



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2023 – 12:40 pm GMT

PDB ID : 8BZ7  
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](mailto: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>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

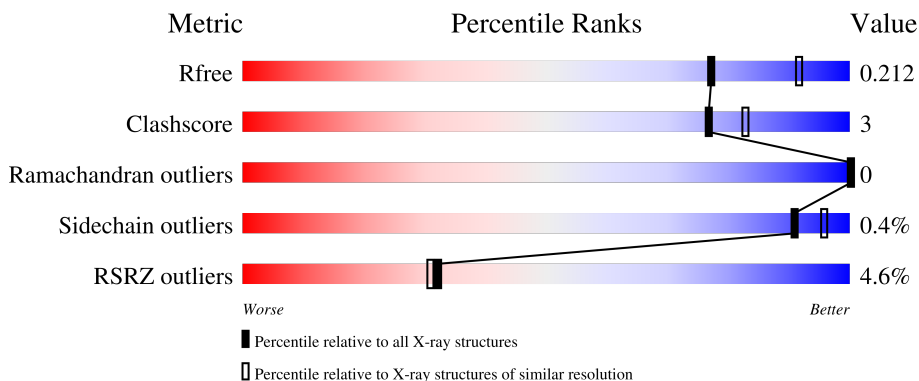
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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.



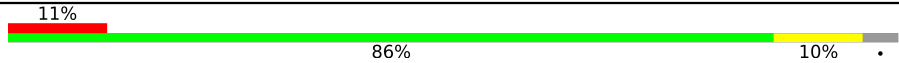
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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  $\geq 3$ , 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	
1	B	624	
1	C	624	
1	D	624	
1	E	624	

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Mol	Chain	Length	Quality of chain
1	F	624	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into three segments: a red segment on the left labeled '11%', a large green segment in the middle labeled '86%', and a yellow segment on the right labeled '10%'. A small grey dot is visible at the far right end of the bar.</p>

## 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.

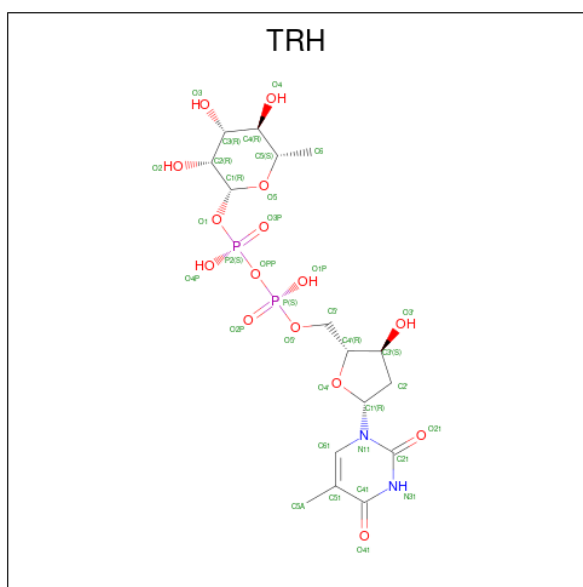
- Molecule 1 is a protein called Glycosyltransferase.

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

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 (three-letter code: TRH) (formula:  $C_{16}H_{26}N_2O_{15}P_2$ ) (labeled as "Ligand of Interest" by depositor).

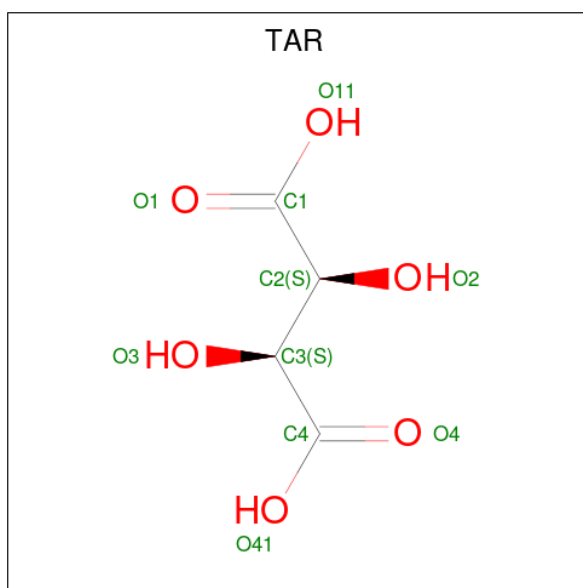


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	N	O			P
2	A	1	35	16	2	15	2	0	0
2	B	1	35	16	2	15	2	0	0
2	C	1	35	16	2	15	2	0	0
2	D	1	35	16	2	15	2	0	0
2	E	1	35	16	2	15	2	0	0
2	F	1	35	16	2	15	2	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: C<sub>4</sub>H<sub>6</sub>O<sub>6</sub>).



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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 7 is water.

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

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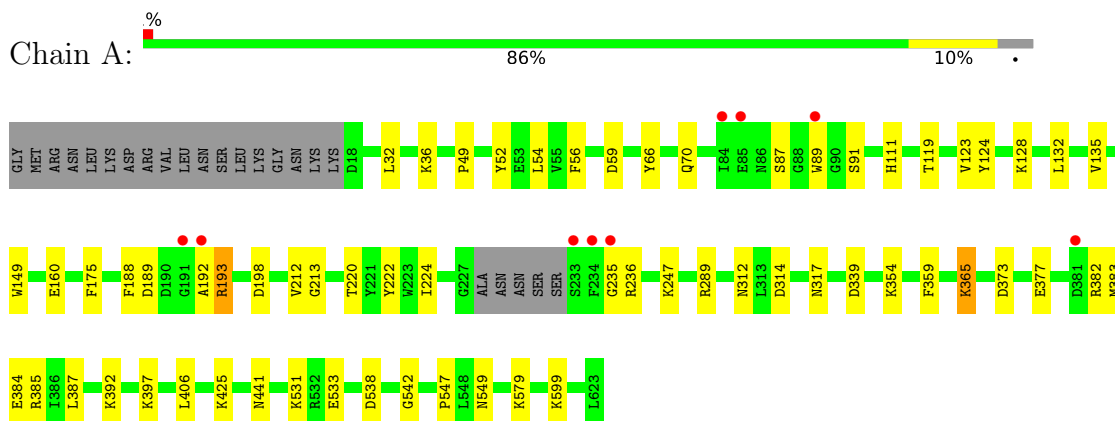
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
7	B	238	Total 238	O 238	0	0
7	C	201	Total 201	O 201	0	0
7	D	204	Total 204	O 204	0	0
7	E	180	Total 180	O 180	0	0
7	F	126	Total 126	O 126	0	0



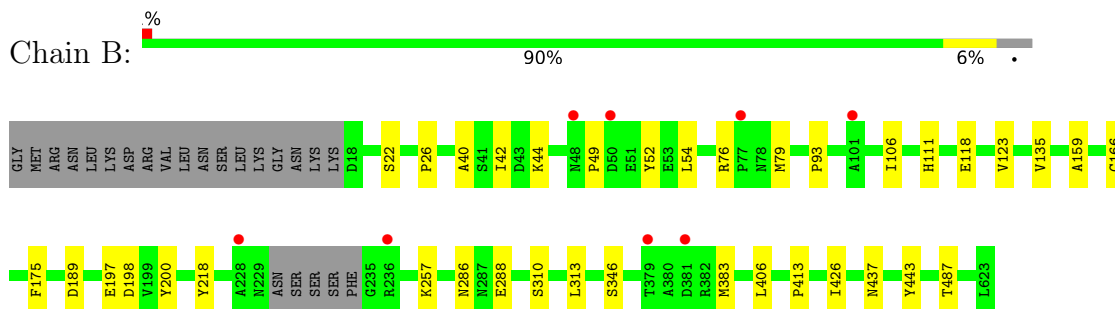
### 3 Residue-property plots [i](#)

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.

