



wwPDB X-ray Structure Validation Summary Report

Feb 28, 2014 – 06:09 AM 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 validation summary 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/ValidationPDFNotes.html>

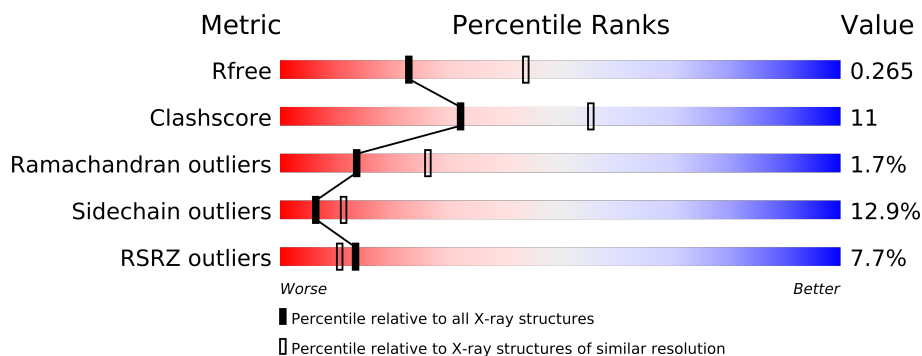
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1323
EDS	:	stable22639
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22683

1 Overall quality at a glance

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}	66092	1718 (2.60-2.60)
Clashscore	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)
RSRZ outliers	66119	1718 (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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	842	
1	B	842	
1	C	842	
1	D	842	

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 26533 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

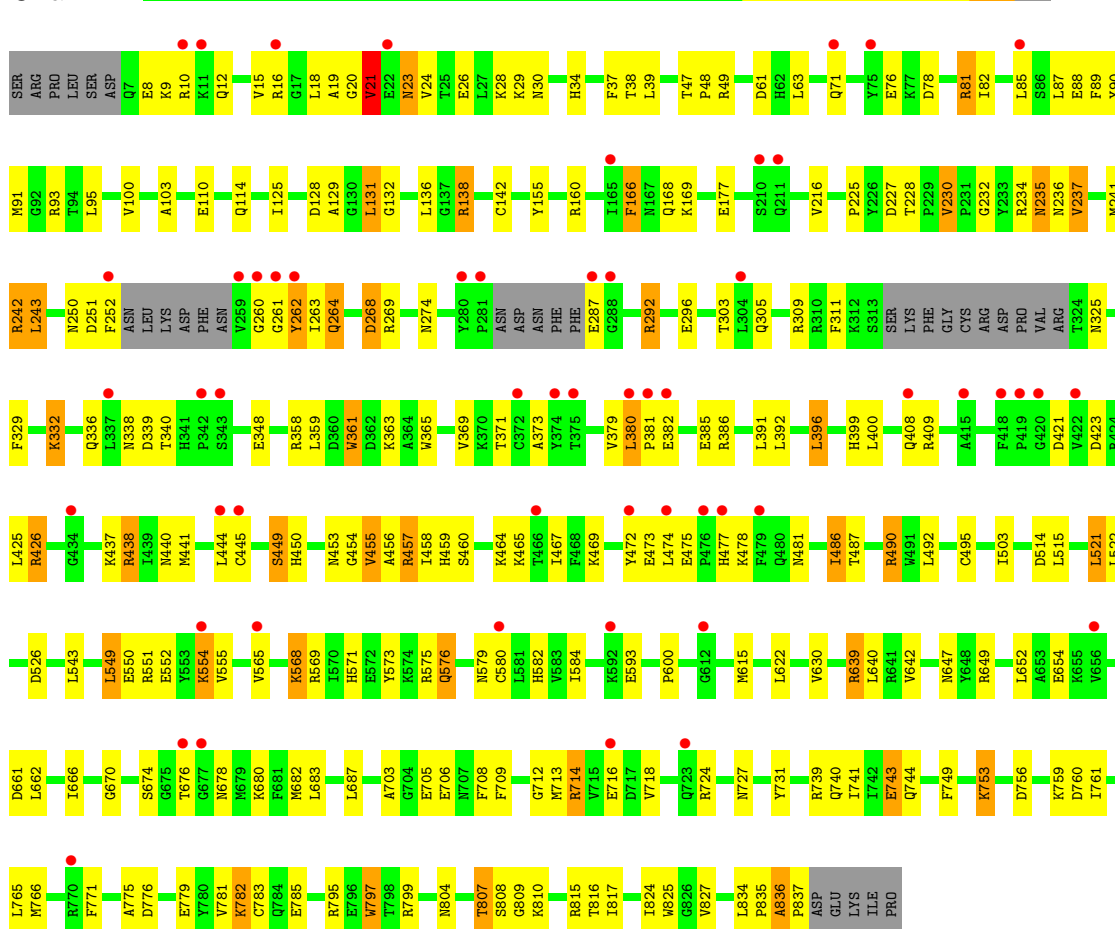
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	23	Total	O	0	0
			23	23		
3	B	35	Total	O	0	0
			35	35		
3	C	26	Total	O	0	0
			26	26		
3	D	26	Total	O	0	0
			26	26		

