



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 10:14 AM UTC

PDB ID : 8BZ7 / pdb_00008bz7
Title : Crystal structure of the *L. monocytogenes* RmlT in complex with TDP-rhamnose
Authors : Cereija, T.B.; Morais-Cabral, J.H.
Deposited on : 2022-12-14
Resolution : 2.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

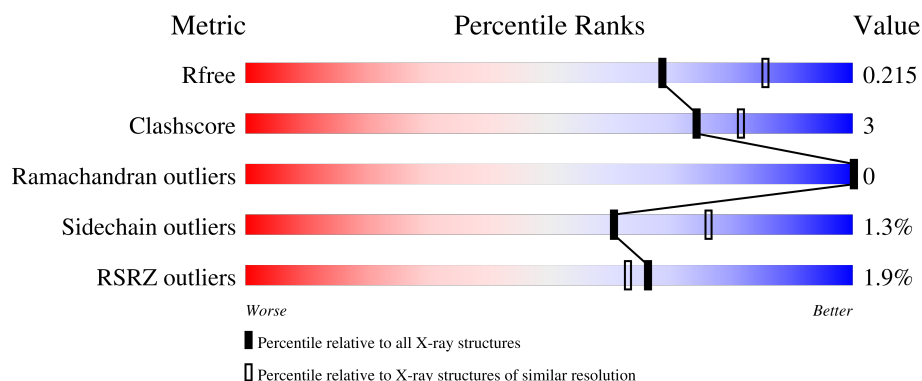
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	624	2% 86% 10% .
1	B	624	2% 89% 7% .
1	C	624	2% 91% 6% .
1	D	624	2% 88% 8% . .
1	E	624	2% 87% 8% .

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Mol	Chain	Length	Quality of chain
1	F	624	3% 86% 10%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 30744 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

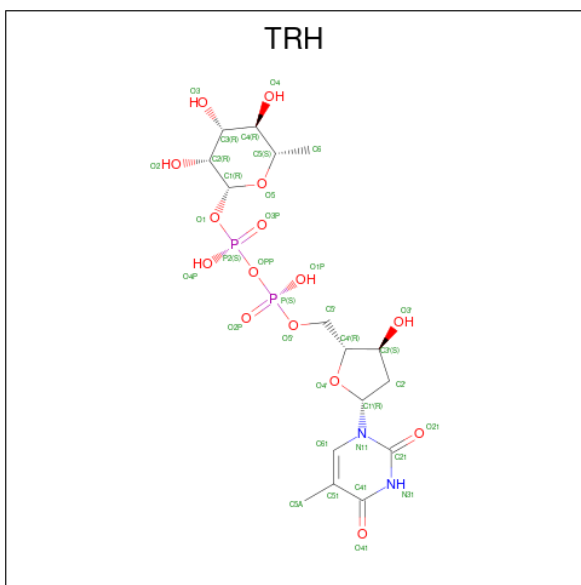
- Molecule 1 is a protein called Glycosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	601	Total	C	N	O	S	0	2	0
			4895	3125	812	946	12			
1	B	601	Total	C	N	O	S	0	1	0
			4877	3109	811	945	12			
1	C	600	Total	C	N	O	S	0	1	0
			4873	3107	810	944	12			
1	D	599	Total	C	N	O	S	0	1	0
			4869	3106	809	942	12			
1	E	598	Total	C	N	O	S	0	1	0
			4860	3100	807	941	12			
1	F	598	Total	C	N	O	S	0	1	0
			4860	3100	807	941	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP A0A401AAP7
B	0	GLY	-	expression tag	UNP A0A401AAP7
C	0	GLY	-	expression tag	UNP A0A401AAP7
D	0	GLY	-	expression tag	UNP A0A401AAP7
E	0	GLY	-	expression tag	UNP A0A401AAP7
F	0	GLY	-	expression tag	UNP A0A401AAP7

- Molecule 2 is 2'-DEOXY-THYMIDINE-BETA-L-RHAMNOSE (CCD ID: TRH) (formula: $C_{16}H_{26}N_2O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).

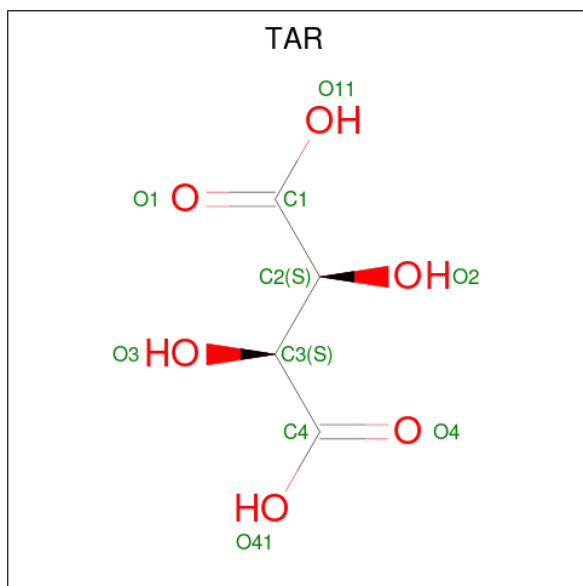


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 35	C 16	N 2	O 15	P 2	0	0
2	B	1	Total 35	C 16	N 2	O 15	P 2	0	0
2	C	1	Total 35	C 16	N 2	O 15	P 2	0	0
2	D	1	Total 35	C 16	N 2	O 15	P 2	0	0
2	E	1	Total 35	C 16	N 2	O 15	P 2	0	0
2	F	1	Total 35	C 16	N 2	O 15	P 2	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

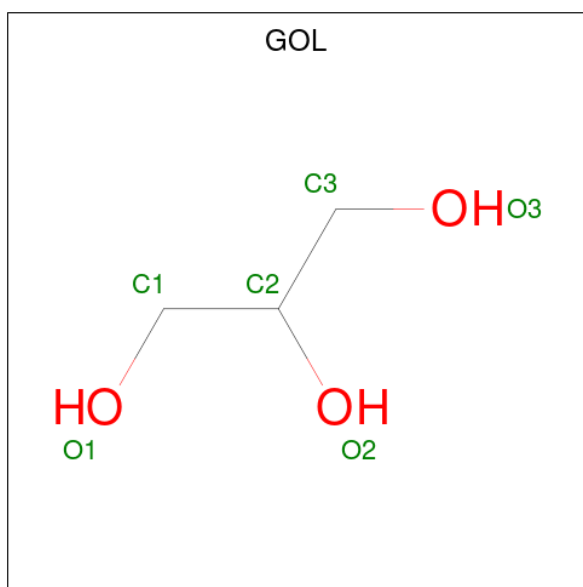
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Mg 1 1	0	0
3	B	2	Total Mg 2 2	0	0
3	C	1	Total Mg 1 1	0	0
3	D	2	Total Mg 2 2	0	0
3	E	2	Total Mg 2 2	0	0
3	F	1	Total Mg 1 1	0	0

- Molecule 4 is D(-)-TARTARIC ACID (CCD ID: TAR) (formula: $C_4H_6O_6$).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	D	1	Total	C	O	0	0
			6	3	3		
5	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Cl	0	0
			1	1		
6	F	1	Total	Cl	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	244	Total	O	0	0
			244	244		

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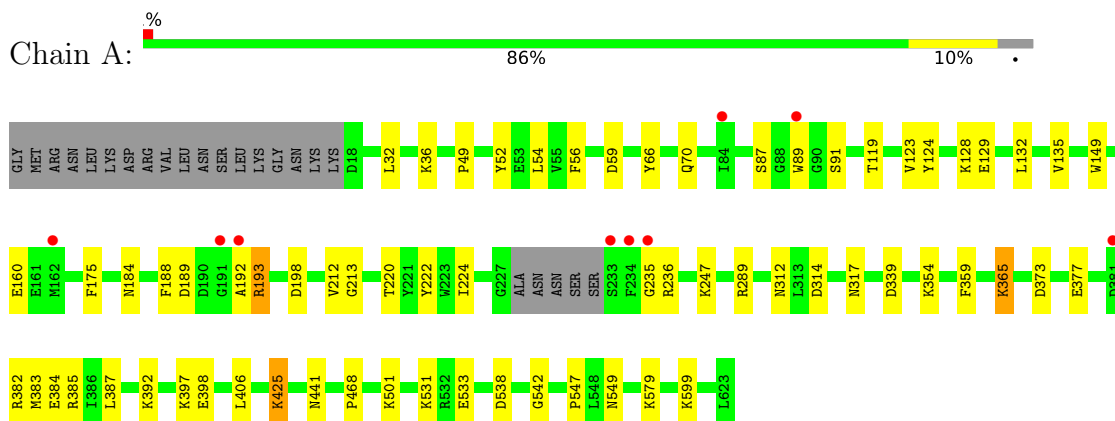
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	238	Total 238	O 238	0	0
7	C	201	Total 201	O 201	0	0
7	D	204	Total 204	O 204	0	0
7	E	180	Total 180	O 180	0	0
7	F	126	Total 126	O 126	0	0

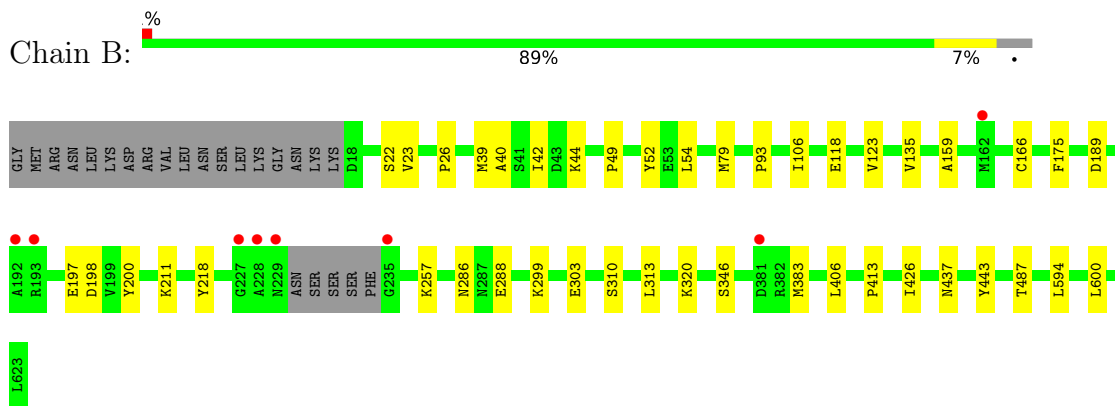
3 Residue-property plots [i](#)

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.

