



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:20 PM UTC

PDB ID : 8QKB / pdb_00008qkb
Title : Crystal structure of human cathepsin L in complex with the vinyl sulfone inhibitor K777
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 : 2023-09-14
Resolution : 1.60 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)
Xtrriage (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

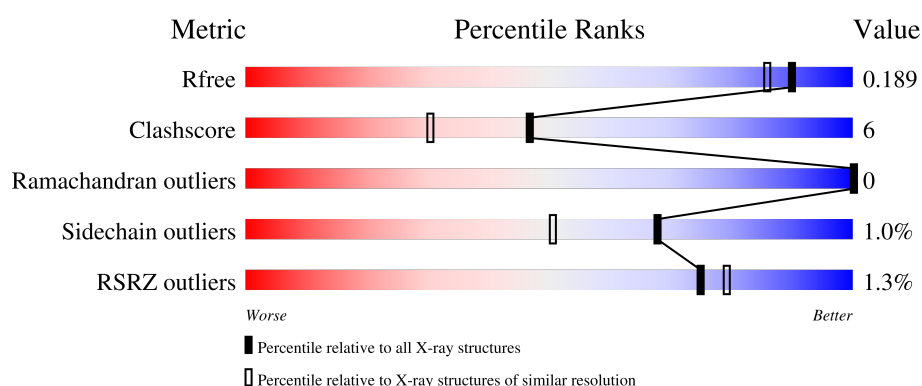
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	2% 90% 8% .
1	B	220	% 87% 12%
1	C	220	2% 87% 11% .
1	D	220	93% 6%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 8065 atoms, of which 200 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.

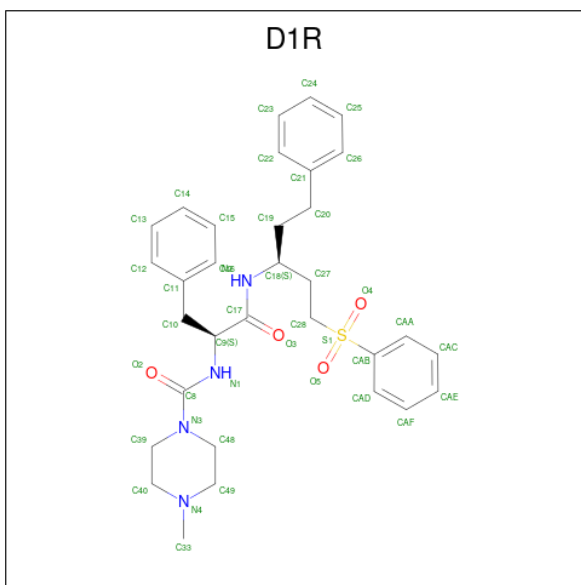
- Molecule 1 is a protein called Cathepsin L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	2	0
			1709	1068	283	344	14			
1	B	220	Total	C	N	O	S	0	4	0
			1726	1079	285	347	15			
1	C	216	Total	C	N	O	S	0	2	0
			1676	1051	278	332	15			
1	D	220	Total	C	N	O	S	0	8	0
			1754	1094	290	354	16			

There are 4 discrepancies between the modelled and reference sequences:

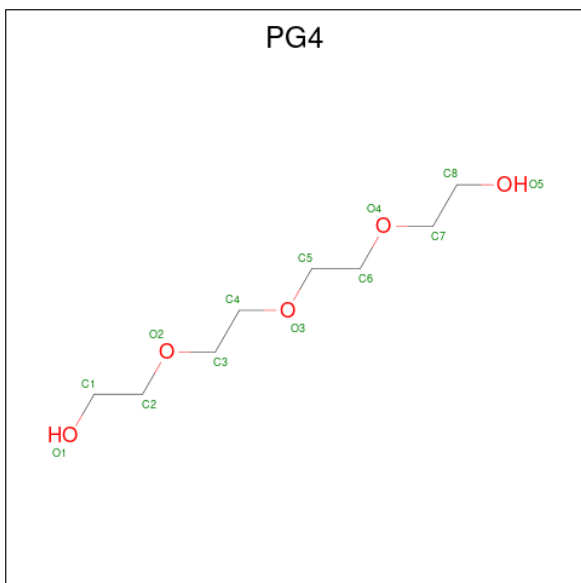
Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ALA	THR	engineered mutation	UNP P07711
B	110	ALA	THR	engineered mutation	UNP P07711
C	110	ALA	THR	engineered mutation	UNP P07711
D	110	ALA	THR	engineered mutation	UNP P07711

- Molecule 2 is NALPHA-[(4-METHYLPIPERAZIN-1-YL)CARBONYL]-N-{(1S)-3-PHENYL-L-1-[2-(PHENYLSULFONYL)ETHYL]PROPYL}-L-PHENYLALANINAMIDE (CCD ID: D1R) (formula: C₃₂H₄₀N₄O₄S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			41	32	4	4	1		
2	B	1	Total	C	N	O	S	0	0
			41	32	4	4	1		
2	C	1	Total	C	N	O	S	0	0
			41	32	4	4	1		
2	D	1	Total	C	N	O	S	0	0
			41	32	4	4	1		

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	A	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	B	1	Total	C	H	O	0	0
			10	2	6	2		
4	C	1	Total	C	H	O	0	0
			10	2	6	2		
4	D	1	Total	C	H	O	0	0
			10	2	6	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



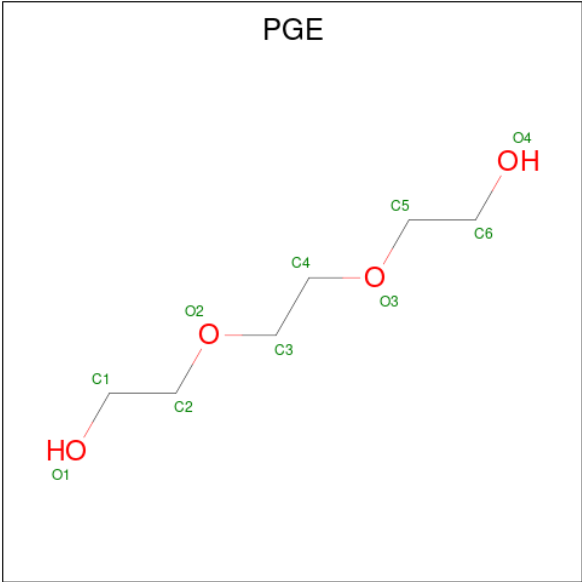
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	A	1	Total	C	H	O	0	0
			17	4	10	3		
5	C	1	Total	C	H	O	0	0
			17	4	10	3		
5	D	1	Total	C	H	O	0	0
			17	4	10	3		
5	D	1	Total	C	H	O	0	0
			17	4	10	3		

- Molecule 6 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	B	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	C	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	C	1	Total	C	H	O	S	0	0
			10	2	6	1	1		
6	D	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

- Molecule 7 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



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

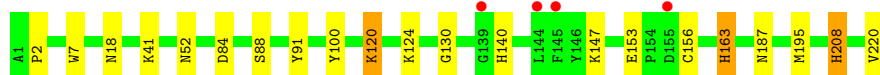
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	158	Total	O	0	0
			158	158		
8	B	183	Total	O	0	0
			183	183		
8	C	145	Total	O	0	0
			145	145		
8	D	200	Total	O	0	0
			200	200		

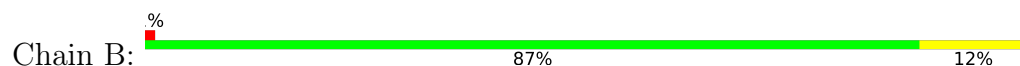
3 Residue-property plots [i](#)

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.

