



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:36 AM UTC

PDB ID : 6MCQ / pdb_00006mcq
Title : L. pneumophila effector kinase LegK7 in complex with human MOB1A
Authors : Beyrakhova, K.A.; Xu, C.; Boniecki, M.T.; Cygler, M.
Deposited on : 2018-09-01
Resolution : 2.57 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

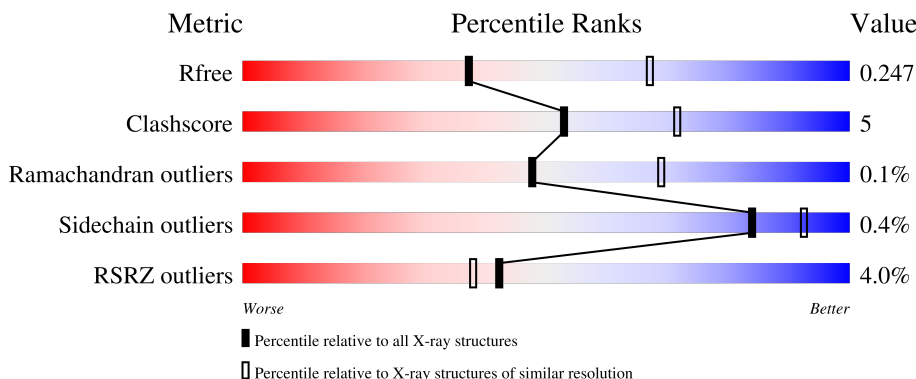
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (2.60-2.56)

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	523	5% 90% 9%
1	C	523	4% 85% 15%
2	B	187	2% 88% 10%
2	D	187	2% 85% 12%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11493 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 LegK7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	1	0
			4164	2680	698	771	15			
1	C	519	Total	C	N	O	S	0	1	0
			4104	2641	692	756	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	SER	-	expression tag	UNP Q5ZU83
A	9	ASN	-	expression tag	UNP Q5ZU83
A	10	ALA	-	expression tag	UNP Q5ZU83
C	8	SER	-	expression tag	UNP Q5ZU83
C	9	ASN	-	expression tag	UNP Q5ZU83
C	10	ALA	-	expression tag	UNP Q5ZU83

- Molecule 2 is a protein called MOB kinase activator 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	183	Total	C	N	O	S	0	1	0
			1461	945	236	271	9			
2	D	182	Total	C	N	O	S	0	0	0
			1418	917	229	263	9			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	30	SER	-	expression tag	UNP Q9H8S9
B	31	ASN	-	expression tag	UNP Q9H8S9
B	32	ALA	-	expression tag	UNP Q9H8S9
D	30	SER	-	expression tag	UNP Q9H8S9
D	31	ASN	-	expression tag	UNP Q9H8S9
D	32	ALA	-	expression tag	UNP Q9H8S9

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



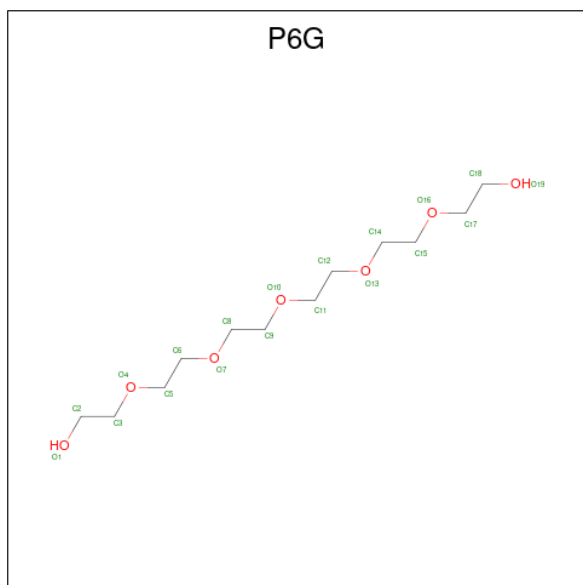
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	C	1	Total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

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

- Molecule 4 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			19	12	7		
4	A	1	Total	C	O	0	0
			19	12	7		
4	B	1	Total	C	O	0	0
			19	12	7		

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		
5	A	1	Total	C	O	0	0
			10	6	4		
5	B	1	Total	C	O	0	0
			13	8	5		
5	C	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Zn	0	0
			1	1		
6	D	1	Total	Zn	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	68	Total	O	0	0
			68	68		
7	B	20	Total	O	0	0
			20	20		

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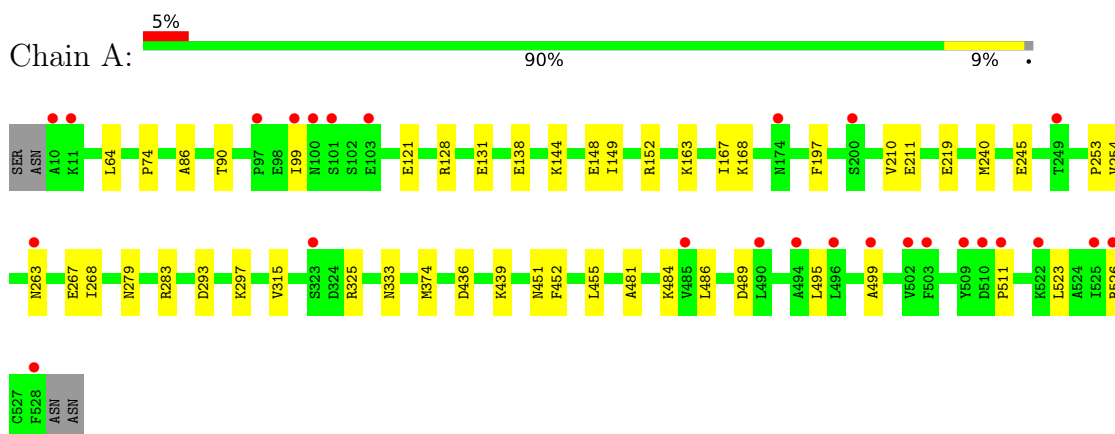
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	25	Total 25	O 25	0	0
7	D	3	Total 3	O 3	0	0

