Full wwPDB X-ray Structure Validation Report ⓘ

Nov 3, 2026 – 06:11 pm GMT

PDB ID	:	34CK / pdb_000034ck
Title	:	Crystal structure of human Cathepsin L in complex with 5,8-dimethoxy-1,2,3 ,4-tetrahydroisoquinolin-4-ol
Authors	:	Falke, S.; Meents, A.
Deposited on	:	2026-09-07
Resolution	:	1.91 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:

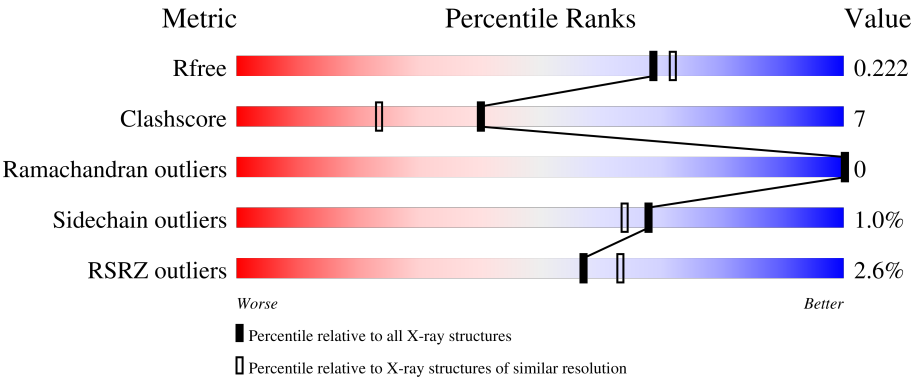
MolProbity	:	4-5-2 with Phenix2.2
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.91 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	1188 (1.92-1.92)
Clashscore	190562	1209 (1.92-1.92)
Ramachandran outliers	187476	1195 (1.92-1.92)
Sidechain outliers	187428	1195 (1.92-1.92)
RSRZ outliers	180081	1188 (1.92-1.92)

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 <=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	89% 11%
1	B	220	5% 86% 13%
1	C	220	5% 78% 19% .
1	D	220	93% 7%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 7527 atoms, of which 42 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.

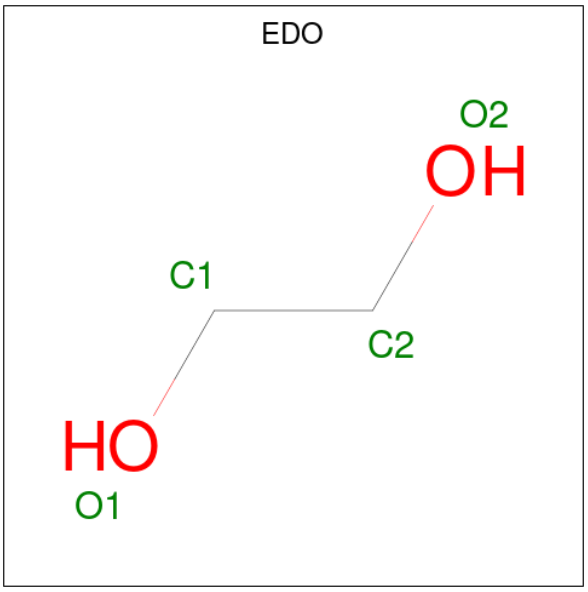
- Molecule 1 is a protein called Cathepsin L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	0	4	0
			1726	1077	286	348	15			
1	B	219	Total	C	N	O	S	0	3	0
			1712	1070	284	344	14			
1	C	213	Total	C	N	O	S	0	4	0
			1678	1051	281	331	15			
1	D	220	Total	C	N	O	S	0	8	0
			1754	1093	292	354	15			

There are 4 discrepancies between the modelled and reference sequences:

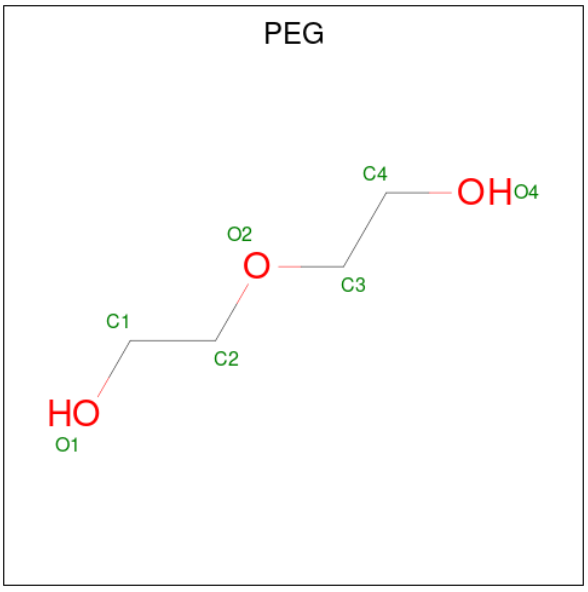
Chain	Residue	Modelled	Actual	Comment	Reference
A	110	ALA	THR	engineered mutation	UNP P07711
B	110	ALA	THR	engineered mutation	UNP P07711
C	110	ALA	THR	engineered mutation	UNP P07711
D	110	ALA	THR	engineered mutation	UNP P07711

