



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:21 AM UTC

PDB ID : 5XNF / pdb_00005xnf
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

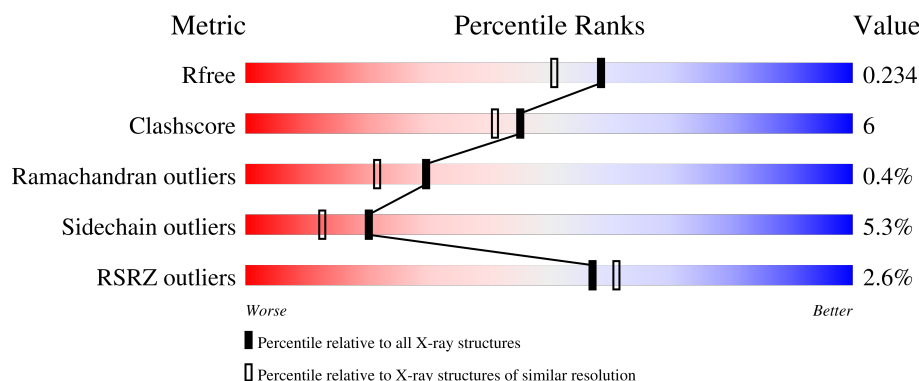
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

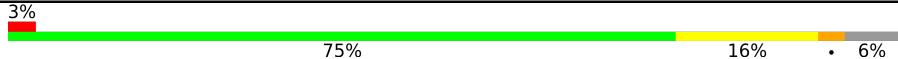
The reported resolution of this entry is 1.90 Å.

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}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (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 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 $\leq 5\%$. 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	 3% 75% 16% • 6%
1	B	371	 2% 76% 15% • 6%

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...

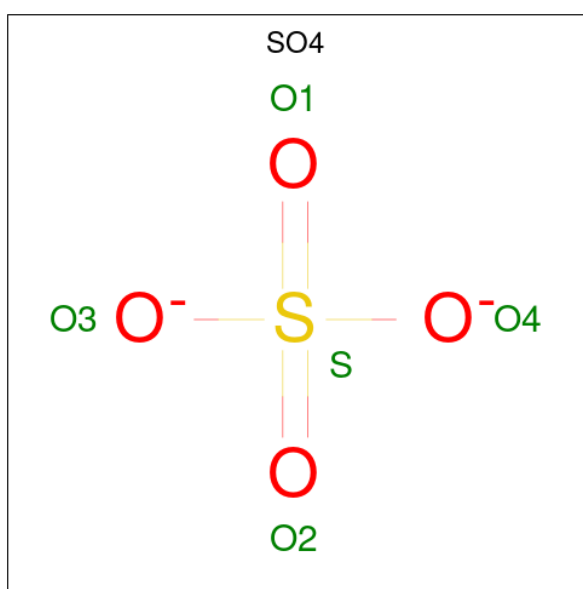
Continued from previous page...

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 (CCD ID: FE) (formula: Fe).

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

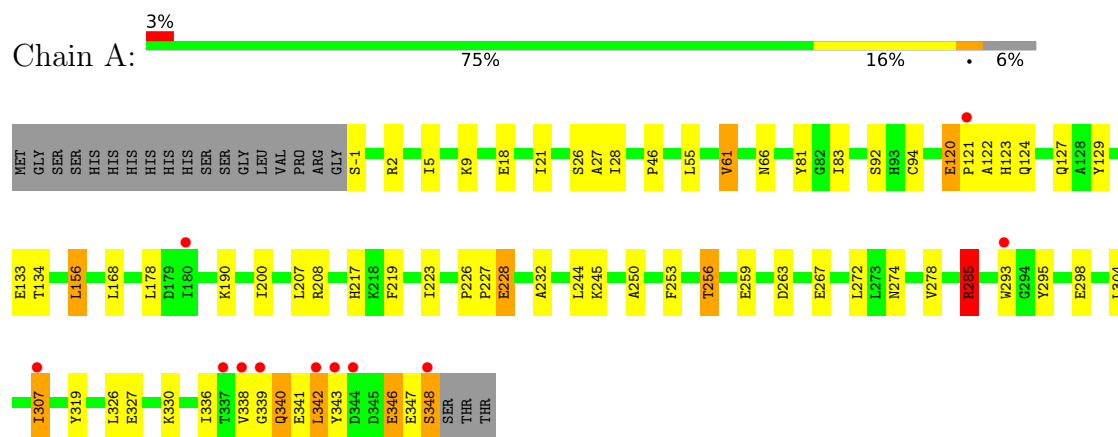
- Molecule 5 is water.