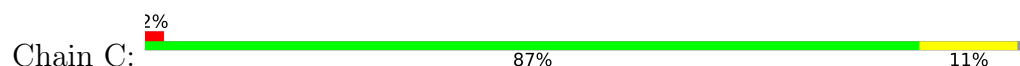
- Molecule 1: Cathepsin L



- 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	56.99Å 62.44Å 67.75Å 105.41° 93.65° 115.53°	Depositor
Resolution (Å)	44.19 – 1.60 44.19 – 1.60	Depositor EDS
% Data completeness (in resolution range)	91.8 (44.19-1.60) 91.8 (44.19-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.00 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.18_3861	Depositor
R, R_{free}	0.157 , 0.187 0.158 , 0.189	Depositor DCC
R_{free} test set	2005 reflections (1.34%)	wwPDB-VP
Wilson B-factor (Å ²)	13.4	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 34.9	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	8065	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.78% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PGE, DMS, EDO, PG4, PEG, D1R

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	0.45	3/1751 (0.2%)	0.53	0/2366
1	B	0.38	1/1768 (0.1%)	0.54	0/2389
1	C	0.42	0/1720	0.54	0/2322
1	D	0.39	0/1796	0.55	0/2425
All	All	0.41	4/7035 (0.1%)	0.54	0/9502

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	D	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	HIS	C-O	-5.41	1.17	1.23
1	B	120	LYS	C-O	-5.38	1.17	1.24
1	A	163	HIS	C-N	-5.36	1.30	1.33
1	A	163	HIS	C-O	-5.09	1.18	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	3	ARG	Sidechain
1	D	148[A]	GLU	Mainchain

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	1709	0	1580	22	0
1	B	1726	0	1595	26	0
1	C	1676	0	1558	17	0
1	D	1754	0	1619	14	0
2	A	41	0	39	3	0
2	B	41	0	39	2	0
2	C	41	0	39	2	0
2	D	41	0	39	1	0
3	A	13	0	18	2	0
4	A	16	24	24	1	0
4	B	20	30	29	5	0
4	C	4	6	6	0	0
4	D	8	12	12	0	0
5	A	14	20	20	3	0
5	C	7	10	10	0	0
5	D	14	20	20	1	0
6	A	4	6	6	0	0
6	B	8	12	12	0	0
6	C	8	12	12	0	0
6	D	4	6	6	1	0
7	B	10	14	14	0	0
7	D	20	28	28	1	0
8	A	158	0	0	1	0
8	B	183	0	0	1	0
8	C	145	0	0	3	0
8	D	200	0	0	2	0
All	All	7865	200	6725	79	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 6.

All (79) 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	1.39	1.00
1:A:195:MET:HE2	8:C:539:HOH:O	1.74	0.87
1:B:108:ASN:HD22	1:D:206:ARG:HH22	1.22	0.86
1:C:41:LYS:HD3	1:C:220:VAL:CG1	2.05	0.84
1:C:123:MET:HE2	8:C:423:HOH:O	1.80	0.81
1:A:153:GLU:H	1:A:208:HIS:CE1	2.01	0.78
1:A:41:LYS:HD2	1:A:220:VAL:HG12	1.68	0.76
1:B:108:ASN:ND2	1:D:206:ARG:HH22	1.83	0.75
1:B:120:LYS:HD3	4:B:308:EDO:H21	1.69	0.75
1:B:5:VAL:HG13	4:B:306:EDO:H11	1.69	0.74
1:B:41:LYS:HD2	1:B:220:VAL:HG12	1.70	0.71
1:A:147:LYS:HD2	1:D:148[A]:GLU:HG3	1.72	0.71
1:D:147:LYS:C	1:D:148[A]:GLU:HG2	2.17	0.70
1:B:68:GLY:HA2	2:B:301:D1R:H332	1.72	0.69
1:C:150:ILE:HD12	1:C:180:ASN:HB3	1.74	0.69
1:A:163:HIS:CD2	2:A:301:D1R:H281	2.29	0.68
1:A:153:GLU:H	1:A:208:HIS:HE1	1.41	0.68
1:A:163:HIS:HD2	2:A:301:D1R:H281	1.60	0.67
1:C:150:ILE:CD1	1:C:180:ASN:HB3	2.27	0.64
1:D:147:LYS:O	1:D:148[A]:GLU:HG2	1.99	0.63
1:B:52:ASN:ND2	1:B:84:ASP:H	1.97	0.62
1:B:163:HIS:ND1	2:B:301:D1R:H281	2.16	0.61
1:B:1:ALA:HB3	1:B:123:MET:HE2	1.82	0.61
1:D:68:GLY:HA2	2:D:602:D1R:H332	1.85	0.59
1:D:52:ASN:ND2	1:D:84:ASP:H	2.02	0.58
1:A:2:PRO:HB3	1:B:159:GLU:HB3	1.86	0.57
1:B:41:LYS:HD2	1:B:220:VAL:CG1	2.35	0.56
1:C:52:ASN:HD22	1:C:84:ASP:H	1.54	0.56
1:B:62:ASN:ND2	1:B:69:LEU:H	2.04	0.56
1:C:52:ASN:ND2	1:C:84:ASP:H	2.03	0.56
1:B:56:CYS:SG	1:B:98[B]:CYS:SG	3.04	0.55
1:B:117:LYS:O	1:B:117:LYS:HG2	2.07	0.55
1:C:183:TRP:CE2	1:C:203:LYS:HG3	2.42	0.55
1:C:163:HIS:ND1	2:C:301:D1R:H281	2.22	0.55
1:B:102:PRO:HG2	1:B:103:LYS:HE2	1.89	0.55
1:D:141:GLU:HG3	1:D:145:PHE:CE2	2.42	0.54
1:A:220:VAL:OXT	4:A:305:EDO:H11	2.08	0.54
1:A:52:ASN:ND2	1:A:84:ASP:H	2.06	0.53
1:B:62:ASN:HD21	1:B:69:LEU:H	1.54	0.53
1:D:52:ASN:HD22	1:D:84:ASP:H	1.55	0.52
1:B:52:ASN:HD22	1:B:84:ASP:H	1.58	0.52
1:A:7:TRP:CE2	1:A:130:GLY:HA2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:HIS:HE1	1:A:187:ASN:OD1	1.93	0.52
1:D:18:ASN:HB3	7:D:605:PGE:H1	1.92	0.52
1:A:18:ASN:H	5:A:306:PEG:H41	1.76	0.51
1:C:148:GLU:HG2	1:C:149:GLY:N	2.26	0.51
1:D:147:LYS:O	1:D:148[A]:GLU:CG	2.60	0.49
1:A:52:ASN:HD22	1:A:84:ASP:H	1.60	0.48
1:C:7:TRP:CE2	1:C:130:GLY:HA2	2.48	0.48
1:D:195[B]:MET:HE1	8:D:740:HOH:O	2.12	0.48
1:A:88:SER:O	3:A:302:PG4:H82	2.14	0.47
1:A:2:PRO:HA	1:B:159:GLU:O	2.14	0.47
1:C:31:THR:O	1:C:35:GLU:HG3	2.15	0.46
1:B:69:LEU:HD12	1:B:72:TYR:CZ	2.50	0.46
3:A:302:PG4:H82	3:A:302:PG4:H61	1.63	0.45
4:B:308:EDO:H22	8:B:541:HOH:O	2.16	0.45
1:B:103:LYS:HE2	1:B:103:LYS:N	2.32	0.44
1:C:120:LYS:O	1:C:124:LYS:HG3	2.18	0.44
1:C:108:ASN:HB3	8:C:506:HOH:O	2.17	0.44
1:A:140:HIS:HD2	8:A:475:HOH:O	2.01	0.43
2:C:301:D1R:HAA	5:D:601:PEG:H31	2.01	0.42
1:B:7:TRP:CE2	1:B:130:GLY:HA2	2.54	0.42
1:A:120:LYS:HG2	1:A:124:LYS:HE3	2.01	0.42
1:B:69:LEU:HD12	1:B:72:TYR:CE2	2.55	0.42
1:C:52:ASN:HD21	1:C:100:TYR:HD1	1.67	0.41
1:A:52:ASN:HD22	1:A:84:ASP:HB2	1.85	0.41
1:A:147:LYS:O	1:A:195:MET:HG2	2.20	0.41
1:B:101:ASN:OD1	1:B:103:LYS:HG2	2.21	0.41
1:B:102:PRO:HG2	1:B:103:LYS:CE	2.50	0.41
1:D:201[A]:MET:HE2	1:D:201[A]:MET:HB3	1.81	0.41
6:D:604:DMS:H21	8:D:900:HOH:O	2.20	0.41
1:B:88:SER:O	4:B:304:EDO:H21	2.21	0.41
1:C:181:LYS:NZ	1:C:204:ASP:OD2	2.50	0.41
2:A:301:D1R:HAA	5:A:308:PEG:H31	2.03	0.40
1:A:52:ASN:HD21	1:A:100:TYR:HD1	1.68	0.40
1:D:133:SER:O	1:D:215:ALA:HA	2.21	0.40
1:B:182:TYR:CZ	1:B:200:LYS:HE2	2.57	0.40
1:A:91:TYR:HB3	5:A:306:PEG:H32	2.02	0.40
4:B:308:EDO:H12	1:C:20:GLY:HA3	2.02	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	220/220 (100%)	215 (98%)	5 (2%)	0	100	100
1	B	222/220 (101%)	216 (97%)	6 (3%)	0	100	100
1	C	214/220 (97%)	208 (97%)	6 (3%)	0	100	100
1	D	226/220 (103%)	219 (97%)	7 (3%)	0	100	100
All	All	882/880 (100%)	858 (97%)	24 (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	180/178 (101%)	178 (99%)	2 (1%)	65	46
1	B	182/178 (102%)	180 (99%)	2 (1%)	65	46
1	C	176/178 (99%)	175 (99%)	1 (1%)	78	66
1	D	186/178 (104%)	184 (99%)	2 (1%)	65	46
All	All	724/712 (102%)	717 (99%)	7 (1%)	68	50

