



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:21 AM UTC

PDB ID : 6X6U / pdb_00006x6u
Title : WOR5 from Pyrococcus furiosus, taurine-bound
Authors : Lanzilotta, W.N.; Mathew, L.G.
Deposited on : 2020-05-29
Resolution : 1.94 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

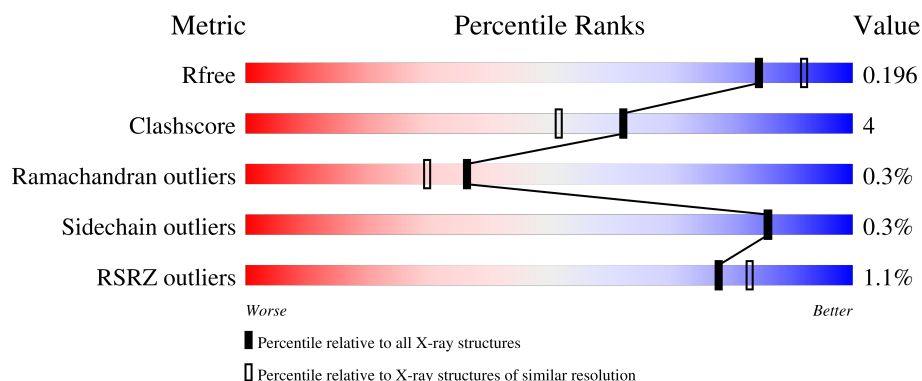
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	623	0.1% 91% 8%
1	C	623	0.1% 89% 11%
2	B	173	2% 91% 6% •
2	D	173	0.1% 91% 5% •

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
6	TAU	A	705	-	X	-	-
6	TAU	C	706	-	X	-	-
7	PO4	A	706	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 13467 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.

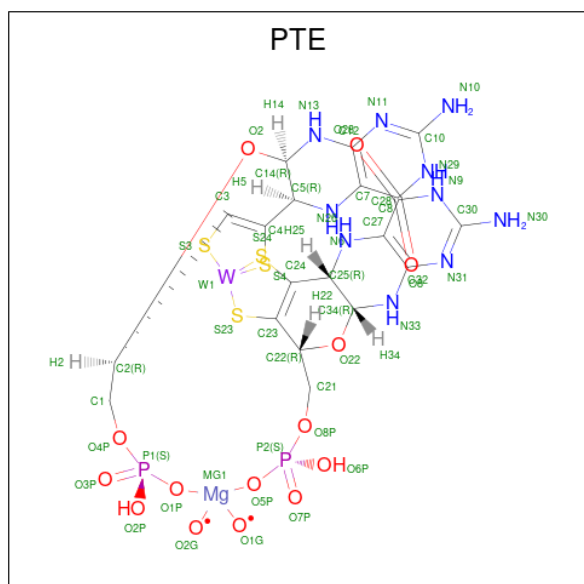
- Molecule 1 is a protein called Formaldehyde:ferredoxin oxidoreductase wor5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	623	Total	C	N	O	S	0	5	0
			4946	3193	813	926	14			
1	C	623	Total	C	N	O	S	0	1	0
			4915	3172	814	915	14			

- Molecule 2 is a protein called Oxidoreductase, Fe-S subunit.

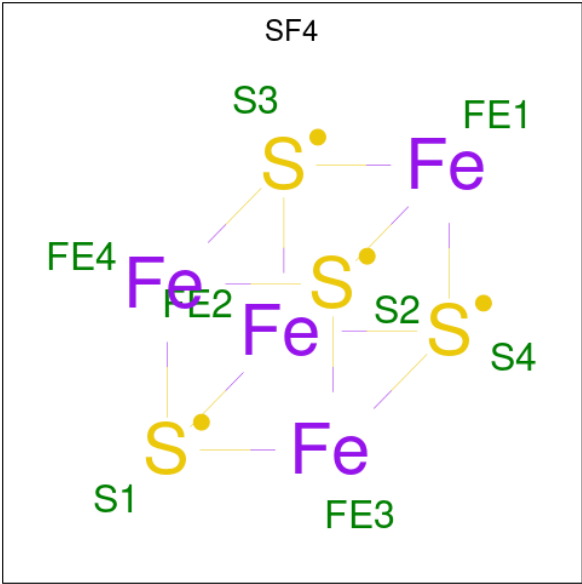
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	167	Total	C	N	O	S	0	1	0
			1262	796	216	234	16			
2	D	167	Total	C	N	O	S	0	0	0
			1256	792	216	232	16			

- Molecule 3 is TUNGSTOPTERIN COFACTOR (CCD ID: PTE) (formula: $C_{20}H_{22}MgN_{10}O_{14}P_2S_4W$).



Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
3	A	1	Total	C	Mg	N	O	P	S	W	0	0
			52	20	1	10	14	2	4	1		
3	C	1	Total	C	Mg	N	O	P	S	W	0	0
			52	20	1	10	14	2	4	1		

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).

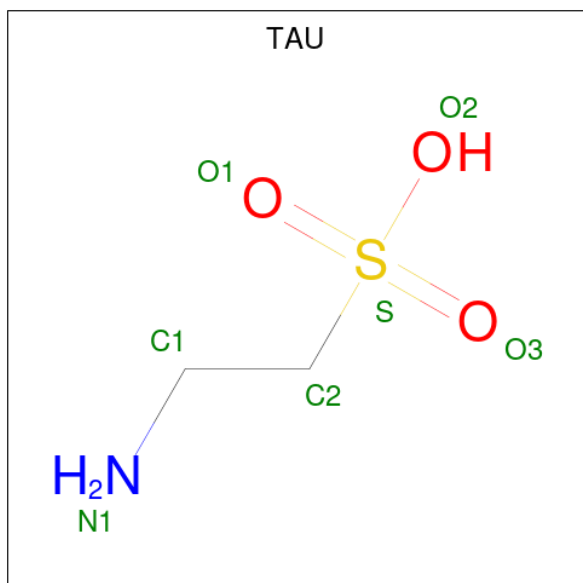


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	B	1	Total	Fe	S	0	0
			8	4	4		
4	C	1	Total	Fe	S	0	0
			8	4	4		
4	D	1	Total	Fe	S	0	0
			8	4	4		
4	D	1	Total	Fe	S	0	0
			8	4	4		
4	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Mg	0	0
			2	2		
5	C	2	Total	Mg	0	0
			2	2		

