



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:40 PM GMT

PDB ID : 1GPA
Title : STRUCTURAL MECHANISM FOR GLYCOGEN PHOSPHORYLASE
CONTROL BY PHOSPHORYLATION AND AMP
Authors : Barford, D.; Hu, S.-H.; Johnson, L.N.
Deposited on : 1990-11-13
Resolution : 2.90 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
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

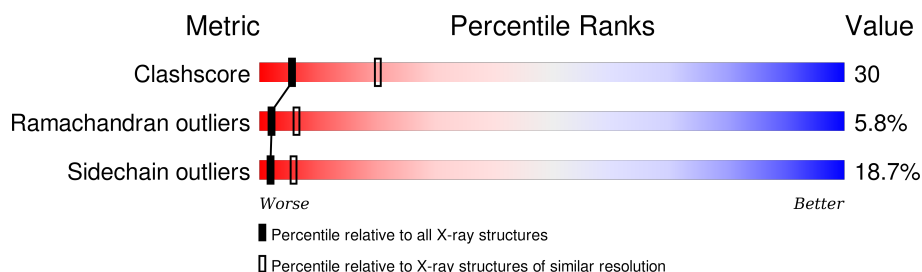
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

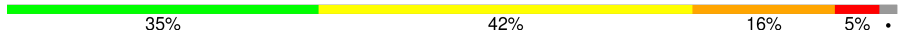
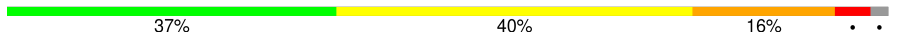
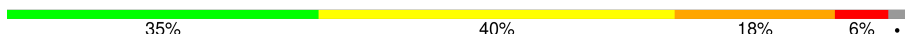
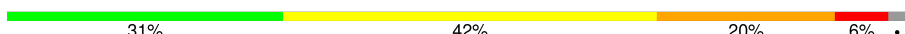
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)

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 ≥ 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.

Note EDS was not executed.

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

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27029 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 A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	828	Total	C	N	O	P	S	44	0	0
			6732	4287	1190	1224	1	30			
1	B	827	Total	C	N	O	P	S	24	0	0
			6733	4286	1189	1227	1	30			
1	C	828	Total	C	N	O	P	S	0	0	0
			6732	4287	1190	1224	1	30			
1	D	828	Total	C	N	O	P	S	0	0	0
			6732	4287	1190	1224	1	30			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	CONFLICT	UNP P00489
B	380	ILE	LEU	CONFLICT	UNP P00489
C	380	ILE	LEU	CONFLICT	UNP P00489
D	380	ILE	LEU	CONFLICT	UNP P00489

- 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		
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		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C₈H₁₀NO₆P).



