Full wwPDB X-ray Structure Validation Report (i)

Jul 4, 2022 – 04:11 pm BST

PDB ID	:	7QLP
Title	:	Structure of beta-lactamase TEM-171 complexed with tazobactam intermediate at 2.3 A resolution
Authors	:	Hakanpaa, J.; Petrova, T.; Samygina, V.R.; Lamzin, V.S.; Egorov, A.M.
Deposited on	:	2021-12-20
Resolution	:	2.30 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 (i) 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 (i)) were used in the production of this report:

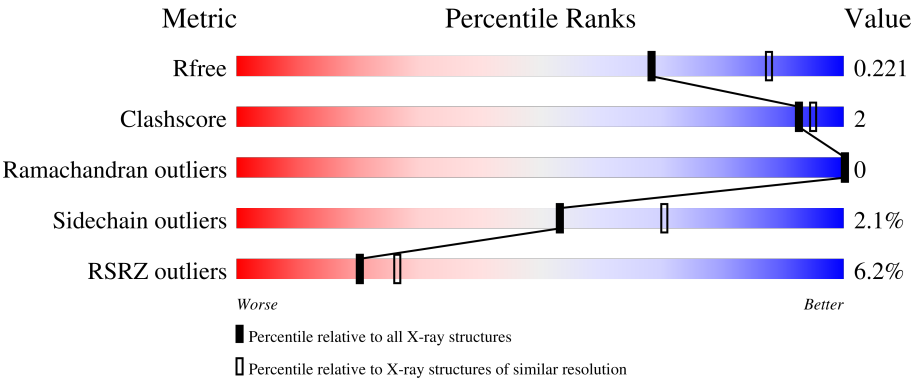
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	263	94% 6%
1	B	263	3% 96%
1	C	263	94% 6%
1	D	263	97%
1	E	263	% 97%

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Mol	Chain	Length	Quality of chain
1	F	263	32% 93% 6%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ACT	A	302	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13092 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.

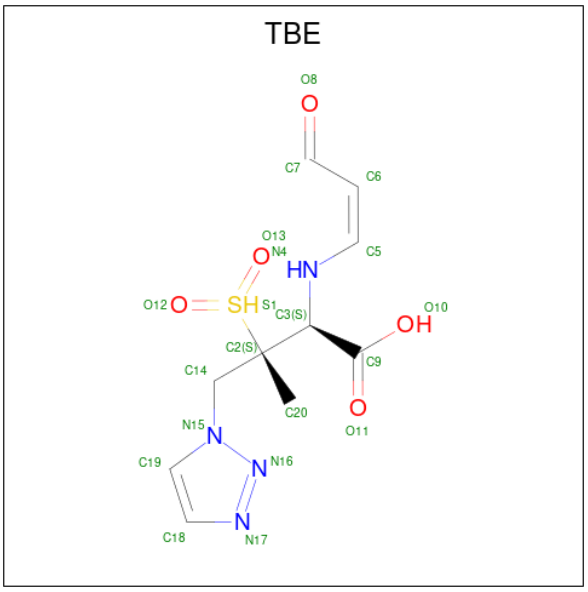
- Molecule 1 is a protein called Beta-lactamase TEM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2028	1266	360	391	11			
1	B	263	Total	C	N	O	S	0	0	0
			2028	1266	360	391	11			
1	C	263	Total	C	N	O	S	0	0	0
			2028	1266	360	391	11			
1	D	263	Total	C	N	O	S	0	0	0
			2028	1266	360	391	11			
1	E	263	Total	C	N	O	S	0	0	0
			2028	1266	360	391	11			
1	F	263	Total	C	N	O	S	0	0	0
			2028	1266	360	391	11			

There are 6 discrepancies between the modelled and reference sequences:

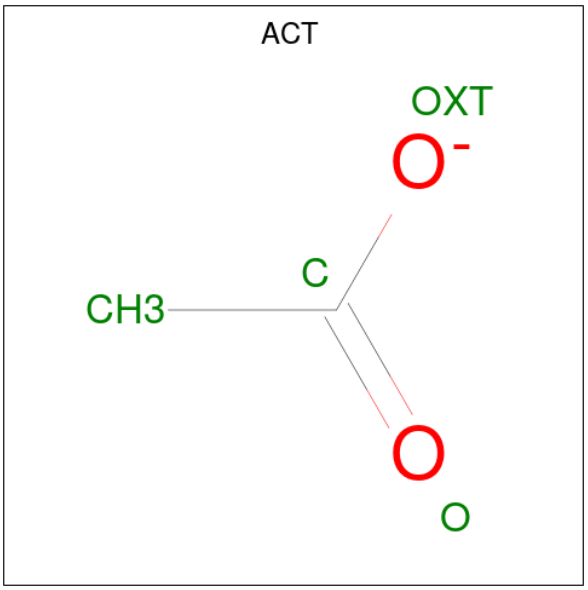
Chain	Residue	Modelled	Actual	Comment	Reference
A	84	ILE	VAL	engineered mutation	UNP P62593
B	84	ILE	VAL	engineered mutation	UNP P62593
C	84	ILE	VAL	engineered mutation	UNP P62593
D	84	ILE	VAL	engineered mutation	UNP P62593
E	84	ILE	VAL	engineered mutation	UNP P62593
F	84	ILE	VAL	engineered mutation	UNP P62593

- Molecule 2 is TAZOBACTAM INTERMEDIATE (three-letter code: TBE) (formula: $C_{10}H_{14}N_4O_5S$) (labeled as "Ligand of Interest" by depositor).



