



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 12:40 am GMT

PDB ID : 1LW5  
Title : X-ray structure of L-Threonine Aldolase (low-specificity) in complex with glycine  
Authors : Kielkopf, C.L.; Burley, S.K.; New York SGX Research Center for Structural Genomics (NYSGXRC)  
Deposited on : 2002-05-30  
Resolution : 2.05 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

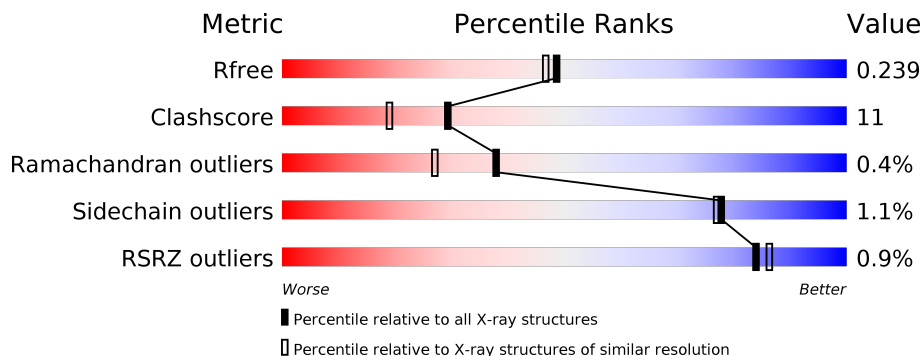
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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))
$R_{free}$	100719	1316 (2.04-2.04)
Clashscore	112137	1394 (2.04-2.04)
Ramachandran outliers	110173	1383 (2.04-2.04)
Sidechain outliers	110143	1383 (2.04-2.04)
RSRZ outliers	101464	1319 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	347	<div> <div style="width: 84%;"></div> <div style="width: 14%;"></div> <div style="width: 2%;"></div> </div> <div>84% 14% .</div>
1	B	347	<div> <div style="width: 79%;"></div> <div style="width: 19%;"></div> <div style="width: 2%;"></div> </div> <div>79% 19% ..</div>
1	C	347	<div> <div style="width: 80%;"></div> <div style="width: 18%;"></div> <div style="width: 2%;"></div> </div> <div>80% 18% .</div>
1	D	347	<div> <div style="width: 79%;"></div> <div style="width: 19%;"></div> <div style="width: 2%;"></div> </div> <div>79% 19% ..</div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11412 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	Se	0	0	0
			2609	1629	465	498	1	3	13			
1	B	343	Total	C	N	O	S	Se		0	1	0
			2621	1637	470	498	3	13				
1	C	343	Total	C	N	O	S	Se		0	0	0
			2596	1622	466	492	3	13				
1	D	344	Total	C	N	O	S	Se		0	0	0
			2616	1635	470	494	3	14				

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	CLONING ARTIFACT	UNP Q9X266
A	-2	PRO	-	CLONING ARTIFACT	UNP Q9X266
A	-1	HIS	-	CLONING ARTIFACT	UNP Q9X266
A	0	MSE	-	CLONING ARTIFACT	UNP Q9X266
B	-3	GLY	-	CLONING ARTIFACT	UNP Q9X266
B	-2	PRO	-	CLONING ARTIFACT	UNP Q9X266
B	-1	HIS	-	CLONING ARTIFACT	UNP Q9X266
B	0	MSE	-	CLONING ARTIFACT	UNP Q9X266
C	-3	GLY	-	CLONING ARTIFACT	UNP Q9X266
C	-2	PRO	-	CLONING ARTIFACT	UNP Q9X266
C	-1	HIS	-	CLONING ARTIFACT	UNP Q9X266
C	0	MSE	-	CLONING ARTIFACT	UNP Q9X266
D	-3	GLY	-	CLONING ARTIFACT	UNP Q9X266
D	-2	PRO	-	CLONING ARTIFACT	UNP Q9X266
D	-1	HIS	-	CLONING ARTIFACT	UNP Q9X266
D	0	MSE	-	CLONING ARTIFACT	UNP Q9X266

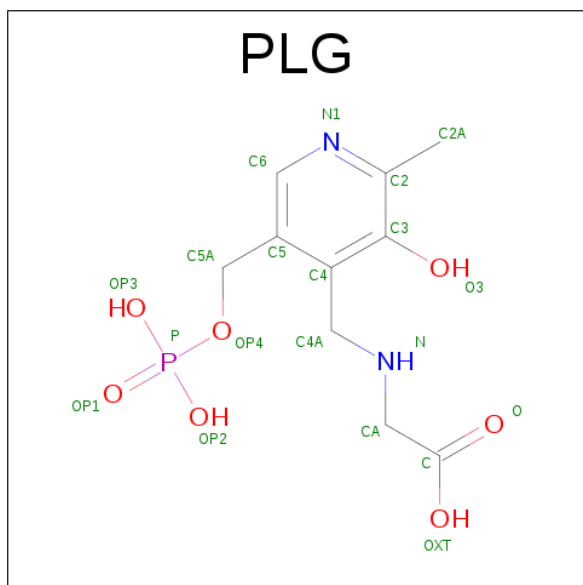
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total Cl 2 2	0	0
3	A	1	Total Cl 1 1	0	0
3	D	3	Total Cl 3 3	0	0

- Molecule 4 is N-GLYCINE-[3-HYDROXY-2-METHYL-5-PHOSPHONOXYMETHYL-PYRIDIN-4-YL-METHANE] (three-letter code: PLG) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>2</sub>O<sub>7</sub>P).