- Molecule 6 is 2-AMINOETHANESULFONIC ACID (CCD ID: TAU) (formula: C₂H₇NO₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	S	0	0
			7	2	1	3	1		
6	C	1	Total	C	N	O	S	0	0
			7	2	1	3	1		

- Molecule 7 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	P	0	0
			5	4	1		
7	A	1	Total	O	P	0	0
			5	4	1		
7	A	1	Total	O	P	0	0
			5	4	1		
7	B	1	Total	O	P	0	0
			5	4	1		
7	C	1	Total	O	P	0	0
			5	4	1		
7	C	1	Total	O	P	0	0
			5	4	1		
7	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Cl	0	0
			1	1		
8	C	1	Total	Cl	0	0
			1	1		
8	D	1	Total	Cl	0	0
			1	1		

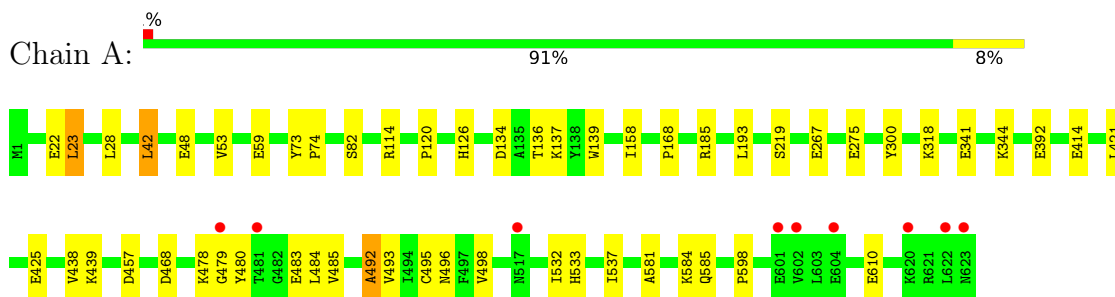
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	273	Total 273	O 273	0	0
9	B	131	Total 131	O 131	0	0
9	C	336	Total 336	O 336	0	0
9	D	108	Total 108	O 108	0	0

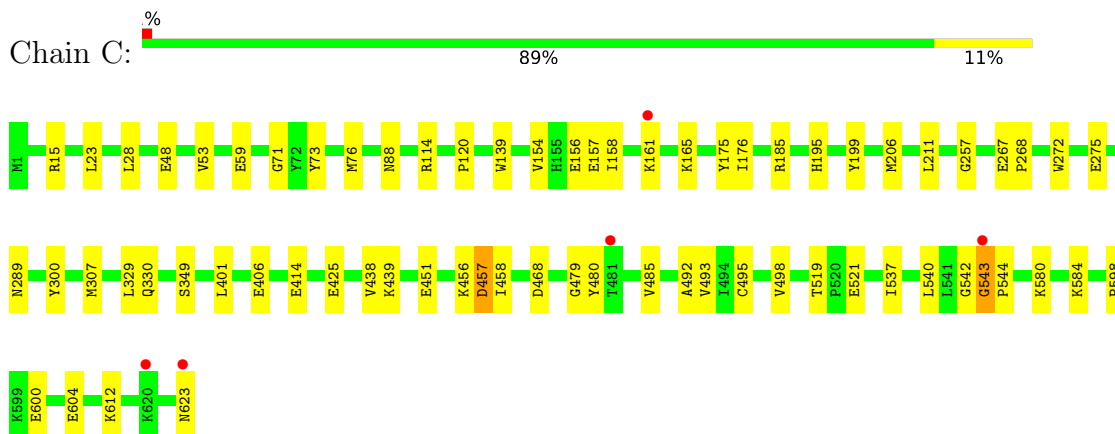
3 Residue-property plots

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

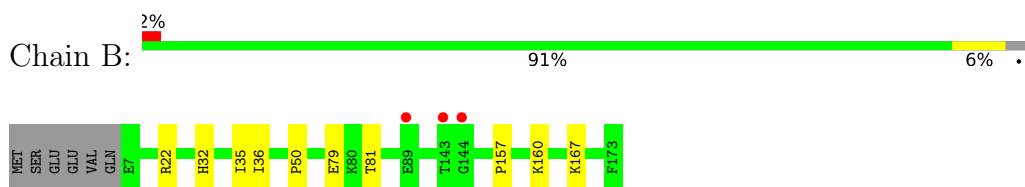
- Molecule 1: Formaldehyde:ferredoxin oxidoreductase wor5



- Molecule 1: Formaldehyde:ferredoxin oxidoreductase wor5

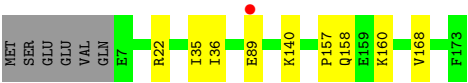


- Molecule 2: Oxidoreductase, Fe-S subunit



- Molecule 2: Oxidoreductase, Fe-S subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	125.15Å 127.50Å 140.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.16 – 1.94 38.16 – 1.94	Depositor EDS
% Data completeness (in resolution range)	94.8 (38.16-1.94) 87.5 (38.16-1.94)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-0.80 (at 1.94Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.170 , 0.196 0.170 , 0.196	Depositor DCC
R_{free} test set	2009 reflections (1.28%)	wwPDB-VP
Wilson B-factor (Å ²)	19.8	Xtriage
Anisotropy	1.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13467	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.20 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1842e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CL, TAU, SF4, PTE, MG, PO4

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	0.49	0/5073	0.67	4/6847 (0.1%)
1	C	0.53	0/5030	0.67	1/6789 (0.0%)
2	B	0.53	0/1293	0.67	2/1760 (0.1%)
2	D	0.51	0/1284	0.60	0/1748
All	All	0.51	0/12680	0.66	7/17144 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	5
All	All	0	6