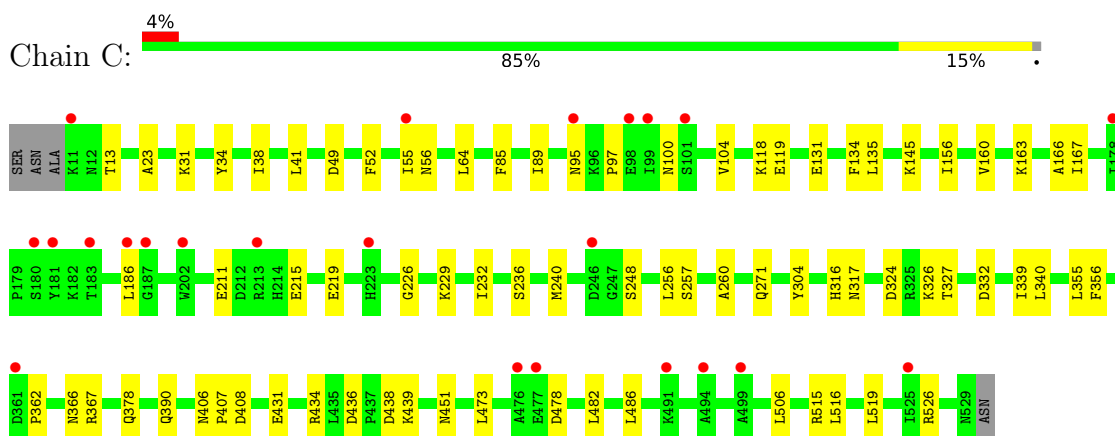
3 Residue-property plots

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.

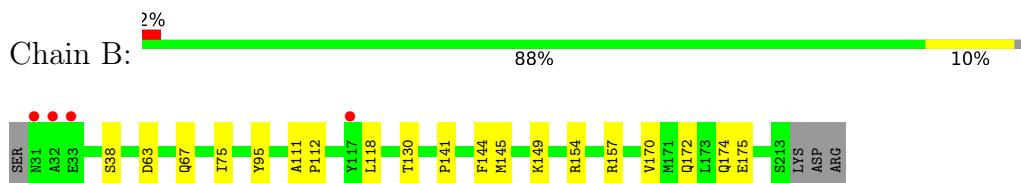
• Molecule 1: LegK7



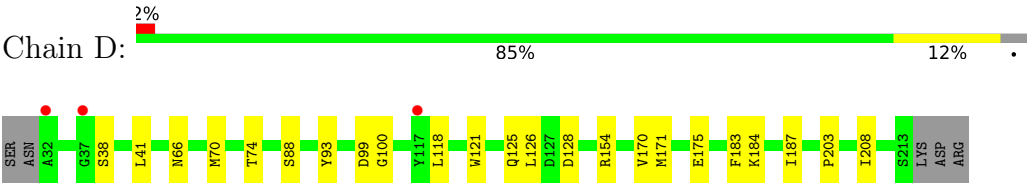
• Molecule 1: LegK7



• Molecule 2: MOB kinase activator 1A



• Molecule 2: MOB kinase activator 1A



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	107.40Å 113.10Å 157.85Å 90.00° 106.00° 90.00°	Depositor
Resolution (Å)	49.49 – 2.57 49.49 – 2.57	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.49-2.57) 99.9 (49.49-2.57)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.199 , 0.245 0.203 , 0.247	Depositor DCC
R_{free} test set	2889 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	58.4	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 63.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11493	wwPDB-VP
Average B, all atoms (Å ²)	72.0	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 43.32 % 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 1.7929e-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: PG4, PEG, P6G, ZN

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	0.15	0/4257	0.34	0/5771
1	C	0.17	0/4196	0.34	0/5698
2	B	0.14	0/1501	0.30	0/2043
2	D	0.15	0/1458	0.32	0/1992
All	All	0.16	0/11412	0.33	0/15504