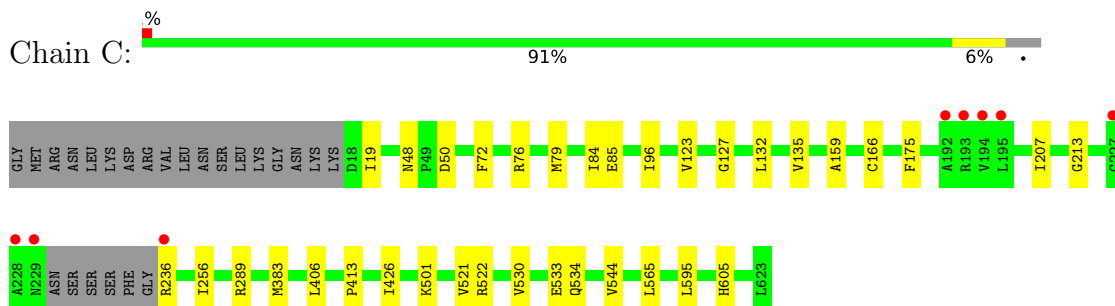
• Molecule 1: Glycosyltransferase



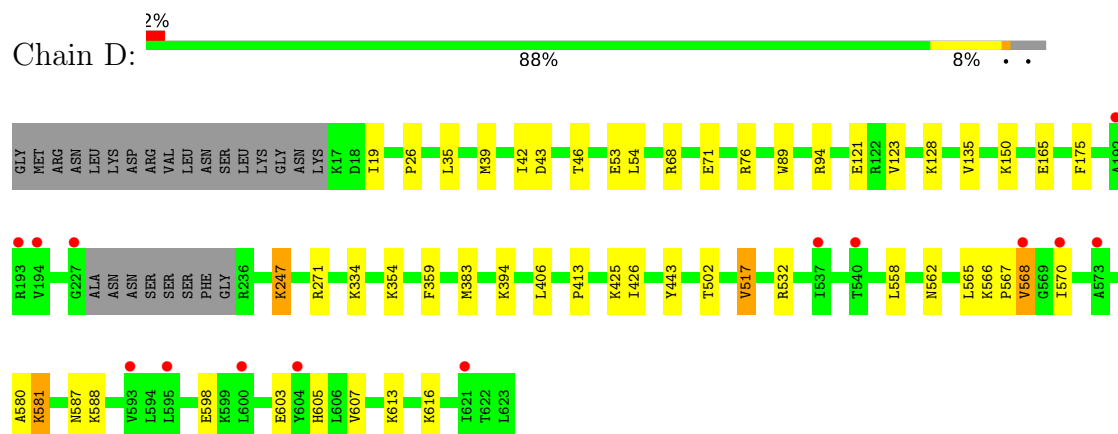
• Molecule 1: Glycosyltransferase



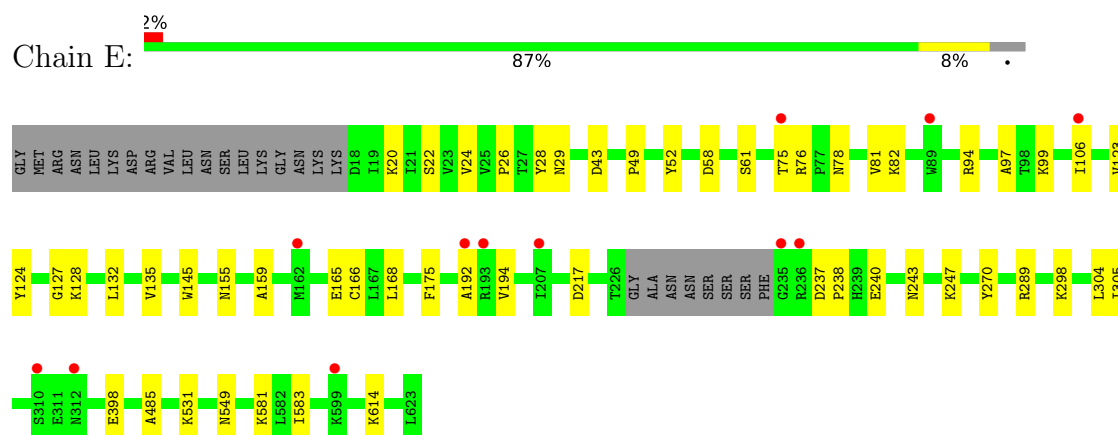
• Molecule 1: Glycosyltransferase



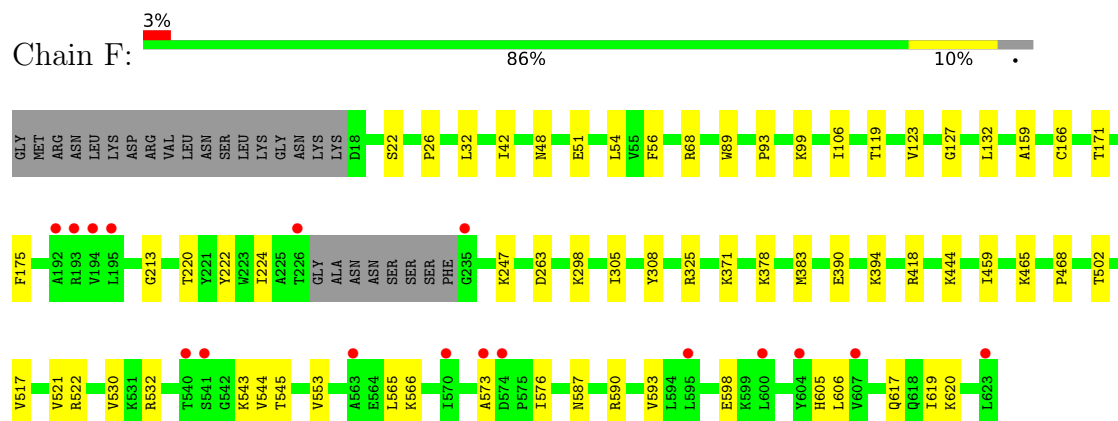
- Molecule 1: Glycosyltransferase



- Molecule 1: Glycosyltransferase



- Molecule 1: Glycosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	86.99Å 291.26Å 92.39Å 90.00° 100.38° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (50.00-2.20) 99.7 (50.00-2.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.187 , 0.215 0.187 , 0.215	Depositor DCC
R_{free} test set	11129 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	30744	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% 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: TAR, TRH, MG, GOL, CL

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	0.47	1/4997 (0.0%)	0.60	0/6748
1	B	0.19	0/4976	0.35	0/6719
1	C	0.17	0/4972	0.34	0/6714
1	D	0.19	0/4968	0.35	0/6707
1	E	0.19	0/4959	0.35	0/6696
1	F	0.17	0/4959	0.34	0/6696
All	All	0.25	1/29831 (0.0%)	0.40	0/40280

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	468	PRO	C-O	-5.71	1.18	1.23

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	4895	0	4828	49	0
1	B	4877	0	4816	23	0
1	C	4873	0	4813	19	0
1	D	4869	0	4815	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4860	0	4802	27	0
1	F	4860	0	4802	33	0
2	A	35	0	24	2	0
2	B	35	0	24	0	0
2	C	35	0	24	0	0
2	D	35	0	24	2	0
2	E	35	0	24	0	0
2	F	35	0	24	1	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	1	0	0	0	0
4	A	10	0	4	1	0
4	B	10	0	4	0	0
4	C	10	0	4	0	0
4	D	10	0	4	0	0
4	E	10	0	4	1	0
4	F	10	0	4	0	0
5	A	12	0	16	1	0
5	B	12	0	16	0	0
5	D	6	0	8	0	0
5	E	6	0	8	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	244	0	0	1	0
7	B	238	0	0	1	0
7	C	201	0	0	1	0
7	D	204	0	0	3	0
7	E	180	0	0	1	0
7	F	126	0	0	1	0
All	All	30744	0	29092	184	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 3.