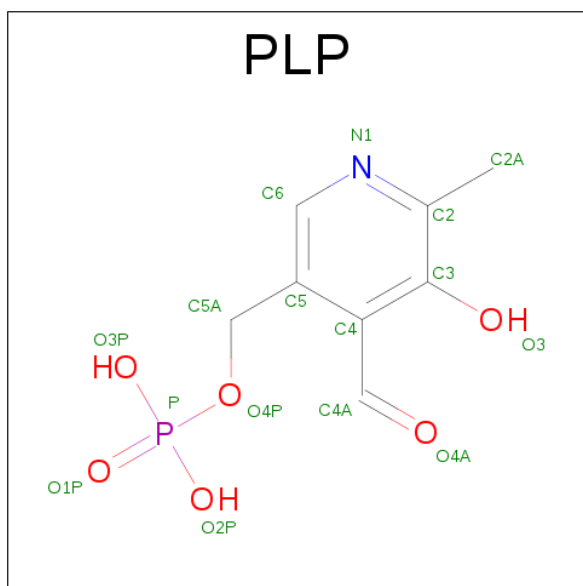
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O P 20 10 2 7 1	0	1
4	C	1	Total C N O P 20 10 2 7 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	D	1	Total	C	N	O	P	0	0
			20	10	2	7	1		

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



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

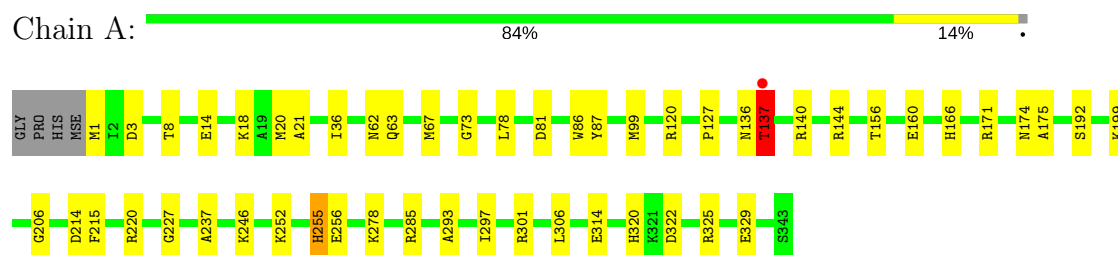
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	205	Total	O	0	0
			205	205		
6	B	225	Total	O	0	0
			225	225		
6	C	227	Total	O	0	0
			227	227		
6	D	226	Total	O	0	0
			226	226		

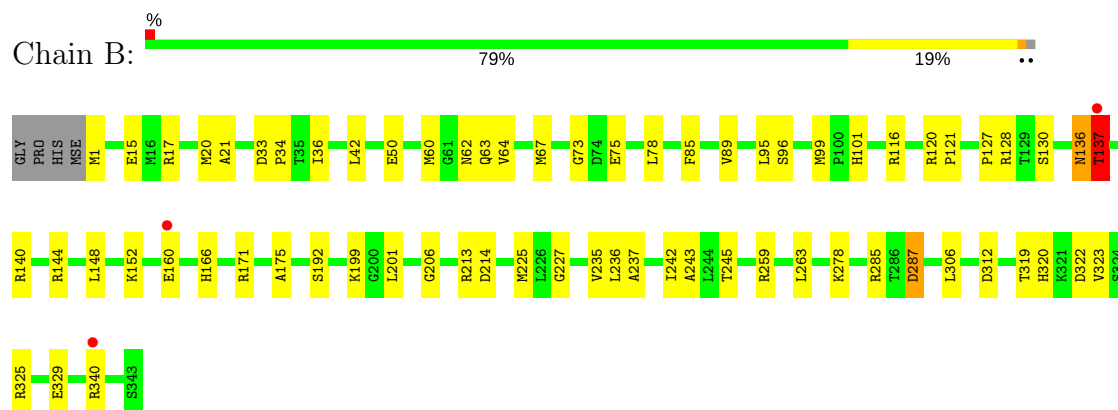
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

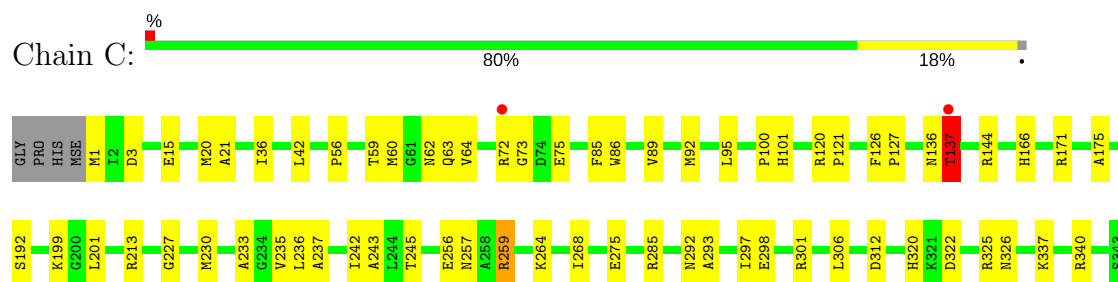
- Molecule 1: L-allo-threonine aldolase



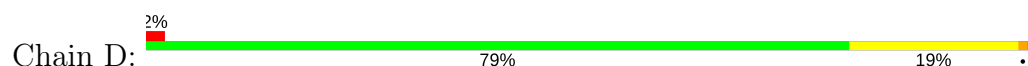
- Molecule 1: L-allo-threonine aldolase

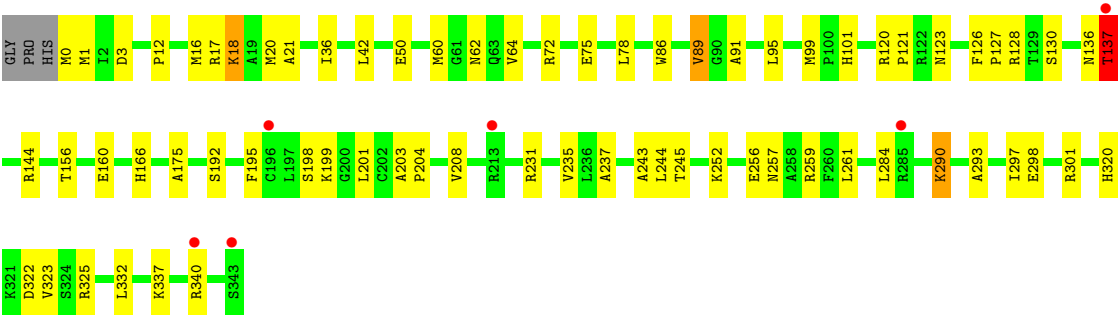


- Molecule 1: L-allo-threonine aldolase



- 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, $\alpha$ , $\beta$ , $\gamma$	96.02Å 100.71Å 150.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.05 29.89 – 2.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.05) 93.7 (29.89-2.05)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 2.04Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.207 , 0.237 0.209 , 0.239	Depositor DCC
$R_{free}$ test set	5953 reflections (6.95%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 51.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.003 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11412	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.12% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PLG, CA, PLP, LLP, CL

