



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:13 PM UTC

PDB ID : 8A4X / pdb_00008a4x
Title : Crystal structure of human Cathepsin L with covalently bound Calpain inhibitor III
Authors : Falke, S.; Lieske, J.; Guenther, S.; Reinke, P.Y.A.; Ewert, W.; Loboda, J.; Karnicar, K.; Usenik, A.; Lindic, N.; Sekirnik, A.; Chapman, H.N.; Hinrichs, W.; Turk, D.; Meents, A.
Deposited on : 2022-06-13
Resolution : 1.80 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](#) ①) 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

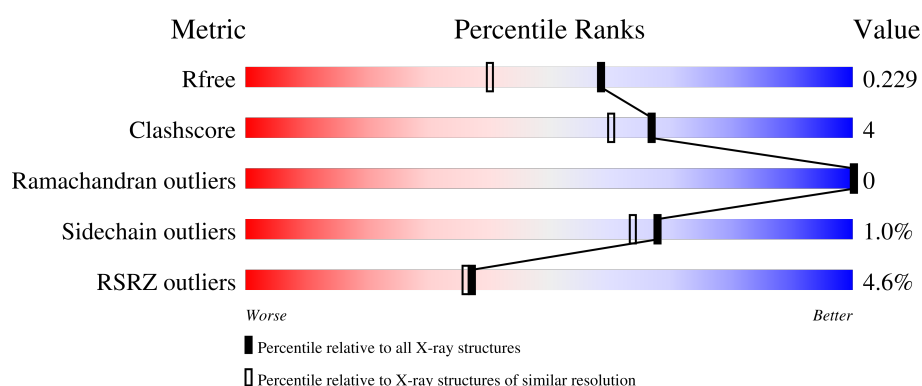
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	220	3% 94% 6%
1	B	220	4% 89% 8% .
1	C	220	10% 82% 15% .
1	D	220	2% 94% 6%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13873 atoms, of which 6541 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.

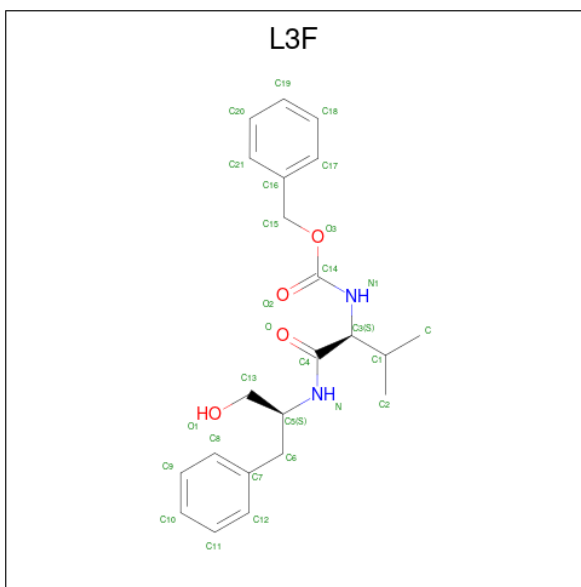
- Molecule 1 is a protein called Cathepsin L.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	220	Total	C	H	N	O	S	0	3	0
			3317	1076	1596	285	346	14			
1	B	213	Total	C	H	N	O	S	0	1	0
			3191	1039	1537	274	327	14			
1	C	212	Total	C	H	N	O	S	0	2	0
			3188	1037	1535	274	328	14			
1	D	220	Total	C	H	N	O	S	0	5	0
			3351	1086	1611	289	350	15			

There are 4 discrepancies between the modelled and reference sequences:

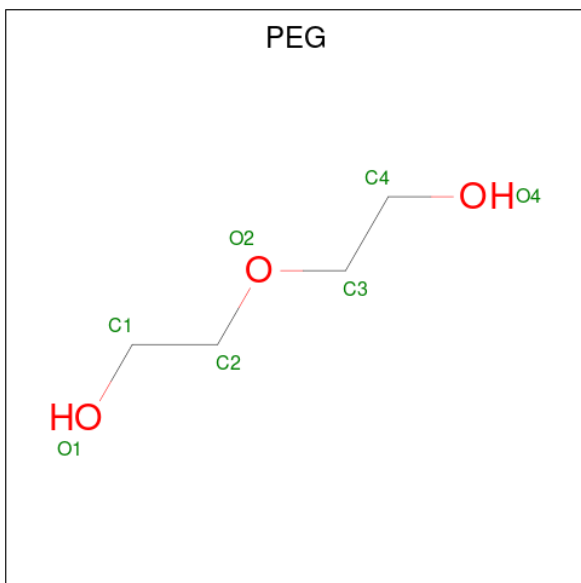
Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ALA	THR	engineered mutation	UNP P07711
B	110	ALA	THR	engineered mutation	UNP P07711
C	110	ALA	THR	engineered mutation	UNP P07711
D	110	ALA	THR	engineered mutation	UNP P07711

- Molecule 2 is (phenylmethyl) N-[(2S)-3-methyl-1-oxidanylidene-1-[(2S)-1-oxidanyl-3-phenyl-propan-2-yl]amino]butan-2-yl]carbamate (CCD ID: L3F) (formula: C₂₂H₂₈N₂O₄) (labeled as "Ligand of Interest" by depositor).