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	4164	0	4069	34	0
1	C	4104	0	3965	53	0
2	B	1461	0	1375	15	0
2	D	1418	0	1296	14	0
3	A	63	0	90	0	0
3	B	7	0	10	0	0
3	C	21	0	30	0	0
3	D	21	0	30	0	0
4	A	38	0	52	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	19	0	26	4	0
5	A	23	0	31	1	0
5	B	13	0	18	0	0
5	C	10	0	13	0	0
5	D	13	0	18	0	0
6	B	1	0	0	0	0
6	D	1	0	0	0	0
7	A	68	0	0	0	0
7	B	20	0	0	0	0
7	C	25	0	0	1	0
7	D	3	0	0	0	0
All	All	11493	0	11023	111	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 (111) 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:168:LYS:HA	1:A:240:MET:HE1	1.62	0.81
1:C:215:GLU:HB2	1:C:326:LYS:HD2	1.62	0.81
1:C:431:GLU:OE1	1:C:434:ARG:NH2	2.20	0.72
1:A:152:ARG:NH1	2:B:172:GLN:OE1	2.26	0.69
1:C:232:ILE:HD13	1:C:257:SER:HB3	1.76	0.68
1:A:486:LEU:HD12	1:A:526:ARG:HH11	1.59	0.67
1:A:163:LYS:HG2	4:A:605:P6G:H151	1.78	0.65
1:C:324:ASP:OD1	1:C:326:LYS:NZ	2.29	0.65
1:A:436:ASP:OD2	1:A:439:LYS:NZ	2.32	0.63
1:C:186:LEU:HD13	1:C:362:PRO:HB2	1.82	0.62
1:C:317:ASN:HB3	2:D:74:THR:HA	1.83	0.61
1:C:49:ASP:HA	1:C:52:PHE:HB3	1.84	0.59
1:A:263[B]:ASN:HD22	1:A:267:GLU:HG3	1.68	0.59
1:A:121:GLU:OE2	1:A:121:GLU:N	2.34	0.59
4:A:609:P6G:H32	2:B:174:GLN:HE22	1.68	0.58
1:A:219:GLU:OE2	1:A:325:ARG:NH1	2.37	0.58
1:C:211:GLU:OE1	1:C:326:LYS:NZ	2.35	0.58
1:A:163:LYS:HZ1	4:A:605:P6G:H32	1.70	0.56
1:C:260:ALA:HA	1:C:316:HIS:HB2	1.87	0.56
1:C:160:VAL:HG11	1:C:256:LEU:HD21	1.87	0.56
2:D:187:ILE:HD13	2:D:208:ILE:HG12	1.88	0.56
1:A:86:ALA:O	1:A:90:THR:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:ALA:HA	1:A:484:LYS:HD3	1.88	0.55
1:A:149:ILE:HD13	4:A:609:P6G:H61	1.90	0.54
1:C:378:GLN:NE2	1:C:438:ASP:OD2	2.36	0.54
1:A:64:LEU:HD22	1:A:74:PRO:HG2	1.89	0.54
1:C:13:THR:HG22	1:C:41:LEU:HD23	1.91	0.53
1:C:163:LYS:O	1:C:166:ALA:N	2.40	0.53
2:B:145:MET:HG2	4:B:303:P6G:H152	1.92	0.52
2:B:63:ASP:O	2:B:67[B]:GLN:HG2	2.09	0.52
1:C:131:GLU:O	1:C:135:LEU:HD12	2.10	0.52
1:A:499:ALA:HB1	1:A:523:LEU:HD21	1.92	0.51
1:A:245:GLU:OE1	1:A:245:GLU:N	2.36	0.51
1:C:356:PHE:HD1	1:C:362:PRO:HA	1.73	0.51
2:B:141:PRO:HD2	2:B:144:PHE:HB2	1.92	0.51
2:D:66:ASN:O	2:D:70:MET:HG2	2.12	0.50
2:D:70:MET:HA	2:D:70:MET:HE2	1.93	0.50
1:A:333:ASN:HA	1:A:374:MET:O	2.11	0.50
2:B:149:LYS:HE2	4:B:303:P6G:H112	1.92	0.50
1:A:167:ILE:HG22	1:A:240:MET:HE3	1.94	0.50
2:D:183:PHE:O	2:D:187:ILE:HG22	2.11	0.50
1:C:356:PHE:CD1	1:C:362:PRO:HA	2.47	0.50
4:A:609:P6G:H32	2:B:174:GLN:NE2	2.26	0.50
1:C:156:ILE:O	1:C:160:VAL:HG22	2.12	0.49
2:D:41:LEU:HD12	2:D:184:LYS:HE3	1.94	0.49
1:A:486:LEU:HD12	1:A:526:ARG:NH1	2.26	0.49
1:C:486:LEU:HD21	1:C:526:ARG:HD2	1.95	0.49
2:B:118:LEU:HD11	2:B:154:ARG:HB3	1.94	0.48
1:C:55:ILE:O	1:C:64:LEU:HD21	2.13	0.48
1:C:486:LEU:CD2	1:C:526:ARG:HD2	2.44	0.47
1:A:489:ASP:HA	1:A:526:ARG:NH2	2.29	0.47
1:A:495:LEU:O	1:A:499:ALA:N	2.47	0.47
2:D:118:LEU:HD11	2:D:154:ARG:HB3	1.97	0.47
1:A:99:ILE:HG12	1:A:138:GLU:OE2	2.14	0.47
1:A:451:ASN:OD1	2:B:38:SER:HB2	2.15	0.47
4:A:605:P6G:H142	1:C:271:GLN:HG2	1.96	0.46
1:A:197:PHE:HB2	4:A:605:P6G:H21	1.97	0.46
1:C:431:GLU:CD	1:C:515:ARG:HH21	2.24	0.46
1:A:128:ARG:HB2	5:A:612:PG4:H51	1.97	0.46
1:A:128:ARG:NH1	1:A:131:GLU:OE1	2.47	0.46
1:C:304:TYR:CZ	1:C:332:ASP:HB3	2.51	0.46
1:C:431:GLU:OE2	1:C:515:ARG:NH2	2.48	0.46
1:A:452:PHE:HB3	1:A:455:LEU:HD22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:PHE:O	1:C:89:ILE:HG13	2.16	0.45
2:B:149:LYS:HE3	4:B:303:P6G:H62	1.98	0.45
1:C:406:ASN:HD22	1:C:407:PRO:N	2.12	0.45
1:C:439:LYS:HD3	1:C:473:LEU:HA	1.97	0.45
2:D:170:VAL:HG13	2:D:175:GLU:HG3	1.99	0.45
2:B:149:LYS:HZ2	4:B:303:P6G:H51	1.81	0.45
1:C:236:SER:HB3	1:C:256:LEU:HB3	1.99	0.45
1:C:327:THR:HG22	1:C:340:LEU:HB3	1.99	0.45
1:C:56:ASN:HA	1:C:64:LEU:HD11	1.97	0.45
1:C:167:ILE:HG22	1:C:240:MET:SD	2.56	0.44
1:C:97:PRO:HG2	1:C:134:PHE:CD2	2.53	0.44
1:C:451:ASN:OD1	2:D:38:SER:HB2	2.17	0.44
1:C:118:LYS:HG2	1:C:119:GLU:HG3	1.99	0.44
1:C:34:TYR:O	1:C:38:ILE:HD12	2.19	0.43
1:C:355:LEU:HG	1:C:366:ASN:HB3	1.99	0.43
1:A:489:ASP:HA	1:A:526:ARG:HH22	1.83	0.43
1:C:23:ALA:HB3	1:C:31:LYS:HE2	2.01	0.43
1:C:100:ASN:O	1:C:104:VAL:HG13	2.18	0.43
1:C:226:GLY:O	1:C:229:LYS:HG3	2.19	0.43
1:A:163:LYS:HZ1	4:A:605:P6G:H52	1.84	0.42
1:C:95:ASN:OD1	1:C:95:ASN:N	2.51	0.42
2:D:93:TYR:CG	2:D:203:PRO:HG3	2.54	0.42
2:D:99:ASP:OD1	2:D:100:GLY:N	2.52	0.42
1:A:211:GLU:HB2	1:A:253:PRO:HG2	2.02	0.42
1:A:293:ASP:OD2	1:A:297:LYS:HE2	2.20	0.42
1:C:145:LYS:HD2	2:D:171:MET:HB3	2.00	0.42
1:C:406:ASN:ND2	1:C:408:ASP:H	2.17	0.42
1:C:478:ASP:OD1	1:C:478:ASP:N	2.52	0.42
2:D:121:TRP:O	2:D:125:GLN:HG2	2.19	0.42
1:C:434:ARG:NH1	1:C:439:LYS:O	2.52	0.42
1:C:163:LYS:O	1:C:167:ILE:HD12	2.20	0.42
1:C:482:LEU:HD23	1:C:519:LEU:HB3	2.01	0.42
1:C:356:PHE:HD1	1:C:362:PRO:CA	2.32	0.42
1:C:506:LEU:HD11	1:C:516:LEU:HD22	2.01	0.42
1:A:210:VAL:HG22	1:A:254:VAL:HG22	2.02	0.42
1:C:215:GLU:OE2	1:C:219:GLU:OE1	2.37	0.41
1:A:268:ILE:HG13	1:A:315:VAL:HG21	2.02	0.41
1:A:279:ASN:O	1:A:283:ARG:HG3	2.20	0.41
1:C:390:GLN:NE2	7:C:702:HOH:O	2.53	0.41
2:B:145:MET:O	2:B:149:LYS:HG3	2.20	0.41
1:C:52:PHE:O	1:C:56:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:436:ASP:OD2	1:C:439:LYS:HG3	2.20	0.41
1:A:144:LYS:O	1:A:148:GLU:HG3	2.21	0.41
2:B:95:TYR:CZ	2:B:157:ARG:HG2	2.56	0.41
2:B:170:VAL:HG13	2:B:175:GLU:HG3	2.03	0.41
2:D:126:LEU:C	2:D:128:ASP:H	2.29	0.41
2:B:111:ALA:N	2:B:112:PRO:HD2	2.36	0.41
1:C:339:ILE:HD13	1:C:339:ILE:HA	1.83	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	518/523 (99%)	500 (96%)	17 (3%)	1 (0%)	43	63
1	C	518/523 (99%)	497 (96%)	21 (4%)	0	100	100
2	B	182/187 (97%)	178 (98%)	4 (2%)	0	100	100
2	D	180/187 (96%)	172 (96%)	8 (4%)	0	100	100
All	All	1398/1420 (98%)	1347 (96%)	50 (4%)	1 (0%)	48	69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	511	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	445/476 (94%)	445 (100%)	0	100	100
1	C	430/476 (90%)	428 (100%)	2 (0%)	81	91
2	B	154/167 (92%)	152 (99%)	2 (1%)	61	81
2	D	144/167 (86%)	143 (99%)	1 (1%)	76	88
All	All	1173/1286 (91%)	1168 (100%)	5 (0%)	84	92

