



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 04:06 AM UTC

PDB ID : 1GPA / pdb_00001gpa
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

<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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

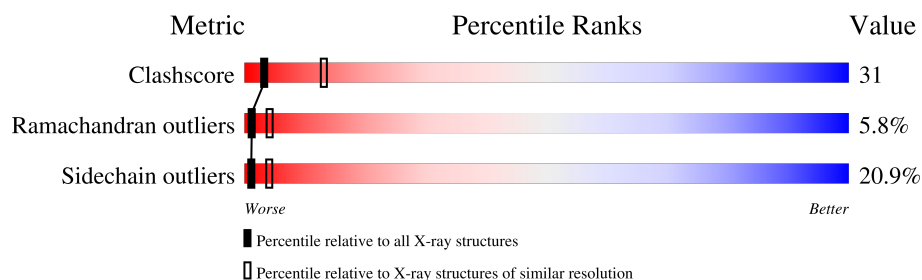
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (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 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 $\leq 5\%$.

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.

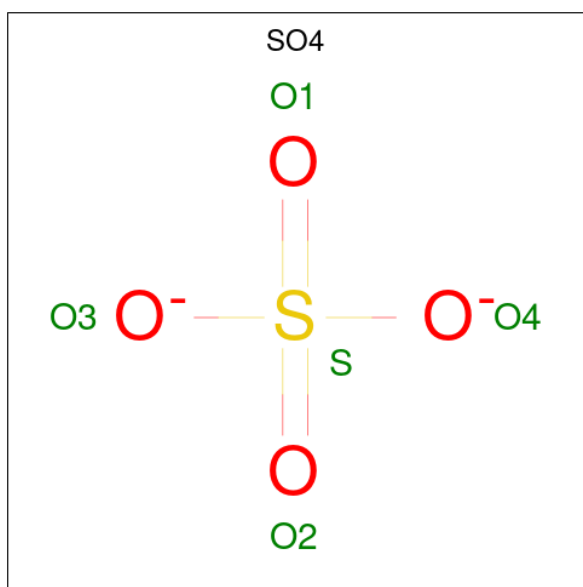
- Molecule 1 is a protein called GLYCOGEN PHOSPHORYLASE A.

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:

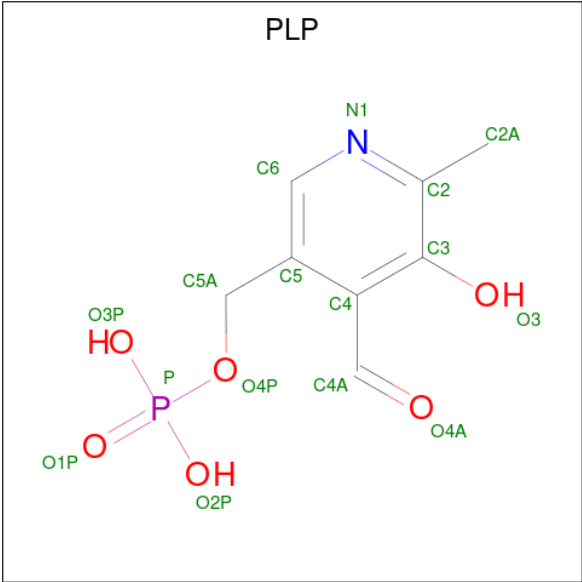
Chain	Residue	Modelled	Actual	Comment	Reference
A	380	ILE	LEU	conflict	UNP P00489
B	380	ILE	LEU	conflict	UNP P00489
C	380	ILE	LEU	conflict	UNP P00489
D	380	ILE	LEU	conflict	UNP P00489

- Molecule 2 is SULFATE ION (CCD ID: 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 (CCD ID: PLP) (formula: C₈H₁₀NO₆P).