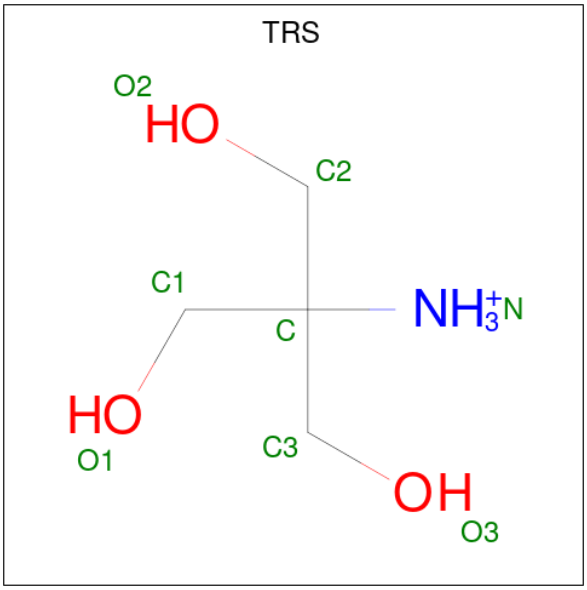
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			20	10	4	5	1		
2	C	1	Total	C	N	O	S	0	0
			20	10	4	5	1		
2	D	1	Total	C	N	O	S	0	0
			20	10	4	5	1		
2	E	1	Total	C	N	O	S	0	0
			20	10	4	5	1		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



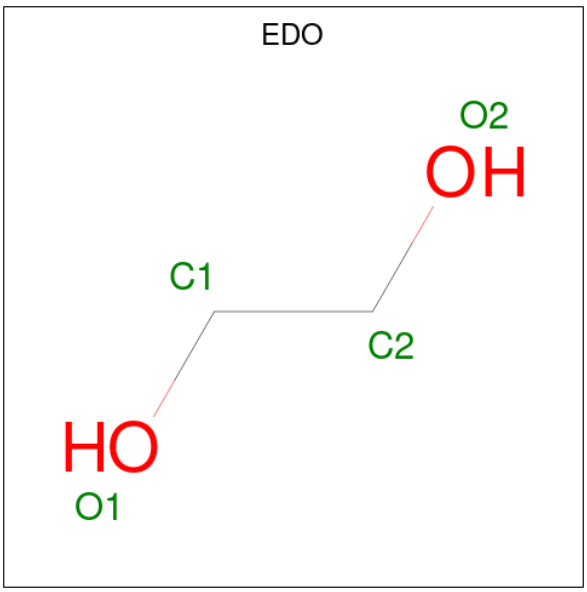
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 8 4 1 3	0	0

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

- Molecule 6 is water.

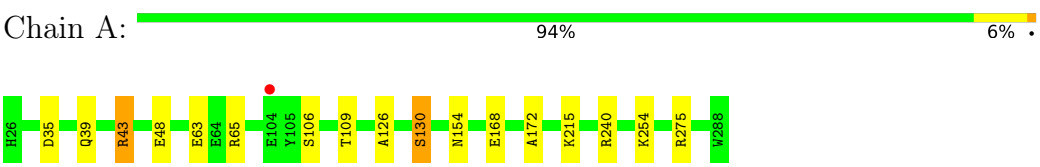
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	212	Total O 212 212	0	2
6	B	57	Total O 57 57	0	0
6	C	233	Total O 233 233	0	6
6	D	167	Total O 167 167	0	0
6	E	149	Total O 149 149	0	3
6	F	10	Total O 10 10	0	0

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.

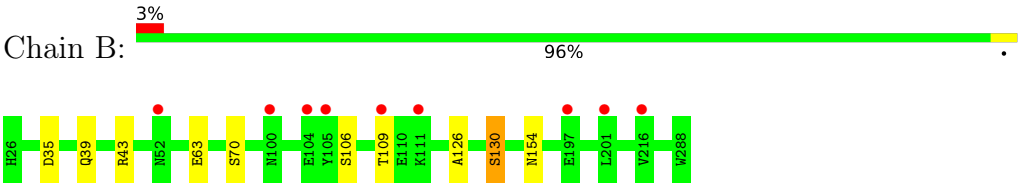
• Molecule 1: Beta-lactamase TEM

Chain A:



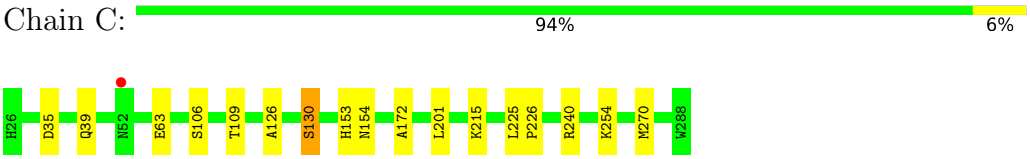
• Molecule 1: Beta-lactamase TEM

Chain B:



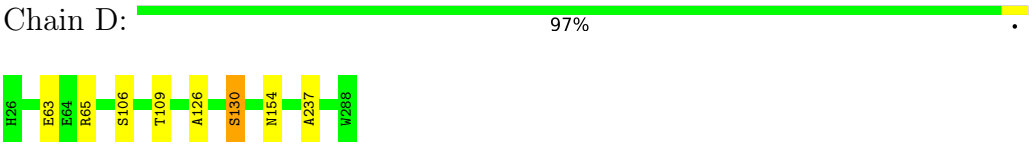
• Molecule 1: Beta-lactamase TEM

Chain C:



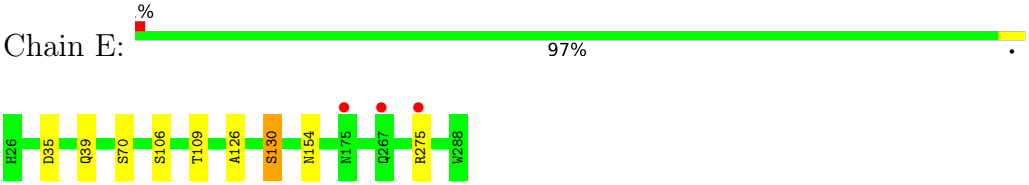
• Molecule 1: Beta-lactamase TEM

Chain D:



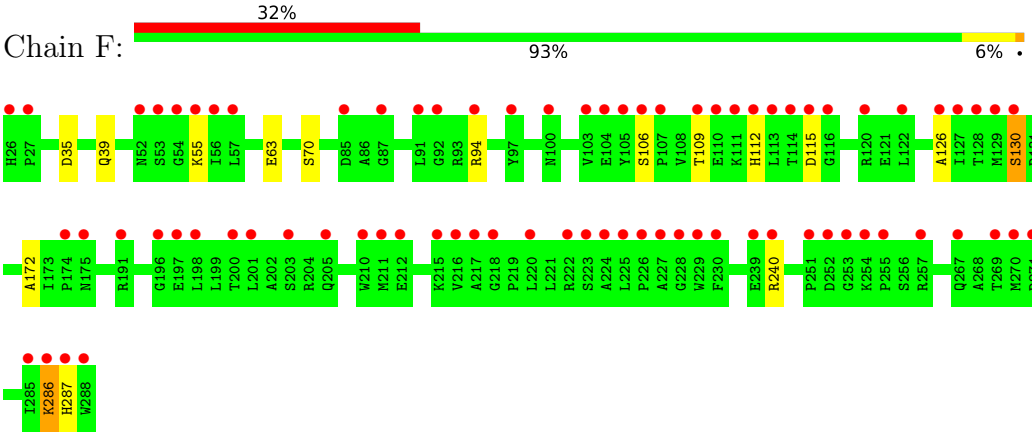
• Molecule 1: Beta-lactamase TEM

Chain E:



• Molecule 1: Beta-lactamase TEM

Chain F:


32%
93%
6%
H26 P27 D35 Q39 N52 S53 G54 K55 I56 L57 E63 S70 D85 A86 G87 L91 G92 R93 R94 Y97 N100 V103 E104 Y105 S106 P107 V108 T109 E110 K111 H112 L113 T114 D115 G116 R120 E121 L122 A126 I127 T128 M129 S130 D131 N132 H153 N154
A172 I173 P174 N175 R191 G196 E197 L198 L199 T200 L201 A202 S203 R204 Q205 W210 M211 E212 K215 V216 A217 G218 P219 L220 L221 R222 S223 A224 L225 P226 A227 G228 W229 F230 E239 R240 P251 D252 G253 K254 P255 S256 R257 Q267 A268 T269 M270 D271 E272 R273 N274 R275
I285 K286 H287 W288

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	89.31Å 89.31Å 501.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.30 15.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.5 (15.00-2.30) 96.9 (15.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.85 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.189 , 0.217 0.196 , 0.221	Depositor DCC
R_{free} test set	4343 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å^2)	33.2	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13092	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TBE, TRS, ACT, EDO

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	0.78	2/2062 (0.1%)	0.86	1/2791 (0.0%)
1	B	0.72	0/2062	0.84	1/2791 (0.0%)
1	C	0.79	0/2062	0.86	0/2791
1	D	0.74	0/2062	0.86	1/2791 (0.0%)
1	E	0.75	0/2062	0.85	0/2791
1	F	0.73	0/2062	0.83	0/2791
All	All	0.75	2/12372 (0.0%)	0.85	3/16746 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	48	GLU	CD-OE1	5.59	1.31	1.25
1	A	168	GLU	CD-OE1	5.29	1.31	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	43	ARG	NE-CZ-NH1	-5.51	117.54	120.30
1	B	43	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	D	65	ARG	NE-CZ-NH2	-5.29	117.65	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2028	0	2035	7	0
1	B	2028	0	2036	3	0
1	C	2028	0	2035	12	0
1	D	2028	0	2035	3	0
1	E	2028	0	2035	3	0
1	F	2028	0	2036	8	0
2	A	20	0	12	0	0
2	C	20	0	12	0	0
2	D	20	0	12	1	0
2	E	20	0	12	1	0
3	A	4	0	3	2	0
4	A	8	0	12	0	0
5	D	4	0	6	0	0
6	A	212	0	0	1	1
6	B	57	0	0	0	0
6	C	233	0	0	7	0
6	D	167	0	0	0	0
6	E	149	0	0	0	0
6	F	10	0	0	3	0
All	All	13092	0	12281	37	1

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 (37) 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:43:ARG:HD3	3:A:302:ACT:O	1.55	1.06
1:F:112:HIS:CE1	6:F:304:HOH:O	2.37	0.77
1:C:201:LEU:HD12	6:C:493:HOH:O	1.89	0.72
1:F:115:ASP:HB2	6:F:302:HOH:O	1.90	0.71
1:C:215:LYS:CE	6:C:589:HOH:O	2.46	0.64
1:C:215:LYS:HE3	6:C:589:HOH:O	1.98	0.62
1:A:65:ARG:O	3:A:302:ACT:H1	2.07	0.55
1:A:215:LYS:HE3	6:A:563:HOH:O	2.10	0.51
1:C:201:LEU:CD1	6:C:493:HOH:O	2.50	0.50
1:F:94:ARG:NH1	6:F:302:HOH:O	2.44	0.50
1:C:215:LYS:HE2	6:C:589:HOH:O	2.12	0.47
1:C:270:MET:HE1	6:C:506:HOH:O	2.13	0.47
2:E:301:TBE:H19	2:E:301:TBE:O11	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:ALA:O	1:C:240:ARG:HD2	2.16	0.45
1:A:172:ALA:O	1:A:240:ARG:HD2	2.17	0.44
1:B:106:SER:HB3	1:B:109:THR:OG1	2.17	0.44
1:F:106:SER:HB3	1:F:109:THR:OG1	2.17	0.44
1:C:126:ALA:O	1:C:130:SER:HA	2.19	0.43
1:D:106:SER:HB3	1:D:109:THR:OG1	2.18	0.43
1:A:106:SER:HB3	1:A:109:THR:OG1	2.19	0.42
1:E:106:SER:HB3	1:E:109:THR:OG1	2.18	0.42
1:C:106:SER:HB3	1:C:109:THR:OG1	2.19	0.42
1:F:172:ALA:O	1:F:240:ARG:HD2	2.20	0.42
1:F:126:ALA:O	1:F:130:SER:HA	2.19	0.42
1:A:35:ASP:O	1:A:39:GLN:HG2	2.20	0.42
1:E:126:ALA:O	1:E:130:SER:HA	2.20	0.42
1:D:126:ALA:O	1:D:130:SER:HA	2.20	0.41
1:A:126:ALA:O	1:A:130:SER:HA	2.21	0.41
1:E:35:ASP:O	1:E:39:GLN:HG2	2.20	0.41
1:B:126:ALA:O	1:B:130:SER:HA	2.21	0.41
1:B:35:ASP:O	1:B:39:GLN:HG2	2.21	0.41
1:C:153:HIS:HB3	6:C:518:HOH:O	2.21	0.41
1:F:286:LYS:HE2	1:F:287:HIS:CE1	2.55	0.41
1:C:35:ASP:O	1:C:39:GLN:HG2	2.21	0.40
1:C:225:LEU:HA	1:C:226:PRO:HD3	1.95	0.40
1:D:237:ALA:O	2:D:301:TBE:H5	2.21	0.40
1:F:35:ASP:O	1:F:39:GLN:HG2	2.21	0.40