All (184) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89[A]:TRP:CZ3	1:A:193:ARG:HG2	2.08	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89[A]:TRP:CE3	1:A:193:ARG:HG2	2.13	0.84
1:A:189:ASP:OD2	1:A:192:ALA:HB3	1.80	0.81
1:F:48:ASN:HB3	1:F:51:GLU:HG3	1.68	0.75
1:A:382:ARG:NE	1:A:384:GLU:OE2	2.30	0.63
1:D:383:MET:HG3	1:D:406:LEU:HD11	1.81	0.63
1:A:312:ASN:HB2	7:A:999:HOH:O	1.98	0.62
1:F:26:PRO:HB3	1:F:93:PRO:HB2	1.81	0.62
1:F:444:LYS:NZ	7:F:804:HOH:O	2.34	0.60
1:C:236:ARG:O	1:C:289:ARG:NH2	2.30	0.60
1:B:383:MET:HG3	1:B:406:LEU:HD11	1.83	0.59
1:D:413:PRO:HG2	1:D:426:ILE:HB	1.83	0.58
1:A:365:LYS:HE3	1:A:373:ASP:OD1	2.03	0.58
1:D:42:ILE:HG21	1:D:54:LEU:HD11	1.85	0.58
1:E:26:PRO:HG3	1:E:94:ARG:HG3	1.86	0.58
1:A:189:ASP:OD2	1:A:192:ALA:CB	2.50	0.57
1:B:26:PRO:HB3	1:B:93:PRO:HB2	1.85	0.57
1:E:123:VAL:HG13	1:E:135:VAL:HG11	1.85	0.56
1:B:299:LYS:NZ	1:B:303:GLU:OE1	2.31	0.56
1:A:89[A]:TRP:CE3	1:A:193:ARG:CG	2.87	0.56
1:C:383:MET:HG3	1:C:406:LEU:HD11	1.87	0.56
1:A:89[A]:TRP:CZ3	1:A:193:ARG:CG	2.87	0.56
1:C:521:VAL:HG23	1:C:522:ARG:HG3	1.88	0.56
1:E:127:GLY:HA2	1:E:132:LEU:HD12	1.88	0.56
1:F:123:VAL:HG11	1:F:175:PHE:CG	2.42	0.55
1:C:533:GLU:HG3	1:C:534:GLN:HG3	1.87	0.55
1:A:123:VAL:HG13	1:A:135:VAL:HG11	1.89	0.55
1:A:377:GLU:HG3	1:A:441:ASN:ND2	2.22	0.54
1:A:382:ARG:NH1	1:A:384:GLU:OE2	2.39	0.54
1:A:533:GLU:H	1:A:533:GLU:CD	2.15	0.54
1:D:502:THR:O	1:D:517:VAL:HA	2.08	0.54
1:A:89[B]:TRP:CZ2	2:A:701:TRH:HC63	2.42	0.54
1:D:562:ASN:HA	1:D:580:ALA:H	1.72	0.53
1:D:425:LYS:NZ	7:D:808:HOH:O	2.38	0.53
1:F:565:LEU:HD21	1:F:606:LEU:HD12	1.89	0.53
1:A:531:LYS:HE2	1:A:549:ASN:HA	1.91	0.53
1:E:237:ASP:HB3	1:E:240:GLU:HB2	1.91	0.53
1:D:150:LYS:HE3	1:D:165:GLU:OE1	2.08	0.52
1:A:387:LEU:HB2	1:A:392:LYS:HG3	1.91	0.52
1:F:530:VAL:HG21	1:F:619:ILE:HD11	1.91	0.52
1:A:59:ASP:OD1	1:A:87:SER:N	2.40	0.51
1:A:198:ASP:OD1	1:A:198:ASP:N	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:581:LYS:HD2	1:E:583:ILE:HD11	1.92	0.51
1:E:531:LYS:HE2	1:E:549:ASN:HA	1.93	0.51
1:B:286:ASN:OD1	1:B:288:GLU:HG2	2.10	0.51
1:B:159:ALA:HB1	1:B:166:CYS:HB2	1.92	0.51
1:F:521:VAL:HG12	1:F:522:ARG:HG3	1.92	0.51
1:D:46:THR:OG1	1:D:121:GLU:HG3	2.11	0.50
1:D:123:VAL:HG11	1:D:175:PHE:CG	2.46	0.50
1:B:123:VAL:HG11	1:B:175:PHE:CG	2.46	0.50
1:B:39:MET:HE1	1:B:79:MET:HE1	1.93	0.50
1:D:89:TRP:HZ2	2:D:701:TRH:HC63	1.76	0.50
1:A:59:ASP:CG	1:A:87:SER:H	2.20	0.50
1:F:502:THR:O	1:F:517:VAL:HA	2.12	0.50
1:F:89:TRP:HZ2	2:F:701:TRH:HC61	1.75	0.50
1:B:320:LYS:NZ	7:B:818:HOH:O	2.44	0.50
1:D:26:PRO:HG3	1:D:94:ARG:HG3	1.93	0.49
1:E:49:PRO:HA	1:E:52:TYR:CE2	2.47	0.49
1:F:605:HIS:HA	1:F:620:LYS:HA	1.94	0.49
1:B:197:GLU:HA	1:B:200:TYR:HD2	1.78	0.49
1:D:43:ASP:CG	1:D:76:ARG:HH12	2.21	0.49
1:A:124:TYR:OH	1:A:128:LYS:HD3	2.13	0.49
1:A:235:GLY:O	1:A:236:ARG:C	2.54	0.49
1:C:123:VAL:HG13	1:C:135:VAL:HG11	1.94	0.49
1:E:243:ASN:O	1:E:247:LYS:HG2	2.12	0.49
1:D:123:VAL:HG11	1:D:175:PHE:CD1	2.47	0.49
1:A:198:ASP:OD2	5:A:705:GOL:O3	2.29	0.48
1:A:377:GLU:CG	1:A:441:ASN:ND2	2.76	0.48
1:B:413:PRO:HG2	1:B:426:ILE:HB	1.95	0.48
1:F:378:LYS:HB2	1:F:383:MET:SD	2.53	0.48
1:C:123:VAL:HG11	1:C:175:PHE:CG	2.48	0.48
1:C:413:PRO:HG2	1:C:426:ILE:HB	1.94	0.48
1:A:66:TYR:O	1:A:70:GLN:HG3	2.13	0.48
1:E:614:LYS:NZ	7:E:813:HOH:O	2.47	0.48
1:F:123:VAL:HG11	1:F:175:PHE:CD1	2.48	0.48
1:A:222:TYR:CE2	1:A:224:ILE:HG12	2.49	0.47
1:D:567:PRO:HG2	1:D:570:ILE:HB	1.97	0.47
1:E:192:ALA:O	1:E:194:VAL:HG23	2.14	0.47
1:D:89:TRP:CZ2	2:D:701:TRH:HC63	2.50	0.47
1:E:270:TYR:CD1	1:E:305:ILE:HG13	2.50	0.47
4:E:704:TAR:O4	4:E:704:TAR:O2	2.29	0.47
1:C:132:LEU:HD13	1:C:213:GLY:HA3	1.96	0.47
1:D:271:ARG:NH2	7:D:825:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:GLY:HA2	1:C:132:LEU:HD12	1.96	0.46
1:C:605:HIS:HE1	7:C:950:HOH:O	1.98	0.46
1:C:544:VAL:HG23	1:C:595:LEU:HD21	1.97	0.46
1:A:383:MET:HG3	1:A:406:LEU:HD11	1.97	0.46
1:A:89[B]:TRP:HZ2	2:A:701:TRH:HC63	1.80	0.46
1:B:54:LEU:HD22	1:B:79:MET:HE2	1.97	0.46
1:D:394:LYS:NZ	7:D:827:HOH:O	2.49	0.46
1:C:72:PHE:HD1	1:C:76:ARG:HH22	1.63	0.46
1:D:35:LEU:HD11	1:D:39:MET:HE2	1.98	0.46
1:D:558:LEU:HD11	1:D:581:LYS:HD2	1.98	0.46
1:D:568:VAL:HG11	1:D:603:GLU:HG2	1.98	0.46
1:F:298:LYS:NZ	1:F:325:ARG:O	2.48	0.45
1:A:531:LYS:HB2	1:A:547:PRO:HG2	1.99	0.45
1:A:54:LEU:HD23	1:A:56:PHE:HE1	1.81	0.45
1:D:354:LYS:HB3	1:D:359:PHE:CE1	2.52	0.45
1:E:24:VAL:HG13	1:E:97:ALA:HB3	1.98	0.45
1:C:159:ALA:HB1	1:C:166:CYS:HB2	1.99	0.45
1:A:123:VAL:HG11	1:A:175:PHE:CG	2.50	0.45
1:D:123:VAL:HG13	1:D:135:VAL:HG11	1.99	0.45
1:F:263:ASP:OD1	1:F:308:TYR:OH	2.32	0.45
1:A:382:ARG:CZ	1:A:397:LYS:HE2	2.47	0.45
1:F:119:THR:HG23	1:F:220:THR:HB	1.99	0.45
1:D:68:ARG:NH1	1:D:71:GLU:OE2	2.47	0.44
1:D:565:LEU:HA	1:D:605:HIS:O	2.17	0.44
1:E:123:VAL:HG11	1:E:175:PHE:CG	2.53	0.44
1:F:22:SER:HB2	1:F:106:ILE:HD13	1.99	0.44
1:D:581:LYS:HB3	1:D:581:LYS:HE2	1.87	0.44
1:A:132:LEU:HD13	1:A:213:GLY:HA3	1.99	0.44
1:D:613:LYS:HA	1:D:613:LYS:HD3	1.76	0.44
1:A:49:PRO:HA	1:A:52:TYR:CE2	2.53	0.44
1:E:49:PRO:O	1:E:78:ASN:ND2	2.50	0.44
1:B:123:VAL:HG13	1:B:135:VAL:HG11	1.98	0.44
1:F:390:GLU:O	1:F:394:LYS:HG3	2.18	0.44
1:A:89[B]:TRP:HA	1:A:89[B]:TRP:CE3	2.53	0.44
1:B:49:PRO:HA	1:B:52:TYR:CE2	2.53	0.44
1:B:257:LYS:HB3	1:B:257:LYS:HE3	1.87	0.44
1:E:135:VAL:HB	1:E:175:PHE:HB2	1.99	0.44
1:F:545:THR:HG23	1:F:590:ARG:HD2	1.99	0.44
1:A:398:GLU:CD	1:A:398:GLU:H	2.26	0.43
1:F:566:LYS:HB2	1:F:605:HIS:CE1	2.52	0.43
1:A:123:VAL:HG11	1:A:175:PHE:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:SER:HB2	1:B:106:ILE:HG12	1.99	0.43
1:F:459:ILE:HG21	1:F:465:LYS:HG3	1.99	0.43
1:B:42:ILE:HG21	1:B:54:LEU:HD21	2.00	0.43
1:A:314:ASP:OD1	1:A:317:ASN:ND2	2.42	0.43
1:A:354:LYS:HB3	1:A:359:PHE:CE1	2.53	0.43
1:B:198:ASP:N	1:B:198:ASP:OD1	2.50	0.43
1:B:310:SER:HA	1:B:313:LEU:HD12	2.01	0.43
4:A:703:TAR:O11	4:A:703:TAR:O3	2.33	0.43
1:C:84:ILE:HD13	1:C:96:ILE:HD12	2.01	0.43
1:C:565:LEU:HA	1:C:605:HIS:O	2.19	0.43
1:E:159:ALA:HB1	1:E:166:CYS:HB2	2.01	0.43
1:B:40:ALA:O	1:B:44:LYS:HG3	2.18	0.42
1:D:566:LYS:HB2	1:D:605:HIS:HB2	2.01	0.42
1:F:553:VAL:HB	1:F:587:ASN:HA	2.01	0.42
1:E:304:LEU:HD23	1:E:304:LEU:HA	1.84	0.42
1:F:54:LEU:HB3	1:F:56:PHE:HE1	1.84	0.42
1:A:160:GLU:OE2	1:A:212:VAL:N	2.48	0.42
1:E:58:ASP:N	1:E:82:LYS:O	2.51	0.42
1:F:543:LYS:HA	1:F:593:VAL:O	2.20	0.42
1:D:566:LYS:O	1:D:605:HIS:N	2.48	0.42
1:E:155:ASN:HD21	1:E:217:ASP:CG	2.27	0.42
1:C:207:ILE:HD11	1:C:256:ILE:HG12	2.01	0.42
1:D:19:ILE:HG21	1:D:53:GLU:HG2	2.00	0.42
1:A:149:TRP:CH2	1:A:425:LYS:HB2	2.54	0.42
1:C:123:VAL:HG11	1:C:175:PHE:CD1	2.54	0.42
1:E:28:TYR:HA	1:E:61:SER:HB3	2.01	0.42
1:F:132:LEU:HD13	1:F:213:GLY:HA3	2.02	0.42
1:A:339:ASP:OD2	1:A:385:ARG:NH2	2.53	0.42
1:A:236:ARG:O	1:A:289:ARG:NH2	2.41	0.42
1:E:165:GLU:HA	1:E:168:LEU:HD13	2.02	0.42
1:F:418:ARG:HB3	1:F:468:PRO:HG2	2.02	0.42
1:A:91:SER:HB3	1:A:188:PHE:HB3	2.01	0.41
1:E:145:TRP:CZ2	1:E:485:ALA:HB2	2.55	0.41
1:A:119:THR:HG23	1:A:220:THR:HB	2.01	0.41
1:C:76:ARG:HD2	1:C:79:MET:CE	2.50	0.41
1:B:437:ASN:HB2	1:B:443:TYR:CE2	2.55	0.41
1:E:22:SER:HB2	1:E:106:ILE:HD13	2.02	0.41
1:F:566:LYS:HB3	1:F:573:ALA:HB1	2.01	0.41
1:A:89[A]:TRP:CH2	1:A:193:ARG:HG2	2.53	0.41
1:C:48:ASN:ND2	1:C:50:ASP:OD1	2.53	0.41
1:E:238:PRO:HG3	1:E:289:ARG:CZ	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:599:LYS:O	1:A:599:LYS:HG3	2.21	0.41
1:D:383:MET:HE1	1:D:443:TYR:CD1	2.55	0.41
1:F:32:LEU:HD13	1:F:68:ARG:HD2	2.01	0.41
1:B:346:SER:O	1:B:487:THR:HG22	2.21	0.41
1:E:29:ASN:H	1:E:61:SER:CB	2.33	0.41
1:F:159:ALA:HB1	1:F:166:CYS:HB2	2.01	0.41
1:A:32:LEU:HG	1:A:36:LYS:HE3	2.03	0.41
1:A:538:ASP:O	1:A:542:GLY:N	2.54	0.41
1:F:532:ARG:NH1	1:F:617:GLN:O	2.43	0.41
1:B:123:VAL:HG11	1:B:175:PHE:CD1	2.55	0.41
1:D:247:LYS:HE2	1:D:247:LYS:HB3	1.94	0.41
1:F:127:GLY:HA2	1:F:132:LEU:HD12	2.03	0.40
1:F:576:ILE:HG21	1:F:598:GLU:HG2	2.03	0.40
1:F:42:ILE:HG21	1:F:54:LEU:HD21	2.04	0.40
1:E:43:ASP:OD1	1:E:76:ARG:NH1	2.54	0.40
1:A:579:LYS:HE2	1:A:579:LYS:HB3	1.85	0.40
1:E:20:LYS:HD3	1:E:124:TYR:CD2	2.56	0.40
1:F:222:TYR:CE2	1:F:224:ILE:HG12	2.57	0.40
1:B:118:GLU:HB2	1:B:218:TYR:CZ	2.56	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	599/624 (96%)	581 (97%)	18 (3%)	0	100	100
1	B	598/624 (96%)	583 (98%)	15 (2%)	0	100	100
1	C	597/624 (96%)	579 (97%)	18 (3%)	0	100	100
1	D	596/624 (96%)	576 (97%)	20 (3%)	0	100	100
1	E	595/624 (95%)	577 (97%)	18 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	595/624 (95%)	573 (96%)	22 (4%)	0	100	100
All	All	3580/3744 (96%)	3469 (97%)	111 (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	535/553 (97%)	528 (99%)	7 (1%)	61	76
1	B	533/553 (96%)	528 (99%)	5 (1%)	70	84
1	C	533/553 (96%)	529 (99%)	4 (1%)	73	85
1	D	533/553 (96%)	521 (98%)	12 (2%)	44	59
1	E	532/553 (96%)	526 (99%)	6 (1%)	65	79
1	F	532/553 (96%)	526 (99%)	6 (1%)	65	79
All	All	3198/3318 (96%)	3158 (99%)	40 (1%)	61	76