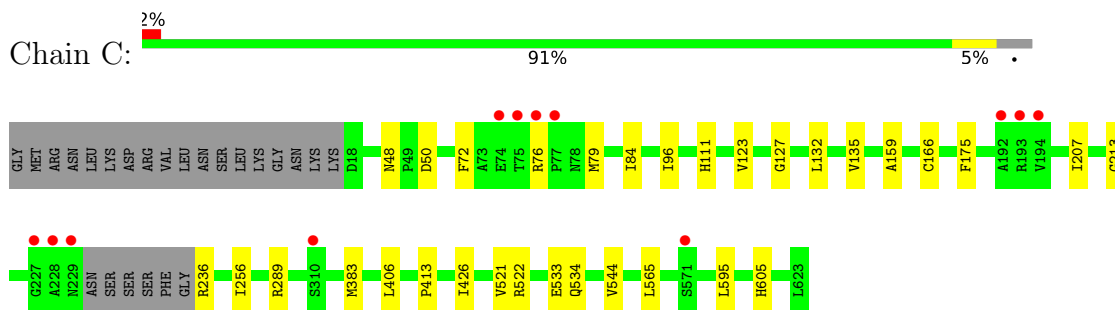
- Molecule 1: Glycosyltransferase



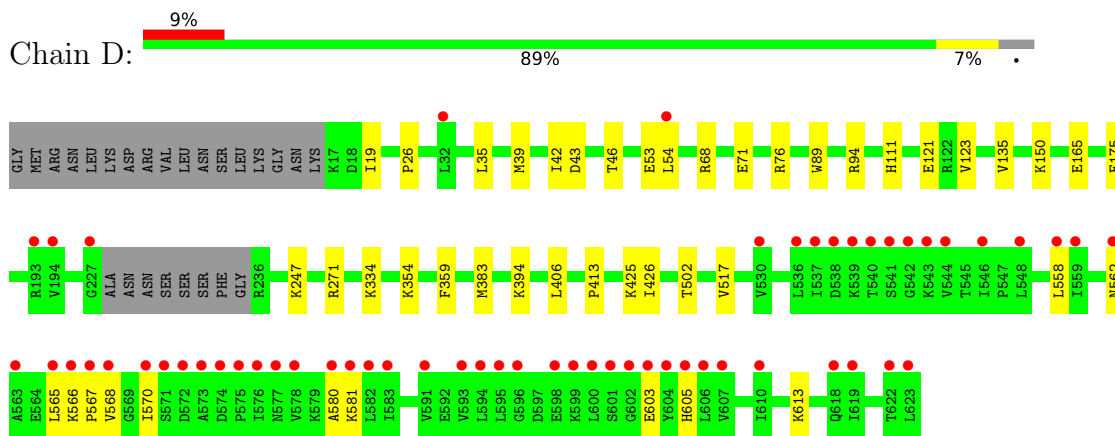
- Molecule 1: Glycosyltransferase



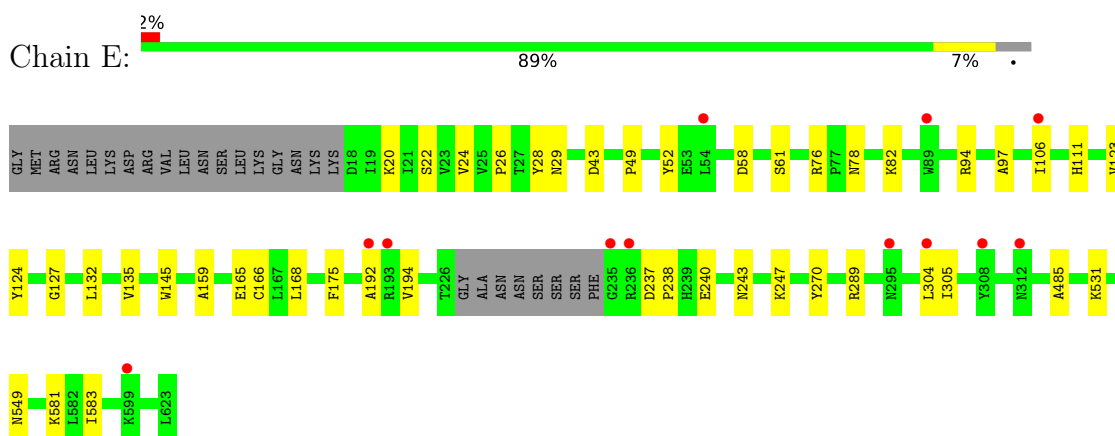
- Molecule 1: Glycosyltransferase



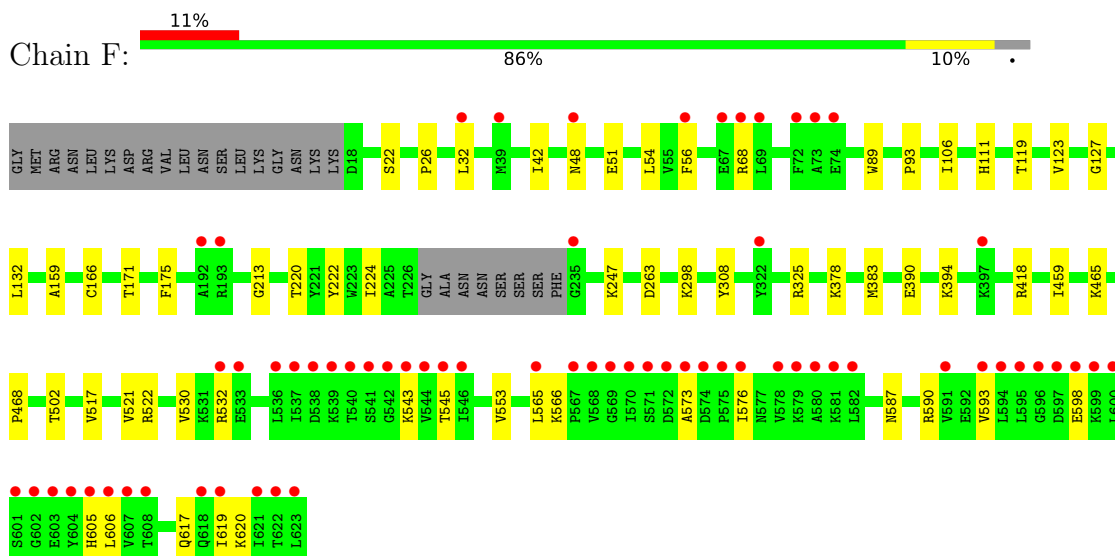
- Molecule 1: Glycosyltransferase



- 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, $R_{free}$	0.187 , 0.215 0.184 , 0.212	Depositor DCC
$R_{free}$ test set	11129 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.6	Xtrriage
Anisotropy	0.360	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 37.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	30744	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtrriage'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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MG, CL, TAR, TRH, GOL

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	0.38	0/4997	0.53	0/6748
1	B	0.29	0/4976	0.50	0/6719
1	C	0.28	0/4972	0.49	0/6714
1	D	0.29	0/4968	0.50	0/6707
1	E	0.28	0/4959	0.49	0/6696
1	F	0.28	0/4959	0.50	0/6696
All	All	0.30	0/29831	0.50	0/40280

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	4895	0	4828	48	0
1	B	4877	0	4816	20	0
1	C	4873	0	4813	19	0
1	D	4869	0	4815	30	0
1	E	4860	0	4802	25	0
1	F	4860	0	4802	32	0
2	A	35	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	0	0
7	C	201	0	0	1	0
7	D	204	0	0	3	0
7	E	180	0	0	0	0
7	F	126	0	0	0	0
All	All	30744	0	29092	176	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 (176) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:89[A]:TRP:CE3	1:A:193:ARG:CG	2.87	0.56
1:D:425:LYS:NZ	7:D:808:HOH:O	2.38	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: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:B:76:ARG:HD2	1:B:79:MET:HE3	1.90	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:N	1:A:198:ASP:OD1	2.42	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:89:TRP:HZ2	2:D:701:TRH:HC63	1.76	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: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:A:533:GLU:H	1:A:533:GLU:CD	2.15	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:A:124:TYR:OH	1:A:128:LYS:HD3	2.13	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: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
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:D:35:LEU:HD11	1:D:39:MET:HE2	1.98	0.46
1:A:89[B]:TRP:HZ2	2:A:701:TRH:HC63	1.80	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:298:LYS:NZ	1:F:325:ARG:O	2.48	0.45
1:A:59:ASP:CG	1:A:87:SER:H	2.20	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:43:ASP:CG	1:D:76:ARG:HH12	2.21	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:A:235:GLY:O	1:A:236:ARG:C	2.54	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:599:LYS:HG3	1:A:599:LYS:O	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	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
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 [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	535/553 (97%)	531 (99%)	4 (1%)	84	91
1	B	533/553 (96%)	531 (100%)	2 (0%)	91	96
1	C	533/553 (96%)	532 (100%)	1 (0%)	93	97
1	D	533/553 (96%)	531 (100%)	2 (0%)	91	96
1	E	532/553 (96%)	531 (100%)	1 (0%)	93	97
1	F	532/553 (96%)	529 (99%)	3 (1%)	86	93
All	All	3198/3318 (96%)	3185 (100%)	13 (0%)	91	96