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	492	ALA	CA-C-N	5.61	131.80	121.70
1	A	492	ALA	C-N-CA	5.61	131.80	121.70
1	A	478	LYS	CA-C-N	-5.35	104.38	120.92
1	A	478	LYS	C-N-CA	-5.35	104.38	120.92
1	C	493	VAL	N-CA-C	5.34	120.44	109.34
2	B	81	THR	CA-C-N	-5.11	111.40	121.41
2	B	81	THR	C-N-CA	-5.11	111.40	121.41

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	479	GLY	Peptide
1	C	479	GLY	Peptide
1	C	492	ALA	Mainchain,Peptide
1	C	542	GLY	Peptide
1	C	543	GLY	Peptide

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	4946	0	4973	37	0
1	C	4915	0	4935	50	0
2	B	1262	0	1238	8	0
2	D	1256	0	1232	7	0
3	A	52	0	20	1	0
3	C	52	0	20	1	0
4	A	8	0	0	0	0
4	B	32	0	0	1	0
4	C	8	0	0	0	0
4	D	32	0	0	0	0
5	A	2	0	0	0	0
5	C	2	0	0	0	0
6	A	7	0	6	2	0
6	C	7	0	6	2	0
7	A	15	0	0	3	0
7	B	5	0	0	1	0
7	C	10	0	0	0	0
7	D	5	0	0	1	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
9	A	273	0	0	4	0
9	B	131	0	0	2	0
9	C	336	0	0	9	0
9	D	108	0	0	1	0
All	All	13467	0	12430	102	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 (102) 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)
6:C:706:TAU:O1	9:C:801:HOH:O	1.54	1.22
6:A:705:TAU:O2	9:A:801:HOH:O	1.63	1.14
1:A:318:LYS:NZ	9:A:802:HOH:O	1.96	0.92
4:B:204:SF4:S3	9:B:301:HOH:O	2.30	0.88
1:C:211:LEU:HG	9:C:857:HOH:O	1.79	0.81
1:A:73:TYR:HE2	1:A:498[A]:VAL:HG13	1.50	0.76
1:C:457[A]:ASP:OD1	1:C:458:ILE:N	2.16	0.76
2:D:168:VAL:HG22	7:D:206:PO4:O3	1.87	0.75
1:C:176:ILE:HG23	1:C:206:MET:HE2	1.72	0.72
1:A:126:HIS:NE2	7:A:706:PO4:O2	2.22	0.72
1:C:15:ARG:NH1	9:C:803:HOH:O	2.16	0.69
1:A:134:ASP:OD1	1:A:136:THR:HG23	1.95	0.67
1:C:425:GLU:OE1	9:C:802:HOH:O	2.14	0.66
1:A:126:HIS:HE2	7:A:706:PO4:P	2.19	0.66
1:A:48[A]:GLU:H	1:A:48[A]:GLU:CD	2.05	0.65
2:B:32:HIS:CE1	9:B:301:HOH:O	2.49	0.63
2:B:167:LYS:HD2	7:B:206:PO4:O4	1.98	0.63
1:A:53:VAL:HG13	1:A:59:GLU:HG2	1.81	0.61
1:A:344:LYS:HD3	1:A:392:GLU:OE1	2.00	0.61
1:C:521:GLU:H	1:C:521:GLU:CD	2.08	0.61
1:C:15:ARG:HG2	1:C:15:ARG:HH11	1.66	0.59
1:A:496:ASN:ND2	9:A:806:HOH:O	2.35	0.59
2:B:79:GLU:H	2:B:79:GLU:CD	2.11	0.58
1:A:581:ALA:O	1:A:584:LYS:HG3	2.04	0.57
1:C:154:VAL:O	1:C:158:ILE:HG12	2.06	0.56
1:A:495:CYS:O	1:A:498[A]:VAL:HG12	2.06	0.56
3:A:701:PTE:S24	6:A:705:TAU:O1	2.65	0.55
1:A:610:GLU:H	1:A:610:GLU:CD	2.14	0.55
1:A:341:GLU:HG2	1:A:344:LYS:HG3	1.88	0.55
1:C:438:VAL:HG12	1:C:439:LYS:HG2	1.89	0.55
1:A:480:TYR:HA	1:A:485:VAL:HG21	1.87	0.54
1:C:480:TYR:HA	1:C:485:VAL:HG21	1.89	0.54
2:B:157:PRO:HA	2:B:160:LYS:HE3	1.90	0.54
1:C:88:ASN:CG	1:C:543:GLY:HA2	2.33	0.54
1:A:438:VAL:HG12	1:A:439:LYS:HG2	1.90	0.53
1:C:519:THR:HB	1:C:521:GLU:OE2	2.09	0.53
1:A:185:ARG:HD2	1:A:414:GLU:OE1	2.09	0.52
1:A:267:GLU:O	1:A:275:GLU:HA	2.09	0.52
1:C:185:ARG:HD2	1:C:414:GLU:OE1	2.09	0.52
1:C:88:ASN:ND2	1:C:543:GLY:HA2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:GLU:H	1:A:22:GLU:CD	2.18	0.51
2:D:35:ILE:HG13	2:D:36:ILE:N	2.24	0.51
