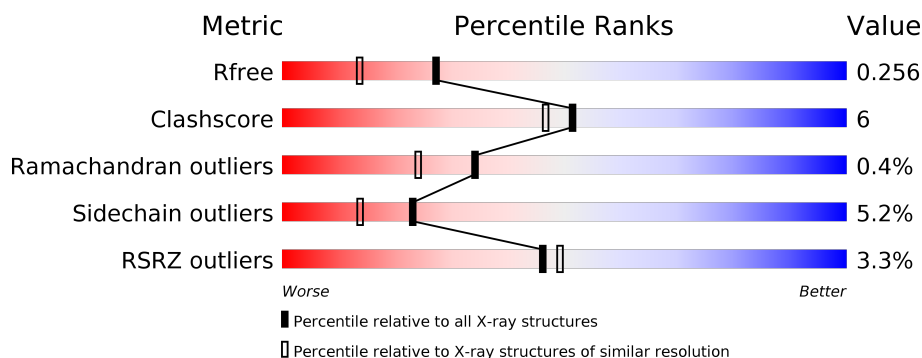
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	371	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>6%</div> </div> </div>
1	B	371	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>6%</div> </div> </div>

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
4	GOL	A	403[A]	-	X	-	-
4	GOL	A	403[B]	-	X	-	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5848 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 N(4)-bis(aminopropyl)spermidine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2835	1812	474	542	7			
1	B	350	Total	C	N	O	S	0	1	0
			2841	1816	474	544	7			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q5JIZ3
A	-18	GLY	-	expression tag	UNP Q5JIZ3
A	-17	SER	-	expression tag	UNP Q5JIZ3
A	-16	SER	-	expression tag	UNP Q5JIZ3
A	-15	HIS	-	expression tag	UNP Q5JIZ3
A	-14	HIS	-	expression tag	UNP Q5JIZ3
A	-13	HIS	-	expression tag	UNP Q5JIZ3
A	-12	HIS	-	expression tag	UNP Q5JIZ3
A	-11	HIS	-	expression tag	UNP Q5JIZ3
A	-10	HIS	-	expression tag	UNP Q5JIZ3
A	-9	SER	-	expression tag	UNP Q5JIZ3
A	-8	SER	-	expression tag	UNP Q5JIZ3
A	-7	GLY	-	expression tag	UNP Q5JIZ3
A	-6	LEU	-	expression tag	UNP Q5JIZ3
A	-5	VAL	-	expression tag	UNP Q5JIZ3
A	-4	PRO	-	expression tag	UNP Q5JIZ3
A	-3	ARG	-	expression tag	UNP Q5JIZ3
A	-2	GLY	-	expression tag	UNP Q5JIZ3
A	-1	SER	-	expression tag	UNP Q5JIZ3
A	0	HIS	-	expression tag	UNP Q5JIZ3
B	-19	MET	-	expression tag	UNP Q5JIZ3
B	-18	GLY	-	expression tag	UNP Q5JIZ3
B	-17	SER	-	expression tag	UNP Q5JIZ3
B	-16	SER	-	expression tag	UNP Q5JIZ3
B	-15	HIS	-	expression tag	UNP Q5JIZ3

*Continued on next page...*

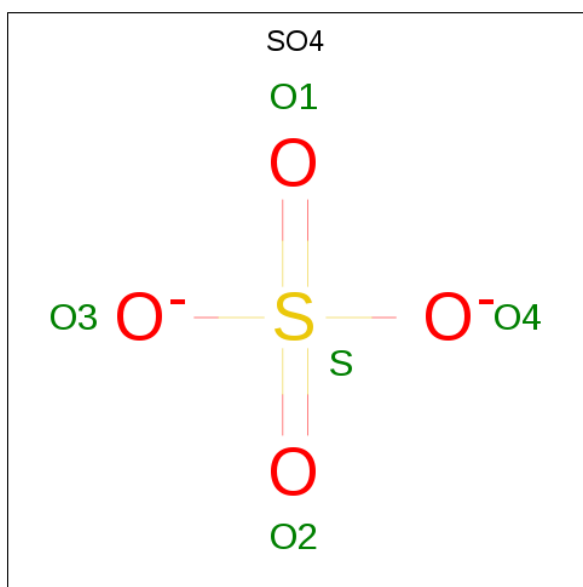
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	expression tag	UNP Q5JIZ3
B	-13	HIS	-	expression tag	UNP Q5JIZ3
B	-12	HIS	-	expression tag	UNP Q5JIZ3
B	-11	HIS	-	expression tag	UNP Q5JIZ3
B	-10	HIS	-	expression tag	UNP Q5JIZ3
B	-9	SER	-	expression tag	UNP Q5JIZ3
B	-8	SER	-	expression tag	UNP Q5JIZ3
B	-7	GLY	-	expression tag	UNP Q5JIZ3
B	-6	LEU	-	expression tag	UNP Q5JIZ3
B	-5	VAL	-	expression tag	UNP Q5JIZ3
B	-4	PRO	-	expression tag	UNP Q5JIZ3
B	-3	ARG	-	expression tag	UNP Q5JIZ3
B	-2	GLY	-	expression tag	UNP Q5JIZ3
B	-1	SER	-	expression tag	UNP Q5JIZ3
B	0	HIS	-	expression tag	UNP Q5JIZ3

