



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 3, 2024 – 02:16 PM JST

PDB ID : 9J4H
Title : Crystal structure of SHMT apo form
Authors : Murayama, K.; Hayashi, H.
Deposited on : 2024-08-09
Resolution : 2.04 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.003 (Gargrove)
Density-Fitness : 1.0.11
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

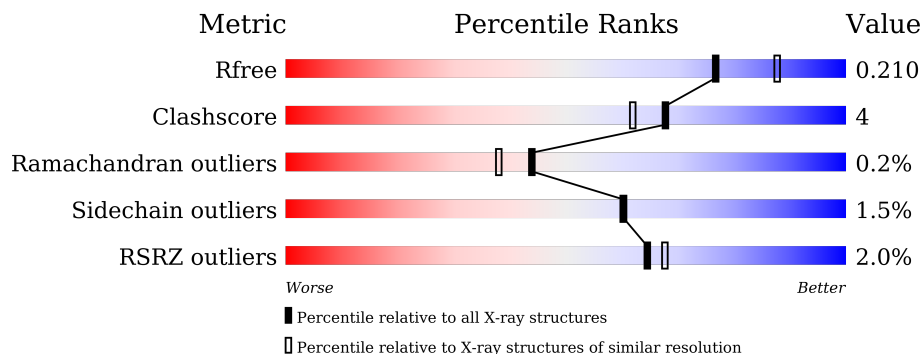
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

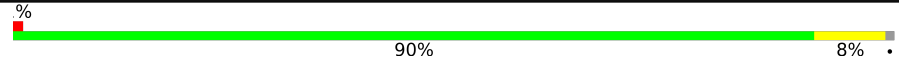
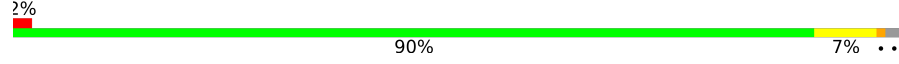
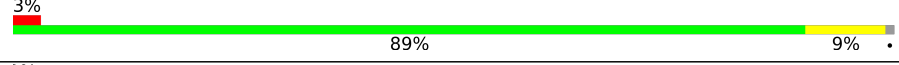
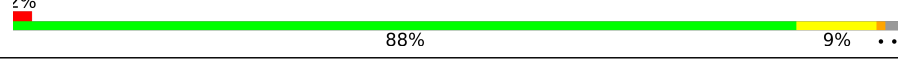
The reported resolution of this entry is 2.04 Å.

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}	164625	2096 (2.04-2.04)
Clashscore	180529	2229 (2.04-2.04)
Ramachandran outliers	177936	2217 (2.04-2.04)
Sidechain outliers	177891	2217 (2.04-2.04)
RSRZ outliers	164620	2096 (2.04-2.04)

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	417	 2% 90% 8%
1	B	417	 2% 90% 7%
1	C	417	 3% 89% 9%
1	D	417	 2% 88% 9%

2 Entry composition i

There are 3 unique types of molecules in this entry. The entry contains 13443 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.

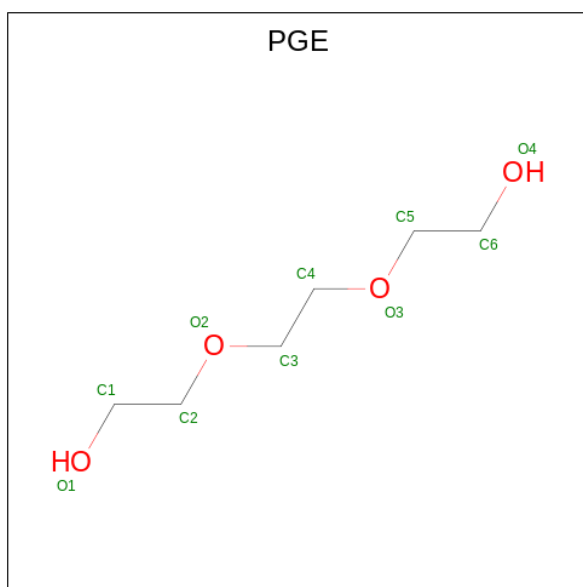
- Molecule 1 is a protein called Serine hydroxymethyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	P	S			
1	A	411	3144	1994	537	604	1	8	0	0	0
1	B	410	3137	1989	536	603	1	8	0	0	0
1	C	412	3155	2001	540	605	1	8	0	0	0
1	D	409	3127	1983	533	602	1	8	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP A0A133CK16
A	-1	PRO	-	expression tag	UNP A0A133CK16
A	0	GLY	-	expression tag	UNP A0A133CK16
A	1	VAL	-	expression tag	UNP A0A133CK16
B	-2	GLY	-	expression tag	UNP A0A133CK16
B	-1	PRO	-	expression tag	UNP A0A133CK16
B	0	GLY	-	expression tag	UNP A0A133CK16
B	1	VAL	-	expression tag	UNP A0A133CK16
C	-2	GLY	-	expression tag	UNP A0A133CK16
C	-1	PRO	-	expression tag	UNP A0A133CK16
C	0	GLY	-	expression tag	UNP A0A133CK16
C	1	VAL	-	expression tag	UNP A0A133CK16
D	-2	GLY	-	expression tag	UNP A0A133CK16
D	-1	PRO	-	expression tag	UNP A0A133CK16
D	0	GLY	-	expression tag	UNP A0A133CK16
D	1	VAL	-	expression tag	UNP A0A133CK16