All (1) 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)
6:A:401:HOH:O	6:A:496:HOH:O[6_445]	2.00	0.20

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	261/263 (99%)	253 (97%)	8 (3%)	0	100	100
1	B	261/263 (99%)	253 (97%)	8 (3%)	0	100	100
1	C	261/263 (99%)	255 (98%)	6 (2%)	0	100	100
1	D	261/263 (99%)	253 (97%)	8 (3%)	0	100	100
1	E	261/263 (99%)	253 (97%)	8 (3%)	0	100	100
1	F	261/263 (99%)	253 (97%)	8 (3%)	0	100	100
All	All	1566/1578 (99%)	1520 (97%)	46 (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	217/217 (100%)	212 (98%)	5 (2%)	50	67
1	B	217/217 (100%)	213 (98%)	4 (2%)	59	75
1	C	217/217 (100%)	213 (98%)	4 (2%)	59	75
1	D	217/217 (100%)	214 (99%)	3 (1%)	67	81
1	E	217/217 (100%)	213 (98%)	4 (2%)	59	75
1	F	217/217 (100%)	210 (97%)	7 (3%)	39	54
All	All	1302/1302 (100%)	1275 (98%)	27 (2%)	53	70

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	GLU
1	A	130	SER
1	A	154	ASN
1	A	254	LYS
1	A	275	ARG

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Mol	Chain	Res	Type
1	B	63	GLU
1	B	70	SER
1	B	130	SER
1	B	154	ASN
1	C	63	GLU
1	C	130	SER
1	C	154	ASN
1	C	254	LYS
1	D	63	GLU
1	D	130	SER
1	D	154	ASN
1	E	70	SER
1	E	130	SER
1	E	154	ASN
1	E	275	ARG
1	F	55	LYS
1	F	63	GLU
1	F	70	SER
1	F	130	SER
1	F	154	ASN
1	F	275	ARG
1	F	286	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	267	GLN
1	F	90	GLN
1	F	287	HIS

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)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	TBE	A	301	1	16,20,20	1.24	2 (12%)	12,27,27	1.46	1 (8%)
2	TBE	C	301	1	16,20,20	1.38	3 (18%)	12,27,27	1.06	1 (8%)
2	TBE	E	301	1	16,20,20	1.52	3 (18%)	12,27,27	1.74	2 (16%)
5	EDO	D	302	-	3,3,3	0.20	0	2,2,2	0.28	0
3	ACT	A	302	-	3,3,3	0.74	0	3,3,3	1.44	0
2	TBE	D	301	1	16,20,20	1.18	2 (12%)	12,27,27	1.21	1 (8%)
4	TRS	A	303	-	7,7,7	0.19	0	9,9,9	0.52	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	TBE	A	301	1	-	4/18/26/26	0/1/1/1
2	TBE	C	301	1	-	3/18/26/26	0/1/1/1
2	TBE	E	301	1	-	5/18/26/26	0/1/1/1
5	EDO	D	302	-	-	1/1/1/1	-
2	TBE	D	301	1	-	3/18/26/26	0/1/1/1
4	TRS	A	303	-	-	3/9/9/9	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	301	TBE	C14-C2	3.85	1.57	1.53
2	E	301	TBE	C6-C7	-2.91	1.35	1.44
2	D	301	TBE	C14-C2	2.71	1.56	1.53
2	C	301	TBE	C6-C7	-2.69	1.36	1.44
2	A	301	TBE	C14-C2	2.56	1.56	1.53
2	C	301	TBE	C14-C2	2.48	1.56	1.53
2	D	301	TBE	C6-C7	-2.44	1.37	1.44
2	A	301	TBE	C2-S1	-2.21	1.82	1.86
2	C	301	TBE	O11-C9	2.18	1.28	1.22
2	E	301	TBE	N16-N15	2.09	1.38	1.34

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	301	TBE	C19-N15-N16	-4.96	108.58	111.72
2	A	301	TBE	C19-N15-N16	-3.97	109.21	111.72
2	D	301	TBE	C19-N15-N16	-3.03	109.81	111.72
2	C	301	TBE	C19-N15-N16	-2.76	109.97	111.72
2	E	301	TBE	C20-C2-C14	-2.28	104.83	112.35