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 12 6 6	0	1

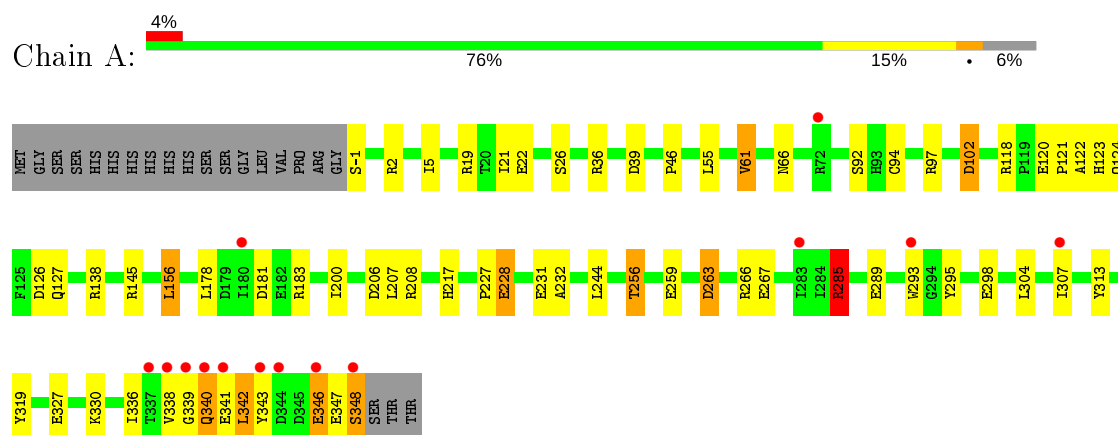
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	74	Total O 74 74	0	0
5	B	75	Total O 75 75	0	0

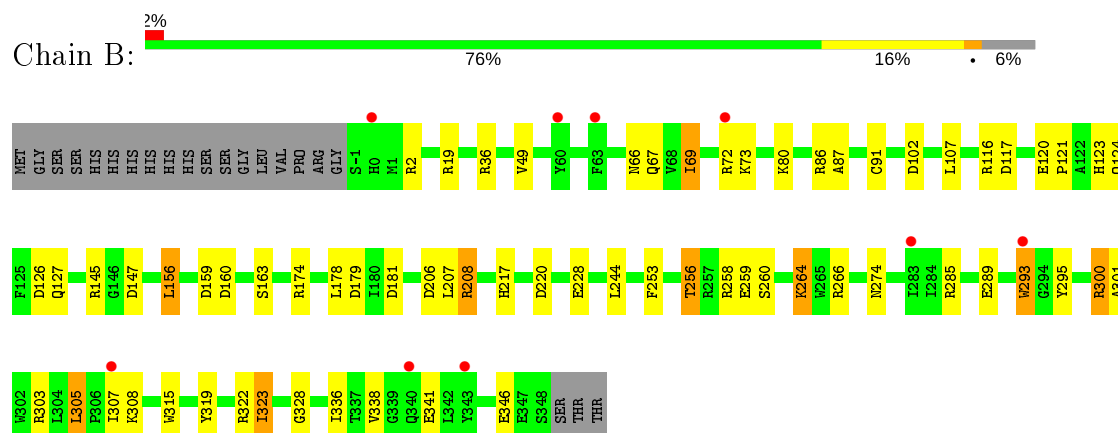
### 3 Residue-property plots [i](#)

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: N(4)-bis(aminopropyl)spermidine synthase



- Molecule 1: N(4)-bis(aminopropyl)spermidine synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.66Å 105.17Å 80.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 45.36 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-1.90) 99.8 (45.36-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, $R_{free}$	0.203 , 0.244 0.212 , 0.256	Depositor DCC
$R_{free}$ test set	2991 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.6	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 41.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5848	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	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 49.22 % 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 7.6913e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: GOL, FE, 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	1.22	6/2895 (0.2%)	1.19	21/3926 (0.5%)
1	B	1.23	6/2904 (0.2%)	1.18	24/3938 (0.6%)
All	All	1.23	12/5799 (0.2%)	1.18	45/7864 (0.6%)

