



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 13, 2025 – 12:12 PM EDT

PDB ID : 9E9J / pdb_00009e9j
Title : L-allo-threonine aldolase from *Thermotoga maritima*, N308E-Y87A-R122G-P121D Mutant
Authors : Wang, S.; Jeffrey, P.D.; Sorigue, D.; Hyster, T.K.
Deposited on : 2024-11-08
Resolution : 2.15 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 Phenix2.0rc1
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.44

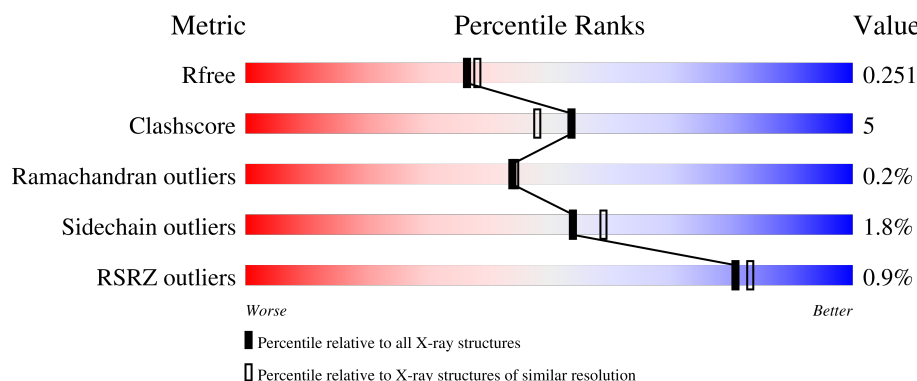
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1881 (2.16-2.16)
Clashscore	180529	2047 (2.16-2.16)
Ramachandran outliers	177936	2027 (2.16-2.16)
Sidechain outliers	177891	2026 (2.16-2.16)
RSRZ outliers	164620	1882 (2.16-2.16)

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	349	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 86% 10% .. </div> </div>
1	B	349	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 85% 13% .. </div> </div>
1	C	349	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 85% 13% .. </div> </div>
1	D	349	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 86% 12% .. </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10958 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	4	0
			2656	1663	471	505	1	16			
1	B	343	Total	C	N	O	P	S	0	4	0
			2656	1663	471	505	1	16			
1	C	343	Total	C	N	O	P	S	0	6	0
			2670	1672	474	507	1	16			
1	D	344	Total	C	N	O	P	S	0	4	0
			2666	1669	474	506	1	16			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	87	ALA	TYR	engineered mutation	UNP Q9X266
A	121	ASP	PRO	engineered mutation	UNP Q9X266
A	122	GLY	ARG	engineered mutation	UNP Q9X266
A	308	GLU	ASN	engineered mutation	UNP Q9X266
A	340	SER	-	expression tag	UNP Q9X266
A	341	GLN	-	expression tag	UNP Q9X266
A	342	VAL	-	expression tag	UNP Q9X266
A	343	GLN	-	expression tag	UNP Q9X266
A	344	HIS	-	expression tag	UNP Q9X266
A	345	HIS	-	expression tag	UNP Q9X266
A	346	HIS	-	expression tag	UNP Q9X266
A	347	HIS	-	expression tag	UNP Q9X266
A	348	HIS	-	expression tag	UNP Q9X266
A	349	HIS	-	expression tag	UNP Q9X266
B	87	ALA	TYR	engineered mutation	UNP Q9X266
B	121	ASP	PRO	engineered mutation	UNP Q9X266
B	122	GLY	ARG	engineered mutation	UNP Q9X266
B	308	GLU	ASN	engineered mutation	UNP Q9X266
B	340	SER	-	expression tag	UNP Q9X266
B	341	GLN	-	expression tag	UNP Q9X266
B	342	VAL	-	expression tag	UNP Q9X266

