



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:05 PM UTC

PDB ID : 2FM1 / pdb_00002fm1
Title : Crystal structure of L-ALLO-threonine aldolase (tm1744) from *Thermotoga maritima* at 2.25 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2006-01-06
Resolution : 2.25 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

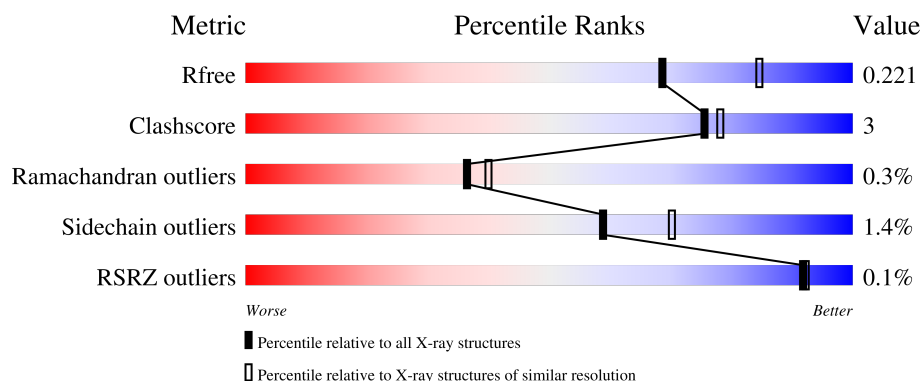
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	355	90% 6% ..
1	B	355	90% 6% ..
1	C	355	89% 7% .
1	D	355	86% 10% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11599 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 L-allo-threonine aldolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	P	S	0	0	0
			2633	1645	469	502	1	16			
1	B	343	Total	C	N	O	P	S	0	2	0
			2630	1645	471	497	1	16			
1	C	343	Total	C	N	O	P	S	0	1	0
			2633	1648	466	502	1	16			
1	D	345	Total	C	N	O	P	S	0	0	0
			2625	1645	464	499	1	16			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	GB 4982322
A	-10	GLY	-	expression tag	GB 4982322
A	-9	SER	-	expression tag	GB 4982322
A	-8	ASP	-	expression tag	GB 4982322
A	-7	LYS	-	expression tag	GB 4982322
A	-6	ILE	-	expression tag	GB 4982322
A	-5	HIS	-	expression tag	GB 4982322
A	-4	HIS	-	expression tag	GB 4982322
A	-3	HIS	-	expression tag	GB 4982322
A	-2	HIS	-	expression tag	GB 4982322
A	-1	HIS	-	expression tag	GB 4982322
A	0	HIS	-	expression tag	GB 4982322
A	199	LLP	LYS	modified residue	GB 4982322
B	-11	MET	-	expression tag	GB 4982322
B	-10	GLY	-	expression tag	GB 4982322
B	-9	SER	-	expression tag	GB 4982322
B	-8	ASP	-	expression tag	GB 4982322
B	-7	LYS	-	expression tag	GB 4982322
B	-6	ILE	-	expression tag	GB 4982322
B	-5	HIS	-	expression tag	GB 4982322
B	-4	HIS	-	expression tag	GB 4982322

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	HIS	-	expression tag	GB 4982322
B	-2	HIS	-	expression tag	GB 4982322
B	-1	HIS	-	expression tag	GB 4982322
B	0	HIS	-	expression tag	GB 4982322
B	199	LLP	LYS	modified residue	GB 4982322
C	-11	MET	-	expression tag	GB 4982322
C	-10	GLY	-	expression tag	GB 4982322
C	-9	SER	-	expression tag	GB 4982322
C	-8	ASP	-	expression tag	GB 4982322
C	-7	LYS	-	expression tag	GB 4982322
C	-6	ILE	-	expression tag	GB 4982322
C	-5	HIS	-	expression tag	GB 4982322
C	-4	HIS	-	expression tag	GB 4982322
C	-3	HIS	-	expression tag	GB 4982322
C	-2	HIS	-	expression tag	GB 4982322
C	-1	HIS	-	expression tag	GB 4982322
C	0	HIS	-	expression tag	GB 4982322
C	199	LLP	LYS	modified residue	GB 4982322
D	-11	MET	-	expression tag	GB 4982322
D	-10	GLY	-	expression tag	GB 4982322
D	-9	SER	-	expression tag	GB 4982322
D	-8	ASP	-	expression tag	GB 4982322
D	-7	LYS	-	expression tag	GB 4982322
D	-6	ILE	-	expression tag	GB 4982322
D	-5	HIS	-	expression tag	GB 4982322
D	-4	HIS	-	expression tag	GB 4982322
D	-3	HIS	-	expression tag	GB 4982322
D	-2	HIS	-	expression tag	GB 4982322
D	-1	HIS	-	expression tag	GB 4982322
D	0	HIS	-	expression tag	GB 4982322
D	199	LLP	LYS	modified residue	GB 4982322