1:C:457[A]:ASP:CG	1:C:458:ILE:H	2.16	0.50
1:A:344:LYS:HD3	1:A:392:GLU:CD	2.37	0.50
1:A:219:SER:HB3	7:A:706:PO4:O1	2.12	0.49
1:C:623:ASN:C	9:C:804:HOH:O	2.55	0.49
2:B:35:ILE:HG13	2:B:36:ILE:N	2.26	0.49
1:C:580:LYS:O	1:C:580:LYS:HD3	2.13	0.48
1:C:600:GLU:O	1:C:604:GLU:HG3	2.14	0.48
1:C:623:ASN:O	9:C:804:HOH:O	2.20	0.48
3:C:701:PTE:S24	6:C:706:TAU:O3	2.71	0.48
1:A:492:ALA:N	1:A:493:VAL:HA	2.29	0.48
2:B:167:LYS:HE3	1:C:289:ASN:O	2.14	0.48
1:C:23:LEU:HD13	1:C:28:LEU:HD21	1.96	0.48
1:A:120:PRO:HB3	1:A:139:TRP:CE3	2.49	0.47
1:C:157:GLU:OE2	1:C:161:LYS:NZ	2.44	0.47
1:C:457[A]:ASP:OD1	1:C:458:ILE:HG13	2.14	0.47
1:C:156:GLU:OE2	2:D:158:GLN:NE2	2.46	0.47
1:C:195:HIS:CE1	1:C:307:MET:HE2	2.49	0.47
2:D:89:GLU:OE1	2:D:89:GLU:N	2.48	0.47
1:C:604:GLU:OE1	1:C:612:LYS:NZ	2.39	0.46
1:A:158:ILE:HG22	1:A:168:PRO:HG2	1.97	0.46
1:C:53:VAL:HG13	1:C:59:GLU:HG2	1.98	0.46
1:C:267:GLU:O	1:C:275:GLU:HA	2.17	0.45
1:A:483:GLU:HG2	9:A:833:HOH:O	2.16	0.45
1:A:484:LEU:HD12	1:A:532:ILE:HG13	1.99	0.45
1:A:74:PRO:HB2	1:A:498[B]:VAL:HG11	1.99	0.44
1:A:23:LEU:HD13	1:A:28:LEU:HD21	2.00	0.44
1:C:268:PRO:HB3	1:C:272:TRP:CE2	2.53	0.44
1:C:206:MET:HE3	9:C:857:HOH:O	2.17	0.44
1:C:71:GLY:HA2	1:C:76:MET:HE1	1.99	0.44
1:C:329:LEU:HD23	1:C:349:SER:HB3	2.00	0.44
1:A:537:ILE:HG13	1:A:598:PRO:HG2	2.00	0.43
1:A:300:TYR:CD2	2:B:22:ARG:HD2	2.53	0.43
1:C:300:TYR:CD2	2:D:22:ARG:HD2	2.52	0.43
1:C:401:LEU:HD22	1:C:406:GLU:HG2	2.00	0.43
1:A:533:HIS:ND1	1:A:598:PRO:HB3	2.34	0.42
1:C:165:LYS:HE2	9:C:956:HOH:O	2.20	0.42
1:C:451:GLU:HG2	1:C:456:LYS:HG2	2.01	0.42
2:D:140:LYS:NZ	9:D:301:HOH:O	1.91	0.42
2:D:157:PRO:HA	2:D:160:LYS:HE3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:TYR:HE2	1:C:498:VAL:HG23	1.85	0.42
1:C:175:TYR:HA	1:C:206:MET:CE	2.49	0.42
1:A:584:LYS:HG3	1:A:585:GLN:N	2.34	0.42
1:C:580:LYS:HD2	1:C:584:LYS:HE3	2.02	0.42
1:C:604:GLU:HG2	1:C:612:LYS:HE3	2.02	0.42
1:C:257:GLY:HA3	1:C:330:GLN:OE1	2.20	0.42
1:C:157:GLU:O	1:C:161:LYS:HD3	2.20	0.41
1:C:537:ILE:HG13	1:C:598:PRO:HG2	2.03	0.41
1:A:42[A]:LEU:HD21	1:A:82:SER:C	2.45	0.41
1:C:495:CYS:O	1:C:498:VAL:HG22	2.21	0.41
1:A:137:LYS:HE3	1:A:137:LYS:HB3	1.53	0.41
1:C:199:TYR:CZ	1:C:468:ASP:HA	2.56	0.41
1:A:421:LEU:O	1:A:425[B]:GLU:HG3	2.21	0.41
1:C:48:GLU:HB2	9:C:924:HOH:O	2.21	0.41
1:C:120:PRO:HB3	1:C:139:TRP:CE3	2.56	0.41
1:C:195:HIS:NE2	1:C:307:MET:HE2	2.37	0.40
1:C:540:LEU:HD23	1:C:540:LEU:HA	1.90	0.40
1:A:193:LEU:HG	2:B:50:PRO:HG2	2.03	0.40
1:C:175:TYR:C	1:C:206:MET:HE2	2.47	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	626/623 (100%)	598 (96%)	26 (4%)	2 (0%)	36	30
1	C	622/623 (100%)	593 (95%)	26 (4%)	3 (0%)	24	15
2	B	166/173 (96%)	159 (96%)	7 (4%)	0	100	100
2	D	165/173 (95%)	159 (96%)	6 (4%)	0	100	100
All	All	1579/1592 (99%)	1509 (96%)	65 (4%)	5 (0%)	36	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	457	ASP
1	C	457[A]	ASP
1	C	457[B]	ASP
1	C	544	PRO
1	A	468	ASP