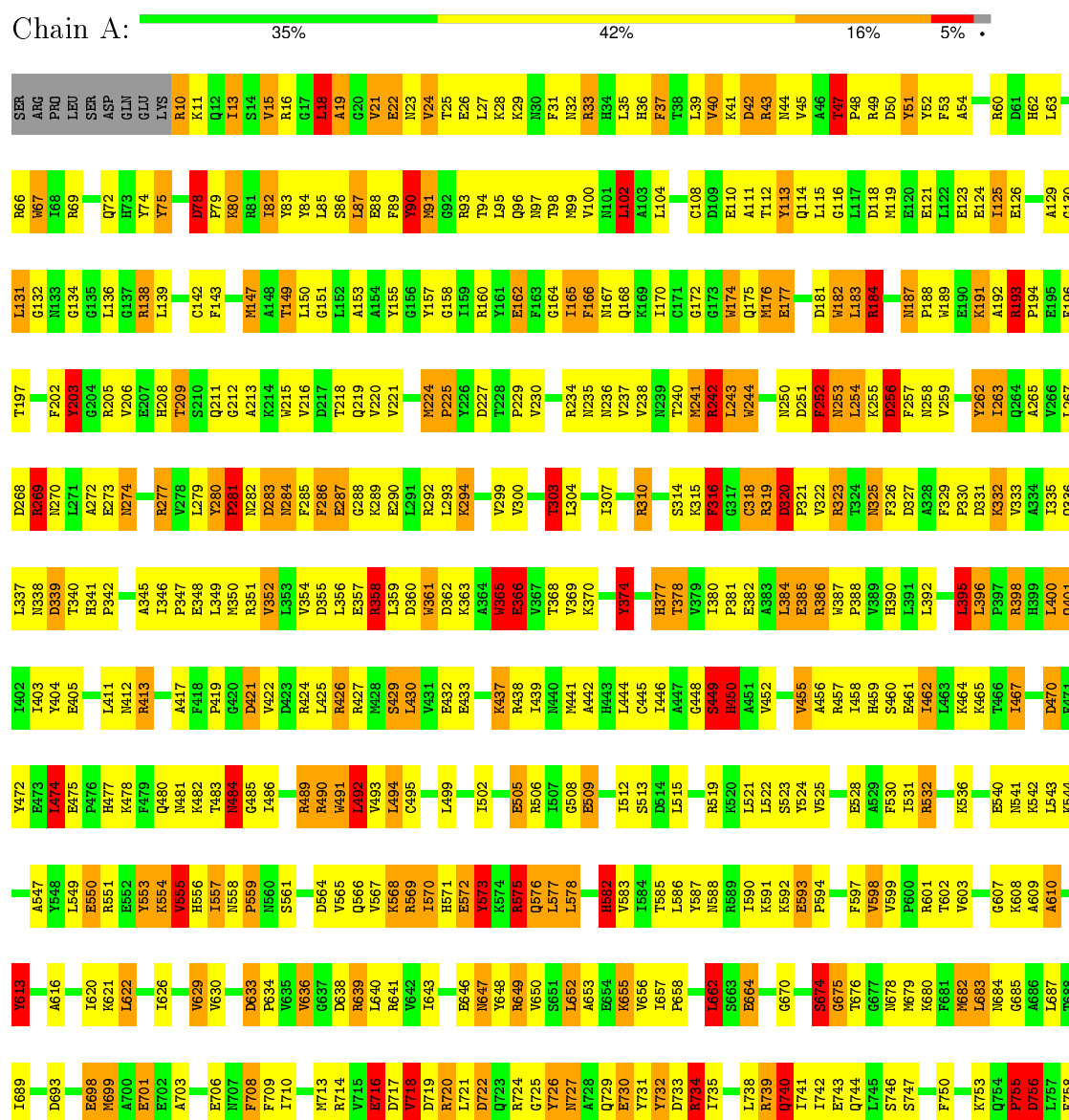
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

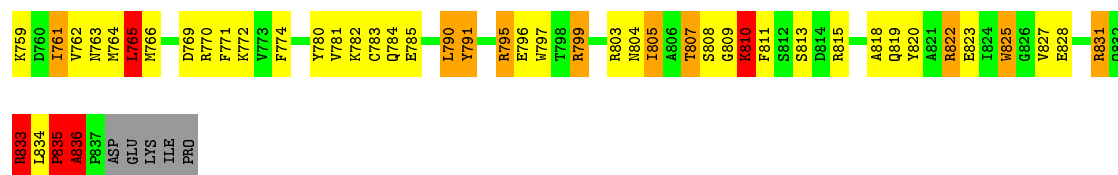
3 Residue-property plots

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.

Note EDS was not executed.

