



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:49 AM UTC

PDB ID : 1LW5 / pdb_00001lw5
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

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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

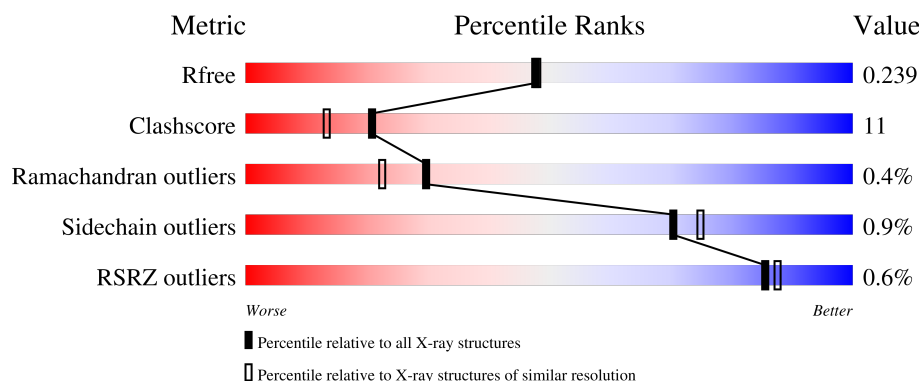
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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}	180053	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (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	347	 82% 16% ..
1	B	347	 77% 22% .
1	C	347	 77% 21% ..
1	D	347	 78% 19% ..

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PLP	B	1003[B]	-	X	-	-

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

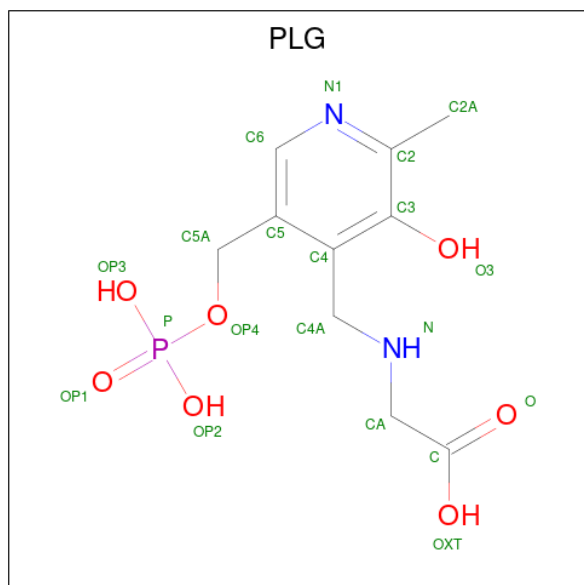
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	2	Total Cl 2 2	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] (CCD ID: PLG) (formula: C₁₀H₁₅N₂O₇P).



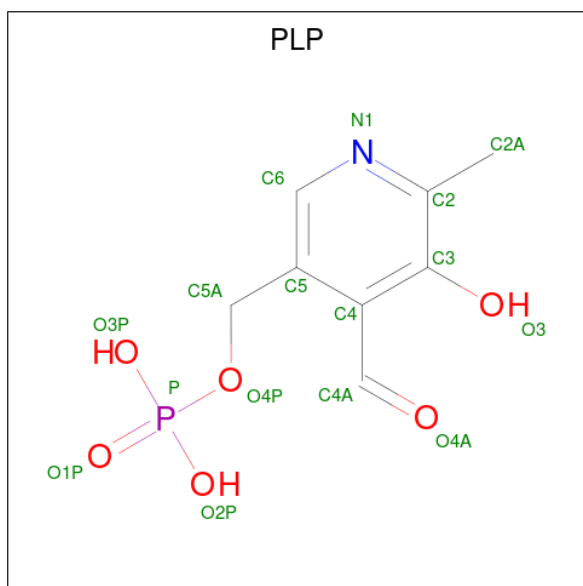
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O P 20 10 2 7 1	0	1
4	C	1	Total C N O P 20 10 2 7 1	0	0

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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 (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



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

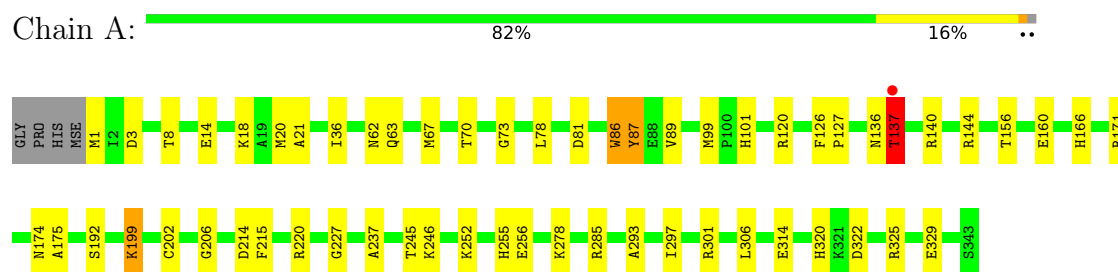
- Molecule 6 is water.

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		

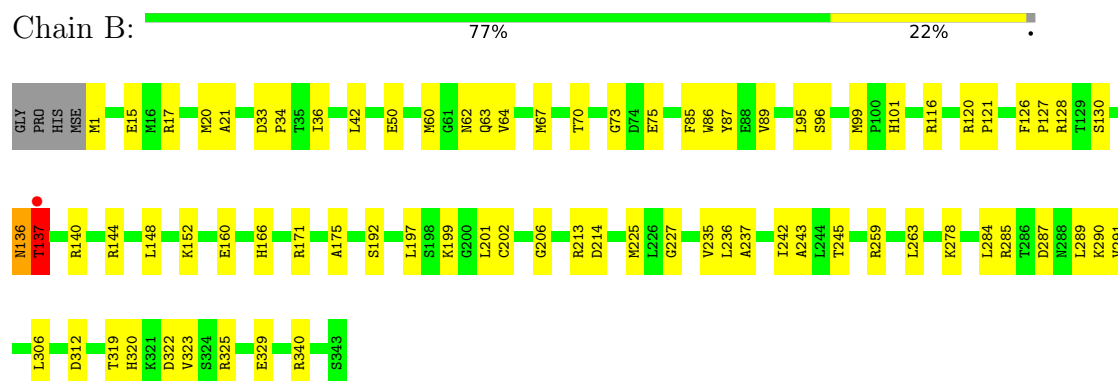
3 Residue-property plots

These plots are drawn for all protein, RNA, 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.