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	520/516 (101%)	516 (99%)	4 (1%)	73	71
1	C	513/516 (99%)	512 (100%)	1 (0%)	87	87
2	B	142/149 (95%)	142 (100%)	0	100	100
2	D	141/149 (95%)	141 (100%)	0	100	100
All	All	1316/1330 (99%)	1311 (100%)	5 (0%)	86	84

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	42[A]	LEU
1	A	42[B]	LEU
1	A	114	ARG
1	C	114	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	53	ASN
1	C	522	GLN
2	D	53	ASN
2	D	68	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 28 ligands modelled in this entry, 7 are monoatomic - leaving 21 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	$\# Z > 2$
4	SF4	D	203	2	0,12,12	-	-	-		
7	PO4	D	206	-	4,4,4	0.73	0	6,6,6	1.51	2 (33%)
7	PO4	A	708	-	4,4,4	0.85	0	6,6,6	0.95	0
7	PO4	C	708	-	4,4,4	0.75	0	6,6,6	1.87	1 (16%)
4	SF4	A	702	1	0,12,12	-	-	-		
6	TAU	A	705	3	6,6,6	4.51	2 (33%)	7,8,8	2.83	4 (57%)
4	SF4	B	202	2	0,12,12	-	-	-		
4	SF4	D	201	2	0,12,12	-	-	-		
3	PTE	C	701	1,6,9,5	46,60,60	2.34	7 (15%)	42,98,98	1.98	15 (35%)
4	SF4	B	204	2,9	0,12,12	-	-	-		
7	PO4	B	206	-	4,4,4	1.11	0	6,6,6	2.05	2 (33%)
4	SF4	D	202	2	0,12,12	-	-	-		
4	SF4	C	702	1	0,12,12	-	-	-		
4	SF4	B	203	2	0,12,12	-	-	-		
7	PO4	C	707	-	4,4,4	1.03	0	6,6,6	0.88	0
4	SF4	B	201	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	PO4	A	707	-	4,4,4	0.88	0	6,6,6	0.61	0
4	SF4	D	204	2	0,12,12	-	-	-	-	-
7	PO4	A	706	-	4,4,4	0.83	0	6,6,6	1.66	2 (33%)
6	TAU	C	706	3	6,6,6	4.68	2 (33%)	7,8,8	4.14	5 (71%)
3	PTE	A	701	1,6,9,5	46,60,60	2.41	6 (13%)	42,98,98	1.92	12 (28%)

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
4	SF4	B	204	2,9	-	-	0/6/5/5
4	SF4	D	203	2	-	-	0/6/5/5
4	SF4	C	702	1	-	-	0/6/5/5
4	SF4	D	204	2	-	-	0/6/5/5
6	TAU	A	705	3	-	2/4/4/4	-
4	SF4	B	203	2	-	-	0/6/5/5
6	TAU	C	706	3	-	1/4/4/4	-
4	SF4	B	202	2	-	-	0/6/5/5
4	SF4	D	201	2	-	-	0/6/5/5
3	PTE	C	701	1,6,9,5	-	0/12/100/100	-
3	PTE	A	701	1,6,9,5	-	0/12/100/100	-
4	SF4	D	202	2	-	-	0/6/5/5
4	SF4	B	201	2	-	-	0/6/5/5
4	SF4	A	702	1	-	-	0/6/5/5

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	PTE	P2-O5P	9.63	1.65	1.50
3	C	701	PTE	P2-O5P	9.57	1.65	1.50
6	C	706	TAU	C2-S	-9.54	1.64	1.77
6	A	705	TAU	C2-S	-9.11	1.64	1.77
3	A	701	PTE	P1-O1P	8.70	1.64	1.50
3	C	701	PTE	P1-O1P	7.36	1.62	1.50
6	C	706	TAU	O3-S	6.06	1.62	1.45
6	A	705	TAU	O3-S	5.89	1.61	1.45
3	C	701	PTE	C7-C12	5.67	1.48	1.38
3	A	701	PTE	C7-C12	5.32	1.47	1.38
3	A	701	PTE	C27-C32	4.73	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	701	PTE	C27-C32	4.64	1.46	1.38
3	A	701	PTE	C8-N9	-3.00	1.33	1.38
3	C	701	PTE	C8-N9	-2.84	1.33	1.38
3	C	701	PTE	C27-C28	2.62	1.49	1.41
3	C	701	PTE	C4-S4	-2.45	1.66	1.74
3	A	701	PTE	C27-C28	2.39	1.49	1.41

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	706	TAU	O2-S-O3	-5.76	97.00	111.40
3	A	701	PTE	C30-N31-C32	5.41	122.90	113.36
6	C	706	TAU	O3-S-C2	5.33	114.78	106.73
3	C	701	PTE	C30-N31-C32	5.19	122.53	113.36
6	C	706	TAU	O2-S-C2	4.93	115.64	106.00
6	A	705	TAU	O3-S-O1	-4.79	98.25	113.82
6	A	705	TAU	O1-S-C2	4.30	113.23	106.73
3	C	701	PTE	O2-C14-N13	4.12	112.35	108.61
3	A	701	PTE	C10-N11-C12	4.04	120.49	113.36
3	C	701	PTE	C10-N11-C12	3.91	120.27	113.36
7	C	708	PO4	O4-P-O2	3.88	119.97	107.91
7	B	206	PO4	O3-P-O2	3.78	119.68	107.91
6	C	706	TAU	O1-S-C2	-3.77	101.03	106.73
6	C	706	TAU	O2-S-O1	3.75	120.79	111.40
3	A	701	PTE	O8-C8-C7	-3.46	118.93	127.26
3	A	701	PTE	O22-C22-C23	3.28	113.72	109.09
3	C	701	PTE	O28-C28-C27	-3.20	119.55	127.26
3	C	701	PTE	O22-C34-N33	3.09	111.41	108.61
3	C	701	PTE	O8-C8-C7	-3.01	120.01	127.26
7	A	706	PO4	O3-P-O1	-2.97	100.44	110.95
3	A	701	PTE	O28-C28-C27	-2.96	120.11	127.26
7	D	206	PO4	O3-P-O1	-2.94	100.56	110.95
6	A	705	TAU	O3-S-C2	2.90	111.11	106.73
3	A	701	PTE	C23-C24-S24	2.84	123.74	119.62
3	C	701	PTE	C28-C27-N26	2.78	123.84	116.27
3	A	701	PTE	C28-C27-N26	2.73	123.70	116.27
3	A	701	PTE	C24-C23-S23	2.65	123.47	119.62
7	B	206	PO4	O4-P-O3	-2.60	99.83	107.91
3	C	701	PTE	C8-C7-N6	2.57	123.28	116.27
3	A	701	PTE	C7-C8-N9	2.56	119.16	112.13
3	A	701	PTE	C27-C28-N29	2.49	118.97	112.13
3	A	701	PTE	C8-C7-N6	2.38	122.77	116.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	701	PTE	C27-C28-N29	2.34	118.56	112.13
6	A	705	TAU	O2-S-O3	2.32	117.21	111.40
3	C	701	PTE	C23-C24-S24	2.32	122.99	119.62
3	C	701	PTE	C7-C8-N9	2.24	118.30	112.13
3	A	701	PTE	O2-C14-N13	2.19	110.59	108.61
3	C	701	PTE	O22-C34-C25	-2.18	107.51	108.96
3	C	701	PTE	O2-C14-C5	-2.17	107.52	108.96
3	C	701	PTE	C30-N29-C28	-2.17	121.18	125.11
7	A	706	PO4	O4-P-O1	2.13	118.50	110.95
3	C	701	PTE	C24-C23-S23	2.09	122.66	119.62
7	D	206	PO4	O2-P-O1	2.05	118.19	110.95