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



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

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



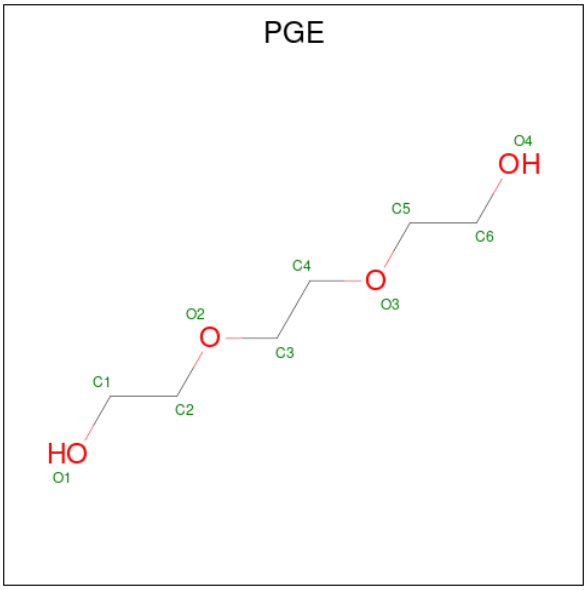
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0

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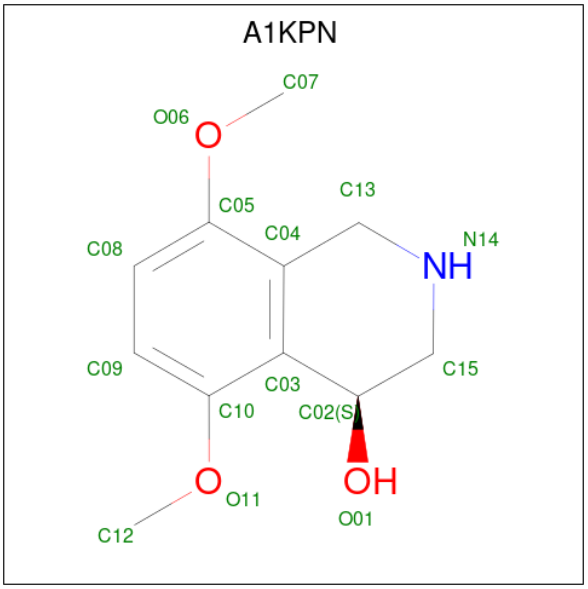
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0
3	C	1	Total C H O 17 4 10 3	0	0
3	C	1	Total C H O 17 4 10 3	0	0
3	D	1	Total C H O 17 4 10 3	0	0

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



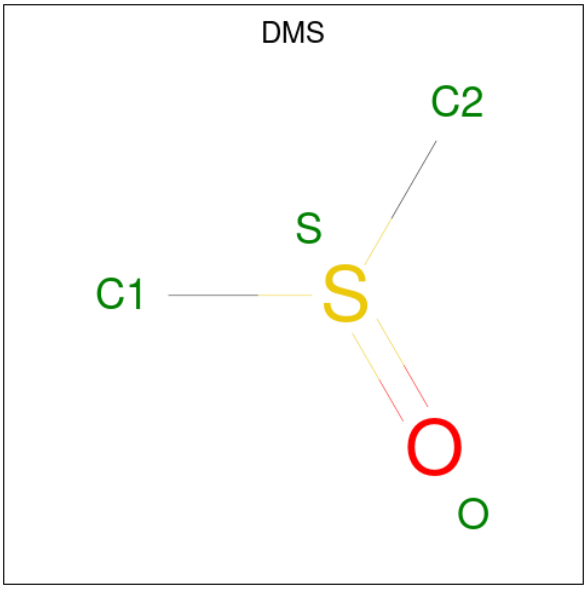
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 6 4	0	0
4	B	1	Total C O 10 6 4	0	0
4	D	1	Total C O 10 6 4	0	0

- Molecule 5 is (4 {S})-5,8-dimethoxy-1,2,3,4-tetrahydroisoquinolin-4-ol (CCD ID: A1KPN) (formula: $C_{11}H_{15}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
5	C	1	15	11	1	3	0	0

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



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

- Molecule 7 is water.

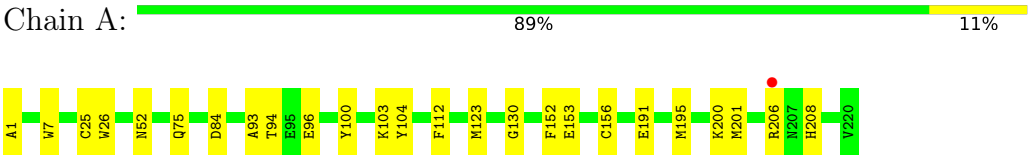
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	115	Total O 115 115	0	0
7	B	123	Total O 123 123	0	0
7	C	93	Total O 93 93	0	0
7	D	160	Total O 160 160	0	0

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.