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	0.31	0/2613	0.63	2/3514 (0.1%)
1	B	0.32	0/2631	0.66	5/3535 (0.1%)
1	C	0.30	0/2615	0.64	3/3516 (0.1%)
1	D	0.36	1/2634 (0.0%)	0.68	5/3536 (0.1%)
All	All	0.33	1/10493 (0.0%)	0.66	15/14101 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	18	LYS	CD-CE	8.21	1.71	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	THR	N-CA-C	-9.85	84.40	111.00
1	D	137	THR	N-CA-C	-9.72	84.76	111.00
1	B	137	THR	N-CA-C	-9.47	85.42	111.00
1	C	137	THR	N-CA-C	-9.18	86.21	111.00
1	D	18	LYS	CA-CB-CG	-7.95	95.91	113.40
1	D	18	LYS	CB-CG-CD	7.20	130.33	111.60
1	D	137	THR	N-CA-CB	6.30	122.28	110.30
1	B	137	THR	N-CA-CB	5.88	121.46	110.30
1	C	137	THR	N-CA-CB	5.87	121.46	110.30
1	B	160	GLU	CA-CB-CG	5.71	125.96	113.40
1	B	136	ASN	C-N-CA	5.49	135.42	121.70
1	B	206	GLY	N-CA-C	5.36	126.49	113.10
1	D	18	LYS	CD-CE-NZ	5.28	123.84	111.70
1	C	136	ASN	C-N-CA	5.09	134.42	121.70
1	A	206	GLY	N-CA-C	5.07	125.78	113.10

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	2609	0	2579	50	0
1	B	2621	0	2610	70	0
1	C	2596	0	2577	73	0
1	D	2616	0	2614	60	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	D	3	0	0	0	0
4	B	20	0	11	4	0
4	C	20	0	11	3	0
4	D	20	0	11	2	0
5	B	15	0	6	3	0
6	A	205	0	0	3	0
6	B	225	0	0	7	0
6	C	227	0	0	12	0
6	D	226	0	0	5	0
All	All	11412	0	10419	227	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 11.

