



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 06:11 AM UTC

PDB ID : 8FMH / pdb_00008fmh
Title : Structure of CBASS Cap5 from *Pseudomonas syringae* as an activated tetramer with the cyclic dinucleotide 3'2'-c-dGAMP ligand (2 tetramers in the AU)
Authors : Rechkoblit, O.; Kreitler, D.F.; Aggarwal, A.K.
Deposited on : 2022-12-23
Resolution : 1.87 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

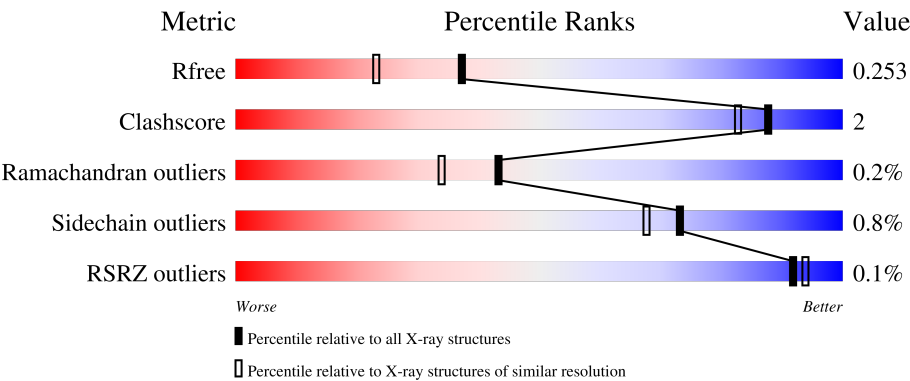
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	388	91%5%
1	B	388	84%7%9%
1	C	388	91%6%
1	D	388	89%8%

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Mol	Chain	Length	Quality of chain
1	E	388	88% 6% 5%
1	F	388	86% 9%
1	G	388	90% 5% 5%
1	H	388	85% 6% 9%

2 Entry composition

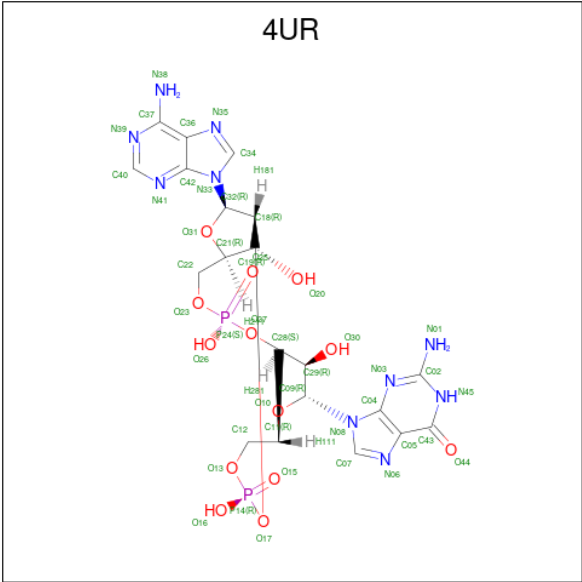
There are 8 unique types of molecules in this entry. The entry contains 44977 atoms, of which 21583 are hydrogens and 0 are deuteriums.

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 SAVED domain-containing protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	369	Total	C	H	N	O	S	0	0	0
			5610	1792	2768	509	531	10			
1	B	352	Total	C	H	N	O	S	0	0	0
			5331	1709	2636	473	503	10			
1	C	366	Total	C	H	N	O	S	0	0	0
			5517	1765	2721	502	519	10			
1	D	357	Total	C	H	N	O	S	0	0	0
			5427	1738	2683	485	511	10			
1	E	367	Total	C	H	N	O	S	0	0	0
			5568	1775	2749	504	530	10			
1	F	353	Total	C	H	N	O	S	0	0	0
			5226	1683	2562	466	506	9			
1	G	369	Total	C	H	N	O	S	0	0	0
			5555	1777	2736	509	523	10			
1	H	353	Total	C	H	N	O	S	0	0	0
			5158	1672	2520	460	496	10			

- Molecule 2 is 3'2'-cGAMP (CCD ID: 4UR) (formula: C₂₀H₂₄N₁₀O₁₃P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	P	0	0
			67	20	22	10	13	2		
2	B	1	Total	C	H	N	O	P	0	0
			67	20	22	10	13	2		
2	C	1	Total	C	H	N	O	P	0	0
			67	20	22	10	13	2		
2	D	1	Total	C	H	N	O	P	0	0
			67	20	22	10	13	2		
2	E	1	Total	C	H	N	O	P	0	0
			67	20	22	10	13	2		
2	F	1	Total	C	H	N	O	P	0	0
			67	20	22	10	13	2		
2	G	1	Total	C	H	N	O	P	0	0
			67	20	22	10	13	2		
2	H	1	Total	C	H	N	O	P	0	0
			67	20	22	10	13	2		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

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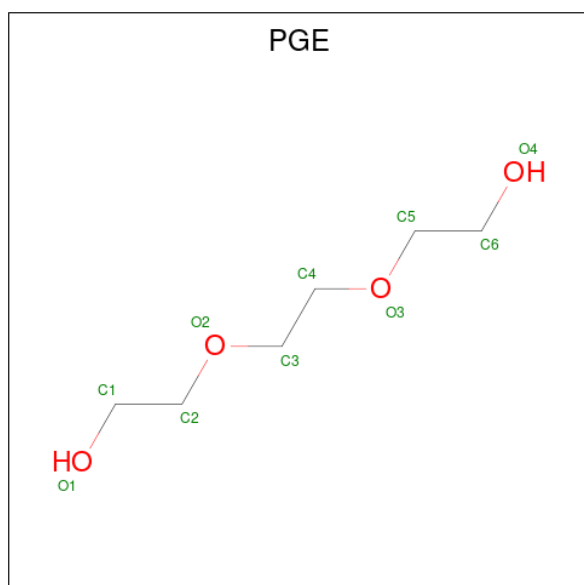
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	1	Total 1	Zn 1	0	0
3	F	1	Total 1	Zn 1	0	0
3	G	1	Total 1	Zn 1	0	0
3	H	1	Total 1	Zn 1	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

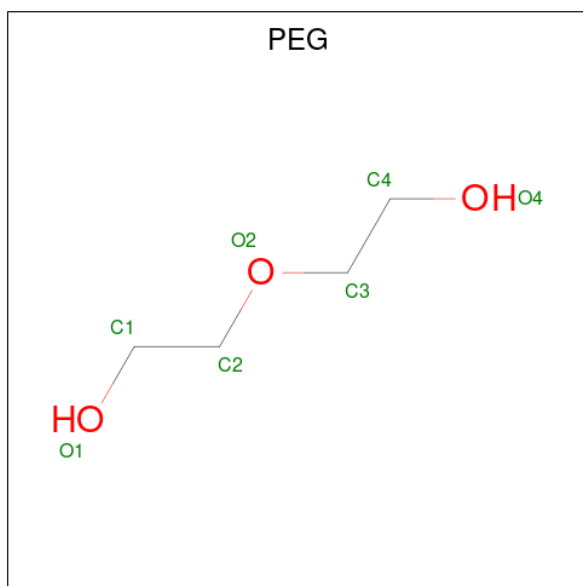
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	Mg 2	0	0
4	B	1	Total 1	Mg 1	0	0
4	C	2	Total 2	Mg 2	0	0
4	E	2	Total 2	Mg 2	0	0
4	F	1	Total 1	Mg 1	0	0
4	G	2	Total 2	Mg 2	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C₆H₁₄O₄).



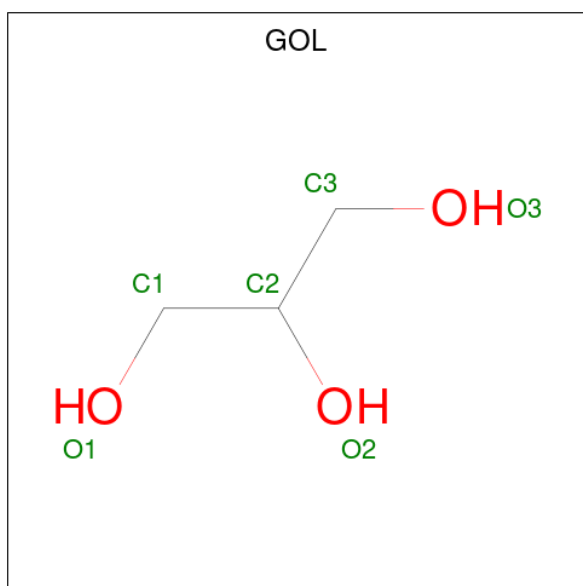
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	G	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	142	Total	O	0	0
			142	142		
8	B	124	Total	O	0	0
			124	124		
8	C	168	Total	O	0	0
			168	168		
8	D	125	Total	O	0	0
			125	125		
8	E	127	Total	O	0	0
			127	127		
8	F	76	Total	O	0	0
			76	76		
8	G	112	Total	O	0	0
			112	112		
8	H	102	Total	O	0	0
			102	102		