- Molecule 2 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C₆H₁₄O₄).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 10 6 4	0	0
2	B	1	Total C O 10 6 4	0	0
2	C	1	Total C O 10 6 4	0	0
2	D	1	Total C O 10 6 4	0	0

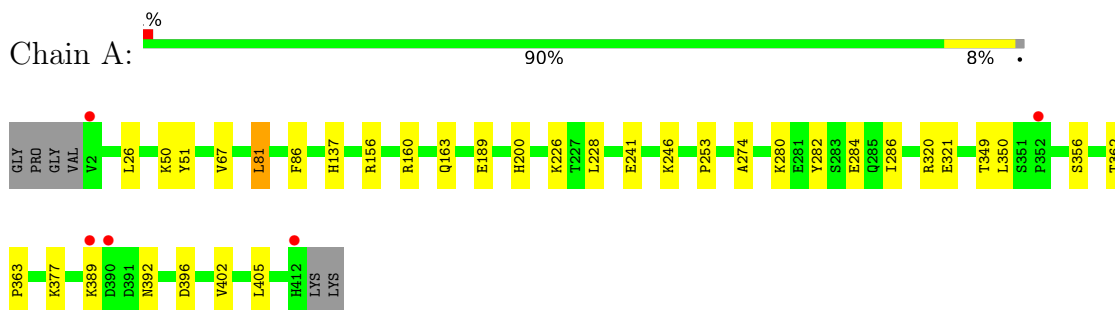
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	296	Total O 296 296	0	0
3	B	210	Total O 210 210	0	0
3	C	145	Total O 145 145	0	0
3	D	189	Total O 189 189	0	0

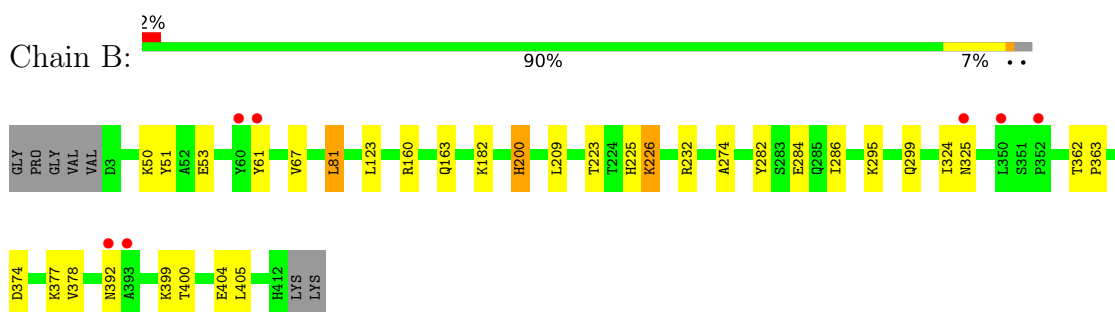
3 Residue-property plots [i](#)

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.