All (227) 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:B:199[A]:LLP:NZ	4:B:1000[A]:PLG:H4A2	1.50	1.24
1:A:99:MSE:HE3	1:C:100:PRO:HG3	1.28	1.14
1:C:259:ARG:HG2	1:C:259:ARG:HH21	1.19	1.07
1:A:14:GLU:OE2	1:A:18:LYS:NZ	1.88	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199[B]:LLP:NZ	5:B:1003[B]:PLP:C4A	2.20	1.05
1:B:199[A]:LLP:NZ	4:B:1000[A]:PLG:C4A	2.27	0.98
1:D:12:PRO:HG3	1:D:204:PRO:HG3	1.48	0.95
6:C:1215:HOH:O	1:D:72:ARG:HB3	1.64	0.95
1:C:259:ARG:HH21	1:C:259:ARG:CG	1.83	0.91
1:B:1:MSE:HE3	1:B:306:LEU:HD21	1.53	0.90
1:D:101:HIS:HE1	6:D:1224:HOH:O	1.59	0.85
1:D:137:THR:HA	1:D:144:ARG:O	1.76	0.85
1:B:116:ARG:NH1	6:B:1192:HOH:O	2.08	0.85
1:B:199[B]:LLP:CE	5:B:1003[B]:PLP:C4A	2.55	0.84
1:A:1:MSE:HE3	1:A:306:LEU:HD21	1.63	0.81
1:C:230:MSE:HE3	6:C:1078:HOH:O	1.78	0.81
1:C:56:PRO:HG3	1:C:230:MSE:HE2	1.62	0.81
1:A:174:ASN:HD22	1:A:255:HIS:HE1	1.30	0.80
1:B:21:ALA:HB2	1:C:21:ALA:HB2	1.65	0.78
1:B:15:GLU:HG2	1:B:242:ILE:HD13	1.67	0.77
1:C:137:THR:HG23	1:C:175:ALA:HB2	1.67	0.76
1:C:1:MSE:HE3	1:C:306:LEU:HD21	1.68	0.75
4:C:1001:PLG:HA1	6:C:1143:HOH:O	1.87	0.74
1:A:156:THR:O	1:A:160:GLU:HG3	1.86	0.74
1:B:214:ASP:HB2	6:B:1153:HOH:O	1.87	0.74
1:C:259:ARG:NH2	1:C:259:ARG:HG2	1.95	0.74
1:D:156:THR:O	1:D:160:GLU:HG3	1.88	0.73
1:B:199[A]:LLP:NZ	4:B:1000[A]:PLG:C4	2.50	0.73
1:B:137:THR:HA	1:B:144:ARG:O	1.88	0.73
1:A:21:ALA:HB2	1:D:21:ALA:HB2	1.70	0.72
1:C:137:THR:HA	1:C:144:ARG:O	1.90	0.71
1:A:36:ILE:HD13	1:A:237:ALA:HB2	1.73	0.71
1:A:137:THR:HG23	1:A:175:ALA:HB2	1.72	0.70
1:B:42:LEU:HD21	1:B:245:THR:CG2	2.22	0.69
4:D:1002:PLG:HA1	6:D:1102:HOH:O	1.92	0.68
1:A:137:THR:CG2	1:A:175:ALA:HB2	2.24	0.68
1:B:320:HIS:HD2	1:B:322:ASP:H	1.43	0.67
1:C:75:GLU:OE2	1:C:101:HIS:HD2	1.77	0.67
1:A:137:THR:HA	1:A:144:ARG:O	1.96	0.66
1:B:73:GLY:O	1:B:127:PRO:HB3	1.96	0.66
1:B:1:MSE:CE	1:B:306:LEU:HD21	2.26	0.66
1:C:42:LEU:HD21	1:C:245:THR:CG2	2.27	0.65
1:D:337:LYS:HD3	1:D:340:ARG:NH1	2.13	0.64
1:C:137:THR:CG2	1:C:175:ALA:HB2	2.28	0.64
1:C:320:HIS:HD2	1:C:322:ASP:H	1.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199[B]:LLP:HE3	5:B:1003[B]:PLP:C4A	2.28	0.64
1:C:36:ILE:HD13	1:C:237:ALA:HB2	1.80	0.63
1:D:257:ASN:ND2	1:D:325:ARG:HE	1.96	0.63
1:D:290:LYS:HA	1:D:290:LYS:HE3	1.81	0.62
1:A:99:MSE:HE1	1:C:85:PHE:CD2	2.34	0.62
1:C:137:THR:OG1	1:C:171:ARG:HB2	1.98	0.62
1:C:298:GLU:HG2	6:C:1127:HOH:O	1.99	0.62
1:C:62:ASN:ND2	1:C:166:HIS:HE1	1.97	0.62
1:A:1:MSE:CE	1:A:306:LEU:HD21	2.30	0.61
1:C:73:GLY:O	1:C:127:PRO:HB3	2.01	0.61
1:A:137:THR:OG1	1:A:171:ARG:HB2	2.00	0.61
6:C:1046:HOH:O	1:D:72:ARG:NH1	2.34	0.61
1:B:62:ASN:ND2	1:B:166:HIS:HE1	1.99	0.61
1:C:326:ASN:ND2	6:C:1077:HOH:O	2.33	0.60
1:A:21:ALA:HB2	1:D:21:ALA:CB	2.31	0.60
1:A:62:ASN:ND2	1:A:166:HIS:HE1	1.99	0.60
1:A:252:LYS:O	1:A:256:GLU:HG3	2.01	0.60
1:B:36:ILE:HD13	1:B:237:ALA:HB2	1.83	0.60
1:A:325:ARG:O	1:A:329:GLU:HG3	2.01	0.60
1:B:325:ARG:O	1:B:329:GLU:HG3	2.01	0.60
1:D:75:GLU:HG3	1:D:127:PRO:CG	2.32	0.60
1:D:199:LLP:CE	4:D:1002:PLG:H4A2	2.31	0.59
1:A:87:TYR:CD1	1:C:126:PHE:HE1	2.19	0.59
1:C:259:ARG:NH2	1:C:259:ARG:CG	2.54	0.59
1:C:1:MSE:CE	1:C:306:LEU:HD21	2.33	0.59
1:B:225:MSE:HA	1:C:89:VAL:HG11	1.85	0.58
1:A:73:GLY:O	1:A:127:PRO:HB3	2.04	0.58
1:A:320:HIS:HD2	1:A:322:ASP:H	1.50	0.57
1:B:120:ARG:HH22	1:D:86:TRP:HA	1.68	0.57
1:A:81:ASP:O	1:A:140:ARG:HD3	2.05	0.57
1:D:201:LEU:HB3	1:D:243:ALA:HB1	1.86	0.57
1:A:86:TRP:HA	1:C:120:ARG:HH22	1.68	0.57
1:A:120:ARG:HH22	1:C:86:TRP:HA	1.70	0.57
1:B:225:MSE:HA	1:C:89:VAL:CG1	2.35	0.57
1:A:293:ALA:O	1:A:297:ILE:HG12	2.05	0.56
1:B:50:GLU:HG2	6:B:1076:HOH:O	2.05	0.56
1:D:320:HIS:HD2	1:D:322:ASP:H	1.54	0.56
1:D:42:LEU:HD21	1:D:245:THR:CG2	2.35	0.56
1:C:62:ASN:HD22	1:C:166:HIS:HE1	1.54	0.56
1:D:137:THR:CA	1:D:144:ARG:O	2.51	0.56
1:A:99:MSE:HE1	1:C:85:PHE:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:257:ASN:ND2	1:C:325:ARG:HE	2.04	0.55
1:D:75:GLU:HG3	1:D:127:PRO:HG2	1.88	0.55
1:B:285:ARG:HB3	1:B:287:ASP:OD1	2.06	0.55
1:C:89:VAL:HG22	1:C:89:VAL:O	2.07	0.55
1:A:278:LYS:HG3	6:A:1086:HOH:O	2.07	0.55
1:D:0:MSE:HE3	1:D:1:MSE:HG2	1.88	0.55
1:C:15:GLU:HG2	1:C:242:ILE:HD13	1.88	0.55
1:B:323:VAL:O	1:B:323:VAL:HG23	2.07	0.54
1:B:340:ARG:HD3	6:B:1144:HOH:O	2.07	0.54
1:B:225:MSE:CA	1:C:89:VAL:HG11	2.37	0.54
1:B:320:HIS:H	1:B:323:VAL:CG2	2.21	0.54
1:C:275:GLU:H	1:C:275:GLU:CD	2.11	0.54
1:B:62:ASN:HD22	1:B:166:HIS:HE1	1.54	0.54
1:B:225:MSE:HG3	1:C:89:VAL:HG13	1.89	0.54
1:A:285:ARG:HD2	1:A:314:GLU:HG2	1.90	0.53
1:C:56:PRO:HG3	1:C:230:MSE:CE	2.36	0.53
1:D:36:ILE:HD13	1:D:237:ALA:HB2	1.90	0.53
1:B:42:LEU:HD21	1:B:245:THR:HG23	1.90	0.53
1:A:137:THR:HG21	1:A:171:ARG:O	2.08	0.53
1:C:337:LYS:HG2	1:C:340:ARG:HH21	1.73	0.53
1:B:17:ARG:HA	1:B:20:MSE:HE3	1.90	0.52
1:B:75:GLU:OE1	1:B:101:HIS:HD2	1.92	0.52
1:C:42:LEU:HD21	1:C:245:THR:HG23	1.91	0.52
1:B:137:THR:CG2	1:B:175:ALA:HB2	2.40	0.52
1:C:199:LLP:CE	4:C:1001:PLG:H4A2	2.40	0.52
1:B:137:THR:CA	1:B:144:ARG:O	2.59	0.51
1:B:166:HIS:HD2	1:B:192:SER:OG	1.92	0.51
1:C:166:HIS:HD2	1:C:192:SER:OG	1.94	0.51
1:A:87:TYR:HD1	1:C:126:PHE:HE1	1.57	0.50
1:D:259:ARG:HD3	6:D:1150:HOH:O	2.11	0.50
