



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 10, 2018 – 09:10 pm GMT

PDB ID : 3E3L
Title : The R-state Glycogen Phosphorylase
Authors : Leonidas, D.D.; Zographos, S.E.; Oikonomakos, N.G.
Deposited on : 2008-08-07
Resolution : 2.59 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

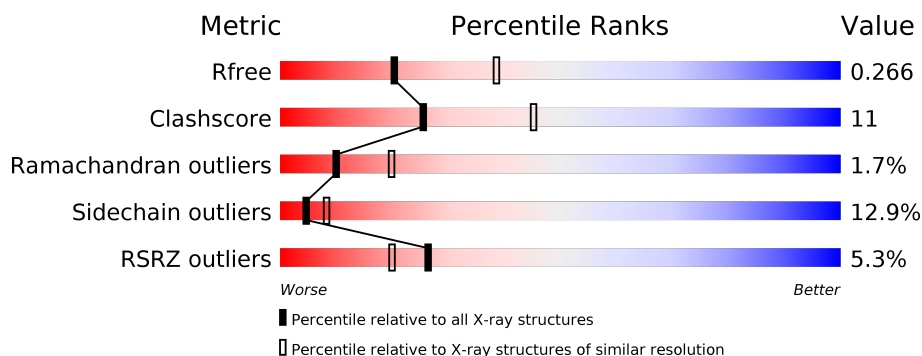
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	111664	2767 (2.60-2.60)
Clashscore	122126	3110 (2.60-2.60)
Ramachandran outliers	120053	3062 (2.60-2.60)
Sidechain outliers	120020	3062 (2.60-2.60)
RSRZ outliers	108989	2706 (2.60-2.60)

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 $\leq 5\%$. 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	842	<div> <div>4%</div> <div> <div></div> <div>66%</div> <div>25%</div> <div>5%</div> <div>.</div> </div> </div>
1	B	842	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>23%</div> <div>.</div> <div>.</div> </div> </div>
1	C	842	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>21%</div> <div>.</div> <div>.</div> </div> </div>
1	D	842	<div> <div>7%</div> <div> <div></div> <div>60%</div> <div>30%</div> <div>6%</div> <div>.</div> <div>.</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 26533 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 Glycogen phosphorylase, muscle form.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	810	Total	C	N	O	P	S	0	0	0
			6601	4206	1164	1201	1	29			
1	B	811	Total	C	N	O	P	S	0	0	0
			6608	4208	1165	1205	1	29			
1	C	807	Total	C	N	O	P	S	0	0	0
			6578	4192	1161	1195	1	29			
1	D	806	Total	C	N	O	P	S	0	0	0
			6576	4190	1159	1197	1	29			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