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	HIS
1	A	193	ARG
1	A	247	LYS
1	A	365	LYS
1	B	111	HIS
1	B	189	ASP
1	C	111	HIS
1	D	111	HIS
1	D	334	LYS
1	E	111	HIS
1	F	111	HIS
1	F	171	THR
1	F	247	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides 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
5	GOL	B	706	-	5,5,5	0.06	0	5,5,5	0.31	0
4	TAR	C	703	-	9,9,9	1.28	2 (22%)	12,12,12	1.04	0
5	GOL	B	705	-	5,5,5	0.12	0	5,5,5	0.30	0
5	GOL	E	705	-	5,5,5	0.09	0	5,5,5	0.30	0
4	TAR	F	704	-	9,9,9	1.19	2 (22%)	12,12,12	1.15	0
4	TAR	B	704	-	9,9,9	1.20	2 (22%)	12,12,12	1.10	0
2	TRH	F	701	3	34,37,37	0.37	0	52,57,57	0.68	0
2	TRH	E	701	3	34,37,37	0.33	0	52,57,57	0.49	0
4	TAR	D	705	-	9,9,9	1.07	2 (22%)	12,12,12	1.04	0
2	TRH	D	701	3	34,37,37	0.34	0	52,57,57	0.51	0
4	TAR	A	703	-	9,9,9	1.29	2 (22%)	12,12,12	1.16	0
5	GOL	A	704	-	5,5,5	0.08	0	5,5,5	0.33	0
4	TAR	E	704	-	9,9,9	1.13	1 (11%)	12,12,12	1.03	0
2	TRH	C	701	3	34,37,37	0.34	0	52,57,57	0.83	4 (7%)
2	TRH	A	701	3	34,37,37	0.35	0	52,57,57	0.55	0
5	GOL	A	705	-	5,5,5	0.15	0	5,5,5	0.23	0
5	GOL	D	706	-	5,5,5	0.11	0	5,5,5	0.18	0
2	TRH	B	701	3	34,37,37	0.39	0	52,57,57	0.78	2 (3%)

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
5	GOL	B	706	-	-	2/4/4/4	-
4	TAR	C	703	-	-	10/12/12/12	-
5	GOL	B	705	-	-	0/4/4/4	-
5	GOL	E	705	-	-	2/4/4/4	-
4	TAR	F	704	-	-	4/12/12/12	-
4	TAR	B	704	-	-	10/12/12/12	-
2	TRH	F	701	3	-	4/21/53/53	0/3/3/3
2	TRH	E	701	3	-	4/21/53/53	0/3/3/3
4	TAR	D	705	-	-	10/12/12/12	-
2	TRH	D	701	3	-	8/21/53/53	0/3/3/3
4	TAR	A	703	-	-	10/12/12/12	-
5	GOL	A	704	-	-	2/4/4/4	-
4	TAR	E	704	-	-	6/12/12/12	-
2	TRH	C	701	3	-	3/21/53/53	0/3/3/3
2	TRH	A	701	3	-	2/21/53/53	0/3/3/3
5	GOL	A	705	-	-	2/4/4/4	-
5	GOL	D	706	-	-	3/4/4/4	-
2	TRH	B	701	3	-	7/21/53/53	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	703	TAR	O11-C1	-2.75	1.21	1.30
4	F	704	TAR	O11-C1	-2.60	1.22	1.30
4	A	703	TAR	O11-C1	-2.53	1.22	1.30
4	A	703	TAR	O41-C4	-2.45	1.22	1.30
4	E	704	TAR	O11-C1	-2.43	1.22	1.30
4	B	704	TAR	O41-C4	-2.41	1.22	1.30
4	D	705	TAR	O11-C1	-2.26	1.23	1.30
4	B	704	TAR	O11-C1	-2.21	1.23	1.30
4	C	703	TAR	O41-C4	-2.15	1.23	1.30
4	F	704	TAR	O41-C4	-2.03	1.23	1.30
4	D	705	TAR	O41-C4	-2.00	1.24	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	701	TRH	P2-O1-C1	3.59	133.61	119.74
2	B	701	TRH	O5-C1-O1	2.74	114.95	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	TRH	P2-O1-C1	2.53	129.51	119.74
2	C	701	TRH	O5-C1-O1	2.27	114.34	111.36
2	C	701	TRH	OPP-P2-O1	2.20	106.92	102.48
2	C	701	TRH	O1-C1-C2	-2.12	104.50	108.38

There are no chirality outliers.

All (89) 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	C	701	TRH	C1-O1-P2-OPP
2	C	701	TRH	O5-C1-O1-P2
2	D	701	TRH	C1-O1-P2-O4P
2	D	701	TRH	O5-C1-O1-P2
2	E	701	TRH	O5-C1-O1-P2
2	F	701	TRH	C1-O1-P2-O4P
4	A	703	TAR	C1-C2-C3-C4
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	A	703	TAR	C1-C2-C3-O3
4	B	704	TAR	O2-C2-C3-O3
4	A	703	TAR	O2-C2-C3-C4
4	C	703	TAR	C1-C2-C3-O3
4	C	703	TAR	O2-C2-C3-C4
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

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

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Mol	Chain	Res	Type	Atoms
4	D	705	TAR	C2-C3-C4-O4
2	F	701	TRH	C4'-C5'-O5'-P
4	D	705	TAR	C2-C3-C4-O41
2	B	701	TRH	C4'-C5'-O5'-P
4	A	703	TAR	O1-C1-C2-C3
2	B	701	TRH	C5'-O5'-P-OPP
2	D	701	TRH	C5'-O5'-P-OPP
2	D	701	TRH	C1-O1-P2-O3P
2	E	701	TRH	C1-O1-P2-OPP
2	D	701	TRH	C4'-C5'-O5'-P
2	B	701	TRH	C5'-O5'-P-O1P
2	B	701	TRH	C5'-O5'-P-O2P
2	D	701	TRH	C5'-O5'-P-O2P
2	A	701	TRH	C4'-C5'-O5'-P