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Chain	Residue	Modelled	Actual	Comment	Reference
B	343	GLN	-	expression tag	UNP Q9X266
B	344	HIS	-	expression tag	UNP Q9X266
B	345	HIS	-	expression tag	UNP Q9X266
B	346	HIS	-	expression tag	UNP Q9X266
B	347	HIS	-	expression tag	UNP Q9X266
B	348	HIS	-	expression tag	UNP Q9X266
B	349	HIS	-	expression tag	UNP Q9X266
C	87	ALA	TYR	engineered mutation	UNP Q9X266
C	121	ASP	PRO	engineered mutation	UNP Q9X266
C	122	GLY	ARG	engineered mutation	UNP Q9X266
C	308	GLU	ASN	engineered mutation	UNP Q9X266
C	340	SER	-	expression tag	UNP Q9X266
C	341	GLN	-	expression tag	UNP Q9X266
C	342	VAL	-	expression tag	UNP Q9X266
C	343	GLN	-	expression tag	UNP Q9X266
C	344	HIS	-	expression tag	UNP Q9X266
C	345	HIS	-	expression tag	UNP Q9X266
C	346	HIS	-	expression tag	UNP Q9X266
C	347	HIS	-	expression tag	UNP Q9X266
C	348	HIS	-	expression tag	UNP Q9X266
C	349	HIS	-	expression tag	UNP Q9X266
D	87	ALA	TYR	engineered mutation	UNP Q9X266
D	121	ASP	PRO	engineered mutation	UNP Q9X266
D	122	GLY	ARG	engineered mutation	UNP Q9X266
D	308	GLU	ASN	engineered mutation	UNP Q9X266
D	340	SER	-	expression tag	UNP Q9X266
D	341	GLN	-	expression tag	UNP Q9X266
D	342	VAL	-	expression tag	UNP Q9X266
D	343	GLN	-	expression tag	UNP Q9X266
D	344	HIS	-	expression tag	UNP Q9X266
D	345	HIS	-	expression tag	UNP Q9X266
D	346	HIS	-	expression tag	UNP Q9X266
D	347	HIS	-	expression tag	UNP Q9X266
D	348	HIS	-	expression tag	UNP Q9X266
D	349	HIS	-	expression tag	UNP Q9X266

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			7	4	3		

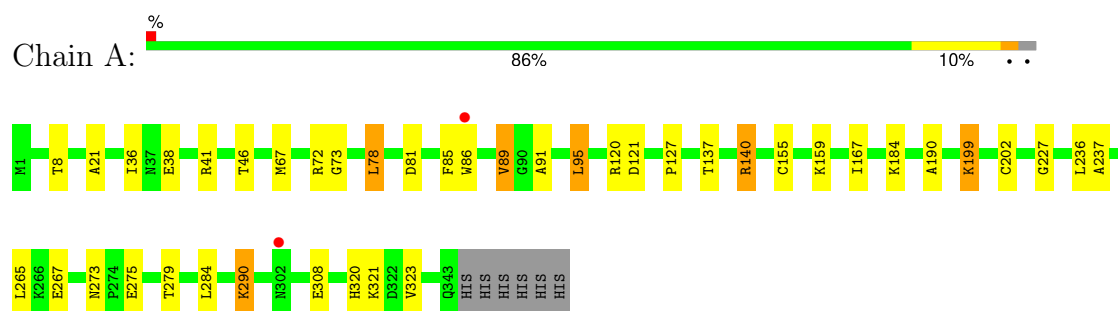
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	75	Total	O	0	0
			75	75		
4	B	78	Total	O	0	0
			78	78		
4	C	62	Total	O	0	0
			62	62		
4	D	84	Total	O	0	0
			84	84		

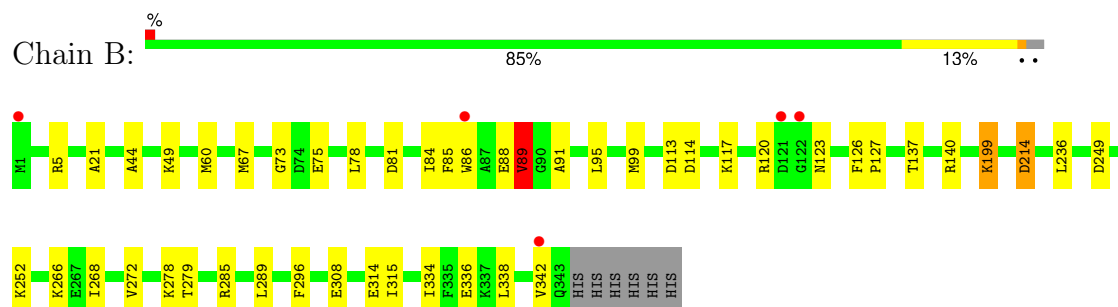
3 Residue-property plots

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 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.