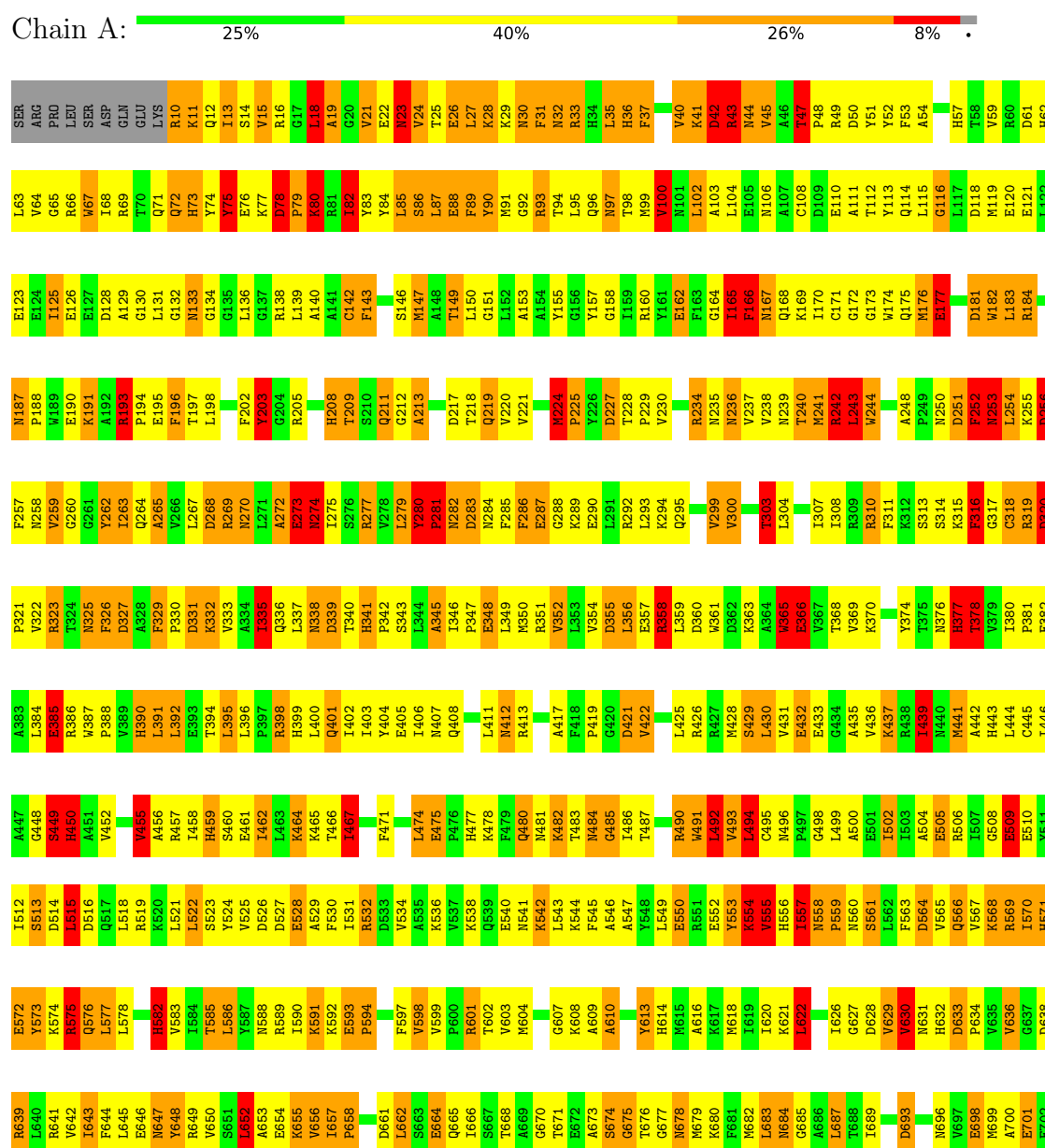
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

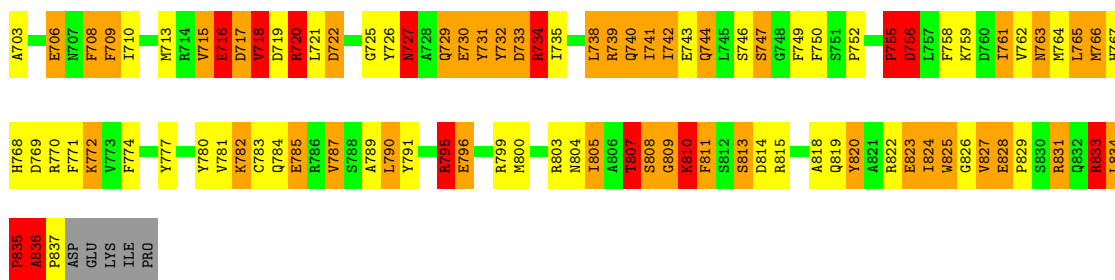
3 Residue-property plots

These plots are drawn for all protein, RNA, 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. 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. 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.