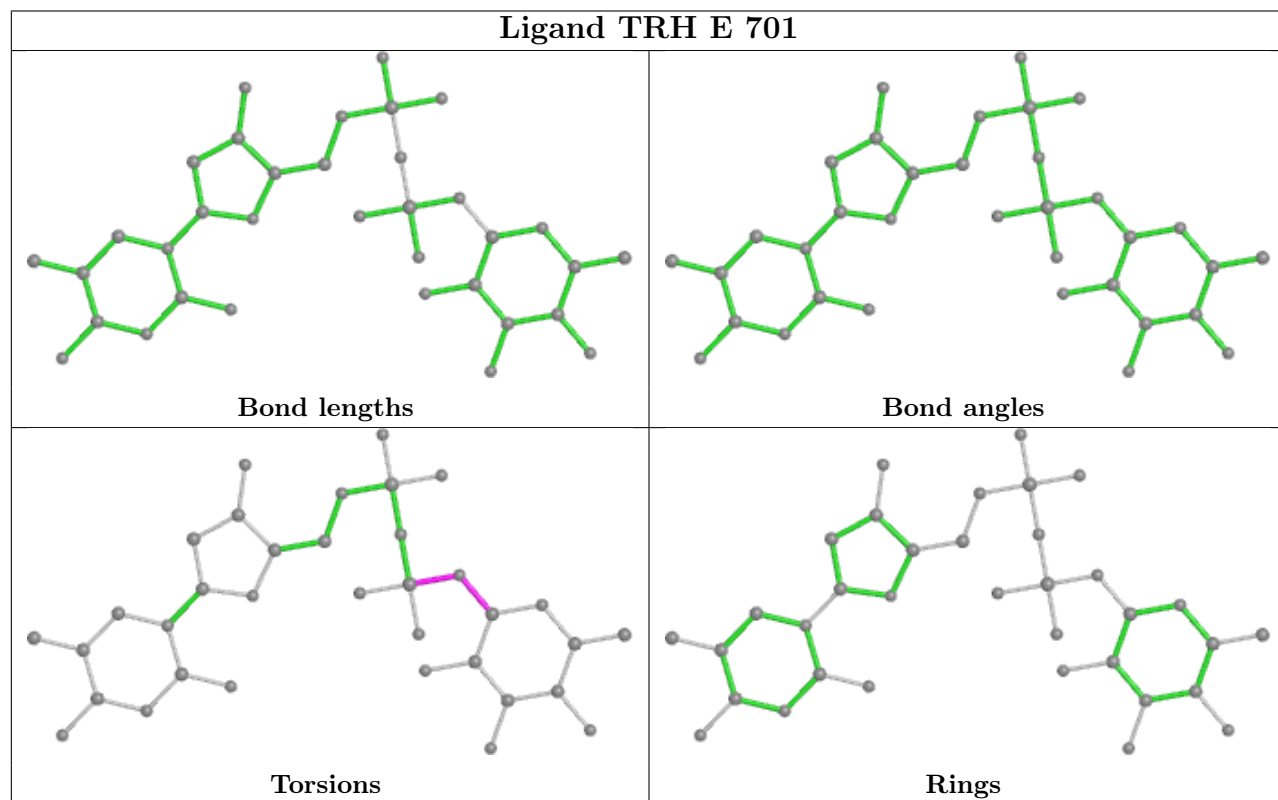
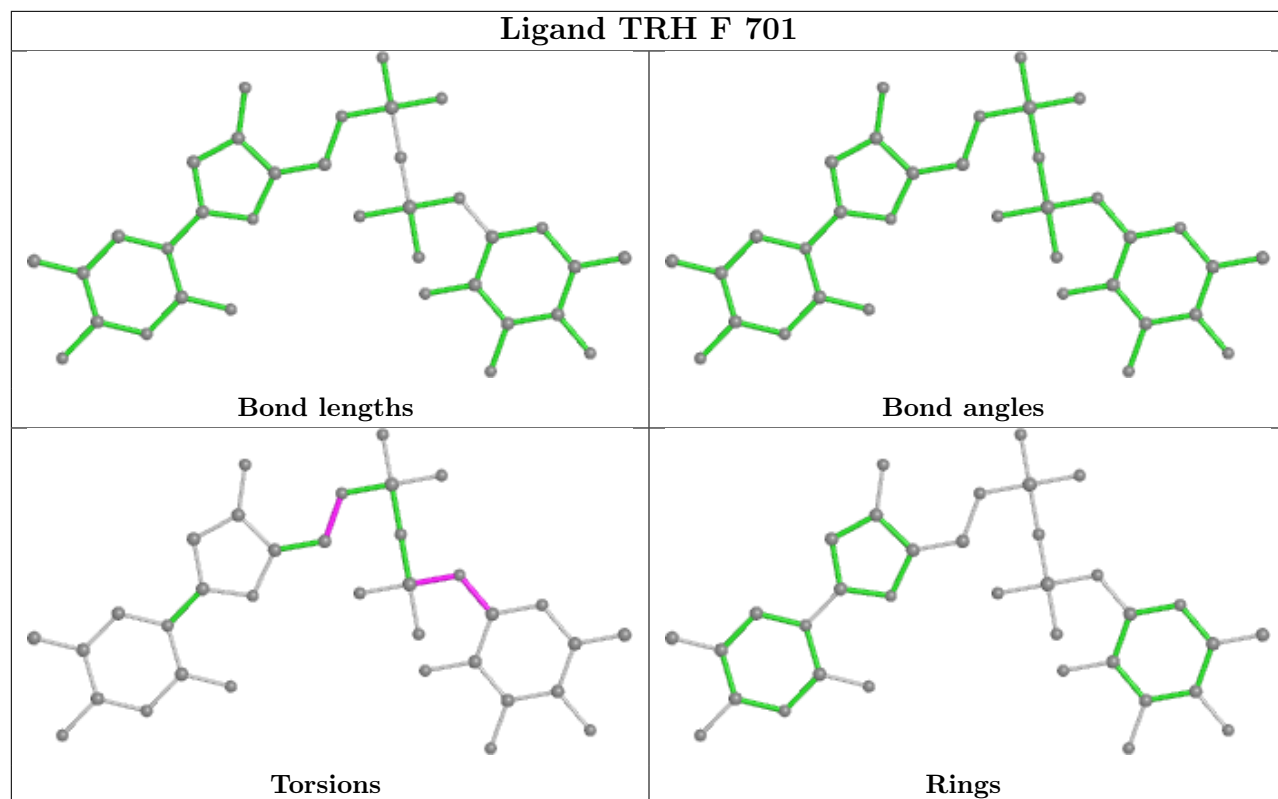
There are no ring outliers.