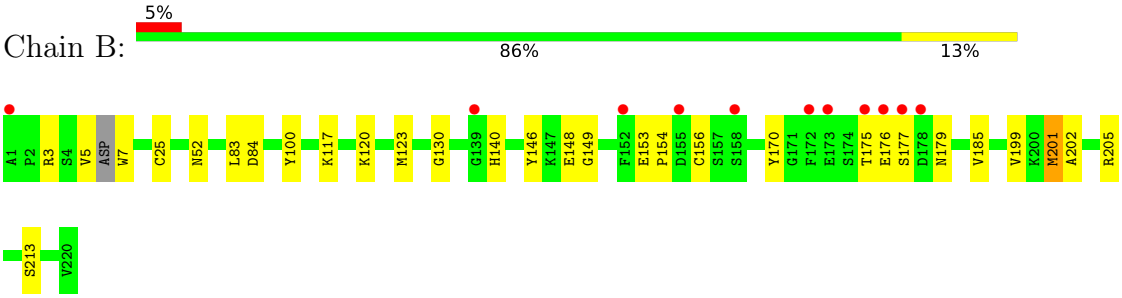
• Molecule 1: Cathepsin L

Chain A:



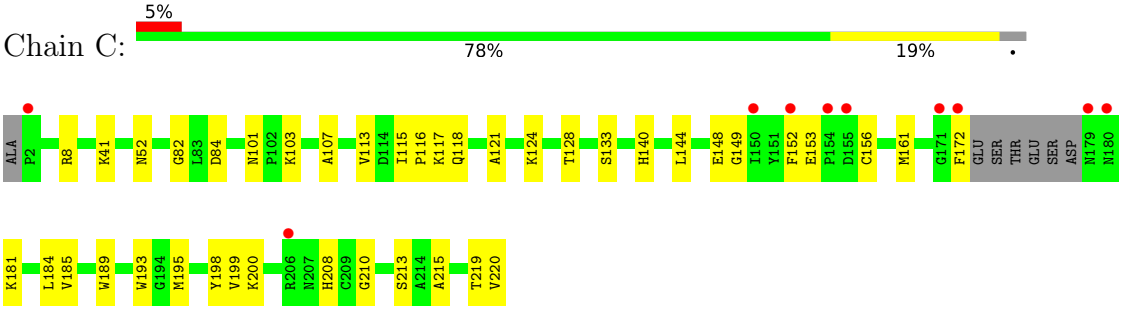
• Molecule 1: Cathepsin L

Chain B:



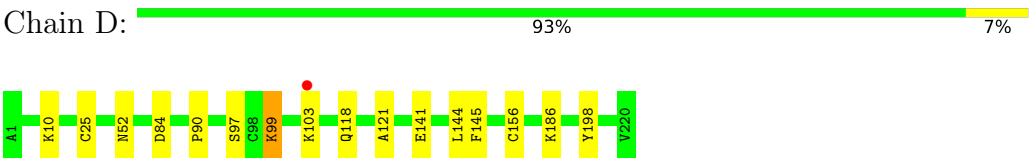
• Molecule 1: Cathepsin L

Chain C:



• Molecule 1: Cathepsin L

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	57.00Å 62.51Å 67.33Å 105.38° 93.79° 115.52°	Depositor
Resolution (Å)	53.32 – 1.91 53.32 – 1.91	Depositor EDS
% Data completeness (in resolution range)	94.3 (53.32-1.91) 94.3 (53.32-1.91)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.30 (at 1.91Å)	Xtriage
Refinement program	PHENIX 2.0-5936_9999	Depositor
R, R_{free}	0.169 , 0.222 0.169 , 0.222	Depositor DCC
R_{free} test set	2873 reflections (1.37%)	wwPDB-VP
Wilson B-factor (Å^2)	22.5	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 41.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7527	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: A1KPN, DMS, PEG, CSO, EDO, PGE

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	0.35	0/1754	0.48	0/2369
1	B	0.46	0/1739	0.57	0/2346
1	C	0.33	0/1705	0.46	0/2299
1	D	0.40	0/1782	0.50	0/2404
All	All	0.39	0/6980	0.50	0/9418

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

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	1726	0	1593	20	0
1	B	1712	0	1584	22	0
1	C	1678	0	1557	35	0
1	D	1754	0	1621	13	0
2	A	4	0	6	2	0
2	B	4	6	6	0	0
2	D	4	6	6	0	0
3	A	14	0	20	2	0
3	B	14	0	20	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	28	20	40	3	0
3	D	7	10	10	0	0
4	A	10	0	14	0	0
4	B	10	0	14	1	0
4	D	10	0	14	0	0
5	C	15	0	0	0	0
6	D	4	0	6	0	0
7	A	115	0	0	1	0
7	B	123	0	0	0	0
7	C	93	0	0	0	0
7	D	160	0	0	1	0
All	All	7485	42	6511	89	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 7.