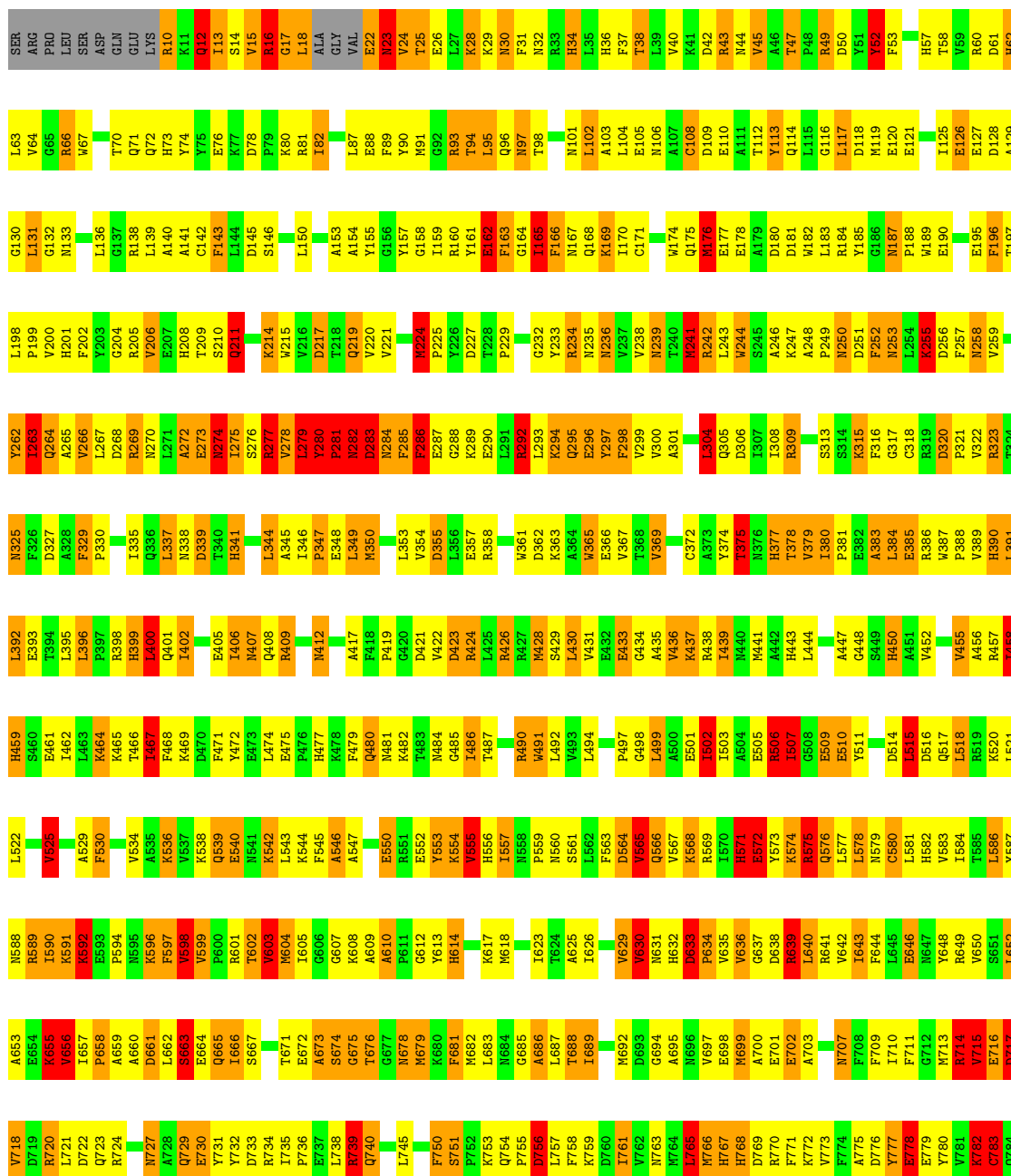
• Molecule 1: GLYCOGEN PHOSPHORYLASE A

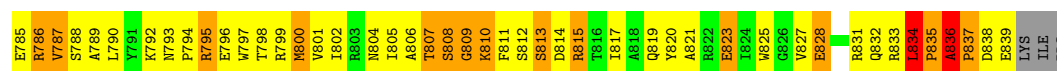