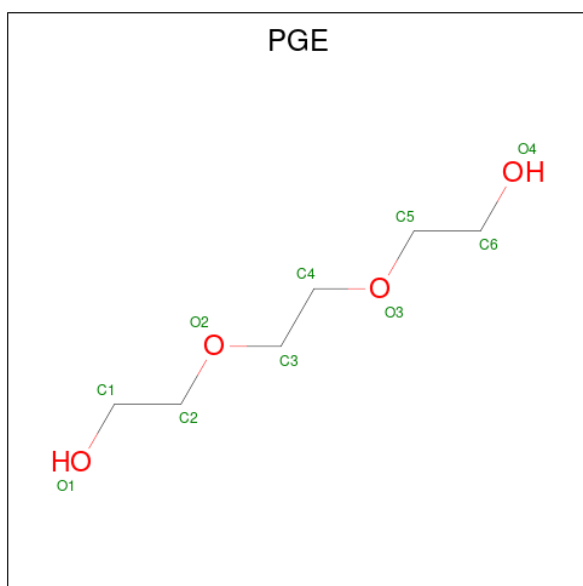
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			55	22	27	2	4		
2	B	1	Total	C	H	N	O	0	0
			55	22	27	2	4		
2	C	1	Total	C	H	N	O	0	0
			55	22	27	2	4		
2	D	1	Total	C	H	N	O	0	0
			55	22	27	2	4		

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



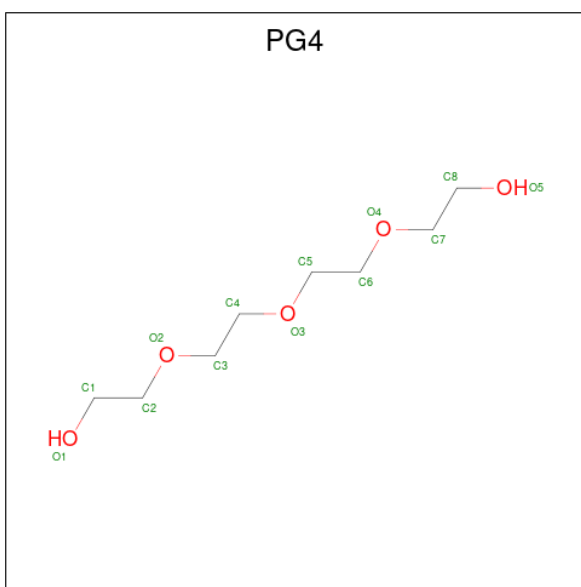
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	B	1	Total	C	H	O	0	0
			17	4	10	3		
3	C	1	Total	C	H	O	0	0
			17	4	10	3		
3	C	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



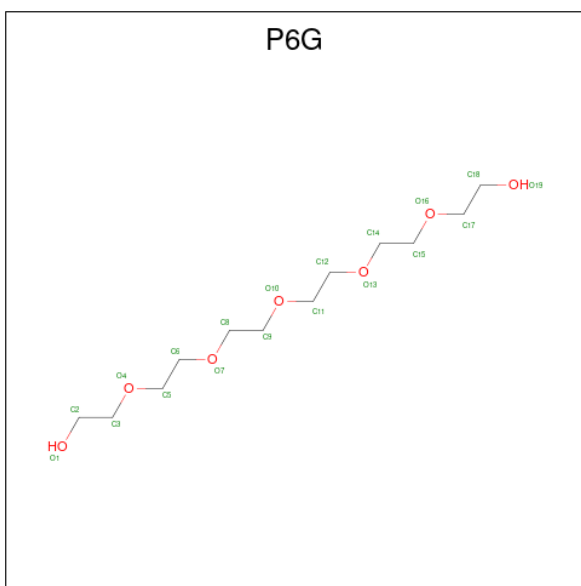
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			24	6	14	4		

- 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	H	O	0	0
			31	8	18	5		

- Molecule 6 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	H	O	0	0
			45	12	26	7		
6	D	1	Total	C	H	O	0	0
			45	12	26	7		

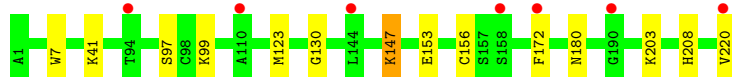
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	97	Total 97	O 97	0	0
7	B	87	Total 87	O 87	0	0
7	C	57	Total 57	O 57	0	0
7	D	101	Total 101	O 101	0	0

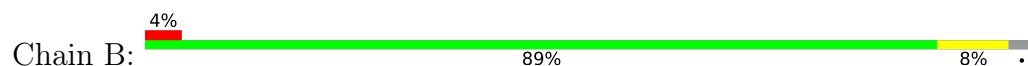
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

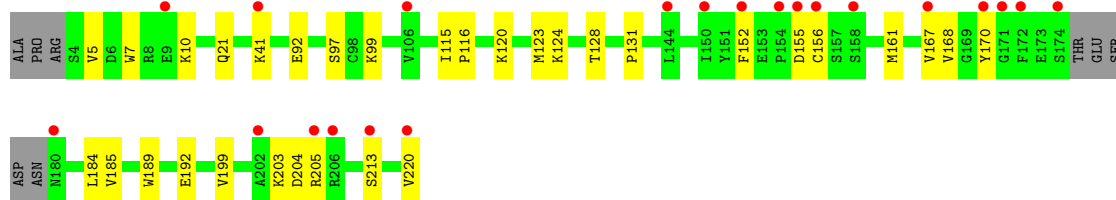
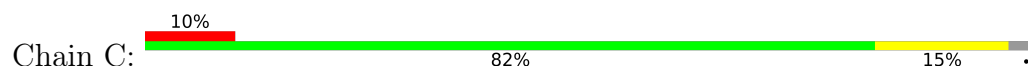
• Molecule 1: Cathepsin L



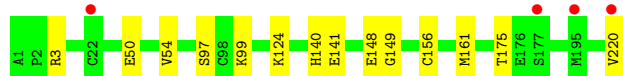
• Molecule 1: Cathepsin L



• Molecule 1: Cathepsin L



• Molecule 1: Cathepsin L



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	56.95Å 62.25Å 67.11Å 105.47° 93.52° 116.06°	Depositor
Resolution (Å)	43.92 – 1.80 43.92 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.3 (43.92-1.80) 88.1 (43.92-1.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.12 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.18-3855_9999	Depositor
R, R_{free}	0.192 , 0.226 0.195 , 0.229	Depositor DCC
R_{free} test set	1989 reflections (2.91%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 44.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13873	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.18% 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: PGE, P6G, PG4, PEG, L3F

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	0.14	0/1763	0.34	0/2381
1	B	0.15	0/1695	0.33	0/2287
1	C	0.15	0/1693	0.35	0/2284
1	D	0.15	0/1782	0.34	0/2406
All	All	0.15	0/6933	0.34	0/9358

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	1721	1596	1593	10	0
1	B	1654	1537	1535	9	0
1	C	1653	1535	1531	24	0
1	D	1740	1611	1606	9	0
2	A	28	27	0	0	0
2	B	28	27	0	0	0
2	C	28	27	0	0	0
2	D	28	27	0	0	0
3	A	7	10	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	28	40	40	0	0
3	C	14	20	20	0	0
4	A	10	14	14	0	0
5	A	13	18	18	0	0
6	C	19	26	26	0	0
6	D	19	26	26	0	0
7	A	97	0	0	0	0
7	B	87	0	0	1	0
7	C	57	0	0	0	0
7	D	101	0	0	1	0
All	All	7332	6541	6419	49	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 4.