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	705	TAU	N1-C1-C2-S
6	C	706	TAU	N1-C1-C2-S
6	A	705	TAU	C1-C2-S-O3

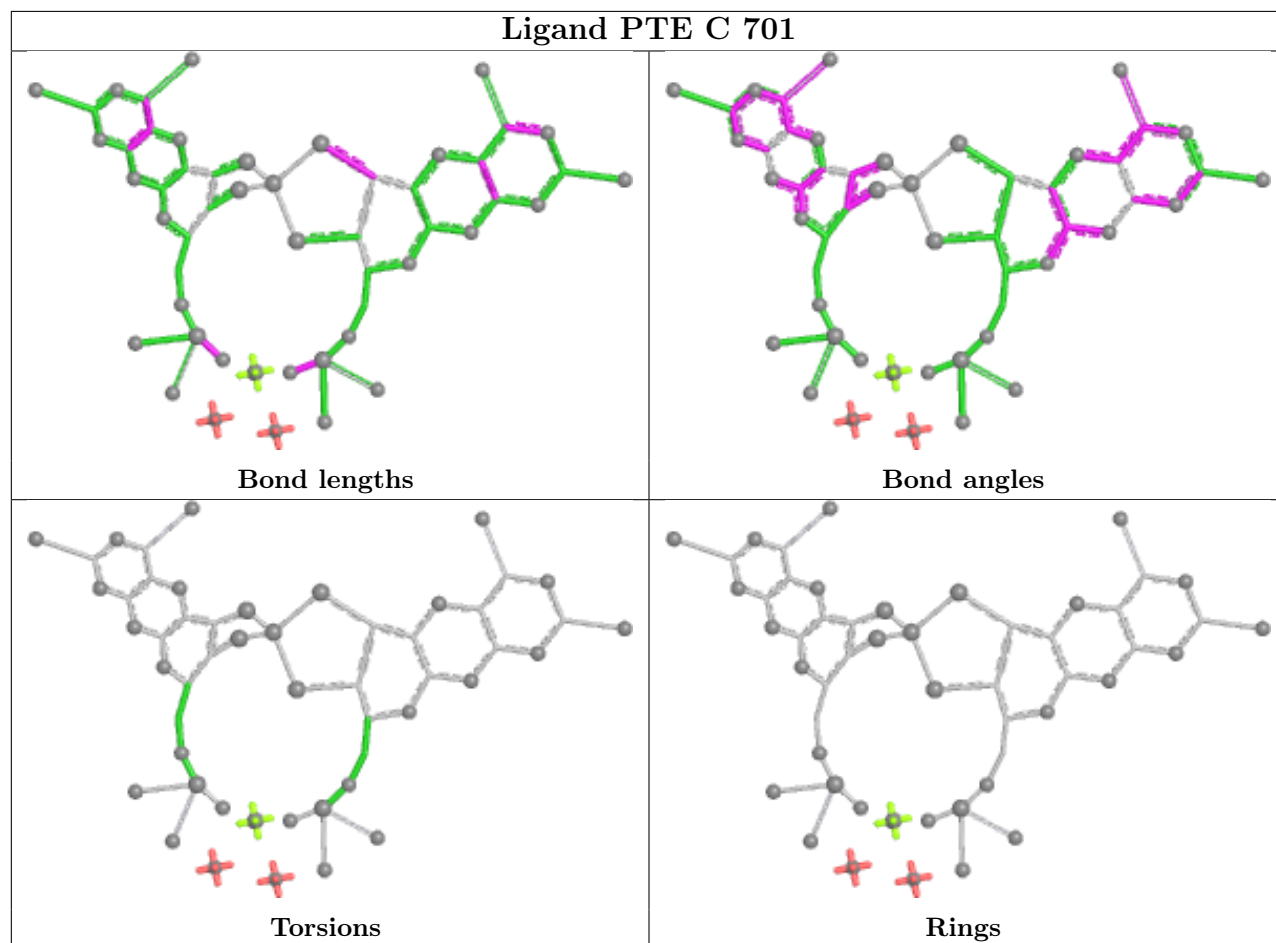
There are no ring outliers.

