



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:03 PM UTC

PDB ID : 6L7L / pdb_00006171
Title : Crystal structure of Ribonucleotide reductase R1 subunit, RRM1 in complex with 5-chloro-2-(N-((1S,2R)-2-(2,3-dihydro-1H-inden-4-yl)-1-(5-oxo-4,5-dihydro-1,3,4-oxadiazol-2-yl)propyl)sulfamoyl)benzamide
Authors : Miyahara, S.; Chong, K.T.; Suzuki, T.
Deposited on : 2019-11-01
Resolution : 2.17 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

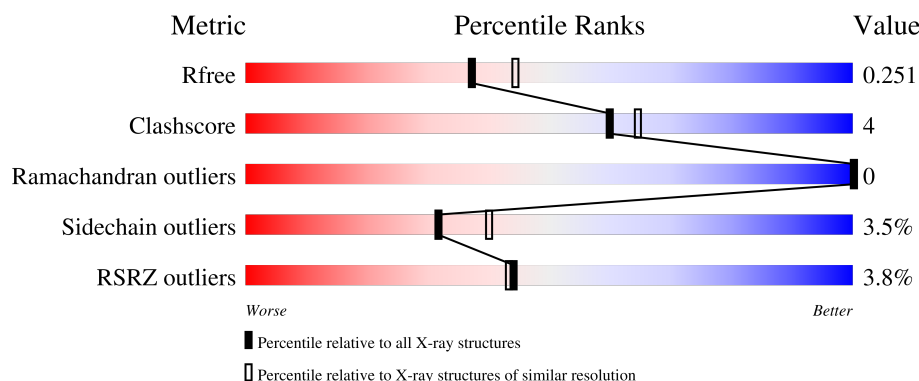
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

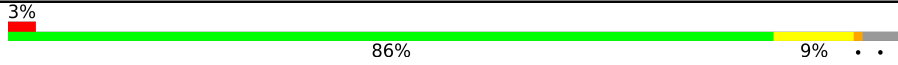
The reported resolution of this entry is 2.17 Å.

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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	669	
1	E	669	

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
5	ACT	A	808	-	-	X	-
5	ACT	E	806	-	-	X	-
5	ACT	E	807	-	-	X	-
5	ACT	E	808	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10456 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 Ribonucleoside-diphosphate reductase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	644	Total	C	N	O	S	0	0	0
			5096	3257	853	957	29			
1	E	629	Total	C	N	O	S	0	0	0
			5019	3206	843	943	27			

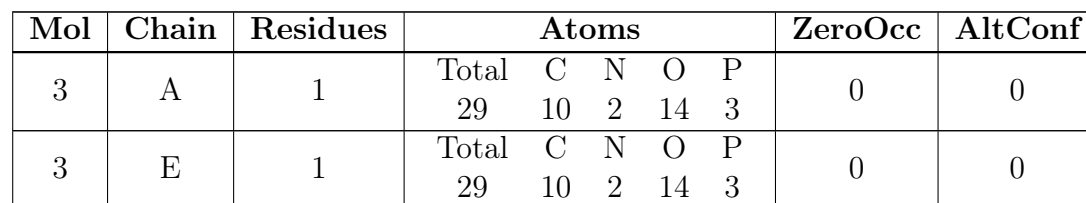
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	74	GLY	-	expression tag	UNP P23921
E	74	GLY	-	expression tag	UNP P23921

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	E	1	Total	Mg	0	0
			1	1		

- Molecule 3 is THYMIDINE-5'-TRIPHOSPHATE (CCD ID: TTP) (formula: C₁₀H₁₇N₂O₁₄P₃).



-
- The ORTEP diagram shows the chemical structure of E60, a complex organic molecule. The structure features a central sulfonamide group (S20) linked to a benzene ring (C23-C28) and a pyrazole ring (N16, N17, C13, C15). The benzene ring is substituted with a chlorine atom (Cl) at C26 and a sulfonamide group (N31, O30, O21) at C29. The pyrazole ring is substituted with a carboxylate group (O18, O14, C15) at C13 and a chiral center (C12(S), C10(R)) at C12. The chiral center is further substituted with a cyclopentyl group (C1-C5) and a methyl group (C11). The displacement ellipsoids are drawn at the 50% probability level, and the structure is shown with thermal ellipsoids at the 50% probability level.

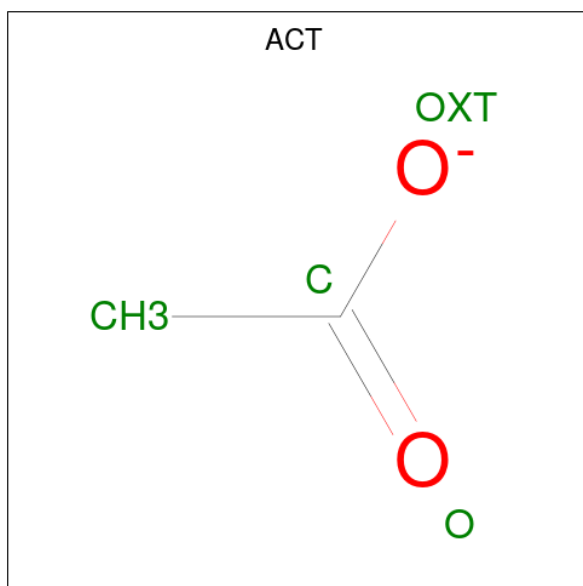
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	O	S	0	0
			32	21	1	4	5	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	E	1	Total	C	Cl	N	O	S	
			32	21	1	4	5	1	
								0	0

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



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

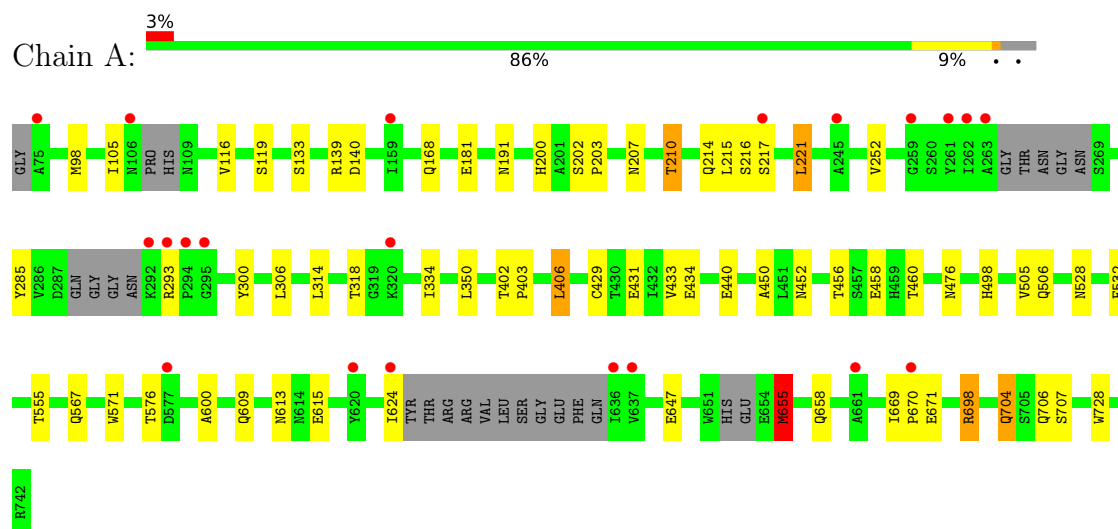
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	89	Total 89	O 89	0	0
6	E	88	Total 88	O 88	0	0