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	228	GLU	CD-OE1	-6.93	1.18	1.25
1	A	289	GLU	CD-OE1	-6.23	1.18	1.25
1	B	315	TRP	CB-CG	-6.08	1.39	1.50
1	B	163	SER	CB-OG	-5.91	1.34	1.42
1	A	313	TYR	CB-CG	5.62	1.60	1.51
1	A	92	SER	CB-OG	-5.62	1.34	1.42
1	B	289	GLU	CD-OE1	-5.62	1.19	1.25
1	A	231	GLU	CG-CD	5.50	1.60	1.51
1	B	87	ALA	C-O	5.23	1.33	1.23
1	B	274	ASN	N-CA	5.21	1.56	1.46
1	A	22	GLU	CD-OE2	5.20	1.31	1.25
1	B	328	GLY	C-O	-5.09	1.15	1.23

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	285	ARG	NE-CZ-NH2	-14.13	113.23	120.30
1	B	303	ARG	NE-CZ-NH2	-7.77	116.42	120.30
1	B	145	ARG	NE-CZ-NH1	7.69	124.14	120.30
1	A	118	ARG	NE-CZ-NH2	-7.65	116.47	120.30
1	A	118	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	B	303	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	A	285	ARG	NE-CZ-NH1	7.42	124.01	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	206	ASP	CB-CG-OD1	7.32	124.88	118.30
1	B	174	ARG	NE-CZ-NH2	7.31	123.95	120.30
1	B	145	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	A	102	ASP	CB-CG-OD1	6.90	124.51	118.30
1	A	145	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	179	ASP	CB-CG-OD2	6.82	124.43	118.30
1	A	266	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	B	147	ASP	CB-CG-OD1	-6.58	112.38	118.30
1	B	181	ASP	CB-CG-OD1	6.49	124.14	118.30
1	B	208	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	97	ARG	NE-CZ-NH2	6.33	123.46	120.30
1	A	92	SER	CB-CA-C	-6.31	98.11	110.10
1	A	181	ASP	CB-CG-OD1	6.23	123.91	118.30
1	A	19	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	B	179	ASP	CB-CG-OD1	-6.09	112.82	118.30
1	B	86	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	B	266	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	B	160	ASP	CB-CG-OD1	6.00	123.70	118.30
1	B	19	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	A	138	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	B	220	ASP	CB-CG-OD1	-5.88	113.01	118.30
1	A	39	ASP	CB-CG-OD1	5.81	123.53	118.30
1	B	300	ARG	NE-CZ-NH1	-5.79	117.41	120.30
1	A	183	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	A	263	ASP	CB-CG-OD1	5.65	123.39	118.30
1	A	206	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	19	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	A	126	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	B	126	ASP	CB-CG-OD2	-5.53	113.32	118.30
1	B	145	ARG	CD-NE-CZ	5.36	131.10	123.60
1	B	126	ASP	CB-CG-OD1	5.29	123.06	118.30
1	B	322	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	A	36	ARG	NE-CZ-NH1	5.21	122.90	120.30
1	A	266	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	B	147	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	36	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	B	266	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	145	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	2835	0	2806	36	0
1	B	2841	0	2812	28	0
2	A	1	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
4	A	12	0	16	1	0
5	A	74	0	0	1	0
5	B	75	0	0	0	0
All	All	5848	0	5634	63	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 6.