All (49) 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:C:41:LYS:HD3	1:C:220:VAL:HG12	1.68	0.76
1:C:123:MET:HE3	1:C:170:TYR:HE2	1.59	0.67
1:C:123:MET:HE3	1:C:170:TYR:CE2	2.37	0.60
1:C:155:ASP:O	1:C:155:ASP:OD1	2.23	0.56
1:B:3:ARG:HG2	1:B:172:PHE:CE1	2.49	0.48
1:C:5:VAL:HB	1:C:170:TYR:CE1	2.49	0.48
1:D:97:SER:O	1:D:99:LYS:HE3	2.14	0.47
1:D:3:ARG:HH11	1:D:3:ARG:HB2	1.79	0.47
1:A:7:TRP:CE2	1:A:130:GLY:HA2	2.50	0.47
1:B:7:TRP:CE2	1:B:130:GLY:HA2	2.49	0.46
1:D:220:VAL:HG23	1:D:220:VAL:O	2.14	0.46
1:A:153:GLU:H	1:A:208:HIS:CE1	2.34	0.46
1:A:147[B]:LYS:HD2	1:D:148:GLU:HB3	1.98	0.46
1:A:123:MET:HE2	1:A:203:LYS:CE	2.46	0.45
1:A:41:LYS:HD2	1:A:220:VAL:HG12	1.99	0.45
1:A:123:MET:HE2	1:A:203:LYS:HE2	1.99	0.45
1:C:124:LYS:HE2	1:C:128:THR:HG21	1.99	0.45
1:C:203:LYS:NZ	1:C:204:ASP:OD2	2.50	0.44
1:C:7:TRP:CE3	1:C:10:LYS:HD2	2.53	0.44
1:B:141:GLU:HG2	1:B:145:PHE:CE2	2.53	0.44
1:C:192:GLU:H	1:C:192:GLU:CD	2.25	0.44
1:B:181:LYS:HE3	1:B:204:ASP:OD2	2.18	0.43
1:C:115:ILE:HG23	1:C:116:PRO:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:LYS:HD2	1:C:120:LYS:N	2.33	0.43
1:B:173:GLU:OE1	1:B:180:ASN:HB2	2.18	0.43
1:C:152:PHE:CD1	1:C:205:ARG:NH1	2.86	0.43
1:C:170:TYR:CD1	1:C:170:TYR:N	2.86	0.43
1:D:161:MET:HE2	1:D:161:MET:HB2	1.94	0.43
1:C:161:MET:CE	1:C:213:SER:HB2	2.49	0.43
1:B:58:GLY:N	1:B:59:PRO:CD	2.82	0.42
1:C:124:LYS:CE	1:C:128:THR:HG21	2.49	0.42
1:D:148:GLU:HG3	1:D:149:GLY:N	2.34	0.42
1:C:5:VAL:CG2	1:C:170:TYR:CE1	3.02	0.42
1:C:21:GLN:OE1	1:D:141:GLU:HG3	2.20	0.42
1:A:123:MET:HE2	1:A:203:LYS:NZ	2.35	0.41
1:B:200:LYS:NZ	7:B:408:HOH:O	2.53	0.41
1:B:185:VAL:HB	1:B:199:VAL:HG13	2.01	0.41
1:A:41:LYS:CD	1:A:220:VAL:HG12	2.50	0.41
1:D:50:GLU:O	1:D:54:VAL:HG23	2.20	0.41
1:C:189:TRP:O	1:C:192:GLU:OE1	2.39	0.41
1:C:185:VAL:HB	1:C:199:VAL:HG13	2.03	0.41
1:A:97:SER:O	1:A:99:LYS:HE2	2.21	0.41
1:A:172:PHE:HA	1:A:180:ASN:O	2.20	0.41
1:B:120:LYS:NZ	1:C:92:GLU:OE2	2.54	0.41
1:C:168:VAL:CG2	1:C:184:LEU:HG	2.51	0.41
1:D:140:HIS:HD2	7:D:436:HOH:O	2.04	0.41
1:C:97:SER:O	1:C:99:LYS:HE2	2.20	0.41
1:C:152:PHE:CD2	1:C:152:PHE:C	2.99	0.40
1:C:131:PRO:HA	1:C:167:VAL:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	221/220 (100%)	216 (98%)	5 (2%)	0	100	100
1	B	210/220 (96%)	205 (98%)	5 (2%)	0	100	100
1	C	210/220 (96%)	203 (97%)	7 (3%)	0	100	100
1	D	223/220 (101%)	214 (96%)	9 (4%)	0	100	100
All	All	864/880 (98%)	838 (97%)	26 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	181/178 (102%)	178 (98%)	3 (2%)	53	45
1	B	173/178 (97%)	172 (99%)	1 (1%)	78	77
1	C	173/178 (97%)	172 (99%)	1 (1%)	78	77
1	D	183/178 (103%)	180 (98%)	3 (2%)	55	47
All	All	710/712 (100%)	702 (99%)	8 (1%)	68	60

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	147[A]	LYS
1	A	147[B]	LYS
1	A	156	CYS
1	B	156	CYS
1	C	156	CYS
1	D	124	LYS
1	D	156	CYS
1	D	175	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	66	ASN
1	B	75	GLN
1	C	19	GLN
1	C	75	GLN
1	C	78	GLN
1	C	108	ASN
1	C	118	GLN
1	C	180	ASN
1	D	21	GLN

5.3.3 RNA [i](#)

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](#)