1:D:16:MSE:O	1:D:20:MSE:HG3	2.12	0.50
1:A:63:GLN:O	1:A:67:MSE:HG3	2.12	0.50
1:B:278:LYS:HB2	6:B:1107:HOH:O	2.12	0.50
1:B:148:LEU:O	1:B:152:LYS:HG3	2.11	0.49
1:D:137:THR:CG2	1:D:175:ALA:HB2	2.42	0.49
1:D:3:ASP:O	1:D:320:HIS:HE1	1.96	0.49
1:C:213:ARG:HB3	1:C:213:ARG:NH1	2.26	0.49
1:D:337:LYS:HA	1:D:340:ARG:HH11	1.76	0.49
1:B:120:ARG:HH22	1:D:86:TRP:CA	2.25	0.49
1:C:257:ASN:HD22	1:C:325:ARG:HE	1.61	0.48
1:D:195:PHE:CE1	1:D:208:VAL:HB	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199[A]:LLP:CE	4:B:1000[A]:PLG:H4A2	2.36	0.48
1:C:89:VAL:HG22	6:C:1017:HOH:O	2.12	0.48
1:B:120:ARG:NH2	1:D:86:TRP:HA	2.27	0.48
1:C:256:GLU:OE2	6:C:1206:HOH:O	2.20	0.48
1:D:62:ASN:OD1	1:D:166:HIS:HE1	1.96	0.48
1:D:298:GLU:CD	1:D:301:ARG:HH21	2.17	0.48
1:A:137:THR:CA	1:A:144:ARG:O	2.62	0.48
1:D:42:LEU:HD21	1:D:245:THR:HG23	1.96	0.47
1:B:285:ARG:HG3	1:B:285:ARG:HH11	1.79	0.47
1:A:20:MSE:SE	1:D:235:VAL:HG11	2.65	0.47
1:A:285:ARG:CD	1:A:314:GLU:HG2	2.45	0.47
1:B:236:LEU:HD11	1:C:236:LEU:HD11	1.97	0.47
1:A:227:GLY:HA3	1:D:60:MSE:HB2	1.97	0.47
1:A:1:MSE:HE1	1:A:301:ARG:HG3	1.96	0.47
1:A:8:THR:HB	1:D:231:ARG:HD2	1.96	0.47
1:B:259:ARG:NE	6:B:1123:HOH:O	2.48	0.47
1:B:63:GLN:O	1:B:67:MSE:HG3	2.14	0.47
1:D:320:HIS:H	1:D:323:VAL:CG2	2.27	0.47
1:A:99:MSE:HB3	1:A:99:MSE:HE2	1.83	0.47
1:B:320:HIS:CD2	1:B:322:ASP:H	2.27	0.46
1:D:166:HIS:HD2	1:D:192:SER:OG	1.97	0.46
1:A:137:THR:OG1	1:A:137:THR:O	2.33	0.46
1:B:235:VAL:HG11	1:C:20:MSE:SE	2.65	0.46
1:C:298:GLU:HG2	1:C:301:ARG:HH22	1.81	0.46
1:B:259:ARG:NH1	1:B:263:LEU:HD11	2.31	0.46
1:D:284:LEU:C	1:D:284:LEU:HD23	2.36	0.46
1:D:75:GLU:OE2	1:D:101:HIS:HD2	1.99	0.45
1:C:62:ASN:HD22	1:C:166:HIS:CE1	2.35	0.45
1:C:264:LYS:O	1:C:268:ILE:HG13	2.16	0.45
1:D:137:THR:HG22	1:D:175:ALA:HB2	1.98	0.45
1:A:220:ARG:HD3	6:A:1163:HOH:O	2.17	0.45
1:B:319:THR:HA	1:B:323:VAL:HG21	1.99	0.45
1:A:246:LYS:HB3	1:A:246:LYS:NZ	2.32	0.45
1:C:337:LYS:HG2	1:C:340:ARG:NH2	2.32	0.45
1:A:62:ASN:HD22	1:A:166:HIS:HE1	1.64	0.45
1:A:171:ARG:NH1	1:A:199:LLP:O3	2.50	0.45
1:B:62:ASN:HD22	1:B:166:HIS:CE1	2.34	0.44
1:D:252:LYS:O	1:D:256:GLU:HG3	2.17	0.44
1:A:136:ASN:O	1:A:137:THR:HG23	2.16	0.44
1:A:14:GLU:CD	1:A:18:LYS:NZ	2.65	0.44
1:B:140:ARG:HD3	6:B:1221:HOH:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:292:ASN:HB2	1:C:312:ASP:O	2.18	0.44
1:D:257:ASN:HD22	1:D:325:ARG:HE	1.61	0.44
1:C:137:THR:CA	1:C:144:ARG:O	2.64	0.44
1:D:136:ASN:O	1:D:137:THR:HG23	2.17	0.44
1:C:293:ALA:O	1:C:297:ILE:HG12	2.16	0.44
1:D:293:ALA:O	1:D:297:ILE:HG12	2.17	0.44
1:C:320:HIS:CD2	1:C:322:ASP:H	2.30	0.44
1:C:75:GLU:OE2	1:C:101:HIS:CD2	2.65	0.44
1:D:0:MSE:HG3	1:D:1:MSE:H	1.83	0.44
1:B:95:LEU:HD22	1:C:95:LEU:HD22	1.99	0.44
1:D:0:MSE:N	6:D:1207:HOH:O	2.50	0.43
1:D:320:HIS:CD2	1:D:322:ASP:H	2.33	0.43
4:C:1001:PLG:HA1	6:C:1118:HOH:O	2.18	0.43
1:C:285:ARG:HG3	1:C:285:ARG:HH11	1.84	0.43
1:C:3:ASP:O	1:C:320:HIS:HE1	2.02	0.43
1:B:136:ASN:O	1:B:137:THR:HG23	2.18	0.43
1:D:50:GLU:HG3	6:D:1037:HOH:O	2.19	0.43
1:C:60:MSE:O	1:C:64:VAL:HG22	2.18	0.42
1:C:92:MSE:SE	1:C:100:PRO:HB3	2.69	0.42
1:D:75:GLU:HG2	1:D:99:MSE:HB2	2.01	0.42
1:B:128:ARG:HH11	1:B:130:SER:HB3	1.83	0.42
1:B:60:MSE:O	1:B:64:VAL:HG22	2.19	0.42
1:D:17:ARG:HA	1:D:20:MSE:CE	2.50	0.42
1:C:201:LEU:HB3	1:C:243:ALA:HB1	2.01	0.42
1:C:72:ARG:HB3	6:C:1215:HOH:O	2.18	0.42
1:B:137:THR:HG23	1:B:175:ALA:HB2	2.01	0.42
1:D:128:ARG:NH1	1:D:130:SER:HB3	2.34	0.42
1:B:20:MSE:SE	1:C:235:VAL:HG11	2.69	0.42
1:B:225:MSE:CB	1:C:89:VAL:HG11	2.50	0.42
1:A:320:HIS:CD2	1:A:322:ASP:H	2.33	0.42
1:B:67:MSE:HG2	1:B:96:SER:OG	2.19	0.42
1:D:261:LEU:HD12	1:D:332:LEU:HD21	2.02	0.42
1:A:3:ASP:O	1:A:320:HIS:HE1	2.03	0.42
1:A:99:MSE:CE	1:C:85:PHE:CE2	3.02	0.42
1:D:257:ASN:HA	1:D:257:ASN:HD22	1.67	0.42
1:C:213:ARG:NH2	6:C:1158:HOH:O	2.52	0.41
1:D:323:VAL:HG23	1:D:323:VAL:O	2.20	0.41
1:D:91:ALA:HB1	1:D:95:LEU:HD22	2.01	0.41
1:A:255:HIS:HD2	6:A:1169:HOH:O	2.03	0.41
1:D:123:ASN:HB3	1:D:126:PHE:CD2	2.54	0.41
1:A:166:HIS:HD2	1:A:192:SER:OG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:LEU:HB3	1:B:243:ALA:HB1	2.02	0.41
1:B:33:ASP:HA	1:B:34:PRO:HD3	1.92	0.41
1:B:60:MSE:HB2	1:C:227:GLY:HA3	2.03	0.41
1:C:233:ALA:CB	6:C:1078:HOH:O	2.67	0.41
1:B:120:ARG:HA	1:B:121:PRO:HD3	1.94	0.41
1:B:285:ARG:HG3	1:B:285:ARG:NH1	2.35	0.41
1:B:137:THR:OG1	1:B:171:ARG:HB2	2.20	0.41
1:D:60:MSE:O	1:D:64:VAL:HG22	2.21	0.41
1:B:85:PHE:HD1	1:D:99:MSE:HE1	1.86	0.41
1:D:198:SER:HA	1:D:203:ALA:O	2.20	0.41
1:B:213:ARG:HG3	1:B:214:ASP:N	2.35	0.41
1:B:227:GLY:HA3	1:C:60:MSE:HB2	2.02	0.41
1:B:75:GLU:HG3	1:B:99:MSE:HB2	2.02	0.41
1:A:214:ASP:OD1	1:A:215:PHE:N	2.54	0.40
1:C:59:THR:O	1:C:63:GLN:HG2	2.21	0.40
1:D:120:ARG:HA	1:D:121:PRO:HD3	1.87	0.40
1:B:75:GLU:OE1	1:B:101:HIS:CD2	2.74	0.40
1:C:120:ARG:HA	1:C:121:PRO:HD3	1.87	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	340/347 (98%)	331 (97%)	8 (2%)	1 (0%)	44	35
1	B	340/347 (98%)	331 (97%)	8 (2%)	1 (0%)	44	35
1	C	340/347 (98%)	333 (98%)	6 (2%)	1 (0%)	44	35
1	D	341/347 (98%)	333 (98%)	6 (2%)	2 (1%)	28	17
All	All	1361/1388 (98%)	1328 (98%)	28 (2%)	5 (0%)	38	27