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	75	ILE
2	B	130	THR
1	C	248	SER
1	C	367	ARG
2	D	88	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	65	ASN
1	A	192	ASN
1	A	214	HIS
1	A	390	GLN
1	A	498	GLN
2	B	125	GLN
1	C	22	ASN
1	C	30	GLN
1	C	65	ASN
1	C	137	ASN
1	C	318	ASN
1	C	406	ASN
1	C	409	HIS
2	D	125	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 2 are monoatomic - leaving 24 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	P6G	B	303	-	18,18,18	0.55	0	17,17,17	0.28	0
3	PEG	C	604	-	6,6,6	0.50	0	5,5,5	0.31	0
3	PEG	A	603	-	6,6,6	0.51	0	5,5,5	0.29	0
3	PEG	A	606	-	6,6,6	0.50	0	5,5,5	0.27	0
3	PEG	A	604	-	6,6,6	0.49	0	5,5,5	0.22	0
5	PG4	B	304	-	12,12,12	0.54	0	11,11,11	0.21	0
3	PEG	B	302	-	6,6,6	0.50	0	5,5,5	0.31	0
3	PEG	D	305	-	6,6,6	0.50	0	5,5,5	0.24	0
3	PEG	D	304	-	6,6,6	0.50	0	5,5,5	0.24	0
3	PEG	A	611	-	6,6,6	0.50	0	5,5,5	0.27	0
3	PEG	C	602	-	6,6,6	0.51	0	5,5,5	0.23	0
3	PEG	A	602	-	6,6,6	0.51	0	5,5,5	0.27	0
3	PEG	A	610	-	6,6,6	0.50	0	5,5,5	0.29	0
4	P6G	A	605	-	18,18,18	0.55	0	17,17,17	0.21	0
5	PG4	A	608	-	12,12,12	0.54	0	11,11,11	0.23	0
4	P6G	A	609	-	18,18,18	0.55	0	17,17,17	0.26	0
5	PG4	D	302	-	12,12,12	0.54	0	11,11,11	0.27	0
5	PG4	A	612	-	9,9,12	0.52	0	8,8,11	0.36	0
3	PEG	A	607	-	6,6,6	0.48	0	5,5,5	0.36	0
3	PEG	C	603	-	6,6,6	0.50	0	5,5,5	0.20	0
3	PEG	D	303	-	6,6,6	0.50	0	5,5,5	0.30	0
5	PG4	C	601	-	9,9,12	0.51	0	8,8,11	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PEG	A	601	-	6,6,6	0.50	0	5,5,5	0.30	0
3	PEG	A	613	-	6,6,6	0.50	0	5,5,5	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	P6G	B	303	-	-	10/16/16/16	-
3	PEG	C	604	-	-	2/4/4/4	-
3	PEG	A	603	-	-	1/4/4/4	-
3	PEG	A	606	-	-	2/4/4/4	-
3	PEG	A	604	-	-	0/4/4/4	-
5	PG4	B	304	-	-	5/10/10/10	-
3	PEG	B	302	-	-	2/4/4/4	-
3	PEG	D	305	-	-	1/4/4/4	-
3	PEG	D	304	-	-	3/4/4/4	-
3	PEG	A	611	-	-	1/4/4/4	-
3	PEG	C	602	-	-	0/4/4/4	-
3	PEG	A	602	-	-	2/4/4/4	-
3	PEG	A	610	-	-	1/4/4/4	-
4	P6G	A	605	-	-	13/16/16/16	-
5	PG4	A	608	-	-	6/10/10/10	-
4	P6G	A	609	-	-	11/16/16/16	-
5	PG4	D	302	-	-	3/10/10/10	-
5	PG4	A	612	-	-	5/7/7/10	-
3	PEG	A	607	-	-	2/4/4/4	-
3	PEG	C	603	-	-	2/4/4/4	-
3	PEG	D	303	-	-	3/4/4/4	-
5	PG4	C	601	-	-	4/7/7/10	-
3	PEG	A	601	-	-	2/4/4/4	-
3	PEG	A	613	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (83) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	303	P6G	C5-C6-O7-C8
5	B	304	PG4	O3-C5-C6-O4
4	A	609	P6G	O13-C14-C15-O16
4	A	609	P6G	O10-C11-C12-O13
3	A	607	PEG	C1-C2-O2-C3
4	A	605	P6G	O7-C8-C9-O10
5	A	612	PG4	O1-C1-C2-O2
3	A	613	PEG	O1-C1-C2-O2
3	D	303	PEG	O2-C3-C4-O4
3	D	304	PEG	O2-C3-C4-O4
5	A	612	PG4	O2-C3-C4-O3
3	B	302	PEG	O1-C1-C2-O2
5	B	304	PG4	O2-C3-C4-O3
5	C	601	PG4	O2-C3-C4-O3
4	A	605	P6G	O10-C11-C12-O13
3	A	607	PEG	O1-C1-C2-O2
4	A	605	P6G	O16-C17-C18-O19
4	A	605	P6G	O13-C14-C15-O16
5	B	304	PG4	C5-C6-O4-C7
3	C	603	PEG	O2-C3-C4-O4
3	C	604	PEG	O2-C3-C4-O4
4	A	605	P6G	O1-C2-C3-O4
5	C	601	PG4	O1-C1-C2-O2
3	A	606	PEG	C4-C3-O2-C2
5	A	608	PG4	O4-C7-C8-O5
3	A	602	PEG	C1-C2-O2-C3
3	C	603	PEG	C4-C3-O2-C2
5	A	612	PG4	C1-C2-O2-C3
5	A	608	PG4	O3-C5-C6-O4
4	A	605	P6G	C12-C11-O10-C9
5	A	612	PG4	C3-C4-O3-C5
5	C	601	PG4	C3-C4-O3-C5
3	D	304	PEG	C1-C2-O2-C3
3	A	611	PEG	C1-C2-O2-C3
5	D	302	PG4	C5-C6-O4-C7
3	D	305	PEG	C4-C3-O2-C2
3	D	303	PEG	O1-C1-C2-O2
4	B	303	P6G	C14-C15-O16-C17
4	A	605	P6G	C5-C6-O7-C8
4	B	303	P6G	O7-C8-C9-O10
4	B	303	P6G	C15-C14-O13-C12
4	A	605	P6G	C15-C14-O13-C12