15 ligands 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	$\# Z > 2$
3	PEG	B	304	-	6,6,6	0.18	0	5,5,5	0.11	0
3	PEG	C	303	-	6,6,6	0.18	0	5,5,5	0.16	0
2	L3F	A	301	1	29,29,29	0.15	0	37,37,37	0.15	0
2	L3F	C	301	1	29,29,29	0.14	0	37,37,37	0.18	0
3	PEG	B	305	-	6,6,6	0.18	0	5,5,5	0.04	0
5	PG4	A	304	-	12,12,12	0.19	0	11,11,11	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	L3F	D	301	1	29,29,29	0.14	0	37,37,37	0.22	0
3	PEG	B	303	-	6,6,6	0.20	0	5,5,5	0.07	0
6	P6G	D	302	-	18,18,18	0.16	0	17,17,17	0.19	0
6	P6G	C	304	-	18,18,18	0.16	0	17,17,17	0.15	0
3	PEG	A	302	-	6,6,6	0.21	0	5,5,5	0.08	0
3	PEG	B	302	-	6,6,6	0.18	0	5,5,5	0.11	0
2	L3F	B	301	1	29,29,29	0.15	0	37,37,37	0.16	0
3	PEG	C	302	-	6,6,6	0.17	0	5,5,5	0.09	0
4	PGE	A	303	-	9,9,9	0.31	0	8,8,8	0.27	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	B	304	-	-	3/4/4/4	-
3	PEG	C	303	-	-	4/4/4/4	-
2	L3F	A	301	1	-	2/27/27/27	0/2/2/2
2	L3F	C	301	1	-	4/27/27/27	0/2/2/2
3	PEG	B	305	-	-	2/4/4/4	-
5	PG4	A	304	-	-	3/10/10/10	-
2	L3F	D	301	1	-	2/27/27/27	0/2/2/2
3	PEG	B	303	-	-	1/4/4/4	-
6	P6G	D	302	-	-	4/16/16/16	-
6	P6G	C	304	-	-	7/16/16/16	-
3	PEG	A	302	-	-	2/4/4/4	-
3	PEG	B	302	-	-	2/4/4/4	-
2	L3F	B	301	1	-	3/27/27/27	0/2/2/2
3	PEG	C	302	-	-	1/4/4/4	-
4	PGE	A	303	-	-	3/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

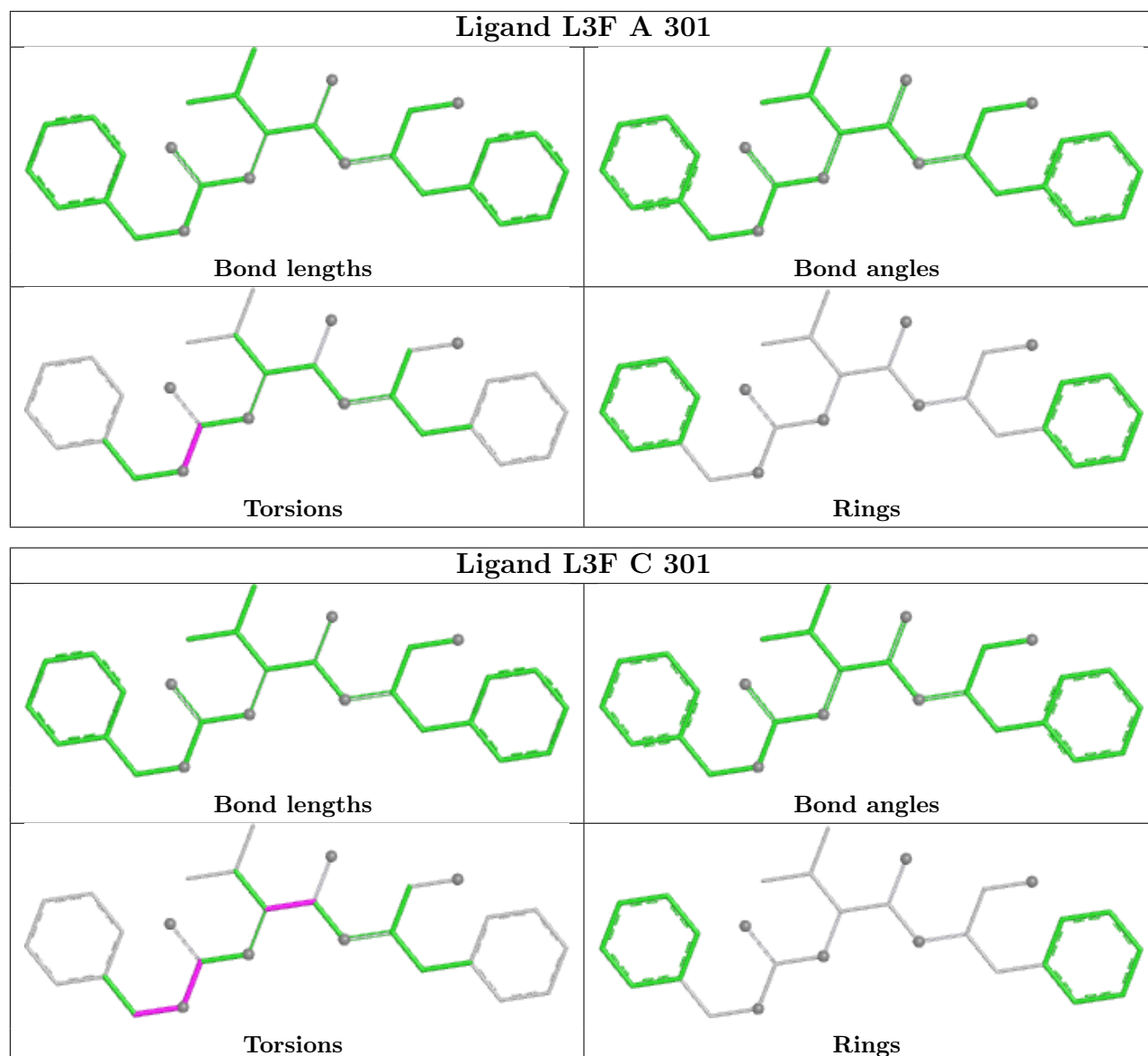
All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	L3F	O2-C14-O3-C15
2	B	301	L3F	N1-C14-O3-C15
2	D	301	L3F	N1-C14-O3-C15
2	D	301	L3F	O2-C14-O3-C15
2	A	301	L3F	N1-C14-O3-C15
2	A	301	L3F	O2-C14-O3-C15
5	A	304	PG4	O2-C3-C4-O3
6	D	302	P6G	O7-C8-C9-O10
6	C	304	P6G	O13-C14-C15-O16
2	C	301	L3F	N1-C14-O3-C15
3	C	303	PEG	O2-C3-C4-O4
2	C	301	L3F	O2-C14-O3-C15
4	A	303	PGE	O1-C1-C2-O2
4	A	303	PGE	O3-C5-C6-O4
6	C	304	P6G	O16-C17-C18-O19
6	D	302	P6G	O10-C11-C12-O13
3	C	303	PEG	O1-C1-C2-O2
3	C	302	PEG	O2-C3-C4-O4
3	B	304	PEG	O2-C3-C4-O4
5	A	304	PG4	O1-C1-C2-O2
6	C	304	P6G	O10-C11-C12-O13
3	A	302	PEG	O2-C3-C4-O4
6	D	302	P6G	C9-C8-O7-C6
6	C	304	P6G	C6-C5-O4-C3
5	A	304	PG4	C5-C6-O4-C7
3	B	303	PEG	O1-C1-C2-O2
6	C	304	P6G	C15-C14-O13-C12
3	B	305	PEG	C1-C2-O2-C3
4	A	303	PGE	C3-C4-O3-C5
3	B	302	PEG	O2-C3-C4-O4
3	B	305	PEG	O1-C1-C2-O2
3	B	304	PEG	O1-C1-C2-O2
3	A	302	PEG	C4-C3-O2-C2
3	C	303	PEG	C4-C3-O2-C2
6	C	304	P6G	C8-C9-O10-C11
2	C	301	L3F	C16-C15-O3-C14
3	B	304	PEG	C4-C3-O2-C2
6	C	304	P6G	O1-C2-C3-O4
6	D	302	P6G	C12-C11-O10-C9
3	C	303	PEG	C1-C2-O2-C3
2	B	301	L3F	C16-C15-O3-C14
3	B	302	PEG	C4-C3-O2-C2
2	C	301	L3F	N1-C3-C4-O