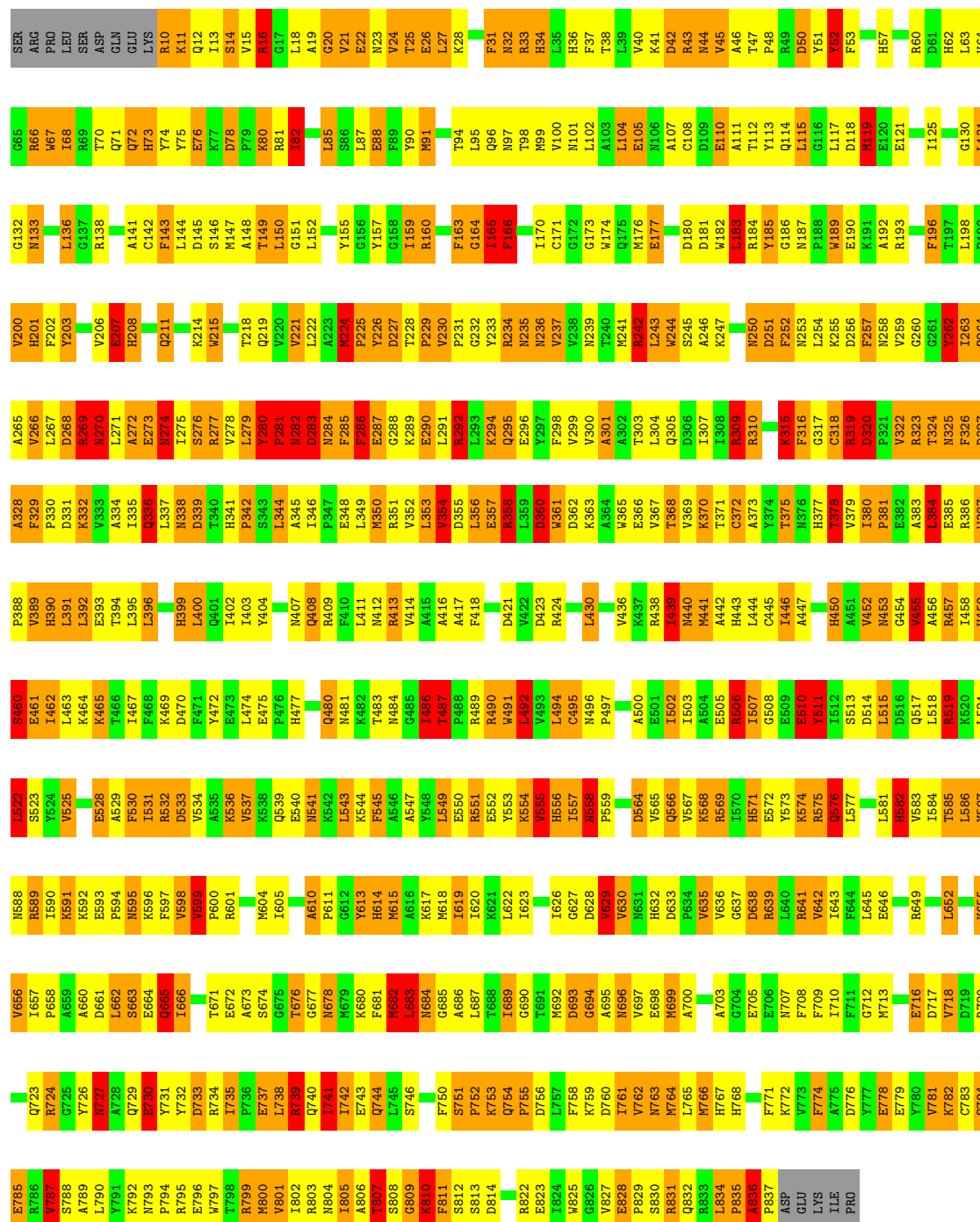
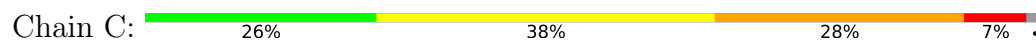
• Molecule 1: GLYCOGEN PHOSPHORYLASE A

Chain B: 26% 42% 23% 7% .