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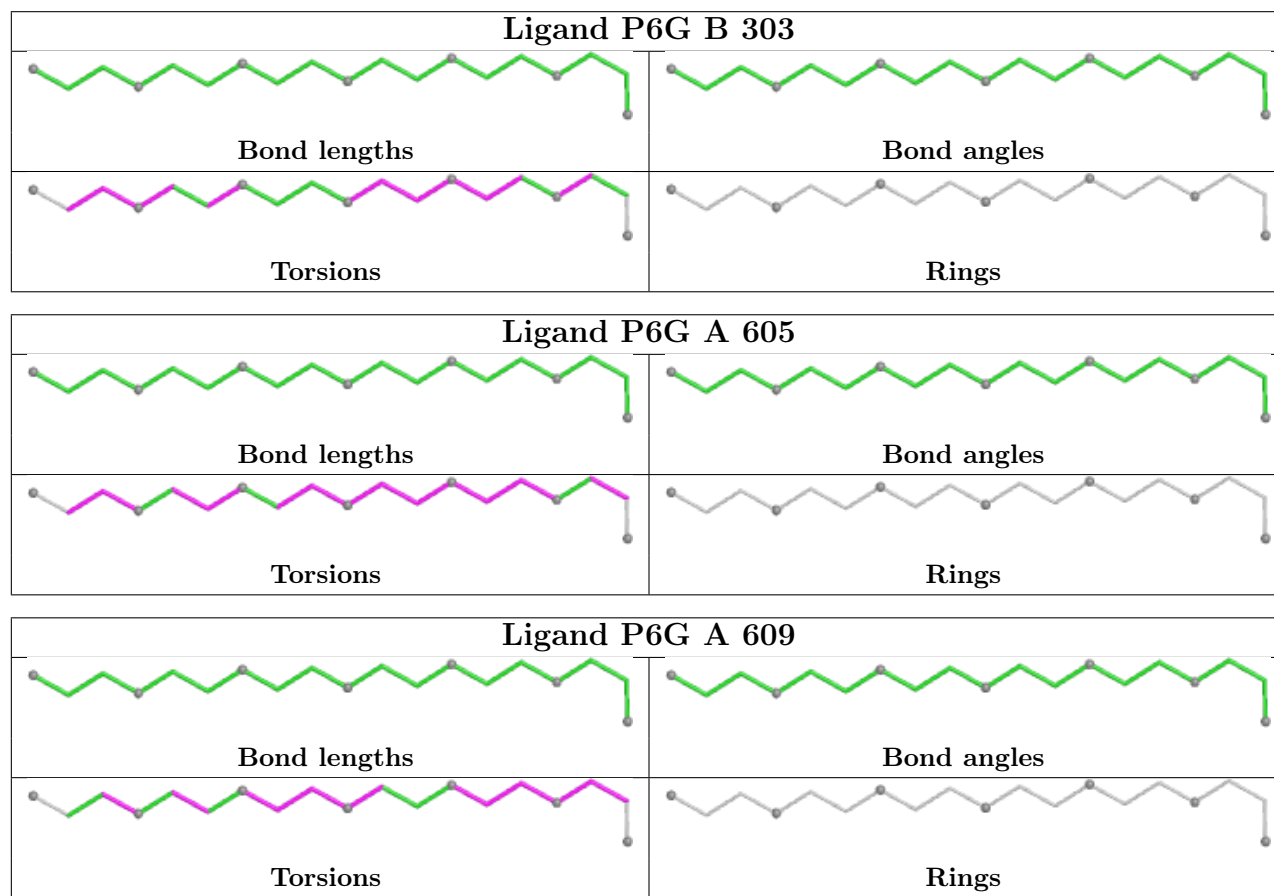
Mol	Chain	Res	Type	Atoms
3	A	606	PEG	O1-C1-C2-O2
4	A	609	P6G	C18-C17-O16-C15
5	A	608	PG4	C4-C3-O2-C2
5	D	302	PG4	C4-C3-O2-C2
4	A	609	P6G	C8-C9-O10-C11
4	B	303	P6G	O16-C17-C18-O19
4	B	303	P6G	C9-C8-O7-C6
3	A	601	PEG	C1-C2-O2-C3
3	B	302	PEG	C1-C2-O2-C3
3	C	604	PEG	C4-C3-O2-C2
4	A	605	P6G	C18-C17-O16-C15
4	A	609	P6G	C12-C11-O10-C9
4	A	609	P6G	C11-C12-O13-C14
4	B	303	P6G	C2-C3-O4-C5
3	D	303	PEG	C4-C3-O2-C2
4	B	303	P6G	C8-C9-O10-C11
4	A	605	P6G	C6-C5-O4-C3
4	A	605	P6G	C9-C8-O7-C6
3	A	601	PEG	O2-C3-C4-O4
4	A	609	P6G	C5-C6-O7-C8
3	A	602	PEG	O2-C3-C4-O4
4	B	303	P6G	O4-C5-C6-O7
5	D	302	PG4	O3-C5-C6-O4
4	A	609	P6G	C2-C3-O4-C5
4	B	303	P6G	C18-C17-O16-C15
4	A	609	P6G	O4-C5-C6-O7
5	B	304	PG4	C8-C7-O4-C6
4	A	609	P6G	C6-C5-O4-C3
4	A	605	P6G	O4-C5-C6-O7
3	A	603	PEG	C1-C2-O2-C3
4	A	609	P6G	O1-C2-C3-O4
5	A	612	PG4	C4-C3-O2-C2
5	A	608	PG4	C1-C2-O2-C3
3	A	610	PEG	O1-C1-C2-O2
5	B	304	PG4	O1-C1-C2-O2
5	A	608	PG4	C3-C4-O3-C5
4	A	605	P6G	C8-C9-O10-C11
3	A	613	PEG	O2-C3-C4-O4
3	D	304	PEG	C4-C3-O2-C2
5	C	601	PG4	O3-C5-C6-O4
5	A	608	PG4	O2-C3-C4-O3