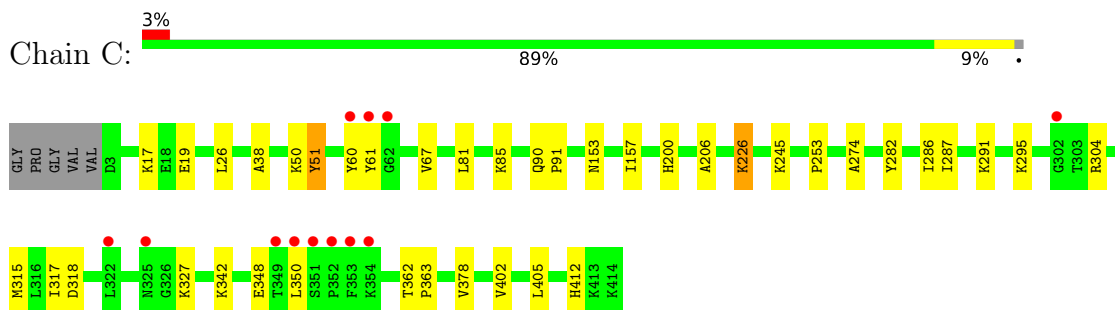
- Molecule 1: Serine hydroxymethyltransferase



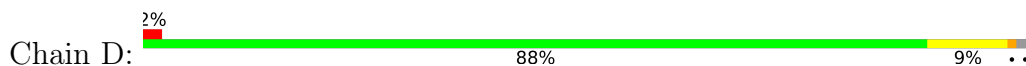
- Molecule 1: Serine hydroxymethyltransferase

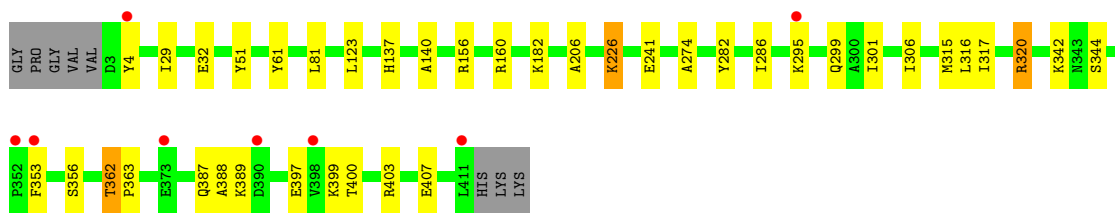


- Molecule 1: Serine hydroxymethyltransferase



- Molecule 1: Serine hydroxymethyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	276.92Å 68.09Å 95.34Å 90.00° 110.61° 90.00°	Depositor
Resolution (Å)	47.67 – 2.04 47.67 – 2.04	Depositor EDS
% Data completeness (in resolution range)	98.9 (47.67-2.04) 98.9 (47.67-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.05Å)	Xtrriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.196 , 0.210 0.196 , 0.210	Depositor DCC
R_{free} test set	104132 reflections (1.92%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtrriage
Anisotropy	0.307	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 35.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.006 for -h-2*1,-k,l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13443	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, LLP

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	0.27	0/3180	0.43	0/4313
1	B	0.26	0/3173	0.43	0/4303
1	C	0.26	0/3191	0.44	0/4325
1	D	0.26	0/3162	0.42	0/4288
All	All	0.26	0/12706	0.43	0/17229

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3144	0	3130	24	0
1	B	3137	0	3121	17	0
1	C	3155	0	3147	24	0
1	D	3127	0	3114	31	0
2	A	10	0	14	0	0
2	B	10	0	14	0	0
2	C	10	0	14	0	0
2	D	10	0	14	0	0
3	A	296	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	210	0	0	1	0
3	C	145	0	0	2	0
3	D	189	0	0	5	0
All	All	13443	0	12568	89	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 4.