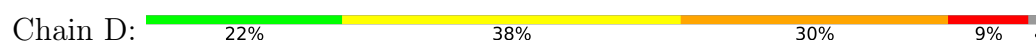




• Molecule 1: GLYCOGEN PHOSPHORYLASE A



• Molecule 1: GLYCOGEN PHOSPHORYLASE A



A818	L757	V697	V635	E572	E510	I446	V379	S314	D251	E190	D128	V64	SER
Q819	F758	E698	V636	V673	Y511	I446	I380	X315	F252	K191	A129	W67	ARG
Y820	K759	M699	K639	K574	I512	S449	A383	G316	N253	K192	G130	W67	PRO
A821	D760	A700	R639	R575	S513	S449	A383	G317	K253	R193	L131	I68	LEU
R822	D761	E701	L640	L576	D514	A451	E385	C318	K255	P194	N133	R69	SER
E823	V762	E702	R641	L577	L515	V452	E385	R319	K256	E195	G132	T70	ASP
T823	K763	A703	V642	L578	D516	R453	R386	D320	F257	F196	Q71	Q71	GLN
K825	K764	G704	L643	N579	Q517	G454	W387	P321	N258	L197	L136	Q72	GLU
	L765	E705	F644		L518	V455	P388	V322	V259	L198	G137	H73	LYS
E828	M766	E706	L645	H582	R519	A456	V389	R323	G260	P199	R138	Y74	K11
P829	K767	N707	E646	V583	K520	R457	H390	T324	G261	V200	L139	Y75	K11
S830	H768	F708	N647	I584	L521	I458	L391	N325	Y262	H201	A140	E76	Q12
R831	D769	F709	V648	T586	L522	H459	L392	F326	T263	F202	A141	K77	I13
Q832	K770	L710	R649	L586	S523	S460		D327	Q264	Y203	C142	D78	S14
R833	F771	F711	V650	V587	Y524	E461	L395	A328	A285	G204	F143	P79	V15
L834	K772	G712	S651	N588	V525	I462	L396	F329		R205	L144	K80	R16
P835	V773	M713	L652	R589	D526	L463	P397	P330	D268	V206	D145	R81	G17
A836	F774	R714	A653	I590	D527	K464	R398	D331	R269	E207	S146	I82	
P837	A775	V715	E654	K591	E528	K465	H399	K332	N270	H208	M147	Y83	
ASP	D776	E716	K655	K592	A529	T466	L400		L271	T209	A148	Y84	
GLU	Y777	D717	V656	E593	F530	I467	Q401	I335	A272	S210	T149	L85	V21
LYS	E778	D718	P657	P594	I531	F468	I402	Q336	E273	Q211	L150	S86	E22
ILE	E779	D719	P658	N595	R532	K469	L403	L337	N274	G212	G151	L87	N23
PRO	Y780	L720	A659	V598	Y534	D470	E405	N338	R277	A213	L152	F88	N24
	Y781	R721	A660	V599	Y534	F471	E406	D339	V276	K214	A153	F88	
	K782	D722	D661	V600	A535	Y472	I406	T340	L279	W215	A154	Y90	K28
G783	Q783	Q723	L662	R601	K536	E473	N407	H341	Y280	D217	Y155	M91	R29
Q784	K784	R724	S663	K601	V537	E474	Q408	P342	Y281	G156	G156		N30
E785	G785	G725	E664	T602	K538	E475	R409	S343	P281	T218	Y157	T94	F31
R786	G786	Y726	Q665	V603	Q539	P476	F410	L344	N282	G158	G158	Q96	N32
Y787	N727	N727	L666	N604	E540	H477	L411		D283	I159	R160	N97	R33
S788	A728	A728	S667	L605	N541	K478	N412	E348	N284	R161	Y161	N97	H34
A789	Q729	Q729	T668	R608	K542		R413	L349	F285	E162	Y162	T98	L35
L790	E730	E730	A669	A609	L543	T483	V414	M350	F286	R351	F163	M99	H36
Y791	V731	V731		K544	F544	N484	A417	R351	E287	P225	V100	V100	
K792	D732	D732	E672	K611	F545	G485		V352	G283	Y226	N101	N101	L39
N793	D733	D733	A673	G612	L549	T487	D421	L353	K289	D227	I165	L102	V40
V794	R734	R734	S674	G612	E550	T487		V354	E290	T228	F166	A103	K41
R795	L735	L735	G675	H614	R551	P488		D355	L291	T229	M167	L104	D42
E796	P736	P736	T676	H614	E552	R489	R424	L356	R292	P230	Q168	E105	R43
W797	E737	E737	G677	N615	Y553	R490	L425	E357	L293	P231	K169	N106	N44
L798	L738	L738	N678	A616	Y553	W491	R426	R358	K294	G232	I170	A107	N44
R799	R739	R739	N679	K617	K554	L492	R427	L359	Q295	Y233	C108	A107	V45
H800	Q740	Q740	K680	N618	Y555	V493	M428	D360	F296	R234	D109	T47	A46
V801	L741	L741	F681	L619	H556	L494	S429	W361	Y297	N235	W174	E110	P48
I802	L742	L742	M682	L620	E557	C495	L430	A364	F298	N236	Q175	A111	R49
R803	E743	E743	L683	K621	N558	N496	V431		V299	V237	M176	T112	D50
N804	Q744	Q744	N684	L622	P559	P497	E432	A364	V299	V238	E177	Y113	Y51
T805	L745	L745	G685	T623	N560	G498	E433		A302	N239	A179	Q114	Y52
A806	S746	S746	A686	T624	S561	L499	G434	T368	T303	T240	D180	F53	F53
T807	S747	S747	L687	K625	L582	A500	A435	V369	L304	M241	D181	A54	
S808	G748	G748	T688	T626	F563	E501	V436	K370	Q305	R242	D181	D118	L55
G809	F749	F749	L689	G627	D584	I502	K437	T371	D306	L243	W182	A56	A56
K810	F750	F750	G690	D628	V585	I503	R438	C372	I307	W244	L183	H57	H57
F811	S751	S751	T691	V629	O566	A504	I439	A373	I308	S245	R194	T58	T58
S812	V752	V752	M692	V630	Y567	E505	M440	Y374	R309	A246	Y185	E123	V59
S813	K753	K753	S693	N631	K586	R586		T376	R310	K247	G186	E124	R60
D814	Q754	Q754	G694	H632	R569	I507	H443	N376	F311	A248	N157	I125	D61
R815	P755	P755	A695	L570	L570	L444	K444	H377	K312	P249	P188	E126	H62
	D756	D756	N696	P634	H571	E509	C445	T378	S313	N250	W189	E127	L63