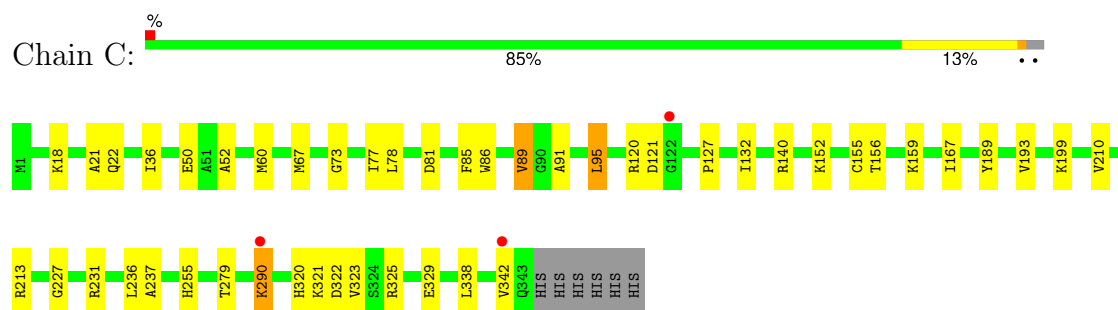
- Molecule 1: L-allo-threonine aldolase



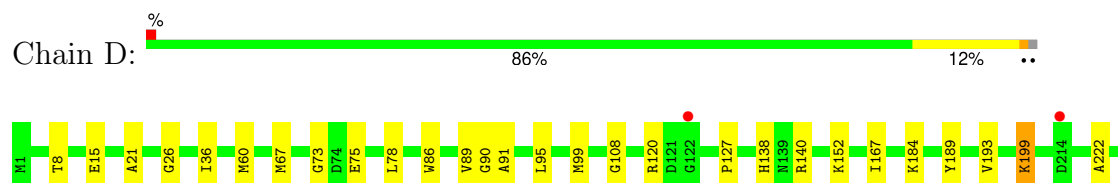
- Molecule 1: L-allo-threonine aldolase



- Molecule 1: L-allo-threonine aldolase



- Molecule 1: L-allo-threonine aldolase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	61.00Å 130.36Å 164.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.33 – 2.15 29.33 – 2.15	Depositor EDS
% Data completeness (in resolution range)	97.7 (29.33-2.15) 97.6 (29.33-2.15)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.32 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.17_3644	Depositor
R, R_{free}	0.203 , 0.252 0.203 , 0.251	Depositor DCC
R_{free} test set	3713 reflections (5.17%)	wwPDB-VP
Wilson B-factor (Å ²)	27.4	Xtriage
Anisotropy	0.405	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10958	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.03 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.9235e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: PEG, CA, 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	0.33	0/2683	0.54	0/3623
1	B	0.32	0/2683	0.53	0/3623
1	C	0.32	0/2703	0.50	0/3649
1	D	0.34	0/2694	0.54	0/3638
All	All	0.33	0/10763	0.52	0/14533

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	2656	0	2681	28	0
1	B	2656	0	2681	32	0
1	C	2670	0	2700	31	0
1	D	2666	0	2688	30	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	D	7	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	75	0	0	1	0
4	B	78	0	0	3	0
4	C	62	0	0	2	0
4	D	84	0	0	2	0
All	All	10958	0	10760	103	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 5.