All (89) 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:392:ASN:ND2	3:A:602:HOH:O	2.24	0.69
1:C:304:ARG:HB3	1:C:318:ASP:HB3	1.78	0.65
1:B:377:LYS:HD3	1:B:405:LEU:HD21	1.80	0.64
1:A:156:ARG:NH1	1:A:189:GLU:OE1	2.31	0.62
1:B:295:LYS:O	1:B:299:GLN:HG3	2.00	0.61
1:C:19:GLU:HG3	1:C:412:HIS:CD2	2.38	0.59
1:D:362:THR:H	1:D:363:PRO:HD3	1.67	0.57
1:B:200:HIS:HD2	1:B:226:LLP:O3	1.89	0.55
1:D:81:LEU:HD22	1:D:206:ALA:HB1	1.88	0.55
1:B:50:LYS:HG2	1:B:67:VAL:HG21	1.89	0.54
1:C:81:LEU:HD11	1:C:274:ALA:HB3	1.89	0.54
1:C:50:LYS:HG2	1:C:67:VAL:HG21	1.91	0.53
1:A:241:GLU:H	1:A:241:GLU:CD	2.12	0.52
1:B:378:VAL:HG12	1:B:405:LEU:HD13	1.91	0.52
1:C:362:THR:N	1:C:363:PRO:HD3	2.25	0.52
1:C:51:TYR:HB3	1:C:61:TYR:CE1	2.44	0.52
1:D:182:LYS:HD3	3:D:609:HOH:O	2.10	0.51
1:D:306:ILE:HD13	1:D:316:LEU:HB3	1.92	0.51
1:A:282:TYR:CZ	1:A:286:ILE:HD11	2.46	0.50
1:B:282:TYR:CZ	1:B:286:ILE:HD11	2.47	0.50
1:D:342:LYS:HE3	1:D:353:PHE:CD2	2.46	0.50
1:A:320:ARG:HB2	1:A:356:SER:OG	2.12	0.49
1:C:315:MET:HG3	1:C:317:ILE:HD11	1.95	0.49
1:C:327:LYS:HB2	1:C:342:LYS:HD3	1.94	0.49
1:C:348:GLU:HG3	1:C:350:LEU:H	1.78	0.49
1:C:291:LYS:O	1:C:295:LYS:HG2	2.14	0.48
1:D:320:ARG:HB2	1:D:356:SER:OG	2.13	0.48
1:A:86:PHE:HZ	1:A:241:GLU:HG3	1.79	0.48
1:C:85:LYS:NZ	3:C:616:HOH:O	2.46	0.48
1:A:86:PHE:CZ	1:A:241:GLU:HG3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:HIS:NE2	1:D:356:SER:HB2	2.29	0.47
1:A:321:GLU:HB2	3:A:753:HOH:O	2.14	0.47
1:A:163:GLN:NE2	3:A:607:HOH:O	2.35	0.47
1:D:389:LYS:HA	1:D:389:LYS:HD2	1.74	0.47
1:B:324:ILE:HG22	1:B:325:ASN:O	2.15	0.47
1:C:253:PRO:HB2	1:D:123:LEU:HD21	1.97	0.46
1:D:301:ILE:HG22	1:D:387:GLN:NE2	2.31	0.46
1:D:61:TYR:N	3:D:602:HOH:O	2.25	0.46
1:A:246:LYS:NZ	3:A:618:HOH:O	2.47	0.46
1:A:389:LYS:HE2	3:A:859:HOH:O	2.14	0.46
1:B:81:LEU:HD11	1:B:274:ALA:HB3	1.98	0.46
1:C:153:ASN:O	1:C:157:ILE:HG12	2.15	0.46
1:C:81:LEU:HD22	1:C:206:ALA:HB1	1.98	0.45
1:D:81:LEU:HD11	1:D:274:ALA:HB3	1.99	0.45
1:D:295:LYS:NZ	3:D:614:HOH:O	2.49	0.45
1:D:295:LYS:O	1:D:299:GLN:HG3	2.16	0.45
1:A:160:ARG:NE	1:A:189:GLU:OE2	2.48	0.45
1:D:295:LYS:HD3	1:D:295:LYS:HA	1.80	0.44
1:C:226:LLP:NZ	1:C:226:LLP:O3	2.33	0.44
1:C:282:TYR:CZ	1:C:286:ILE:HD11	2.52	0.44
1:C:51:TYR:HB3	1:C:61:TYR:HE1	1.82	0.44
1:C:287:ILE:HG22	1:C:291:LYS:HE2	1.99	0.44
1:A:356:SER:HB2	1:D:137:HIS:CE1	2.53	0.43
1:C:26:LEU:HD12	1:C:402:VAL:HG22	2.00	0.43
1:D:282:TYR:CZ	1:D:286:ILE:HD11	2.53	0.43
1:C:378:VAL:HG12	1:C:405:LEU:HD13	1.99	0.43
1:A:81:LEU:HD11	1:A:274:ALA:HB3	2.01	0.43
1:D:29:ILE:HB	1:D:32:GLU:HG3	2.01	0.43
1:D:399:LYS:HG2	3:D:604:HOH:O	2.19	0.43
1:A:349:THR:HG22	1:D:140:ALA:HB2	2.00	0.43
1:D:315:MET:HG3	1:D:317:ILE:HD11	2.01	0.43
1:B:53:GLU:OE2	1:B:61:TYR:OH	2.31	0.42
1:D:362:THR:N	1:D:363:PRO:CD	2.82	0.42
1:B:209:LEU:HD11	1:B:284:GLU:HG3	2.00	0.42
1:B:374:ASP:O	1:B:378:VAL:HG13	2.19	0.42
1:A:253:PRO:HB2	1:B:123:LEU:HD21	2.02	0.42
1:D:403:ARG:O	1:D:407:GLU:HG3	2.20	0.42
1:A:356:SER:HB2	1:D:137:HIS:NE2	2.34	0.42
1:C:362:THR:N	1:C:363:PRO:CD	2.82	0.42
1:D:320:ARG:HB2	1:D:356:SER:HG	1.84	0.42
1:D:397:GLU:O	1:D:400:THR:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:GLN:N	1:C:91:PRO:CD	2.83	0.41
1:A:280:LYS:NZ	1:A:284:GLU:OE2	2.48	0.41
1:A:362:THR:N	1:A:363:PRO:CD	2.84	0.41
1:B:362:THR:N	1:B:363:PRO:CD	2.83	0.41
3:C:602:HOH:O	1:D:226:LLP:H5'1	2.20	0.41
1:A:26:LEU:HG	1:A:402:VAL:HG13	2.02	0.41
1:A:377:LYS:HD3	1:A:405:LEU:HD21	2.02	0.41
1:D:226:LLP:NZ	1:D:226:LLP:O3	2.37	0.41
1:A:50:LYS:HG2	1:A:67:VAL:HG11	2.02	0.41
3:B:720:HOH:O	1:C:245:LYS:HD3	2.21	0.41
1:D:160:ARG:HD3	3:D:655:HOH:O	2.20	0.41
1:A:362:THR:N	1:A:363:PRO:HD3	2.36	0.40
1:C:38:ALA:HB2	1:D:4:TYR:HB2	2.04	0.40
1:D:156:ARG:O	1:D:160:ARG:HG3	2.20	0.40
1:B:160:ARG:HA	1:B:163:GLN:OE1	2.21	0.40
1:B:223:THR:HB	1:B:225:HIS:CE1	2.57	0.40
1:B:226:LLP:O3	1:B:226:LLP:NZ	2.42	0.40
1:B:400:THR:O	1:B:404:GLU:HG3	2.22	0.40