3 Residue-property plots

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

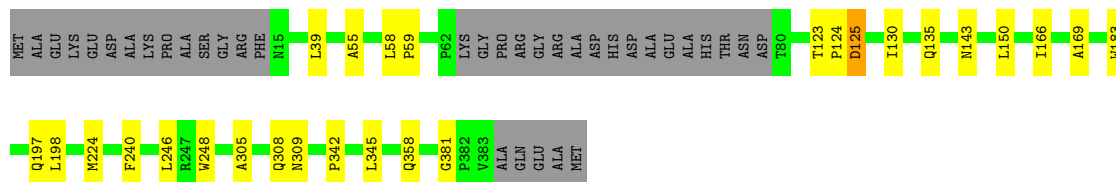
- Molecule 1: SAVED domain-containing protein

Chain A: 



- Molecule 1: SAVED domain-containing protein

Chain B: 



- Molecule 1: SAVED domain-containing protein

Chain C: 



- Molecule 1: SAVED domain-containing protein

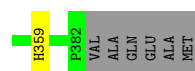
Chain D: 



- Molecule 1: SAVED domain-containing protein

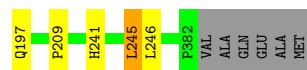
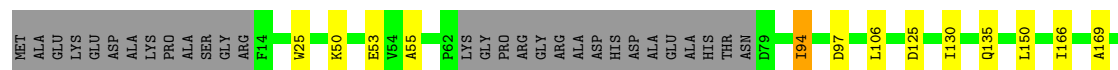
Chain E: 





- Molecule 1: SAVED domain-containing protein

Chain F: 86% 9%



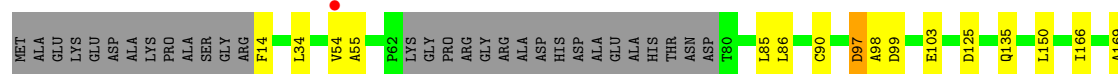
- Molecule 1: SAVED domain-containing protein

Chain G: 90% 5% 5%



- Molecule 1: SAVED domain-containing protein

Chain H: 85% 6% 9%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.97Å 295.68Å 84.05Å 90.00° 113.79° 90.00°	Depositor
Resolution (Å)	38.45 – 1.87 38.45 – 1.87	Depositor EDS
% Data completeness (in resolution range)	61.0 (38.45-1.87) 61.1 (38.45-1.87)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 1.87Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.210 , 0.253 0.210 , 0.253	Depositor DCC
R_{free} test set	7516 reflections (3.03%)	wwPDB-VP
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.120 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	44977	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% 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, PEG, ZN, GOL, 4UR, MG

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	0/2912	0.30	0/3972
1	B	0.15	0/2760	0.33	0/3768
1	C	0.15	0/2864	0.31	0/3908
1	D	0.14	0/2811	0.31	0/3836
1	E	0.16	0/2886	0.33	0/3937
1	F	0.14	0/2727	0.30	0/3729
1	G	0.13	0/2888	0.28	0/3940
1	H	0.15	0/2701	0.32	0/3696
All	All	0.15	0/22549	0.31	0/30786

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	2842	2768	2766	8	1
1	B	2695	2636	2632	15	0
1	C	2796	2721	2720	8	0
1	D	2744	2683	2681	6	0
1	E	2819	2749	2748	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2664	2562	2560	10	0
1	G	2819	2736	2735	11	0
1	H	2638	2520	2518	13	0
2	A	45	22	24	0	0
2	B	45	22	24	0	0
2	C	45	22	24	0	0
2	D	45	22	24	0	0
2	E	45	22	24	0	0
2	F	45	22	24	1	0
2	G	45	22	24	0	0
2	H	45	22	24	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
4	E	2	0	0	0	0
4	F	1	0	0	0	0
4	G	2	0	0	0	0
5	C	10	14	14	0	0
6	G	7	10	10	0	0
7	G	6	8	8	0	0
8	A	142	0	0	0	0
8	B	124	0	0	0	0
8	C	168	0	0	0	1
8	D	125	0	0	0	0
8	E	127	0	0	0	1
8	F	76	0	0	1	0
8	G	112	0	0	1	0
8	H	102	0	0	0	1
All	All	23394	21583	21584	87	2

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 2.

All (87) 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:E:66:ARG:HG3	1:E:98:ALA:HB1	1.76	0.66
1:E:66:ARG:CG	1:E:98:ALA:HB1	2.25	0.66
2:F:401:4UR:N41	8:F:503:HOH:O	2.31	0.62
1:G:289:LEU:HD21	1:G:336:HIS:CG	2.36	0.61
1:F:241:HIS:O	1:F:245:LEU:N	2.36	0.58
1:H:166:ILE:HD11	1:H:197:GLN:HG3	1.88	0.56
1:A:297:LEU:HD22	1:A:320:LEU:HD13	1.87	0.55
1:D:229:ILE:HD12	1:D:235:ARG:HD2	1.90	0.53
1:G:377:THR:OG1	1:G:378:LEU:N	2.41	0.53
1:F:94:ILE:HD12	1:F:106:LEU:HD11	1.90	0.53
1:H:135:GLN:O	1:H:169:ALA:HA	2.09	0.53
1:B:166:ILE:HD11	1:B:197:GLN:HG3	1.90	0.52
1:D:125:ASP:OD1	1:D:125:ASP:C	2.51	0.52
1:E:66:ARG:HD3	1:E:101:TYR:O	2.10	0.51
1:B:39:LEU:HD13	1:B:55:ALA:HB2	1.93	0.51
1:D:42:ASP:N	1:D:42:ASP:OD1	2.44	0.51
1:G:95:ASP:OD1	8:G:501:HOH:O	2.19	0.51
1:F:166:ILE:HD11	1:F:197:GLN:HG3	1.93	0.51
1:E:23:ILE:HG21	1:E:80:THR:HG22	1.92	0.50
1:A:223:MET:HE1	1:A:337:VAL:HG11	1.93	0.50
1:F:50:LYS:O	1:F:53:GLU:N	2.41	0.50
1:F:125:ASP:OD1	1:F:125:ASP:C	2.57	0.48
1:B:143:ASN:O	1:B:143:ASN:ND2	2.46	0.48
1:B:305:ALA:O	1:B:308:GLN:NE2	2.44	0.48
1:D:166:ILE:HD11	1:D:197:GLN:HG3	1.94	0.48
1:A:223:MET:HE3	1:A:349:PHE:CD1	2.48	0.47
1:G:289:LEU:HB3	1:G:292:ALA:HB2	1.96	0.47
1:E:66:ARG:HG2	1:E:98:ALA:HB1	1.96	0.47
1:B:358:GLN:HG2	1:B:381:GLY:HA2	1.97	0.47
1:G:159:LEU:HD21	1:G:236:LEU:HD22	1.97	0.47
1:E:333:ASP:HB3	1:E:334:PRO:HD2	1.96	0.46
1:A:88:PRO:HB2	1:C:88:PRO:HB2	1.97	0.46
1:F:130:ILE:HD11	1:F:209:PRO:HG2	1.97	0.46
1:G:354:THR:HG23	1:G:355:THR:N	2.31	0.46
1:H:166:ILE:HG21	1:H:193:GLU:HG2	1.98	0.46
1:C:354:THR:HG23	1:C:355:THR:N	2.30	0.46
1:E:88:PRO:HB2	1:G:88:PRO:HB2	1.98	0.46
1:B:240:PHE:HA	1:B:246:LEU:HD23	1.98	0.45
1:E:110:HIS:NE2	1:E:114:LEU:HD11	2.32	0.45
1:H:34:LEU:HD12	1:H:90:CYS:HB3	1.97	0.45
1:E:201:ARG:NH2	1:H:196:GLN:OE1	2.50	0.45
1:H:55:ALA:HB3	1:H:85:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:TRP:CE3	1:B:224:MET:HG3	2.52	0.44
1:E:65:PRO:CB	1:E:98:ALA:HB2	2.47	0.44
1:D:241:HIS:O	1:D:245:LEU:N	2.49	0.44
1:E:200:ARG:HG3	1:H:192:TYR:HB2	1.99	0.44
1:H:97:ASP:O	1:H:98:ALA:C	2.60	0.44
1:C:25:TRP:CZ2	1:C:50:LYS:CG	3.01	0.44
1:A:17:ASN:HD21	1:A:19:GLU:HB3	1.83	0.43
1:B:150:LEU:N	1:B:246:LEU:HD12	2.33	0.43
1:F:150:LEU:N	1:F:246:LEU:HD12	2.33	0.43
1:B:135:GLN:O	1:B:169:ALA:HA	2.18	0.43
1:H:55:ALA:HB1	1:H:86:LEU:O	2.18	0.43
1:B:125:ASP:OD1	1:B:125:ASP:C	2.61	0.43
1:E:297:LEU:HD22	1:E:320:LEU:HD12	1.99	0.43
1:C:328:GLU:OE2	1:C:357:HIS:HB3	2.19	0.42
1:D:65:PRO:HD2	2:H:401:4UR:C02	2.50	0.42
1:E:320:LEU:HD23	1:E:324:LEU:HD11	2.01	0.42
1:E:73:ALA:O	1:E:74:GLU:C	2.61	0.42
1:G:226:GLY:O	1:G:230:GLY:N	2.53	0.42
1:A:377:THR:OG1	1:A:378:LEU:N	2.49	0.42
1:F:135:GLN:O	1:F:169:ALA:HA	2.20	0.42
1:G:279:GLN:NE2	1:G:296:GLU:OE2	2.48	0.42
1:H:150:LEU:HA	1:H:246:LEU:HD12	2.02	0.42
1:E:66:ARG:HD2	1:E:102:PRO:HA	2.01	0.42
1:E:74:GLU:O	1:E:75:ALA:C	2.62	0.42
1:B:58:LEU:HD12	1:B:59:PRO:HD2	2.03	0.41
1:E:94:ILE:HG13	1:E:95:ASP:N	2.35	0.41
1:B:342:PRO:HD2	1:B:345:LEU:HD22	2.02	0.41
1:C:377:THR:OG1	1:C:378:LEU:N	2.53	0.41
1:E:66:ARG:N	1:E:98:ALA:HB1	2.34	0.41
1:F:130:ILE:HD13	1:F:197:GLN:CB	2.49	0.41
1:A:33:GLU:OE1	1:A:110:HIS:ND1	2.46	0.41
1:B:248:TRP:CE3	1:B:309:ASN:HA	2.56	0.41
1:C:349:PHE:CD1	1:C:349:PHE:C	2.99	0.41
1:E:24:VAL:HG12	1:E:85:LEU:HB2	2.03	0.41
1:G:145:ILE:O	1:G:167:LYS:NZ	2.48	0.41
1:G:65:PRO:O	1:G:66:ARG:HB2	2.21	0.41
1:H:257:SER:O	1:H:300:PRO:HD3	2.21	0.41
1:B:130:ILE:HD12	1:B:198:LEU:HD23	2.02	0.40
1:C:351:ALA:O	1:C:354:THR:HG22	2.21	0.40
1:C:25:TRP:CZ2	1:C:50:LYS:HG2	2.55	0.40
1:F:25:TRP:CZ2	1:F:55:ALA:HB3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:14:PHE:HA	1:H:99:ASP:O	2.21	0.40
1:B:123:THR:N	1:B:124:PRO:CD	2.84	0.40
1:A:130:ILE:HB	1:A:211:LEU:HD23	2.03	0.40
1:E:200:ARG:CG	1:H:192:TYR:HB2	2.52	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASP:OD2	8:C:519:HOH:O[1_454]	1.58	0.62
8:E:614:HOH:O	8:H:598:HOH:O[1_454]	1.88	0.32