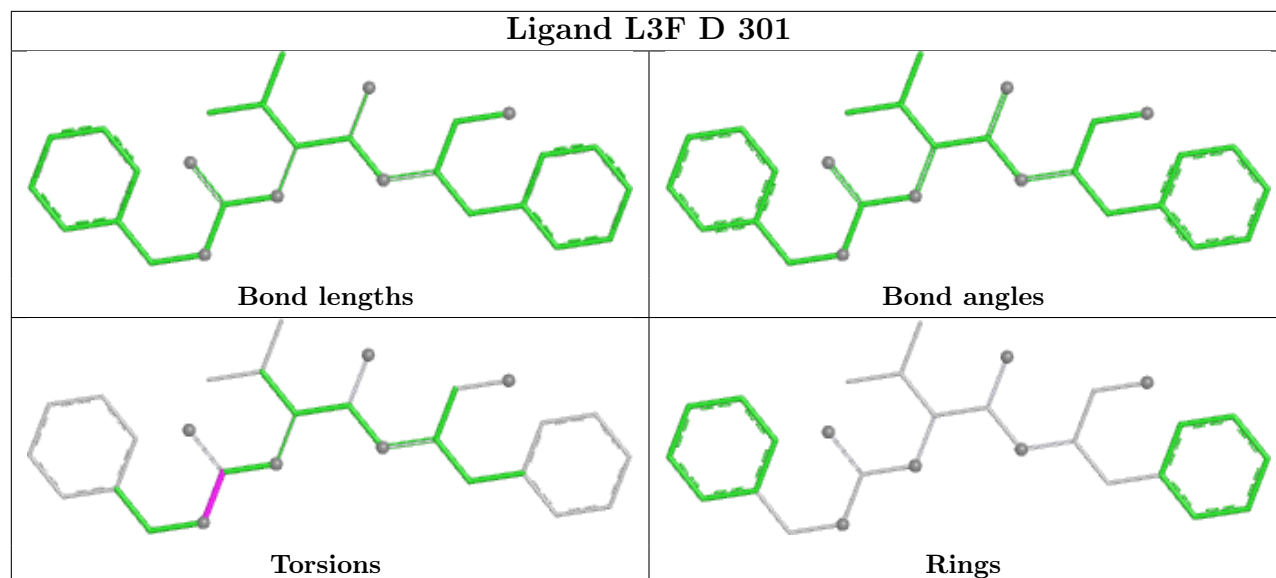
There are no ring outliers.

No monomer is involved in short contacts.

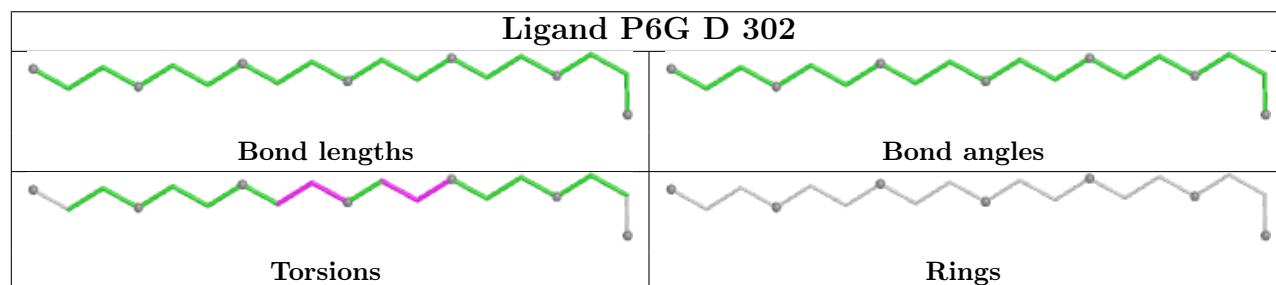
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