All (89) 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	1.34	1.02
1:C:124:LYS:HE3	1:C:128:THR:HG21	1.49	0.93
1:C:161:MET:HE1	1:C:213:SER:HB2	1.50	0.92
1:A:103:LYS:HE2	2:A:301:EDO:H21	1.61	0.81
1:C:161:MET:CE	1:C:213:SER:HB2	2.09	0.81
1:C:144:LEU:HD22	1:D:144:LEU:HD13	1.68	0.75
1:B:153:GLU:OE1	1:B:154:PRO:HD2	1.88	0.73
1:B:148:GLU:HG2	1:B:149:GLY:N	2.05	0.71
1:C:144:LEU:CD2	1:D:144:LEU:HD13	2.24	0.67
1:B:202:ALA:HB1	1:B:205:ARG:HD3	1.76	0.66
1:D:118:GLN:HE21	1:D:121:ALA:HB2	1.59	0.66
1:B:140:HIS:CD2	1:B:153:GLU:HG2	2.29	0.66
1:B:185:VAL:HG21	1:B:201:MET:HG3	1.77	0.66
1:B:52:ASN:ND2	1:B:84:ASP:H	1.95	0.65
1:C:140:HIS:CD2	1:C:153:GLU:HG2	2.33	0.64
1:A:7:TRP:CE2	1:A:130:GLY:HA2	2.33	0.64
1:C:124:LYS:HD2	1:C:124:LYS:O	1.98	0.64
1:C:52:ASN:ND2	1:C:84:ASP:H	1.95	0.63
1:B:153:GLU:OE1	1:B:153:GLU:HA	1.98	0.63
1:A:52:ASN:ND2	1:A:84:ASP:H	1.98	0.62
1:B:52:ASN:HD22	1:B:84:ASP:H	1.48	0.60
1:C:189:TRP:CE2	3:C:304:PEG:H42	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:120:LYS:HE2	1:B:120:LYS:H	1.67	0.59
1:B:120:LYS:H	1:B:120:LYS:CE	2.16	0.59
1:C:161:MET:HE3	1:C:210:GLY:O	2.03	0.57
1:D:52:ASN:ND2	1:D:84:ASP:H	2.02	0.57
1:D:141:GLU:HG3	1:D:145:PHE:CE2	2.39	0.57
1:C:172:PHE:HA	1:C:181:LYS:HA	1.88	0.56
1:C:52:ASN:HD22	1:C:84:ASP:H	1.53	0.56
1:B:148:GLU:HG2	1:B:149:GLY:H	1.71	0.55
1:C:161:MET:HE1	1:C:213:SER:CB	2.30	0.55
1:C:152:PHE:HA	1:C:208:HIS:NE2	2.22	0.54
1:A:52:ASN:HD22	1:A:84:ASP:H	1.54	0.54
1:A:103:LYS:CE	2:A:301:EDO:H21	2.35	0.54
1:D:52:ASN:HD22	1:D:84:ASP:H	1.54	0.53
1:C:153:GLU:H	1:C:208:HIS:CE1	2.25	0.53
1:A:75[B]:GLN:HG2	1:A:112:PHE:HE2	1.74	0.53
1:C:101:ASN:OD1	1:C:103:LYS:HG3	2.08	0.53
1:A:52:ASN:HD21	1:A:100:TYR:HD1	1.57	0.53
1:B:175:THR:HG23	1:B:176:GLU:CD	2.35	0.52
1:A:104:TYR:CE2	3:A:302:PEG:H42	2.44	0.52
1:B:177:SER:OG	1:B:179:ASN:HB2	2.11	0.51
1:C:148:GLU:HG2	1:C:149:GLY:N	2.26	0.50
1:B:5:VAL:HG13	3:B:303:PEG:H11	1.94	0.50
1:A:195:MET:HE1	1:A:200:LYS:HE3	1.94	0.50
1:B:146:TYR:CZ	1:B:199:VAL:HG23	2.47	0.49
1:A:1:ALA:HB3	1:A:123:MET:HE2	1.94	0.49
1:B:123:MET:HE3	1:B:170:TYR:CE1	2.47	0.49
1:A:96:GLU:HA	1:A:96:GLU:OE1	2.13	0.49
1:A:75[B]:GLN:CG	1:A:112:PHE:HE2	2.25	0.48
1:C:124:LYS:HE3	1:C:128:THR:CG2	2.33	0.48
1:C:117:LYS:N	1:C:117:LYS:HD3	2.29	0.48
1:C:8:ARG:NH2	1:C:184:LEU:HD21	2.29	0.48
1:A:153:GLU:H	1:A:208:HIS:CE1	2.32	0.47
1:C:113:VAL:HG23	1:C:219[B]:THR:CG2	2.44	0.47
1:B:117:LYS:HG2	1:B:213:SER:HA	1.97	0.47
1:B:185:VAL:CG2	1:B:201:MET:HG3	2.44	0.47
1:C:148:GLU:HG2	1:C:149:GLY:H	1.79	0.47
1:D:118:GLN:NE2	1:D:121:ALA:HB2	2.27	0.46
3:C:305:PEG:H12	1:D:144:LEU:HD21	1.97	0.46
1:B:3:ARG:HH12	1:B:175:THR:HA	1.80	0.45
1:B:52:ASN:HD21	1:B:100:TYR:HD1	1.63	0.45
1:C:195:MET:HE1	1:C:200:LYS:HE2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:MET:HE1	1:A:200:LYS:CE	2.47	0.45
1:C:185:VAL:HB	1:C:199:VAL:HG13	1.98	0.44
1:A:191:GLU:HG2	7:A:491:HOH:O	2.18	0.44
1:C:118:GLN:HG3	1:C:121:ALA:H	1.83	0.43
1:D:90:PRO:HB3	7:D:514:HOH:O	2.18	0.43
1:D:103[B]:LYS:O	1:D:103[B]:LYS:HD3	2.19	0.43
1:B:52:ASN:ND2	1:B:83:LEU:HD12	2.32	0.43
1:B:7:TRP:CE2	1:B:130:GLY:HA2	2.53	0.43
1:C:115:ILE:HG23	1:C:116:PRO:HD2	2.00	0.43
1:C:189:TRP:CZ2	3:C:304:PEG:H42	2.54	0.43
1:C:124:LYS:HD2	1:C:124:LYS:C	2.43	0.43
1:D:186:LYS:HB2	1:D:198:TYR:CE2	2.54	0.42
1:D:97:SER:O	1:D:99[A]:LYS:HE3	2.20	0.41
1:A:104:TYR:CD2	3:A:302:PEG:H42	2.55	0.41
1:A:201[B]:MET:HE3	1:A:201[B]:MET:HB3	1.94	0.41
1:A:93:ALA:O	1:A:94[B]:THR:HG23	2.21	0.41
1:C:133:SER:O	1:C:215:ALA:HA	2.21	0.41
1:C:193:TRP:CH2	1:C:199:VAL:HB	2.56	0.41
1:C:117:LYS:HE2	1:C:117:LYS:HB2	1.85	0.41
1:C:82:GLY:HA2	1:C:107:ALA:O	2.21	0.41
1:D:10:LYS:HA	1:D:10:LYS:HD2	1.92	0.41
1:C:8:ARG:HD3	1:C:198:TYR:CZ	2.55	0.41
1:C:115:ILE:CG2	1:C:116:PRO:HD2	2.51	0.40
4:B:304:PGE:H4	4:B:304:PGE:H2	1.85	0.40
1:A:25[B]:CSO:SG	1:A:26:TRP:N	2.94	0.40
1:A:152:PHE:HA	1:A:208:HIS:CE1	2.57	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	220/220 (100%)	216 (98%)	4 (2%)	0	100	100
1	B	216/220 (98%)	208 (96%)	8 (4%)	0	100	100
1	C	211/220 (96%)	204 (97%)	7 (3%)	0	100	100
1	D	224/220 (102%)	216 (96%)	8 (4%)	0	100	100
All	All	871/880 (99%)	844 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	180/177 (102%)	178 (99%)	2 (1%)	65	60
1	B	178/177 (101%)	176 (99%)	2 (1%)	65	60
1	C	174/177 (98%)	173 (99%)	1 (1%)	78	75
1	D	184/177 (104%)	181 (98%)	3 (2%)	55	44
All	All	716/708 (101%)	708 (99%)	8 (1%)	68	60