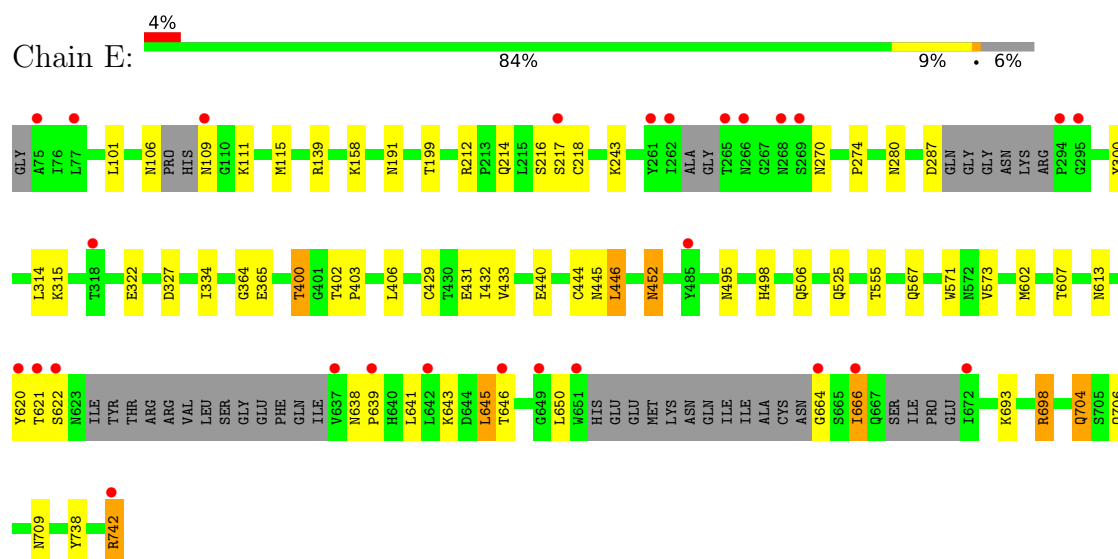
3 Residue-property plots [i](#)

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: Ribonucleoside-diphosphate reductase large subunit



- Molecule 1: Ribonucleoside-diphosphate reductase large subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.90Å 130.43Å 76.61Å 90.00° 93.15° 90.00°	Depositor
Resolution (Å)	76.49 – 2.17 76.49 – 2.17	Depositor EDS
% Data completeness (in resolution range)	87.0 (76.49-2.17) 87.0 (76.49-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.191 , 0.247 0.199 , 0.251	Depositor DCC
R_{free} test set	3240 reflections (4.42%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 26.9	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	0.95	EDS
Total number of atoms	10456	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TTP, E6O, ACT

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	0.92	2/5204 (0.0%)	1.03	6/7051 (0.1%)
1	E	0.92	0/5124	1.03	4/6932 (0.1%)
All	All	0.92	2/10328 (0.0%)	1.03	10/13983 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	ARG	CA-C	7.83	1.59	1.52
1	A	505	VAL	N-CA	-5.08	1.40	1.46

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	655	MET	N-CA-C	6.50	119.19	111.71
1	A	698	ARG	CB-CA-C	-6.25	100.42	110.79
1	A	221	LEU	N-CA-C	6.14	118.40	109.07
1	A	334	ILE	N-CA-C	6.05	114.62	107.73
1	A	314	LEU	N-CA-C	5.78	118.36	111.71
1	A	252	VAL	N-CA-C	5.57	117.56	112.43
1	E	446	LEU	N-CA-C	5.57	118.80	109.95
1	E	364	GLY	CA-C-N	5.29	128.15	120.79
1	E	364	GLY	C-N-CA	5.29	128.15	120.79
1	E	334	ILE	N-CA-C	5.21	113.67	107.73

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	5096	0	5019	38	0
1	E	5019	0	4971	45	0
2	A	1	0	0	0	0
2	E	1	0	0	0	0
3	A	29	0	13	1	0
3	E	29	0	13	0	0
4	A	32	0	0	0	0
4	E	32	0	0	0	0
5	A	20	0	15	4	0
5	E	20	0	15	4	0
6	A	89	0	0	3	0
6	E	88	0	0	4	0
All	All	10456	0	10046	87	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 4.