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	129	GLU
1	A	184	ASN
1	A	193	ARG
1	A	247	LYS
1	A	365	LYS
1	A	425	LYS
1	A	501	LYS
1	B	23	VAL
1	B	189	ASP
1	B	211	LYS
1	B	594	LEU
1	B	600	LEU
1	C	19	ILE

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Mol	Chain	Res	Type
1	C	85	GLU
1	C	501	LYS
1	C	530	VAL
1	D	128	LYS
1	D	247	LYS
1	D	334	LYS
1	D	517	VAL
1	D	532	ARG
1	D	568	VAL
1	D	581	LYS
1	D	587	ASN
1	D	588	LYS
1	D	598	GLU
1	D	607	VAL
1	D	616	LYS
1	E	75	THR
1	E	81	VAL
1	E	99	LYS
1	E	128	LYS
1	E	298	LYS
1	E	398	GLU
1	F	99	LYS
1	F	171	THR
1	F	247	LYS
1	F	305	ILE
1	F	371	LYS
1	F	544	VAL

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	432	ASN
1	A	587	ASN
1	A	605	HIS
1	A	617	GLN
1	B	70	GLN
1	B	83	GLN
1	B	143	ASN
1	B	243	ASN
1	B	250	ASN
1	B	285	ASN
1	B	432	ASN

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Mol	Chain	Res	Type
1	B	456	ASN
1	B	611	GLN
1	C	143	ASN
1	C	184	ASN
1	C	259	GLN
1	C	295	ASN
1	C	312	ASN
1	C	534	GLN
1	C	577	ASN
1	C	617	GLN
1	D	83	GLN
1	D	86	ASN
1	D	250	ASN
1	D	437	ASN
1	D	562	ASN
1	E	70	GLN
1	E	86	ASN
1	E	255	ASN
1	E	280	GLN
1	E	295	ASN
1	E	605	HIS
1	F	617	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, 11 are monoatomic - leaving 18 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
2	TRH	A	701	3	36,37,37	0.37	0	54,57,57	0.54	0
4	TAR	E	704	-	9,9,9	1.16	1 (11%)	12,12,12	1.00	0
4	TAR	A	703	-	9,9,9	1.33	2 (22%)	12,12,12	1.15	0
5	GOL	D	706	-	5,5,5	0.11	0	5,5,5	0.17	0
5	GOL	E	705	-	5,5,5	0.09	0	5,5,5	0.29	0
4	TAR	F	704	-	9,9,9	1.23	2 (22%)	12,12,12	1.12	0
4	TAR	C	703	-	9,9,9	1.32	2 (22%)	12,12,12	1.03	0
2	TRH	D	701	3	36,37,37	0.44	0	54,57,57	0.51	0
2	TRH	C	701	3	36,37,37	0.48	0	54,57,57	0.72	3 (5%)
5	GOL	A	704	-	5,5,5	0.08	0	5,5,5	0.32	0
5	GOL	A	705	-	5,5,5	0.16	0	5,5,5	0.23	0
4	TAR	D	705	-	9,9,9	1.11	2 (22%)	12,12,12	1.02	0
2	TRH	F	701	3	36,37,37	0.50	0	54,57,57	0.64	0
5	GOL	B	705	-	5,5,5	0.13	0	5,5,5	0.30	0
2	TRH	B	701	3	36,37,37	0.51	0	54,57,57	0.75	2 (3%)
2	TRH	E	701	3	36,37,37	0.43	0	54,57,57	0.49	0
4	TAR	B	704	-	9,9,9	1.24	2 (22%)	12,12,12	1.07	0
5	GOL	B	706	-	5,5,5	0.06	0	5,5,5	0.30	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRH	A	701	3	-	2/21/53/53	0/3/3/3
4	TAR	E	704	-	-	6/12/12/12	-
4	TAR	A	703	-	-	10/12/12/12	-
5	GOL	D	706	-	-	3/4/4/4	-
5	GOL	E	705	-	-	2/4/4/4	-
4	TAR	F	704	-	-	4/12/12/12	-
4	TAR	C	703	-	-	10/12/12/12	-
2	TRH	D	701	3	-	5/21/53/53	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TRH	C	701	3	-	5/21/53/53	0/3/3/3
5	GOL	A	704	-	-	2/4/4/4	-
5	GOL	A	705	-	-	2/4/4/4	-
4	TAR	D	705	-	-	10/12/12/12	-
2	TRH	F	701	3	-	5/21/53/53	0/3/3/3
5	GOL	B	705	-	-	0/4/4/4	-
2	TRH	B	701	3	-	5/21/53/53	0/3/3/3
2	TRH	E	701	3	-	2/21/53/53	0/3/3/3
4	TAR	B	704	-	-	10/12/12/12	-
5	GOL	B	706	-	-	2/4/4/4	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	703	TAR	O11-C1	-2.86	1.21	1.30
4	F	704	TAR	O11-C1	-2.70	1.22	1.30
4	A	703	TAR	O11-C1	-2.64	1.22	1.30
4	A	703	TAR	O41-C4	-2.55	1.22	1.30
4	E	704	TAR	O11-C1	-2.53	1.22	1.30
4	B	704	TAR	O41-C4	-2.51	1.22	1.30
4	D	705	TAR	O11-C1	-2.35	1.23	1.30
4	B	704	TAR	O11-C1	-2.30	1.23	1.30
4	C	703	TAR	O41-C4	-2.24	1.23	1.30
4	F	704	TAR	O41-C4	-2.12	1.23	1.30
4	D	705	TAR	O41-C4	-2.09	1.24	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	TRH	P2-O1-C1	3.04	133.61	121.21
2	B	701	TRH	O5-C1-O1	2.74	114.95	111.36
2	C	701	TRH	O5-C1-O1	2.27	114.34	111.36
2	C	701	TRH	O1-C1-C2	-2.12	104.50	108.38
2	B	701	TRH	P2-O1-C1	2.04	129.51	121.21

There are no chirality outliers.

All (85) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	TRH	O5-C1-O1-P2
2	B	701	TRH	C1-O1-P2-O4P
2	B	701	TRH	C1-O1-P2-OPP
2	C	701	TRH	C1-O1-P2-OPP
2	C	701	TRH	O5-C1-O1-P2
2	D	701	TRH	O5-C1-O1-P2
2	E	701	TRH	O5-C1-O1-P2
2	F	701	TRH	C1-O1-P2-O4P
2	F	701	TRH	C1-O1-P2-OPP
4	A	703	TAR	O2-C2-C3-O3
4	B	704	TAR	O1-C1-C2-O2
4	B	704	TAR	O11-C1-C2-O2
4	B	704	TAR	C1-C2-C3-C4
4	C	703	TAR	C1-C2-C3-C4
4	C	703	TAR	O2-C2-C3-O3
4	D	705	TAR	O1-C1-C2-O2
4	D	705	TAR	O11-C1-C2-O2
4	D	705	TAR	C1-C2-C3-C4
5	A	705	GOL	O1-C1-C2-C3
5	D	706	GOL	O1-C1-C2-O2
5	D	706	GOL	O1-C1-C2-C3
5	E	705	GOL	O1-C1-C2-O2
5	E	705	GOL	O1-C1-C2-C3
4	B	704	TAR	O2-C2-C3-O3
4	A	703	TAR	C1-C2-C3-C4
4	A	703	TAR	C1-C2-C3-O3
4	A	703	TAR	O1-C1-C2-O2
4	A	703	TAR	O11-C1-C2-O2
4	B	704	TAR	O3-C3-C4-O4
4	B	704	TAR	O3-C3-C4-O41
4	C	703	TAR	O1-C1-C2-O2
4	C	703	TAR	O11-C1-C2-O2
4	C	703	TAR	O3-C3-C4-O4
4	C	703	TAR	O3-C3-C4-O41
4	D	705	TAR	O3-C3-C4-O4
4	D	705	TAR	O3-C3-C4-O41
4	E	704	TAR	O3-C3-C4-O4
4	E	704	TAR	O3-C3-C4-O41
4	F	704	TAR	O1-C1-C2-O2
4	F	704	TAR	O11-C1-C2-O2
4	B	704	TAR	C1-C2-C3-O3
4	D	705	TAR	O2-C2-C3-O3
4	A	703	TAR	O2-C2-C3-C4