3 Residue-property plots

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.

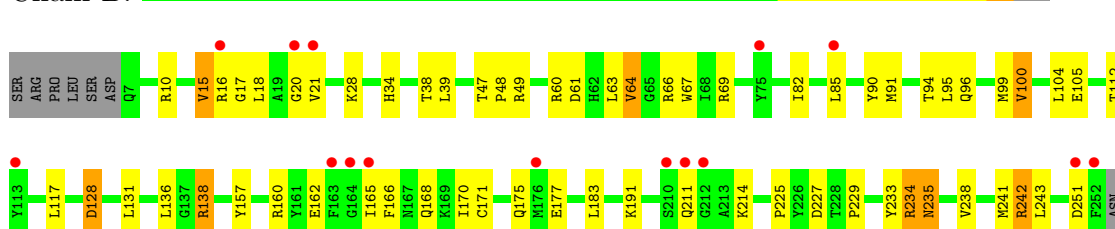
- Molecule 1: Glycogen phosphorylase, muscle form

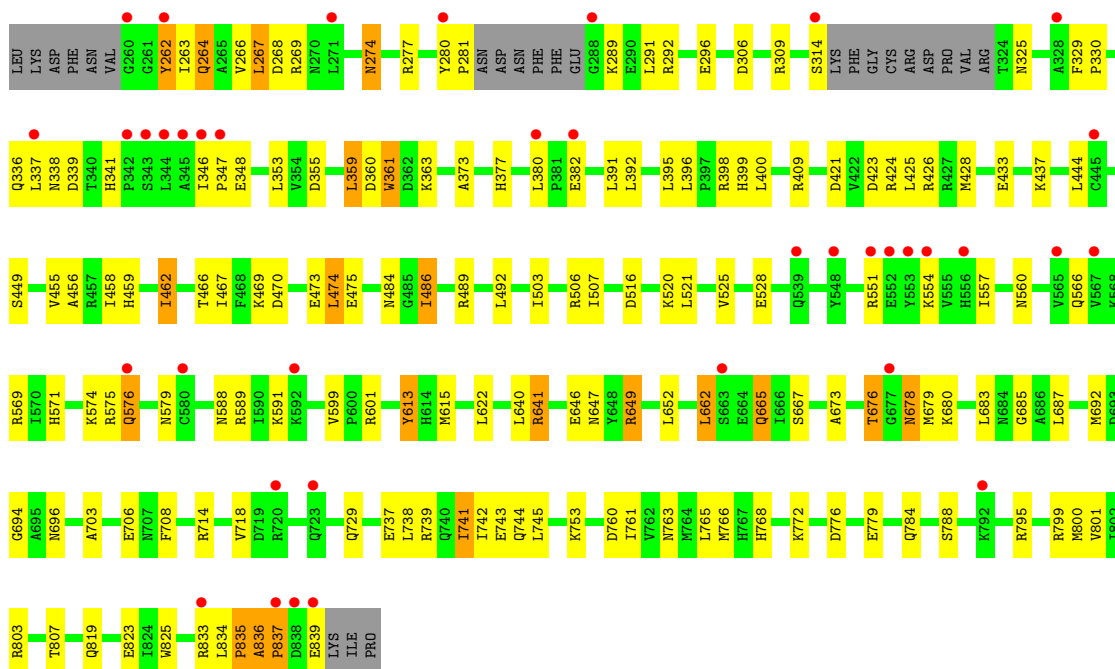
Chain A:



- Molecule 1: Glycogen phosphorylase, muscle form

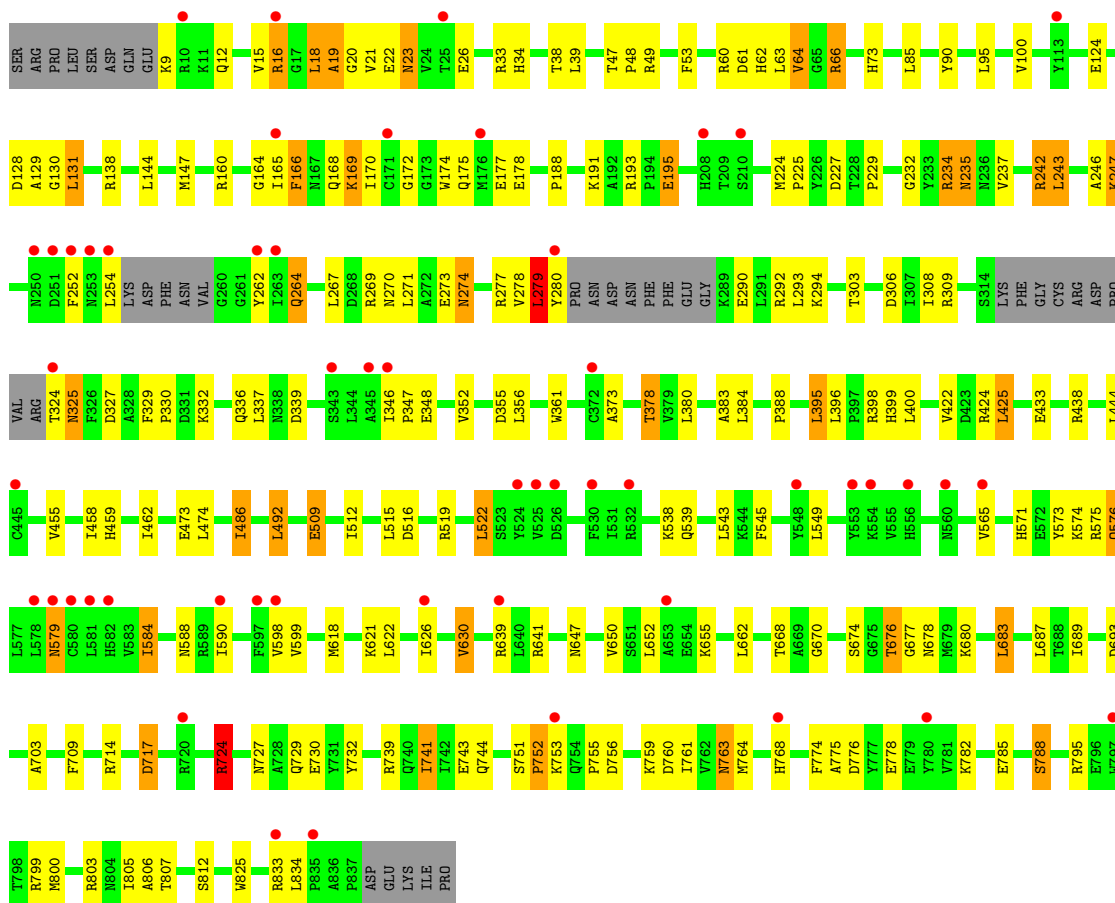
Chain B:





• Molecule 1: Glycogen phosphorylase, muscle form

Chain C:



• Molecule 1: Glycogen phosphorylase, muscle form

W825	T676	V598	I531	K437	ASP	W244	Y90	SER
G826	G677	V599	R532	K437	PRO	S245	M91	ARG
V827	M678	P600	D533	L444	VAL	A246		PRO
E828	M679	R601	V534	L444	ARG	K247	L95	LEU
P829	G680	G602	A535	S449			Q96	SER
S830	P681	V603	K536	S449	T324			ASP
R831	D756	M604	V537			Y250		ASP
Q832	L757	L605	K538	V455	F329	D251	Y100	GLN
R833	L758	L605	Q539	A456	P330	F252	Y113	E8
			Q539	A456	D331	ASN		K9
A836	A686	Y613	N541	T458	K332	LEU	D128	R10
P837	L687	K617	K542	H459	I335	LYS	A129	S14
ASP	L689		L543		Q336	ASP	G130	V15
GLU			F544		L337	PHE	L131	R16
LYS			A546		N338	ASN		
ILE	M692	I623		E473		VAL	L136	
R770	D693	I623	A546	E473	H341	GLY	G137	V21
	G694	I626	L549	L474		GLY	R138	E22
Y777	A695	G627	L549	L474		GLY		E22
	G696	D628		T483	A345	Y262		T25
Y780	P697	V629	Y553	T486	E348	I263	F143	T25
E698	W781	K630	K554	T486		Q264		R33
K782	M699	N631	V555	T487		R269	S146	H34
C783		H632	H556	P488	V352		A147	L35
Q784	E702		I557	R489		N274	A148	H36
	A703	V636	N558	R490	R358		T149	F37
R789	G704			W491				T38
L790	E705	R639	S561	L492	W361	R277	R160	L39
Y791	W706	L640	L562	V493	D362	L279	Y161	V40
K792	E707	R641	F563	L494	K363	Y280		
N793	F708	V642	D564	C495		PRO	G164	R43
W794	F709	L643	V565		A373	ASN	T185	
R795		F644	Q566	L499		ASP	F166	T47
E796	M713	L645	V567	A500	V379	ASN	Q168	F48
W797	E714	E646		E501		PHE		R49
L798	W715	L647	H571	L502	E382	PHE		D50
R799	E716	V648	E572	L503			C171	L55
M800		R649	Y573		V389	E287		
W801	Q723	P650	K574	I507		C288		
L802	R724	S651	K574	G508	L392	K289	Q175	V59
R803	G725	L652	Q576	E509	L291	E290	M176	R60
N804	Y726	A653	L577	E510	L396	L291	K191	
L805	N727	E654	L578	L511		R292		
A806	A728	K655	N579	L512	H399	Q295	T209	L63
	Q729	V656	C580	S513	L400		S210	V64
T807	E730		L581	D514			Q211	
S808	W731	A659	H582	L515	I403	V299	G212	I68
G809	Y732	A660	V583	D516	Y404	A301		
X810	Y733	D661	L584	Q517	E405		D227	Q72
F811	R734	L662	T585	L518			T228	
S812		S663	L586			L304	T228	
S813	I735	E664			F418		T228	
D814		Q665	Y587	L521	P419	I308	T229	Y75
R815	L738	R665	N588	L522	G420	R309	V230	E76
R739	T816	L666	R589	S523	D421	R310	F231	K77
L817	Q740	S667	T590	Y524	V422		N235	
A818	Y741	K591	K591	V525	D423	S314	W236	
	I742	G670	K592	D526	R424	LYS	V237	
Q819	E743	T671		D527	L425	PHE		L85
	Q744	S674	N595	E528	R426			

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 5.3.0037	Depositor
R, R_{free}	0.207 , 0.266 0.208 , 0.265	Depositor DCC
R_{free} test set	5654 reflections (5.27%)	DCC
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 , 23.0	EDS
Estimated twinning fraction	0.013 for -h-l,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 112933 reflections	Xtriage
F_o, F_c correlation	0.93	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.

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6601	0	6556	153	0
1	B	6608	0	6556	118	0
1	C	6578	0	6539	137	0
1	D	6576	0	6530	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	26181	598	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 11.

The worst 5 of 598 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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%)	14	28
1	B	802/842 (95%)	754 (94%)	37 (5%)	11 (1%)	16	32
1	C	798/842 (95%)	746 (94%)	43 (5%)	9 (1%)	21	42
1	D	797/842 (95%)	698 (88%)	78 (10%)	21 (3%)	8	13
All	All	3198/3368 (95%)	2943 (92%)	201 (6%)	54 (2%)	14	26

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%)	5	9
1	B	700/730 (96%)	609 (87%)	91 (13%)	6	11
1	C	697/730 (96%)	626 (90%)	71 (10%)	11	19
1	D	697/730 (96%)	593 (85%)	104 (15%)	4	7
All	All	2793/2920 (96%)	2432 (87%)	361 (13%)	6	11