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

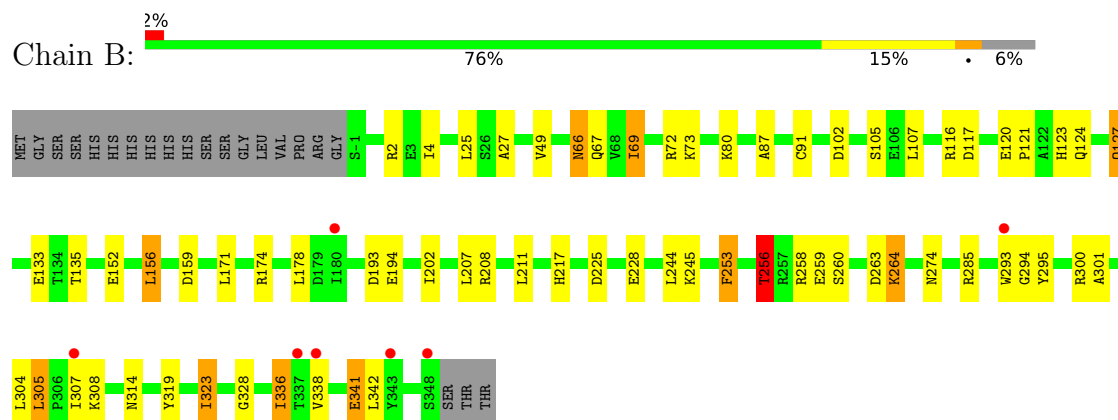
3 Residue-property plots

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: 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, α , β , γ	89.66Å 105.17Å 80.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.90 50.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (50.00-1.90) 99.8 (50.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 1.89Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.203 , 0.244 (Not available) , 0.234	Depositor DCC
R_{free} test set	2991 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: FE, SO₄, GOL

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	1.54	14/2895 (0.5%)	1.31	14/3926 (0.4%)
1	B	1.57	20/2904 (0.7%)	1.29	9/3938 (0.2%)
All	All	1.56	34/5799 (0.6%)	1.30	23/7864 (0.3%)

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	274	ASN	N-CA	8.30	1.56	1.46
1	B	87	ALA	C-O	7.43	1.33	1.23
1	B	225	ASP	C-O	-7.06	1.17	1.24
1	B	152	GLU	N-CA	-6.33	1.38	1.46
1	B	328	GLY	C-O	-6.32	1.15	1.24
1	B	25	LEU	N-CA	-6.31	1.38	1.46
1	B	105	SER	N-CA	-6.11	1.39	1.46
1	A	28	ILE	C-O	-6.06	1.17	1.24
1	A	219	PHE	N-CA	6.04	1.53	1.45
1	B	133	GLU	N-CA	-6.01	1.39	1.46
1	B	256	THR	C-O	5.97	1.31	1.23
1	A	274	ASN	N-CA	5.94	1.53	1.46
1	B	253	PHE	N-CA	-5.91	1.38	1.46
1	B	194	GLU	C-O	-5.81	1.17	1.24
1	B	4	ILE	C-O	-5.78	1.17	1.24
1	A	272	LEU	C-O	5.77	1.30	1.24
1	A	134	THR	N-CA	5.75	1.53	1.46
1	A	18	GLU	N-CA	-5.74	1.39	1.46
1	A	223	ILE	N-CA	-5.71	1.39	1.46
1	B	263	ASP	N-CA	5.69	1.53	1.46
1	B	202	ILE	C-O	-5.57	1.18	1.24
1	B	102	ASP	N-CA	5.57	1.53	1.46
1	B	135	THR	N-CA	-5.56	1.39	1.46
1	B	304	LEU	C-O	-5.53	1.16	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	285	ARG	CD-NE	-5.35	1.38	1.46
1	B	336	ILE	CA-C	-5.30	1.46	1.52
1	A	83	ILE	C-O	-5.28	1.17	1.23
1	A	278	VAL	N-CA	5.24	1.54	1.45
1	B	314	ASN	C-O	-5.17	1.18	1.23
1	A	129	TYR	CA-C	5.14	1.59	1.52
1	A	168	LEU	N-CA	5.11	1.52	1.46
1	B	193	ASP	C-O	-5.09	1.18	1.24
1	A	326	LEU	N-CA	-5.07	1.39	1.45
1	A	253	PHE	N-CA	-5.05	1.39	1.45

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	92	SER	CB-CA-C	-7.64	98.11	110.79
1	A	228	GLU	N-CA-C	7.28	120.53	109.62
1	B	171	LEU	CA-C-N	-7.24	112.87	120.03
1	B	171	LEU	C-N-CA	-7.24	112.87	120.03
1	B	245	LYS	N-CA-C	6.81	118.70	111.28
1	A	285	ARG	NE-CZ-NH2	-6.63	113.23	119.20
1	B	294	GLY	N-CA-C	-5.87	106.63	115.32
1	A	9	LYS	N-CA-C	5.76	118.34	111.71
1	A	228	GLU	CA-CB-CG	-5.63	102.84	114.10
1	A	250	ALA	CA-C-N	5.59	125.45	121.65
1	A	250	ALA	C-N-CA	5.59	125.45	121.65
1	A	120	GLU	N-CA-C	-5.55	102.42	110.08
1	A	133	GLU	N-CA-C	-5.46	105.41	111.36
1	A	27	ALA	N-CA-C	5.42	116.87	111.07
1	B	211	LEU	CA-C-N	-5.42	114.67	120.03
1	B	211	LEU	C-N-CA	-5.42	114.67	120.03
1	A	226	PRO	CA-C-N	-5.38	114.24	119.78
1	A	226	PRO	C-N-CA	-5.38	114.24	119.78
1	A	307	ILE	N-CA-CB	5.30	116.30	110.53
1	B	174	ARG	NE-CZ-NH2	5.28	123.95	119.20
1	B	27	ALA	N-CA-C	5.20	116.95	111.28
1	B	66	ASN	N-CA-C	5.09	118.76	112.24
1	A	245	LYS	N-CA-C	5.03	117.49	111.71