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	367/388 (95%)	350 (95%)	17 (5%)	0	100	100
1	B	348/388 (90%)	338 (97%)	10 (3%)	0	100	100
1	C	364/388 (94%)	353 (97%)	11 (3%)	0	100	100
1	D	353/388 (91%)	338 (96%)	15 (4%)	0	100	100
1	E	365/388 (94%)	348 (95%)	15 (4%)	2 (0%)	24	13
1	F	349/388 (90%)	329 (94%)	18 (5%)	2 (1%)	21	10
1	G	367/388 (95%)	353 (96%)	14 (4%)	0	100	100
1	H	349/388 (90%)	329 (94%)	18 (5%)	2 (1%)	21	10
All	All	2862/3104 (92%)	2738 (96%)	118 (4%)	6 (0%)	43	34

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	54	VAL
1	E	73	ALA
1	E	74	GLU
1	H	97	ASP
1	F	245	LEU
1	F	94	ILE

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	296/317 (93%)	293 (99%)	3 (1%)	68	60
1	B	282/317 (89%)	281 (100%)	1 (0%)	84	79
1	C	288/317 (91%)	287 (100%)	1 (0%)	86	82
1	D	288/317 (91%)	285 (99%)	3 (1%)	68	60
1	E	294/317 (93%)	289 (98%)	5 (2%)	53	40
1	F	275/317 (87%)	274 (100%)	1 (0%)	84	79
1	G	290/317 (92%)	288 (99%)	2 (1%)	76	69
1	H	266/317 (84%)	264 (99%)	2 (1%)	73	68
All	All	2279/2536 (90%)	2261 (99%)	18 (1%)	73	68

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	PHE
1	A	320	LEU
1	A	322	ILE
1	B	125	ASP
1	C	287	ASP
1	D	58	LEU
1	D	61	SER
1	D	372	ASP
1	E	23	ILE
1	E	77	THR

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Mol	Chain	Res	Type
1	E	218	ASP
1	E	320	LEU
1	E	359	HIS
1	F	97	ASP
1	G	348	GLU
1	G	379	GLN
1	H	103	GLU
1	H	125	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	184	GLN
1	A	185	ASN
1	A	197	GLN
1	A	308	GLN
1	A	314	HIS
1	A	321	GLN
1	A	356	GLN
1	B	104	ASN
1	B	197	GLN
1	B	308	GLN
1	B	370	ASN
1	C	56	HIS
1	C	71	HIS
1	C	137	GLN
1	C	185	ASN
1	D	138	HIS
1	D	376	GLN
1	E	184	GLN
1	E	185	ASN
1	E	321	GLN
1	E	356	GLN
1	F	137	GLN
1	F	251	GLN
1	F	359	HIS
1	F	376	GLN
1	G	71	HIS
1	G	164	GLN
1	G	185	ASN
1	G	326	GLN

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Mol	Chain	Res	Type
1	H	184	GLN
1	H	251	GLN
1	H	379	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](#)

Of 29 ligands modelled in this entry, 18 are monoatomic - leaving 11 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	GOL	G	403	-	5,5,5	0.84	0	5,5,5	1.07	0
2	4UR	A	401	-	51,51,51	0.36	0	76,80,80	0.48	0
5	PGE	C	402	-	9,9,9	0.33	0	8,8,8	0.35	0
2	4UR	B	401	-	51,51,51	0.35	0	76,80,80	0.57	0
2	4UR	E	401	-	51,51,51	0.36	0	76,80,80	0.49	0
2	4UR	C	401	-	51,51,51	0.36	0	76,80,80	0.52	0
2	4UR	G	401	-	51,51,51	0.36	0	76,80,80	0.48	0
2	4UR	D	401	-	51,51,51	0.36	0	76,80,80	0.49	0
2	4UR	F	401	-	51,51,51	0.36	0	76,80,80	0.50	0
2	4UR	H	401	-	51,51,51	0.36	0	76,80,80	0.50	0
6	PEG	G	402	-	6,6,6	0.09	0	5,5,5	0.16	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
7	GOL	G	403	-	-	0/4/4/4	-
2	4UR	A	401	-	-	3/30/62/62	0/6/7/7
5	PGE	C	402	-	-	5/7/7/7	-
2	4UR	B	401	-	-	3/30/62/62	0/6/7/7
2	4UR	E	401	-	-	3/30/62/62	0/6/7/7
2	4UR	C	401	-	-	3/30/62/62	0/6/7/7
2	4UR	G	401	-	-	3/30/62/62	0/6/7/7
2	4UR	D	401	-	-	3/30/62/62	0/6/7/7
2	4UR	F	401	-	-	4/30/62/62	0/6/7/7
2	4UR	H	401	-	-	3/30/62/62	0/6/7/7
6	PEG	G	402	-	-	3/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	4UR	C28-O27-P24-O26
2	B	401	4UR	C28-O27-P24-O26
2	G	401	4UR	C28-O27-P24-O26
2	H	401	4UR	C28-O27-P24-O26
6	G	402	PEG	O2-C3-C4-O4
5	C	402	PGE	O2-C3-C4-O3
5	C	402	PGE	O1-C1-C2-O2
5	C	402	PGE	O3-C5-C6-O4
5	C	402	PGE	C4-C3-O2-C2
5	C	402	PGE	C6-C5-O3-C4
2	H	401	4UR	C11-C12-O13-P14
2	C	401	4UR	C28-O27-P24-O26
2	D	401	4UR	C28-O27-P24-O26
2	E	401	4UR	C28-O27-P24-O26
2	F	401	4UR	C28-O27-P24-O26
2	C	401	4UR	C11-C12-O13-P14
6	G	402	PEG	C4-C3-O2-C2