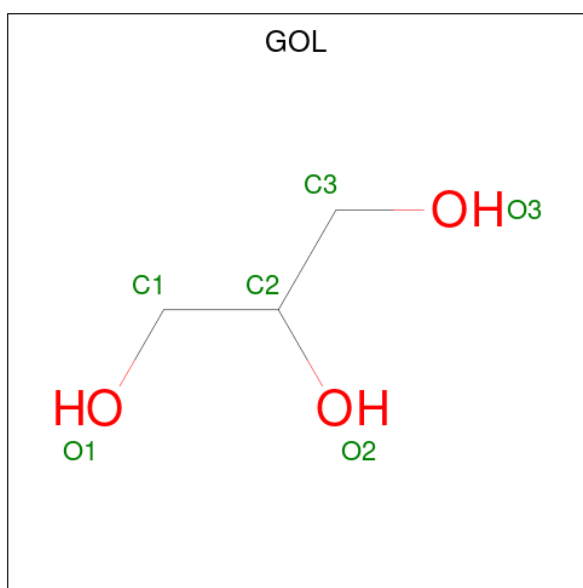
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ca 2 2	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Cl	0	0
			3	3		
3	B	3	Total	Cl	0	0
			3	3		
3	C	2	Total	Cl	0	0
			2	2		
3	D	2	Total	Cl	0	0
			2	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Na	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	258	Total	O	0	0
			258	258		

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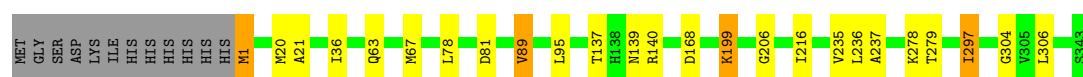
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	261	Total 261	O 261	0	0
6	C	273	Total 273	O 273	0	0
6	D	267	Total 267	O 267	0	0

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.

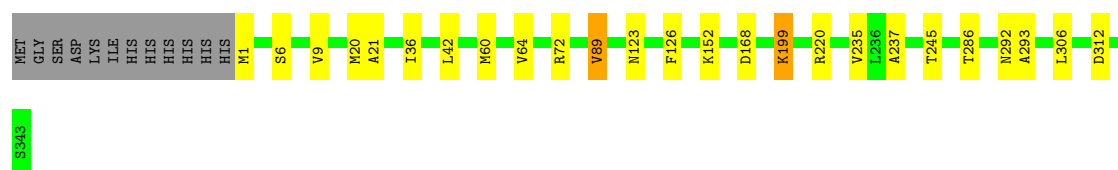
- Molecule 1: L-allo-threonine aldolase

Chain A: 



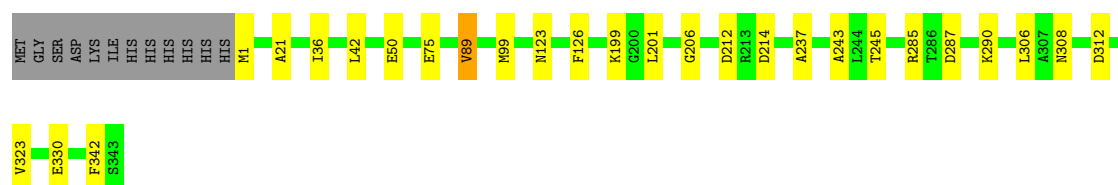
- Molecule 1: L-allo-threonine aldolase

Chain B: 