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120	LYS
1	A	156	CYS

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Mol	Chain	Res	Type
1	B	156	CYS
1	B	160	ASP
1	C	156	CYS
1	D	156	CYS
1	D	174	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	80	ASN
1	A	163	HIS
1	A	180	ASN
1	A	208	HIS
1	B	52	ASN
1	B	62	ASN
1	B	75	GLN
1	B	108	ASN
1	C	52	ASN
1	D	52	ASN
1	D	75	GLN
1	D	80	ASN
1	D	179	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

31 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	$\# Z > 2$
4	EDO	B	308	-	3,3,3	0.84	0	2,2,2	0.22	0
4	EDO	A	303	-	3,3,3	0.47	0	2,2,2	0.34	0
6	DMS	C	305	-	3,3,3	1.06	0	3,3,3	0.74	0
7	PGE	D	607	-	9,9,9	0.29	0	8,8,8	0.33	0
7	PGE	D	605	-	9,9,9	0.33	0	8,8,8	0.48	0
4	EDO	A	305	-	3,3,3	0.43	0	2,2,2	0.58	0
4	EDO	A	307	-	3,3,3	0.45	0	2,2,2	0.32	0
5	PEG	D	603	-	6,6,6	0.17	0	5,5,5	0.38	0
4	EDO	B	307	-	3,3,3	0.51	0	2,2,2	0.28	0
5	PEG	A	306	-	6,6,6	0.65	0	5,5,5	0.90	0
4	EDO	C	304	-	3,3,3	0.45	0	2,2,2	0.38	0
2	D1R	C	301	1	44,44,44	2.11	11 (25%)	57,59,59	2.36	14 (24%)
6	DMS	A	309	-	3,3,3	0.67	0	3,3,3	0.46	0
4	EDO	B	304	-	3,3,3	0.42	0	2,2,2	0.45	0
6	DMS	B	305	-	3,3,3	0.66	0	3,3,3	0.62	0
4	EDO	B	303	-	3,3,3	0.44	0	2,2,2	0.47	0
7	PGE	B	302	-	9,9,9	0.31	0	8,8,8	0.43	0
2	D1R	B	301	1	44,44,44	2.42	13 (29%)	57,59,59	2.70	19 (33%)
4	EDO	B	306	-	3,3,3	0.42	0	2,2,2	0.35	0
2	D1R	A	301	1	44,44,44	2.53	9 (20%)	57,59,59	2.45	15 (26%)
4	EDO	D	606	-	3,3,3	0.41	0	2,2,2	0.63	0
5	PEG	C	302	-	6,6,6	0.14	0	5,5,5	0.24	0
2	D1R	D	602	1	44,44,44	2.30	13 (29%)	57,59,59	2.13	16 (28%)
3	PG4	A	302	-	12,12,12	0.32	0	11,11,11	1.39	1 (9%)
6	DMS	C	303	-	3,3,3	0.64	0	3,3,3	0.55	0
4	EDO	D	608	-	3,3,3	0.49	0	2,2,2	0.24	0
5	PEG	A	308	-	6,6,6	0.14	0	5,5,5	0.31	0
6	DMS	D	604	-	3,3,3	0.64	0	3,3,3	0.70	0
5	PEG	D	601	-	6,6,6	0.75	0	5,5,5	1.00	0
6	DMS	B	309	-	3,3,3	0.61	0	3,3,3	0.25	0
4	EDO	A	304	-	3,3,3	0.48	0	2,2,2	0.35	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	EDO	B	308	-	-	1/1/1/1	-
4	EDO	A	303	-	-	1/1/1/1	-
7	PGE	D	607	-	-	1/7/7/7	-
7	PGE	D	605	-	-	3/7/7/7	-
4	EDO	A	305	-	-	1/1/1/1	-
4	EDO	A	307	-	-	1/1/1/1	-
5	PEG	D	603	-	-	2/4/4/4	-
4	EDO	B	307	-	-	1/1/1/1	-
5	PEG	A	306	-	-	3/4/4/4	-
4	EDO	C	304	-	-	1/1/1/1	-
2	D1R	C	301	1	-	5/37/47/47	0/4/4/4
4	EDO	B	304	-	-	0/1/1/1	-
4	EDO	B	303	-	-	0/1/1/1	-
7	PGE	B	302	-	-	3/7/7/7	-
2	D1R	B	301	1	-	8/37/47/47	0/4/4/4
4	EDO	B	306	-	-	0/1/1/1	-
2	D1R	A	301	1	-	6/37/47/47	0/4/4/4
4	EDO	D	606	-	-	0/1/1/1	-
5	PEG	C	302	-	-	1/4/4/4	-
2	D1R	D	602	1	-	5/37/47/47	0/4/4/4
3	PG4	A	302	-	-	6/10/10/10	-
4	EDO	D	608	-	-	0/1/1/1	-
5	PEG	A	308	-	-	1/4/4/4	-
5	PEG	D	601	-	-	2/4/4/4	-
4	EDO	A	304	-	-	0/1/1/1	-