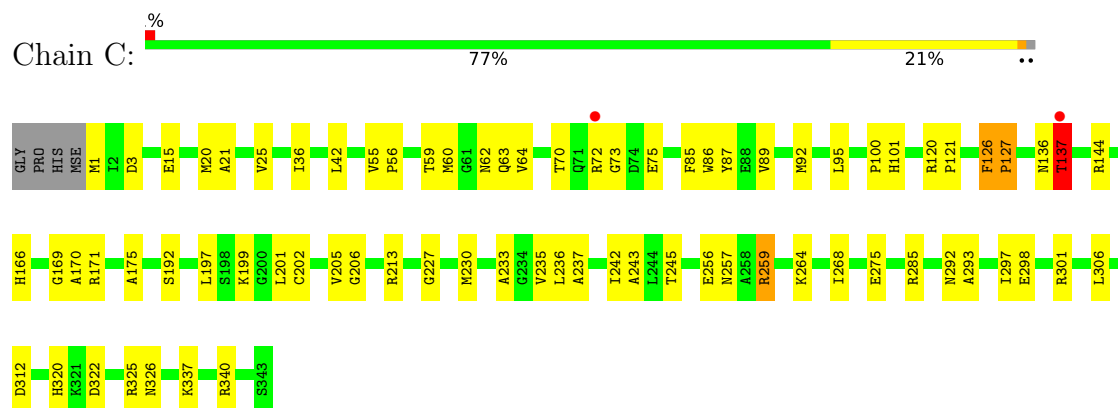
- Molecule 1: L-allo-threonine aldolase



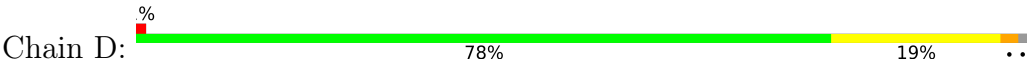
- Molecule 1: L-allo-threonine aldolase



- 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	96.02Å 100.71Å 150.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.05 20.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.05) 93.6 (20.00-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.04Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.237 0.209 , 0.239	Depositor DCC
R_{free} test set	5953 reflections (6.95%)	wwPDB-VP
Wilson B-factor (Å ²)	23.3	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	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 ²)	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.*

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: PLP, CA, PLG, 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	0.38	0/2613	0.99	10/3514 (0.3%)
1	B	0.40	0/2631	1.03	13/3535 (0.4%)
1	C	0.38	0/2615	1.00	15/3516 (0.4%)
1	D	0.43	1/2634 (0.0%)	1.03	14/3536 (0.4%)
All	All	0.40	1/10493 (0.0%)	1.01	52/14101 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	18	LYS	CD-CE	6.44	1.71	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	206	GLY	N-CA-C	14.56	125.78	111.95
1	D	206	GLY	N-CA-C	13.77	125.03	111.95
1	B	206	GLY	N-CA-C	12.68	126.49	112.29
1	A	137	THR	N-CA-C	-12.39	84.40	110.80
1	D	137	THR	N-CA-C	-12.22	84.76	110.80
1	B	137	THR	N-CA-C	-11.92	85.42	110.80
1	C	137	THR	N-CA-C	-11.54	86.21	110.80
1	C	206	GLY	N-CA-C	11.44	125.10	112.29
1	D	18	LYS	CA-CB-CG	-9.10	95.91	114.10
1	D	18	LYS	CB-CG-CD	8.27	130.33	111.30
1	B	136	ASN	CA-C-N	7.27	135.42	121.54
1	B	136	ASN	C-N-CA	7.27	135.42	121.54
1	A	126	PHE	N-CA-C	7.20	120.24	110.31
1	D	137	THR	N-CA-CB	6.97	122.28	110.49
1	A	202	CYS	N-CA-C	6.83	123.05	113.56
1	D	202	CYS	N-CA-C	6.77	122.97	113.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	136	ASN	CA-C-N	6.74	134.42	121.54
1	C	136	ASN	C-N-CA	6.74	134.42	121.54
1	A	70	THR	N-CA-C	6.55	118.49	109.18
1	C	202	CYS	N-CA-C	6.53	122.64	113.56
1	B	137	THR	N-CA-CB	6.49	121.46	110.49
1	C	137	THR	N-CA-CB	6.49	121.46	110.49
1	C	126	PHE	N-CA-C	6.47	119.65	110.40
1	C	25	VAL	N-CA-C	6.47	116.71	108.82
1	C	70	THR	N-CA-C	6.39	119.13	109.41
1	D	136	ASN	CA-C-N	6.37	133.72	121.54
1	D	136	ASN	C-N-CA	6.37	133.72	121.54
1	B	87	TYR	N-CA-C	6.34	120.33	112.59
1	B	202	CYS	N-CA-C	6.34	122.37	113.56
1	B	126	PHE	N-CA-C	6.29	119.82	110.32
1	D	70	THR	N-CA-C	6.18	118.81	109.41
1	B	70	THR	N-CA-C	6.07	119.09	109.81
1	B	160	GLU	CA-CB-CG	5.93	125.96	114.10
1	C	127	PRO	N-CA-C	-5.75	103.17	111.22
1	C	55	VAL	CA-C-N	5.70	125.38	119.56
1	C	55	VAL	C-N-CA	5.70	125.38	119.56
1	A	245	THR	N-CA-C	5.57	119.80	112.89
1	B	136	ASN	N-CA-C	5.54	117.67	108.20
1	D	18	LYS	CG-CD-CE	5.53	124.02	111.30
1	D	25	VAL	N-CA-C	5.51	116.84	108.80
1	A	87	TYR	N-CA-C	5.50	119.56	112.41
1	D	138	HIS	N-CA-C	-5.49	100.85	109.25
1	C	197	LEU	N-CA-C	-5.47	106.97	113.97
1	C	205	VAL	N-CA-C	5.40	115.48	108.35
1	D	86	TRP	N-CA-C	5.37	119.96	113.41
1	C	87	TYR	N-CA-C	5.19	118.93	112.59
1	B	86	TRP	N-CA-C	5.17	119.64	112.45
1	A	86	TRP	N-CA-C	5.04	119.45	112.45
1	A	101	HIS	CA-C-N	5.03	125.26	119.83
1	A	101	HIS	C-N-CA	5.03	125.26	119.83
1	D	126	PHE	N-CA-C	5.02	117.91	110.32
1	B	197	LEU	N-CA-C	-5.00	107.56	113.97