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	137	THR
1	A	137	THR
1	C	137	THR
1	D	137	THR
1	D	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	271/269 (101%)	269 (99%)	2 (1%)	87	87
1	B	275/269 (102%)	271 (98%)	4 (2%)	70	68
1	C	271/269 (101%)	270 (100%)	1 (0%)	93	93
1	D	275/269 (102%)	270 (98%)	5 (2%)	64	60
All	All	1092/1076 (102%)	1080 (99%)	12 (1%)	78	77

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	78	LEU
1	A	255	HIS
1	B	78	LEU
1	B	89	VAL
1	B	287	ASP
1	B	312	ASP
1	C	259	ARG
1	D	18	LYS
1	D	78	LEU
1	D	89	VAL
1	D	244	LEU
1	D	290	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	161	HIS
1	A	166	HIS
1	A	255	HIS
1	A	257	ASN
1	A	320	HIS
1	B	62	ASN
1	B	101	HIS
1	B	166	HIS
1	B	273	ASN
1	B	320	HIS
1	C	62	ASN
1	C	63	GLN
1	C	101	HIS
1	C	150	ASN
1	C	166	HIS
1	C	257	ASN
1	C	320	HIS
1	C	326	ASN
1	D	101	HIS
1	D	107	ASN
1	D	125	HIS
1	D	161	HIS
1	D	166	HIS
1	D	257	ASN
1	D	308	ASN
1	D	320	HIS
1	D	333	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 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	24,24,25	3.75	6 (25%)	28,32,34	2.35	12 (42%)
1	LLP	B	199[A]	1	8,8,25	0.60	0	5,8,34	1.13	0
1	LLP	B	199[B]	1	8,8,25	0.78	0	5,8,34	0.87	0
1	LLP	C	199	1	8,8,25	0.69	0	5,8,34	0.90	0
1	LLP	D	199	1	8,8,25	0.57	0	5,8,34	0.87	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
1	LLP	A	199	1	-	0/15/17/19	0/1/1/1
1	LLP	B	199[A]	1	-	0/5/7/19	0/0/0/1
1	LLP	B	199[B]	1	-	0/5/7/19	0/0/0/1
1	LLP	C	199	1	-	0/5/7/19	0/0/0/1
1	LLP	D	199	1	-	0/5/7/19	0/0/0/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	LLP	P-OP3	-2.01	1.46	1.54
1	A	199	LLP	C6-N1	3.04	1.40	1.34
1	A	199	LLP	C4'-NZ	3.49	1.37	1.27
1	A	199	LLP	C2-N1	3.70	1.41	1.33
1	A	199	LLP	C4-C5	11.35	1.56	1.42
1	A	199	LLP	C3-C2	12.40	1.49	1.40