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	D1R	CAB-S1	-10.94	1.60	1.76
2	B	301	D1R	O4-S1	-7.07	1.34	1.44
2	B	301	D1R	O5-S1	-6.85	1.34	1.44
2	D	602	D1R	O5-S1	-6.40	1.35	1.44
2	A	301	D1R	O5-S1	-6.17	1.35	1.44
2	A	301	D1R	C28-S1	-5.96	1.66	1.77
2	C	301	D1R	O5-S1	-5.26	1.37	1.44
2	A	301	D1R	O4-S1	-5.14	1.37	1.44
2	D	602	D1R	O3-C17	-5.10	1.13	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	602	D1R	C8-N3	4.99	1.45	1.36
2	B	301	D1R	C17-N2	4.81	1.44	1.34
2	D	602	D1R	O2-C8	-4.62	1.14	1.23
2	B	301	D1R	C8-N3	4.53	1.44	1.36
2	C	301	D1R	C17-N2	4.51	1.43	1.34
2	B	301	D1R	O3-C17	-4.41	1.14	1.23
2	C	301	D1R	C8-N3	4.40	1.44	1.36
2	C	301	D1R	O3-C17	-4.37	1.15	1.23
2	D	602	D1R	O4-S1	-4.18	1.38	1.44
2	D	602	D1R	C17-N2	4.07	1.42	1.34
2	C	301	D1R	O2-C8	-4.07	1.15	1.23
2	B	301	D1R	O2-C8	-3.92	1.16	1.23
2	B	301	D1R	C8-N1	3.61	1.43	1.35
2	C	301	D1R	C28-S1	3.55	1.84	1.77
2	C	301	D1R	C8-N1	3.52	1.42	1.35
2	D	602	D1R	C8-N1	3.39	1.42	1.35
2	D	602	D1R	CAD-CAB	-3.33	1.33	1.38
2	C	301	D1R	O4-S1	-3.28	1.39	1.44
2	B	301	D1R	C28-S1	3.24	1.83	1.77
2	D	602	D1R	C48-N3	-3.19	1.41	1.47
2	A	301	D1R	CAD-CAB	-3.17	1.34	1.38
2	D	602	D1R	C28-S1	3.16	1.83	1.77
2	A	301	D1R	O3-C17	-3.06	1.17	1.23
2	C	301	D1R	C48-N3	-2.72	1.42	1.47
2	B	301	D1R	C18-N2	-2.65	1.41	1.46
2	B	301	D1R	C49-N4	-2.57	1.40	1.46
2	C	301	D1R	CAD-CAB	-2.56	1.34	1.38
2	D	602	D1R	CAB-S1	2.55	1.80	1.76
2	B	301	D1R	C22-C21	-2.47	1.34	1.38
2	B	301	D1R	CAF-CAD	-2.39	1.34	1.38
2	A	301	D1R	O2-C8	-2.39	1.18	1.23
2	A	301	D1R	C48-N3	-2.22	1.43	1.47
2	B	301	D1R	C16-C11	-2.18	1.34	1.38
2	D	602	D1R	CAF-CAE	-2.17	1.33	1.38
2	C	301	D1R	C16-C11	-2.11	1.34	1.38
2	A	301	D1R	C16-C11	-2.04	1.34	1.38
2	D	602	D1R	CAA-CAB	-2.02	1.35	1.38

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	D1R	O5-S1-O4	-11.72	105.89	118.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	301	D1R	O5-S1-O4	-10.44	107.26	118.45
2	B	301	D1R	O5-S1-O4	-9.27	108.51	118.45
2	B	301	D1R	O4-S1-CAB	7.73	115.73	108.33
2	B	301	D1R	C48-C49-N4	6.81	121.80	110.86
2	A	301	D1R	O5-S1-CAB	-6.78	101.84	108.33
2	D	602	D1R	O5-S1-O4	-6.32	111.68	118.45
2	B	301	D1R	C33-N4-C40	6.31	122.65	110.63
2	C	301	D1R	C48-C49-N4	5.79	120.16	110.86
2	C	301	D1R	O4-S1-CAB	5.02	113.14	108.33
2	D	602	D1R	O5-S1-CAB	-4.98	103.56	108.33
2	D	602	D1R	O4-S1-CAB	4.98	113.10	108.33
2	B	301	D1R	C49-C48-N3	4.94	120.23	110.42
2	D	602	D1R	C48-C49-N4	4.90	118.73	110.86
2	C	301	D1R	C49-C48-N3	4.90	120.15	110.42
2	A	301	D1R	C28-S1-CAB	4.86	111.67	105.09
2	D	602	D1R	C49-C48-N3	4.59	119.55	110.42
2	A	301	D1R	CAF-CAD-CAB	4.39	123.44	118.95
2	D	602	D1R	C33-N4-C40	4.32	118.87	110.63
2	B	301	D1R	C28-S1-CAB	4.12	110.67	105.09
2	C	301	D1R	C33-N4-C49	-4.06	102.89	110.63
2	D	602	D1R	C28-S1-CAB	4.04	110.57	105.09
2	C	301	D1R	O5-S1-CAB	-3.83	104.66	108.33
2	B	301	D1R	O5-S1-CAB	-3.79	104.70	108.33
2	C	301	D1R	C49-N4-C40	3.65	115.34	109.54
2	B	301	D1R	C27-C28-S1	-3.63	104.87	114.14
2	A	301	D1R	O5-S1-C28	3.61	114.10	108.18
3	A	302	PG4	C3-O2-C2	3.59	128.99	113.26
2	B	301	D1R	C39-C40-N4	3.36	116.26	110.86
2	B	301	D1R	C27-C18-C19	-3.24	107.14	112.41
2	D	602	D1R	C27-C18-N2	3.23	115.80	110.50
2	A	301	D1R	N1-C8-N3	3.12	122.80	117.23
2	B	301	D1R	C26-C21-C22	2.99	122.68	118.23
2	C	301	D1R	C28-S1-CAB	2.99	109.13	105.09
2	A	301	D1R	C49-C48-N3	2.97	116.32	110.42
2	B	301	D1R	C39-N3-C8	2.94	132.49	121.83
2	A	301	D1R	C49-N4-C40	2.91	114.17	109.54
2	A	301	D1R	C27-C18-N2	2.91	115.27	110.50
2	D	602	D1R	C27-C28-S1	-2.89	106.78	114.14
2	C	301	D1R	C27-C28-S1	-2.72	107.21	114.14
2	D	602	D1R	CAC-CAA-CAB	-2.60	116.29	118.95
2	A	301	D1R	O4-S1-C28	2.54	112.34	108.18
2	C	301	D1R	O4-S1-C28	2.46	112.20	108.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	D1R	C27-C18-C19	-2.44	108.44	112.41
2	D	602	D1R	CAF-CAD-CAB	2.38	121.39	118.95
2	B	301	D1R	C10-C9-C17	-2.31	104.38	110.30
2	C	301	D1R	CAC-CAA-CAB	-2.30	116.60	118.95
2	A	301	D1R	C15-C14-C13	-2.27	116.76	119.87
2	C	301	D1R	C33-N4-C40	2.26	114.94	110.63
2	B	301	D1R	C19-C18-N2	-2.20	106.88	110.50
2	B	301	D1R	C13-C12-C11	2.19	123.69	120.61
2	B	301	D1R	C15-C14-C13	-2.17	116.90	119.87
2	A	301	D1R	C39-C40-N4	2.16	114.33	110.86
2	D	602	D1R	C17-C9-N1	-2.16	105.26	111.11
2	C	301	D1R	C39-C40-N4	2.15	114.31	110.86
2	A	301	D1R	O4-S1-CAB	2.15	110.39	108.33
2	D	602	D1R	C39-N3-C8	2.14	129.60	121.83
2	D	602	D1R	C27-C18-C19	-2.14	108.93	112.41
2	B	301	D1R	CAC-CAA-CAB	-2.13	116.77	118.95
2	B	301	D1R	C27-C18-N2	2.10	113.95	110.50
2	B	301	D1R	C49-N4-C40	2.09	112.87	109.54
2	C	301	D1R	N1-C8-N3	2.09	120.96	117.23
2	D	602	D1R	C48-N3-C39	-2.08	108.44	112.68
2	A	301	D1R	CAA-CAB-S1	2.04	121.60	119.50
2	D	602	D1R	C19-C18-N2	-2.00	107.22	110.50

There are no chirality outliers.