All (87) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:506:GLN:HE21	1:E:613:ASN:HD22	1.14	0.95
1:A:139:ARG:HH12	1:A:191:ASN:HD22	1.26	0.84
1:A:567:GLN:HE21	1:A:571:TRP:HE1	1.30	0.76
1:A:429:CYS:SG	6:A:986:HOH:O	2.45	0.73
1:E:567:GLN:HE21	1:E:571:TRP:HE1	1.36	0.73
1:E:139:ARG:HH12	1:E:191:ASN:HD22	1.37	0.70
1:A:98:MET:SD	6:A:927:HOH:O	2.50	0.69
5:A:807:ACT:H1	5:A:808:ACT:O	1.93	0.69
1:A:506:GLN:HE21	1:A:613:ASN:HD22	1.45	0.65
1:A:528:ASN:HD21	1:A:698:ARG:HG3	1.63	0.63
5:E:807:ACT:OXT	5:E:808:ACT:H1	2.00	0.62
1:A:207:ASN:O	1:A:210:THR:HB	2.00	0.60
1:A:567:GLN:NE2	1:A:571:TRP:HE1	1.99	0.60
1:E:525:GLN:HE22	1:E:693:LYS:HZ1	1.49	0.59
1:E:525:GLN:HE22	1:E:693:LYS:NZ	2.01	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:452:ASN:HD22	1:E:452:ASN:H	1.50	0.59
1:A:139:ARG:HH12	1:A:191:ASN:ND2	1.97	0.58
1:E:300:TYR:HE2	1:E:406:LEU:HD13	1.70	0.57
5:E:806:ACT:H3	6:E:984:HOH:O	2.03	0.56
1:E:440:GLU:OE1	1:E:498:HIS:HE1	1.88	0.56
1:E:214:GLN:HE22	1:E:216:SER:HB2	1.70	0.56
1:A:300:TYR:HE2	1:A:406:LEU:HD13	1.69	0.56
1:A:698:ARG:HE	1:A:706:GLN:NE2	2.04	0.55
1:E:270:ASN:HB3	1:E:274:PRO:HG2	1.89	0.55
1:E:445:ASN:HD21	1:E:495:ASN:HD21	1.53	0.54
1:A:698:ARG:HE	1:A:706:GLN:HE22	1.55	0.54
1:E:638:ASN:HD22	1:E:639:PRO:CD	2.20	0.54
1:A:202:SER:OG	5:A:806:ACT:H3	2.08	0.54
1:A:402:THR:HB	1:A:403:PRO:HA	1.89	0.54
1:E:638:ASN:HD22	1:E:639:PRO:HD2	1.72	0.53
1:E:506:GLN:NE2	1:E:613:ASN:HD22	1.96	0.52
1:E:433:VAL:H	1:E:704:GLN:HE21	1.56	0.52
1:E:446:LEU:HB3	1:E:602:MET:HE2	1.94	0.50
1:A:456:THR:OG1	1:A:460:THR:OG1	2.28	0.50
1:E:622:SER:HG	1:E:664:GLY:N	2.10	0.50
1:E:641:LEU:HD21	1:E:666:ILE:CD1	2.42	0.50
1:E:218:CYS:HB2	6:E:926:HOH:O	2.13	0.49
1:E:433:VAL:H	1:E:704:GLN:NE2	2.10	0.49
1:E:567:GLN:HE21	1:E:571:TRP:NE1	2.09	0.49
5:E:807:ACT:OXT	5:E:808:ACT:CH3	2.60	0.49
1:A:214:GLN:HE22	1:A:216:SER:HB2	1.78	0.48
1:E:742:ARG:HH11	1:E:742:ARG:HG3	1.79	0.48
1:A:655:MET:CE	1:A:669:ILE:HG21	2.43	0.48
1:A:532:PHE:CE1	1:A:698:ARG:HD3	2.49	0.48
1:A:203:PRO:HG2	1:A:217:SER:HA	1.95	0.48
1:E:106:ASN:CG	1:E:109:ASN:HB3	2.38	0.48
1:A:433:VAL:H	1:A:704:GLN:NE2	2.11	0.48
1:E:139:ARG:HH12	1:E:191:ASN:ND2	2.08	0.47
1:E:698:ARG:HE	1:E:706:GLN:NE2	2.13	0.47
1:A:528:ASN:ND2	1:A:698:ARG:HG3	2.29	0.47
1:A:433:VAL:H	1:A:704:GLN:HE21	1.62	0.46
1:A:450:ALA:HB1	1:A:452:ASN:HD21	1.79	0.46
1:E:109:ASN:HD21	1:E:111:LYS:HE2	1.80	0.46
1:A:140:ASP:OD1	1:A:168:GLN:HG2	2.16	0.46
1:E:432:ILE:HG13	1:E:444:CYS:SG	2.57	0.45
1:E:199:THR:HG21	1:E:607:THR:HB	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:315:LYS:CG	1:E:400:THR:HG21	2.47	0.45
1:A:434:GLU:HG3	1:A:704:GLN:HE22	1.82	0.44
1:E:402:THR:HB	1:E:403:PRO:HA	1.98	0.44
1:E:709:ASN:HD22	1:E:738:TYR:H	1.64	0.44
1:A:506:GLN:HE21	1:A:613:ASN:ND2	2.14	0.44
1:E:498:HIS:HD2	1:E:555:THR:OG1	2.00	0.44
1:A:285:TYR:HD1	1:E:274:PRO:HB2	1.83	0.43
1:E:567:GLN:NE2	1:E:571:TRP:HE1	2.10	0.43
1:E:641:LEU:HD21	1:E:666:ILE:HD11	2.00	0.43
3:A:802:TTP:HM52	1:E:243:LYS:HB2	2.00	0.43
1:E:280:ASN:HD21	1:E:327:ASP:H	1.65	0.43
1:E:452:ASN:H	1:E:452:ASN:ND2	2.16	0.43
1:A:576:THR:HB	5:A:805:ACT:H3	2.01	0.43
1:A:200:HIS:HE1	1:A:476:ASN:HD22	1.66	0.42
5:E:806:ACT:CH3	6:E:984:HOH:O	2.64	0.42
1:A:440:GLU:OE1	1:A:498:HIS:HE1	2.02	0.42
1:E:101:LEU:HD23	1:E:115:MET:HE3	2.02	0.42
1:A:498:HIS:HD2	1:A:555:THR:OG1	2.01	0.42
1:E:641:LEU:HG	1:E:645:LEU:HD22	2.00	0.42
1:E:698:ARG:HE	1:E:706:GLN:HE22	1.67	0.42
1:A:306:LEU:HA	1:A:350:LEU:HB3	2.01	0.41
1:A:202:SER:HB2	1:A:203:PRO:HD3	2.03	0.41
1:A:600:ALA:HB2	1:A:704:GLN:HB2	2.01	0.41
1:A:431:GLU:HB3	1:A:707:SER:OG	2.21	0.41
1:E:452:ASN:ND2	1:E:452:ASN:N	2.68	0.41
1:A:217:SER:HB2	6:A:987:HOH:O	2.20	0.40
1:E:158:LYS:NZ	6:E:908:HOH:O	2.54	0.40
1:E:742:ARG:HH11	1:E:742:ARG:CG	2.33	0.40
1:E:429:CYS:HB2	1:E:431:GLU:OE1	2.20	0.40
1:A:669:ILE:HA	1:A:670:PRO:HD3	1.95	0.40
1:A:728:TRP:CE2	5:A:808:ACT:H3	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	632/669 (94%)	613 (97%)	19 (3%)	0	100	100
1	E	615/669 (92%)	590 (96%)	25 (4%)	0	100	100
All	All	1247/1338 (93%)	1203 (96%)	44 (4%)	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	548/583 (94%)	529 (96%)	19 (4%)	32	40
1	E	544/583 (93%)	525 (96%)	19 (4%)	32	40
All	All	1092/1166 (94%)	1054 (96%)	38 (4%)	32	40