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PLP, SEP, 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	1.44	53/6873 (0.8%)	2.51	530/9300 (5.7%)
1	B	1.37	43/6873 (0.6%)	2.46	464/9298 (5.0%)
1	C	1.49	49/6873 (0.7%)	2.47	487/9300 (5.2%)
1	D	1.40	48/6873 (0.7%)	2.66	513/9300 (5.5%)
All	All	1.43	193/27492 (0.7%)	2.53	1994/37198 (5.4%)

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 193 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	24	VAL	C-N	48.27	1.95	1.33
1	A	47	THR	N-CA	-15.37	1.22	1.45
1	A	756	ASP	N-CA	14.51	1.77	1.46
1	A	543	LEU	N-CA	9.77	1.59	1.46
1	A	262	TYR	CA-C	9.34	1.63	1.52

The worst 5 of 1994 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	251	ASP	CA-CB-CG	57.27	169.87	112.60
1	D	24	VAL	O-C-N	42.80	165.09	121.87
1	D	250	ASN	CA-CB-CG	25.95	138.55	112.60
1	D	24	VAL	CA-C-N	-21.88	79.76	121.54
1	D	24	VAL	C-N-CA	-21.88	79.76	121.54

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	427	1
1	B	6733	0	6667	382	0
1	C	6732	0	6674	412	0
1	D	6732	0	6674	462	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	0	0
3	B	15	0	7	0	0
3	C	15	0	7	1	0
3	D	15	0	6	0	0
All	All	27029	0	26717	1646	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 31.