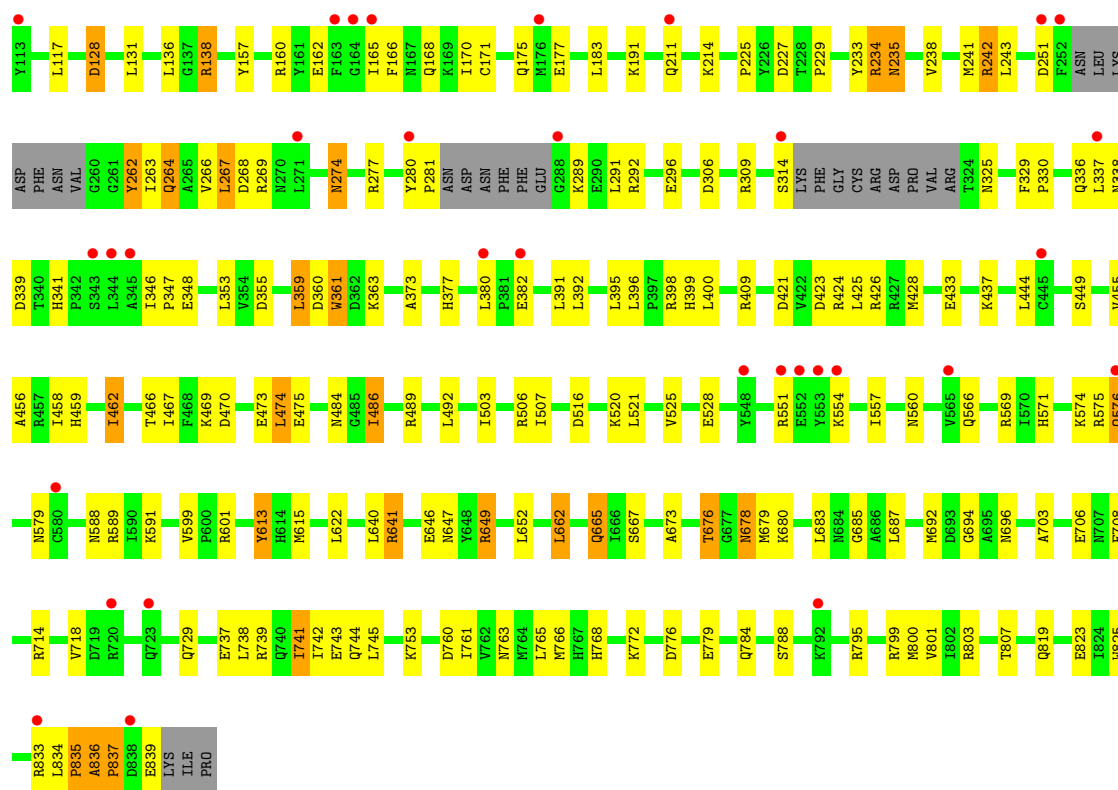
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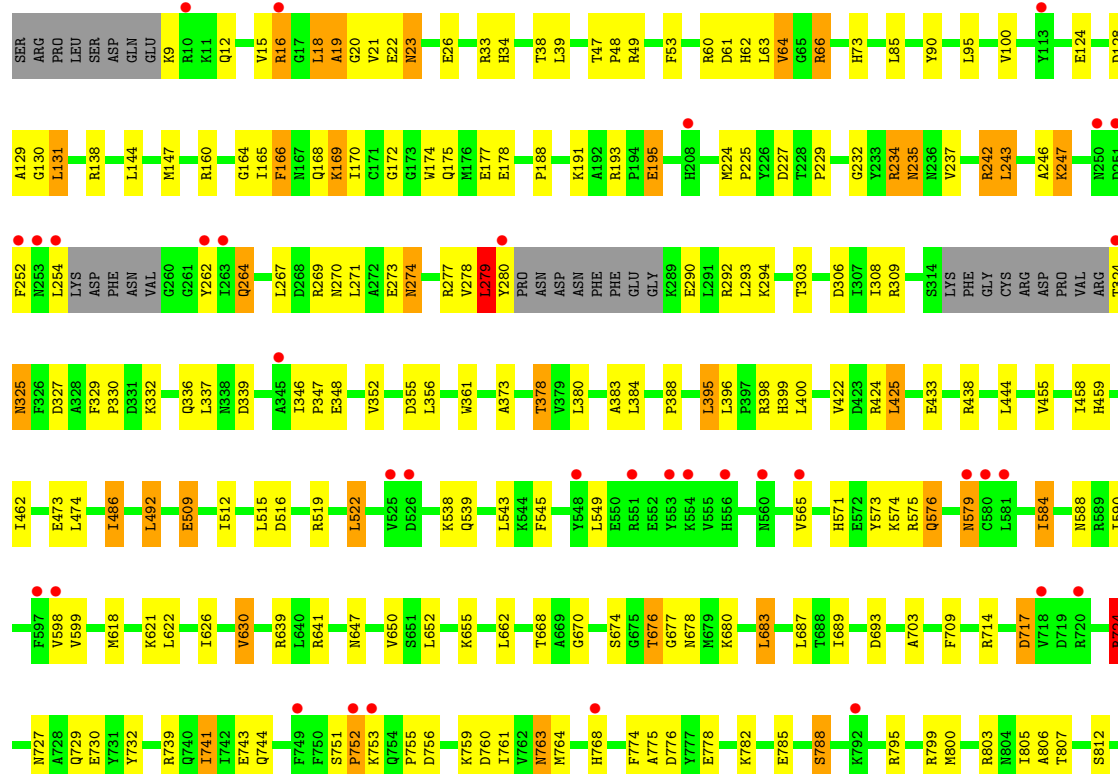
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total	O	0	0
			23	23		
3	B	35	Total	O	0	0
			35	35		
3	C	26	Total	O	0	0
			26	26		
3	D	26	Total	O	0	0
			26	26		