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

Mol	Chain	Res	Type
1	A	156	CYS
1	A	206	ARG
1	B	156	CYS
1	B	201	MET
1	C	156	CYS
1	D	99[A]	LYS
1	D	99[B]	LYS
1	D	156	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	78	GLN
1	B	19	GLN
1	B	52	ASN
1	B	118	GLN
1	C	21	GLN
1	C	52	ASN
1	C	75	GLN
1	C	179	ASN
1	D	21	GLN
1	D	52	ASN
1	D	118	GLN
1	D	179	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	CSO	B	25[B]	1	4,5,7	1.41	1 (25%)	1,5,8	0.86	0
1	CSO	D	25[A]	1	3,6,7	0.70	0	0,6,8	-	-
1	CSO	C	25[A]	1	3,6,7	0.69	0	0,6,8	-	-
1	CSO	A	25[B]	1	4,5,7	0.58	0	1,5,8	0.78	0
1	CSO	B	25[A]	1	3,6,7	0.67	0	0,6,8	-	-
1	CSO	D	25[B]	1	4,5,7	1.61	1 (25%)	1,5,8	1.18	0
1	CSO	A	25[A]	1	3,6,7	0.52	0	0,6,8	-	-
1	CSO	C	25[B]	1	4,5,7	0.64	0	1,5,8	0.31	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CSO	B	25[B]	1	-	0/1/4/7	-
1	CSO	D	25[A]	1	-	1/1/5/7	-
1	CSO	C	25[A]	1	-	1/1/5/7	-
1	CSO	A	25[B]	1	-	0/1/4/7	-
1	CSO	B	25[A]	1	-	0/1/5/7	-
1	CSO	D	25[B]	1	-	0/1/4/7	-
1	CSO	A	25[A]	1	-	1/1/5/7	-
1	CSO	C	25[B]	1	-	0/1/4/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	25[B]	CSO	CB-SG	-2.96	1.75	1.81
1	B	25[B]	CSO	CB-SG	-2.53	1.76	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	25[A]	CSO	N-CA-CB-SG
1	D	25[A]	CSO	N-CA-CB-SG
1	C	25[A]	CSO	N-CA-CB-SG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	25[B]	CSO	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