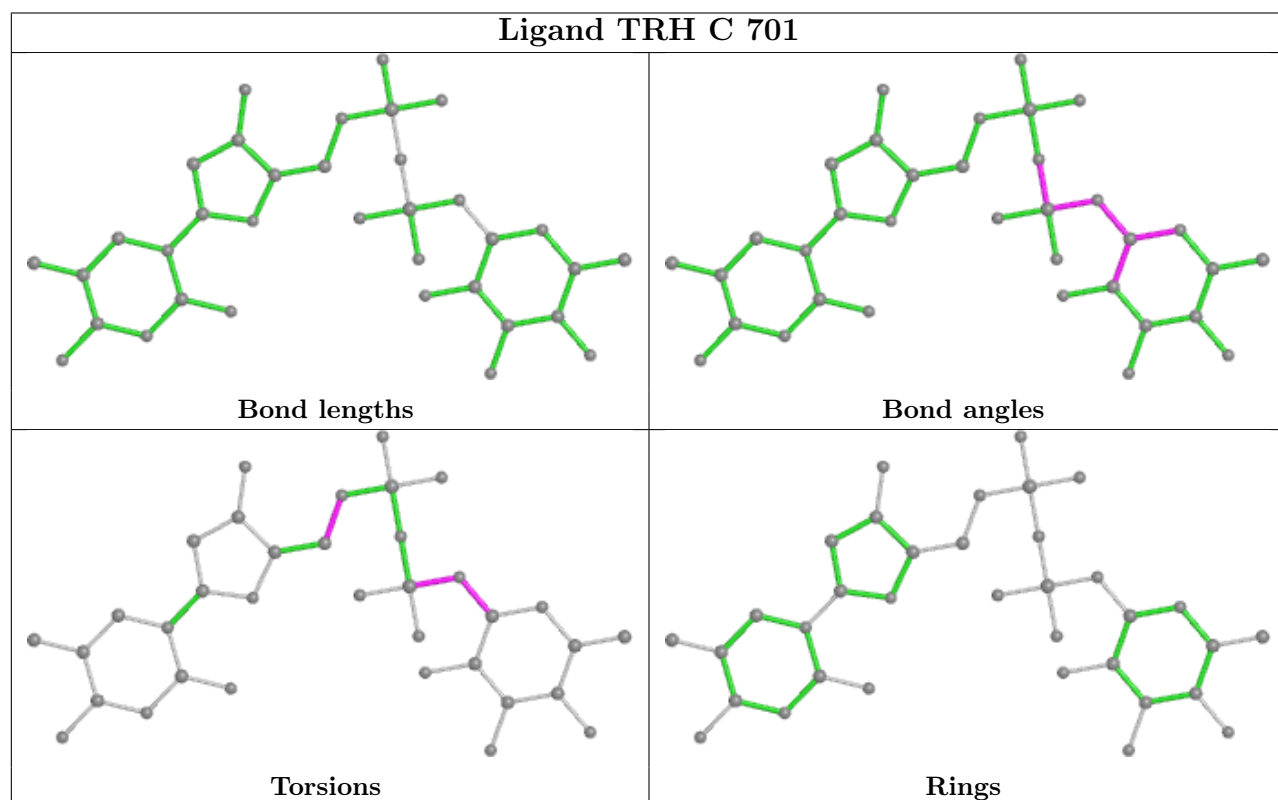
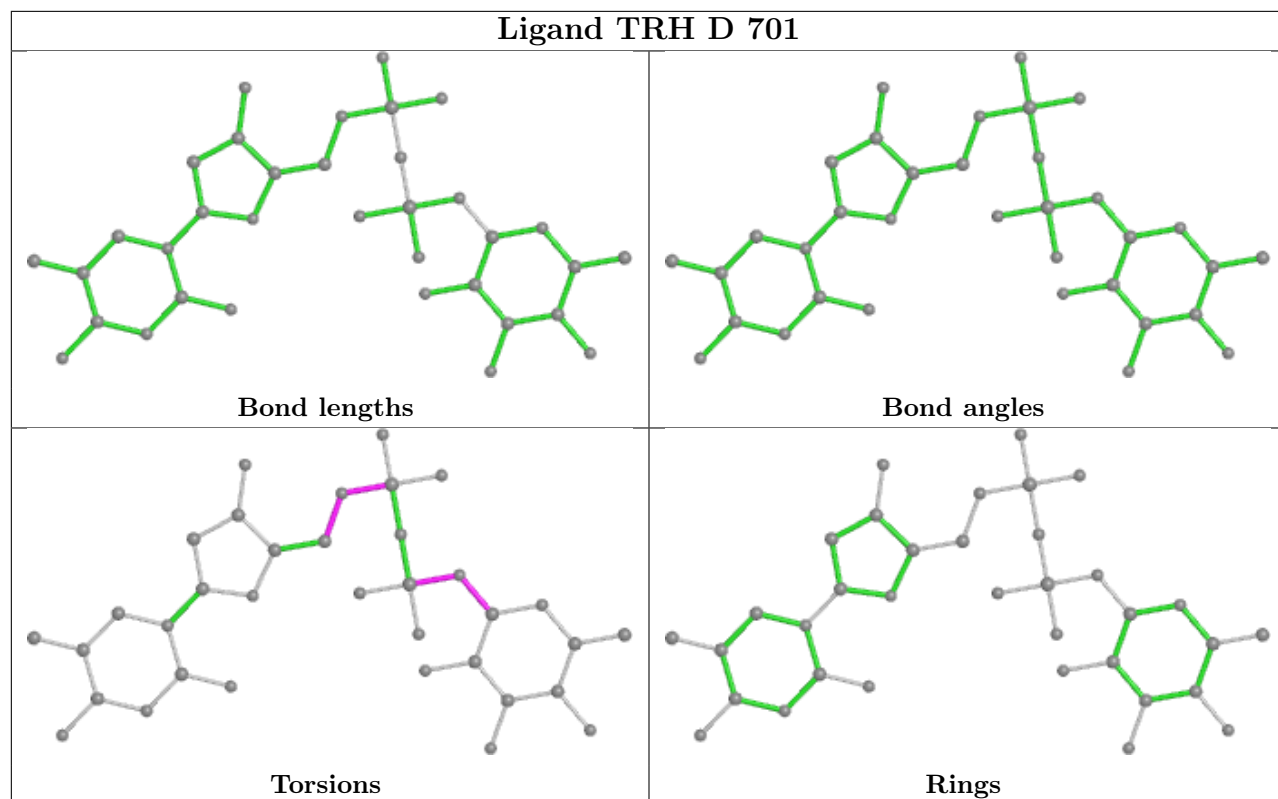
6 monomers are involved in 8 short contacts:

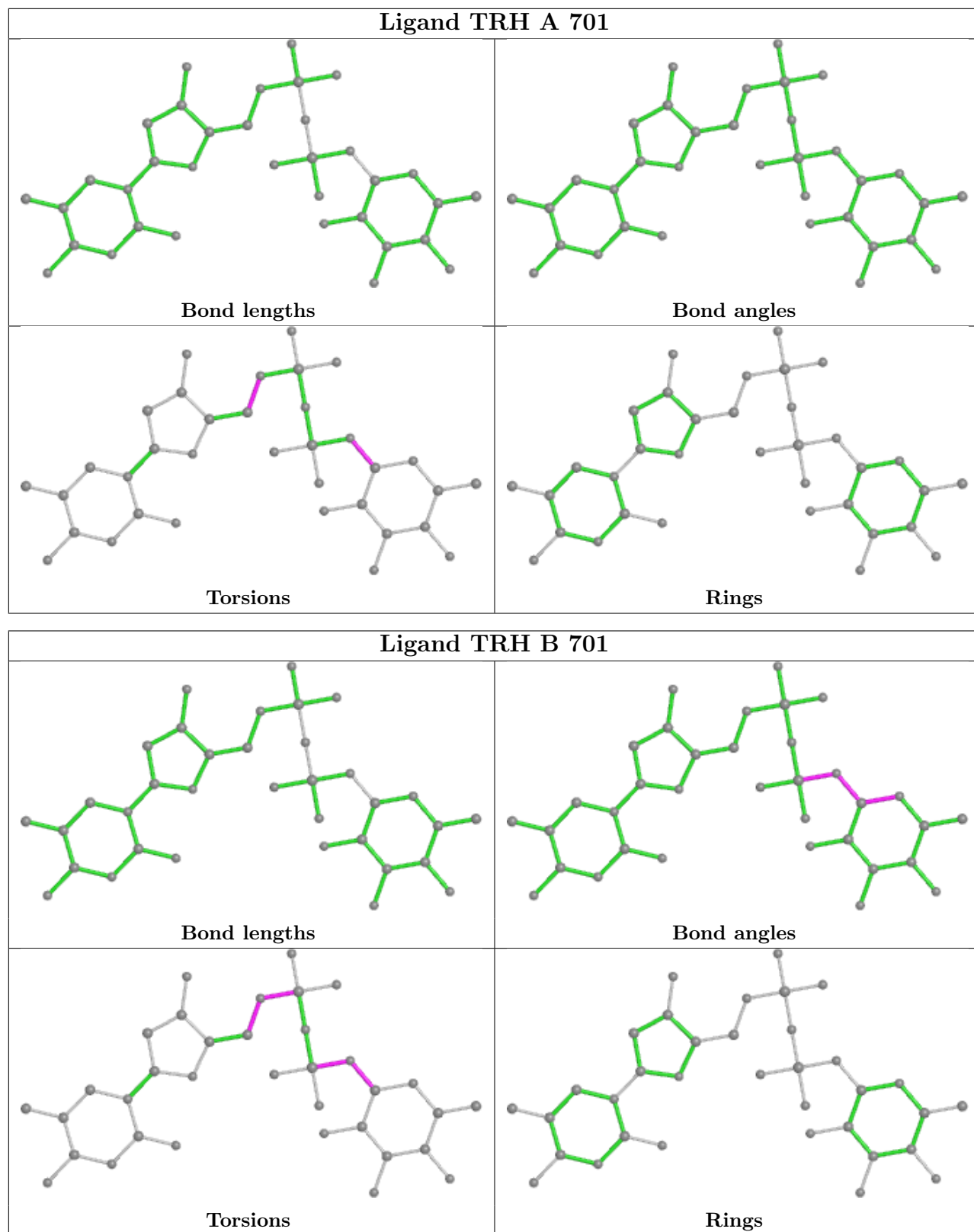
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	701	TRH	1	0
2	D	701	TRH	2	0
4	A	703	TAR	1	0
4	E	704	TAR	1	0
2	A	701	TRH	2	0
5	A	705	GOL	1	0