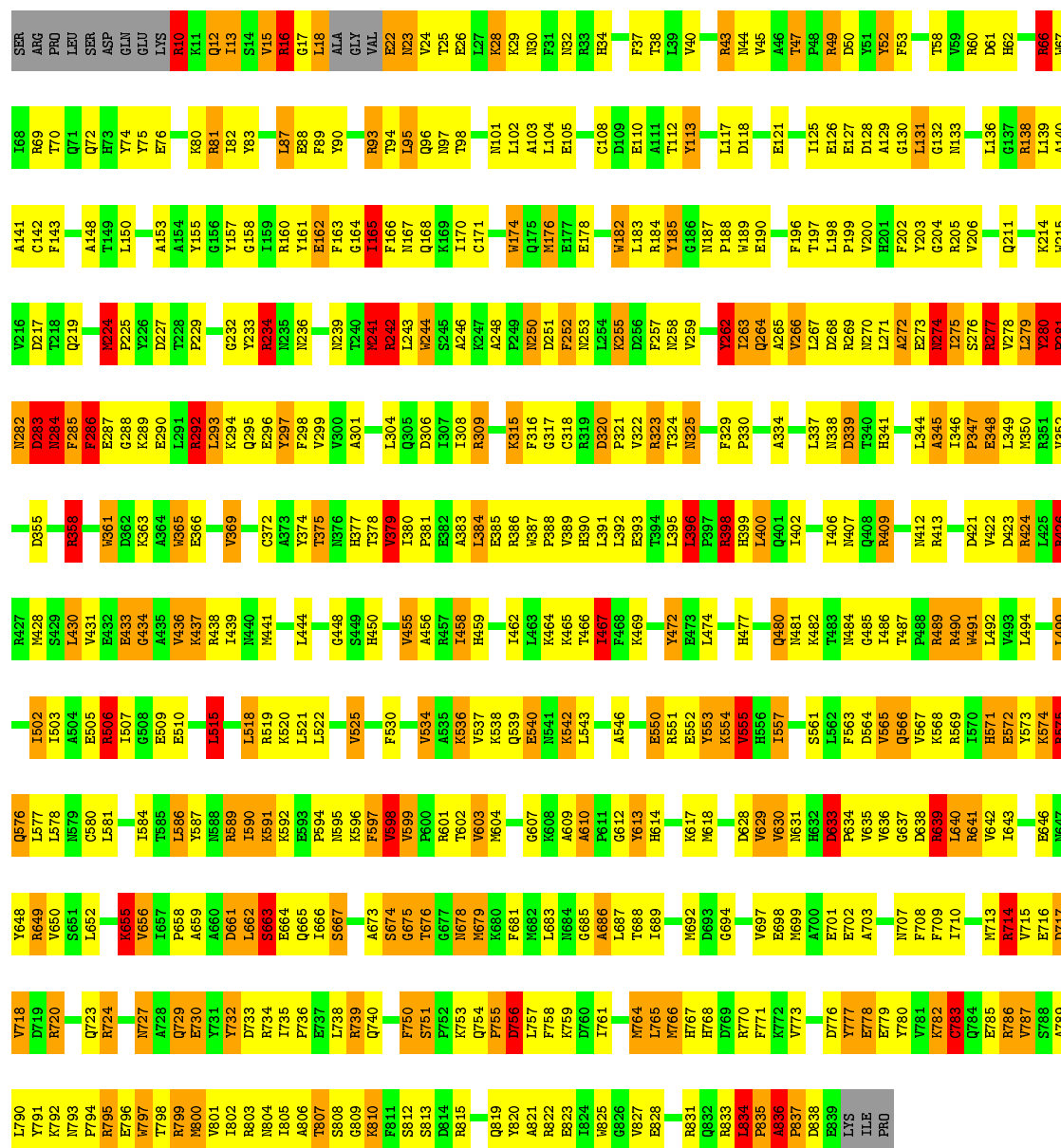
• Molecule 1: GLYCOGEN PHOSPHORYLASE A





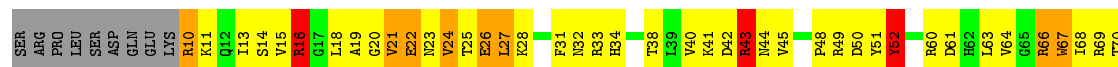
• Molecule 1: GLYCOGEN PHOSPHORYLASE A

Chain B: 37% 40% 16%



• Molecule 1: GLYCOGEN PHOSPHORYLASE A

Chain C: 35% 40% 18% 6%





S808	G809	R810	F811	S812	S813	D814	R815	A818	A821	R822	E823	R824	R825	E828	R831	Q832	R833	L834	P835	A836	P837	ASP	GLU	LYS	ILE	PRO																														
L745	L683	H614	K617	M618	K619	K620	K621	L622	T623	A625	G626	G627	D628	V629	V630	M631	H632	D633	P634	V635	V636	G637	D638	R639	L640	R641	V642	L643	F644	L645	E646	M647	Y648	R649	L652	K655	V656	L657	P658	A659	A660	D661	L662	S663	E664	Q665	L666	S674	G675	T676	G677	M678	M679	R680	F681	M682
S746	M684	L687	T688	I619	K619	K620	K621	L622	T624	A625	G626	G627	D628	V629	V630	M631	H632	D633	P634	V635	V636	G637	D638	R639	L640	R641	V642	L643	F644	L645	E646	M647	Y648	R649	L652	K655	V656	L657	P658	A659	A660	D661	L662	S663	E664	Q665	L666	S674	G675	T676	G677	M678	M679	R680	F681	M682
F750	L687	M618	K619	K620	K621	L622	T623	A625	G626	G627	D628	V629	V630	M631	H632	D633	P634	V635	V636	G637	D638	R639	L640	R641	V642	L643	F644	L645	E646	M647	Y648	R649	L652	K655	V656	L657	P658	A659	A660	D661	L662	S663	E664	Q665	L666	S674	G675	T676	G677	M678	M679	R680	F681	M682		
S751	T688	M619	K564	V555	R556	T557	R558	K559	M560	S561	L562	F563	E564	Q565	V566	V567	V568	R569	L570	H571	E572	V573	Y574	R575	Q576	L577	L578	N579	C580	L581	H582	V583	L584	L585	L586	Y587	R588	R589	L590	K591	K592	E593	P594	N595	V596	V599	P600	R601	T602	V603	M604	L605	A610	F611	G612	V613
P752	L689	I620	R621	R622	R623	T624	A625	G626	G627	D628	V629	V630	M631	H632	D633	P634	V635	V636	G637	D638	R639	L640	R641	V642	L643	F644	L645	E646	M647	Y648	R649	L652	K655	V656	L657	P658	A659	A660	D661	L662	S663	E664	Q665	L666	S674	G675	T676	G677	M678	M679	R680	F681	M682			
K753	G690	K620	K621	L622	T623	A625	G626	G627	D628	V629	V630	M631	H632	D633	P634	V635	V636	G637	D638	R639	L640	R641	V642	L643	F644	L645	E646	M647	Y648	R649	L652	K655	V656	L657	P658	A659	A660	D661	L662	S663	E664	Q665	L666	S674	G675	T676	G677	M678	M679	R680	F681	M682				
Q754	T691	M692	D693	A694	A695	L696	M697	E698	V699	A700	E701	E702	A703	G704	E705	E706	N707	F708	R709	I710	F711	G712	M713	R714	V715	E716	D717	K718	L721	D722	Q723	R724	G725	Y726	M727	E730	Y731	F732	D733	R734	I735	F736	E737	L738	R739	Q740	I741	I742	E743	T807						