17 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	$\#\|Z\| > 2$
6	DMS	D	301	-	3,3,3	0.56	0	3,3,3	0.18	0
3	PEG	C	305	-	6,6,6	0.43	0	5,5,5	0.62	0
3	PEG	C	302	-	6,6,6	0.24	0	5,5,5	0.28	0
4	PGE	A	304	-	9,9,9	0.34	0	8,8,8	0.62	0
3	PEG	C	304	-	6,6,6	0.27	0	5,5,5	0.43	0
3	PEG	A	303	-	6,6,6	0.22	0	5,5,5	0.28	0
3	PEG	B	303	-	6,6,6	0.23	0	5,5,5	0.37	0
5	A1KPN	C	301	-	16,16,16	1.91	7 (43%)	17,22,22	2.19	5 (29%)
2	EDO	D	302	-	3,3,3	0.26	0	2,2,2	0.41	0
4	PGE	D	304	-	9,9,9	0.34	0	8,8,8	0.60	0
4	PGE	B	304	-	9,9,9	0.30	0	8,8,8	0.62	0
3	PEG	D	303	-	6,6,6	0.31	0	5,5,5	0.37	0
3	PEG	A	302	-	6,6,6	0.30	0	5,5,5	0.35	0
3	PEG	B	302	-	6,6,6	0.24	0	5,5,5	0.24	0
2	EDO	A	301	-	3,3,3	0.28	0	2,2,2	0.29	0
2	EDO	B	301	-	3,3,3	0.32	0	2,2,2	0.21	0
3	PEG	C	303	-	6,6,6	0.23	0	5,5,5	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
3	PEG	C	305	-	-	4/4/4/4	-
3	PEG	C	302	-	-	3/4/4/4	-
4	PGE	A	304	-	-	4/7/7/7	-
3	PEG	C	304	-	-	3/4/4/4	-
3	PEG	A	303	-	-	2/4/4/4	-
3	PEG	B	303	-	-	1/4/4/4	-
5	A1KPN	C	301	-	-	2/4/14/14	0/2/2/2
2	EDO	D	302	-	-	1/1/1/1	-
4	PGE	D	304	-	-	3/7/7/7	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGE	B	304	-	-	4/7/7/7	-
3	PEG	D	303	-	-	2/4/4/4	-
3	PEG	A	302	-	-	1/4/4/4	-
3	PEG	B	302	-	-	1/4/4/4	-
2	EDO	A	301	-	-	1/1/1/1	-
2	EDO	B	301	-	-	1/1/1/1	-
3	PEG	C	303	-	-	2/4/4/4	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	301	A1KPN	O06-C05	-4.21	1.30	1.37
5	C	301	A1KPN	O06-C07	-3.20	1.33	1.42
5	C	301	A1KPN	C15-N14	-2.51	1.43	1.46
5	C	301	A1KPN	C10-C03	2.28	1.43	1.39
5	C	301	A1KPN	C03-C02	2.26	1.56	1.52
5	C	301	A1KPN	C15-C02	2.13	1.54	1.52
5	C	301	A1KPN	O11-C10	-2.12	1.33	1.37

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	301	A1KPN	O11-C10-C03	4.80	120.59	115.54
5	C	301	A1KPN	O11-C10-C09	-4.20	117.17	124.37
5	C	301	A1KPN	O06-C05-C04	3.58	119.14	115.35
5	C	301	A1KPN	C10-C03-C02	3.43	125.61	119.75
5	C	301	A1KPN	O06-C05-C08	-2.87	119.45	124.37

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	304	PGE	C4-C3-O2-C2
5	C	301	A1KPN	C03-C10-O11-C12
5	C	301	A1KPN	C09-C10-O11-C12
3	C	305	PEG	O1-C1-C2-O2
3	B	303	PEG	O2-C3-C4-O4
3	C	302	PEG	O1-C1-C2-O2
4	D	304	PGE	O1-C1-C2-O2
4	A	304	PGE	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	B	304	PGE	O2-C3-C4-O3
3	A	302	PEG	O1-C1-C2-O2
2	A	301	EDO	O1-C1-C2-O2
2	B	301	EDO	O1-C1-C2-O2
2	D	302	EDO	O1-C1-C2-O2
3	C	305	PEG	O2-C3-C4-O4
3	A	303	PEG	O2-C3-C4-O4
3	C	302	PEG	O2-C3-C4-O4
3	D	303	PEG	O1-C1-C2-O2
3	B	302	PEG	C1-C2-O2-C3
4	B	304	PGE	C6-C5-O3-C4
3	C	304	PEG	C1-C2-O2-C3
3	C	305	PEG	C4-C3-O2-C2
3	C	303	PEG	C1-C2-O2-C3
3	D	303	PEG	C4-C3-O2-C2
3	C	305	PEG	C1-C2-O2-C3
4	D	304	PGE	O3-C5-C6-O4
3	C	303	PEG	C4-C3-O2-C2
3	A	303	PEG	C1-C2-O2-C3
4	A	304	PGE	O3-C5-C6-O4
3	C	304	PEG	O2-C3-C4-O4
4	D	304	PGE	C4-C3-O2-C2
4	A	304	PGE	C1-C2-O2-C3
4	A	304	PGE	C3-C4-O3-C5
3	C	302	PEG	C1-C2-O2-C3
4	B	304	PGE	C3-C4-O3-C5
3	C	304	PEG	O1-C1-C2-O2

There are no ring outliers.