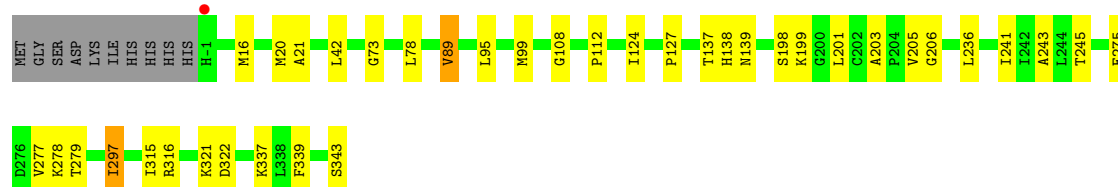
- Molecule 1: L-allo-threonine aldolase

Chain C: 



- Molecule 1: L-allo-threonine aldolase

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	95.61Å 100.41Å 149.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.33 – 2.25 83.33 – 2.25	Depositor EDS
% Data completeness (in resolution range)	96.9 (83.33-2.25) 96.9 (83.33-2.25)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.25Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.142 , 0.216 0.158 , 0.221	Depositor DCC
R_{free} test set	3400 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	25.7	Xtriage
Anisotropy	0.433	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.001 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11599	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, CA, GOL, CL, 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	1.02	2/2649 (0.1%)	1.01	2/3577 (0.1%)
1	B	1.01	0/2652	1.03	0/3582
1	C	1.03	0/2652	1.00	1/3582 (0.0%)
1	D	1.05	2/2643 (0.1%)	1.04	1/3573 (0.0%)
All	All	1.03	4/10596 (0.0%)	1.02	4/14314 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	277	VAL	CA-CB	6.23	1.60	1.53
1	A	297	ILE	CA-CB	5.92	1.60	1.54
1	D	297	ILE	CA-CB	5.24	1.60	1.54
1	A	216	ILE	CA-CB	5.02	1.61	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	GLY	N-CA-C	8.95	121.17	112.04
1	C	206	GLY	N-CA-C	7.67	119.82	112.08
1	D	206	GLY	N-CA-C	5.86	118.02	112.04
1	A	139	ASN	N-CA-C	5.19	116.74	111.14

There are no chirality outliers.

There are no planarity outliers.

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	2633	0	2619	16	0
1	B	2630	0	2620	13	0
1	C	2633	0	2623	16	0
1	D	2625	0	2586	24	0
2	A	2	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	C	6	0	8	0	0
5	D	1	0	0	0	0
6	A	258	0	0	1	0
6	B	261	0	0	0	0
6	C	273	0	0	4	0
6	D	267	0	0	2	0
All	All	11599	0	10456	62	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 3.