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	39	0
1	B	2841	0	2812	29	0
2	A	1	0	0	0	0
3	A	5	0	0	1	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	67	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 (67) 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:A:340:GLN:C	1:A:342:LEU:H	2.16	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: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:A:-1:SER:OG	1:A:2:ARG:NH2	2.47	0.47
1:B:49:VAL:HG11	1:B:300:ARG:HD3	1.95	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:A:346:GLU:C	1:A:348:SER:H	2.23	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:C	1:A:342:LEU:HD23	2.43	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:B:156:LEU:C	1:B:156:LEU:HD12	2.44	0.42
1:A:285:ARG:HG3	1:A:319:TYR:OH	2.20	0.42
1:A:81:TYR:OH	3:A:402:SO4:O1	2.37	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:340:GLN:C	1:A:342:LEU:N	2.79	0.41
1:A:342:LEU:CD2	1:A:343:TYR:CD2	3.04	0.41
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%)	14	6
1	B	349/371 (94%)	335 (96%)	14 (4%)	0	100	100
All	All	697/742 (94%)	670 (96%)	24 (3%)	3 (0%)	30	22

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	295/326 (90%)	281 (95%)	14 (5%)	23	15
1	B	309/326 (95%)	291 (94%)	18 (6%)	18	10
All	All	604/652 (93%)	572 (95%)	32 (5%)	20	12

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

Mol	Chain	Res	Type
1	A	61	VAL
1	A	156	LEU
1	A	190	LYS
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	107	LEU
1	B	116	ARG
1	B	127	GLN
1	B	156	LEU
1	B	159	ASP
1	B	207	LEU
1	B	256	THR
1	B	264	LYS
1	B	305	LEU
1	B	308	LYS
1	B	323	ILE
1	B	341	GLU
1	B	342	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	93	HIS
1	A	124	GLN
1	A	274	ASN
1	B	65	ASN
1	B	67	GLN
1	B	95	GLN
1	B	274	ASN
1	B	286	ASN

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 oligosaccharides 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	2.28	3 (60%)	5,5,5	2.10	2 (40%)
4	GOL	A	403[B]	-	5,5,5	2.52	2 (40%)	5,5,5	1.76	3 (60%)
3	SO4	B	401	-	4,4,4	0.45	0	6,6,6	0.50	0
3	SO4	A	402	-	4,4,4	0.41	0	6,6,6	0.62	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	4.73	1.69	1.51
4	A	403[A]	GOL	O2-C2	2.91	1.51	1.43
4	A	403[A]	GOL	C1-C2	2.76	1.62	1.51
4	A	403[A]	GOL	C3-C2	2.59	1.61	1.51
4	A	403[B]	GOL	C3-C2	2.56	1.61	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	403[A]	GOL	O2-C2-C3	3.44	123.42	109.18
4	A	403[A]	GOL	O1-C1-C2	-2.62	98.57	110.38
4	A	403[B]	GOL	O2-C2-C3	-2.29	99.70	109.18
4	A	403[B]	GOL	O2-C2-C1	2.22	118.37	109.18
4	A	403[B]	GOL	C3-C2-C1	2.07	119.39	111.80

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.

2 monomers are involved in 2 short contacts:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	SO4	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 [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	350/371 (94%)	0.05	11 (3%) 51 55	27, 39, 68, 146	0
1	B	350/371 (94%)	0.04	7 (2%) 65 69	20, 38, 66, 88	1 (0%)
All	All	700/742 (94%)	0.05	18 (2%) 57 61	20, 39, 67, 146	1 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	338	VAL	4.5
1	A	348	SER	4.0
1	B	348	SER	3.7
1	B	338	VAL	3.7
1	B	293	TRP	3.6
1	A	339	GLY	3.4
1	A	342	LEU	3.1
1	A	293	TRP	2.8
1	A	337	THR	2.6
1	B	343	TYR	2.5
1	B	337	THR	2.5
1	A	121	PRO	2.2
1	A	180	ILE	2.2
1	A	307	ILE	2.2
1	B	307	ILE	2.2
1	A	344	ASP	2.1
1	B	180	ILE	2.1
1	A	343	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
3	SO4	B	401	5/5	0.86	0.08	67,68,84,88	0
3	SO4	A	402	5/5	0.88	0.09	59,66,70,77	0
4	GOL	A	403[A]	6/6	0.88	0.58	247,248,257,260	6
4	GOL	A	403[B]	6/6	0.88	0.58	51,64,67,72	6
2	FE	A	401	1/1	0.98	0.10	40,40,40,40	1

6.5 Other polymers [i](#)

There are no such residues in this entry.