All (52) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	D1R	CAD-CAB-S1-C28
2	B	301	D1R	CAA-CAB-S1-O5
2	B	301	D1R	CAD-CAB-S1-O5
2	C	301	D1R	CAA-CAB-S1-O5
2	C	301	D1R	CAD-CAB-S1-O5
2	D	602	D1R	CAA-CAB-S1-O5
2	D	602	D1R	CAD-CAB-S1-O5
2	A	301	D1R	CAA-CAB-S1-C28
2	A	301	D1R	CAD-CAB-S1-C28
2	B	301	D1R	CAA-CAB-S1-C28
2	C	301	D1R	CAA-CAB-S1-C28
2	C	301	D1R	CAD-CAB-S1-C28
2	D	602	D1R	CAA-CAB-S1-C28
2	D	602	D1R	CAD-CAB-S1-C28
2	A	301	D1R	CAD-CAB-S1-O5

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Mol	Chain	Res	Type	Atoms
2	A	301	D1R	CAA-CAB-S1-O5
3	A	302	PG4	O2-C3-C4-O3
3	A	302	PG4	O3-C5-C6-O4
5	D	603	PEG	O1-C1-C2-O2
7	B	302	PGE	O3-C5-C6-O4
5	A	306	PEG	O2-C3-C4-O4
4	B	307	EDO	O1-C1-C2-O2
3	A	302	PG4	C6-C5-O3-C4
5	A	308	PEG	O2-C3-C4-O4
5	A	306	PEG	O1-C1-C2-O2
4	B	308	EDO	O1-C1-C2-O2
4	C	304	EDO	O1-C1-C2-O2
7	D	605	PGE	C1-C2-O2-C3
5	D	603	PEG	C4-C3-O2-C2
7	B	302	PGE	C6-C5-O3-C4
3	A	302	PG4	O1-C1-C2-O2
7	B	302	PGE	C1-C2-O2-C3
5	A	306	PEG	C1-C2-O2-C3
2	A	301	D1R	C27-C18-C19-C20
2	A	301	D1R	C18-C27-C28-S1
2	B	301	D1R	C18-C27-C28-S1
2	C	301	D1R	C18-C27-C28-S1
2	D	602	D1R	C18-C27-C28-S1
3	A	302	PG4	O4-C7-C8-O5
5	D	601	PEG	O1-C1-C2-O2
5	D	601	PEG	C4-C3-O2-C2
4	A	303	EDO	O1-C1-C2-O2
2	B	301	D1R	C27-C18-C19-C20
7	D	607	PGE	C4-C3-O2-C2
5	C	302	PEG	O2-C3-C4-O4
4	A	305	EDO	O1-C1-C2-O2
4	A	307	EDO	O1-C1-C2-O2
2	B	301	D1R	C9-C10-C11-C12
2	B	301	D1R	C9-C10-C11-C16
7	D	605	PGE	C3-C4-O3-C5
3	A	302	PG4	C8-C7-O4-C6
7	D	605	PGE	C6-C5-O3-C4

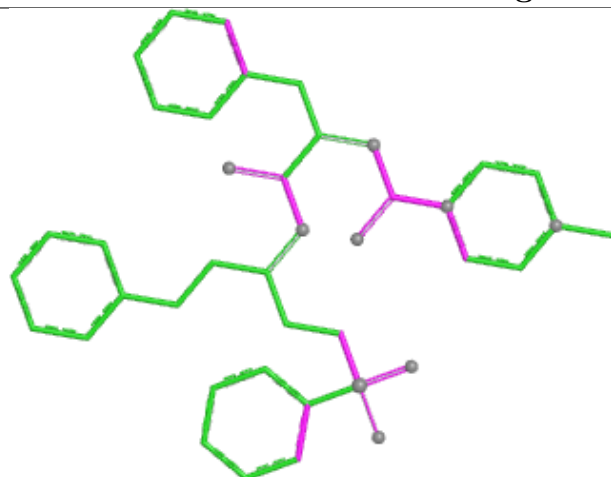
There are no ring outliers.

14 monomers are involved in 20 short contacts:

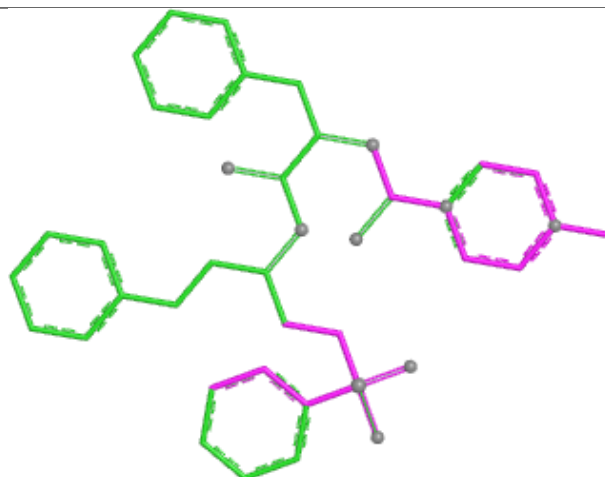
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	308	EDO	3	0
7	D	605	PGE	1	0
4	A	305	EDO	1	0
5	A	306	PEG	2	0
2	C	301	D1R	2	0
4	B	304	EDO	1	0
2	B	301	D1R	2	0
4	B	306	EDO	1	0
2	A	301	D1R	3	0
2	D	602	D1R	1	0
3	A	302	PG4	2	0
5	A	308	PEG	1	0
6	D	604	DMS	1	0
5	D	601	PEG	1	0

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.