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ILE
1	A	116	VAL
1	A	119	SER
1	A	133	SER
1	A	181	GLU
1	A	210	THR
1	A	215	LEU
1	A	221	LEU
1	A	318	THR
1	A	406	LEU
1	A	458	GLU
1	A	609	GLN
1	A	615	GLU
1	A	624	ILE
1	A	647	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	655	MET
1	A	658	GLN
1	A	671	GLU
1	A	704	GLN
1	E	212	ARG
1	E	217	SER
1	E	287	ASP
1	E	314	LEU
1	E	322	GLU
1	E	365	GLU
1	E	400	THR
1	E	452	ASN
1	E	573	VAL
1	E	620	TYR
1	E	621	THR
1	E	643	LYS
1	E	645	LEU
1	E	646	THR
1	E	650	LEU
1	E	666	ILE
1	E	698	ARG
1	E	704	GLN
1	E	742	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	191	ASN
1	A	200	HIS
1	A	207	ASN
1	A	214	GLN
1	A	237	GLN
1	A	418	GLN
1	A	452	ASN
1	A	498	HIS
1	A	506	GLN
1	A	525	GLN
1	A	550	GLN
1	A	567	GLN
1	A	638	ASN
1	A	704	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	706	GLN
1	A	709	ASN
1	A	724	HIS
1	E	160	ASN
1	E	191	ASN
1	E	214	GLN
1	E	270	ASN
1	E	280	ASN
1	E	317	ASN
1	E	323	GLN
1	E	387	GLN
1	E	445	ASN
1	E	452	ASN
1	E	459	HIS
1	E	498	HIS
1	E	506	GLN
1	E	525	GLN
1	E	567	GLN
1	E	595	ASN
1	E	613	ASN
1	E	623	ASN
1	E	638	ASN
1	E	688	GLN
1	E	704	GLN
1	E	706	GLN
1	E	709	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 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	ACT	A	804	-	3,3,3	0.80	0	3,3,3	0.87	0
5	ACT	E	808	-	3,3,3	0.39	0	3,3,3	1.85	2 (66%)
5	ACT	E	804	-	3,3,3	0.82	0	3,3,3	1.43	1 (33%)
5	ACT	A	808	-	3,3,3	0.77	0	3,3,3	1.52	0
4	E6O	E	803	-	35,35,35	2.53	6 (17%)	46,52,52	2.11	10 (21%)
5	ACT	A	807	-	3,3,3	1.22	1 (33%)	3,3,3	0.60	0
3	TTP	E	802	2	29,30,30	2.23	7 (24%)	43,47,47	1.79	11 (25%)
3	TTP	A	802	2	29,30,30	2.21	7 (24%)	43,47,47	1.73	7 (16%)
4	E6O	A	803	-	35,35,35	2.48	6 (17%)	46,52,52	2.09	10 (21%)
5	ACT	E	806	-	3,3,3	1.05	0	3,3,3	2.14	1 (33%)
5	ACT	E	807	-	3,3,3	0.98	0	3,3,3	0.49	0
5	ACT	E	805	-	3,3,3	1.15	0	3,3,3	0.64	0
5	ACT	A	806	-	3,3,3	1.12	0	3,3,3	1.74	2 (66%)
5	ACT	A	805	-	3,3,3	0.81	0	3,3,3	1.42	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TTP	A	802	2	-	3/22/34/34	0/2/2/2
3	TTP	E	802	2	-	2/22/34/34	0/2/2/2
4	E6O	A	803	-	-	6/27/33/33	0/4/4/4
4	E6O	E	803	-	-	6/27/33/33	0/4/4/4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	803	E6O	C23-S20	-12.21	1.60	1.77
4	A	803	E6O	C23-S20	-11.87	1.61	1.77
3	A	802	TTP	PB-O3B	7.19	1.67	1.59
3	E	802	TTP	PB-O3B	7.10	1.67	1.59
3	A	802	TTP	PB-O3A	5.56	1.65	1.59
3	E	802	TTP	PB-O3A	4.83	1.64	1.59
3	E	802	TTP	PA-O3A	4.65	1.64	1.59
3	A	802	TTP	PA-O3A	4.31	1.64	1.59
4	E	803	E6O	O18-C15	3.82	1.28	1.21
3	E	802	TTP	C2-N1	3.73	1.44	1.38
4	A	803	E6O	O18-C15	3.61	1.28	1.21
4	A	803	E6O	C6-C10	-3.56	1.49	1.52
4	E	803	E6O	N16-N17	3.38	1.43	1.36
3	A	802	TTP	C2-N1	3.25	1.43	1.38
4	E	803	E6O	C6-C10	-3.17	1.49	1.52
3	E	802	TTP	C4-C5	3.01	1.49	1.44
3	A	802	TTP	C4-C5	2.82	1.49	1.44
3	E	802	TTP	C6-C5	2.67	1.39	1.34
4	E	803	E6O	C13-N17	2.66	1.36	1.31
4	A	803	E6O	C26-CL	2.59	1.80	1.74
4	A	803	E6O	C13-N17	2.44	1.36	1.31
3	A	802	TTP	C6-C5	2.40	1.38	1.34
3	E	802	TTP	O2-C2	2.37	1.27	1.23
4	E	803	E6O	C28-C23	2.17	1.41	1.39
3	A	802	TTP	O2-C2	2.09	1.26	1.23
4	A	803	E6O	C28-C23	2.04	1.41	1.39
5	A	807	ACT	OXT-C	-2.04	1.21	1.30

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	803	E6O	O22-S20-O21	-9.02	108.57	119.52
4	E	803	E6O	O22-S20-O21	-8.64	109.03	119.52
4	E	803	E6O	C12-C13-N17	5.90	132.55	125.90
3	E	802	TTP	C5M-C5-C4	5.06	124.19	118.78
4	A	803	E6O	C12-C13-N17	5.00	131.54	125.90
3	A	802	TTP	O4-C4-C5	-4.59	119.67	124.92
3	E	802	TTP	O4-C4-C5	-4.27	120.03	124.92
3	A	802	TTP	C4-N3-C2	-4.24	121.78	127.34
4	A	803	E6O	O14-C15-N16	4.23	112.80	107.89
4	E	803	E6O	C13-C12-N19	4.22	116.43	108.79
3	A	802	TTP	C5M-C5-C4	4.21	123.28	118.78
4	E	803	E6O	O14-C15-N16	4.20	112.75	107.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	802	TTP	C5-C4-N3	3.84	118.66	115.32
3	A	802	TTP	N3-C2-N1	3.81	119.85	114.89
3	E	802	TTP	C4-N3-C2	-3.80	122.36	127.34
3	A	802	TTP	C5M-C5-C6	-3.47	118.15	122.85
3	A	802	TTP	C5-C4-N3	3.37	118.26	115.32
3	E	802	TTP	C5M-C5-C6	-3.34	118.33	122.85
3	E	802	TTP	N3-C2-N1	3.17	119.02	114.89
4	A	803	E6O	O14-C15-O18	3.04	125.18	120.63
5	E	806	ACT	OXT-C-CH3	2.99	127.58	115.05
4	E	803	E6O	O22-S20-C23	2.91	112.48	107.68
4	A	803	E6O	O22-S20-C23	2.85	112.39	107.68
4	E	803	E6O	C4-C3-C2	2.74	112.57	110.27
3	E	802	TTP	O3A-PB-O1B	-2.68	102.65	110.70
4	E	803	E6O	O22-S20-N19	2.56	111.53	106.88
4	A	803	E6O	C13-C12-N19	2.54	113.40	108.79
4	A	803	E6O	O22-S20-N19	2.53	111.47	106.88
3	E	802	TTP	O3G-PG-O2G	2.46	117.02	107.80
4	A	803	E6O	C25-C24-C23	2.41	119.97	117.55
4	E	803	E6O	O14-C15-O18	2.41	124.23	120.63
5	E	808	ACT	OXT-C-CH3	2.37	124.98	115.05
3	E	802	TTP	C1'-N1-C2	2.35	122.26	117.66
4	E	803	E6O	C2-C6-C10	-2.28	119.59	122.25
3	E	802	TTP	O5'-C5'-C4'	2.24	116.60	108.99
4	A	803	E6O	O30-C29-C24	-2.23	117.61	120.24
5	A	806	ACT	OXT-C-O	-2.22	113.80	122.03
5	E	808	ACT	O-C-CH3	-2.16	113.65	122.53
3	E	802	TTP	C1'-N1-C6	-2.15	117.14	120.74
3	A	802	TTP	C5-C6-N1	-2.12	121.01	123.31
4	E	803	E6O	C12-N19-S20	-2.06	115.51	121.06
5	A	806	ACT	OXT-C-CH3	2.03	123.56	115.05
4	A	803	E6O	C28-C23-C24	-2.02	118.89	121.25
5	E	804	ACT	OXT-C-CH3	2.01	123.47	115.05