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	LLP	C3-C2-N1	-3.57	116.06	120.75
1	A	199	LLP	C5-C6-N1	-3.00	118.79	123.87
1	A	199	LLP	C4-C4'-NZ	-2.98	110.17	124.66
1	A	199	LLP	C3-C4-C4'	-2.21	116.29	120.52
1	A	199	LLP	O-C-CA	-2.05	119.36	125.02
1	A	199	LLP	O3-C3-C2	-2.00	113.59	117.78
1	A	199	LLP	O3-C3-C4	2.07	125.26	119.59
1	A	199	LLP	OP4-C5'-C5	2.53	114.41	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	LLP	C5-C4-C4'	3.07	125.95	121.36
1	A	199	LLP	C6-N1-C2	3.89	126.75	119.26
1	A	199	LLP	CE-NZ-C4'	4.40	131.81	119.03
1	A	199	LLP	C2'-C2-C3	6.60	128.83	120.96

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	199	LLP	1	0
1	B	199[A]	LLP	4	0
1	B	199[B]	LLP	3	0
1	C	199	LLP	1	0
1	D	199	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 12 are monoatomic - leaving 4 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	PLG	B	1000[A]	-	17,20,20	4.85	5 (29%)	23,28,28	2.88	10 (43%)
5	PLP	B	1003[B]	-	15,15,16	5.19	5 (33%)	20,22,23	2.61	9 (45%)
4	PLG	C	1001	-	17,20,20	4.62	6 (35%)	23,28,28	2.95	10 (43%)
4	PLG	D	1002	-	17,20,20	4.79	5 (29%)	23,28,28	2.92	10 (43%)

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	PLG	B	1000[A]	-	-	0/10/12/12	0/1/1/1
5	PLP	B	1003[B]	-	-	0/6/6/8	0/1/1/1
4	PLG	C	1001	-	-	0/10/12/12	0/1/1/1
4	PLG	D	1002	-	-	0/10/12/12	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1003[B]	PLP	C4A-C4	-2.30	1.47	1.51
4	C	1001	PLG	C4A-C4	-2.04	1.49	1.51
4	C	1001	PLG	C3-C4	2.44	1.43	1.40
4	B	1000[A]	PLG	C3-C4	2.81	1.44	1.40
4	D	1002	PLG	C3-C4	2.83	1.44	1.40
4	C	1001	PLG	C6-N1	2.99	1.40	1.34
4	D	1002	PLG	C6-N1	3.08	1.41	1.34
4	B	1000[A]	PLG	C6-N1	3.18	1.41	1.34
5	B	1003[B]	PLP	C6-N1	3.48	1.41	1.34
5	B	1003[B]	PLP	C2-N1	3.63	1.41	1.33
4	B	1000[A]	PLG	C2-N1	3.77	1.41	1.33
4	D	1002	PLG	C2-N1	3.93	1.42	1.33
4	C	1001	PLG	C2-N1	4.01	1.42	1.33
4	C	1001	PLG	C5-C4	11.33	1.56	1.40
5	B	1003[B]	PLP	C3-C2	11.87	1.49	1.40
4	B	1000[A]	PLG	C5-C4	11.89	1.57	1.40
4	D	1002	PLG	C5-C4	12.04	1.57	1.40
4	C	1001	PLG	C3-C2	13.50	1.50	1.40
4	D	1002	PLG	C3-C2	13.94	1.50	1.40
4	B	1000[A]	PLG	C3-C2	14.42	1.50	1.40
5	B	1003[B]	PLP	C5-C4	14.80	1.57	1.40