All (62) 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:D:339:PHE:O	1:D:343:SER:HB3	1.76	0.84
1:A:1:MET:HE2	1:A:306:LEU:HG	1.69	0.75
1:C:290:LYS:NZ	6:C:601:HOH:O	2.21	0.72
1:A:21:ALA:HB2	1:D:21:ALA:HB2	1.78	0.66
1:C:36:ILE:HD13	1:C:237:ALA:HB2	1.76	0.66
1:B:21:ALA:HB2	1:C:21:ALA:HB2	1.77	0.66
1:D:337:LYS:HD2	6:D:409:HOH:O	1.95	0.65
1:C:42:LEU:HD21	1:C:245:THR:CG2	2.28	0.64
1:A:1:MET:HE3	1:A:304:GLY:C	2.27	0.60
1:D:339:PHE:O	1:D:343:SER:CB	2.50	0.58
1:A:1:MET:HE3	1:A:304:GLY:HA2	1.86	0.58
1:C:1:MET:HE2	1:C:306:LEU:HD21	1.86	0.57
1:A:36:ILE:HD13	1:A:237:ALA:HB2	1.86	0.57
1:D:139:ASN:OD1	1:D:316:ARG:NH1	2.40	0.55
1:B:1:MET:HE2	1:B:306:LEU:HD21	1.90	0.54
1:C:1:MET:CE	1:C:306:LEU:HD21	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:LYS:HE3	1:D:322:ASP:OD1	2.08	0.52
1:C:214:ASP:HB2	6:C:471:HOH:O	2.08	0.52
1:B:1:MET:CE	1:B:306:LEU:HD21	2.41	0.51
1:B:20:MET:HG2	1:B:235:VAL:O	2.11	0.51
1:D:201:LEU:HB3	1:D:243:ALA:HB1	1.93	0.50
1:A:95:LEU:HD22	1:D:95:LEU:HD22	1.92	0.50
1:D:297:ILE:HD11	1:D:315:ILE:HG12	1.94	0.50
1:B:42:LEU:HD21	1:B:245:THR:CG2	2.42	0.49
1:C:330:GLU:HG2	6:C:397:HOH:O	2.12	0.49
1:A:1:MET:HE3	1:A:304:GLY:CA	2.42	0.48
1:A:137:THR:HG21	1:A:279:THR:HG21	1.95	0.47
1:D:275:GLU:O	1:D:278:LYS:NZ	2.47	0.47
1:A:278:LYS:HG3	6:A:355:HOH:O	2.15	0.47
1:A:63:GLN:O	1:A:67:MET:HG3	2.15	0.46
1:A:81:ASP:O	1:A:140:ARG:HD3	2.15	0.46
1:B:168:ASP:OD2	1:B:199:LLP:N1	2.48	0.46
1:D:205:VAL:HB	1:D:236:LEU:HD22	1.98	0.45
1:C:50:GLU:HG2	1:C:212:ASP:HA	1.99	0.45
1:B:6:SER:O	1:B:9:VAL:HG22	2.16	0.45
1:D:16:MET:O	1:D:20:MET:HG3	2.16	0.45
1:A:20:MET:HG2	1:A:235:VAL:O	2.18	0.44
1:C:285:ARG:HH11	1:C:285:ARG:HG3	1.82	0.44
1:A:168:ASP:OD2	1:A:199:LLP:N1	2.51	0.44
1:D:42:LEU:HD21	1:D:245:THR:CG2	2.48	0.44
1:D:108:GLY:HA2	1:D:138:HIS:CD2	2.52	0.44
1:D:73:GLY:O	1:D:127:PRO:HB3	2.18	0.44
1:B:286:THR:HG21	1:B:293:ALA:HA	1.99	0.44
1:B:292:ASN:HB2	1:B:312:ASP:O	2.18	0.44
1:C:123:ASN:HB3	1:C:126:PHE:CD2	2.53	0.44
1:C:201:LEU:HB3	1:C:243:ALA:HB1	1.99	0.43
1:A:21:ALA:HB2	1:D:21:ALA:CB	2.47	0.42
1:B:123:ASN:HB3	1:B:126:PHE:CD2	2.53	0.42
1:D:198:SER:HA	1:D:203:ALA:O	2.19	0.42
1:A:235:VAL:HG21	1:D:20:MET:HE1	2.01	0.42
1:B:36:ILE:HD13	1:B:237:ALA:HB2	2.02	0.42
1:C:42:LEU:HD21	1:C:245:THR:HG21	2.02	0.42
1:C:75:GLU:HG3	1:C:99:MET:HB2	2.02	0.41
1:D:337:LYS:HE2	6:D:410:HOH:O	2.21	0.41
1:A:236:LEU:HD11	1:D:236:LEU:HD11	2.02	0.41
1:D:321:LYS:HE2	1:D:321:LYS:HB3	1.93	0.41
1:B:60:MET:O	1:B:64:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ARG:HG2	1:D:124:ILE:HD11	2.02	0.41
1:D:241:ILE:O	1:D:245:THR:HG23	2.21	0.41
1:D:137:THR:HG21	1:D:279:THR:HG21	2.03	0.40
1:C:290:LYS:HG3	1:C:342:PHE:O	2.22	0.40
1:C:308:ASN:HB2	6:C:402:HOH:O	2.21	0.40

There are no symmetry-related clashes.

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	340/355 (96%)	332 (98%)	7 (2%)	1 (0%)	36	40
1	B	342/355 (96%)	335 (98%)	6 (2%)	1 (0%)	36	40
1	C	341/355 (96%)	335 (98%)	5 (2%)	1 (0%)	36	40
1	D	342/355 (96%)	335 (98%)	6 (2%)	1 (0%)	36	40
All	All	1365/1420 (96%)	1337 (98%)	24 (2%)	4 (0%)	36	40

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	89	VAL
1	A	89	VAL
1	C	89	VAL
1	D	89	VAL

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	274/291 (94%)	270 (98%)	4 (2%)	57	68
1	B	273/291 (94%)	270 (99%)	3 (1%)	65	75
1	C	275/291 (94%)	271 (98%)	4 (2%)	57	68
1	D	269/291 (92%)	265 (98%)	4 (2%)	57	68
All	All	1091/1164 (94%)	1076 (99%)	15 (1%)	59	70