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	303	P6G	4	0
4	A	605	P6G	5	0
4	A	609	P6G	3	0
5	A	612	PG4	1	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	519/523 (99%)	0.09	26 (5%) 34 29	35, 59, 130, 178	1 (0%)
1	C	519/523 (99%)	0.33	23 (4%) 39 34	24, 71, 141, 182	1 (0%)
2	B	183/187 (97%)	-0.10	4 (2%) 62 58	21, 59, 98, 125	1 (0%)
2	D	182/187 (97%)	0.21	3 (1%) 70 67	52, 75, 110, 121	0
All	All	1403/1420 (98%)	0.17	56 (3%) 42 38	21, 67, 130, 182	3 (0%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	10	ALA	4.0
2	B	117	TYR	3.9
1	C	186	LEU	3.8
1	C	223[A]	HIS	3.6
1	C	99	ILE	3.5
1	A	525	ILE	3.4
1	A	99	ILE	3.2
1	A	249	THR	2.8
1	A	11	LYS	2.8
1	C	525	ILE	2.8
1	A	100	ASN	2.7
1	C	202	TRP	2.7
2	D	32	ALA	2.7
1	A	502	VAL	2.7
1	C	476	ALA	2.7
1	A	174	ASN	2.6
1	A	101	SER	2.6
1	C	491	LYS	2.6
1	C	180	SER	2.6
1	A	526	ARG	2.5
2	D	37	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	477	GLU	2.5
1	A	200	SER	2.5
1	A	496	LEU	2.5
1	A	528	PHE	2.5
2	B	31	ASN	2.4
1	A	494	ALA	2.4
1	C	187	GLY	2.4
1	A	510	ASP	2.4
1	C	181	TYR	2.4
1	C	178	ILE	2.4
1	C	101	SER	2.4
1	A	499	ALA	2.4
1	C	55	ILE	2.3
2	B	33	GLU	2.3
1	C	98	GLU	2.3
1	A	323	SER	2.2
1	A	509	TYR	2.2
1	C	361	ASP	2.2
1	A	485	VAL	2.1
1	C	246	ASP	2.1
1	C	213	ARG	2.1
1	A	97	PRO	2.1
1	A	503	PHE	2.1
1	C	499	ALA	2.1
1	A	490	LEU	2.1
1	A	522	LYS	2.1
1	C	11	LYS	2.1
1	C	494	ALA	2.0
2	B	32	ALA	2.0
1	C	95	ASN	2.0
1	A	511	PRO	2.0
2	D	117	TYR	2.0
1	A	103	GLU	2.0
1	A	263[A]	ASN	2.0
1	C	183	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