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	53	0
1	B	2621	0	2610	72	0
1	C	2596	0	2577	74	0
1	D	2616	0	2614	59	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	4	0
All	All	11412	0	10419	232	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 (232) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:56:PRO:HG3	1:C:230:MSE:HE2	1.62	0.81
1:C:230:MSE:HE3	6:C:1078:HOH:O	1.78	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:HG2	1:C:259:ARG:NH2	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:21:ALA:HB2	1:D:21:ALA:CB	2.31	0.60
1:C:326:ASN:ND2	6:C:1077:HOH:O	2.33	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:CG	1:C:259:ARG:NH2	2.54	0.59
1:C:1:MSE:CE	1:C:306:LEU:HD21	2.33	0.59
1:C:275:GLU:H	1:C:275:GLU:CD	2.11	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:89:VAL:HG22	1:C:89:VAL:O	2.07	0.55
1:A:14:GLU:CD	1:A:18:LYS:NZ	2.65	0.54
1:B:323:VAL:HG23	1:B:323:VAL:O	2.07	0.54
1:B:225:MSE:CA	1:C:89:VAL:HG11	2.37	0.54
1:B:340:ARG:HD3	6:B:1144:HOH:O	2.07	0.54
1:B:320:HIS:H	1:B:323:VAL:CG2	2.21	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:D:298:GLU:CD	1:D:301:ARG:HH21	2.17	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:D:284:LEU:HD23	1:D:284:LEU:C	2.36	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:3:ASP:O	1:D:320:HIS:HE1	1.96	0.49
1:D:137:THR:CG2	1:D:175:ALA:HB2	2.42	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
1:B:199[A]:LLP:CE	4:B:1000[A]:PLG:H4A2	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:137:THR:CA	1:A:144:ARG:O	2.62	0.48
1:A:14:GLU:HG3	1:A:18:LYS:HZ3	1.77	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:227:GLY:HA3	1:D:60:MSE:HB2	1.97	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: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:63:GLN:O	1:B:67:MSE:HG3	2.14	0.47
1:B:259:ARG:NE	6:B:1123:HOH:O	2.48	0.47
1:D:320:HIS:H	1:D:323:VAL:CG2	2.27	0.47
1:A:99:MSE:HE2	1:A:99:MSE:HB3	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: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:A:14:GLU:CD	1:A:18:LYS:HZ3	2.22	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:NZ	1:A:246:LYS:HB3	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:B:140:ARG:HD3	6:B:1221:HOH:O	2.18	0.44
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:60:MSE:O	1:B:64:VAL:HG22	2.19	0.42
1:B:128:ARG:HH11	1:B:130:SER:HB3	1.83	0.42
1:D:17:ARG:HA	1:D:20:MSE:CE	2.50	0.42
1:C:72:ARG:HB3	6:C:1215:HOH:O	2.18	0.42
1:C:201:LEU:HB3	1:C:243:ALA:HB1	2.01	0.42
1:B:137:THR:HG23	1:B:175:ALA:HB2	2.01	0.42
1:A:14:GLU:CG	1:A:18:LYS:HZ3	2.32	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:HD22	1:D:257:ASN:HA	1.67	0.42
1:C:213:ARG:NH2	6:C:1158:HOH:O	2.52	0.41
1:D:91:ALA:HB1	1:D:95:LEU:HD22	2.01	0.41
1:D:323:VAL:HG23	1:D:323:VAL:O	2.20	0.41
1:A:255:HIS:HD2	6:A:1169:HOH:O	2.03	0.41
1:B:289:LEU:C	1:B:291:VAL:H	2.29	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
1:B:33:ASP:HA	1:B:34:PRO:HD3	1.92	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:MSE:HB2	1:C:227:GLY:HA3	2.03	0.41
1:B:201:LEU:HB3	1:B:243:ALA:HB1	2.02	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:85:PHE:HD1	1:D:99:MSE:HE1	1.86	0.41
1:B:137:THR:OG1	1:B:171:ARG:HB2	2.20	0.41
1:C:169:GLY:O	1:C:170:ALA:C	2.62	0.41
1:D:60:MSE:O	1:D:64:VAL:HG22	2.21	0.41
1:D:198:SER:HA	1:D:203:ALA:O	2.20	0.41
1:B:75:GLU:HG3	1:B:99:MSE:HB2	2.02	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:284:LEU:HD23	1:B:284:LEU:C	2.46	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%)	36	30
1	B	340/347 (98%)	331 (97%)	8 (2%)	1 (0%)	36	30
1	C	340/347 (98%)	333 (98%)	6 (2%)	1 (0%)	36	30
1	D	341/347 (98%)	333 (98%)	6 (2%)	2 (1%)	21	13
All	All	1361/1388 (98%)	1328 (98%)	28 (2%)	5 (0%)	30	22

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%)	76	80
1	B	275/269 (102%)	272 (99%)	3 (1%)	65	68
1	C	271/269 (101%)	270 (100%)	1 (0%)	84	88
1	D	275/269 (102%)	271 (98%)	4 (2%)	57	58
All	All	1092/1076 (102%)	1082 (99%)	10 (1%)	70	75

All (10) residues with a non-rotameric sidechain are listed below:

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	63	GLN
1	A	166	HIS
1	A	174	ASN
1	A	255	HIS
1	A	257	ASN
1	A	308	ASN
1	A	320	HIS
1	B	62	ASN
1	B	101	HIS
1	B	166	HIS
1	B	174	ASN
1	B	273	ASN
1	B	320	HIS
1	C	62	ASN
1	C	101	HIS
1	C	166	HIS
1	C	174	ASN
1	C	257	ASN
1	C	308	ASN
1	C	320	HIS
1	C	326	ASN
1	D	22	GLN
1	D	63	GLN
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	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	B	199[B]	1	7,8,25	0.49	0	3,8,34	0.45	0
1	LLP	A	199	1	23,24,25	3.19	6 (26%)	25,32,34	2.50	10 (40%)
1	LLP	B	199[A]	1	7,8,25	0.45	0	3,8,34	1.04	0
1	LLP	C	199	1	7,8,25	0.51	0	3,8,34	0.41	0
1	LLP	D	199	1	7,8,25	0.54	0	3,8,34	0.39	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	B	199[B]	1	-	1/6/7/19	-
1	LLP	A	199	1	-	5/16/17/19	0/1/1/1
1	LLP	B	199[A]	1	-	1/6/7/19	-
1	LLP	C	199	1	-	1/6/7/19	-
1	LLP	D	199	1	-	1/6/7/19	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	199	LLP	C4-C5	10.51	1.56	1.42
1	A	199	LLP	C3-C2	8.07	1.49	1.41
1	A	199	LLP	C2-N1	4.34	1.41	1.33
1	A	199	LLP	C6-N1	3.20	1.40	1.34
1	A	199	LLP	C4'-NZ	3.11	1.37	1.27
1	A	199	LLP	P-OP3	-2.22	1.46	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	LLP	C2'-C2-C3	6.86	128.83	120.80
1	A	199	LLP	C6-N1-C2	4.17	126.75	119.20
1	A	199	LLP	CE-NZ-C4'	4.09	131.81	118.72
1	A	199	LLP	C3-C2-N1	-3.88	116.06	120.96
1	A	199	LLP	C5-C6-N1	-3.10	118.79	123.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	199	LLP	C4-C4'-NZ	-3.01	110.17	124.04
1	A	199	LLP	C5-C4-C4'	2.91	125.95	121.47
1	A	199	LLP	OP4-C5'-C5	2.70	114.41	109.36
1	A	199	LLP	C3-C4-C4'	-2.28	116.29	120.40
1	A	199	LLP	O3-C3-C4	2.16	125.26	119.44

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 10 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
5	PLP	B	1003[B]	-	15,15,16	4.78	6 (40%)	21,22,23	2.62	9 (42%)
4	PLG	D	1002	-	20,20,20	3.82	6 (30%)	26,28,28	3.64	10 (38%)
4	PLG	B	1000[A]	-	20,20,20	3.84	6 (30%)	26,28,28	3.51	10 (38%)
4	PLG	C	1001	-	20,20,20	3.67	6 (30%)	26,28,28	3.67	9 (34%)

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
5	PLP	B	1003[B]	-	-	3/6/6/8	0/1/1/1
4	PLG	D	1002	-	-	3/12/12/12	0/1/1/1
4	PLG	B	1000[A]	-	-	3/12/12/12	0/1/1/1
4	PLG	C	1001	-	-	2/12/12/12	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1003[B]	PLP	C5-C4	15.21	1.57	1.40
4	D	1002	PLG	C5-C4	12.04	1.57	1.40
4	B	1000[A]	PLG	C5-C4	11.88	1.57	1.40
4	C	1001	PLG	C5-C4	11.32	1.56	1.40
4	B	1000[A]	PLG	C3-C2	9.42	1.50	1.41
4	D	1002	PLG	C3-C2	9.10	1.50	1.41
4	C	1001	PLG	C3-C2	8.81	1.50	1.41
5	B	1003[B]	PLP	C3-C2	7.71	1.49	1.41
4	C	1001	PLG	C2-N1	4.70	1.42	1.33
4	D	1002	PLG	C2-N1	4.61	1.42	1.33
4	B	1000[A]	PLG	C2-N1	4.42	1.41	1.33
5	B	1003[B]	PLP	C2-N1	4.26	1.41	1.33
5	B	1003[B]	PLP	C6-N1	3.67	1.41	1.34
4	B	1000[A]	PLG	C6-N1	3.35	1.41	1.34
4	D	1002	PLG	C6-N1	3.25	1.41	1.34
4	C	1001	PLG	C6-N1	3.15	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1002	PLG	C3-C4	3.08	1.44	1.40
4	B	1000[A]	PLG	C3-C4	3.07	1.44	1.40
4	C	1001	PLG	C3-C4	2.66	1.43	1.40
5	B	1003[B]	PLP	C4A-C4	-2.32	1.47	1.51
4	D	1002	PLG	P-OP3	-2.17	1.46	1.54
5	B	1003[B]	PLP	P-O3P	-2.12	1.46	1.54
4	B	1000[A]	PLG	P-OP3	-2.08	1.47	1.54
4	C	1001	PLG	P-OP3	-2.03	1.47	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1001	PLG	C4A-N-CA	14.36	129.44	112.72
4	D	1002	PLG	C4A-N-CA	14.06	129.09	112.72
4	B	1000[A]	PLG	C4A-N-CA	13.15	128.03	112.72
4	D	1002	PLG	C2A-C2-C3	6.79	128.74	120.80
4	B	1000[A]	PLG	C2A-C2-C3	6.73	128.68	120.80
4	C	1001	PLG	C2A-C2-C3	6.70	128.64	120.80
5	B	1003[B]	PLP	C2A-C2-C3	6.03	127.86	120.80
5	B	1003[B]	PLP	C4A-C4-C5	5.40	126.50	120.94
5	B	1003[B]	PLP	C6-N1-C2	4.23	126.87	119.20
4	D	1002	PLG	C6-N1-C2	4.23	126.87	119.20
4	B	1000[A]	PLG	C6-N1-C2	4.16	126.74	119.20
4	C	1001	PLG	C4A-C4-C5	4.15	124.26	119.75
4	B	1000[A]	PLG	C4A-C4-C5	4.13	124.25	119.75
4	C	1001	PLG	C6-N1-C2	4.05	126.55	119.20
4	D	1002	PLG	C4A-C4-C5	3.92	124.01	119.75
4	D	1002	PLG	C3-C2-N1	-3.72	116.27	120.96
5	B	1003[B]	PLP	C3-C2-N1	-3.68	116.32	120.96
4	C	1001	PLG	C3-C2-N1	-3.68	116.32	120.96
4	B	1000[A]	PLG	C3-C2-N1	-3.66	116.34	120.96
5	B	1003[B]	PLP	C5-C6-N1	-3.27	118.52	123.83
4	C	1001	PLG	C5-C6-N1	-3.09	118.81	123.83
4	D	1002	PLG	C5-C6-N1	-3.06	118.85	123.83
4	B	1000[A]	PLG	C5-C6-N1	-3.06	118.86	123.83
5	B	1003[B]	PLP	C4A-C4-C3	-2.99	115.54	120.52
5	B	1003[B]	PLP	O3-C3-C4	2.96	125.83	118.10
4	B	1000[A]	PLG	C4-C4A-N	2.84	116.74	111.50
4	D	1002	PLG	O3-C3-C4	2.77	126.21	118.18
4	B	1000[A]	PLG	O3-C3-C4	2.71	126.03	118.18
4	B	1000[A]	PLG	C6-C5-C4	2.70	120.11	118.06
4	C	1001	PLG	C6-C5-C4	2.65	120.07	118.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1001	PLG	O3-C3-C4	2.60	125.72	118.18
4	D	1002	PLG	C6-C5-C4	2.54	119.98	118.06
4	D	1002	PLG	C4-C4A-N	2.52	116.16	111.50
5	B	1003[B]	PLP	O4P-C5A-C5	2.42	113.89	109.36
5	B	1003[B]	PLP	O3-C3-C2	-2.11	113.20	117.58
4	C	1001	PLG	C4-C4A-N	2.11	115.40	111.50
4	D	1002	PLG	O3-C3-C2	-2.09	113.24	117.58
4	B	1000[A]	PLG	O3-C3-C2	-2.03	113.36	117.58