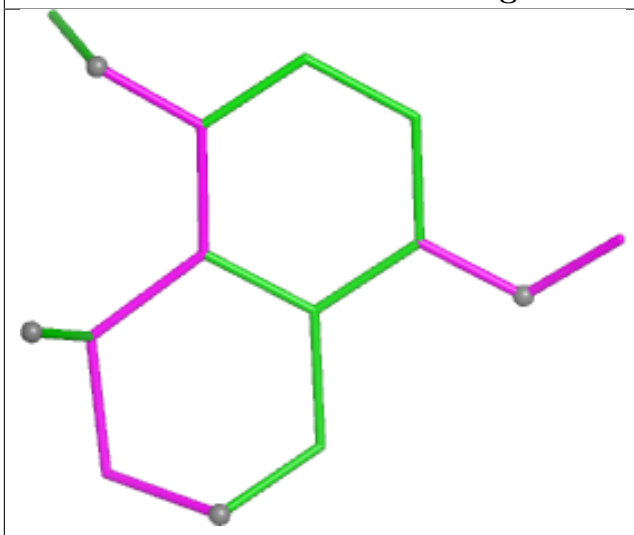
6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	305	PEG	1	0
3	C	304	PEG	2	0
3	B	303	PEG	1	0
4	B	304	PGE	1	0
3	A	302	PEG	2	0
2	A	301	EDO	2	0

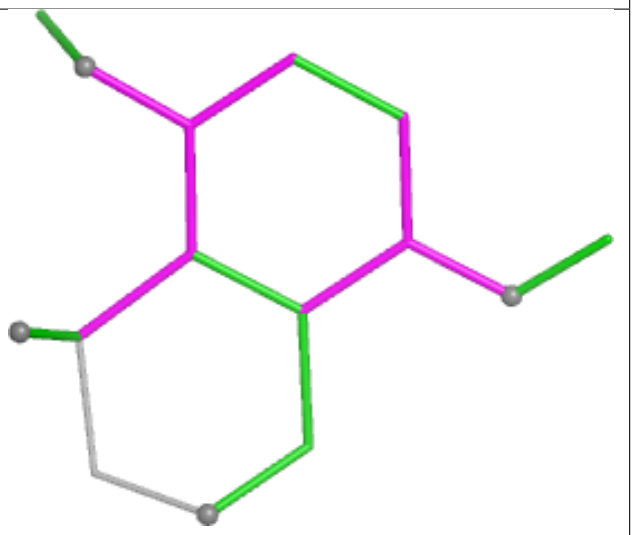
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 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.