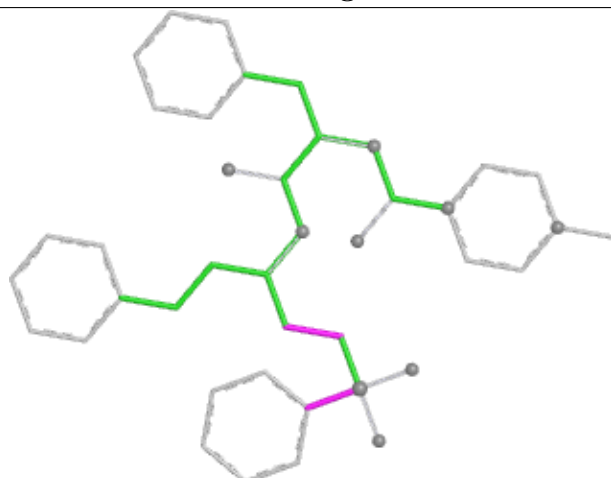
Ligand D1R C 301



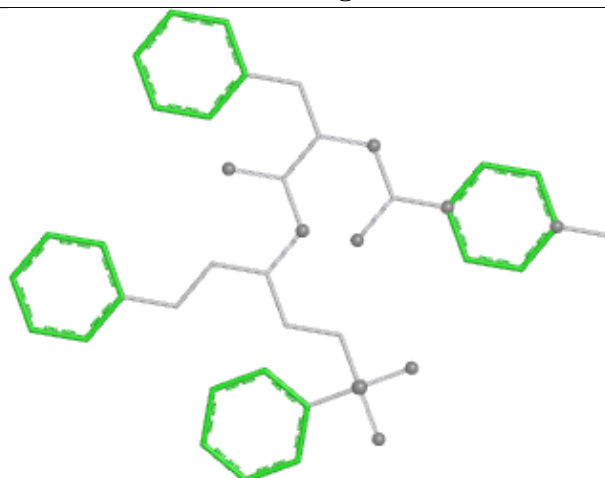
Bond lengths



Bond angles

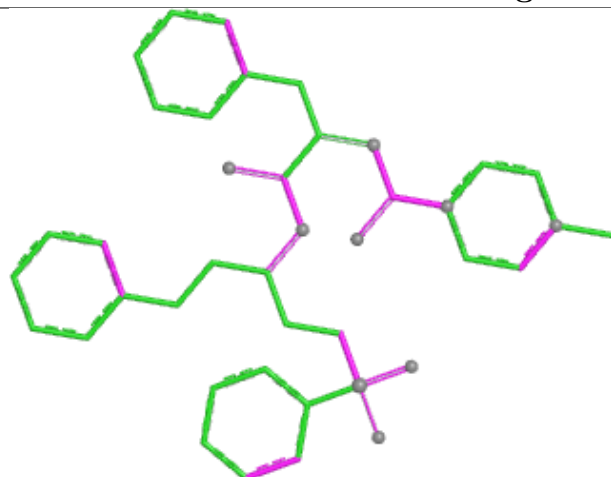


Torsions

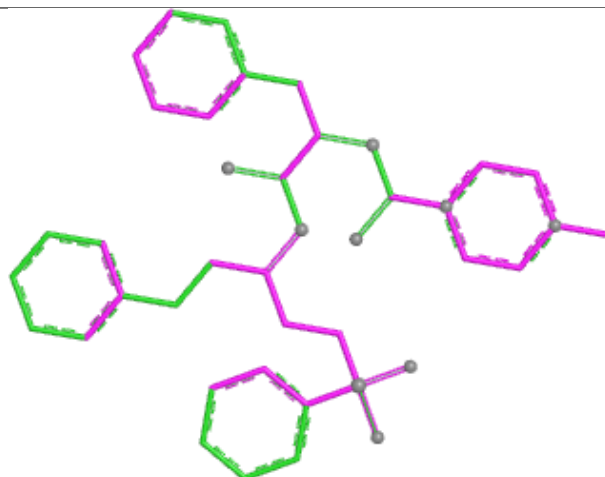


Rings

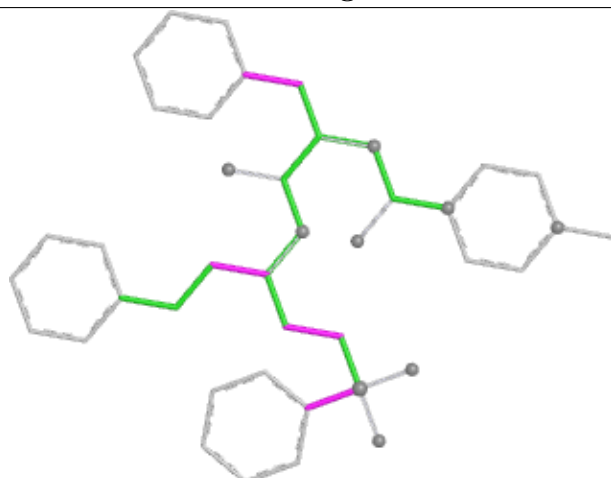
Ligand D1R B 301



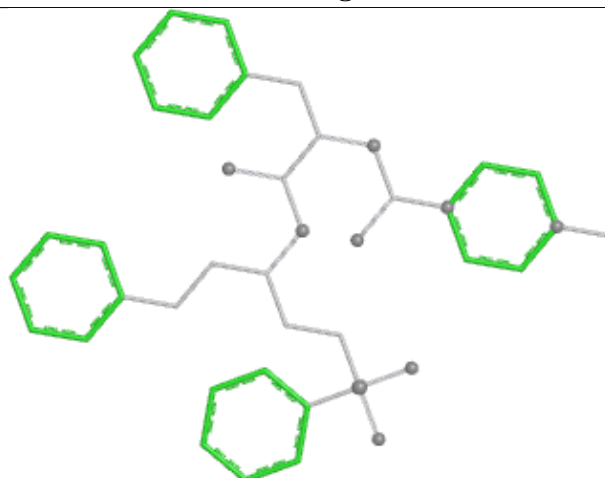
Bond lengths



Bond angles

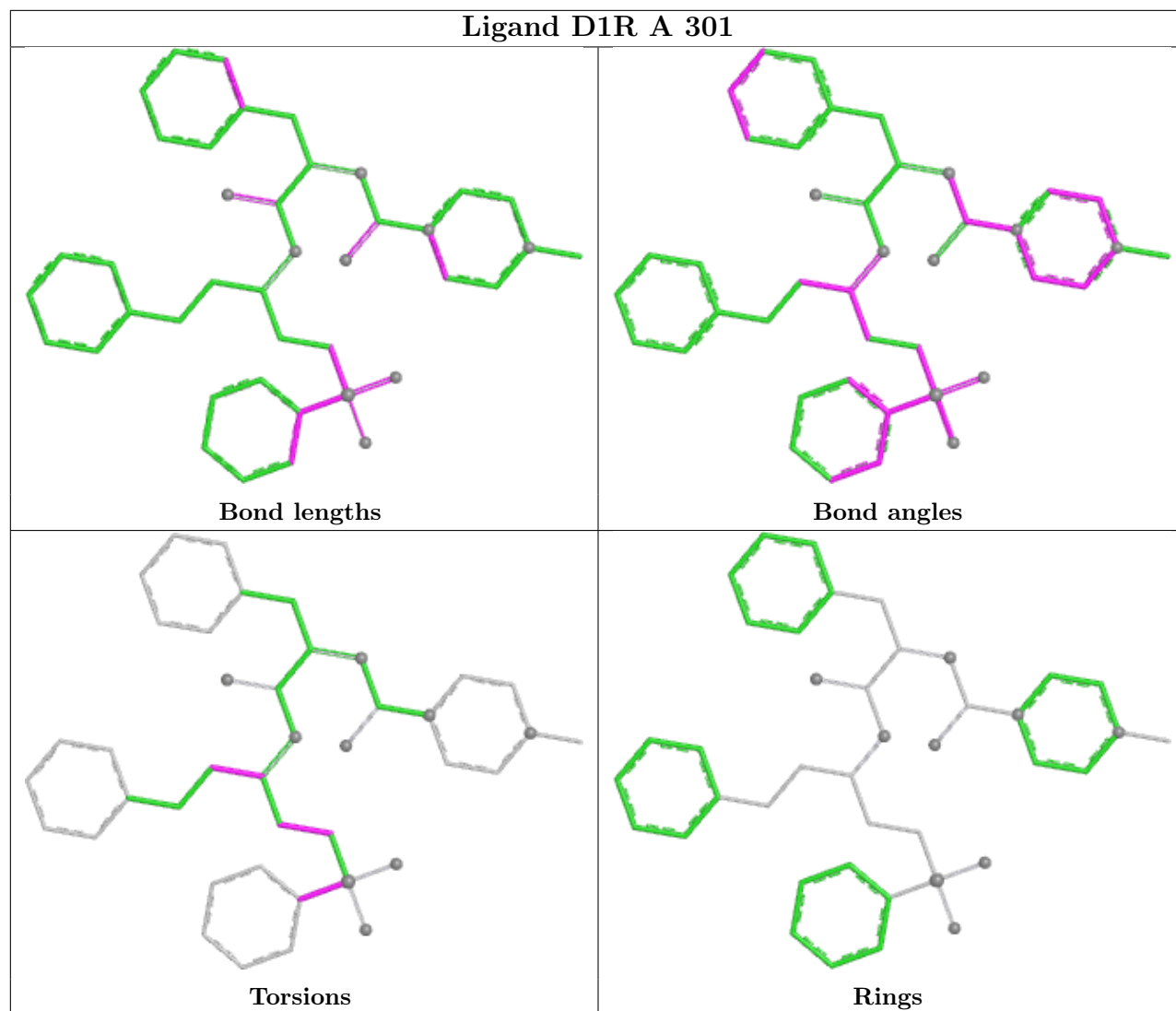


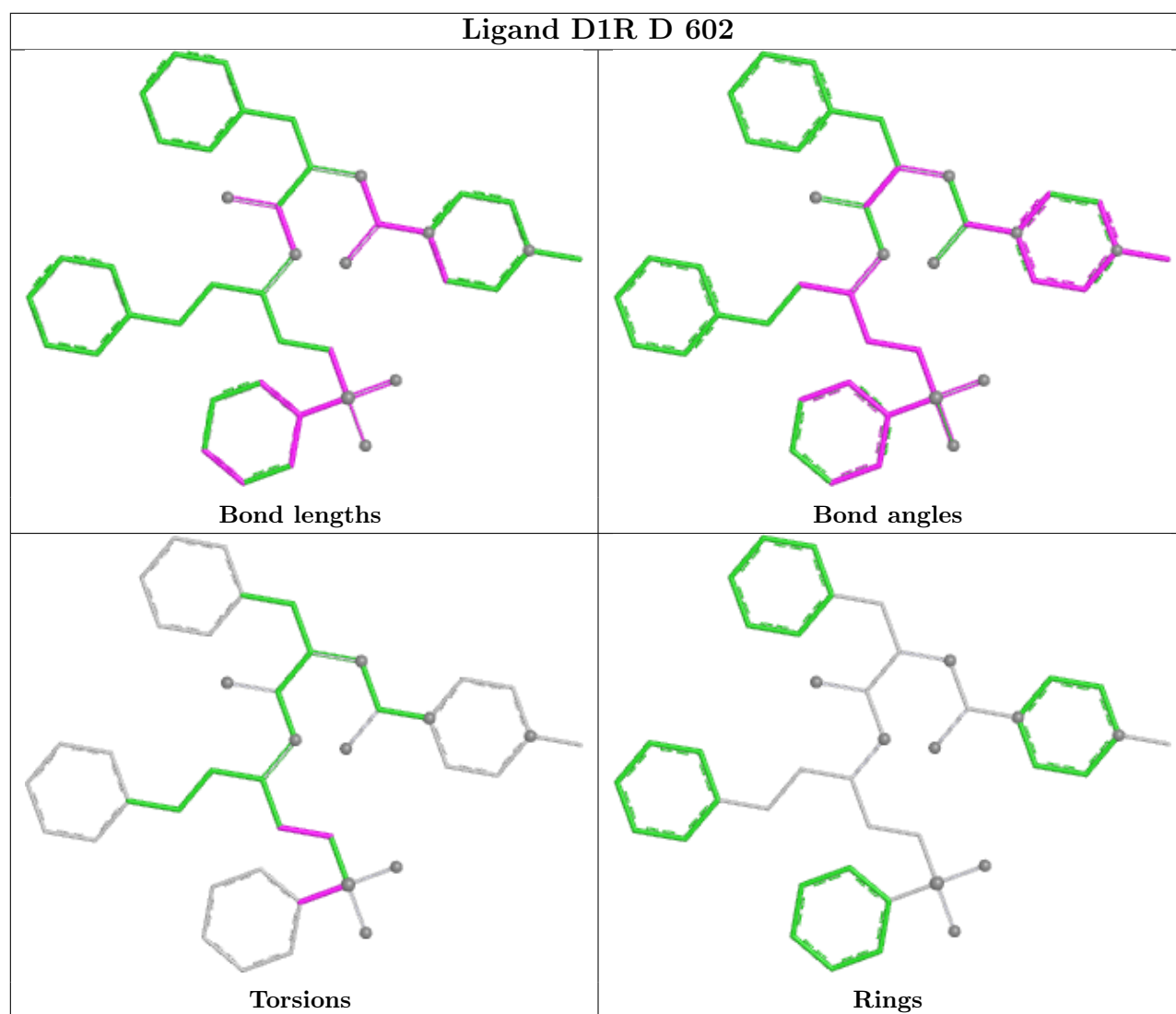
Torsions



Rings

Ligand D1R A 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 [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	220/220 (100%)	-0.03	4 (1%) 67 71	7, 16, 29, 40	2 (0%)
1	B	220/220 (100%)	-0.31	2 (0%) 81 84	5, 12, 27, 41	4 (1%)
1	C	216/220 (98%)	-0.07	4 (1%) 66 70	8, 17, 31, 43	2 (0%)
1	D	220/220 (100%)	-0.44	1 (0%) 87 90	5, 12, 24, 33	8 (3%)
All	All	876/880 (99%)	-0.21	11 (1%) 75 79	5, 14, 28, 43	16 (1%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	145	PHE	2.7
1	C	1	ALA	2.6
1	C	174	SER	2.6
1	A	144	LEU	2.5
1	B	178	ASP	2.5
1	B	175	THR	2.5
1	A	139	GLY	2.3
1	D	103[A]	LYS	2.2
1	C	104	TYR	2.2
1	A	155	ASP	2.2
1	C	173	GLU	2.2

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 ⓘ

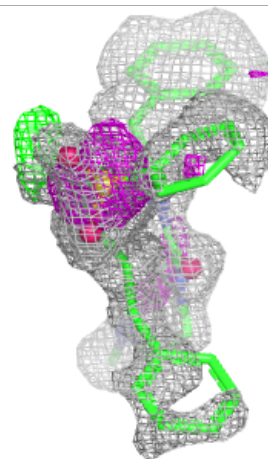
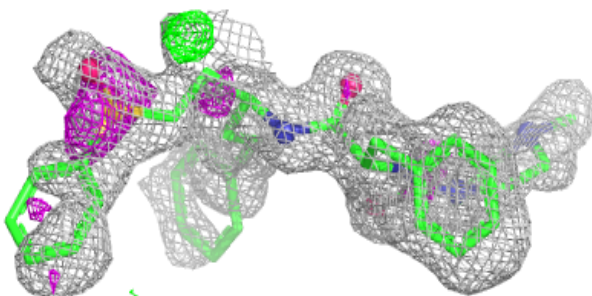
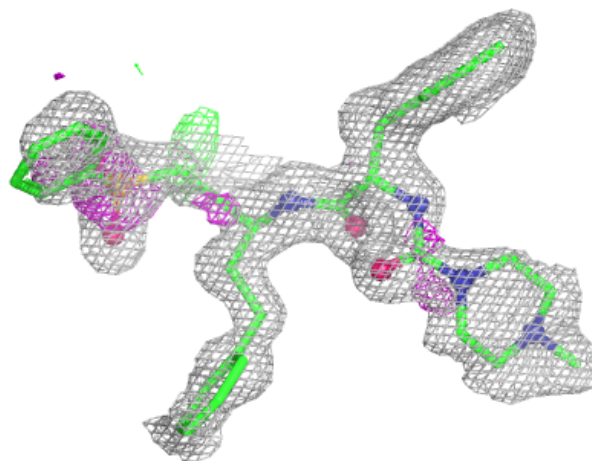