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

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	601/624 (96%)	0.12	9 (1%) 73 72	27, 48, 86, 120	0
1	B	601/624 (96%)	0.18	8 (1%) 77 75	31, 51, 80, 111	0
1	C	600/624 (96%)	0.10	12 (2%) 65 63	35, 51, 79, 136	0
1	D	599/624 (95%)	0.48	58 (9%) 7 6	31, 54, 116, 166	0
1	E	598/624 (95%)	0.16	12 (2%) 65 63	31, 59, 96, 131	0
1	F	598/624 (95%)	0.60	66 (11%) 5 4	35, 64, 120, 165	0
All	All	3597/3744 (96%)	0.27	165 (4%) 32 31	27, 54, 97, 166	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	569	GLY	10.0
1	F	573	ALA	9.6
1	D	595	LEU	8.5
1	F	571	SER	8.5
1	F	595	LEU	7.8
1	D	573	ALA	7.7
1	D	568	VAL	7.5
1	F	623	LEU	7.4
1	F	604	TYR	7.4
1	F	568	VAL	7.0
1	F	600	LEU	6.8
1	F	574	ASP	6.0
1	D	537	ILE	5.8
1	D	598	GLU	5.7
1	D	604	TYR	5.6
1	D	570	ILE	5.6
1	D	542	GLY	5.4
1	D	577	ASN	5.4
1	F	602	GLY	5.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	544	VAL	5.3
1	A	234	PHE	5.2
1	F	575	PRO	5.1
1	F	537	ILE	4.9
1	F	235	GLY	4.9
1	D	536	LEU	4.9
1	F	579	LYS	4.8
1	D	566	LYS	4.8
1	D	593	VAL	4.7
1	D	623	LEU	4.7
1	D	546	ILE	4.7
1	A	89[A]	TRP	4.6
1	F	622	THR	4.6
1	C	228	ALA	4.6
1	F	543	LYS	4.6
1	D	544	VAL	4.5
1	D	567	PRO	4.5
1	C	227	GLY	4.4
1	D	578	VAL	4.3
1	F	621	ILE	4.3
1	F	619	ILE	4.3
1	A	191	GLY	4.3
1	F	594	LEU	4.3
1	D	607	VAL	4.2
1	F	597	ASP	4.2
1	F	580	ALA	4.1
1	D	572	ASP	4.1
1	D	606	LEU	4.1
1	D	602	GLY	4.1
1	F	538	ASP	4.0
1	F	541	SER	3.9
1	D	558	LEU	3.9
1	D	576	ILE	3.9
1	F	533	GLU	3.9
1	F	599	LYS	3.8
1	F	578	VAL	3.8
1	D	571	SER	3.7
1	D	530	VAL	3.7
1	D	596	GLY	3.7
1	E	89	TRP	3.7
1	C	229	ASN	3.7
1	F	540	THR	3.7

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	536	LEU	3.6
1	F	606	LEU	3.6
1	A	85	GLU	3.6
1	D	575	PRO	3.6
1	D	574	ASP	3.6
1	D	594	LEU	3.5
1	F	576	ILE	3.5
1	C	193	ARG	3.4
1	A	235	GLY	3.4
1	F	565	LEU	3.4
1	A	192	ALA	3.4
1	F	593	VAL	3.4
1	D	599	LYS	3.4
1	F	603	GLU	3.3
1	F	570	ILE	3.3
1	F	572	ASP	3.2
1	E	304	LEU	3.2
1	D	580	ALA	3.2
1	D	562	ASN	3.2
1	F	542	GLY	3.2
1	B	77	PRO	3.1
1	F	192	ALA	3.1
1	F	581	LYS	3.1
1	F	69	LEU	3.0
1	F	607	VAL	3.0
1	A	84	ILE	3.0
1	D	581	LYS	3.0
1	F	605	HIS	3.0
1	D	619	ILE	3.0
1	F	322	TYR	2.9
1	A	233	SER	2.9
1	D	618	GLN	2.9
1	F	598	GLU	2.9
1	D	541	SER	2.9
1	D	591	VAL	2.9
1	D	565	LEU	2.9
1	D	622	THR	2.9
1	D	601	SER	2.9
1	F	193	ARG	2.8
1	D	582	LEU	2.8
1	D	605	HIS	2.8
1	F	545	THR	2.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	591	VAL	2.8
1	F	39	MET	2.8
1	B	48	ASN	2.8
1	F	32	LEU	2.7
1	D	538	ASP	2.7
1	F	596	GLY	2.7
1	D	600	LEU	2.7
1	F	608	THR	2.7
1	D	548	LEU	2.7
1	B	50	ASP	2.7
1	B	379	THR	2.7
1	F	74	GLU	2.7
1	D	610	ILE	2.7
1	F	546	ILE	2.7
1	B	381	ASP	2.7
1	F	397	LYS	2.7
1	C	571	SER	2.6
1	F	567	PRO	2.6
1	D	603	GLU	2.6
1	E	235	GLY	2.6
1	E	308	TYR	2.6
1	F	68	ARG	2.5
1	D	540	THR	2.5
1	B	101	ALA	2.5
1	C	192	ALA	2.5
1	F	67	GLU	2.5
1	F	532	ARG	2.4
1	C	76	ARG	2.4
1	E	312	ASN	2.4
1	F	72	PHE	2.4
1	D	193	ARG	2.4
1	C	194	VAL	2.4
1	F	582	LEU	2.4
1	F	618	GLN	2.4
1	E	295	ASN	2.4
1	D	54	LEU	2.4
1	E	193	ARG	2.3
1	D	583	ILE	2.3
1	E	106	ILE	2.3
1	B	236	ARG	2.3
1	C	310	SER	2.3
1	F	539	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	236	ARG	2.3
1	D	559	ILE	2.3
1	E	192	ALA	2.3
1	D	194	VAL	2.2
1	D	563	ALA	2.2
1	B	228	ALA	2.2
1	A	381	ASP	2.2
1	F	56	PHE	2.1
1	C	75	THR	2.1
1	D	32	LEU	2.1
1	F	73	ALA	2.1
1	C	77	PRO	2.1
1	E	599	LYS	2.1
1	F	48	ASN	2.1
1	F	601	SER	2.1
1	C	74	GLU	2.0
1	D	543	LYS	2.0
1	E	54	LEU	2.0
1	D	227	GLY	2.0
1	D	539	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 monosaccharides 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<sup>th</sup> 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.