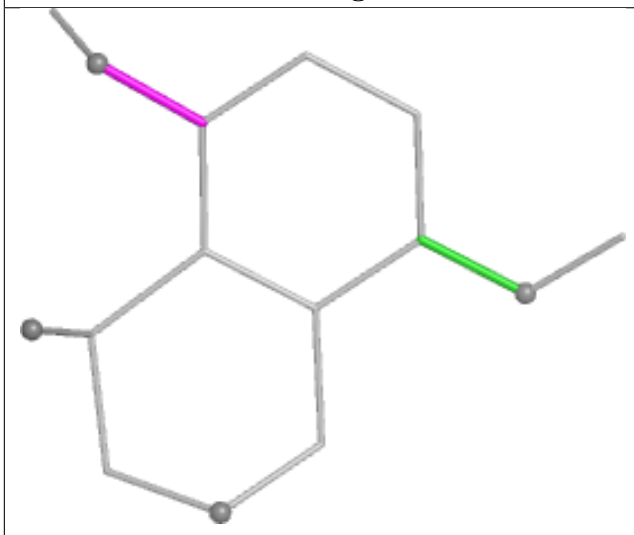
Ligand A1KPN C 301



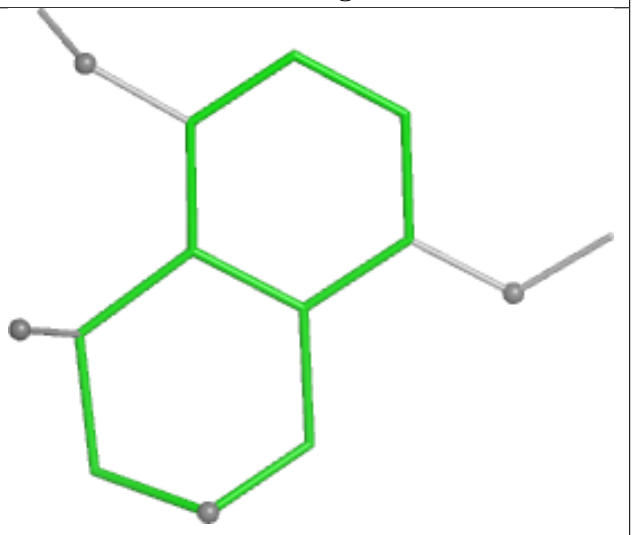
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	219/220 (99%)	-0.03	1 (0%)	87	91	10, 24, 40, 62	3 (1%)
1	B	218/220 (99%)	0.11	11 (5%)	34	38	14, 23, 52, 85	2 (0%)
1	C	212/220 (96%)	0.31	10 (4%)	36	41	14, 27, 55, 83	3 (1%)
1	D	219/220 (99%)	-0.23	1 (0%)	87	91	8, 20, 36, 44	7 (3%)
All	All	868/880 (98%)	0.04	23 (2%)	57	63	8, 24, 46, 85	15 (1%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	103[A]	LYS	3.7
1	C	152	PHE	3.1
1	C	206[A]	ARG	3.1
1	B	152	PHE	3.1
1	B	178	ASP	3.0
1	B	173	GLU	3.0
1	B	177	SER	2.9
1	C	150	ILE	2.9
1	B	176	GLU	2.7
1	B	172	PHE	2.7
1	C	172	PHE	2.7
1	C	154	PRO	2.6
1	C	179	ASN	2.6
1	B	175	THR	2.4
1	C	171	GLY	2.4
1	B	1	ALA	2.4
1	C	180	ASN	2.3
1	A	206	ARG	2.2
1	B	155	ASP	2.2
1	B	139	GLY	2.2
1	B	158	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	155	ASP	2.1
1	C	2	PRO	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	CSO	D	25[A]	7/8	0.87	0.09	15,16,22,26	7
1	CSO	D	25[B]	6/8	0.87	0.09	15,16,17,18	6
1	CSO	B	25[A]	7/8	0.93	0.08	17,18,33,36	7
1	CSO	B	25[B]	6/8	0.93	0.08	17,18,22,22	6
1	CSO	A	25[A]	7/8	0.93	0.10	18,19,23,25	7
1	CSO	A	25[B]	6/8	0.93	0.10	18,19,20,22	6
1	CSO	C	25[A]	7/8	0.96	0.06	19,21,27,33	7
1	CSO	C	25[B]	6/8	0.96	0.06	19,21,22,23	6

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, 95^{th} 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	A	303	7/7	0.75	0.14	33,41,48,56	0
3	PEG	C	302	7/7	0.77	0.16	36,49,59,65	0
4	PGE	A	304	10/10	0.77	0.15	41,48,50,63	0
4	PGE	D	304	10/10	0.78	0.15	42,47,52,52	0
5	A1KPN	C	301	15/15	0.79	0.14	33,42,52,52	15
3	PEG	A	302	7/7	0.81	0.13	27,36,41,52	0
4	PGE	B	304	10/10	0.81	0.14	37,49,57,64	0
2	EDO	B	301	4/4	0.82	0.15	33,42,51,51	0

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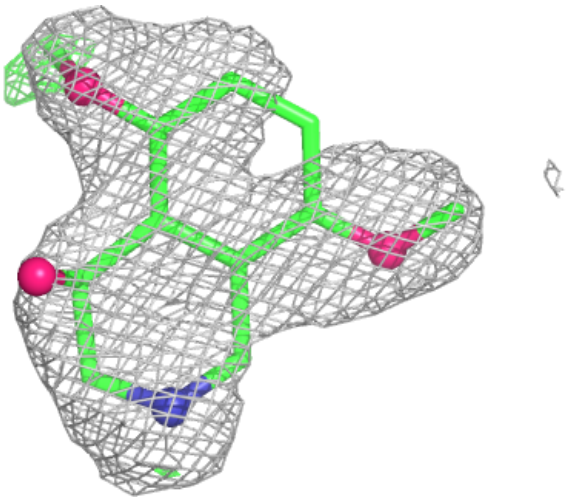
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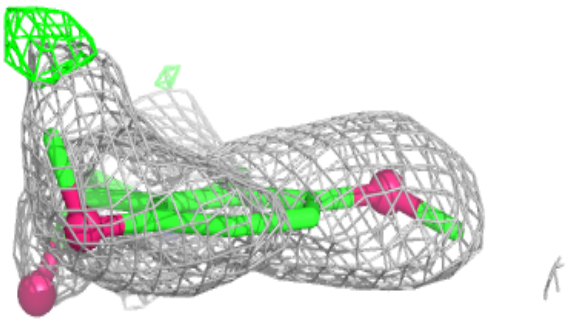
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PEG	C	303	7/7	0.82	0.11	33,36,48,54	0
3	PEG	B	302	7/7	0.82	0.14	41,50,54,59	0
3	PEG	B	303	7/7	0.83	0.13	36,40,51,53	0
3	PEG	C	304	7/7	0.83	0.11	37,48,55,61	0
2	EDO	D	302	4/4	0.83	0.14	38,47,56,66	0
3	PEG	C	305	7/7	0.89	0.08	38,48,57,60	0
3	PEG	D	303	7/7	0.90	0.07	34,41,51,61	0
2	EDO	A	301	4/4	0.91	0.11	34,40,45,46	0
6	DMS	D	301	4/4	0.92	0.14	37,39,50,58	0

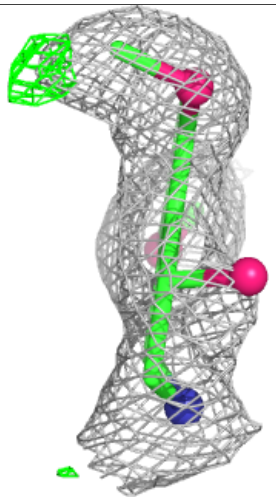
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1KPN 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)







6.5 Other polymers (i)

There are no such residues in this entry.