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 chains 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	4.12	5 (20%)	30,32,34	1.53	4 (13%)
1	LLP	B	680	1	24,24,25	3.89	5 (20%)	30,32,34	1.32	4 (13%)
1	LLP	C	680	1	24,24,25	4.02	5 (20%)	30,32,34	1.15	3 (10%)
1	LLP	D	680	1	24,24,25	4.03	4 (16%)	30,32,34	2.60	7 (23%)

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 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	680	LLP	O-C	18.39	1.24	1.11
1	D	680	LLP	O-C	18.13	1.23	1.11
1	C	680	LLP	O-C	17.98	1.23	1.11
1	B	680	LLP	O-C	17.13	1.23	1.11
1	A	680	LLP	O3-C3	-6.02	1.22	1.37

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	680	LLP	C-CA-N	-11.82	102.03	113.83
1	A	680	LLP	C-CA-N	-5.02	108.81	113.83
1	D	680	LLP	C6-C5-C4	4.48	121.50	118.10
1	A	680	LLP	C6-C5-C4	3.68	120.90	118.10
1	B	680	LLP	C6-C5-C4	3.38	120.67	118.10

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	0.18	0	6,6,6	0.30	0
2	SO4	A	901	-	4,4,4	0.11	0	6,6,6	0.45	0
2	SO4	A	902	-	4,4,4	0.08	0	6,6,6	0.44	0
2	SO4	B	900	-	4,4,4	0.15	0	6,6,6	0.21	0
2	SO4	B	901	-	4,4,4	0.12	0	6,6,6	0.39	0
2	SO4	B	902	-	4,4,4	0.12	0	6,6,6	0.23	0
2	SO4	C	901	-	4,4,4	0.14	0	6,6,6	0.50	0
2	SO4	C	902	-	4,4,4	0.17	0	6,6,6	0.19	0
2	SO4	D	900	-	4,4,4	0.07	0	6,6,6	0.35	0
2	SO4	D	901	-	4,4,4	0.18	0	6,6,6	0.21	0
2	SO4	D	902	-	4,4,4	0.15	0	6,6,6	0.22	0
2	SO4	D	903	-	4,4,4	0.26	0	6,6,6	0.25	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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	810/842 (96%)	0.49	55 (6%) 17 14	29, 46, 62, 74	0
1	B	811/842 (96%)	0.44	53 (6%) 18 15	28, 46, 66, 78	0
1	C	807/842 (95%)	0.50	52 (6%) 19 16	23, 48, 71, 83	0
1	D	806/842 (95%)	0.73	89 (11%) 6 4	34, 53, 87, 102	0
All	All	3234/3368 (96%)	0.54	249 (7%) 13 10	23, 48, 73, 102	0

The worst 5 of 249 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	75	TYR	6.7
1	A	252	PHE	6.6
1	D	288	GLY	6.4
1	D	252	PHE	6.1
1	C	324	THR	5.8

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

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	LLP	B	680	24/25	0.20	-0.15	37,38,40,42	0
1	LLP	D	680	24/25	0.24	-0.17	51,58,62,63	0
1	LLP	A	680	24/25	0.18	-0.18	28,31,36,39	0
1	LLP	C	680	24/25	0.20	-0.21	40,42,48,49	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	A	901	5/5	0.18	0.58	82,83,83,84	0
2	SO4	C	901	5/5	0.16	-0.46	74,76,77,77	0
2	SO4	B	901	5/5	0.13	-0.71	76,77,79,79	0
2	SO4	B	900	5/5	0.15	-0.75	81,81,82,83	0
2	SO4	D	900	5/5	0.15	-0.90	88,89,89,90	0
2	SO4	B	902	5/5	0.11	-1.09	58,58,58,60	0
2	SO4	D	901	5/5	0.13	-1.14	83,84,84,85	0
2	SO4	A	902	5/5	0.12	-1.15	79,80,81,81	0
2	SO4	C	902	5/5	0.11	-1.30	64,64,65,65	0
2	SO4	A	900	5/5	0.11	-1.37	71,72,72,73	0
2	SO4	D	902	5/5	0.13	-1.47	77,77,78,78	0
2	SO4	D	903	5/5	0.10	-1.65	68,69,69,70	0

6.5 Other polymers

There are no such residues in this entry.