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	803	E6O	C24-C23-S20-N19
4	E	803	E6O	C24-C23-S20-N19
4	A	803	E6O	C28-C23-S20-N19
4	E	803	E6O	C28-C23-S20-N19
4	A	803	E6O	C23-C24-C29-N31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	803	E6O	C23-C24-C29-O30
4	A	803	E6O	C24-C23-S20-O22
4	A	803	E6O	C28-C23-S20-O22
4	E	803	E6O	C24-C23-S20-O22
4	E	803	E6O	C23-C24-C29-N31
4	E	803	E6O	C23-C24-C29-O30
4	E	803	E6O	C28-C23-S20-O22
3	E	802	TTP	PA-O3A-PB-O2B
3	A	802	TTP	PB-O3A-PA-O1A
3	A	802	TTP	PB-O3A-PA-O2A
3	A	802	TTP	PG-O3B-PB-O1B
3	E	802	TTP	PA-O3A-PB-O1B

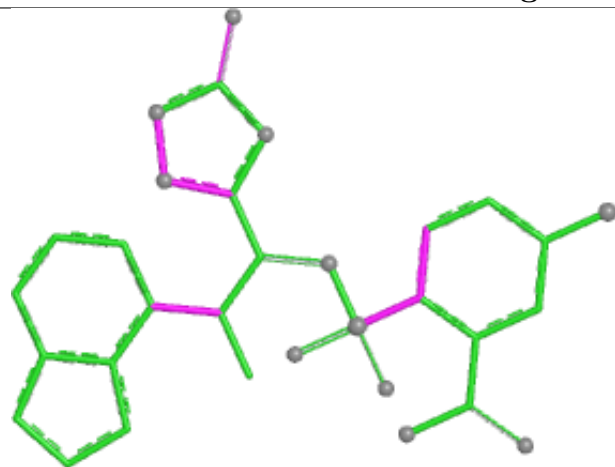
There are no ring outliers.

8 monomers are involved in 9 short contacts:

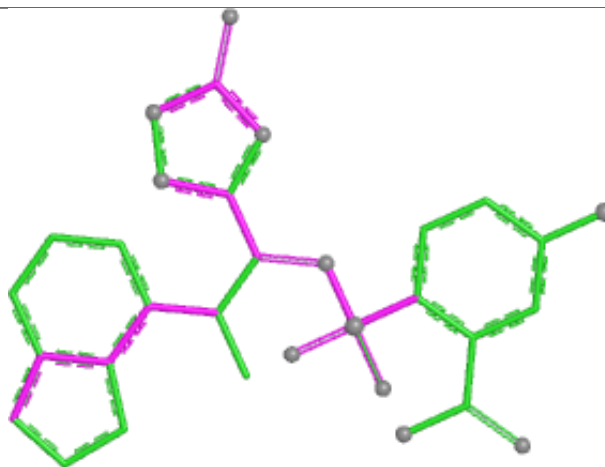
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	808	ACT	2	0
5	A	808	ACT	2	0
5	A	807	ACT	1	0
3	A	802	TTP	1	0
5	E	806	ACT	2	0
5	E	807	ACT	2	0
5	A	806	ACT	1	0
5	A	805	ACT	1	0