All (63) 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:228:GLU:OE2	1:A:256:THR:HG22	1.64	0.97
1:A:208:ARG:NH1	1:A:338:VAL:O	2.07	0.88
1:B:228:GLU:OE1	1:B:256:THR:HG22	1.79	0.82
1:A:342:LEU:HD22	1:A:343:TYR:CE2	2.22	0.74
1:B:123:HIS:ND1	1:B:295:TYR:CZ	2.54	0.72
1:A:124:GLN:HE22	1:A:298:GLU:HG3	1.56	0.69
1:A:55:LEU:HB3	1:A:61:VAL:HG13	1.77	0.65
1:A:156:LEU:HD13	1:A:178:LEU:HD23	1.79	0.64
1:B:285:ARG:HA	1:B:319:TYR:CD2	2.31	0.64
1:A:66:ASN:HA	1:A:307:ILE:HD12	1.79	0.63
1:A:121:PRO:HG3	1:A:293:TRP:CZ3	2.34	0.63
1:B:124:GLN:HB2	1:B:127:GLN:HG3	1.80	0.62
1:B:256:THR:HG23	1:B:259:GLU:H	1.65	0.62
1:A:256:THR:HG23	1:A:259:GLU:H	1.65	0.62
1:B:121:PRO:HG3	1:B:293:TRP:CE3	2.36	0.60
1:A:285:ARG:HA	1:A:319:TYR:CD2	2.37	0.59
1:B:66:ASN:HA	1:B:307:ILE:HG22	1.85	0.59
1:B:338:VAL:CG1	1:B:341:GLU:HB2	2.33	0.58
1:A:267:GLU:HG2	5:A:558:HOH:O	2.05	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:ASP:OD1	1:B:117:ASP:N	2.40	0.54
1:A:120:GLU:HG2	1:A:121:PRO:HD2	1.90	0.54
1:B:253:PHE:HE1	1:B:323:ILE:HD13	1.73	0.53
1:A:123:HIS:ND1	1:A:295:TYR:CZ	2.77	0.53
1:B:67:GLN:HB2	1:B:69:ILE:HD12	1.92	0.52
1:A:342:LEU:HD22	1:A:343:TYR:CZ	2.44	0.52
1:B:121:PRO:HG3	1:B:293:TRP:CZ3	2.44	0.51
1:A:120:GLU:HG2	1:A:121:PRO:CD	2.41	0.50
1:A:121:PRO:HG3	1:A:293:TRP:CE3	2.46	0.50
1:B:256:THR:CG2	1:B:259:GLU:H	2.25	0.50
1:B:260:SER:HA	1:B:264:LYS:HE2	1.92	0.50
1:A:120:GLU:CG	1:A:121:PRO:HD2	2.43	0.49
1:B:120:GLU:OE2	1:B:123:HIS:CE1	2.67	0.48
1:B:124:GLN:HB2	1:B:127:GLN:CG	2.42	0.48
1:A:340:GLN:C	1:A:342:LEU:H	2.16	0.48
1:B:123:HIS:ND1	1:B:295:TYR:OH	2.46	0.48
1:A:256:THR:CG2	1:A:259:GLU:H	2.26	0.48
1:B:301:ALA:O	1:B:305:LEU:HB2	2.15	0.47
1:B:49:VAL:HG11	1:B:300:ARG:HD3	1.95	0.47
1:A:-1:SER:OG	1:A:2:ARG:NH2	2.47	0.47
1:A:217:HIS:HA	1:A:244:LEU:O	2.14	0.47
1:A:208:ARG:HA	1:A:336:ILE:HD12	1.97	0.47
1:B:217:HIS:HA	1:B:244:LEU:O	2.15	0.47
1:B:338:VAL:HG11	1:B:341:GLU:HB2	1.96	0.46
1:A:26:SER:HB2	4:A:403[B]:GOL:H12	1.98	0.45
1:A:46:PRO:HG3	1:A:348:SER:HB2	1.99	0.45
1:A:124:GLN:HB2	1:A:127:GLN:HB2	1.99	0.45
1:A:285:ARG:HA	1:A:319:TYR:CG	2.52	0.45
1:B:208:ARG:HA	1:B:336:ILE:HB	2.00	0.44
1:A:227:PRO:HD2	1:A:232:ALA:HB1	1.99	0.43
1:A:342:LEU:HD22	1:A:343:TYR:CD2	2.53	0.42
1:A:94:CYS:HB3	1:B:91:CYS:SG	2.60	0.42
1:A:285:ARG:HG3	1:A:319:TYR:OH	2.20	0.42
1:A:346:GLU:C	1:A:348:SER:H	2.23	0.42
1:A:122:ALA:HB3	1:A:127:GLN:HB3	2.01	0.42
1:A:338:VAL:HG12	1:A:339:GLY:N	2.34	0.42
1:B:120:GLU:OE2	1:B:123:HIS:NE2	2.53	0.41
1:B:285:ARG:HA	1:B:319:TYR:CG	2.55	0.41
1:A:342:LEU:HD23	1:A:343:TYR:CG	2.56	0.41
1:B:123:HIS:CE1	1:B:295:TYR:OH	2.74	0.41
1:A:342:LEU:CD2	1:A:343:TYR:CD2	3.04	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:256:THR:HG23	1:B:258:ARG:N	2.36	0.41
1:B:156:LEU:HD13	1:B:178:LEU:HD23	2.02	0.40
1:A:5:ILE:HD13	1:A:21:ILE:HG13	2.02	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	348/371 (94%)	335 (96%)	10 (3%)	3 (1%)	17	7
1	B	349/371 (94%)	335 (96%)	14 (4%)	0	100	100
All	All	697/742 (94%)	670 (96%)	24 (3%)	3 (0%)	34	24