All (103) 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:155:CYS:SG	1:A:159:LYS:NZ	2.50	0.85
1:A:21:ALA:HB2	1:B:21:ALA:HB2	1.72	0.71
1:B:86[B]:TRP:CD2	1:B:140:ARG:HD2	2.27	0.69
1:C:21:ALA:HB2	1:D:21:ALA:HB2	1.82	0.61
1:D:297:ILE:HD11	1:D:315[A]:ILE:HG12	1.82	0.61
1:A:91:ALA:HB1	1:A:95[A]:LEU:HD22	1.85	0.59
1:D:75:GLU:HG3	1:D:99:MET:HB2	1.85	0.59
1:A:86[B]:TRP:HA	1:C:120:ARG:HH22	1.69	0.58
1:B:285:ARG:HD2	1:B:314:GLU:HG2	1.87	0.57
1:B:214:ASP:HB3	4:B:576:HOH:O	2.04	0.56
1:C:213:ARG:HD3	4:C:551:HOH:O	2.06	0.56
1:A:73:GLY:O	1:A:127:PRO:HB3	2.06	0.55
1:C:73:GLY:O	1:C:127:PRO:HB3	2.06	0.55
1:D:36:ILE:HD13	1:D:237:ALA:HB2	1.88	0.55
1:A:46:THR:O	1:A:184:LYS:HG2	2.06	0.55
1:A:86[A]:TRP:HA	1:C:120:ARG:HH22	1.71	0.54
1:B:99:MET:HG3	1:D:90:GLY:HA2	1.87	0.54
1:A:36:ILE:HD13	1:A:237:ALA:HB2	1.90	0.53
1:D:184:LYS:HG3	4:D:578:HOH:O	2.07	0.53
1:C:155:CYS:SG	1:C:159:LYS:HE3	2.49	0.53
1:C:78[A]:LEU:HD11	1:C:85:PHE:HB2	1.91	0.53
1:C:325:ARG:O	1:C:329:GLU:HG3	2.10	0.52
1:C:227:GLY:HA3	1:D:60:MET:HB2	1.91	0.52
1:B:91:ALA:HB1	1:B:95[A]:LEU:HD22	1.90	0.52
1:D:167:ILE:HB	1:D:193:VAL:HG22	1.92	0.52
1:C:338:LEU:O	1:C:342:VAL:HG22	2.09	0.52
1:C:320:HIS:CE1	1:C:323:VAL:HG23	2.44	0.52
1:C:95[B]:LEU:HD22	1:D:95[B]:LEU:HD22	1.92	0.52
1:A:120:ARG:HH22	1:C:86[B]:TRP:HA	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:LEU:HB3	1:B:342:VAL:HG12	1.92	0.51
1:B:123:ASN:HB3	1:B:126:PHE:CD2	2.46	0.51
1:D:320:HIS:CE1	1:D:323:VAL:HG23	2.45	0.50
1:A:320:HIS:CE1	1:A:323:VAL:HG23	2.46	0.50
1:A:236:LEU:HD11	1:B:236:LEU:HD11	1.92	0.50
1:B:137:THR:HG21	1:B:279:THR:HG21	1.93	0.49
1:C:91:ALA:HB1	1:C:95[A]:LEU:HD22	1.94	0.49
1:D:278:LYS:HG3	4:D:565:HOH:O	2.12	0.49
1:C:86[B]:TRP:CD2	1:C:140:ARG:HD2	2.47	0.49
1:B:44:ALA:HB1	1:B:49:LYS:O	2.13	0.49
1:A:8:THR:HG22	1:A:199:LLP:HG3	1.94	0.48
1:C:167:ILE:HB	1:C:193:VAL:HG22	1.94	0.48
1:B:84:ILE:HG13	4:B:502:HOH:O	2.13	0.48
1:D:86[B]:TRP:CE3	1:D:140:ARG:HD2	2.49	0.48
1:A:86[B]:TRP:CD2	1:A:140:ARG:HD2	2.49	0.48
1:B:99:MET:HG3	1:D:90:GLY:CA	2.43	0.48
1:D:152:LYS:HG3	1:D:189:TYR:CE1	2.49	0.47
1:B:199:LLP:NZ	1:B:199:LLP:O3	2.44	0.47
1:D:91:ALA:HB1	1:D:95[A]:LEU:HD22	1.96	0.47
1:B:113:ASP:O	1:B:117:LYS:HE2	2.15	0.47
1:C:152:LYS:HG3	1:C:189:TYR:CE1	2.50	0.47
1:A:137:THR:HG21	1:A:279:THR:HG21	1.96	0.47
1:A:227:GLY:HA3	1:B:60:MET:HB2	1.97	0.47
1:D:265:LEU:HD13	1:D:284:LEU:HD12	1.96	0.47
1:B:81:ASP:O	1:B:140:ARG:HD3	2.14	0.47