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1002	PLG	C3-C2-N1	-3.41	116.27	120.75
5	B	1003[B]	PLP	C3-C2-N1	-3.38	116.32	120.75
4	C	1001	PLG	C3-C2-N1	-3.37	116.32	120.75
4	B	1000[A]	PLG	C3-C2-N1	-3.36	116.34	120.75
5	B	1003[B]	PLP	C5-C6-N1	-3.16	118.52	123.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1001	PLG	C5-C6-N1	-2.99	118.81	123.87
4	D	1002	PLG	C5-C6-N1	-2.97	118.85	123.87
4	B	1000[A]	PLG	C5-C6-N1	-2.96	118.86	123.87
5	B	1003[B]	PLP	C4A-C4-C3	-2.90	115.54	120.54
5	B	1003[B]	PLP	O3-C3-C2	-2.19	113.20	117.78
4	D	1002	PLG	O3-C3-C2	-2.17	113.24	117.78
4	B	1000[A]	PLG	O3-C3-C2	-2.11	113.36	117.78
4	C	1001	PLG	C4-C4A-N	2.02	115.40	111.91
4	C	1001	PLG	C-CA-N	2.24	115.79	111.91
5	B	1003[B]	PLP	O4P-C5A-C5	2.27	113.89	109.32
4	D	1002	PLG	C4-C4A-N	2.45	116.16	111.91
4	D	1002	PLG	C6-C5-C4	2.49	119.98	118.13
4	C	1001	PLG	O3-C3-C4	2.58	125.72	118.10
4	C	1001	PLG	C6-C5-C4	2.61	120.07	118.13
4	B	1000[A]	PLG	C6-C5-C4	2.66	120.11	118.13
4	B	1000[A]	PLG	O3-C3-C4	2.68	126.03	118.10
4	D	1002	PLG	O3-C3-C4	2.74	126.21	118.10
4	B	1000[A]	PLG	C4-C4A-N	2.79	116.74	111.91
5	B	1003[B]	PLP	O3-C3-C4	2.83	125.83	118.14
4	C	1001	PLG	C6-N1-C2	3.78	126.55	119.26
4	B	1000[A]	PLG	C6-N1-C2	3.88	126.74	119.26
4	D	1002	PLG	C6-N1-C2	3.95	126.87	119.26
5	B	1003[B]	PLP	C6-N1-C2	3.95	126.87	119.26
4	D	1002	PLG	C4A-C4-C5	4.66	124.01	119.75
4	B	1000[A]	PLG	C4A-C4-C5	4.91	124.25	119.75
4	C	1001	PLG	C4A-C4-C5	4.93	124.26	119.75
5	B	1003[B]	PLP	C4A-C4-C5	5.59	126.50	120.86
5	B	1003[B]	PLP	C2A-C2-C3	5.78	127.86	120.96
4	C	1001	PLG	C2A-C2-C3	6.44	128.64	120.96
4	B	1000[A]	PLG	C2A-C2-C3	6.47	128.68	120.96
4	D	1002	PLG	C2A-C2-C3	6.52	128.74	120.96
4	B	1000[A]	PLG	CA-N-C4A	7.10	128.03	112.18
4	D	1002	PLG	CA-N-C4A	7.58	129.09	112.18
4	C	1001	PLG	CA-N-C4A	7.74	129.44	112.18

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1000[A]	PLG	4	0
5	B	1003[B]	PLP	3	0
4	C	1001	PLG	3	0
4	D	1002	PLG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	329/347 (94%)	-0.10	1 (0%) 93 94	17, 25, 35, 46	0
1	B	329/347 (94%)	-0.04	3 (0%) 84 86	16, 23, 37, 44	0
1	C	329/347 (94%)	-0.04	2 (0%) 89 91	14, 25, 36, 46	1 (0%)
1	D	329/347 (94%)	-0.07	6 (1%) 69 73	15, 24, 39, 48	0
All	All	1316/1388 (94%)	-0.06	12 (0%) 84 86	14, 24, 37, 48	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	THR	4.4
1	D	137	THR	3.8
1	C	137	THR	3.4
1	B	137	THR	3.3
1	B	340	ARG	3.2
1	C	72	ARG	3.2
1	D	340	ARG	2.9
1	D	343	SER	2.4
1	B	160	GLU	2.1
1	D	196	CYS	2.1
1	D	285	ARG	2.1
1	D	213	ARG	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	LLP	A	199	24/25	0.96	0.17	-	17,23,27,30	0
1	LLP	C	199	9/25	0.95	0.22	-	17,21,28,32	0
1	LLP	D	199	9/25	0.95	0.22	-	21,22,26,33	0
1	LLP	B	199[A]	9/25	0.97	0.20	-	18,21,29,32	9
1	LLP	B	199[B]	9/25	0.97	0.20	-	17,22,30,31	9

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PLG	B	1000[A]	20/20	0.95	0.20	1.71	21,25,31,31	20
4	PLG	C	1001	20/20	0.96	0.17	0.64	21,25,30,31	0
4	PLG	D	1002	20/20	0.95	0.17	0.60	20,22,37,37	0
5	PLP	B	1003[B]	15/16	0.96	0.14	0.47	23,25,27,29	15
2	CA	D	1009	1/1	0.96	0.07	-1.77	25,25,25,25	0
2	CA	C	1004	1/1	0.99	0.06	-2.23	22,22,22,22	0
2	CA	A	1006	1/1	0.95	0.08	-2.45	21,21,21,21	0
2	CA	A	1005	1/1	0.95	0.07	-2.85	23,23,23,23	0
2	CA	B	1007	1/1	0.99	0.04	-4.94	22,22,22,22	0
3	CL	D	1015	1/1	0.96	0.06	-	38,38,38,38	0
3	CL	D	1011	1/1	0.93	0.12	-	30,30,30,30	0
3	CL	A	1010	1/1	0.96	0.06	-	27,27,27,27	0
2	CA	B	1008	1/1	0.94	0.08	-	31,31,31,31	0
3	CL	B	1012	1/1	0.99	0.10	-	36,36,36,36	0
3	CL	D	1014	1/1	0.97	0.08	-	37,37,37,37	0
3	CL	B	1013	1/1	0.99	0.08	-	34,34,34,34	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.