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

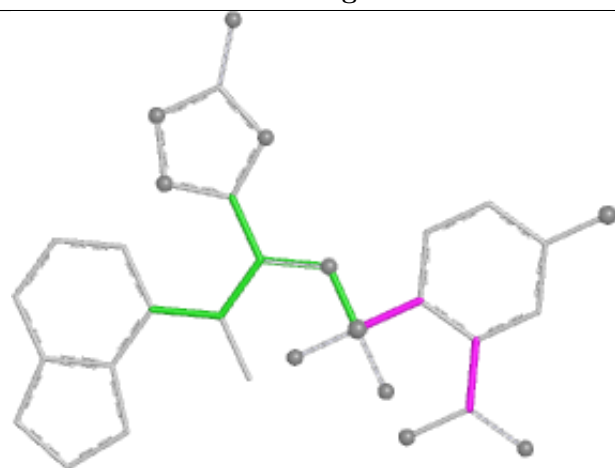
Ligand E6O E 803



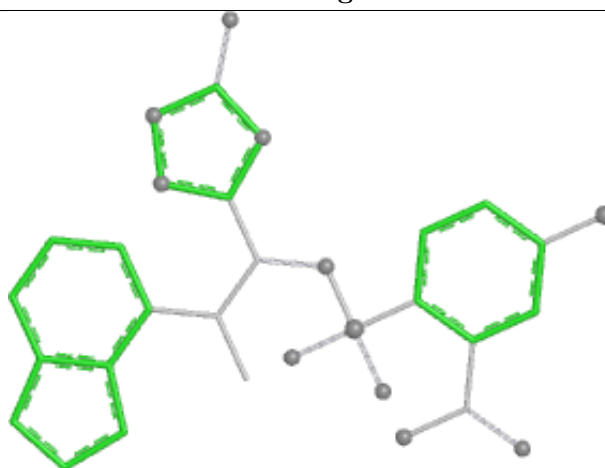
Bond lengths



Bond angles

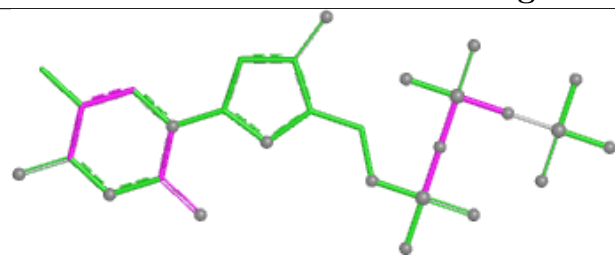


Torsions

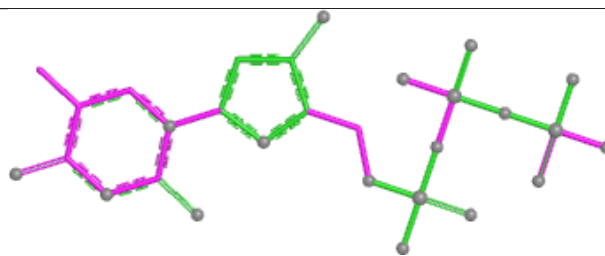


Rings

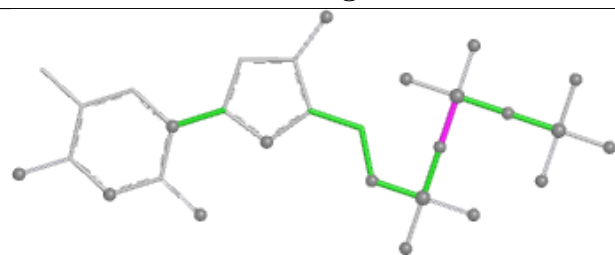
Ligand TTP E 802



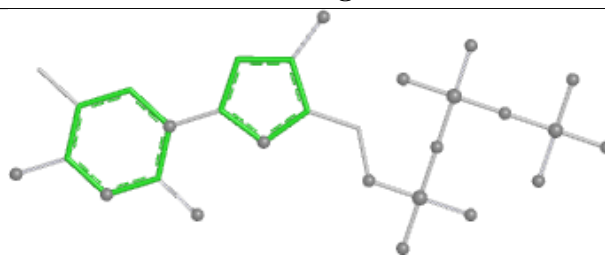
Bond lengths



Bond angles

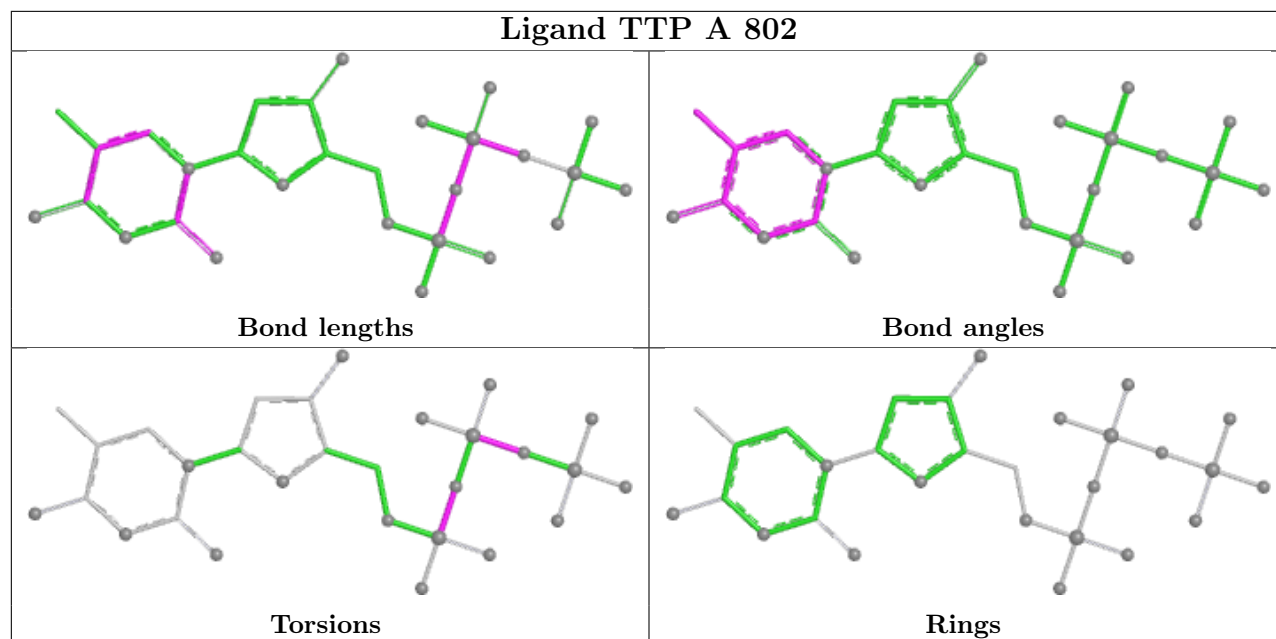


Torsions

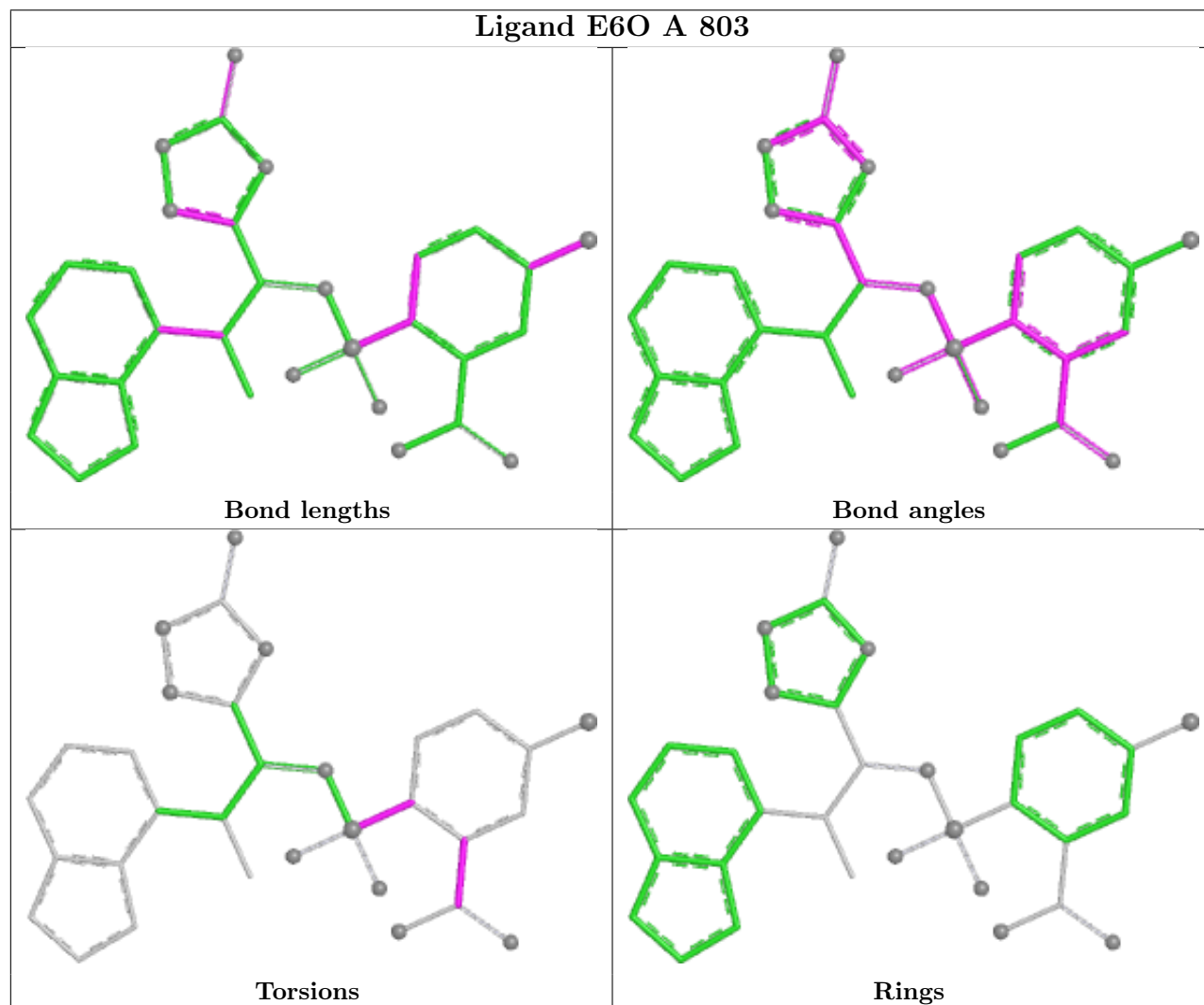


Rings

Ligand TTP A 802



Ligand E6O A 803



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	644/669 (96%)	0.13	21 (3%)	49 48	22, 35, 64, 79	0
1	E	629/669 (94%)	0.12	27 (4%)	40 39	21, 36, 64, 77	0
All	All	1273/1338 (95%)	0.13	48 (3%)	44 43	21, 36, 64, 79	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	620	TYR	4.6
1	E	651	TRP	4.5
1	A	636	ILE	4.4
1	E	268	ASN	4.2
1	A	259	GLY	3.8
1	E	294	PRO	3.7
1	E	261	TYR	3.5
1	A	261	TYR	3.4
1	A	263	ALA	3.2
1	E	295	GLY	3.2
1	E	666	ILE	3.2
1	A	320	LYS	3.2
1	A	293	ARG	3.1
1	E	637	VAL	3.1
1	A	624	ILE	3.1
1	A	106	ASN	3.0
1	A	294	PRO	2.9
1	E	742	ARG	2.9
1	E	485	TYR	2.8
1	E	265	THR	2.8
1	E	269	SER	2.7
1	A	75	ALA	2.7
1	E	664	GLY	2.6
1	E	649	GLY	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	292	LYS	2.6
1	A	262	ILE	2.5