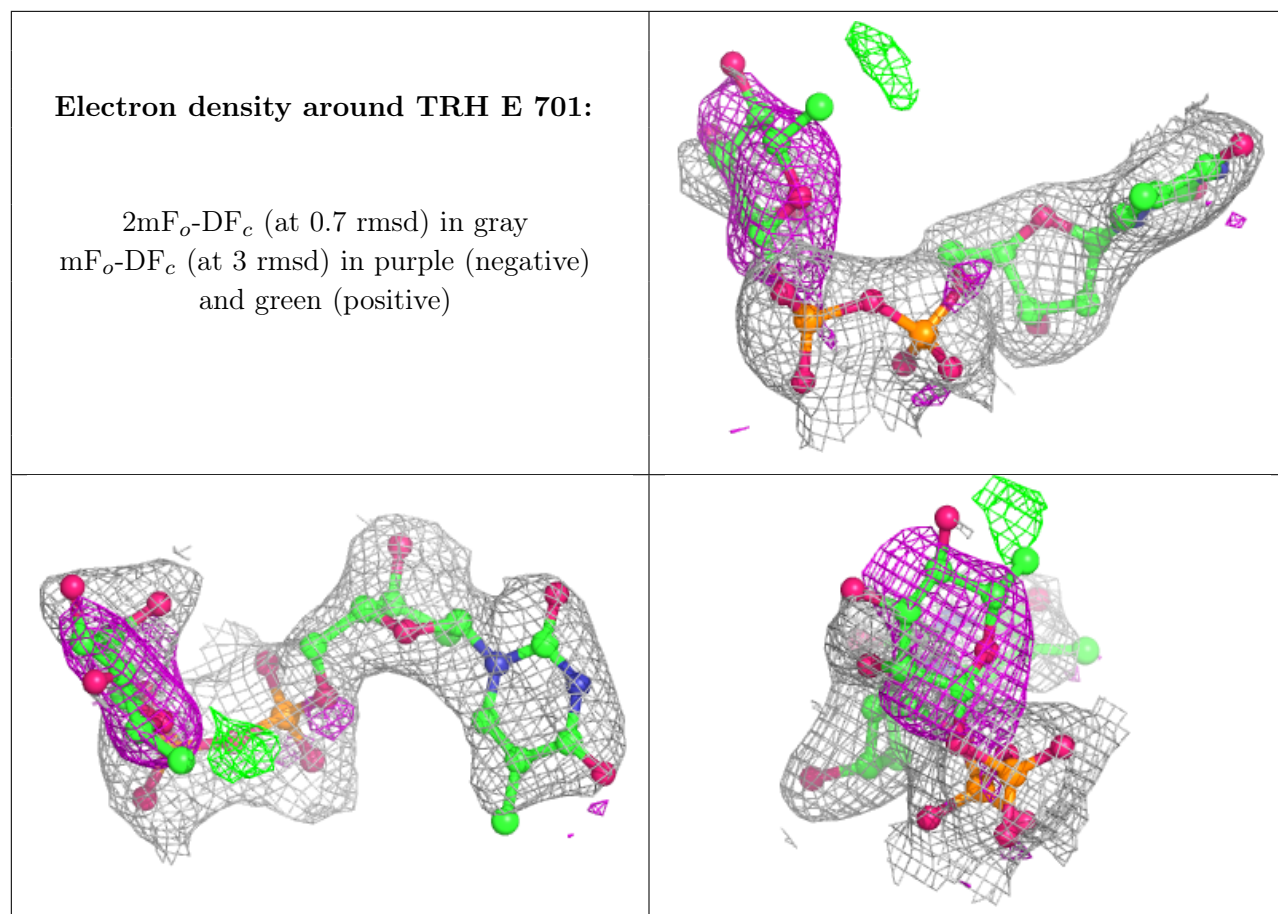
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
3	MG	A	702	1/1	0.74	0.09	53,53,53,53	0
5	GOL	A	705	6/6	0.75	0.22	56,64,66,68	0
5	GOL	A	704	6/6	0.77	0.19	50,59,62,66	0

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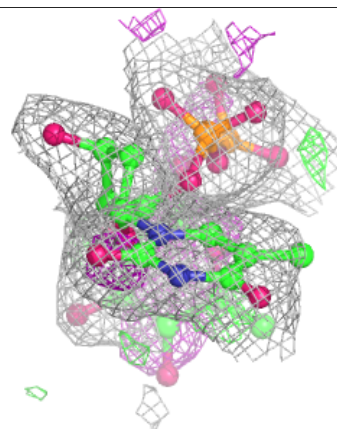
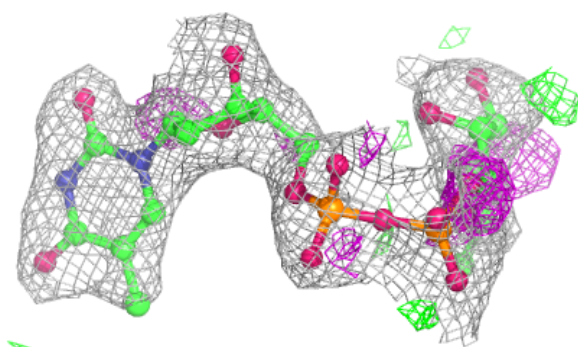
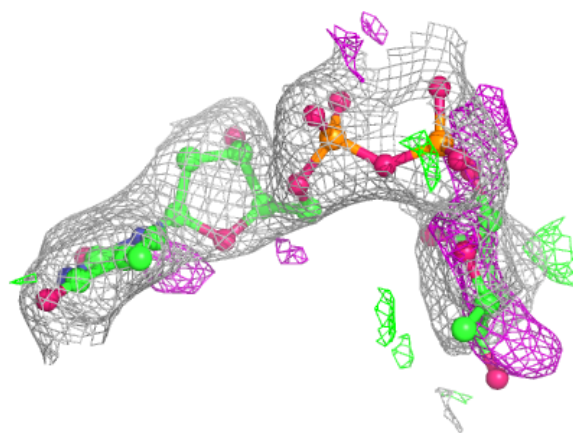
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	GOL	B	706	6/6	0.78	0.23	49,60,68,69	0
4	TAR	D	705	10/10	0.82	0.21	46,54,59,62	0
4	TAR	C	703	10/10	0.82	0.19	47,56,60,61	0
3	MG	B	702	1/1	0.85	0.12	52,52,52,52	0
4	TAR	E	704	10/10	0.85	0.19	54,58,65,67	0
4	TAR	F	704	10/10	0.85	0.22	47,51,61,61	0
5	GOL	E	705	6/6	0.86	0.14	69,71,72,75	0
2	TRH	E	701	35/35	0.87	0.24	62,72,82,83	0
3	MG	D	702	1/1	0.87	0.15	50,50,50,50	0
2	TRH	A	701	35/35	0.88	0.19	53,70,82,84	0
4	TAR	B	704	10/10	0.89	0.15	43,54,59,64	0
5	GOL	B	705	6/6	0.89	0.21	56,61,64,65	0
3	MG	C	702	1/1	0.89	0.10	49,49,49,49	0
5	GOL	D	706	6/6	0.89	0.18	51,56,57,59	0
4	TAR	A	703	10/10	0.89	0.17	43,49,57,57	0
2	TRH	F	701	35/35	0.90	0.17	53,68,77,81	0
2	TRH	D	701	35/35	0.91	0.18	51,60,76,79	0
2	TRH	B	701	35/35	0.92	0.18	44,59,71,73	0
2	TRH	C	701	35/35	0.93	0.16	42,57,84,89	0
3	MG	F	702	1/1	0.93	0.06	53,53,53,53	0
3	MG	E	702	1/1	0.95	0.12	62,62,62,62	0
3	MG	B	703	1/1	0.95	0.28	39,39,39,39	0
6	CL	F	703	1/1	0.95	0.13	51,51,51,51	0
3	MG	D	703	1/1	0.98	0.29	31,31,31,31	0
6	CL	D	704	1/1	0.98	0.11	50,50,50,50	0
3	MG	E	703	1/1	0.98	0.18	27,27,27,27	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.

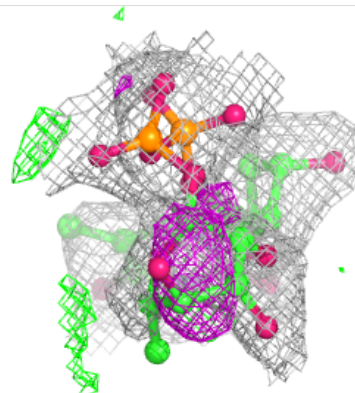
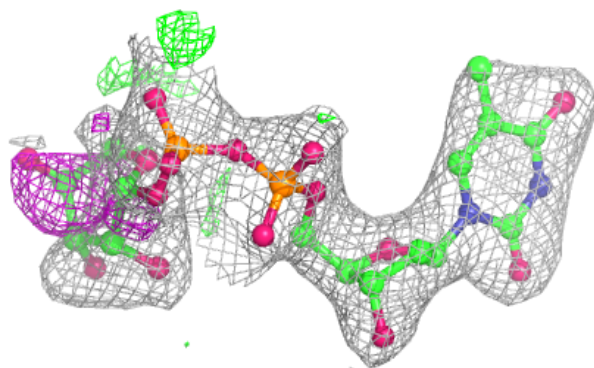
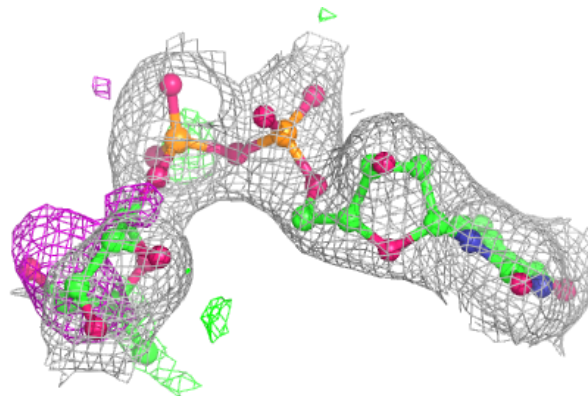