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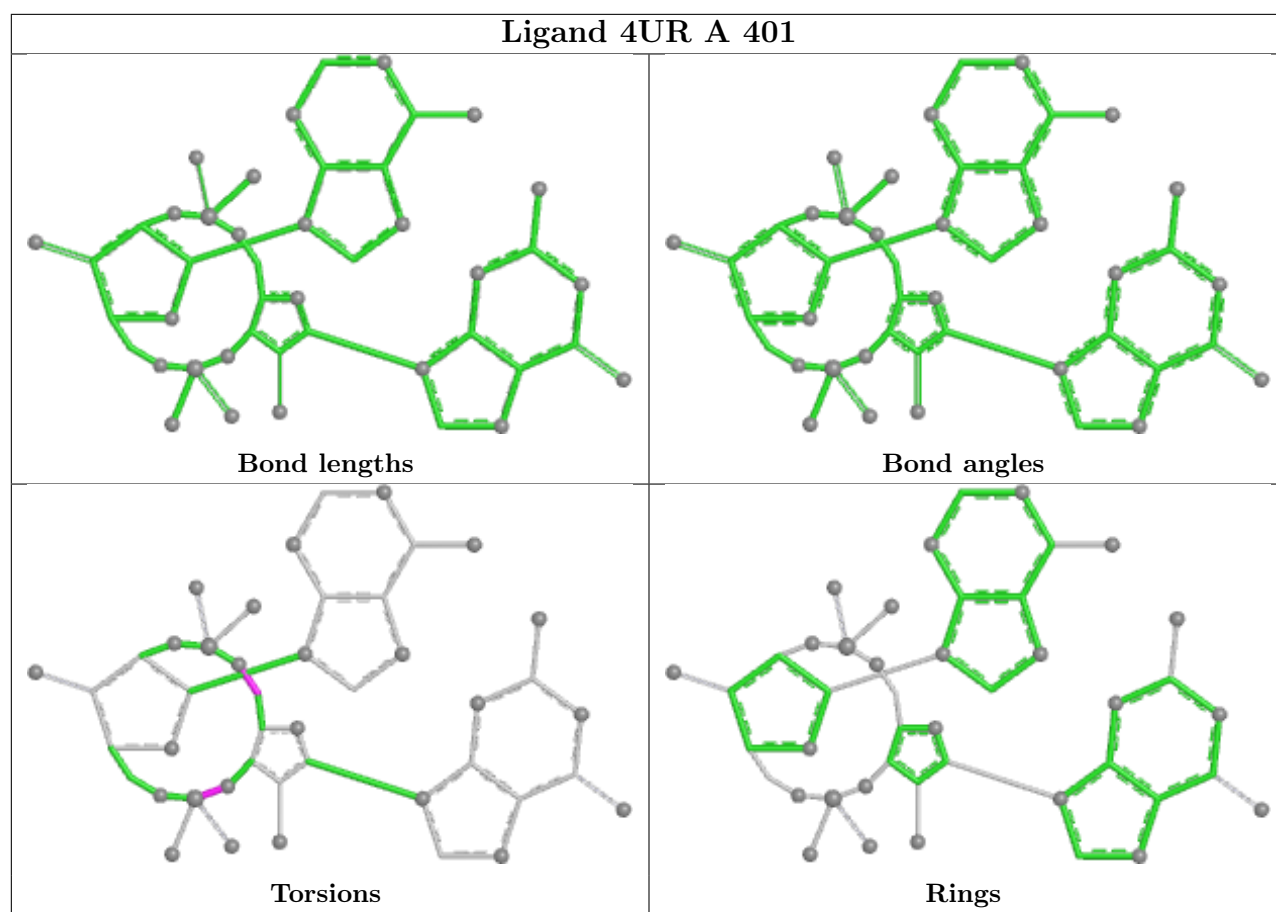
Mol	Chain	Res	Type	Atoms
2	A	401	4UR	C11-C12-O13-P14
2	B	401	4UR	C11-C12-O13-P14
2	D	401	4UR	C11-C12-O13-P14
2	E	401	4UR	C11-C12-O13-P14
2	F	401	4UR	C11-C12-O13-P14
2	G	401	4UR	C11-C12-O13-P14
6	G	402	PEG	O1-C1-C2-O2
2	A	401	4UR	C28-O27-P24-O25
2	B	401	4UR	C28-O27-P24-O25
2	C	401	4UR	C28-O27-P24-O25
2	D	401	4UR	C28-O27-P24-O25
2	E	401	4UR	C28-O27-P24-O25
2	F	401	4UR	C28-O27-P24-O25
2	G	401	4UR	C28-O27-P24-O25
2	H	401	4UR	C28-O27-P24-O25
2	F	401	4UR	O10-C11-C12-O13

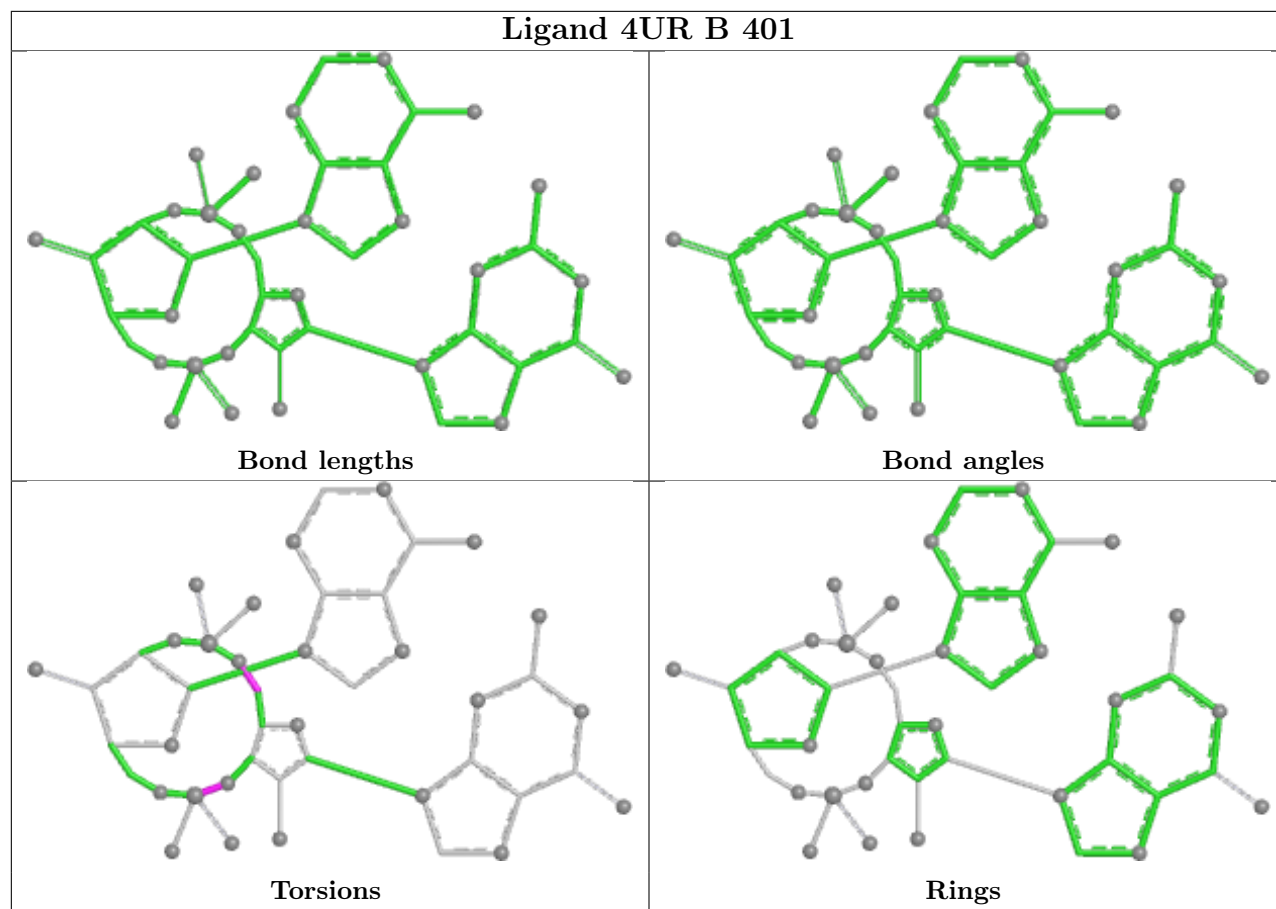
There are no ring outliers.

2 monomers are involved in 2 short contacts:

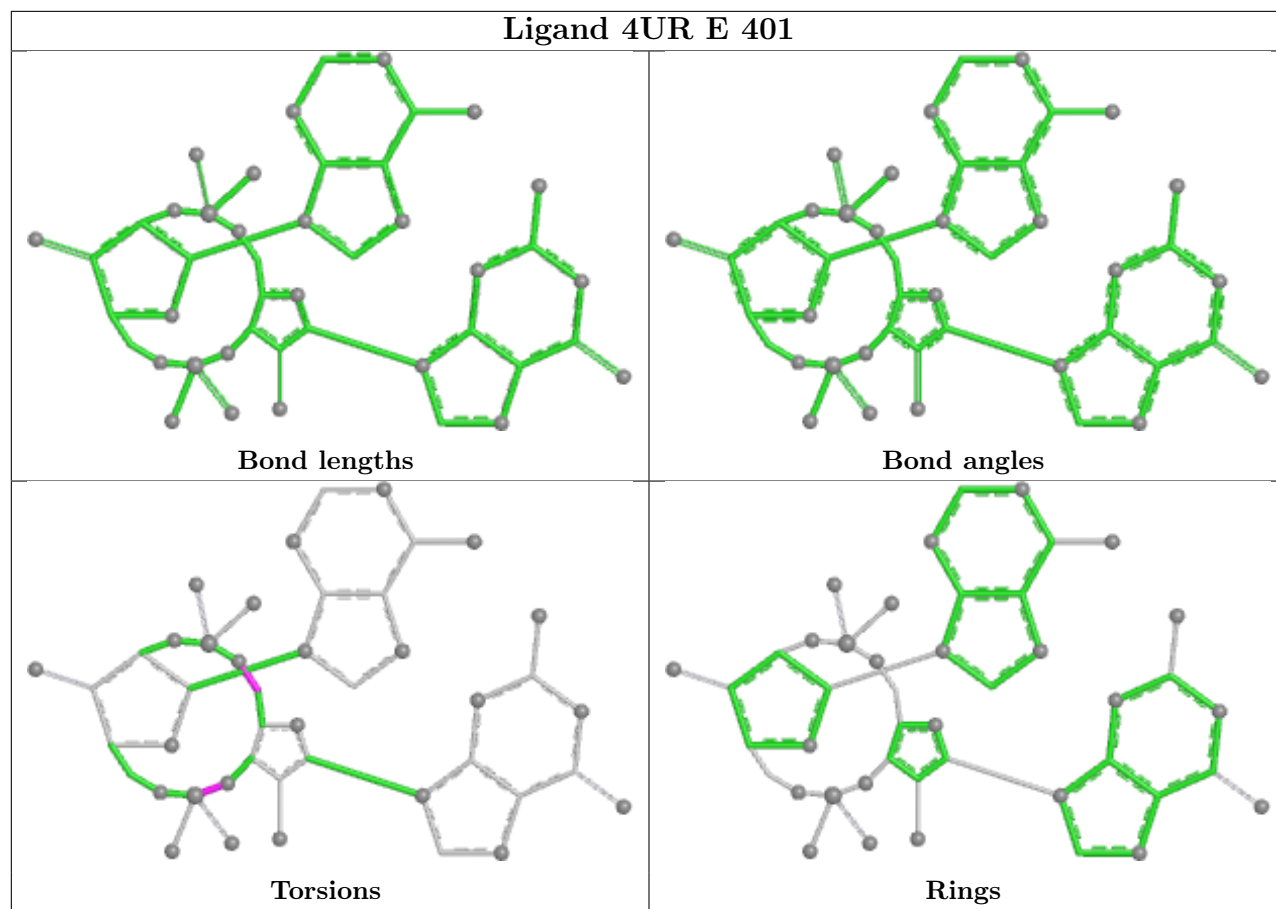
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	401	4UR	1	0
2	H	401	4UR	1	0