1	A	637	VAL	2.5
1	E	672	ILE	2.5
1	A	661	ALA	2.5
1	E	75	ALA	2.5
1	A	159	ILE	2.5
1	E	318	THR	2.4
1	E	109	ASN	2.4
1	E	262	ILE	2.4
1	A	217	SER	2.4
1	E	621	THR	2.4
1	E	620	TYR	2.3
1	E	642	LEU	2.3
1	E	622	SER	2.2
1	E	217	SER	2.2
1	E	646	THR	2.2
1	A	245	ALA	2.2
1	E	266	ASN	2.2
1	A	577	ASP	2.1
1	A	670	PRO	2.1
1	E	639	PRO	2.1
1	E	77	LEU	2.1
1	A	295	GLY	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](#)

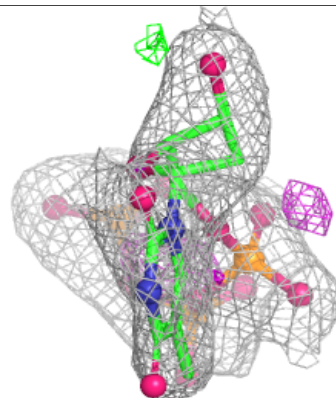
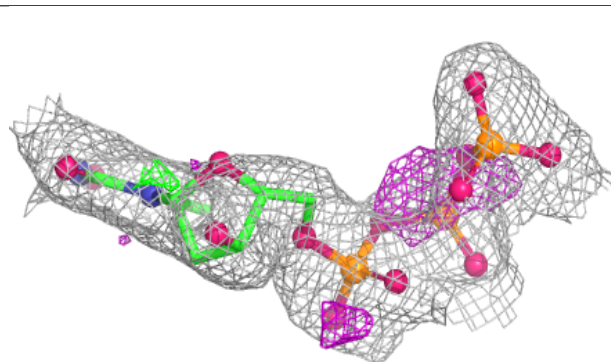
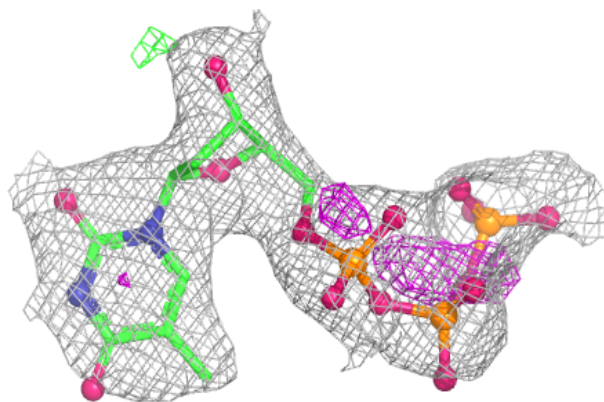
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ACT	E	808	4/4	0.74	0.16	36,37,38,43	0
5	ACT	A	805	4/4	0.76	0.18	41,42,46,48	0
5	ACT	A	806	4/4	0.81	0.15	34,35,38,43	0
3	TTP	E	802	29/29	0.82	0.13	46,59,91,95	0
2	MG	A	801	1/1	0.83	0.11	63,63,63,63	0
5	ACT	E	805	4/4	0.86	0.12	38,41,44,45	0
5	ACT	E	807	4/4	0.86	0.12	33,35,37,40	0
2	MG	E	801	1/1	0.86	0.08	59,59,59,59	0
5	ACT	E	806	4/4	0.87	0.12	33,33,34,41	0
5	ACT	A	807	4/4	0.87	0.12	34,36,36,39	0
3	TTP	A	802	29/29	0.87	0.11	41,61,94,96	0
5	ACT	A	804	4/4	0.90	0.12	26,26,28,29	0
4	E6O	E	803	32/32	0.92	0.09	42,48,55,58	0
5	ACT	A	808	4/4	0.93	0.09	36,36,36,39	0
5	ACT	E	804	4/4	0.94	0.08	28,29,30,30	0
4	E6O	A	803	32/32	0.95	0.07	41,44,54,55	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.