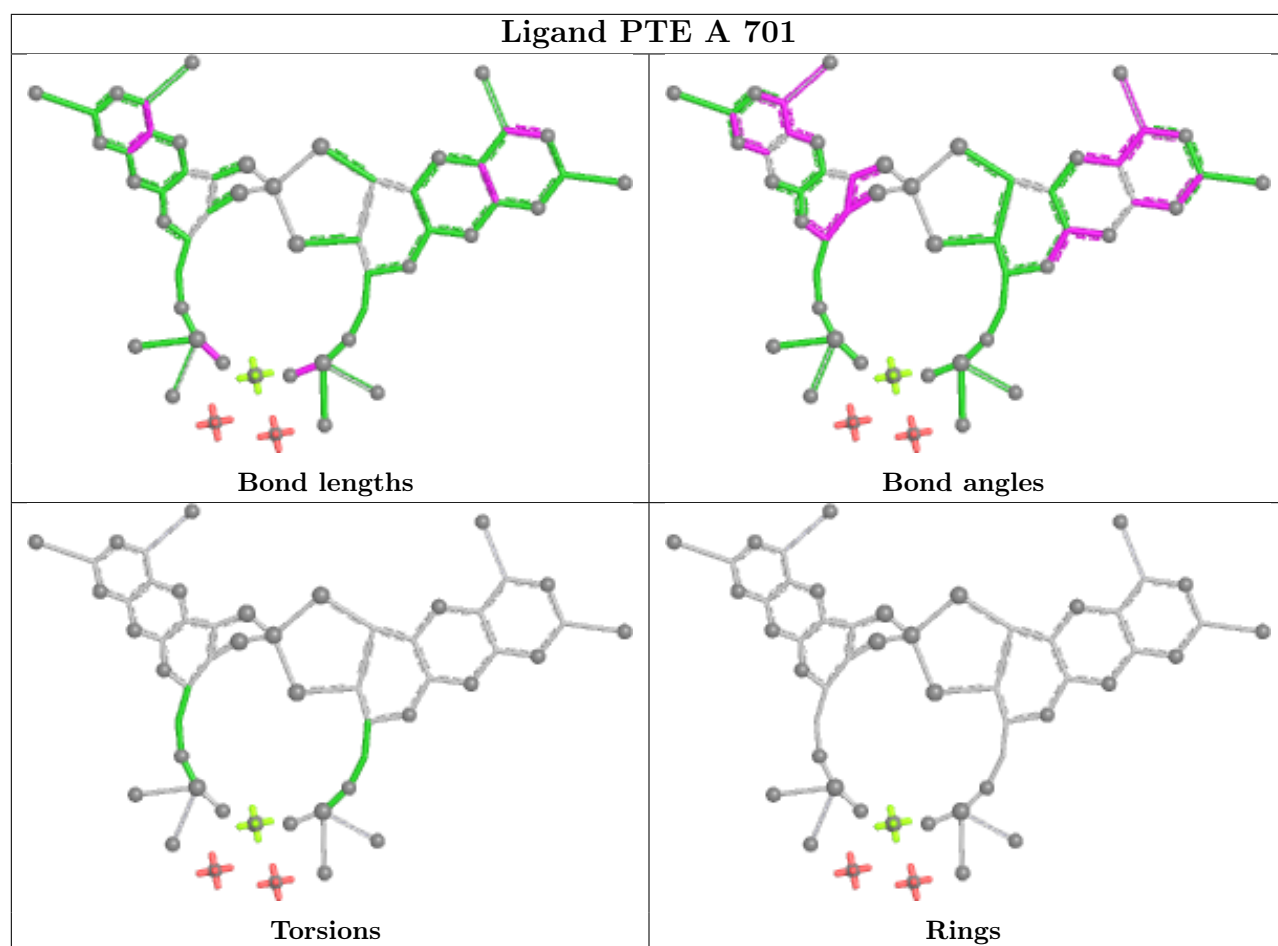
8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	206	PO4	1	0
6	A	705	TAU	2	0
3	C	701	PTE	1	0
4	B	204	SF4	1	0
7	B	206	PO4	1	0
7	A	706	PO4	3	0
6	C	706	TAU	2	0
3	A	701	PTE	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	623/623 (100%)	0.06	9 (1%) 73 79	15, 28, 44, 52	5 (0%)
1	C	623/623 (100%)	-0.12	5 (0%) 82 87	16, 26, 39, 49	1 (0%)
2	B	167/173 (96%)	-0.06	3 (1%) 67 74	16, 25, 38, 49	1 (0%)
2	D	167/173 (96%)	-0.12	1 (0%) 85 89	16, 24, 37, 52	0
All	All	1580/1592 (99%)	-0.04	18 (1%) 78 83	15, 26, 42, 52	7 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	620	LYS	4.6
1	C	543	GLY	4.6
1	A	481	THR	4.5
1	A	620	LYS	3.6
1	A	623	ASN	3.2
1	C	623	ASN	2.9
2	B	144	GLY	2.9
2	D	89	GLU	2.7
1	A	602	VAL	2.7
1	C	161	LYS	2.5
1	A	479	GLY	2.5
1	A	517	ASN	2.4
2	B	143	THR	2.3
1	A	601	GLU	2.3
1	A	604	GLU	2.3
2	B	89	GLU	2.3
1	C	481	THR	2.3
1	A	622	LEU	2.2