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	78	LEU
1	A	89	VAL
1	A	297	ILE
1	B	72	ARG
1	B	89	VAL
1	B	152	LYS
1	C	89	VAL
1	C	287	ASP
1	C	312	ASP
1	C	323	VAL
1	D	78	LEU
1	D	89	VAL
1	D	99	MET
1	D	112	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	71	GLN
1	A	174	ASN
1	A	273	ASN
1	B	63	GLN
1	B	107	ASN
1	B	308	ASN
1	B	326	ASN
1	C	71	GLN
1	C	174	ASN

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Mol	Chain	Res	Type
1	D	71	GLN
1	D	150	ASN
1	D	308	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	A	199	1	23,24,25	1.79	6 (26%)	25,32,34	1.97	5 (20%)
1	LLP	D	199	1	23,24,25	1.65	5 (21%)	25,32,34	2.30	7 (28%)
1	LLP	C	199	1	23,24,25	1.67	6 (26%)	25,32,34	2.51	9 (36%)
1	LLP	B	199	1	23,24,25	1.81	5 (21%)	25,32,34	2.12	4 (16%)

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	199	1	-	6/16/17/19	0/1/1/1
1	LLP	D	199	1	-	8/16/17/19	0/1/1/1
1	LLP	C	199	1	-	7/16/17/19	0/1/1/1
1	LLP	B	199	1	-	5/16/17/19	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	199	LLP	O3-C3	-5.65	1.24	1.36
1	A	199	LLP	O3-C3	-5.35	1.24	1.36
1	D	199	LLP	O3-C3	-4.84	1.25	1.36
1	C	199	LLP	O3-C3	-4.68	1.26	1.36
1	A	199	LLP	C2-N1	3.19	1.39	1.33
1	C	199	LLP	C2-N1	2.76	1.38	1.33
1	D	199	LLP	C4-C4'	2.70	1.52	1.46
1	A	199	LLP	C4-C4'	2.69	1.52	1.46
1	A	199	LLP	C6-N1	2.65	1.39	1.34
1	C	199	LLP	C4-C4'	2.60	1.52	1.46
1	C	199	LLP	C6-N1	2.56	1.39	1.34
1	D	199	LLP	P-OP3	-2.51	1.45	1.54
1	D	199	LLP	C2-N1	2.47	1.38	1.33
1	B	199	LLP	C4'-NZ	2.47	1.35	1.27
1	B	199	LLP	C4-C4'	2.45	1.51	1.46
1	B	199	LLP	C2-N1	2.35	1.38	1.33
1	B	199	LLP	P-OP2	-2.35	1.46	1.54
1	C	199	LLP	P-OP3	-2.34	1.46	1.54
1	C	199	LLP	C2'-C2	2.16	1.53	1.50
1	A	199	LLP	P-OP3	-2.14	1.46	1.54
1	D	199	LLP	C6-N1	2.14	1.38	1.34
1	A	199	LLP	C4'-NZ	2.05	1.34	1.27

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	LLP	OP4-C5'-C5	8.67	125.61	109.36
1	B	199	LLP	OP4-C5'-C5	8.22	124.76	109.36
1	D	199	LLP	OP4-C5'-C5	7.99	124.33	109.36
1	A	199	LLP	OP4-C5'-C5	6.67	121.86	109.36
1	B	199	LLP	C4-C4'-NZ	-4.52	103.17	124.04
1	C	199	LLP	C4-C4'-NZ	-4.06	105.32	124.04
1	D	199	LLP	C4-C4'-NZ	-4.05	105.33	124.04
1	A	199	LLP	C4-C4'-NZ	-3.57	107.56	124.04
1	C	199	LLP	OP3-P-OP2	3.43	120.65	107.80
1	C	199	LLP	OP2-P-OP4	-3.29	98.09	106.67
1	D	199	LLP	C5'-C5-C6	-2.86	114.71	119.36
1	A	199	LLP	C5-C6-N1	-2.77	119.32	123.83
1	D	199	LLP	OP3-P-OP2	2.73	118.04	107.80
1	C	199	LLP	CD-CE-NZ	-2.70	103.69	110.83
1	C	199	LLP	C2'-C2-N1	2.52	122.39	117.64
1	C	199	LLP	C5-C6-N1	-2.41	119.90	123.83
1	C	199	LLP	C3-C2-N1	-2.34	118.01	120.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	199	LLP	CD-CE-NZ	-2.33	104.66	110.83
1	D	199	LLP	C3-C4-C4'	-2.28	116.28	120.40
1	D	199	LLP	C5-C6-N1	-2.27	120.15	123.83
1	C	199	LLP	C3-C4-C5	2.18	120.02	118.28
1	A	199	LLP	OP2-P-OP1	2.17	119.30	110.83
1	B	199	LLP	C5'-C5-C6	-2.16	115.85	119.36
1	B	199	LLP	OP2-P-OP4	-2.05	101.31	106.67
1	A	199	LLP	C3-C4-C4'	-2.02	116.75	120.40