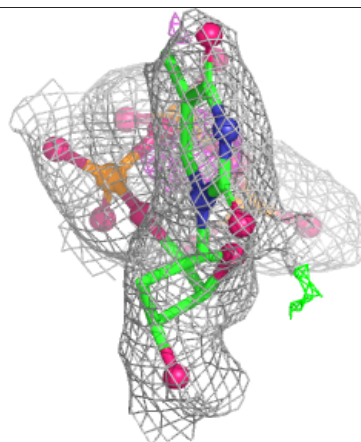
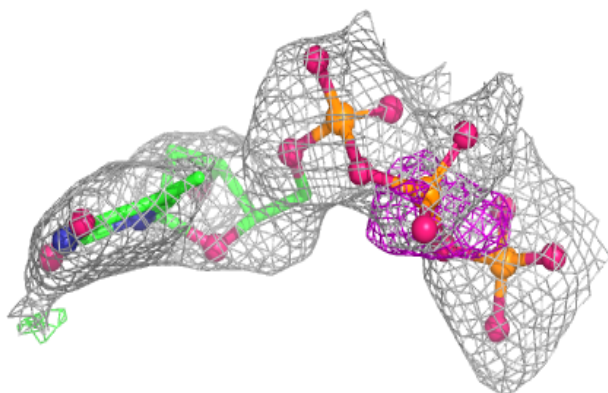
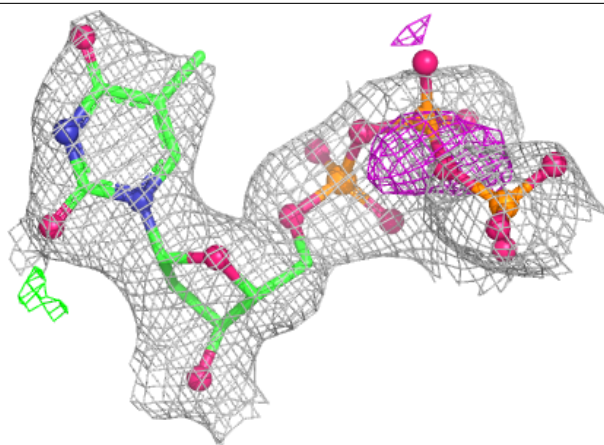
Electron density around TTP E 802:

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

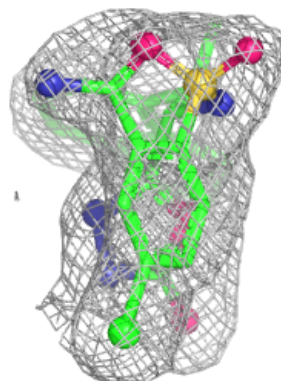
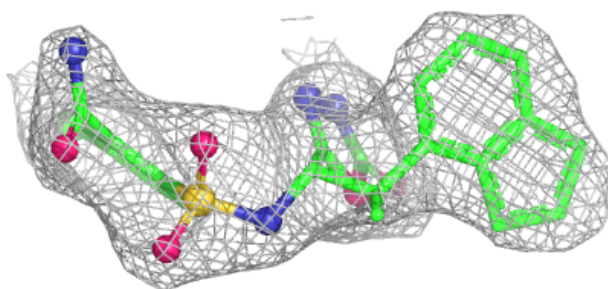
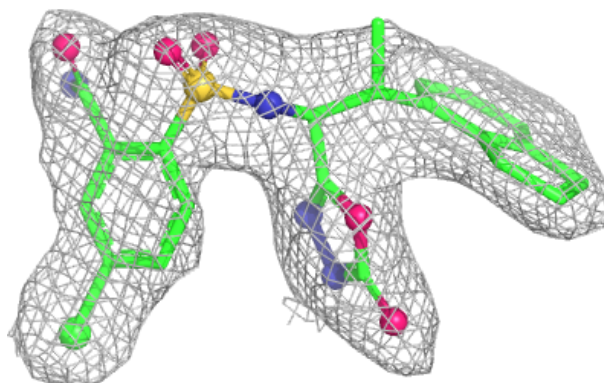


Electron density around TTP A 802:

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

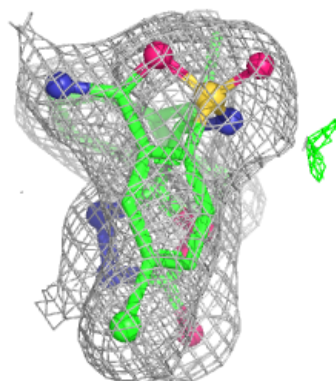
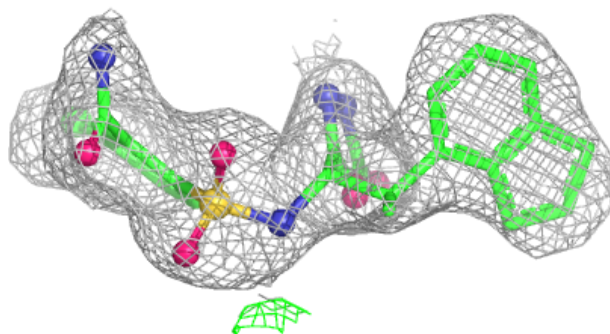
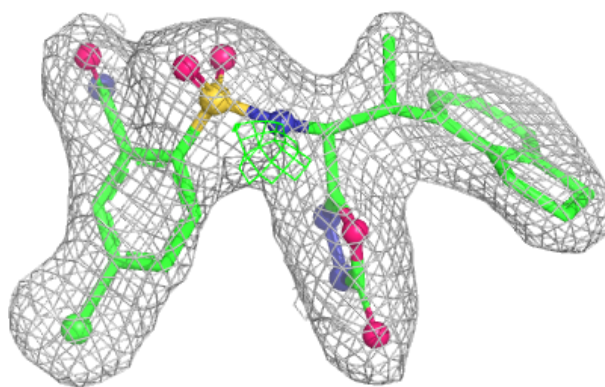
**Electron density around E6O E 803:**

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



Electron density around E6O A 803:

$2mF_o - DF_c$ (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.