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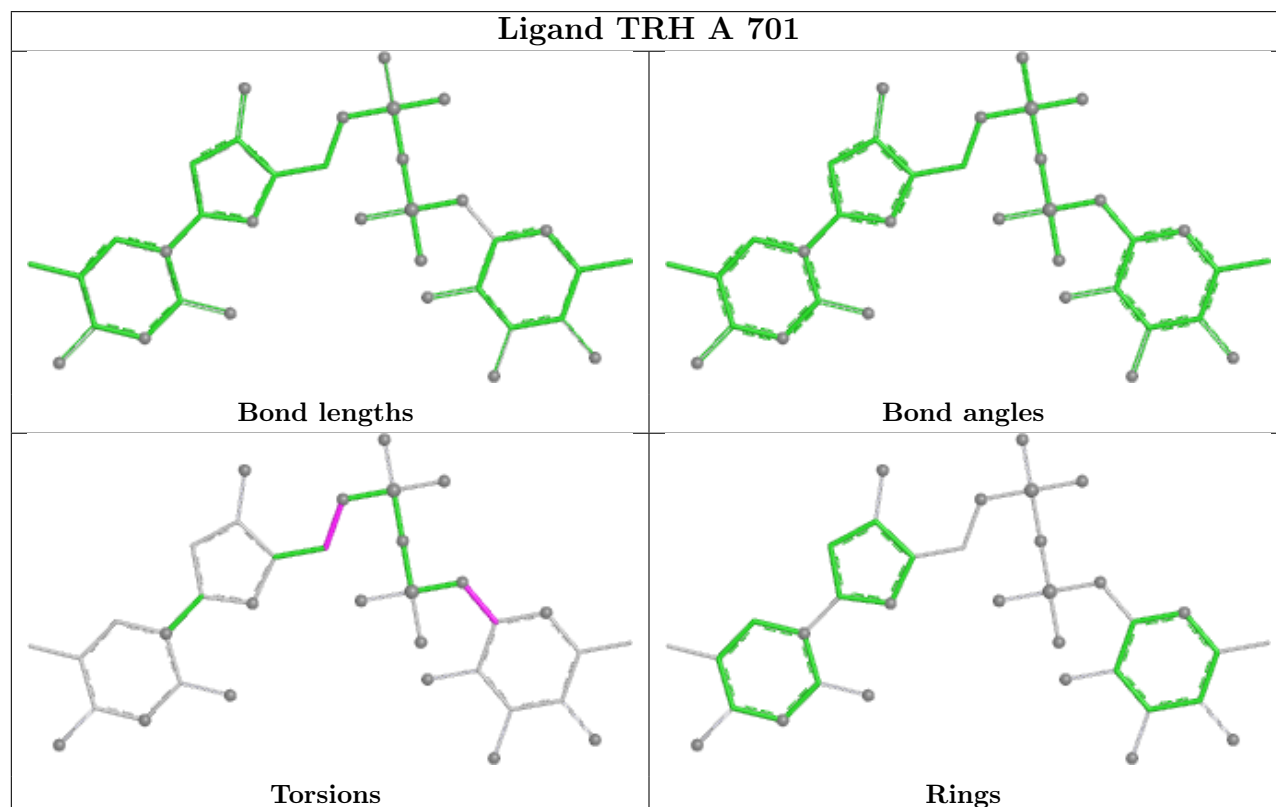
Mol	Chain	Res	Type	Atoms
4	B	704	TAR	O2-C2-C3-C4
4	C	703	TAR	C1-C2-C3-O3
4	C	703	TAR	O2-C2-C3-C4
4	E	704	TAR	O1-C1-C2-O2
4	E	704	TAR	O11-C1-C2-O2
4	A	703	TAR	O3-C3-C4-O4
4	A	703	TAR	O3-C3-C4-O41
4	F	704	TAR	O3-C3-C4-O4
4	F	704	TAR	O3-C3-C4-O41
5	A	704	GOL	O1-C1-C2-O2
2	F	701	TRH	C2-C1-O1-P2
5	A	704	GOL	O1-C1-C2-C3
5	B	706	GOL	O1-C1-C2-C3
5	D	706	GOL	C1-C2-C3-O3
4	E	704	TAR	C2-C3-C4-O4
5	A	705	GOL	O1-C1-C2-O2
4	D	705	TAR	C1-C2-C3-O3
2	B	701	TRH	C2-C1-O1-P2
2	E	701	TRH	C2-C1-O1-P2
4	B	704	TAR	C2-C3-C4-O4
4	B	704	TAR	C2-C3-C4-O41
4	E	704	TAR	C2-C3-C4-O41
4	D	705	TAR	O2-C2-C3-C4
2	D	701	TRH	C2-C1-O1-P2
5	B	706	GOL	O1-C1-C2-O2
4	A	703	TAR	O11-C1-C2-C3
4	C	703	TAR	C2-C3-C4-O4
2	B	701	TRH	C1-O1-P2-O3P
2	D	701	TRH	C1-O1-P2-O4P
2	F	701	TRH	C1-O1-P2-O3P
4	C	703	TAR	C2-C3-C4-O41
4	D	705	TAR	C2-C3-C4-O4
2	C	701	TRH	C4'-C5'-O5'-P
4	D	705	TAR	C2-C3-C4-O41
2	F	701	TRH	C4'-C5'-O5'-P
2	C	701	TRH	C1-O1-P2-O3P
2	D	701	TRH	C1-O1-P2-O3P
2	B	701	TRH	C4'-C5'-O5'-P
2	D	701	TRH	C4'-C5'-O5'-P
4	A	703	TAR	O1-C1-C2-C3
2	A	701	TRH	C4'-C5'-O5'-P
2	C	701	TRH	P-OPP-P2-O4P

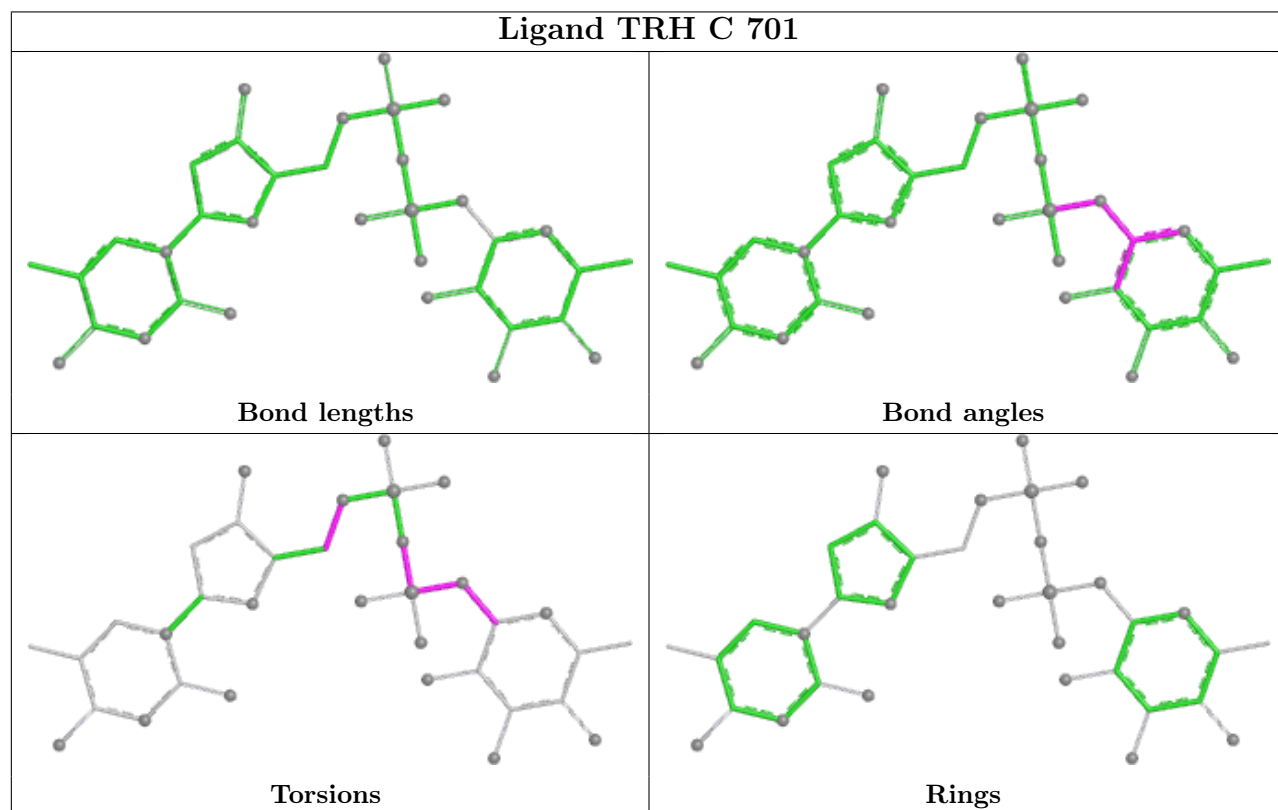
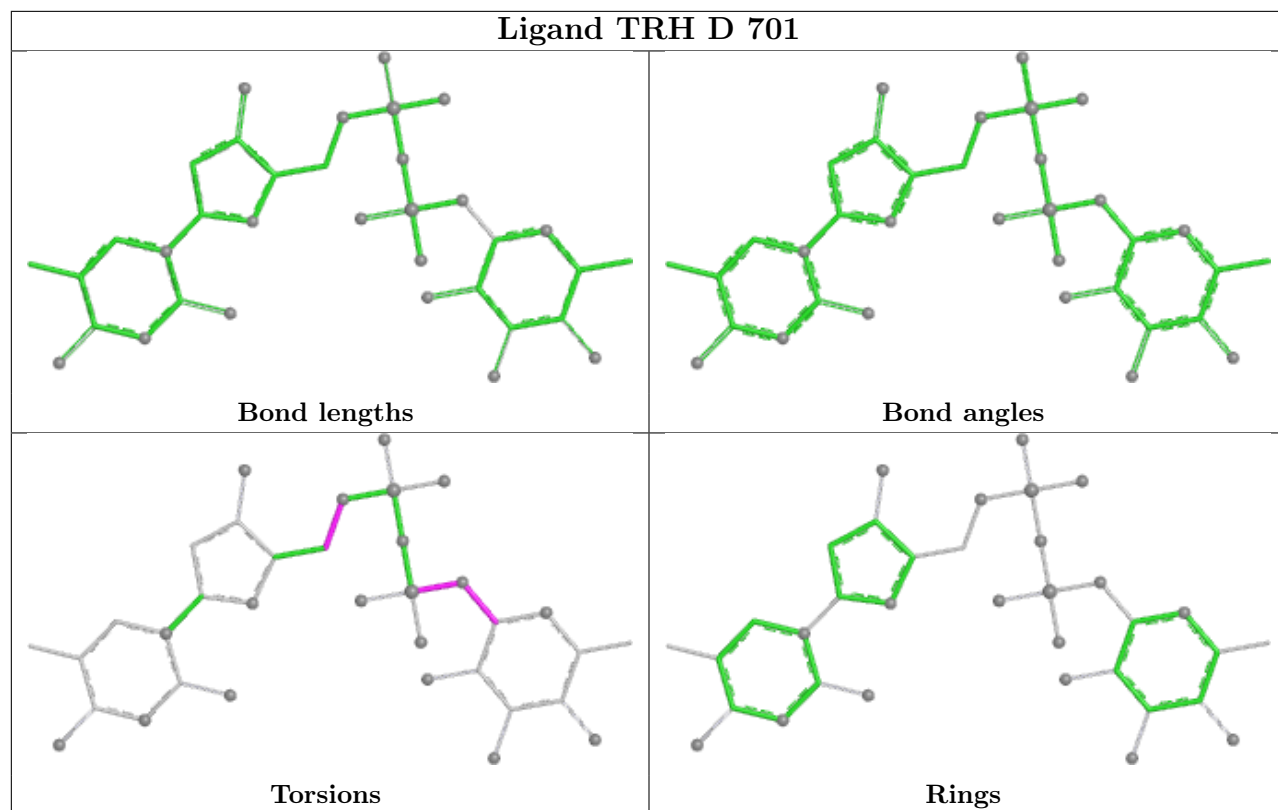
There are no ring outliers.