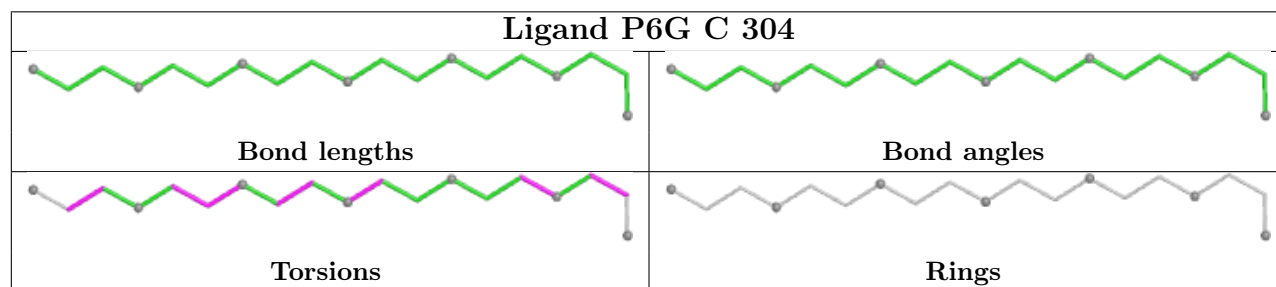
Ligand L3F D 301



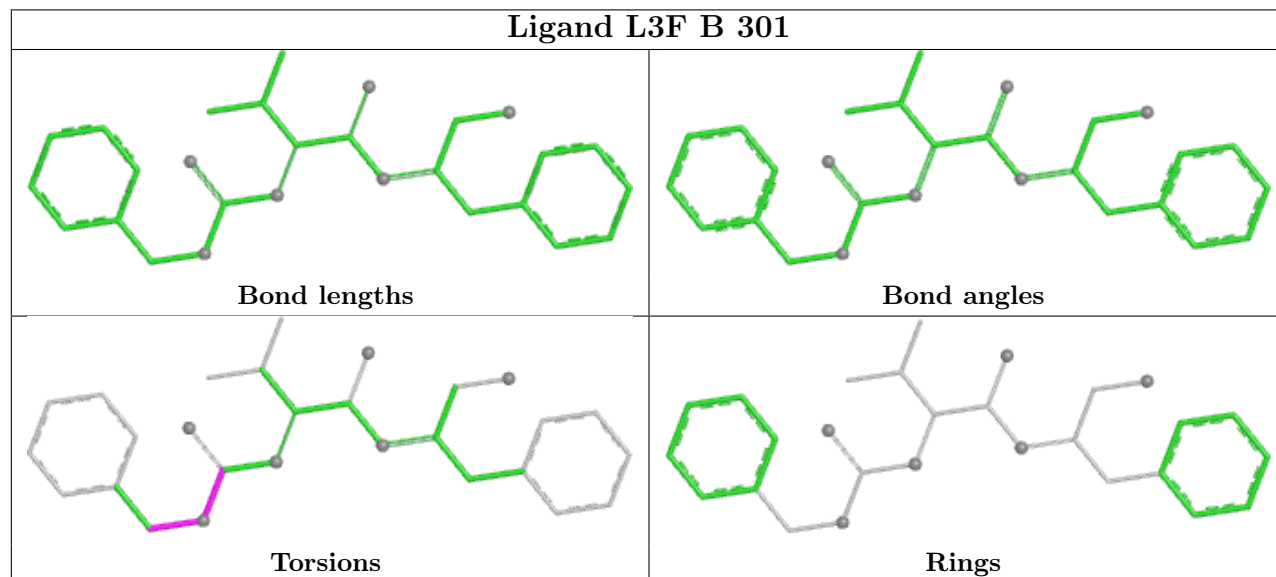
Ligand P6G D 302



Ligand P6G C 304



Ligand L3F B 301



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	220/220 (100%)	0.64	7 (3%)	50	50	15, 34, 50, 72	3 (1%)
1	B	213/220 (96%)	0.67	8 (3%)	44	44	19, 34, 57, 75	1 (0%)
1	C	212/220 (96%)	1.03	21 (9%)	13	11	25, 42, 72, 101	2 (0%)
1	D	220/220 (100%)	0.56	4 (1%)	67	68	13, 33, 53, 62	5 (2%)
All	All	865/880 (98%)	0.72	40 (4%)	37	36	13, 35, 62, 101	11 (1%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	206[A]	ARG	4.2
1	C	174	SER	4.2
1	C	172	PHE	4.2
1	B	172	PHE	3.9
1	C	220	VAL	3.1
1	C	150	ILE	3.1
1	C	180	ASN	3.1
1	A	158	SER	2.9
1	C	156	CYS	2.9
1	C	154	PRO	2.9
1	C	158	SER	2.8
1	C	167	VAL	2.8
1	B	144	LEU	2.8
1	B	94	THR	2.6
1	D	22	CYS	2.5
1	C	106	VAL	2.5
1	B	139	GLY	2.4
1	B	173	GLU	2.4
1	B	2	PRO	2.3
1	C	9	GLU	2.3
1	C	41	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	220	VAL	2.3
1	C	144	LEU	2.3
1	B	158	SER	2.2
1	C	213	SER	2.2
1	C	171	GLY	2.2
1	D	177	SER	2.2
1	A	190	GLY	2.2
1	C	170	TYR	2.2
1	C	152	PHE	2.1
1	A	144	LEU	2.1
1	C	205	ARG	2.1
1	A	110	ALA	2.1
1	C	202	ALA	2.1
1	B	152	PHE	2.1
1	A	172	PHE	2.1
1	A	220	VAL	2.1
1	C	155	ASP	2.0
1	D	195[A]	MET	2.0
1	A	94	THR	2.0

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

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(Å ²)	Q<0.9
3	PEG	B	305	7/7	0.76	0.15	36,49,63,66	0
6	P6G	C	304	19/19	0.76	0.15	38,50,59,65	0
5	PG4	A	304	13/13	0.77	0.16	39,55,70,70	0
3	PEG	B	304	7/7	0.80	0.13	42,54,64,68	0