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	199	LLP	O-C-CA-CB
1	B	199	LLP	O-C-CA-CB
1	C	199	LLP	O-C-CA-CB
1	D	199	LLP	C4-C5-C5'-OP4
1	D	199	LLP	C6-C5-C5'-OP4
1	D	199	LLP	O-C-CA-CB
1	C	199	LLP	C4-C4'-NZ-CE
1	A	199	LLP	CG-CD-CE-NZ
1	C	199	LLP	CG-CD-CE-NZ
1	A	199	LLP	C3-C4-C4'-NZ
1	C	199	LLP	C3-C4-C4'-NZ
1	D	199	LLP	C3-C4-C4'-NZ
1	B	199	LLP	C3-C4-C4'-NZ
1	B	199	LLP	C5-C4-C4'-NZ
1	A	199	LLP	C4-C4'-NZ-CE
1	D	199	LLP	CD-CE-NZ-C4'
1	D	199	LLP	C-CA-CB-CG
1	A	199	LLP	CD-CE-NZ-C4'
1	B	199	LLP	CD-CE-NZ-C4'
1	C	199	LLP	CD-CE-NZ-C4'
1	C	199	LLP	C5-C4-C4'-NZ
1	B	199	LLP	C4-C4'-NZ-CE
1	D	199	LLP	C5-C4-C4'-NZ
1	D	199	LLP	CG-CD-CE-NZ
1	A	199	LLP	C-CA-CB-CG
1	C	199	LLP	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	199	LLP	1	0
1	B	199	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 13 are monoatomic - leaving 1 for Mogul analysis.

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	$\# Z > 2$
4	GOL	C	346	-	5,5,5	0.39	0	5,5,5	0.35	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
4	GOL	C	346	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	346	GOL	C1-C2-C3-O3
4	C	346	GOL	O2-C2-C3-O3

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	342/355 (96%)	-0.47	0	100 100	19, 25, 37, 50	0
1	B	342/355 (96%)	-0.49	0	100 100	18, 25, 35, 49	2 (0%)
1	C	342/355 (96%)	-0.54	0	100 100	17, 25, 37, 54	1 (0%)
1	D	344/355 (96%)	-0.52	1 (0%)	90 90	19, 25, 36, 67	0
All	All	1370/1420 (96%)	-0.50	1 (0%)	92 92	17, 25, 36, 67	3 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	-1	HIS	2.3

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	B	199	24/25	0.97	0.05	19,26,30,35	0
1	LLP	C	199	24/25	0.97	0.05	21,25,29,36	0
1	LLP	A	199	24/25	0.98	0.05	18,25,29,36	0
1	LLP	D	199	24/25	0.98	0.05	19,25,31,36	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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
4	GOL	C	346	6/6	0.71	0.15	47,53,55,63	0
5	NA	D	344	1/1	0.92	0.06	39,39,39,39	0
3	CL	C	344	1/1	0.93	0.10	58,58,58,58	0
2	CA	A	345	1/1	0.98	0.04	32,32,32,32	0
2	CA	A	344	1/1	0.98	0.02	27,27,27,27	0
3	CL	B	344	1/1	0.99	0.02	28,28,28,28	0
3	CL	B	345	1/1	0.99	0.08	32,32,32,32	0
3	CL	B	346	1/1	0.99	0.10	30,30,30,30	0
3	CL	A	346	1/1	0.99	0.07	31,31,31,31	0
3	CL	C	345	1/1	0.99	0.07	34,34,34,34	0
3	CL	D	345	1/1	0.99	0.08	34,34,34,34	0
3	CL	D	346	1/1	0.99	0.06	34,34,34,34	0
3	CL	A	347	1/1	0.99	0.02	32,32,32,32	0
3	CL	A	348	1/1	0.99	0.02	33,33,33,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.