P755	D693	A694	A695	L696	M697	E698	V699	A700	E701	E702	A703	G704	E705	E706	N707	F708	R709	I710	F711	G712	M713	R714	V715	E716	D717	K718	L721	D722	Q723	R724	G725	Y726	M727	E730	Y731	F732	D733	R734	I735	F736	E737	L738	R739	Q740	I741	I742	E743	T807								
D756	L693	A694	A695	L696	M697	E698	V699	A700	E701	E702	A703	G704	E705	E706	N707	F708	R709	I710	F711	G712	M713	R714	V715	E716	D717	K718	L721	D722	Q723	R724	G725	Y726	M727	E730	Y731	F732	D733	R734	I735	F736	E737	L738	R739	Q740	I741	I742	E743	T807								
L757	L694	A695	L696	M697	E698	V699	A700	E701	E702	A703	G704	E705	E706	N707	F708	R709	I710	F711	G712	M713	R714	V715	E716	D717	K718	L721	D722	Q723	R724	G725	Y726	M727	E730	Y731	F732	D733	R734	I735	F736	E737	L738	R739	Q740	I741	I742	E743	T807									
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D760	V697	E698	V699	A700	E701	E702	A703	G704	E705	E706	N707	F708	R709	I710	F711	G712	M713	R714	V715	E716	D717	K718	L721	D722	Q723	R724	G725	Y726	M727	E730	Y731	F732	D733	R734	I735	F736	E737	L738	R739	Q740	I741	I742	E743	T807												
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V762	M699	A700	E701	E702	A703	G704	E705	E706	N707	F708	R709	I710	F711	G712	M713	R714	V715	E716	D717	K718	L721	D722	Q723	R724	G725	Y726	M727	E730	Y731	F732	D733	R734	I735	F736	E737	L738	R739	Q740	I741	I742	E743	T807														
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R780	E716	D717	K718	L721	D722	Q723	R724	G725	Y726	M727	E730	Y731	F732	D733	R734	I735	F736	E737	L738	R739	Q740	I741	I742	E743	T807																															
F781	D717	K718	L721	D722	Q723	R724	G725	Y726	M727	E730	Y731	F732	D733	R734	I735	F736	E737	L738	R739	Q740	I741	I742	E743	T807																																
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Q783	D722	Q723	R724	G725	Y726	M727	E730	Y731	F732	D733	R734	I735	F736	E737	L738	R739	Q740	I741	I742	E743	T807																																			
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E785	L721	D722	Q723	R724	G725	Y726	M727	E730	Y731	F732	D733	R734	I735	F736	E737	L738	R739	Q740	I741	I742	E743	T807																																		
R786	D722	Q723	R724	G725	Y726	M727	E730	Y731	F732	D733	R734	I735	F736	E737	L738	R739	Q740	I741	I742	E743	T807																																			
F787	Q723	R724	G725	Y726	M727	E730	Y731	F732	D733	R734	I735	F736	E737	L738	R739	Q740	I741	I742	E743	T807																																				
S788	R724	G725	Y726	M727	E730	Y731	F732	D733	R734	I735	F736	E737	L738	R739	Q740	I741	I742	E743	T807																																					
A789																																																								