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	EDO	B	303	4/4	0.78	0.15	34,41,48,50	0
7	PGE	D	605	10/10	0.78	0.14	30,40,46,46	0
5	PEG	D	603	7/7	0.79	0.13	28,36,49,52	0
4	EDO	B	304	4/4	0.79	0.14	28,36,48,58	0
7	PGE	B	302	10/10	0.81	0.12	28,38,46,55	0
5	PEG	C	302	7/7	0.81	0.14	25,41,49,50	0
4	EDO	C	304	4/4	0.83	0.12	28,38,46,52	0
4	EDO	D	608	4/4	0.83	0.16	27,35,42,48	0
3	PG4	A	302	13/13	0.84	0.14	30,36,48,50	0
4	EDO	A	304	4/4	0.84	0.12	29,34,42,50	0
5	PEG	A	306	7/7	0.84	0.11	20,34,45,54	0
5	PEG	A	308	7/7	0.84	0.12	29,36,47,47	0
4	EDO	A	307	4/4	0.86	0.10	32,41,51,51	0
4	EDO	B	307	4/4	0.86	0.15	26,36,44,49	0
4	EDO	A	303	4/4	0.87	0.11	21,35,43,50	0
7	PGE	D	607	10/10	0.87	0.11	24,32,42,49	0
4	EDO	D	606	4/4	0.88	0.14	14,25,35,35	0
2	D1R	A	301	41/41	0.88	0.13	18,27,38,43	0
6	DMS	C	303	4/4	0.88	0.12	30,37,45,46	0
4	EDO	B	306	4/4	0.89	0.14	24,33,35,40	0
5	PEG	D	601	7/7	0.89	0.12	29,39,46,48	0
6	DMS	D	604	4/4	0.89	0.16	25,31,45,45	0
4	EDO	A	305	4/4	0.90	0.11	30,39,46,47	0
2	D1R	D	602	41/41	0.90	0.12	13,20,35,43	0
6	DMS	A	309	4/4	0.90	0.12	30,36,43,48	0
2	D1R	B	301	41/41	0.90	0.12	17,22,36,41	0
6	DMS	B	305	4/4	0.91	0.11	24,36,46,46	0
2	D1R	C	301	41/41	0.91	0.11	16,23,36,40	0
6	DMS	C	305	4/4	0.92	0.11	34,43,51,51	0
4	EDO	B	308	4/4	0.93	0.20	20,32,40,47	0
6	DMS	B	309	4/4	0.93	0.12	20,24,33,33	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.