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1000[A]	PLG	C-CA-N-C4A
4	D	1002	PLG	C-CA-N-C4A
5	B	1003[B]	PLP	C4-C5-C5A-O4P
5	B	1003[B]	PLP	C6-C5-C5A-O4P
4	B	1000[A]	PLG	C5-C4-C4A-N
4	D	1002	PLG	C5-C4-C4A-N
4	C	1001	PLG	C5-C4-C4A-N
4	C	1001	PLG	C3-C4-C4A-N
4	B	1000[A]	PLG	C3-C4-C4A-N
4	D	1002	PLG	C3-C4-C4A-N
5	B	1003[B]	PLP	C5A-O4P-P-O2P

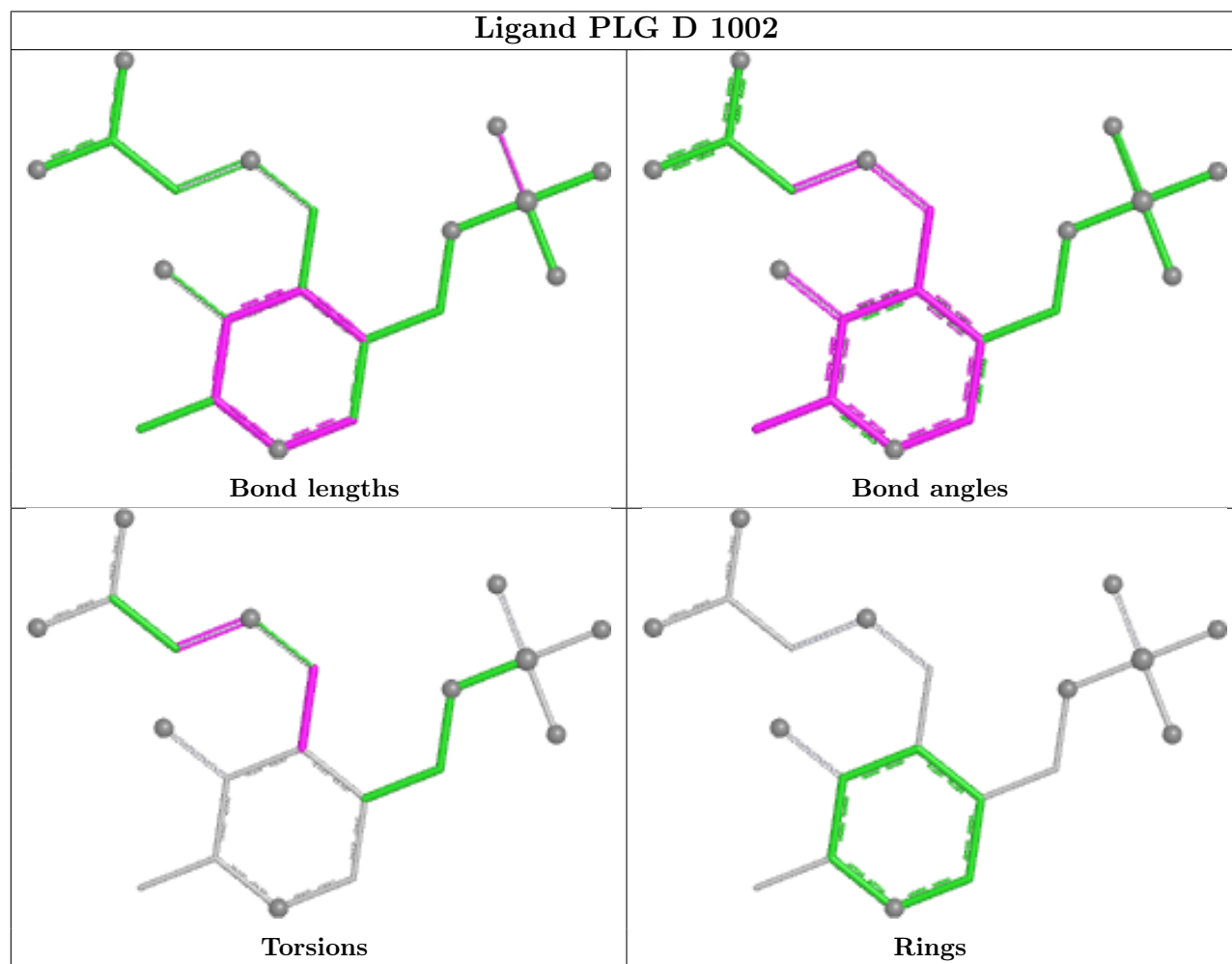
There are no ring outliers.