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	TBE	C6-C5-N4-C3
2	A	301	TBE	N4-C5-C6-C7
2	A	301	TBE	C5-C6-C7-O8
2	C	301	TBE	C6-C5-N4-C3
2	C	301	TBE	N4-C5-C6-C7
2	C	301	TBE	C5-C6-C7-O8
2	D	301	TBE	C6-C5-N4-C3
2	D	301	TBE	N4-C5-C6-C7
2	D	301	TBE	C5-C6-C7-O8
2	E	301	TBE	C9-C3-N4-C5
2	E	301	TBE	C6-C5-N4-C3
2	E	301	TBE	C2-C14-N15-N16
2	E	301	TBE	C5-C6-C7-O8
4	A	303	TRS	C2-C-C1-O1
4	A	303	TRS	C3-C-C1-O1
4	A	303	TRS	N-C-C1-O1
5	D	302	EDO	O1-C1-C2-O2
2	A	301	TBE	N15-C14-C2-C20
2	E	301	TBE	N15-C14-C2-C20

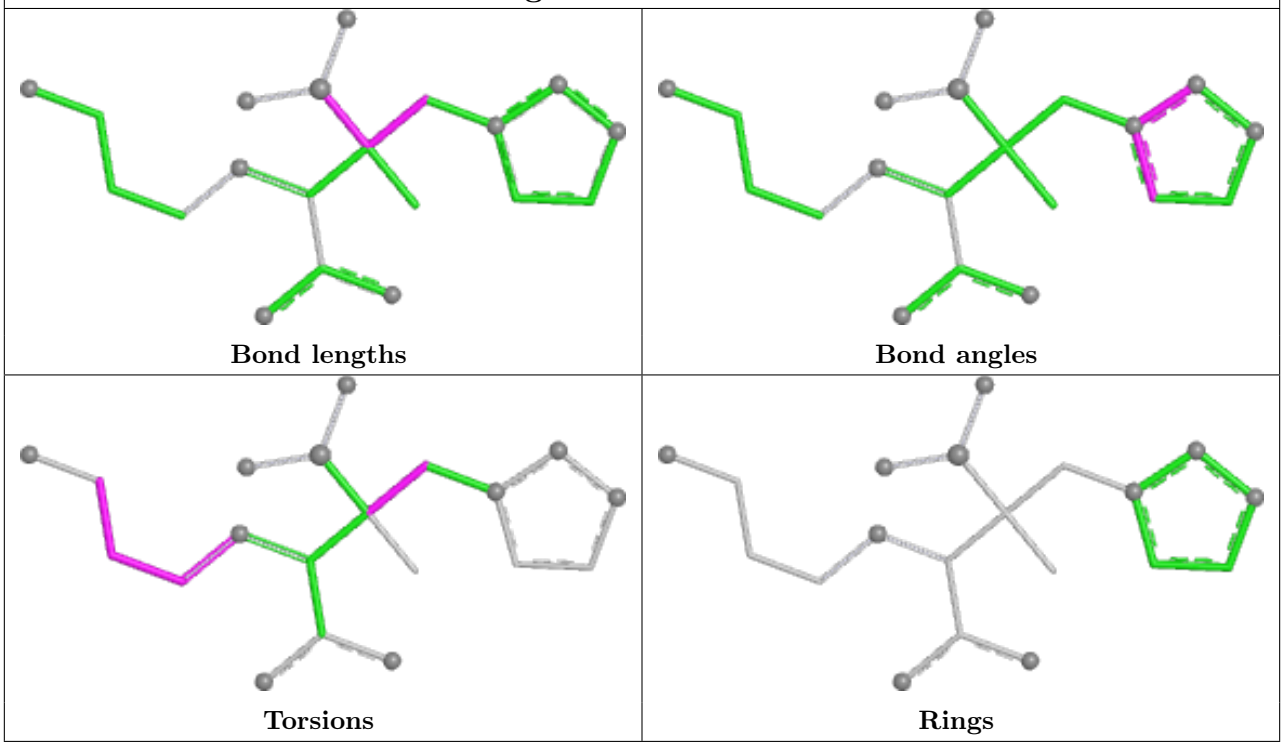
There are no ring outliers.

3 monomers are involved in 4 short contacts:

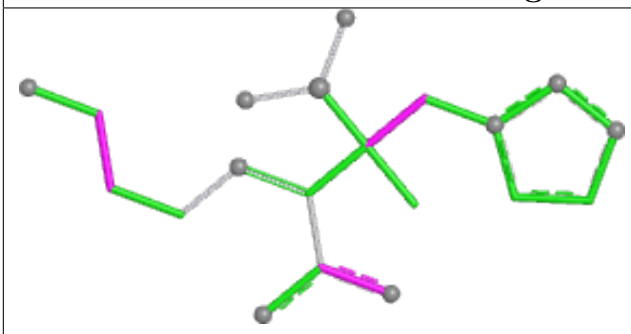
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	301	TBE	1	0
3	A	302	ACT	2	0
2	D	301	TBE	1	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