**Electron density around TRH A 701:**

$2mF_o-DF_c$  (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:**

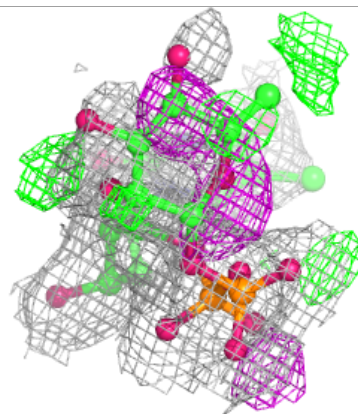
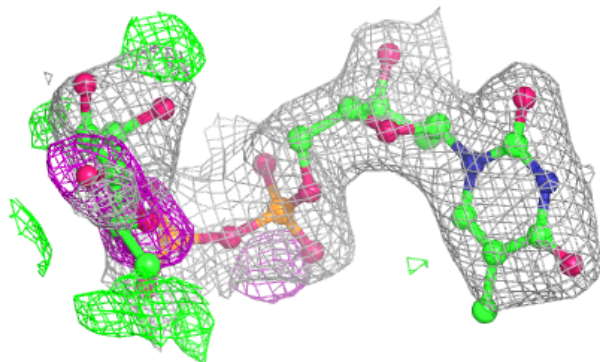
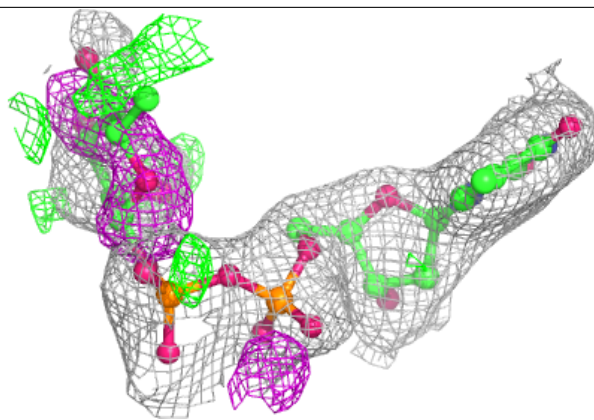
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



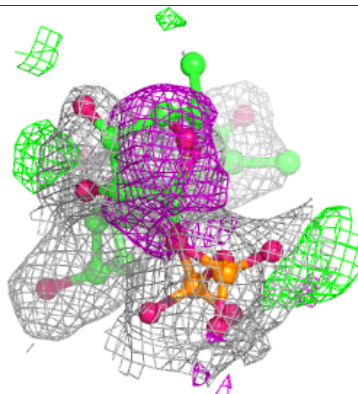
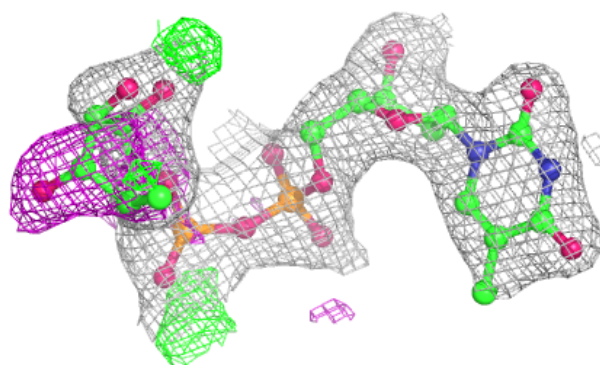
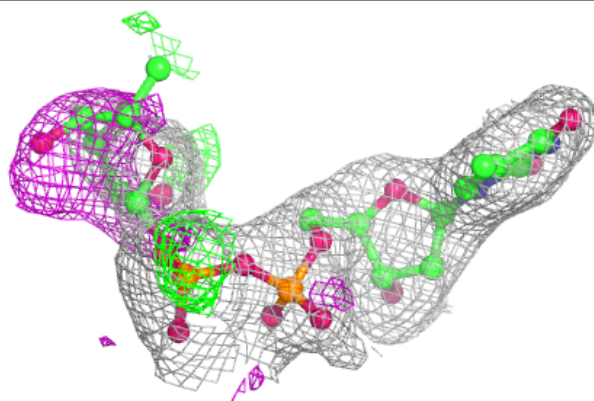


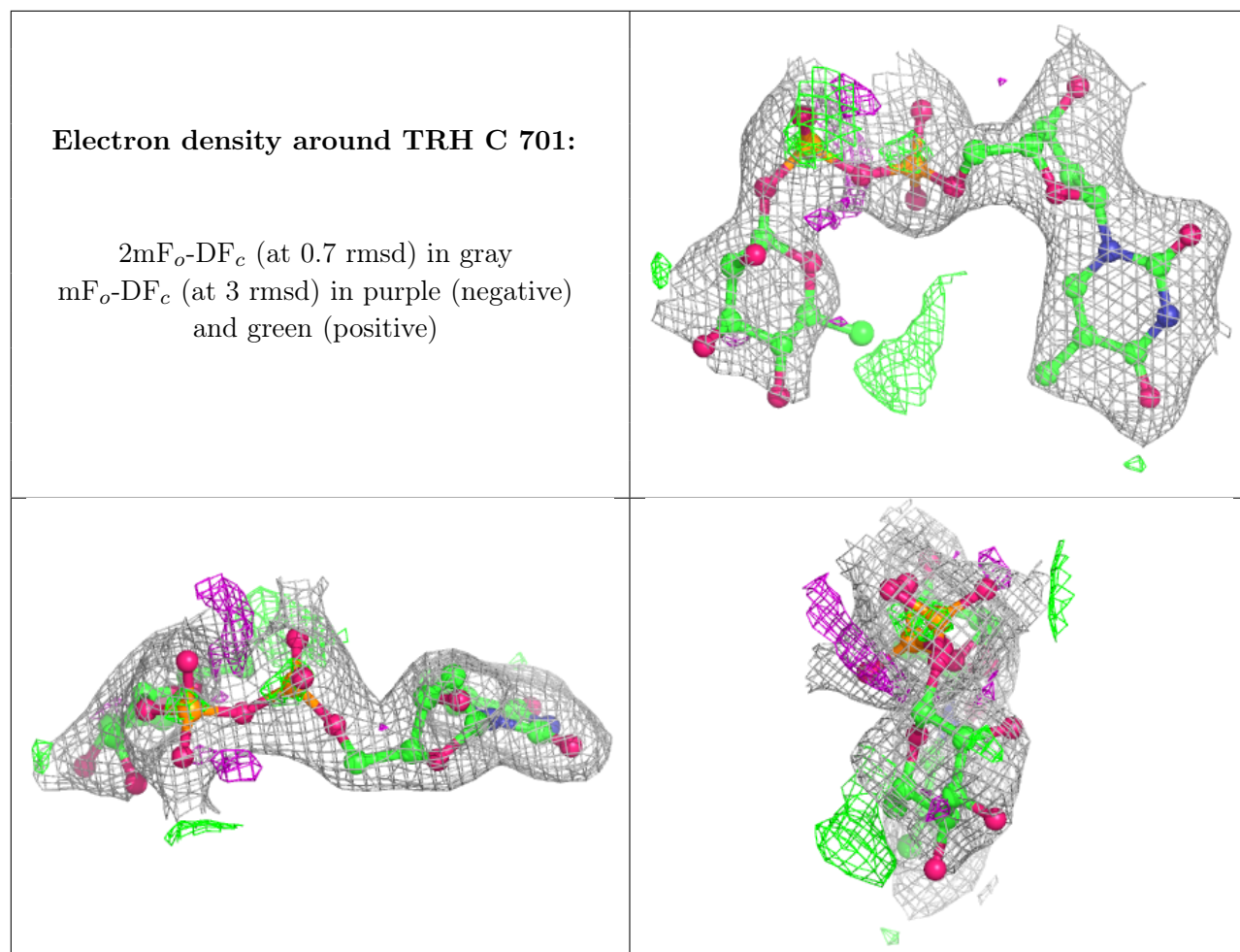
**Electron density around TRH D 701:**

$2mF_o-DF_c$  (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.