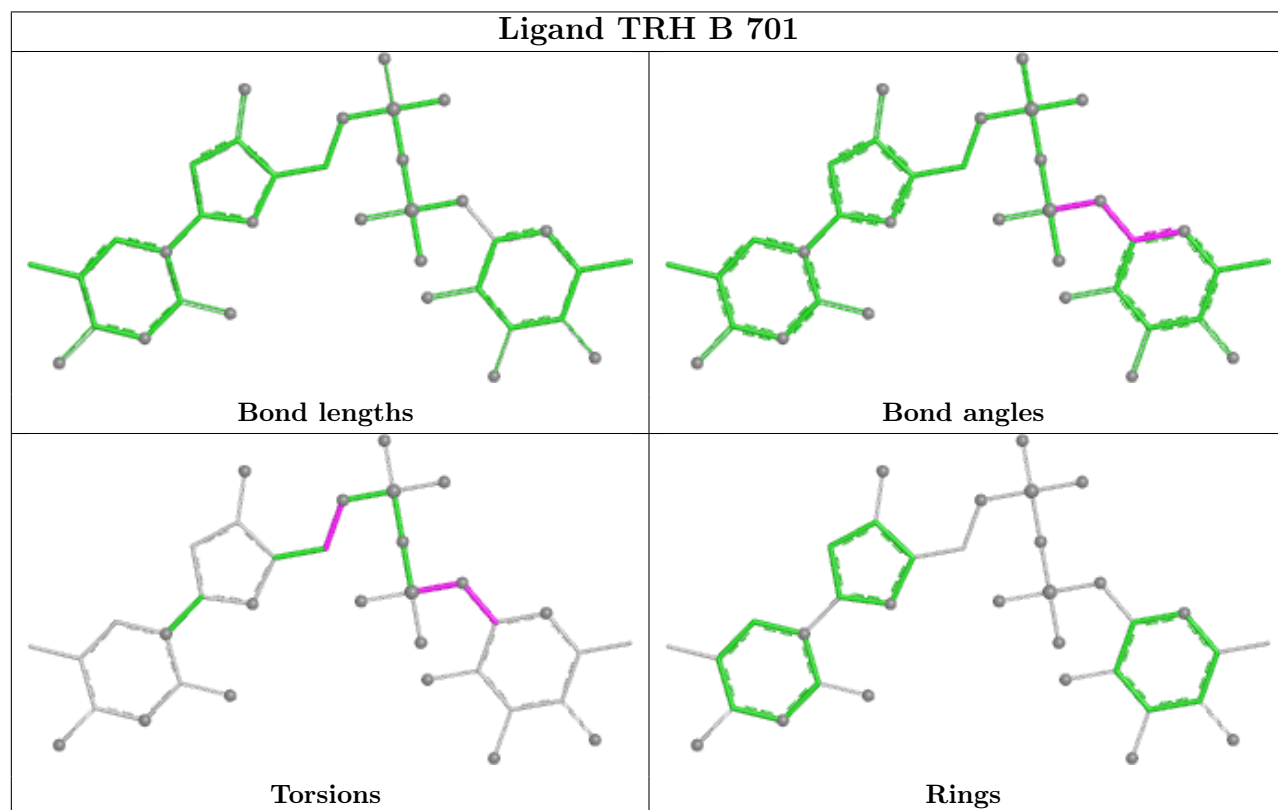
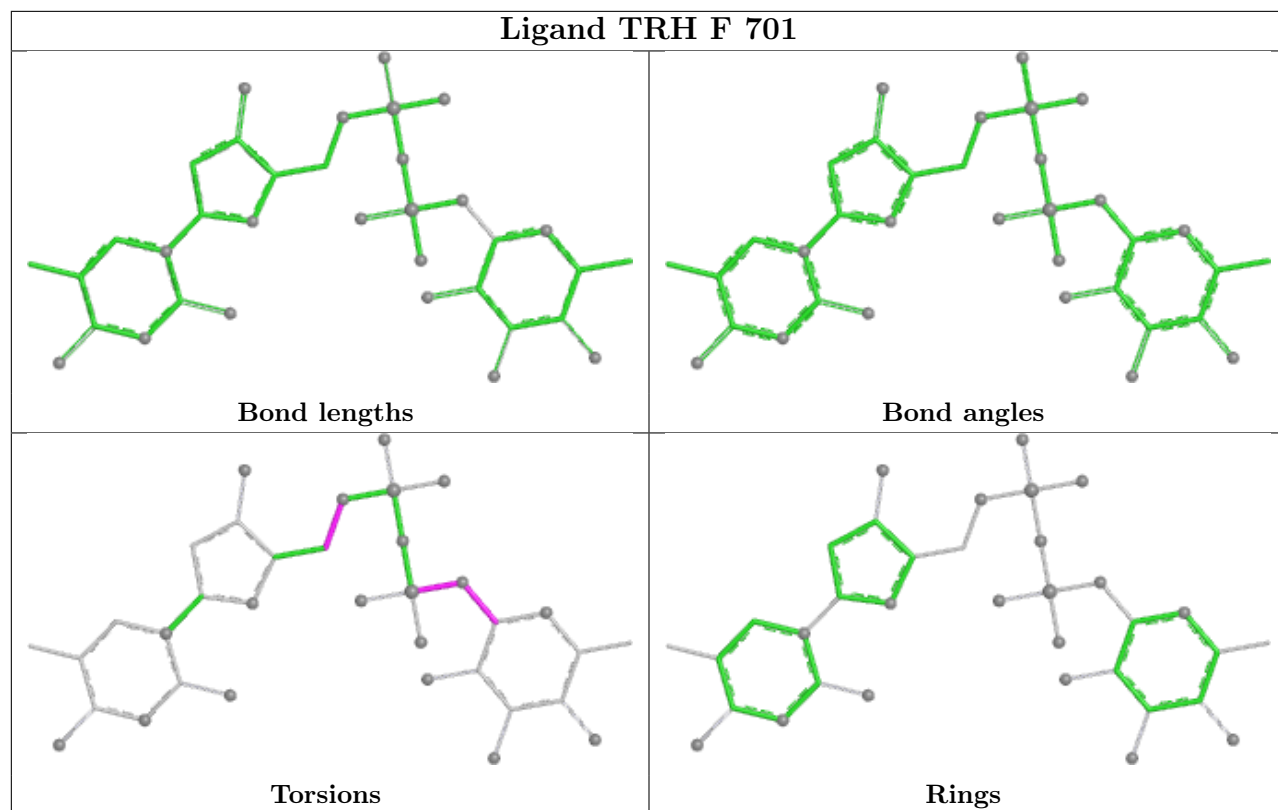
6 monomers are involved in 8 short contacts:

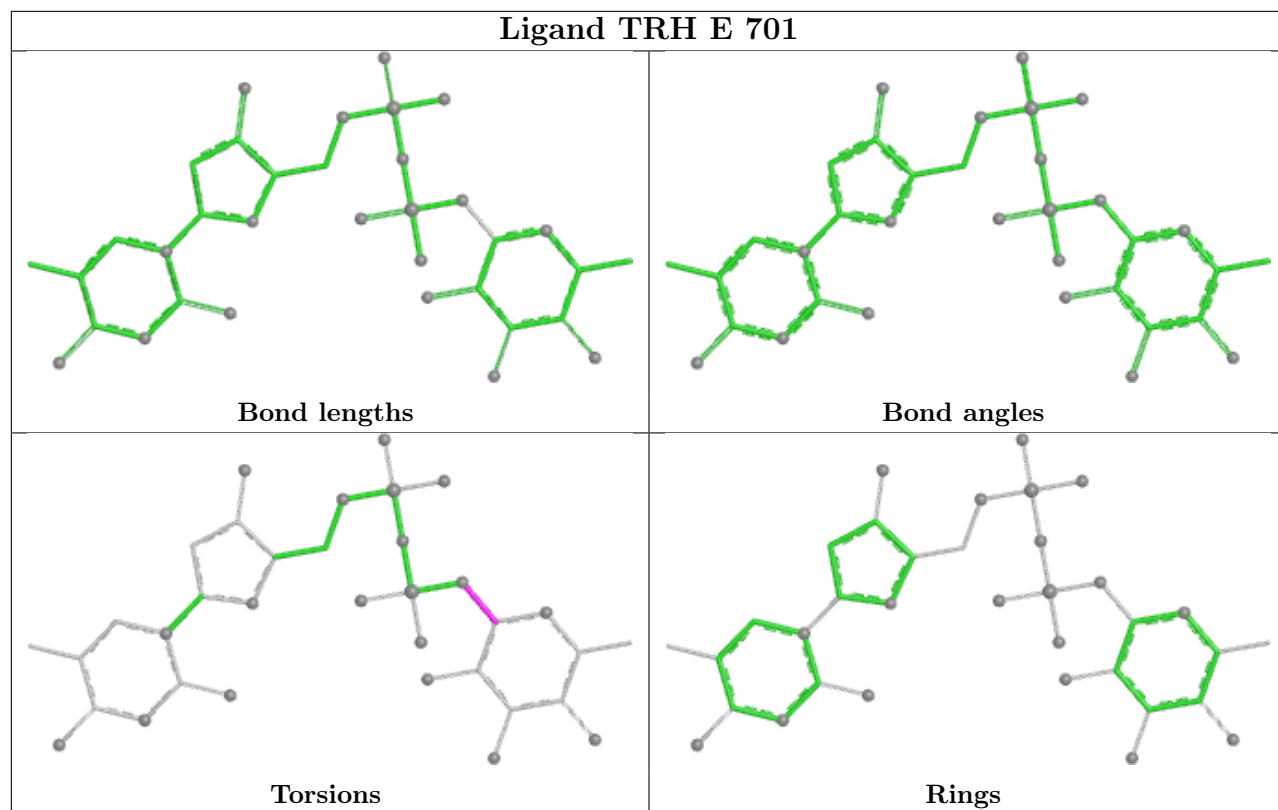
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	TRH	2	0
4	E	704	TAR	1	0
4	A	703	TAR	1	0
2	D	701	TRH	2	0
5	A	705	GOL	1	0
2	F	701	TRH	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	601/624 (96%)	-0.15	9 (1%) 72 69	20, 48, 86, 120	2 (0%)
1	B	601/624 (96%)	-0.17	8 (1%) 75 73	21, 51, 80, 111	1 (0%)
1	C	600/624 (96%)	-0.11	8 (1%) 75 73	20, 51, 79, 136	1 (0%)
1	D	599/624 (95%)	0.03	14 (2%) 61 58	19, 54, 116, 166	1 (0%)
1	E	598/624 (95%)	0.00	12 (2%) 65 62	20, 59, 96, 131	1 (0%)
1	F	598/624 (95%)	0.18	17 (2%) 55 52	21, 64, 120, 165	1 (0%)
All	All	3597/3744 (96%)	-0.04	68 (1%) 66 63	19, 54, 97, 166	7 (0%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	89[A]	TRP	5.3
1	C	228	ALA	5.0
1	E	235	GLY	4.4
1	B	228	ALA	4.3
1	E	192	ALA	3.8
1	F	235	GLY	3.8
1	C	194	VAL	3.6
1	F	623	LEU	3.6
1	F	570	ILE	3.6
1	F	194	VAL	3.5
1	D	194	VAL	3.5
1	F	600	LEU	3.3
1	F	540	THR	3.1
1	C	192	ALA	3.1
1	E	312	ASN	3.1
1	F	192	ALA	3.1
1	E	75	THR	3.0
1	C	227	GLY	3.0
1	F	607	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	E	89	TRP	3.0
1	A	191	GLY	2.9
1	B	235	GLY	2.9
1	F	595	LEU	2.9
1	D	568	VAL	2.9
1	A	84	ILE	2.9
1	F	574	ASP	2.8
1	D	540	THR	2.8
1	B	192	ALA	2.8
1	D	193	ARG	2.7
1	B	227	GLY	2.6
1	D	570	ILE	2.5
1	F	604	TYR	2.5
1	C	193	ARG	2.5
1	A	235	GLY	2.5
1	D	621	ILE	2.4
1	D	604	TYR	2.4
1	F	193	ARG	2.4
1	D	595	LEU	2.4
1	D	573	ALA	2.3
1	E	207	ILE	2.3
1	B	381	ASP	2.3
1	F	563	ALA	2.3
1	F	195	LEU	2.3
1	F	226	THR	2.3
1	D	600	LEU	2.2
1	C	229	ASN	2.2
1	E	236	ARG	2.2
1	F	573	ALA	2.2
1	C	236	ARG	2.2
1	B	229	ASN	2.2
1	E	310	SER	2.2
1	A	162	MET	2.1
1	B	162	MET	2.1
1	E	162	MET	2.1
1	D	227	GLY	2.1
1	F	541	SER	2.1
1	E	106	ILE	2.1
1	A	234	PHE	2.1
1	A	192	ALA	2.1
1	D	593	VAL	2.1
1	A	233	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	193	ARG	2.0
1	D	192	ALA	2.0
1	A	381	ASP	2.0
1	C	195	LEU	2.0
1	D	537	ILE	2.0
1	E	193	ARG	2.0
1	E	599	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

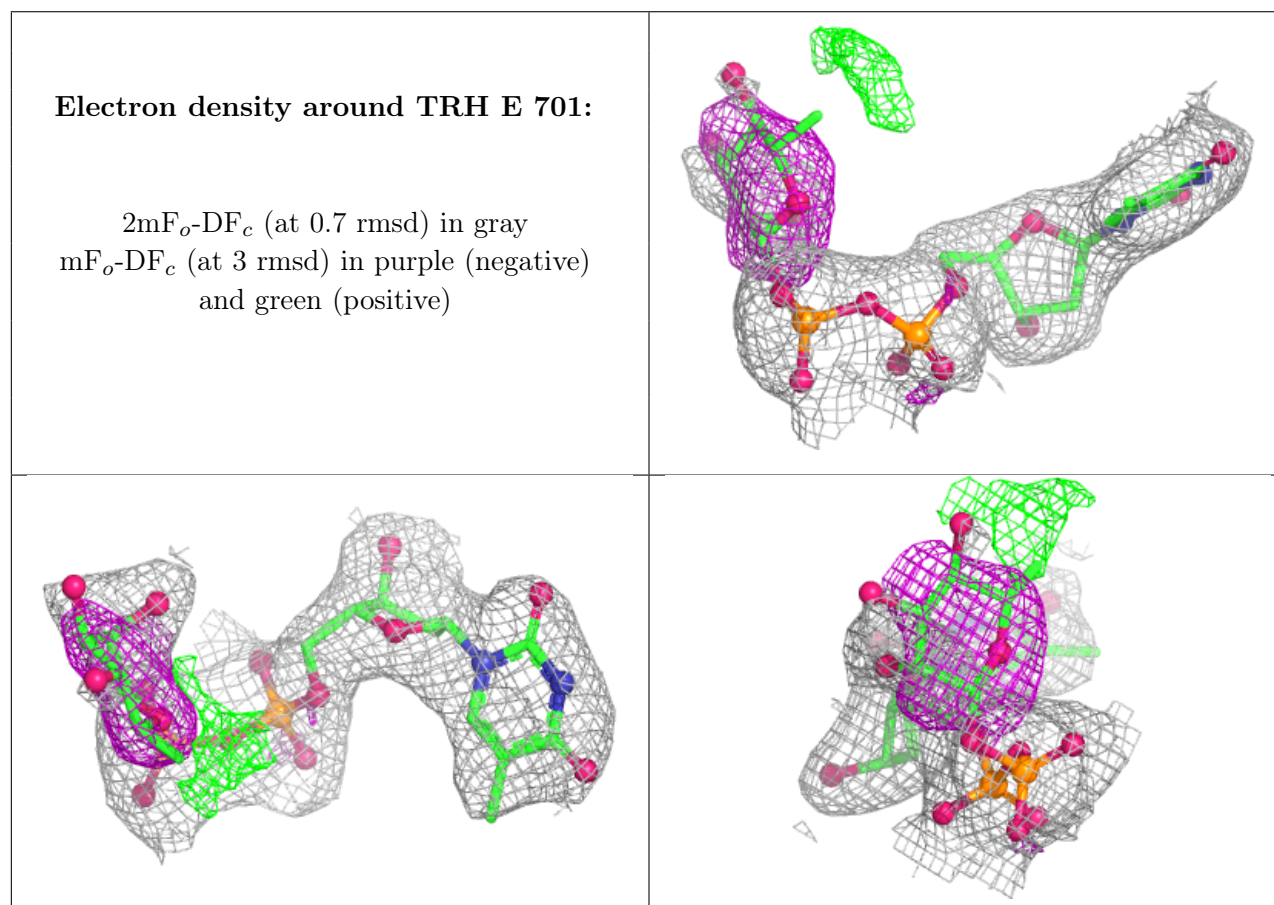
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	704	6/6	0.74	0.16	50,59,62,66	0
5	GOL	B	706	6/6	0.76	0.14	49,60,68,69	0
5	GOL	A	705	6/6	0.78	0.17	56,64,66,68	0
4	TAR	F	704	10/10	0.80	0.12	47,51,61,61	0
4	TAR	E	704	10/10	0.81	0.11	54,58,65,67	0
5	GOL	E	705	6/6	0.81	0.15	69,71,72,75	0
5	GOL	B	705	6/6	0.82	0.15	56,61,64,65	0
4	TAR	D	705	10/10	0.84	0.11	46,54,59,62	0
4	TAR	C	703	10/10	0.84	0.12	47,56,60,61	0
5	GOL	D	706	6/6	0.85	0.14	51,56,57,59	0
2	TRH	E	701	35/35	0.85	0.13	62,72,82,83	0
4	TAR	B	704	10/10	0.86	0.10	43,54,59,64	0
2	TRH	A	701	35/35	0.88	0.13	53,70,82,84	0
4	TAR	A	703	10/10	0.89	0.09	43,49,57,57	0
3	MG	B	702	1/1	0.89	0.08	52,52,52,52	0
3	MG	A	702	1/1	0.90	0.09	53,53,53,53	0