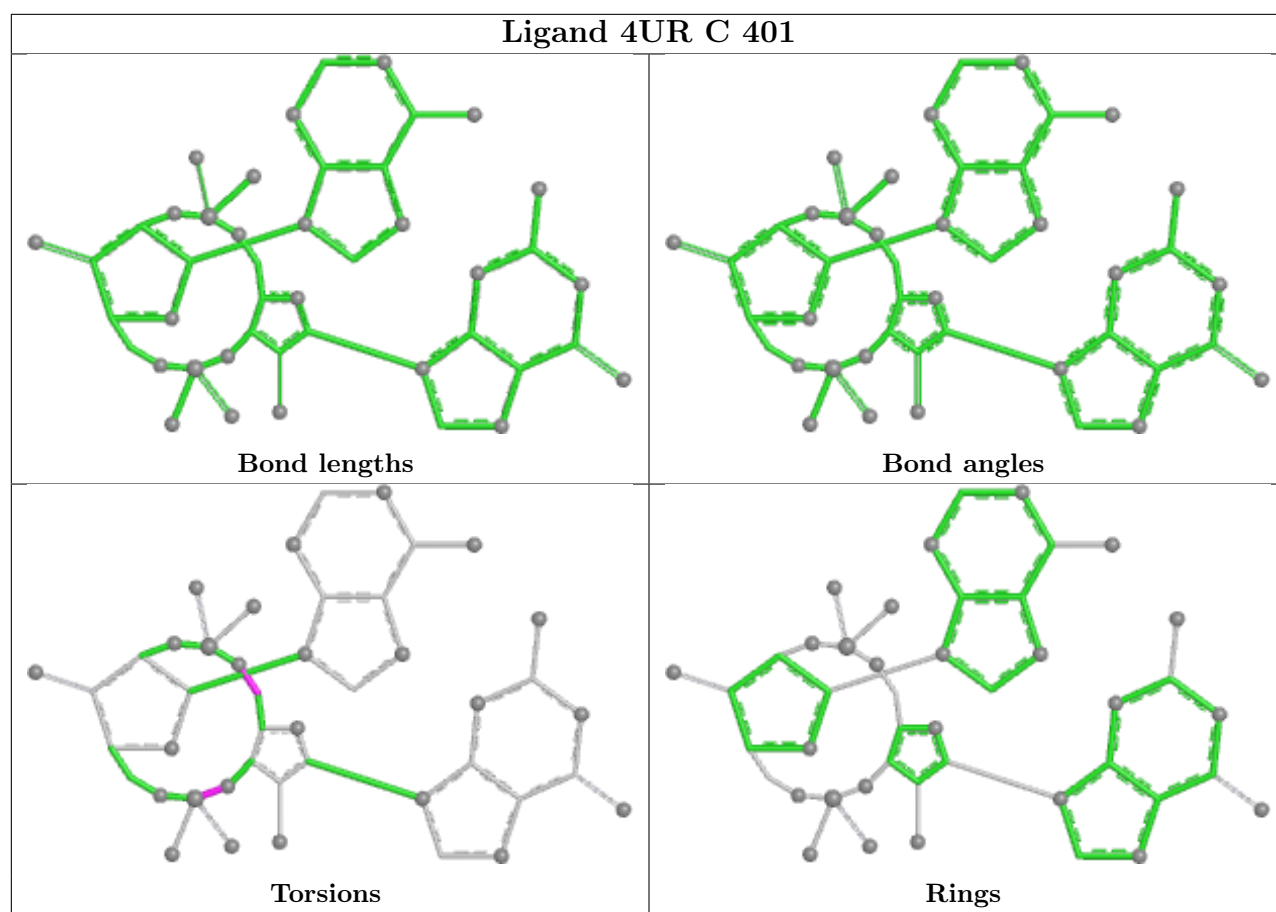
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