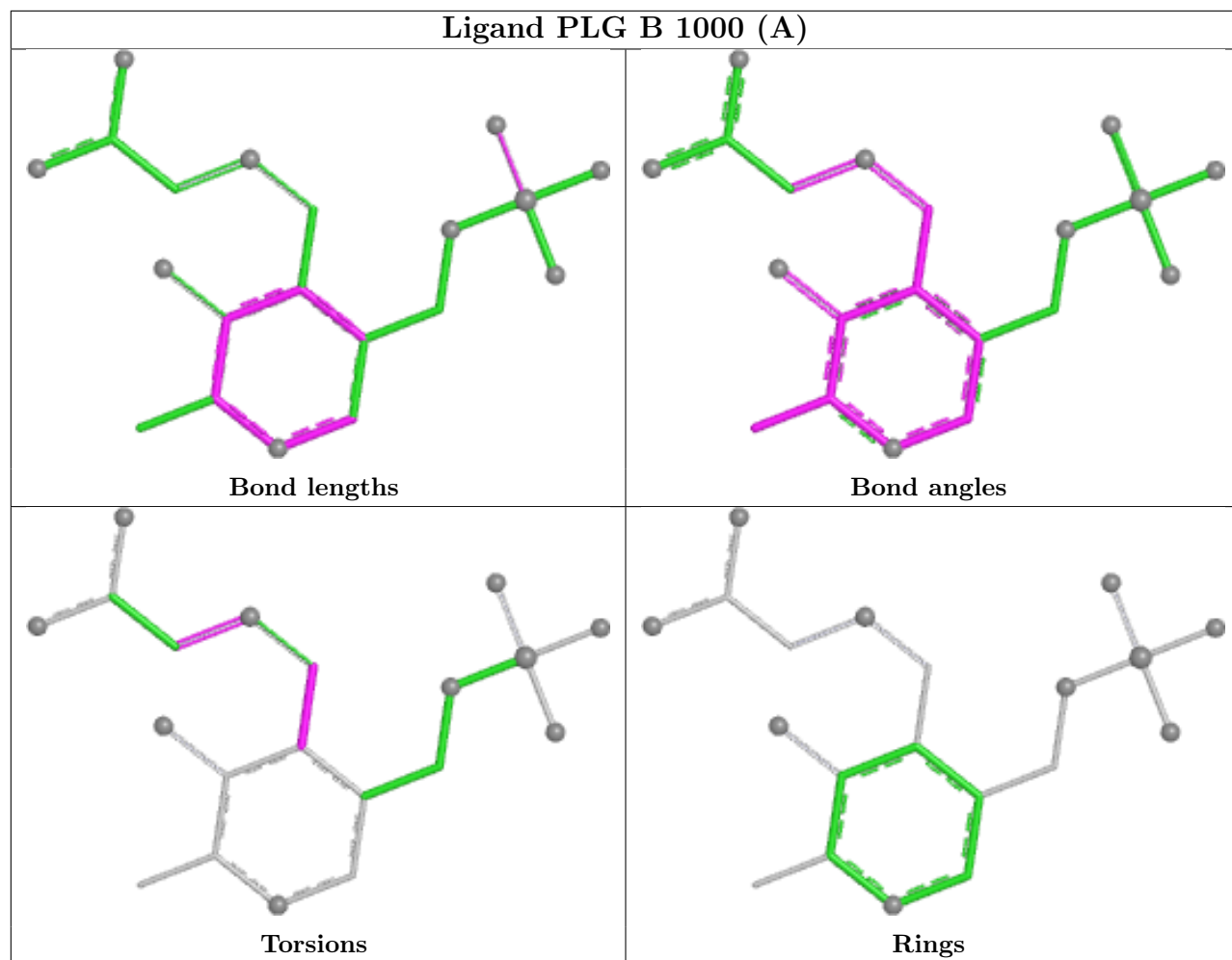
4 monomers are involved in 12 short contacts:

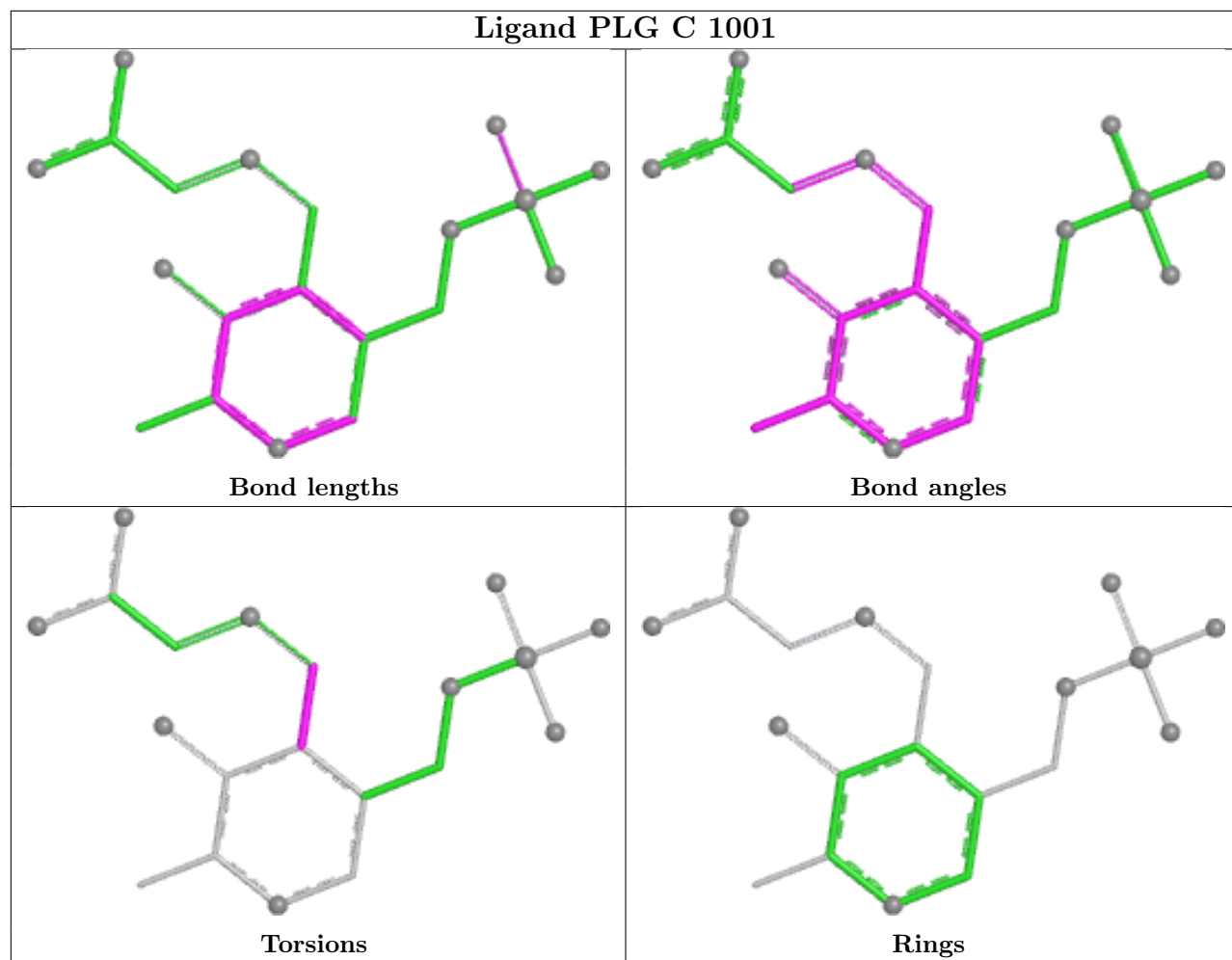
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1003[B]	PLP	3	0
4	D	1002	PLG	2	0
4	B	1000[A]	PLG	4	0
4	C	1001	PLG	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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	329/347 (94%)	-0.15	1 (0%) 90 92	17, 25, 35, 46	0
1	B	329/347 (94%)	-0.16	1 (0%) 90 92	16, 23, 37, 44	0
1	C	329/347 (94%)	-0.10	2 (0%) 85 87	7, 25, 36, 46	1 (0%)
1	D	329/347 (94%)	-0.12	4 (1%) 76 78	15, 24, 39, 48	0
All	All	1316/1388 (94%)	-0.13	8 (0%) 85 87	7, 24, 37, 48	1 (0%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	137	THR	5.9
1	B	137	THR	4.9
1	D	137	THR	4.7
1	C	137	THR	4.1
1	C	72	ARG	3.8
1	D	213	ARG	2.7
1	D	340	ARG	2.4
1	D	86	TRP	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	D	199	9/25	0.91	0.09	21,22,26,33	0
1	LLP	B	199[B]	9/25	0.94	0.09	17,22,30,31	9
1	LLP	C	199	9/25	0.94	0.08	17,21,28,32	0
1	LLP	B	199[A]	9/25	0.94	0.09	18,21,29,32	9

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
1	LLP	A	199	24/25	0.95	0.07	17,23,27,30	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

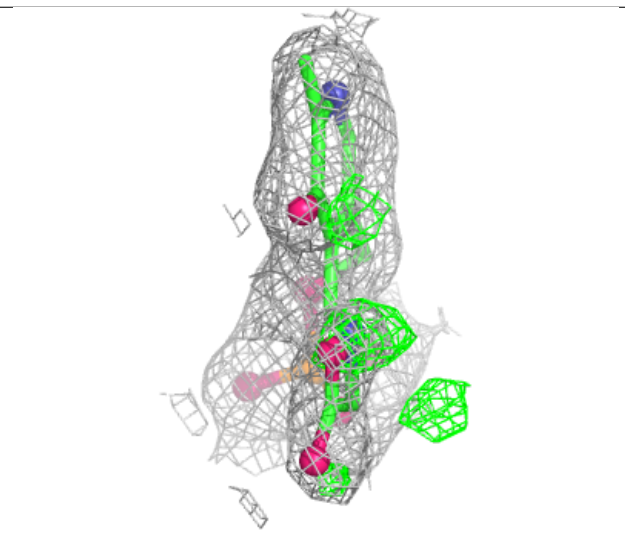
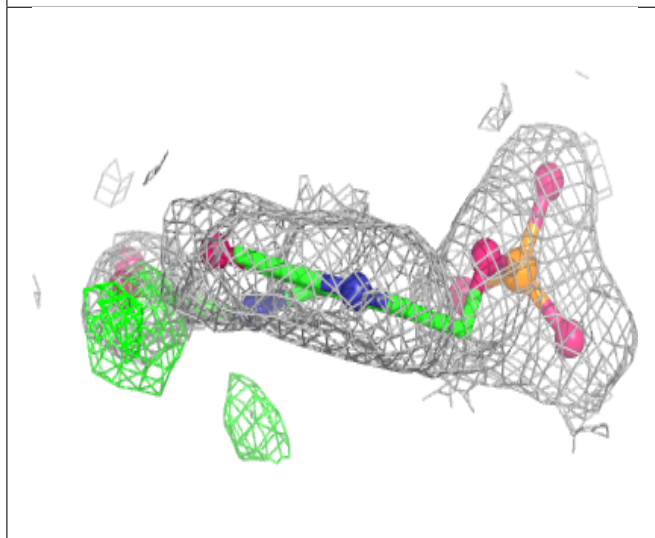
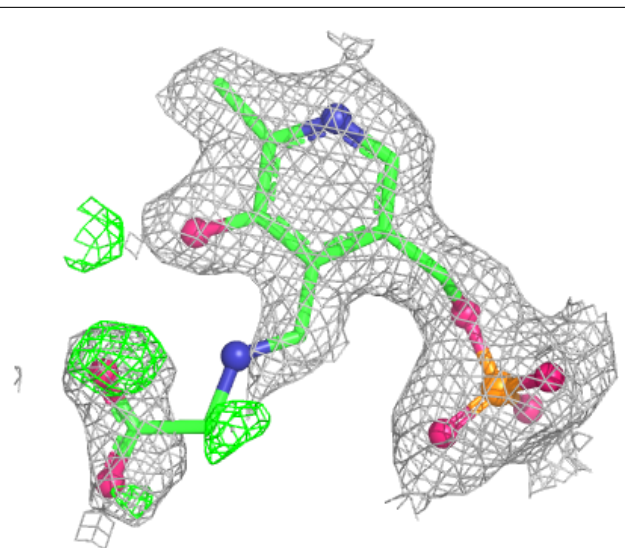
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	B	1008	1/1	0.86	0.08	31,31,31,31	0
3	CL	D	1011	1/1	0.88	0.09	30,30,30,30	0
4	PLG	B	1000[A]	20/20	0.89	0.12	21,25,31,31	20
2	CA	A	1006	1/1	0.90	0.10	21,21,21,21	0
2	CA	A	1005	1/1	0.94	0.07	23,23,23,23	0
2	CA	D	1009	1/1	0.94	0.04	25,25,25,25	0
5	PLP	B	1003[B]	15/16	0.94	0.09	23,25,27,29	15
4	PLG	D	1002	20/20	0.95	0.08	20,22,37,37	0
3	CL	A	1010	1/1	0.96	0.07	27,27,27,27	0
4	PLG	C	1001	20/20	0.96	0.07	21,25,30,31	0
3	CL	B	1012	1/1	0.97	0.08	36,36,36,36	0
2	CA	C	1004	1/1	0.98	0.04	22,22,22,22	0
3	CL	D	1015	1/1	0.98	0.05	38,38,38,38	0
3	CL	B	1013	1/1	0.98	0.06	34,34,34,34	0
3	CL	D	1014	1/1	0.99	0.03	37,37,37,37	0
2	CA	B	1007	1/1	0.99	0.05	22,22,22,22	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