1:D:67:MET:HE2	1:D:67:MET:HB3	1.77	0.46
1:B:249:ASP:O	1:B:252:LYS:HG2	2.15	0.46
1:D:26:GLY:O	1:D:232:GLN:HA	2.16	0.46
1:B:73:GLY:O	1:B:127:PRO:HB3	2.16	0.46
1:A:202:CYS:SG	1:A:321:LYS:HE3	2.55	0.46
1:B:268:ILE:HG12	1:B:336:GLU:HG3	1.97	0.46
1:B:296:PHE:HB3	1:B:315[A]:ILE:HD11	1.98	0.46
1:D:73:GLY:O	1:D:127:PRO:HB3	2.16	0.46
1:A:120:ARG:HH22	1:C:86[A]:TRP:HA	1.81	0.45
1:A:155:CYS:O	1:A:159:LYS:HG2	2.17	0.45
1:B:81:ASP:HA	1:B:86[A]:TRP:CD1	2.52	0.45
1:B:86[A]:TRP:HA	1:D:120:ARG:HH22	1.81	0.45
1:C:36:ILE:HD13	1:C:237:ALA:HB2	1.97	0.45
1:B:75:GLU:OE2	1:B:120:ARG:NH2	2.49	0.45
1:A:72:ARG:HD2	1:D:67:MET:HE3	1.98	0.45
1:A:78[B]:LEU:HD11	1:A:85:PHE:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:ILE:O	1:B:338:LEU:HG	2.17	0.45
1:A:95[B]:LEU:HD22	1:B:95[B]:LEU:HD22	1.99	0.44
1:A:290:LYS:HE3	1:A:290:LYS:HB2	1.72	0.44
1:C:52:ALA:HB2	1:C:210:VAL:HG12	1.98	0.44
1:C:67:MET:HE2	1:C:67:MET:HB3	1.81	0.44
1:A:267:GLU:OE2	4:A:501:HOH:O	2.21	0.44
1:B:78[A]:LEU:HD11	1:B:85:PHE:HB2	2.00	0.44
1:C:18:LYS:O	1:C:22:GLN:HG2	2.18	0.44
1:B:278:LYS:HG3	4:B:565:HOH:O	2.17	0.43
1:C:236:LEU:HD11	1:D:236:LEU:HD11	1.99	0.43
1:B:266:LYS:HB2	1:B:272:VAL:HG23	2.00	0.43
1:C:60:MET:HB2	1:D:227:GLY:HA3	2.00	0.43
1:D:222:ALA:O	1:D:226:LEU:HG	2.17	0.43
1:C:50:GLU:HG3	4:C:522:HOH:O	2.18	0.43
1:C:231:ARG:CZ	1:D:8:THR:HG21	2.49	0.43
1:A:81:ASP:HA	1:A:86[A]:TRP:CD1	2.54	0.43
1:D:86[B]:TRP:CD2	1:D:140:ARG:HD2	2.53	0.43
1:D:15:GLU:HG2	1:D:242:ILE:HD13	2.00	0.42
1:A:167:ILE:HG13	1:A:190:ALA:HB2	2.01	0.42
1:A:38:GLU:OE2	1:A:41:ARG:NH2	2.50	0.42
1:C:290:LYS:HG3	1:C:342:VAL:HA	2.01	0.42
1:C:77:ILE:HB	1:C:132:ILE:HG12	2.03	0.41
1:C:81:ASP:HA	1:C:86[A]:TRP:CD1	2.56	0.41
1:D:8:THR:HG22	1:D:199:LLP:HE3	2.02	0.41
1:C:255:HIS:CE1	1:C:279:THR:HG22	2.56	0.41
1:D:263:LEU:O	1:D:267:GLU:HG3	2.20	0.41
1:C:321:LYS:NZ	1:C:322:ASP:OD1	2.42	0.41
1:A:273:ASN:HB3	1:A:275:GLU:OE2	2.22	0.40
1:B:114:ASP:HA	1:B:117:LYS:HE2	2.03	0.40
1:D:108:GLY:HA2	1:D:138:HIS:CD2	2.57	0.40
1:B:5:ARG:HG2	1:B:308:GLU:HG3	2.03	0.40
1:B:88:GLU:C	1:B:89:VAL:HG23	2.46	0.40
1:A:265:LEU:HD13	1:A:284:LEU:HD12	2.04	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	344/349 (99%)	338 (98%)	5 (2%)	1 (0%)	37	34
1	B	344/349 (99%)	336 (98%)	7 (2%)	1 (0%)	37	34
1	C	346/349 (99%)	336 (97%)	9 (3%)	1 (0%)	37	34
1	D	345/349 (99%)	339 (98%)	6 (2%)	0	100	100
All	All	1379/1396 (99%)	1349 (98%)	27 (2%)	3 (0%)	44	44