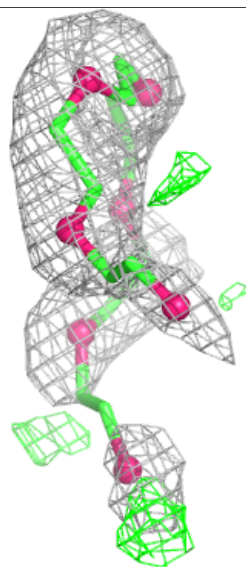
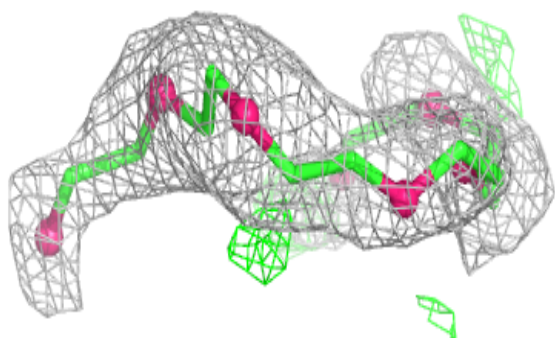
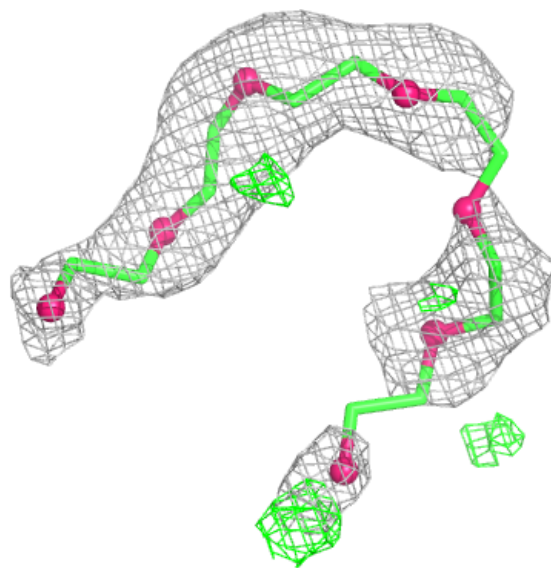
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
5	PG4	D	302	13/13	0.75	0.21	84,100,104,105	0
3	PEG	C	603	7/7	0.77	0.20	87,88,92,92	0
3	PEG	A	601	7/7	0.78	0.16	103,103,105,105	0
3	PEG	A	604	7/7	0.78	0.13	98,99,101,103	0
3	PEG	D	305	7/7	0.80	0.18	85,94,99,100	0
4	P6G	B	303	19/19	0.80	0.19	81,87,100,100	0
3	PEG	D	303	7/7	0.80	0.18	84,86,88,88	0
3	PEG	A	613	7/7	0.81	0.18	100,101,103,104	0
5	PG4	A	612	10/13	0.82	0.21	60,78,81,81	0
4	P6G	A	605	19/19	0.82	0.19	88,92,96,98	0
3	PEG	A	607	7/7	0.83	0.19	66,71,81,84	0
3	PEG	C	604	7/7	0.83	0.15	88,89,93,94	0
5	PG4	A	608	13/13	0.84	0.17	100,107,110,111	0
5	PG4	C	601	10/13	0.85	0.17	59,81,84,85	0
5	PG4	B	304	13/13	0.85	0.16	84,87,92,93	0
3	PEG	C	602	7/7	0.86	0.13	90,92,95,95	0
3	PEG	A	610	7/7	0.87	0.16	73,78,85,86	0
3	PEG	B	302	7/7	0.87	0.13	68,70,72,73	0
3	PEG	A	602	7/7	0.89	0.14	90,97,100,100	0
3	PEG	A	606	7/7	0.90	0.11	73,74,81,82	0
3	PEG	D	304	7/7	0.91	0.12	73,78,80,82	0
3	PEG	A	603	7/7	0.92	0.12	82,82,91,95	0
4	P6G	A	609	19/19	0.92	0.14	51,65,94,94	0
3	PEG	A	611	7/7	0.93	0.11	82,87,92,92	0
6	ZN	B	301	1/1	0.99	0.05	59,59,59,59	0
6	ZN	D	301	1/1	1.00	0.04	70,70,70,70	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.