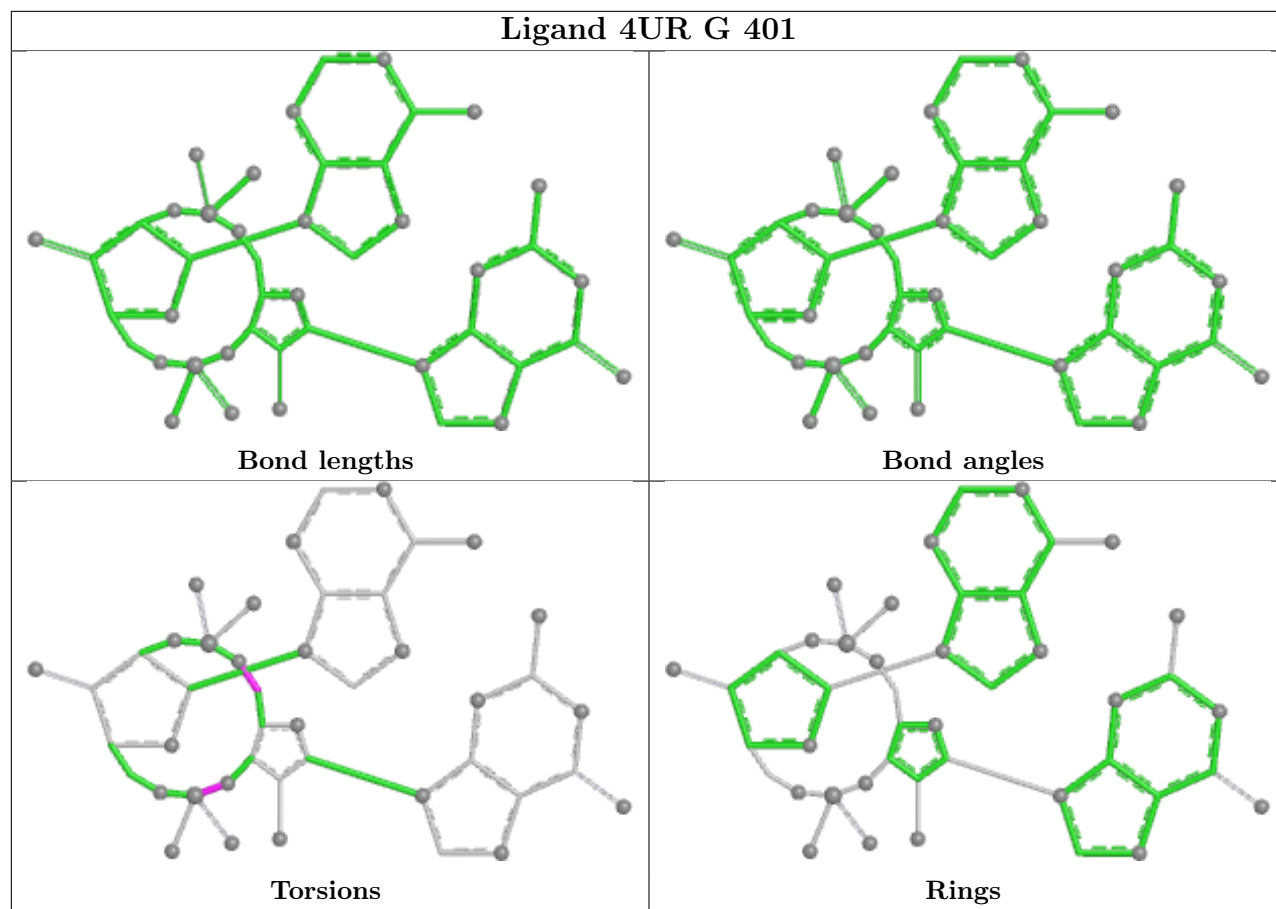


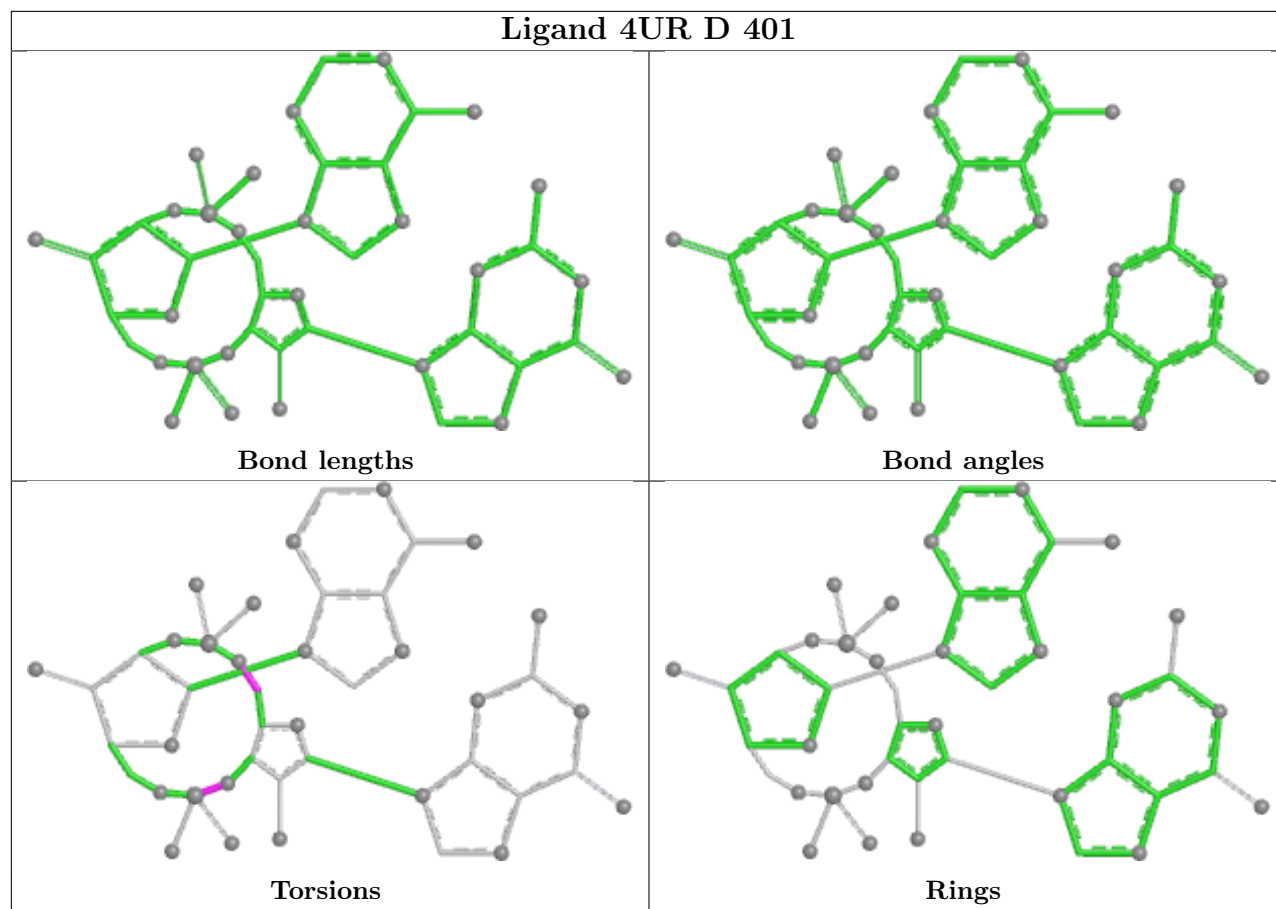


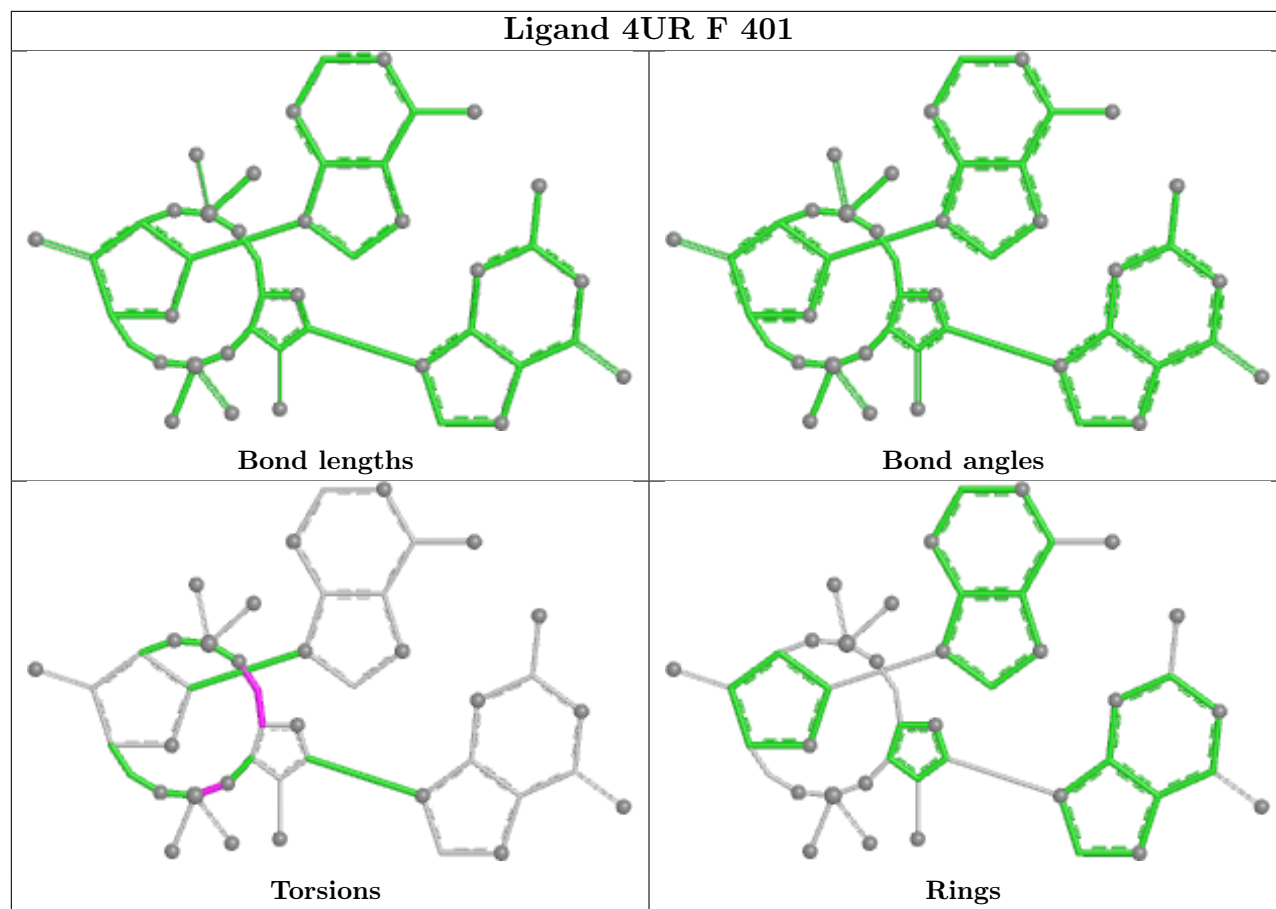
Ligand 4UR E 401

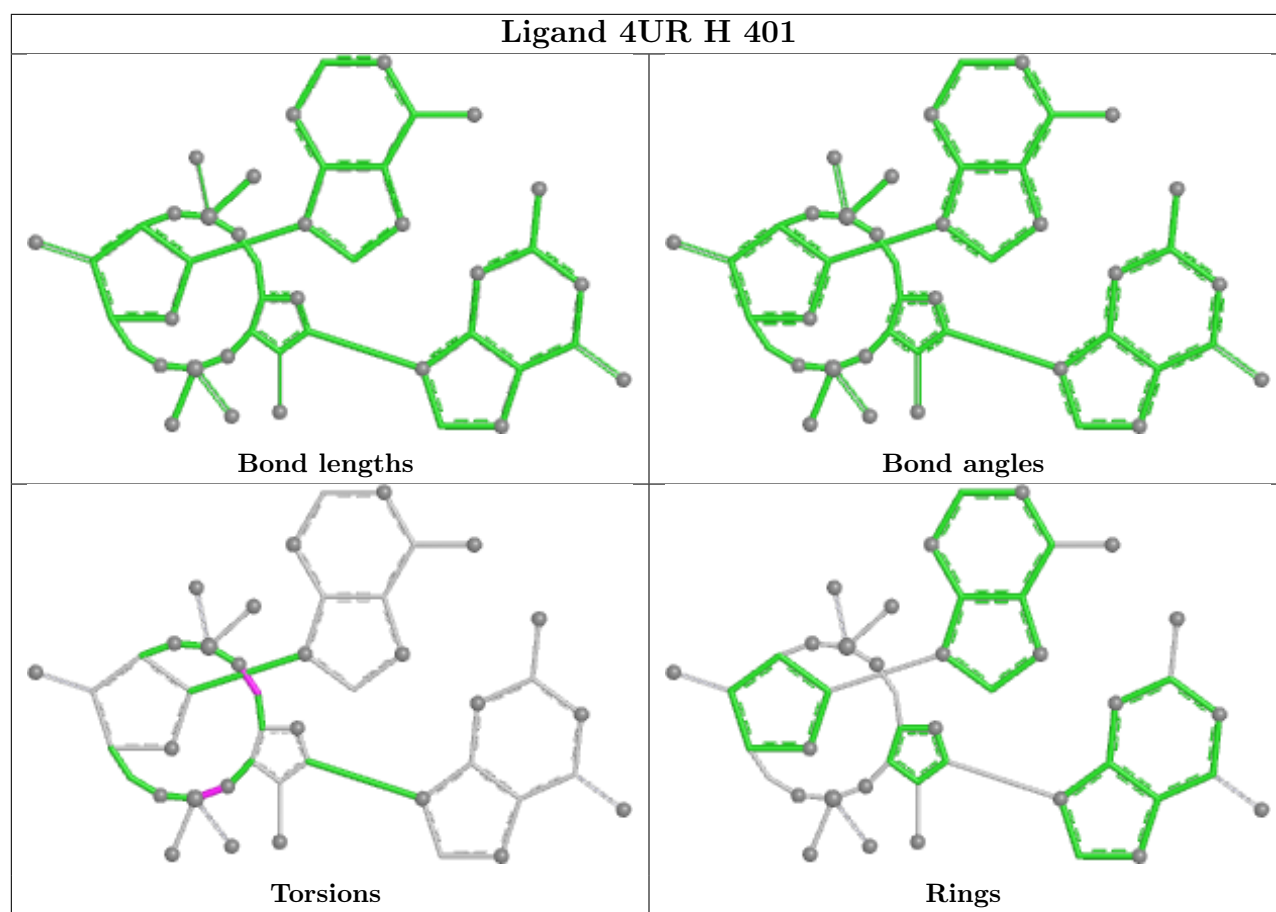












5.7 Other polymers [i](#)

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	369/388 (95%)	-1.23	0	100	100	30, 50, 91, 138	0
1	B	352/388 (90%)	-1.19	0	100	100	29, 50, 102, 124	0
1	C	366/388 (94%)	-1.23	0	100	100	30, 48, 89, 135	0
1	D	357/388 (92%)	-1.17	0	100	100	32, 54, 86, 113	0
1	E	367/388 (94%)	-1.13	1 (0%)	90	93	32, 51, 100, 144	0
1	F	353/388 (90%)	-0.90	0	100	100	39, 66, 103, 134	0
1	G	369/388 (95%)	-0.95	0	100	100	35, 64, 105, 134	0
1	H	353/388 (90%)	-0.98	1 (0%)	90	93	31, 52, 119, 167	0
All	All	2886/3104 (92%)	-1.10	2 (0%)	92	94	29, 54, 102, 167	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	54	VAL	2.8
1	E	75	ALA	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 ⓘ

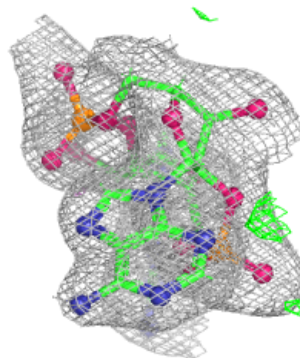
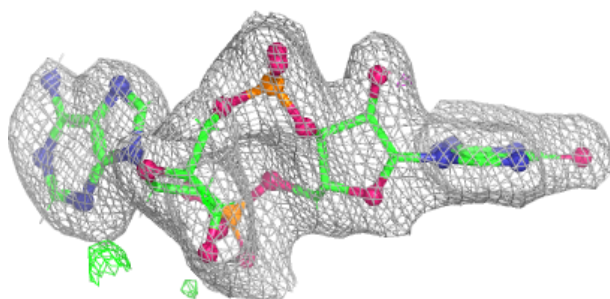
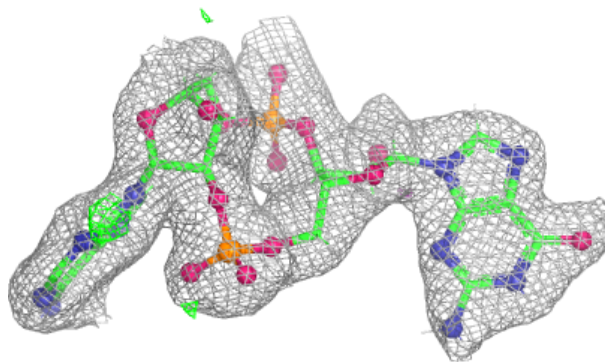
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MG	E	404	1/1	0.98	0.04	83,83,83,83	0
4	MG	F	403	1/1	0.98	0.05	100,100,100,100	0
5	PGE	C	402	10/10	0.98	0.05	55,72,79,81	0
4	MG	A	404	1/1	0.99	0.03	65,65,65,65	0
4	MG	B	403	1/1	0.99	0.04	93,93,93,93	0
4	MG	E	403	1/1	0.99	0.05	87,87,87,87	0