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	119.00Å 190.00Å 88.20Å 90.00° 109.35° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.90)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.176 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	27029	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, SO4, PLP

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	1.12	5/6873 (0.1%)	2.11	267/9300 (2.9%)
1	B	1.07	5/6873 (0.1%)	2.08	259/9298 (2.8%)
1	C	1.11	5/6873 (0.1%)	2.10	264/9300 (2.8%)
1	D	1.09	7/6873 (0.1%)	2.19	266/9300 (2.9%)
All	All	1.10	22/27492 (0.1%)	2.12	1056/37198 (2.8%)

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	11
1	B	0	11
1	C	0	9
1	D	0	15
All	All	0	46

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	24	VAL	C-N	26.58	1.95	1.34
1	A	756	ASP	N-CA	15.44	1.77	1.46
1	A	47	THR	N-CA	-11.92	1.22	1.46
1	D	22	GLU	CD-OE2	6.78	1.33	1.25
1	A	543	LEU	N-CA	6.35	1.59	1.46

The worst 5 of 1056 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	24	VAL	O-C-N	26.50	165.09	122.70
1	D	251	ASP	CA-CB-CG	25.67	169.87	113.40
1	D	24	VAL	CA-C-N	-20.73	71.59	117.20
1	D	575	ARG	NE-CZ-NH1	18.09	129.35	120.30
1	D	281	PRO	O-C-N	17.08	150.02	122.70

There are no chirality outliers.

5 of 46 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	113	TYR	Sidechain
1	A	203	TYR	Sidechain
1	A	320	ASP	Peptide
1	A	380	ILE	Peptide
1	A	51	TYR	Sidechain

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	6732	0	6675	411	1
1	B	6733	0	6667	363	0
1	C	6732	0	6674	391	0
1	D	6732	0	6674	454	1
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	1	0
2	D	10	0	0	0	0
3	A	15	0	7	1	0
3	B	15	0	7	1	0
3	C	15	0	7	1	0
3	D	15	0	6	1	0
All	All	27029	0	26717	1582	1

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 30.

The worst 5 of 1582 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:756:ASP:CA	1:A:756:ASP:N	1.77	1.46
1:C:279:LEU:HD22	1:C:281:PRO:CD	1.62	1.28
1:C:279:LEU:HD22	1:C:281:PRO:CG	1.70	1.22
1:B:283:ASP:OD2	1:B:383:ALA:HB1	1.39	1.21
1:C:283:ASP:OD2	1:C:383:ALA:HB1	1.37	1.19

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:VAL:O	1:D:370:LYS:NZ[2_646]	1.97	0.23

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	825/842 (98%)	656 (80%)	130 (16%)	39 (5%)	3	11
1	B	822/842 (98%)	674 (82%)	105 (13%)	43 (5%)	2	8
1	C	825/842 (98%)	673 (82%)	100 (12%)	52 (6%)	2	5
1	D	825/842 (98%)	635 (77%)	133 (16%)	57 (7%)	1	4
All	All	3297/3368 (98%)	2638 (80%)	468 (14%)	191 (6%)	2	6

5 of 191 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ALA
1	A	166	PHE
1	A	252	PHE
1	A	256	ASP
1	A	265	ALA

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	714/730 (98%)	585 (82%)	129 (18%)	2	6
1	B	715/730 (98%)	600 (84%)	115 (16%)	3	9
1	C	714/730 (98%)	574 (80%)	140 (20%)	1	5
1	D	714/730 (98%)	563 (79%)	151 (21%)	1	4
All	All	2857/2920 (98%)	2322 (81%)	535 (19%)	2	6

5 of 535 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	834	LEU
1	C	360	ASP
1	D	562	LEU
1	C	63	LEU
1	C	235	ASN