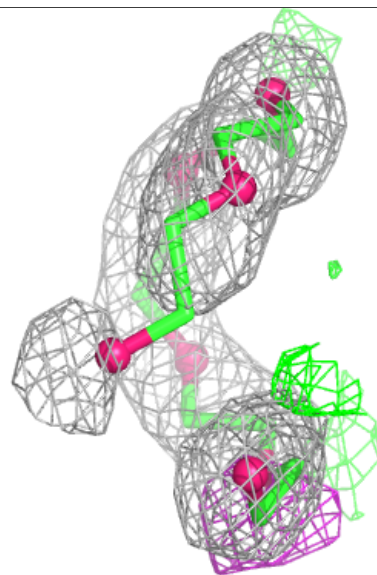
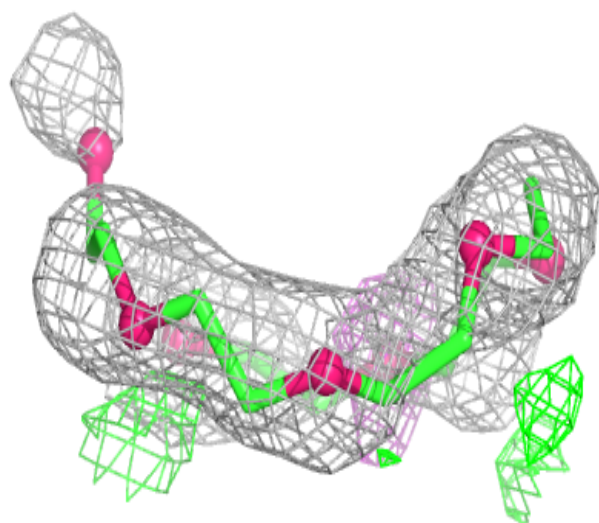
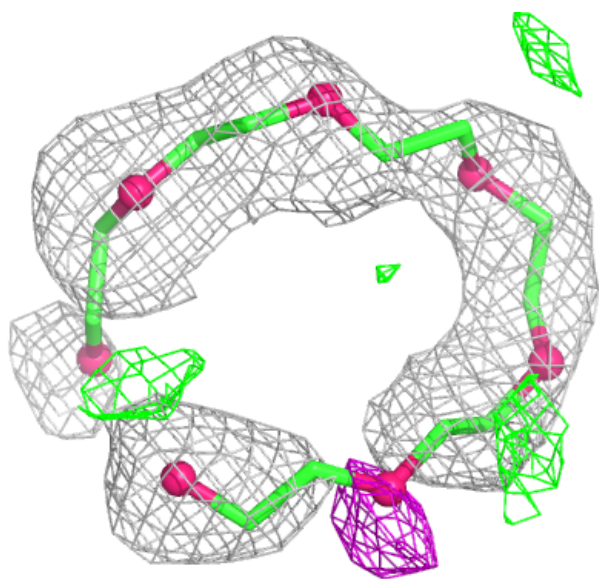
Electron density around P6G B 303:

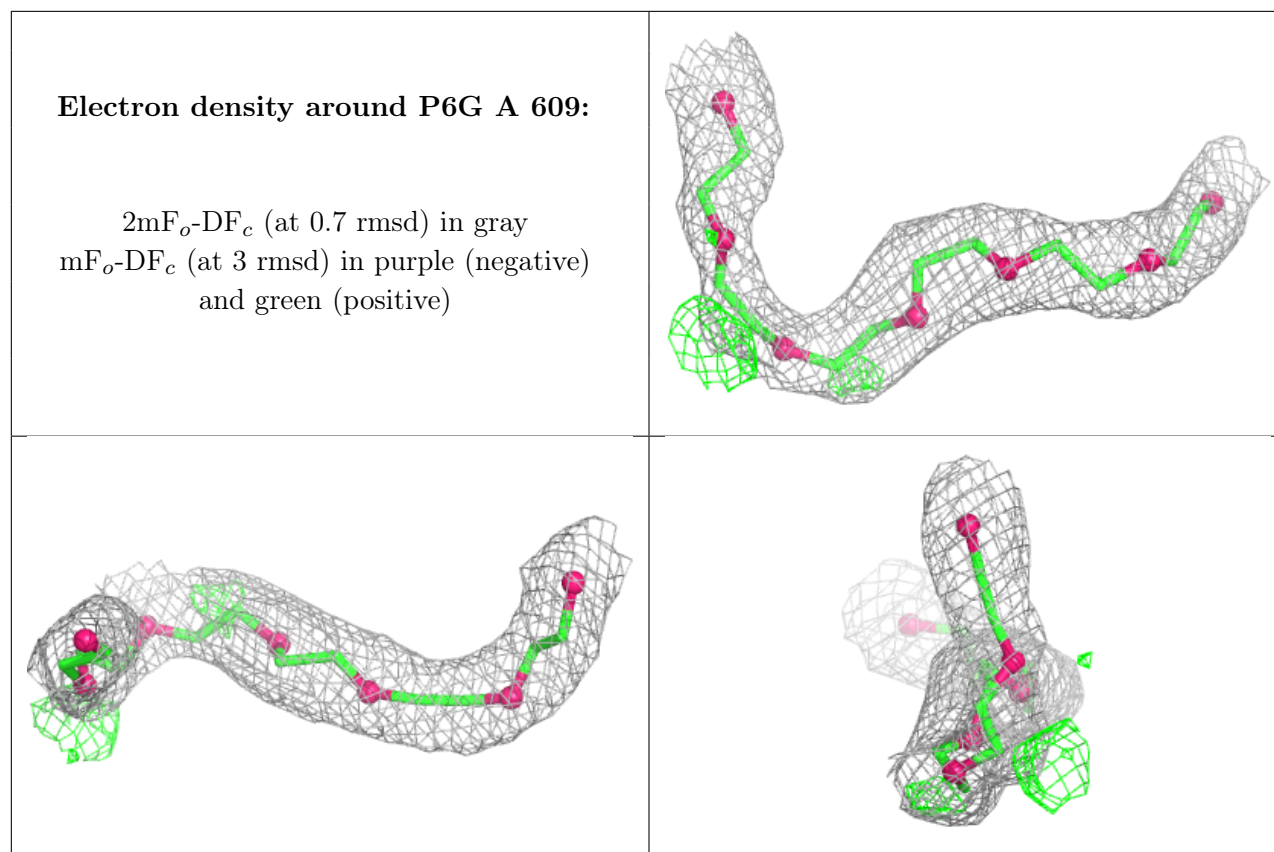
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around P6G A 605:

$2mF_o-DF_c$ (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.