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

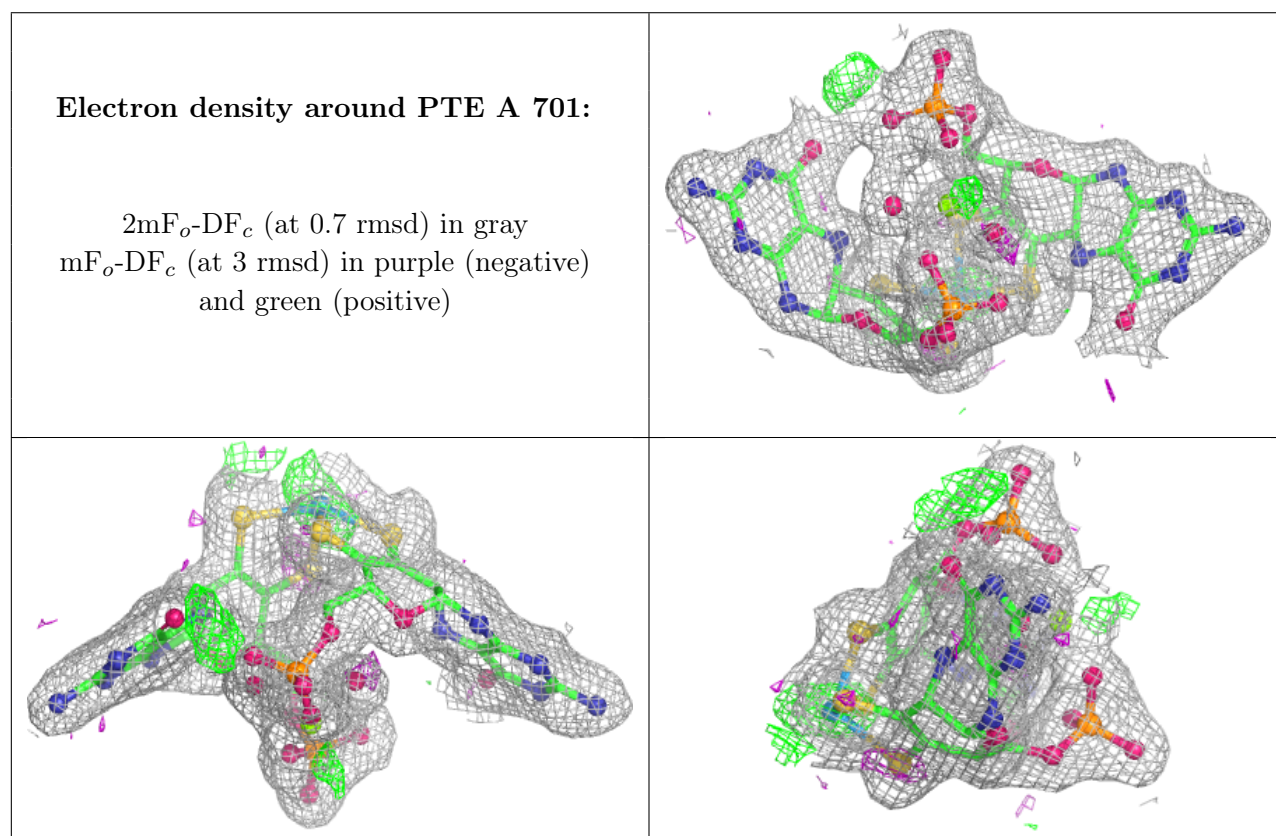
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	PO4	B	206	5/5	0.65	0.22	28,48,60,64	0
7	PO4	D	206	5/5	0.73	0.17	32,39,67,67	0
7	PO4	A	706	5/5	0.82	0.39	41,47,53,53	0
7	PO4	A	707	5/5	0.85	0.13	56,58,61,68	0
7	PO4	C	708	5/5	0.87	0.28	28,36,52,54	0
7	PO4	C	707	5/5	0.89	0.11	45,46,51,52	0
7	PO4	A	708	5/5	0.91	0.25	31,41,50,60	0
6	TAU	C	706	7/7	0.96	0.10	12,21,26,33	0
6	TAU	A	705	7/7	0.96	0.13	14,27,35,44	0
8	CL	B	205	1/1	0.96	0.17	39,39,39,39	0
8	CL	C	705	1/1	0.96	0.06	39,39,39,39	0
5	MG	A	703	1/1	0.97	0.07	24,24,24,24	0
8	CL	D	205	1/1	0.97	0.16	39,39,39,39	0
4	SF4	B	204	8/8	0.98	0.04	21,22,24,25	0
4	SF4	D	203	8/8	0.98	0.04	21,24,25,26	0
4	SF4	B	203	8/8	0.98	0.04	22,24,25,26	0
4	SF4	A	702	8/8	0.99	0.04	18,20,21,22	0
4	SF4	C	702	8/8	0.99	0.03	16,17,19,20	0
4	SF4	D	201	8/8	0.99	0.03	16,16,19,19	0
4	SF4	D	202	8/8	0.99	0.03	18,20,20,21	0
4	SF4	B	201	8/8	0.99	0.03	15,17,19,20	0
4	SF4	D	204	8/8	0.99	0.04	19,21,24,24	0
4	SF4	B	202	8/8	0.99	0.03	18,20,20,22	0
5	MG	A	704	1/1	0.99	0.10	16,16,16,16	0
5	MG	C	703	1/1	0.99	0.06	22,22,22,22	0
5	MG	C	704	1/1	0.99	0.06	13,13,13,13	0
3	PTE	A	701	52/52	0.99	0.05	17,21,24,28	0

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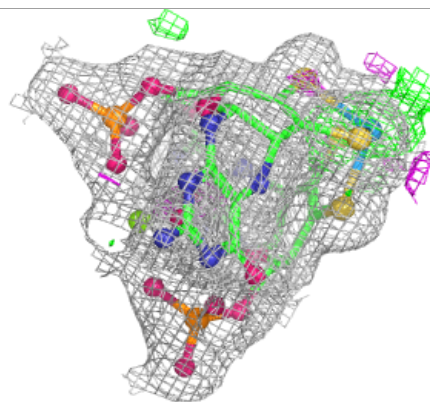
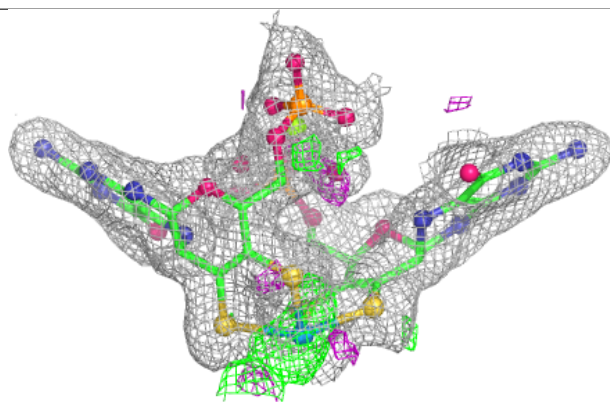
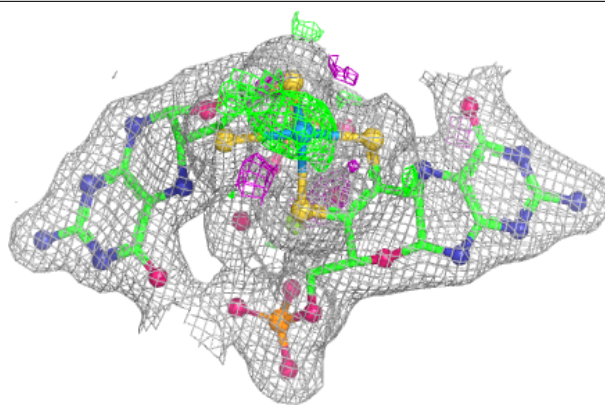
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	PTE	C	701	52/52	1.00	0.04	15,20,22,25	0

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 PTE C 701:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.