The worst 5 of 1646 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:N	1:A:756:ASP:CA	1.77	1.46
1:C:279:LEU:HD22	1:C:281:PRO:CD	1.62	1.28
1:C:24:VAL:C	1:C:25:THR:N	1.95	1.24
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

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

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%)	565 (79%)	149 (21%)	1	4
1	B	715/730 (98%)	586 (82%)	129 (18%)	2	6
1	C	714/730 (98%)	563 (79%)	151 (21%)	1	4
1	D	714/730 (98%)	546 (76%)	168 (24%)	1	3
All	All	2857/2920 (98%)	2260 (79%)	597 (21%)	1	4

5 of 597 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	181	ASP
1	D	676	THR
1	D	251	ASP
1	D	169	LYS
1	D	446	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 100 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	390	HIS
1	C	727	ASN
1	D	804	ASN
1	C	412	ASN
1	C	496	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	C	14	1	8,9,10	1.35	1 (12%)	7,12,14	4.36	2 (28%)
1	SEP	D	14	1	8,9,10	1.26	0	7,12,14	14.68	1 (14%)
1	SEP	A	14	1	8,9,10	1.20	0	7,12,14	3.04	2 (28%)
1	SEP	B	14	1	8,9,10	1.12	0	7,12,14	2.68	2 (28%)

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	C	14	1	-	3/6/8/10	-
1	SEP	D	14	1	-	5/6/8/10	-
1	SEP	A	14	1	-	5/6/8/10	-
1	SEP	B	14	1	-	6/6/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	14	SEP	CA-N	-2.24	1.41	1.48

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	14	SEP	OG-CB-CA	-38.78	70.41	108.14
1	C	14	SEP	OG-CB-CA	11.01	118.86	108.14
1	A	14	SEP	OG-CB-CA	7.29	115.24	108.14
1	B	14	SEP	OG-CB-CA	6.21	114.19	108.14
1	A	14	SEP	O2P-P-OG	2.96	114.38	106.67

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	14	SEP	N-CA-CB-OG
1	A	14	SEP	CA-CB-OG-P
1	A	14	SEP	CB-OG-P-O2P
1	A	14	SEP	CB-OG-P-O3P
1	B	14	SEP	C-CA-CB-OG

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 oligosaccharides 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	D	901	-	4,4,4	0.36	0	6,6,6	0.70	0
3	PLP	D	999	1	15,15,16	1.49	3 (20%)	21,22,23	1.21	2 (9%)
2	SO4	B	901	-	4,4,4	0.40	0	6,6,6	0.41	0
2	SO4	C	902	-	4,4,4	0.50	0	6,6,6	0.43	0
3	PLP	B	999	1	15,15,16	1.33	2 (13%)	21,22,23	1.73	2 (9%)
2	SO4	C	901	-	4,4,4	0.35	0	6,6,6	0.44	0
3	PLP	A	999	1	15,15,16	2.23	4 (26%)	21,22,23	1.54	5 (23%)
3	PLP	C	999	1	15,15,16	1.37	1 (6%)	21,22,23	1.22	2 (9%)
2	SO4	D	902	-	4,4,4	0.61	0	6,6,6	0.31	0
2	SO4	A	901	-	4,4,4	0.46	0	6,6,6	0.48	0
2	SO4	A	902	-	4,4,4	0.47	0	6,6,6	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	B	902	-	4,4,4	0.54	0	6,6,6	0.36	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
3	PLP	A	999	1	-	3/6/6/8	0/1/1/1
3	PLP	D	999	1	-	2/6/6/8	0/1/1/1
3	PLP	B	999	1	-	2/6/6/8	0/1/1/1
3	PLP	C	999	1	-	1/6/6/8	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	PLP	C5-C4	-5.43	1.34	1.40
3	C	999	PLP	C3-C2	-3.85	1.37	1.41
3	A	999	PLP	C3-C2	-3.52	1.37	1.41
3	D	999	PLP	C3-C2	-3.39	1.37	1.41
3	A	999	PLP	C2A-C2	-3.34	1.45	1.50

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	999	PLP	O4P-C5A-C5	5.48	119.62	109.36
3	A	999	PLP	C4A-C4-C5	-4.17	116.64	120.94
3	C	999	PLP	O4P-C5A-C5	3.58	116.08	109.36
3	D	999	PLP	O4P-C5A-C5	2.73	114.47	109.36
3	C	999	PLP	O3P-P-O4P	2.71	113.75	106.67

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	999	PLP	C5A-O4P-P-O2P
3	A	999	PLP	C5A-O4P-P-O3P
3	B	999	PLP	C5A-O4P-P-O2P
3	B	999	PLP	C5A-O4P-P-O3P
3	D	999	PLP	C5A-O4P-P-O2P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	24:VAL	C	25:THR	N	1.95

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.