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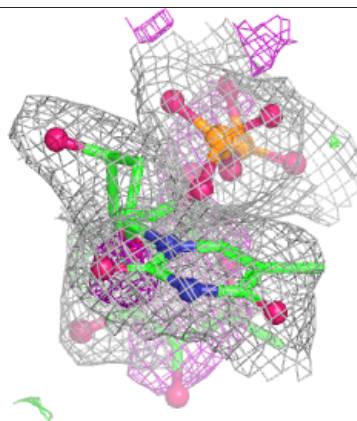
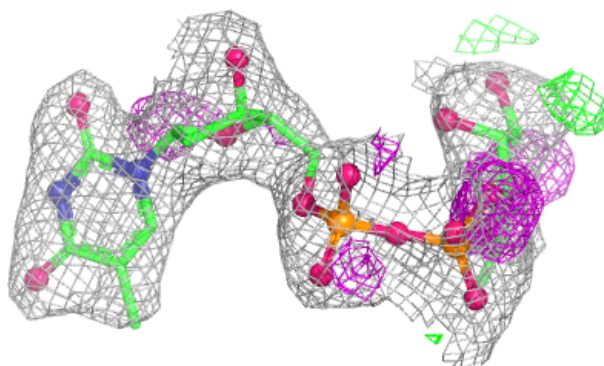
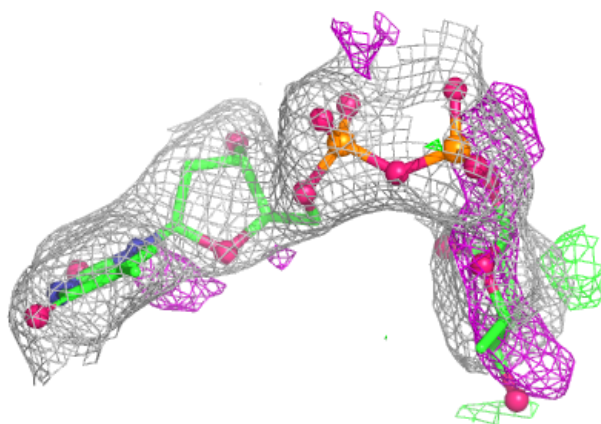
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TRH	F	701	35/35	0.90	0.12	53,68,77,81	0
2	TRH	C	701	35/35	0.91	0.11	42,57,84,89	0
2	TRH	D	701	35/35	0.91	0.11	51,60,76,79	0
2	TRH	B	701	35/35	0.91	0.12	44,59,71,73	0
3	MG	E	703	1/1	0.96	0.06	27,27,27,27	0
6	CL	F	703	1/1	0.96	0.07	51,51,51,51	0
3	MG	B	703	1/1	0.97	0.17	39,39,39,39	0
3	MG	D	702	1/1	0.97	0.06	50,50,50,50	0
3	MG	C	702	1/1	0.98	0.05	49,49,49,49	0
3	MG	D	703	1/1	0.98	0.15	31,31,31,31	0
3	MG	F	702	1/1	0.99	0.03	53,53,53,53	0
6	CL	D	704	1/1	0.99	0.04	50,50,50,50	0
3	MG	E	702	1/1	0.99	0.06	62,62,62,62	0

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

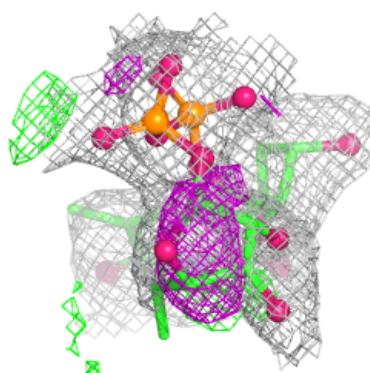
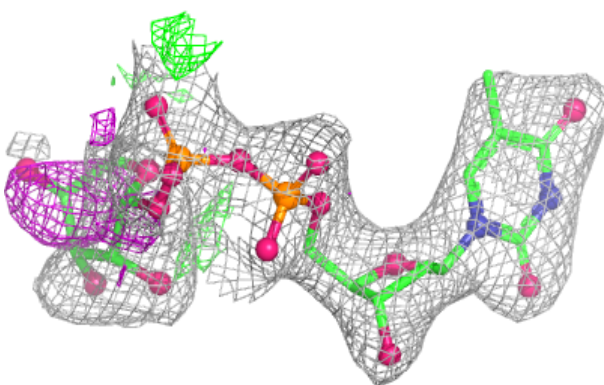
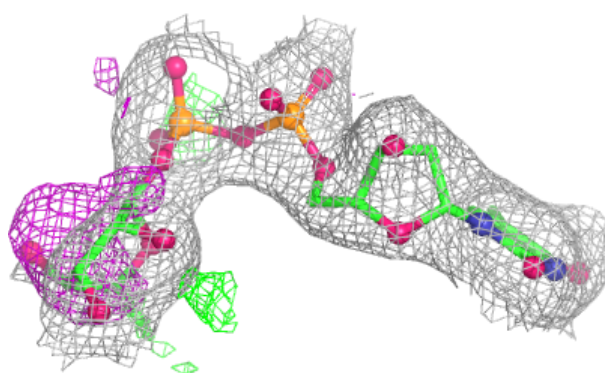


Electron density around TRH A 701:

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

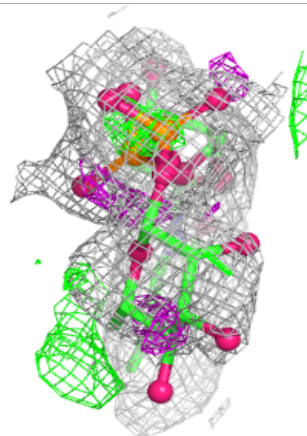
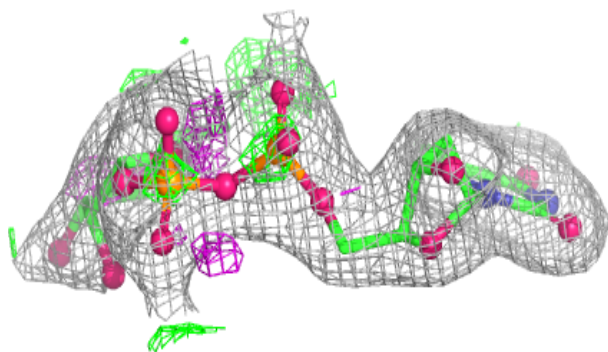
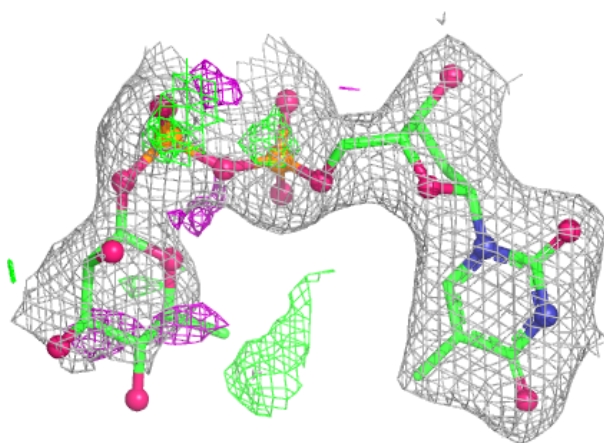
**Electron density around TRH F 701:**

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



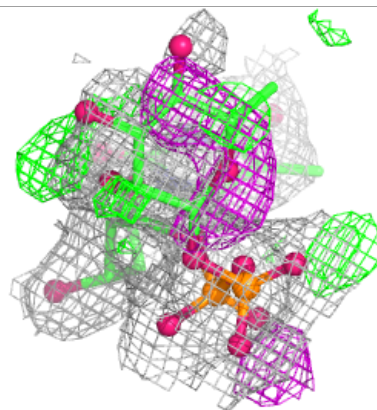
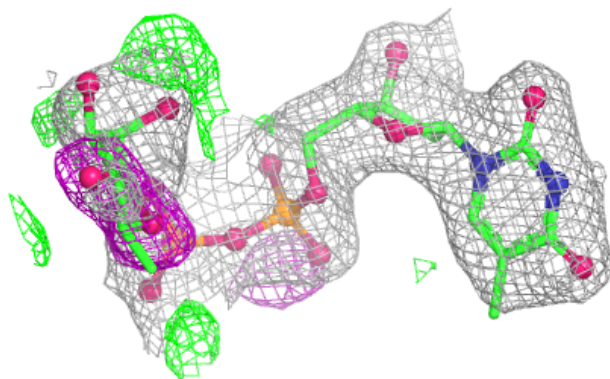
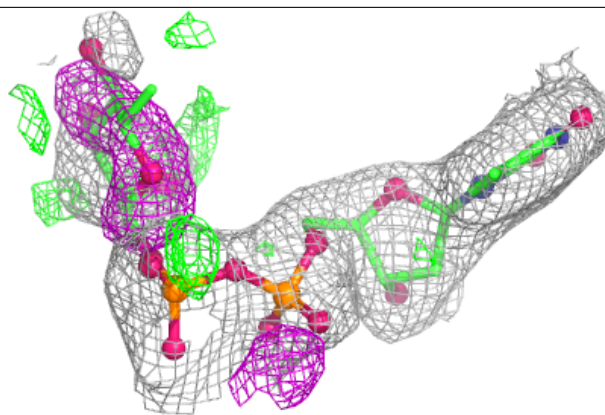
Electron density around TRH C 701:

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

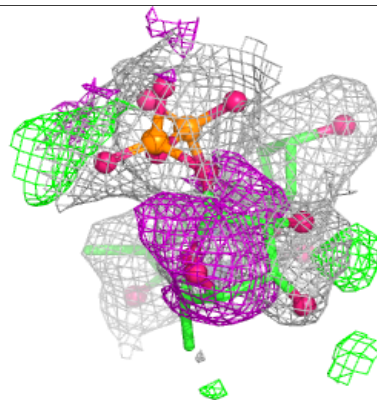
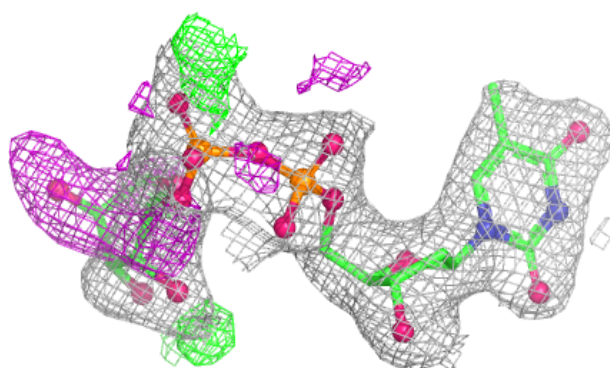
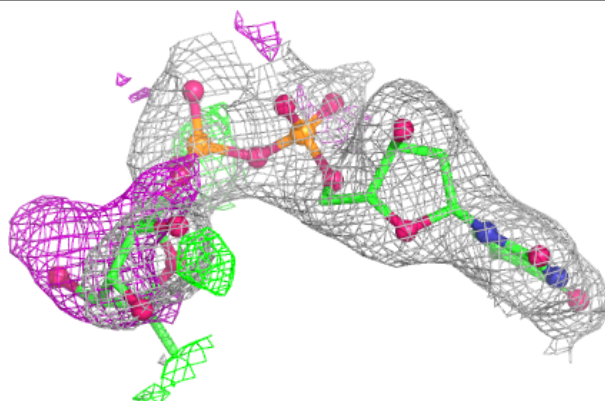


Electron density around TRH D 701:

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

**Electron density around TRH B 701:**

$2mF_o-DF_c$ (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.