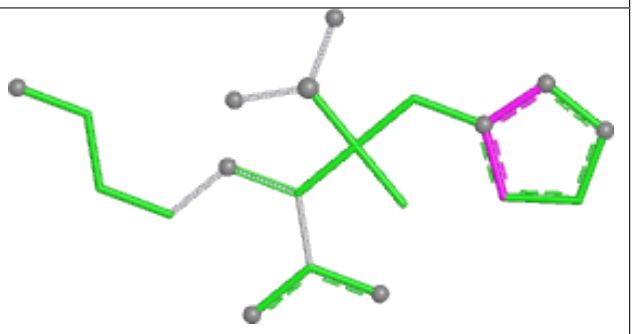
Ligand TBE A 301



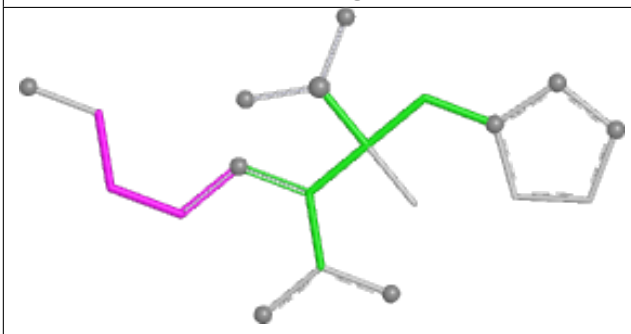
Ligand TBE C 301



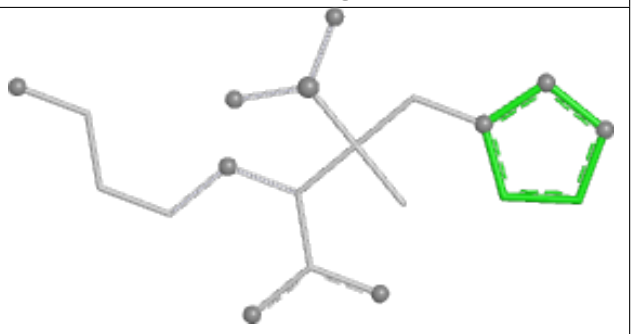
Bond lengths



Bond angles

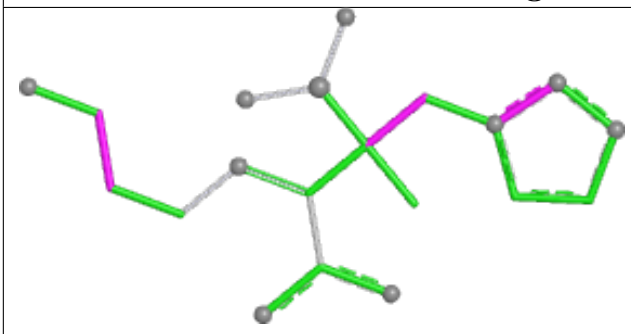


Torsions

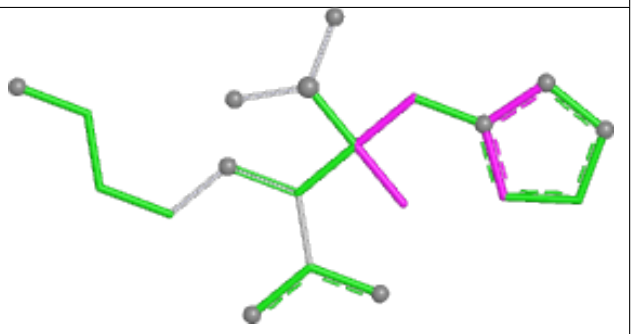


Rings

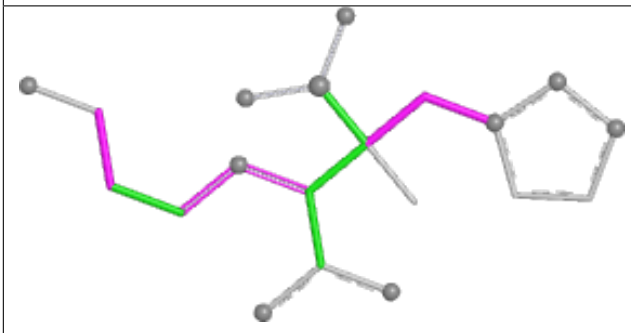
Ligand TBE E 301



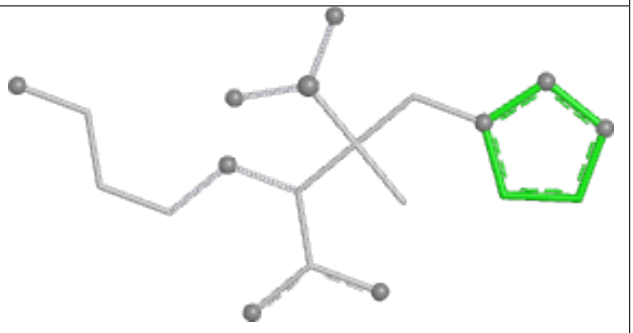
Bond lengths



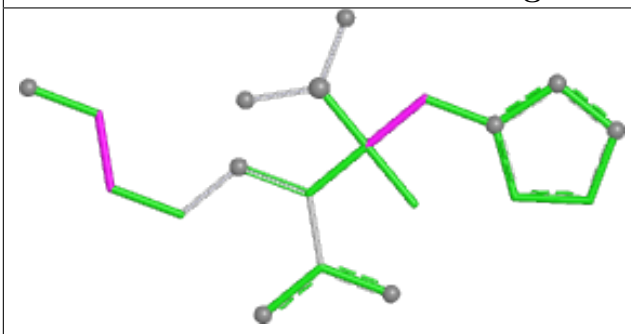
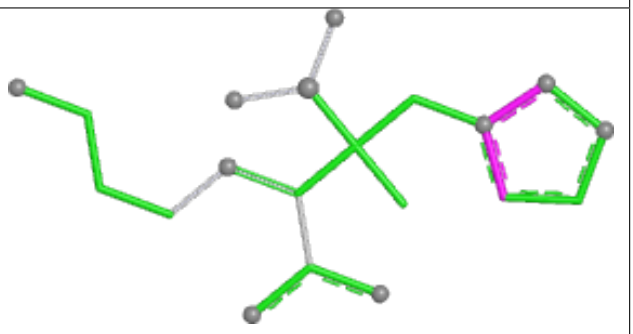
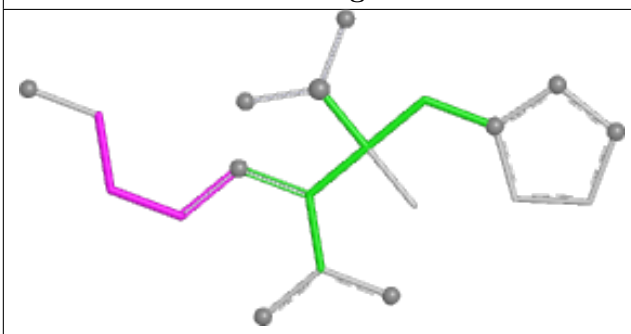
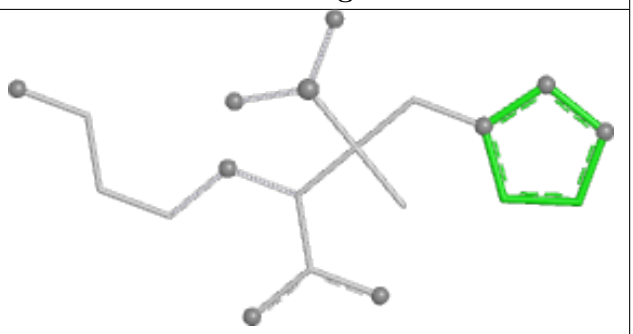
Bond angles