All (3) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	282/284 (99%)	272 (96%)	10 (4%)	31	30
1	B	282/284 (99%)	279 (99%)	3 (1%)	70	75
1	C	284/284 (100%)	278 (98%)	6 (2%)	48	53
1	D	283/284 (100%)	277 (98%)	6 (2%)	48	53
All	All	1131/1136 (100%)	1106 (98%)	25 (2%)	54	51

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	67	MET
1	A	78[A]	LEU
1	A	78[B]	LEU
1	A	89	VAL
1	A	95[A]	LEU
1	A	95[B]	LEU
1	A	121	ASP
1	A	140	ARG
1	A	290	LYS
1	A	308	GLU
1	B	67	MET
1	B	89	VAL
1	B	214	ASP
1	C	89	VAL
1	C	95[A]	LEU
1	C	95[B]	LEU
1	C	121	ASP
1	C	156	THR
1	C	290	LYS
1	D	78[A]	LEU
1	D	78[B]	LEU
1	D	89	VAL
1	D	308	GLU
1	D	315[A]	ILE
1	D	315[B]	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	B	150	ASN
1	B	174	ASN
1	B	333	ASN
1	C	63	GLN
1	C	71	GLN
1	C	174	ASN
1	C	255	HIS
1	D	150	ASN
1	D	343	GLN

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	D	199	1	23,24,25	2.48	6 (26%)	25,32,34	1.47	4 (16%)
1	LLP	A	199	1	23,24,25	2.47	6 (26%)	25,32,34	1.48	5 (20%)
1	LLP	C	199	1	23,24,25	2.57	6 (26%)	25,32,34	1.55	6 (24%)
1	LLP	B	199	1	23,24,25	2.49	6 (26%)	25,32,34	1.63	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	D	199	1	-	4/16/17/19	0/1/1/1
1	LLP	A	199	1	-	4/16/17/19	0/1/1/1
1	LLP	C	199	1	-	5/16/17/19	0/1/1/1
1	LLP	B	199	1	-	5/16/17/19	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	199	LLP	C4-C4'	7.59	1.62	1.46
1	D	199	LLP	C4-C4'	7.54	1.62	1.46
1	A	199	LLP	C4-C4'	7.39	1.62	1.46
1	B	199	LLP	C4-C4'	7.38	1.62	1.46
1	C	199	LLP	C4'-NZ	5.19	1.44	1.27
1	A	199	LLP	C4'-NZ	5.18	1.44	1.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	199	LLP	C4'-NZ	5.17	1.44	1.27
1	D	199	LLP	C4'-NZ	5.04	1.44	1.27
1	D	199	LLP	C2'-C2	4.27	1.57	1.50
1	C	199	LLP	C4-C5	-3.77	1.36	1.42
1	C	199	LLP	C2'-C2	3.67	1.56	1.50
1	B	199	LLP	C2'-C2	3.61	1.56	1.50
1	B	199	LLP	C6-N1	3.56	1.41	1.34
1	A	199	LLP	C2'-C2	3.51	1.56	1.50
1	A	199	LLP	C6-N1	3.36	1.41	1.34
1	A	199	LLP	C4-C5	-3.18	1.37	1.42
1	B	199	LLP	C4-C5	-3.15	1.37	1.42
1	D	199	LLP	C4-C5	-3.06	1.37	1.42
1	C	199	LLP	C6-N1	2.95	1.40	1.34
1	B	199	LLP	C5'-C5	2.66	1.57	1.50
1	A	199	LLP	C5'-C5	2.59	1.57	1.50
1	D	199	LLP	C6-N1	2.56	1.39	1.34
1	C	199	LLP	C5'-C5	2.44	1.57	1.50
1	D	199	LLP	C5'-C5	2.36	1.57	1.50