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	804	ASN
1	C	336	GLN
1	D	614	HIS
1	C	32	ASN
1	C	235	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](#)

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	SEP	A	14	1	8,9,10	1.17	0	8,12,14	3.20	3 (37%)
1	SEP	B	14	1	8,9,10	1.12	0	8,12,14	2.93	3 (37%)
1	SEP	C	14	1	8,9,10	1.27	1 (12%)	8,12,14	4.54	2 (25%)
1	SEP	D	14	1	8,9,10	1.22	0	8,12,14	15.72	1 (12%)

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	SEP	A	14	1	-	0/6/8/10	0/0/0/0
1	SEP	B	14	1	-	0/6/8/10	0/0/0/0
1	SEP	C	14	1	-	0/6/8/10	0/0/0/0
1	SEP	D	14	1	-	0/6/8/10	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	14	SEP	P-O3P	-2.01	1.47	1.54

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	14	SEP	OG-CB-CA	-44.38	70.41	108.27
1	B	14	SEP	O-C-CA	-3.05	117.55	125.49
1	A	14	SEP	O-C-CA	-2.35	119.37	125.49
1	C	14	SEP	O2P-P-OG	2.30	113.19	106.56
1	B	14	SEP	OG-P-O1P	2.49	113.48	107.14

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
1	C	14	SEP	1	0
1	D	14	SEP	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	901	-	4,4,4	0.50	0	6,6,6	0.39	0
2	SO4	A	902	-	4,4,4	0.33	0	6,6,6	0.38	0
3	PLP	A	999	1	15,15,16	2.31	4 (26%)	21,22,23	1.56	3 (14%)
2	SO4	B	901	-	4,4,4	0.36	0	6,6,6	0.30	0
2	SO4	B	902	-	4,4,4	0.48	0	6,6,6	0.53	0
3	PLP	B	999	1	15,15,16	1.41	1 (6%)	21,22,23	1.89	3 (14%)
2	SO4	C	901	-	4,4,4	0.37	0	6,6,6	0.31	0
2	SO4	C	902	-	4,4,4	0.45	0	6,6,6	0.80	0
3	PLP	C	999	1	15,15,16	1.69	1 (6%)	21,22,23	1.28	2 (9%)
2	SO4	D	901	-	4,4,4	0.36	0	6,6,6	0.51	0
2	SO4	D	902	-	4,4,4	0.62	0	6,6,6	0.49	0
3	PLP	D	999	1	15,15,16	1.67	3 (20%)	21,22,23	1.24	2 (9%)

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	901	-	-	0/0/0/0	0/0/0/0
2	SO4	A	902	-	-	0/0/0/0	0/0/0/0
3	PLP	A	999	1	-	0/6/6/8	0/1/1/1
2	SO4	B	901	-	-	0/0/0/0	0/0/0/0
2	SO4	B	902	-	-	0/0/0/0	0/0/0/0
3	PLP	B	999	1	-	0/6/6/8	0/1/1/1
2	SO4	C	901	-	-	0/0/0/0	0/0/0/0
2	SO4	C	902	-	-	0/0/0/0	0/0/0/0
3	PLP	C	999	1	-	0/6/6/8	0/1/1/1
2	SO4	D	901	-	-	0/0/0/0	0/0/0/0
2	SO4	D	902	-	-	0/0/0/0	0/0/0/0
3	PLP	D	999	1	-	0/6/6/8	0/1/1/1

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	999	PLP	C3-C2	-5.49	1.37	1.40
3	A	999	PLP	C5-C4	-5.27	1.34	1.40
3	A	999	PLP	C3-C2	-4.99	1.37	1.40
3	D	999	PLP	C3-C2	-4.80	1.37	1.40
3	B	999	PLP	C3-C2	-3.53	1.38	1.40

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	PLP	C4A-C4-C5	-4.07	116.64	120.88
3	A	999	PLP	C5A-C5-C4	-2.48	118.36	121.65
3	B	999	PLP	O2P-P-O1P	-2.15	103.64	110.58
3	D	999	PLP	O2P-P-O4P	2.21	112.94	106.56
3	B	999	PLP	O2P-P-O4P	2.43	113.56	106.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	PLP	1	0
3	B	999	PLP	1	0
2	C	902	SO4	1	0
3	C	999	PLP	1	0
3	D	999	PLP	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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.