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	408/417 (98%)	392 (96%)	15 (4%)	1 (0%)	44	38
1	B	407/417 (98%)	393 (97%)	14 (3%)	0	100	100
1	C	409/417 (98%)	394 (96%)	15 (4%)	0	100	100
1	D	406/417 (97%)	394 (97%)	10 (2%)	2 (0%)	25	17
All	All	1630/1668 (98%)	1573 (96%)	54 (3%)	3 (0%)	44	38

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	388	ALA
1	A	350	LEU
1	D	362	THR

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	326/330 (99%)	321 (98%)	5 (2%)	60	60
1	B	325/330 (98%)	318 (98%)	7 (2%)	47	43
1	C	327/330 (99%)	323 (99%)	4 (1%)	67	68
1	D	324/330 (98%)	320 (99%)	4 (1%)	67	68
All	All	1302/1320 (99%)	1282 (98%)	20 (2%)	60	60

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	TYR
1	A	81	LEU
1	A	200	HIS
1	A	228	LEU
1	A	396	ASP
1	B	51	TYR
1	B	81	LEU
1	B	182	LYS
1	B	200	HIS
1	B	232	ARG
1	B	392	ASN
1	B	399	LYS
1	C	17	LYS
1	C	51	TYR
1	C	60	TYR
1	C	200	HIS
1	D	51	TYR
1	D	241	GLU
1	D	320	ARG