2	4UR	D	401	45/45	0.99	0.03	41,52,66,72	0
2	4UR	F	401	45/45	0.99	0.04	55,65,79,89	0
4	MG	G	405	1/1	0.99	0.03	60,60,60,60	0
2	4UR	H	401	45/45	0.99	0.03	32,45,60,62	0
6	PEG	G	402	7/7	0.99	0.05	48,59,71,71	0
7	GOL	G	403	6/6	0.99	0.03	51,62,72,74	0
3	ZN	E	402	1/1	1.00	0.01	52,52,52,52	0
3	ZN	F	402	1/1	1.00	0.03	73,73,73,73	0
3	ZN	G	404	1/1	1.00	0.01	50,50,50,50	0
3	ZN	H	402	1/1	1.00	0.03	101,101,101,101	0
4	MG	A	403	1/1	1.00	0.02	49,49,49,49	0
2	4UR	A	401	45/45	1.00	0.02	25,31,38,43	0
2	4UR	E	401	45/45	1.00	0.03	29,35,44,46	0
4	MG	C	404	1/1	1.00	0.04	53,53,53,53	0
4	MG	C	405	1/1	1.00	0.02	60,60,60,60	0
2	4UR	B	401	45/45	1.00	0.02	33,46,58,67	0
2	4UR	G	401	45/45	1.00	0.02	33,42,53,55	0
2	4UR	C	401	45/45	1.00	0.02	26,32,38,41	0
3	ZN	A	402	1/1	1.00	0.01	37,37,37,37	0
4	MG	G	406	1/1	1.00	0.01	60,60,60,60	0
3	ZN	B	402	1/1	1.00	0.01	71,71,71,71	0
3	ZN	C	403	1/1	1.00	0.01	42,42,42,42	0
3	ZN	D	402	1/1	1.00	0.02	56,56,56,56	0

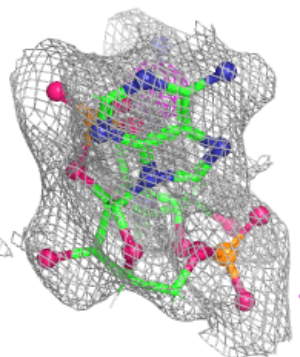
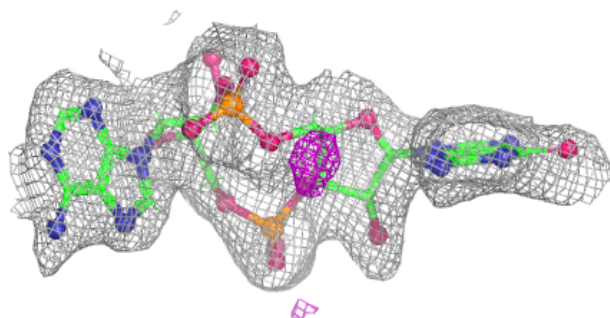
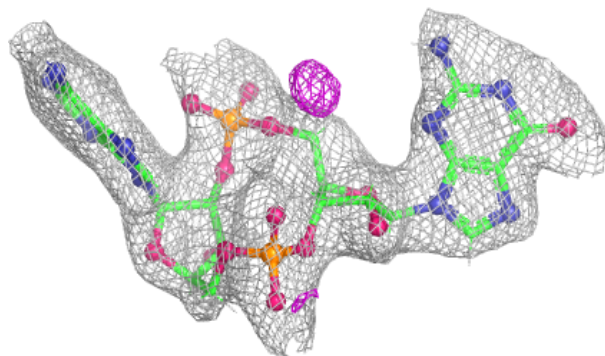
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 4UR D 401:

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

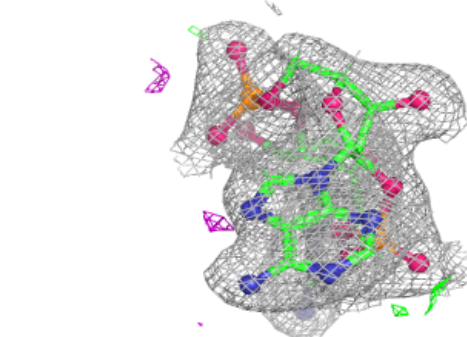
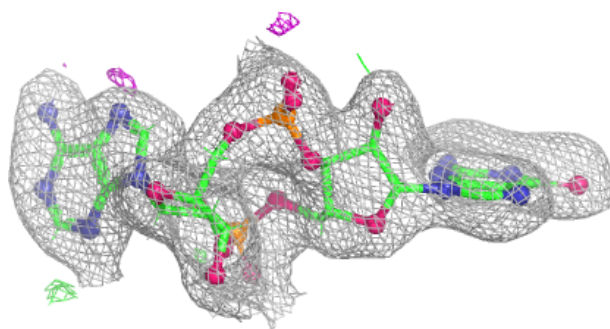
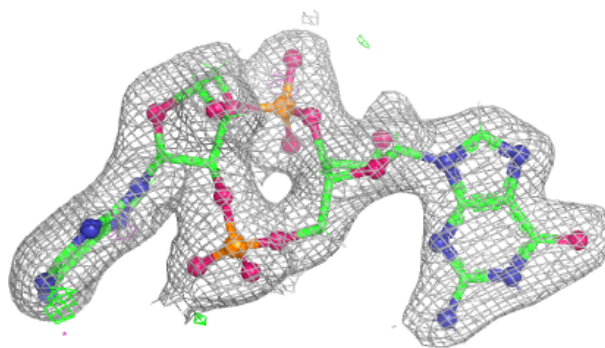
**Electron density around 4UR F 401:**