• Molecule 1: Glycogen phosphorylase, muscle form





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	118.89Å 189.92Å 88.16Å 90.00° 109.27° 90.00°	Depositor
Resolution (Å)	29.59 – 2.59 29.59 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.59-2.59) 99.4 (29.59-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.92 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.207 , 0.266 0.207 , 0.266	Depositor DCC
R_{free} test set	5654 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.013 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	26533	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% of the height of the origin peak. No significant pseudotranslation is detected.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LLP, 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	0.49	0/6721	0.66	0/9091
1	B	0.49	0/6728	0.66	1/9100 (0.0%)
1	C	0.50	1/6697 (0.0%)	0.66	2/9058 (0.0%)
1	D	0.50	0/6695	0.66	1/9055 (0.0%)
All	All	0.49	1/26841 (0.0%)	0.66	4/36304 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	795	ARG	CZ-NH1	6.38	1.41	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	795	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	D	87	LEU	CA-CB-CG	-5.98	101.54	115.30
1	C	279	LEU	CA-CB-CG	5.30	127.48	115.30
1	B	662	LEU	CA-CB-CG	5.26	127.40	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	VAL	Peptide

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	6601	0	6554	153	0
1	B	6608	0	6554	116	0
1	C	6578	0	6537	138	0
1	D	6576	0	6528	203	0
2	A	15	0	0	1	0
2	B	15	0	0	0	0
2	C	10	0	0	0	0
2	D	20	0	0	1	0
3	A	23	0	0	0	0
3	B	35	0	0	0	0
3	C	26	0	0	0	0
3	D	26	0	0	1	0
All	All	26533	0	26173	597	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 11.

The worst 5 of 597 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:712:GLY:H	1:A:779:GLU:HG2	1.22	1.03
1:B:641:ARG:HH11	1:B:641:ARG:HG3	1.24	0.98
1:A:20:GLY:O	1:A:21:VAL:HG13	1.65	0.96
1:D:707:ASN:HA	1:D:800:MET:SD	2.09	0.93
1:C:274:ASN:HD22	1:C:274:ASN:H	1.18	0.92

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	801/842 (95%)	745 (93%)	43 (5%)	13 (2%)	11	21
1	B	802/842 (95%)	754 (94%)	37 (5%)	11 (1%)	12	24
1	C	798/842 (95%)	746 (94%)	43 (5%)	9 (1%)	16	33
1	D	797/842 (95%)	698 (88%)	78 (10%)	21 (3%)	6	10
All	All	3198/3368 (95%)	2943 (92%)	201 (6%)	54 (2%)	10	20

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	VAL
1	A	514	ASP
1	A	551	ARG
1	A	835	PRO
1	B	678	ASN

5.3.2 Protein sidechains ⓘ

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	699/730 (96%)	604 (86%)	95 (14%)	4	7
1	B	700/730 (96%)	609 (87%)	91 (13%)	4	8
1	C	697/730 (96%)	626 (90%)	71 (10%)	8	15
1	D	697/730 (96%)	593 (85%)	104 (15%)	3	5
All	All	2793/2920 (96%)	2432 (87%)	361 (13%)	5	8

5 of 361 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	640	LEU
1	C	195	GLU
1	D	667	SER
1	B	665	GLN
1	B	779	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 89 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	481	ASN
1	C	34	HIS
1	D	576	GLN
1	B	541	ASN
1	B	696	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	LLP	A	680	1	24,24,25	1.83	6 (25%)	28,32,34	1.26	3 (10%)
1	LLP	B	680	1	24,24,25	1.82	6 (25%)	28,32,34	1.26	4 (14%)
1	LLP	C	680	1	24,24,25	1.77	5 (20%)	28,32,34	1.24	3 (10%)
1	LLP	D	680	1	24,24,25	1.77	5 (20%)	28,32,34	1.37	5 (17%)

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
1	LLP	A	680	1	-	0/15/17/19	0/1/1/1
1	LLP	B	680	1	-	0/15/17/19	0/1/1/1
1	LLP	C	680	1	-	0/15/17/19	0/1/1/1
1	LLP	D	680	1	-	0/15/17/19	0/1/1/1

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	680	LLP	O3-C3	-6.27	1.22	1.37
1	D	680	LLP	O3-C3	-5.93	1.23	1.37
1	B	680	LLP	O3-C3	-5.87	1.23	1.37
1	C	680	LLP	O3-C3	-5.76	1.23	1.37
1	A	680	LLP	C3-C2	-2.00	1.39	1.40