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Mol	Chain	Res	Type
1	D	344	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	200	HIS
1	C	337	ASN
1	C	412	HIS

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	LLP	C	226	1	23,24,25	1.95	5 (21%)	25,32,34	1.80	6 (24%)
1	LLP	B	226	1	23,24,25	1.95	5 (21%)	25,32,34	1.48	5 (20%)
1	LLP	A	226	1	23,24,25	1.98	5 (21%)	25,32,34	1.42	4 (16%)
1	LLP	D	226	1	23,24,25	1.97	5 (21%)	25,32,34	1.80	6 (24%)

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	C	226	1	-	3/16/17/19	0/1/1/1
1	LLP	B	226	1	-	3/16/17/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	A	226	1	-	4/16/17/19	0/1/1/1
1	LLP	D	226	1	-	3/16/17/19	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	226	LLP	C4'-NZ	4.89	1.43	1.27
1	A	226	LLP	C4'-NZ	4.88	1.43	1.27
1	B	226	LLP	C4'-NZ	4.88	1.43	1.27
1	C	226	LLP	C4'-NZ	4.85	1.43	1.27
1	C	226	LLP	C4-C5	-4.42	1.36	1.42
1	A	226	LLP	C4-C5	-4.33	1.36	1.42
1	D	226	LLP	C4-C5	-4.32	1.36	1.42
1	B	226	LLP	C4-C5	-4.19	1.36	1.42
1	A	226	LLP	C4-C4'	3.67	1.53	1.46
1	B	226	LLP	C4-C4'	3.60	1.53	1.46
1	C	226	LLP	C4-C4'	3.53	1.53	1.46
1	D	226	LLP	C4-C4'	3.49	1.53	1.46
1	D	226	LLP	C4-C3	-3.41	1.35	1.40
1	B	226	LLP	C4-C3	-3.35	1.35	1.40
1	A	226	LLP	C4-C3	-3.31	1.35	1.40
1	C	226	LLP	C4-C3	-3.25	1.36	1.40
1	D	226	LLP	C3-C2	-2.31	1.38	1.40
1	B	226	LLP	C3-C2	-2.23	1.38	1.40
1	C	226	LLP	C3-C2	-2.22	1.38	1.40
1	A	226	LLP	C3-C2	-2.13	1.38	1.40

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	226	LLP	C4-C4'-NZ	-5.04	101.18	124.31
1	D	226	LLP	C4-C4'-NZ	-4.66	102.92	124.31
1	D	226	LLP	CE-NZ-C4'	3.39	129.30	118.90
1	A	226	LLP	OP2-P-OP4	2.87	114.37	106.73
1	D	226	LLP	OP4-P-OP1	2.80	114.33	106.47
1	B	226	LLP	OP2-P-OP4	2.80	114.18	106.73
1	C	226	LLP	OP3-P-OP4	2.79	114.17	106.73
1	C	226	LLP	OP2-P-OP4	2.76	114.09	106.73
1	B	226	LLP	OP3-P-OP4	2.75	114.06	106.73
1	D	226	LLP	OP2-P-OP4	2.73	114.01	106.73
1	C	226	LLP	OP4-P-OP1	2.65	113.92	106.47
1	D	226	LLP	OP3-P-OP4	2.58	113.59	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	226	LLP	OP4-P-OP1	2.57	113.68	106.47
1	A	226	LLP	OP3-P-OP4	2.55	113.52	106.73
1	A	226	LLP	OP4-P-OP1	2.55	113.62	106.47
1	C	226	LLP	CE-NZ-C4'	2.54	126.70	118.90
1	B	226	LLP	OP4-C5'-C5	2.29	113.72	109.35
1	C	226	LLP	C5-C6-N1	-2.18	120.18	123.82
1	A	226	LLP	C5-C6-N1	-2.13	120.28	123.82
1	B	226	LLP	CD-CE-NZ	2.10	116.08	110.93
1	D	226	LLP	C5-C6-N1	-2.08	120.36	123.82