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

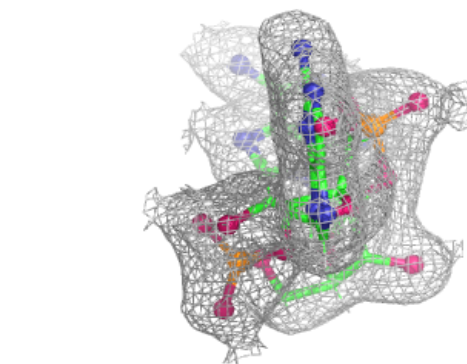
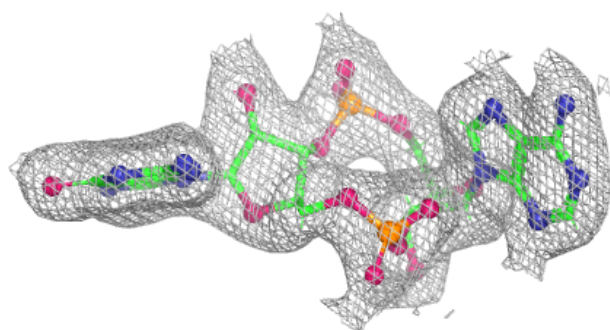
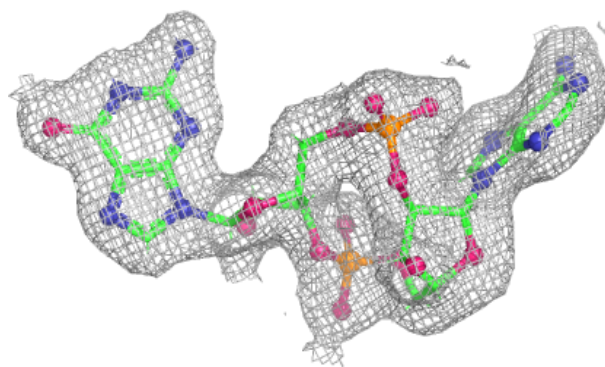


Electron density around 4UR H 401:

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

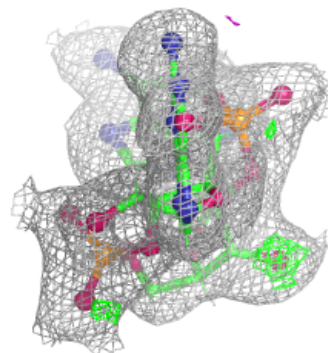
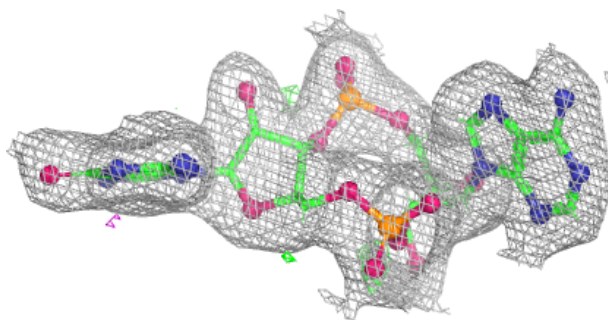
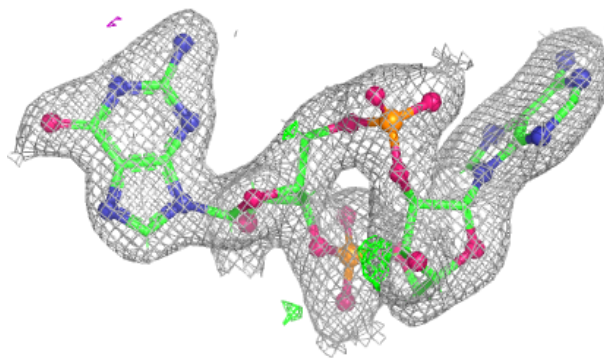
**Electron density around 4UR A 401:**

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

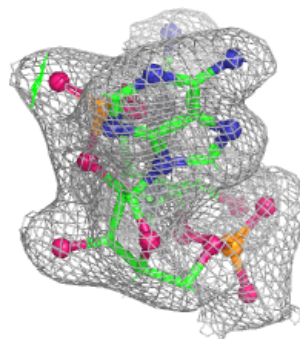
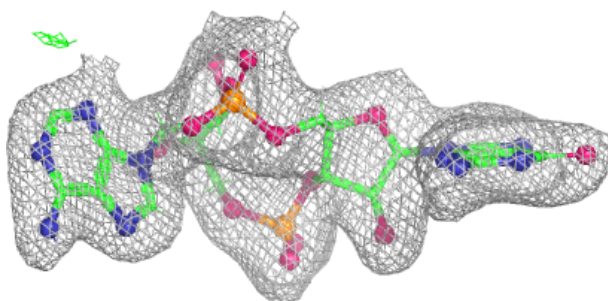
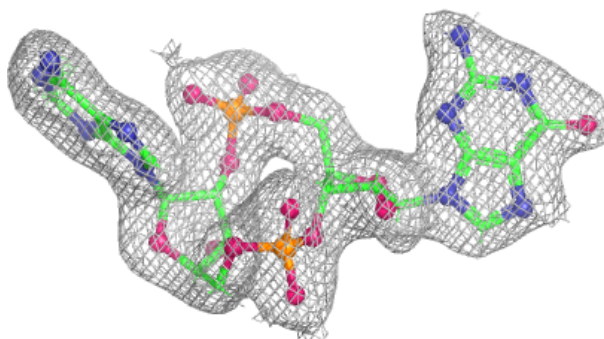


Electron density around 4UR E 401:

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

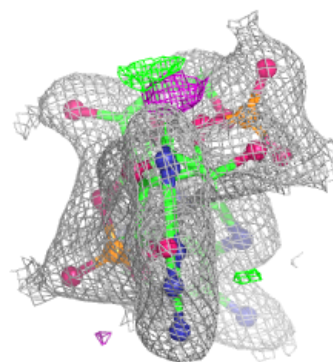
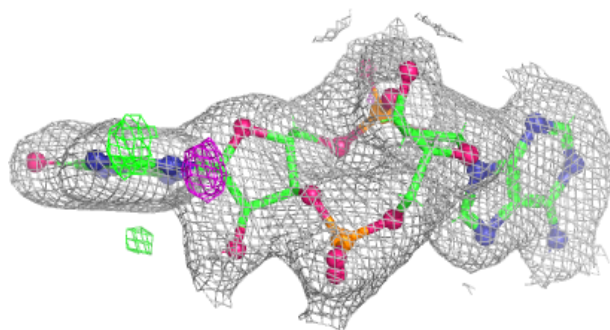
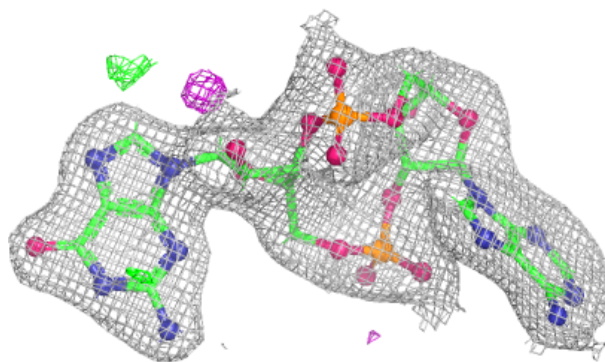
**Electron density around 4UR B 401:**

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

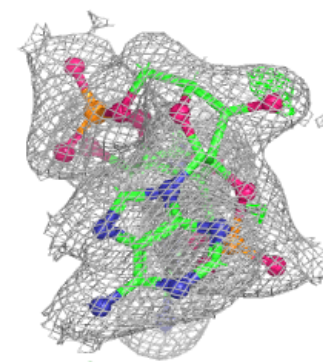
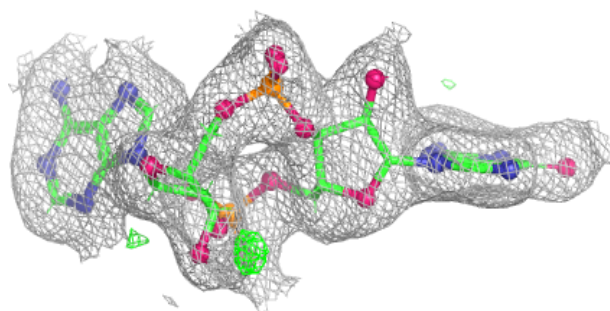
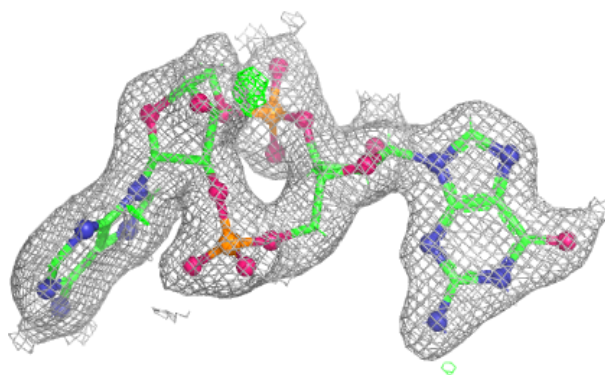


Electron density around 4UR G 401:

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

**Electron density around 4UR C 401:**

$2mF_o-DF_c$ (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.