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	341	GLU
1	A	347	GLU
1	A	346	GLU

### 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.

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	308/326 (94%)	294 (96%)	14 (4%)	27	18
1	B	309/326 (95%)	291 (94%)	18 (6%)	20	10
All	All	617/652 (95%)	585 (95%)	32 (5%)	23	14

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	VAL
1	A	102	ASP
1	A	156	LEU
1	A	200	ILE
1	A	207	LEU
1	A	256	THR
1	A	263	ASP
1	A	285	ARG
1	A	304	LEU
1	A	327	GLU
1	A	330	LYS
1	A	340	GLN
1	A	342	LEU
1	A	348	SER
1	B	2	ARG
1	B	69	ILE
1	B	72	ARG
1	B	73	LYS
1	B	80	LYS
1	B	102	ASP
1	B	107	LEU
1	B	116	ARG
1	B	156	LEU
1	B	159	ASP
1	B	207	LEU
1	B	256	THR
1	B	264	LYS
1	B	293	TRP
1	B	305	LEU
1	B	308	LYS
1	B	323	ILE
1	B	346	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	124	GLN
1	A	127	GLN
1	A	150	ASN
1	B	29	GLN
1	B	65	ASN
1	B	67	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 for Mogul analysis.

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
4	GOL	A	403[A]	-	5,5,5	2.17	3 (60%)	5,5,5	1.97	2 (40%)
3	SO4	B	401	-	4,4,4	0.36	0	6,6,6	0.52	0
4	GOL	A	403[B]	-	5,5,5	2.35	2 (40%)	5,5,5	1.67	2 (40%)
3	SO4	A	402	-	4,4,4	0.31	0	6,6,6	0.73	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
4	GOL	A	403[A]	-	-	2/4/4/4	-
4	GOL	A	403[B]	-	-	4/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	403[B]	GOL	C1-C2	4.40	1.69	1.51
4	A	403[A]	GOL	O2-C2	2.82	1.51	1.43
4	A	403[A]	GOL	C1-C2	2.58	1.62	1.51
4	A	403[A]	GOL	C3-C2	2.42	1.61	1.51
4	A	403[B]	GOL	C3-C2	2.39	1.61	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403[A]	GOL	O2-C2-C3	3.24	123.42	109.12
4	A	403[A]	GOL	O1-C1-C2	-2.43	98.57	110.20
4	A	403[B]	GOL	O2-C2-C3	-2.14	99.70	109.12
4	A	403[B]	GOL	O2-C2-C1	2.10	118.37	109.12

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	403[A]	GOL	C1-C2-C3-O3
4	A	403[B]	GOL	O1-C1-C2-O2
4	A	403[B]	GOL	O1-C1-C2-C3
4	A	403[B]	GOL	C1-C2-C3-O3
4	A	403[B]	GOL	O2-C2-C3-O3
4	A	403[A]	GOL	O2-C2-C3-O3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	403[B]	GOL	1	0



## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	350/371 (94%)	0.18	14 (4%) 38 41	27, 39, 68, 146	0
1	B	350/371 (94%)	0.06	9 (2%) 56 58	25, 38, 66, 88	0
All	All	700/742 (94%)	0.12	23 (3%) 46 49	25, 39, 67, 146	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	339	GLY	10.4
1	A	340	GLN	9.9
1	A	341	GLU	6.5
1	A	337	THR	6.4
1	A	338	VAL	4.8
1	A	344	ASP	4.5
1	A	180	ILE	4.5
1	A	348	SER	4.3
1	A	343	TYR	3.8
1	A	307	ILE	3.4
1	B	343	TYR	3.4
1	B	293	TRP	2.8
1	B	283	ILE	2.7
1	B	307	ILE	2.6
1	A	346	GLU	2.6
1	B	72	ARG	2.5
1	B	60	TYR	2.5
1	B	63	PHE	2.3
1	B	340	GLN	2.3
1	A	293	TRP	2.2
1	B	0	HIS	2.2
1	A	283	ILE	2.1
1	A	72	ARG	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	GOL	A	403[A]	6/6	0.83	0.48	247,248,257,260	6
4	GOL	A	403[B]	6/6	0.83	0.48	51,64,67,72	6
3	SO4	A	402	5/5	0.92	0.12	59,66,70,77	0
3	SO4	B	401	5/5	0.93	0.15	67,68,84,88	0
2	FE	A	401	1/1	0.97	0.04	40,40,40,40	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.