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	226	LLP	C4-C4'-NZ-CE
1	A	226	LLP	O-C-CA-CB
1	B	226	LLP	C4-C4'-NZ-CE
1	B	226	LLP	O-C-CA-CB
1	C	226	LLP	O-C-CA-CB
1	D	226	LLP	O-C-CA-CB
1	A	226	LLP	CG-CD-CE-NZ
1	D	226	LLP	CD-CE-NZ-C4'
1	B	226	LLP	CD-CE-NZ-C4'
1	C	226	LLP	CD-CE-NZ-C4'
1	D	226	LLP	C3-C4-C4'-NZ
1	A	226	LLP	CD-CE-NZ-C4'
1	C	226	LLP	C3-C4-C4'-NZ

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	226	LLP	1	0
1	B	226	LLP	2	0
1	D	226	LLP	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 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	PGE	C	501	-	9,9,9	0.30	0	8,8,8	0.28	0
2	PGE	A	501	-	9,9,9	0.32	0	8,8,8	0.31	0
2	PGE	D	501	-	9,9,9	0.31	0	8,8,8	0.33	0
2	PGE	B	501	-	9,9,9	0.31	0	8,8,8	0.31	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	PGE	C	501	-	-	2/7/7/7	-
2	PGE	A	501	-	-	3/7/7/7	-
2	PGE	D	501	-	-	5/7/7/7	-
2	PGE	B	501	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PGE	O2-C3-C4-O3
2	C	501	PGE	O2-C3-C4-O3
2	B	501	PGE	O2-C3-C4-O3
2	D	501	PGE	O1-C1-C2-O2
2	A	501	PGE	O3-C5-C6-O4
2	D	501	PGE	C3-C4-O3-C5
2	D	501	PGE	O2-C3-C4-O3

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Mol	Chain	Res	Type	Atoms
2	B	501	PGE	O3-C5-C6-O4
2	D	501	PGE	O3-C5-C6-O4
2	D	501	PGE	C1-C2-O2-C3
2	A	501	PGE	C4-C3-O2-C2
2	C	501	PGE	O1-C1-C2-O2
2	B	501	PGE	C4-C3-O2-C2

There are no ring outliers.

No monomer is involved in short contacts.

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

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	410/417 (98%)	-0.45	5 (1%) 76 79	22, 29, 45, 80	0
1	B	409/417 (98%)	-0.19	7 (1%) 69 71	22, 37, 58, 84	0
1	C	411/417 (98%)	0.22	12 (2%) 54 55	28, 45, 71, 106	0
1	D	408/417 (97%)	-0.00	8 (1%) 64 68	25, 39, 64, 99	0
All	All	1638/1668 (98%)	-0.11	32 (1%) 64 68	22, 38, 64, 106	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	353	PHE	4.4
1	C	62	GLY	4.3
1	A	2	VAL	4.1
1	C	352	PRO	3.9
1	A	352	PRO	3.8
1	A	412	HIS	3.5
1	B	60	TYR	3.2
1	C	60	TYR	3.2
1	C	350	LEU	3.1
1	B	352	PRO	3.1
1	C	61	TYR	2.8
1	C	349	THR	2.8
1	C	302	GLY	2.7
1	D	411	LEU	2.6
1	A	389	LYS	2.6
1	B	350	LEU	2.5
1	C	322	LEU	2.4
1	D	352	PRO	2.3
1	D	390	ASP	2.3
1	D	4	TYR	2.3
1	C	351	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	354	LYS	2.1
1	B	392	ASN	2.1
1	D	373	GLU	2.1
1	B	61	TYR	2.1
1	C	325	ASN	2.1
1	D	353	PHE	2.0
1	B	325	ASN	2.0
1	B	393	ALA	2.0
1	D	295	LYS	2.0
1	D	398	VAL	2.0
1	A	390	ASP	2.0

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	C	226	24/25	0.94	0.09	32,39,43,46	0
1	LLP	B	226	24/25	0.95	0.08	29,34,39,40	0
1	LLP	D	226	24/25	0.95	0.07	27,35,39,44	0
1	LLP	A	226	24/25	0.96	0.07	21,28,36,42	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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	PGE	D	501	10/10	0.78	0.14	46,55,59,65	0
2	PGE	B	501	10/10	0.82	0.13	40,47,52,52	0
2	PGE	C	501	10/10	0.84	0.11	45,52,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PGE	A	501	10/10	0.89	0.10	27,35,42,43	0

6.5 Other polymers [i](#)

There are no such residues in this entry.