Torsions



Rings

Ligand TBE D 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	263/263 (100%)	-0.37	1 (0%) 92 95	21, 32, 50, 67	0
1	B	263/263 (100%)	0.09	9 (3%) 45 52	37, 54, 72, 86	0
1	C	263/263 (100%)	-0.41	1 (0%) 92 95	21, 30, 45, 55	0
1	D	263/263 (100%)	-0.32	0 100 100	24, 35, 52, 71	0
1	E	263/263 (100%)	-0.19	3 (1%) 80 85	24, 41, 64, 77	0
1	F	263/263 (100%)	1.53	84 (31%) 0 0	56, 81, 116, 124	0
All	All	1578/1578 (100%)	0.06	98 (6%) 20 26	21, 41, 94, 124	0

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	217	ALA	7.6
1	F	197	GLU	6.7
1	F	196	GLY	6.7
1	F	105	TYR	6.6
1	F	218	GLY	6.5
1	F	252	ASP	6.4
1	F	104	GLU	5.9
1	F	111	LYS	5.6
1	F	216	VAL	5.4
1	F	55	LYS	5.3
1	F	253	GLY	5.2
1	F	254	LYS	5.2
1	F	107	PRO	5.0
1	F	26	HIS	5.0
1	F	56	ILE	4.9
1	F	106	SER	4.8
1	B	52	ASN	4.7
1	F	222	ARG	4.7
1	F	223	SER	4.5

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Mol	Chain	Res	Type	RSRZ
1	F	27	PRO	4.5
1	F	215	LYS	4.4
1	F	112	HIS	4.3
1	F	239	GLU	4.3
1	F	114	THR	4.2
1	F	52	ASN	4.1
1	F	100	ASN	4.1
1	F	210	TRP	4.1
1	F	154	ASN	4.0
1	F	288	TRP	4.0
1	F	201	LEU	4.0
1	F	225	LEU	3.9
1	F	227	ALA	3.9
1	F	113	LEU	3.6
1	F	122	LEU	3.5
1	F	230	PHE	3.5
1	E	175	ASN	3.4
1	F	226	PRO	3.4
1	F	275	ARG	3.4
1	F	92	GLY	3.4
1	F	57	LEU	3.3
1	F	130	SER	3.3
1	F	110	GLU	3.2
1	F	54	GLY	3.2
1	F	127	ILE	3.2
1	F	271	ASP	3.2
1	F	286	LYS	3.1
1	F	87	GLY	3.1
1	F	200	THR	3.1
1	F	257	ARG	3.0
1	F	175	ASN	3.0
1	F	103	VAL	3.0
1	B	201	LEU	3.0
1	F	53	SER	3.0
1	F	132	ASN	2.9
1	F	153	HIS	2.9
1	F	91	LEU	2.9
1	F	272	GLU	2.9
1	F	97	TYR	2.9
1	F	120	ARG	2.9
1	F	255	PRO	2.9
1	E	267	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	224	ALA	2.8
1	F	211	MET	2.8
1	F	240	ARG	2.7
1	F	115	ASP	2.7
1	B	105	TYR	2.7
1	F	129	MET	2.6
1	F	228	GLY	2.6
1	B	109	THR	2.6
1	C	52	ASN	2.5
1	F	128	THR	2.5
1	F	109	THR	2.5
1	F	251	PRO	2.4
1	F	126	ALA	2.4
1	F	269	THR	2.4
1	F	273	ARG	2.4
1	A	104	GLU	2.4
1	F	203	SER	2.3
1	F	85	ASP	2.3
1	F	94	ARG	2.3
1	F	198	LEU	2.3
1	F	212	GLU	2.3
1	B	104	GLU	2.3
1	B	111	LYS	2.2
1	B	216	VAL	2.2
1	F	205	GLN	2.2
1	F	267	GLN	2.2
1	F	287	HIS	2.2
1	F	229	TRP	2.2
1	F	270	MET	2.2
1	F	116	GLY	2.2
1	B	100	ASN	2.1
1	B	197	GLU	2.1
1	F	220	LEU	2.1
1	F	174	PRO	2.1
1	E	275	ARG	2.0
1	F	285	ILE	2.0
1	F	191	ARG	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)

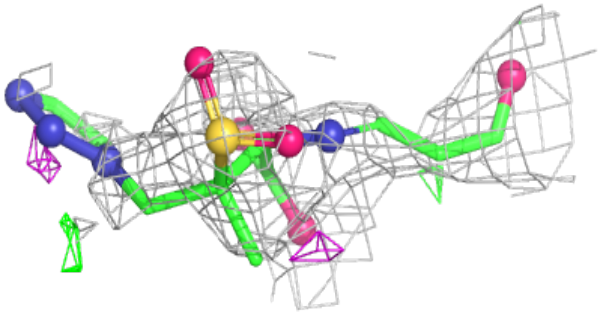
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

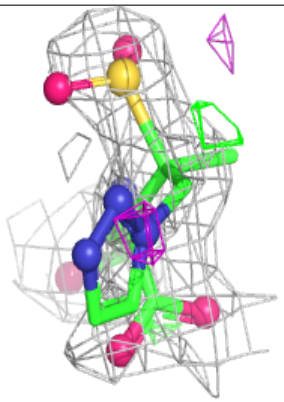
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	TBE	E	301	20/20	0.70	0.31	48,70,81,82	20
4	TRS	A	303	8/8	0.76	0.24	65,71,73,73	0
5	EDO	D	302	4/4	0.80	0.18	60,61,63,64	0
2	TBE	C	301	20/20	0.85	0.18	27,44,55,55	20
2	TBE	A	301	20/20	0.85	0.20	36,50,58,58	20
2	TBE	D	301	20/20	0.87	0.17	36,51,56,56	20
3	ACT	A	302	4/4	0.95	0.17	50,51,52,55	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 TBE E 301:

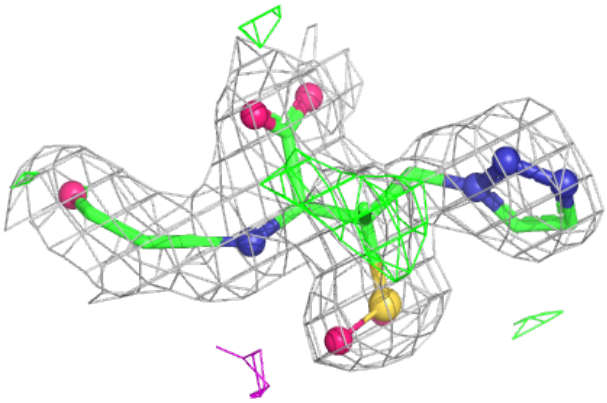
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

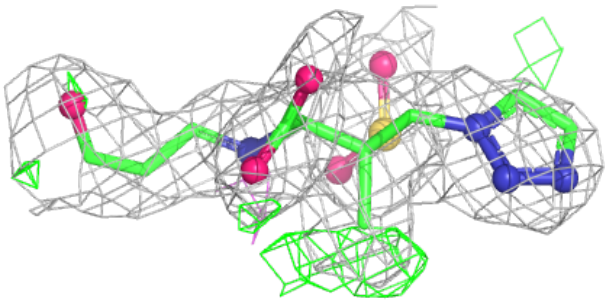


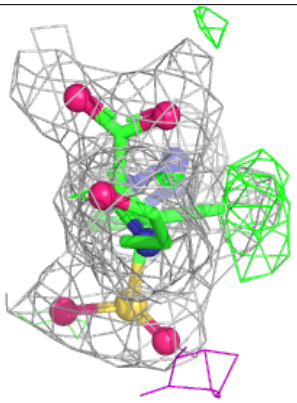


Electron density around TBE C 301:

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

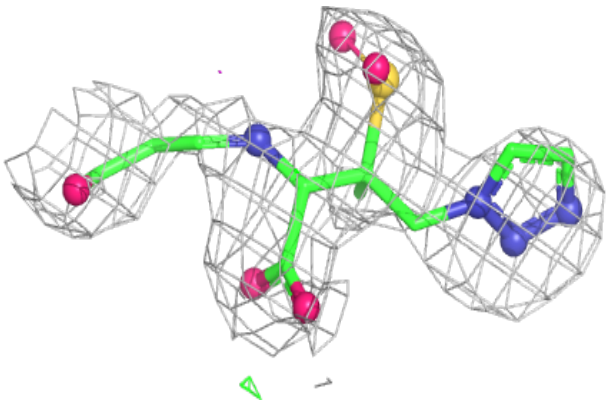


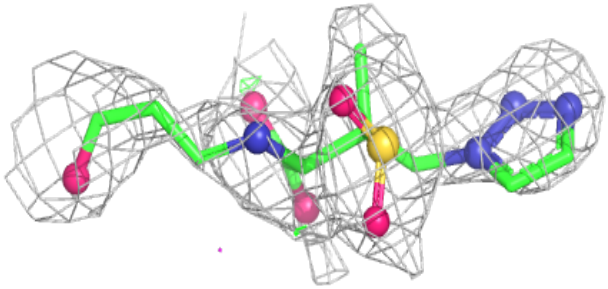


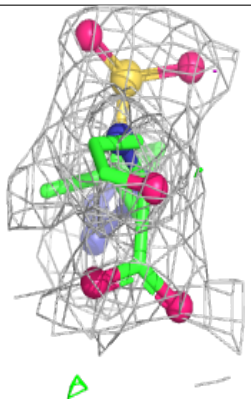


Electron density around TBE A 301:

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

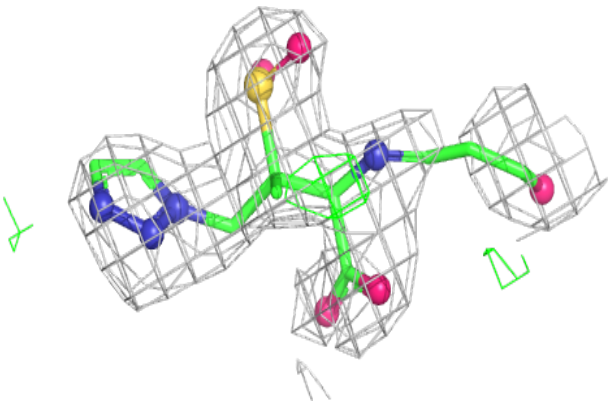


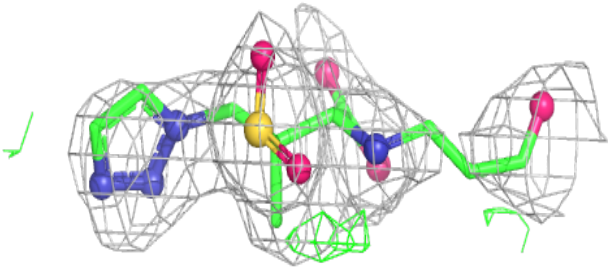


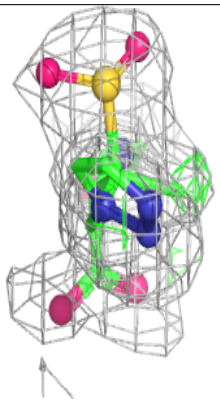


Electron density around TBE D 301:

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







6.5 Other polymers (i)

There are no such residues in this entry.