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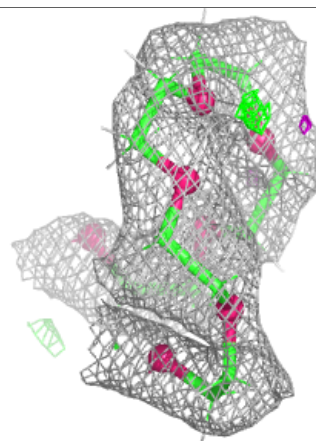
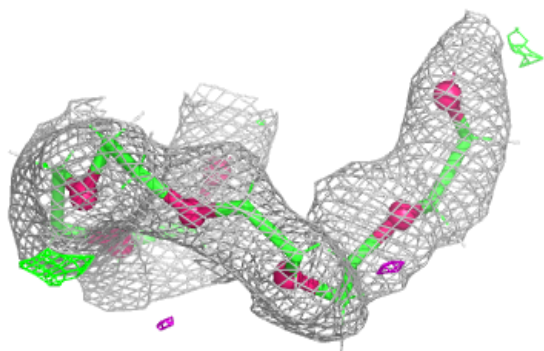
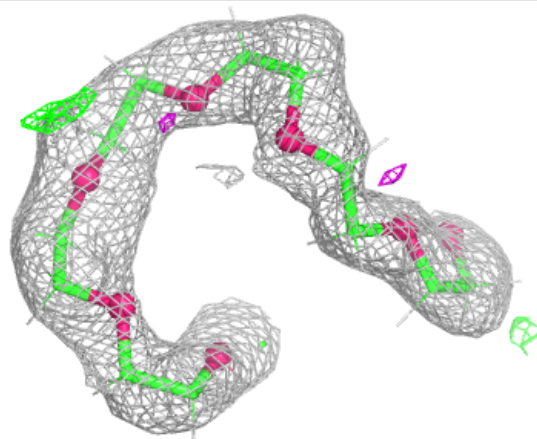
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PGE	A	303	10/10	0.82	0.14	38,52,60,62	0
3	PEG	B	302	7/7	0.83	0.14	46,55,63,63	0
3	PEG	C	302	7/7	0.84	0.14	45,54,63,63	0
6	P6G	D	302	19/19	0.85	0.14	29,45,62,66	0
2	L3F	C	301	28/28	0.86	0.13	27,43,62,70	0
3	PEG	A	302	7/7	0.87	0.13	41,51,63,63	0
2	L3F	B	301	28/28	0.87	0.13	26,39,60,61	0
2	L3F	D	301	28/28	0.87	0.12	21,34,56,61	0
2	L3F	A	301	28/28	0.88	0.12	25,40,64,68	0
3	PEG	C	303	7/7	0.88	0.11	43,52,64,64	0
3	PEG	B	303	7/7	0.89	0.13	34,46,56,62	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.

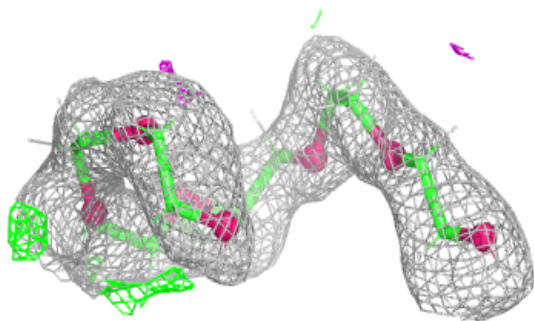
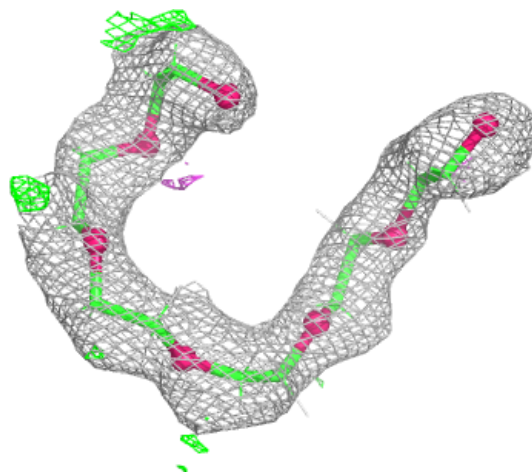
Electron density around P6G C 304:

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



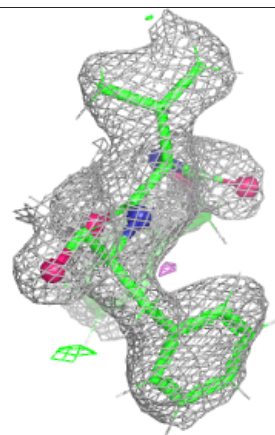
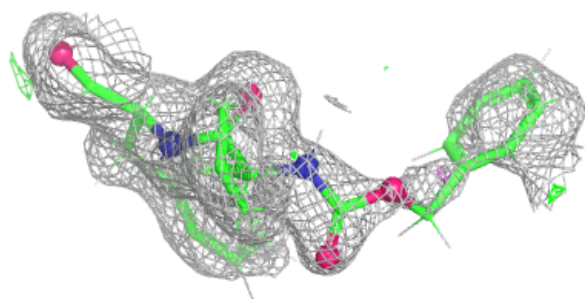
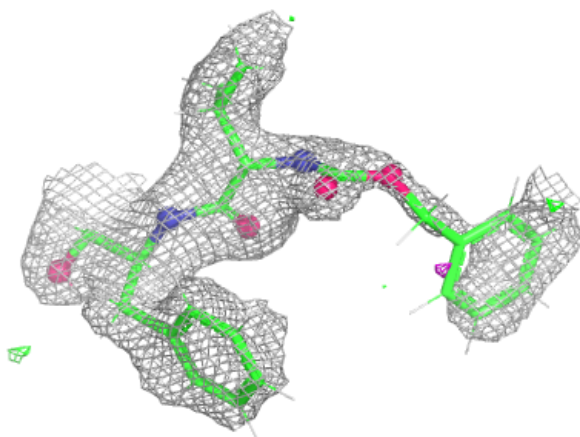
Electron density around P6G D 302:

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



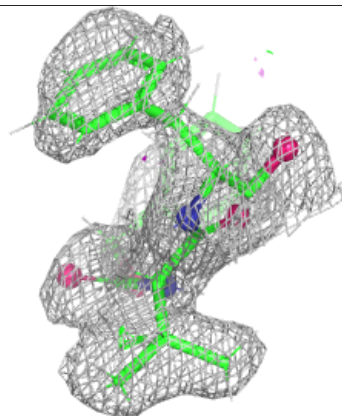
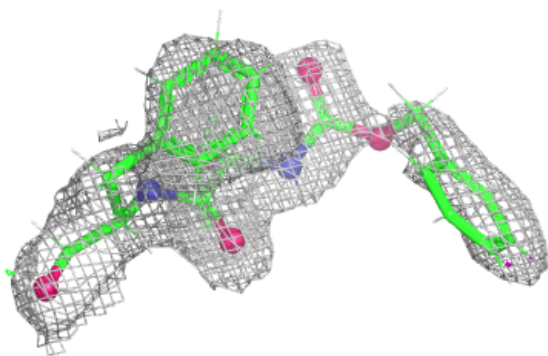
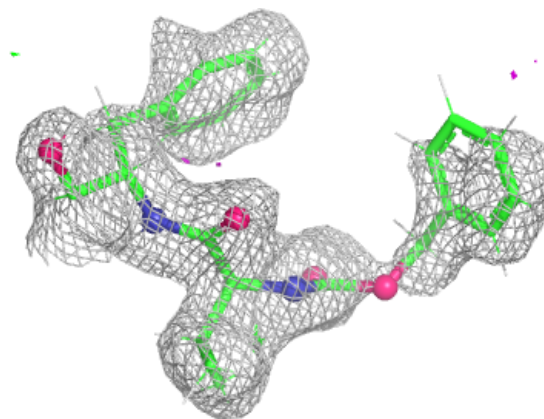
Electron density around L3F C 301:

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

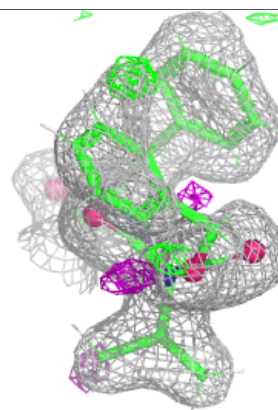
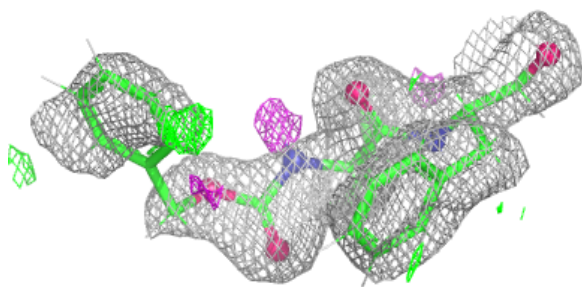
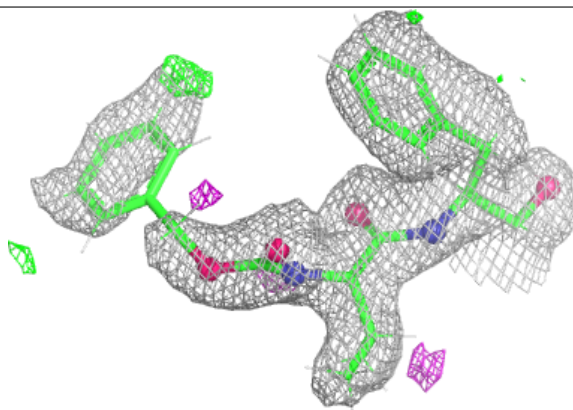


Electron density around L3F B 301:

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

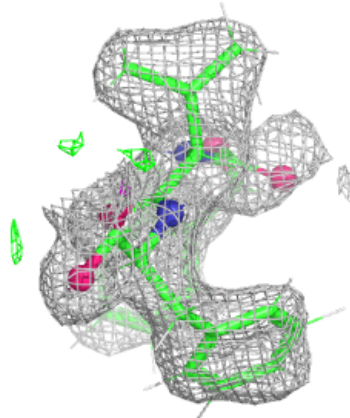
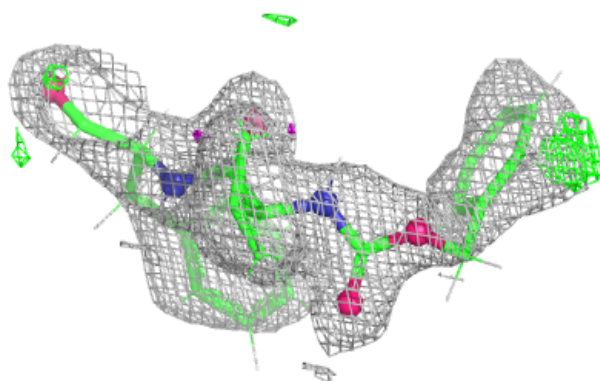
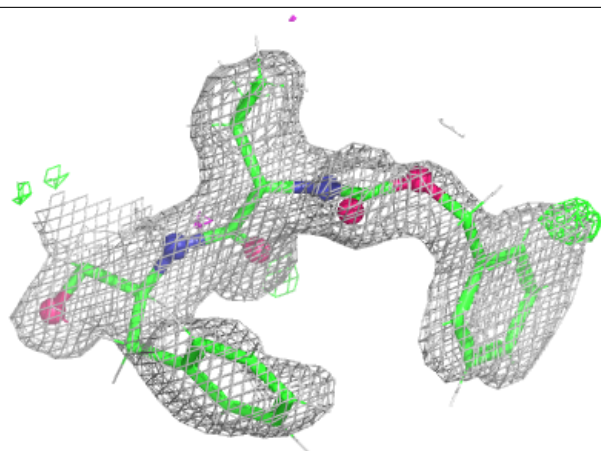
**Electron density around L3F D 301:**

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



Electron density around L3F A 301:

$2mF_o-DF_c$ (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.