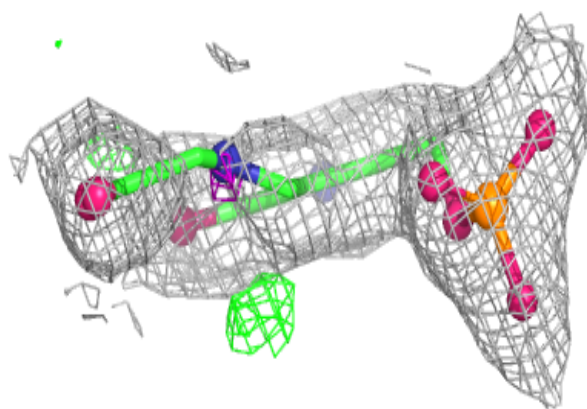
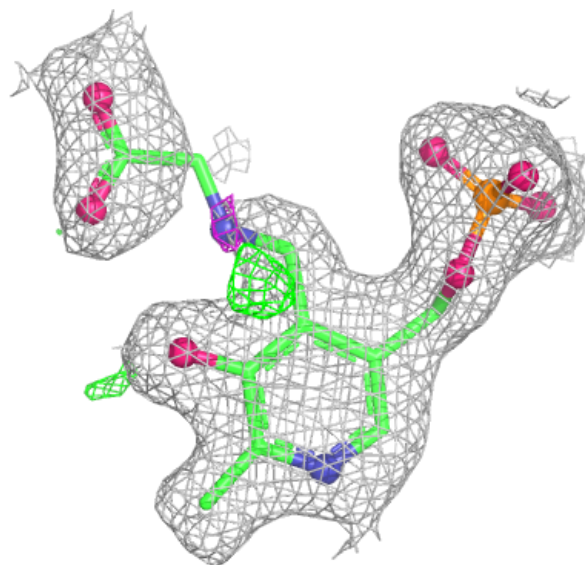
Electron density around PLG B 1000 (A):

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



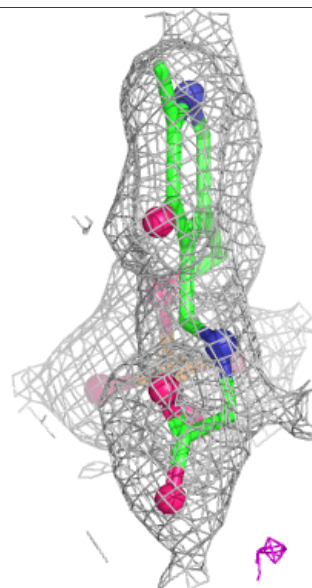
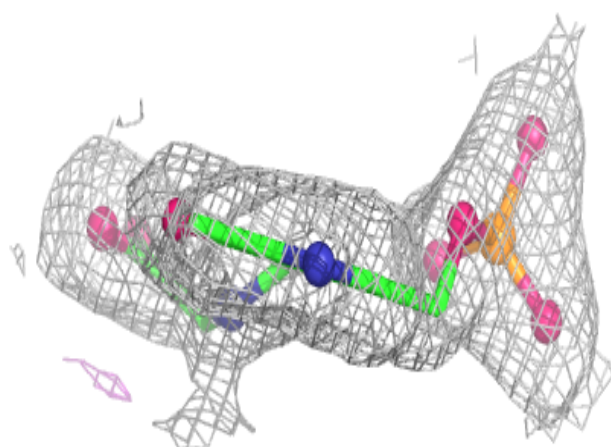
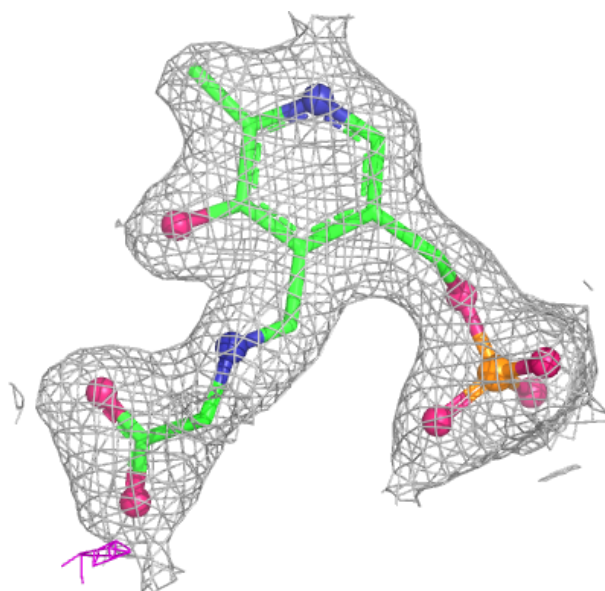
Electron density around PLG D 1002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around PLG C 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.