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	199	LLP	OP4-C5'-C5	4.01	116.86	109.36
1	D	199	LLP	OP4-C5'-C5	3.55	116.00	109.36
1	A	199	LLP	C4-C4'-NZ	-3.49	107.94	124.04
1	B	199	LLP	C4-C4'-NZ	-3.32	108.71	124.04
1	A	199	LLP	OP4-C5'-C5	3.15	115.27	109.36
1	C	199	LLP	C4-C4'-NZ	-3.10	109.75	124.04
1	B	199	LLP	CE-NZ-C4'	-3.08	108.84	118.72
1	D	199	LLP	CE-NZ-C4'	-2.74	109.96	118.72
1	D	199	LLP	C4-C4'-NZ	-2.63	111.92	124.04
1	B	199	LLP	OP4-C5'-C5	2.58	114.19	109.36
1	D	199	LLP	C5-C6-N1	-2.49	119.79	123.83
1	C	199	LLP	OP4-P-OP1	2.42	112.98	106.44
1	C	199	LLP	CE-NZ-C4'	-2.37	111.12	118.72
1	B	199	LLP	C2'-C2-N1	2.30	121.98	117.64
1	A	199	LLP	C4-C3-C2	2.29	121.43	120.14
1	C	199	LLP	C4-C3-C2	2.24	121.40	120.14
1	A	199	LLP	CE-NZ-C4'	-2.20	111.67	118.72
1	B	199	LLP	CG-CD-CE	-2.20	105.73	113.38
1	A	199	LLP	C5'-C5-C6	-2.07	115.99	119.36
1	C	199	LLP	C5-C6-N1	-2.06	120.48	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	LLP	C5-C6-N1	-2.05	120.50	123.83

There are no chirality outliers.

All (18) torsion outliers are listed below:

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

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	199	LLP	1	0
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 5 ligands modelled in this entry, 4 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	$\# Z > 2$
3	PEG	D	401	-	6,6,6	0.17	0	5,5,5	0.12	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	PEG	D	401	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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	342/349 (97%)	-0.12	2 (0%) 85 87	14, 28, 50, 68	4 (1%)
1	B	342/349 (97%)	-0.05	5 (1%) 71 75	13, 29, 52, 67	4 (1%)
1	C	342/349 (97%)	-0.06	3 (0%) 81 83	14, 29, 51, 68	6 (1%)
1	D	343/349 (98%)	-0.14	3 (0%) 81 83	13, 27, 46, 63	4 (1%)
All	All	1369/1396 (98%)	-0.09	13 (0%) 81 83	13, 28, 51, 68	18 (1%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	122	GLY	3.5
1	D	344	HIS	3.3
1	D	214	ASP	2.9
1	B	342	VAL	2.6
1	B	86[A]	TRP	2.6
1	C	342	VAL	2.2
1	B	1	MET	2.2
1	C	290	LYS	2.1
1	B	121	ASP	2.1
1	C	122	GLY	2.1
1	A	302	ASN	2.1
1	D	122	GLY	2.0
1	A	86[A]	TRP	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(\AA^2)	Q<0.9
1	LLP	A	199	24/25	0.94	0.08	14,21,28,30	0
1	LLP	C	199	24/25	0.94	0.08	19,23,30,36	0
1	LLP	B	199	24/25	0.95	0.07	17,22,29,31	0
1	LLP	D	199	24/25	0.95	0.07	15,21,26,32	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(\AA^2)	Q<0.9
3	PEG	D	401	7/7	0.82	0.14	30,40,50,52	0
2	CA	D	402	1/1	0.98	0.06	22,22,22,22	0
2	CA	B	401	1/1	0.98	0.04	24,24,24,24	0
2	CA	A	401	1/1	0.99	0.06	24,24,24,24	0
2	CA	C	401	1/1	0.99	0.04	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.