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	680	LLP	C4-C4'-NZ	-2.77	111.22	124.66
1	A	680	LLP	C5-C6-N1	-2.74	119.20	123.83
1	B	680	LLP	C4-C4'-NZ	-2.57	112.19	124.66
1	D	680	LLP	CE-NZ-C4'	-2.53	111.39	119.08
1	C	680	LLP	CE-NZ-C4'	-2.46	111.60	119.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	680	LLP	3	0
1	B	680	LLP	2	0
1	C	680	LLP	7	0
1	D	680	LLP	2	0

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

12 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	900	-	4,4,4	0.17	0	6,6,6	0.36	0
2	SO4	A	901	-	4,4,4	0.25	0	6,6,6	0.40	0
2	SO4	A	902	-	4,4,4	0.18	0	6,6,6	0.43	0
2	SO4	B	900	-	4,4,4	0.26	0	6,6,6	0.18	0
2	SO4	B	901	-	4,4,4	0.23	0	6,6,6	0.32	0
2	SO4	B	902	-	4,4,4	0.21	0	6,6,6	0.39	0
2	SO4	C	901	-	4,4,4	0.26	0	6,6,6	0.56	0
2	SO4	C	902	-	4,4,4	0.20	0	6,6,6	0.16	0
2	SO4	D	900	-	4,4,4	0.23	0	6,6,6	0.37	0
2	SO4	D	901	-	4,4,4	0.26	0	6,6,6	0.26	0
2	SO4	D	902	-	4,4,4	0.24	0	6,6,6	0.29	0
2	SO4	D	903	-	4,4,4	0.14	0	6,6,6	0.29	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	900	-	-	0/0/0/0	0/0/0/0
2	SO4	A	901	-	-	0/0/0/0	0/0/0/0
2	SO4	A	902	-	-	0/0/0/0	0/0/0/0
2	SO4	B	900	-	-	0/0/0/0	0/0/0/0
2	SO4	B	901	-	-	0/0/0/0	0/0/0/0
2	SO4	B	902	-	-	0/0/0/0	0/0/0/0
2	SO4	C	901	-	-	0/0/0/0	0/0/0/0
2	SO4	C	902	-	-	0/0/0/0	0/0/0/0
2	SO4	D	900	-	-	0/0/0/0	0/0/0/0
2	SO4	D	901	-	-	0/0/0/0	0/0/0/0
2	SO4	D	902	-	-	0/0/0/0	0/0/0/0
2	SO4	D	903	-	-	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	902	SO4	1	0
2	D	900	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	809/842 (96%)	0.18	36 (4%) 34 26	29, 46, 62, 74	0
1	B	810/842 (96%)	0.17	36 (4%) 34 26	28, 46, 66, 78	0
1	C	806/842 (95%)	0.22	37 (4%) 32 25	23, 48, 71, 83	0
1	D	805/842 (95%)	0.42	61 (7%) 14 10	34, 53, 87, 102	0
All	All	3230/3368 (95%)	0.25	170 (5%) 26 20	23, 48, 73, 102	0

The worst 5 of 170 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	288	GLY	7.7
1	A	252	PHE	6.5
1	D	252	PHE	6.4
1	C	252	PHE	6.1
1	A	260	GLY	5.9

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	D	680	24/25	0.94	0.15	51,58,62,63	0
1	LLP	A	680	24/25	0.96	0.19	28,31,36,39	0
1	LLP	B	680	24/25	0.97	0.18	37,38,40,42	0
1	LLP	C	680	24/25	0.97	0.15	40,42,48,49	0

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, 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	SO4	D	900	5/5	0.83	0.21	88,89,89,90	0
2	SO4	A	901	5/5	0.86	0.19	82,83,83,84	0
2	SO4	C	901	5/5	0.86	0.23	74,76,77,77	0
2	SO4	A	902	5/5	0.90	0.16	79,80,81,81	0
2	SO4	B	901	5/5	0.91	0.19	76,77,79,79	0
2	SO4	B	900	5/5	0.92	0.23	81,81,82,83	0
2	SO4	D	901	5/5	0.93	0.17	83,84,84,85	0
2	SO4	D	902	5/5	0.93	0.15	77,77,78,78	0
2	SO4	D	903	5/5	0.94	0.14	68,69,69,70	0
2	SO4	A	900	5/5	0.95	0.13	71,72,72,73	0
2	SO4	B	902	5/5	0.97	0.12	58,58,58,60	0
2	SO4	C	902	5/5	0.98	0.09	64,64,65,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.