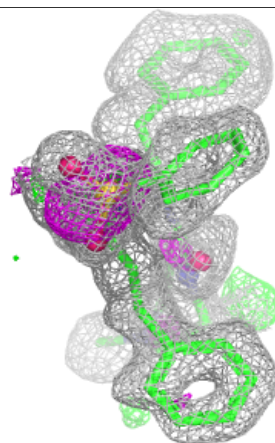
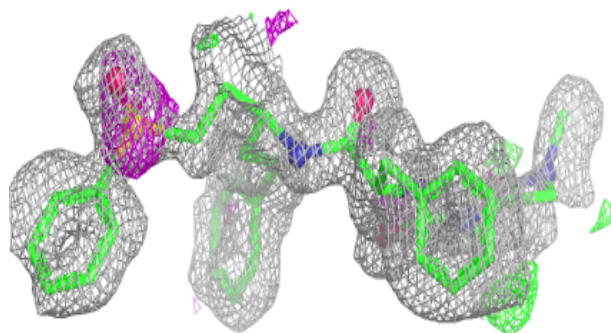
Electron density around D1R A 301:

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



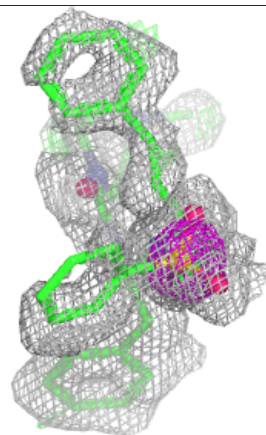
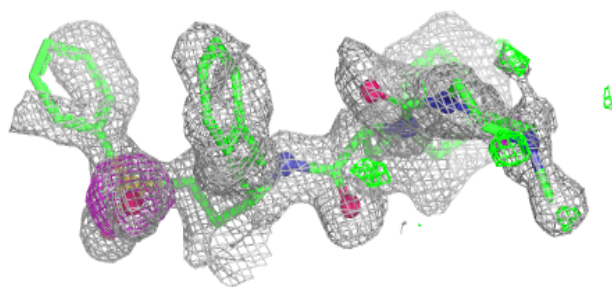
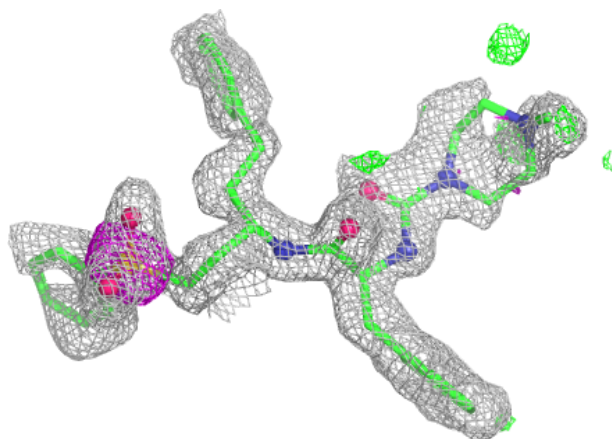
Electron density around D1R D 602:

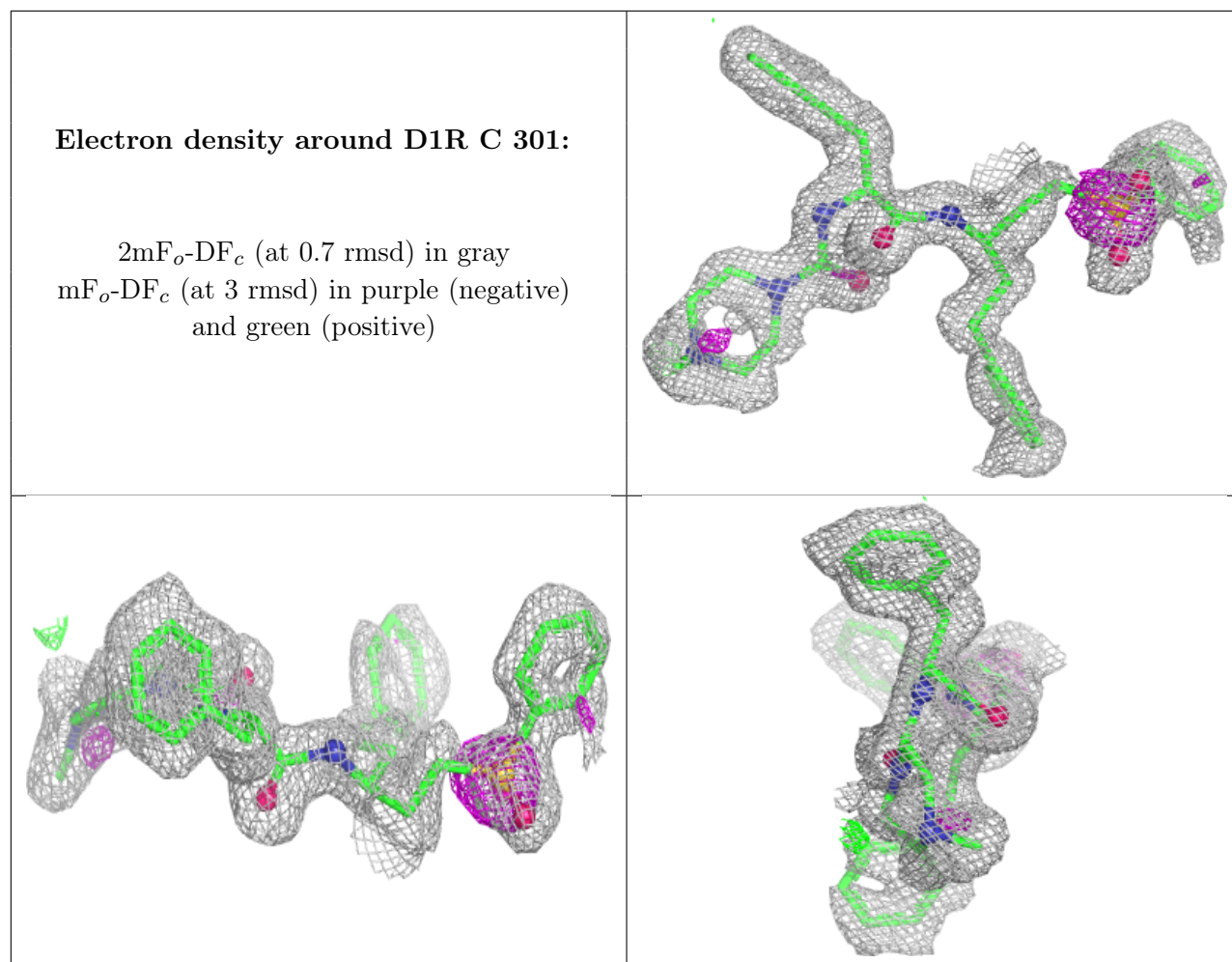
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around D1R 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)





6.5 Other polymers ⓘ

There are no such residues in this entry.