



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:21 PM UTC

PDB ID : 6X1O / pdb_00006x1o
Title : WOR5 from Pyrococcus furiosus, as crystallized
Authors : Mathew, L.G.; Lanzilotta, W.N.
Deposited on : 2020-05-19
Resolution : 2.09 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

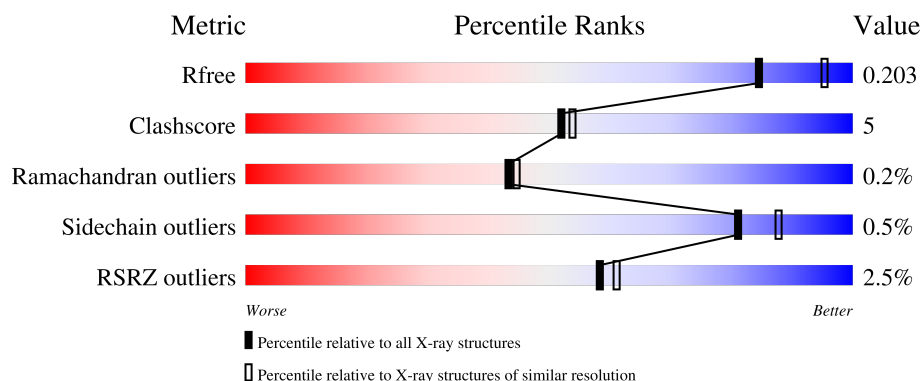
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	624	3% 85% 14% .
1	C	624	2% 88% 12% .
2	B	166	% 93% 6% .
2	D	166	4% 97% ..

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12790 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	1	0
			4931	3182	814	921	14			
1	C	624	Total	C	N	O	S	0	0	0
			4931	3180	815	922	14			

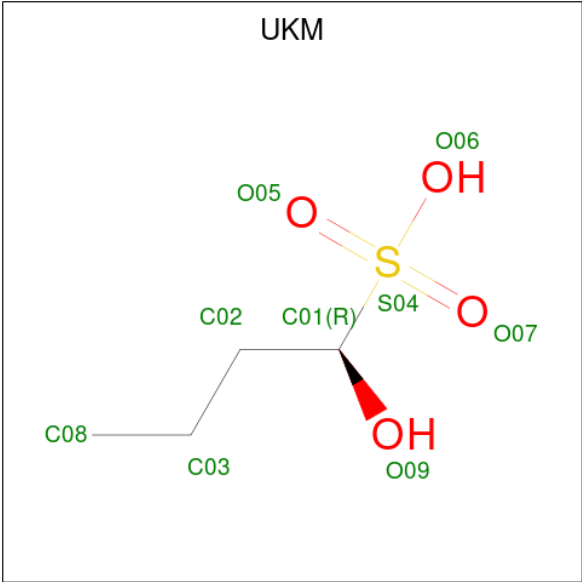
- Molecule 2 is a protein called Oxidoreductase, Fe-S subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	0	0
			1251	789	215	231	16			
2	D	166	Total	C	N	O	S	0	0	0
			1244	786	215	227	16			

There are 2 discrepancies between the modelled and reference sequences:

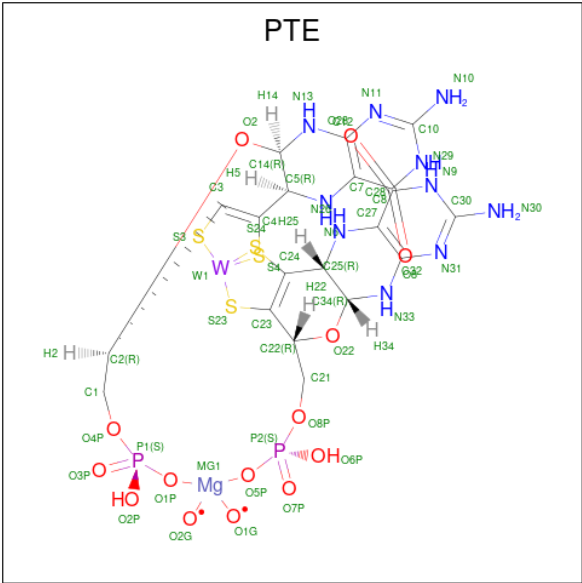
Chain	Residue	Modelled	Actual	Comment	Reference
B	8	ALA	-	expression tag	UNP I6U881
D	8	ALA	-	expression tag	UNP I6U881

- Molecule 3 is (1R)-1-hydroxybutane-1-sulfonic acid (CCD ID: UKM) (formula: C₄H₁₀O₄S).



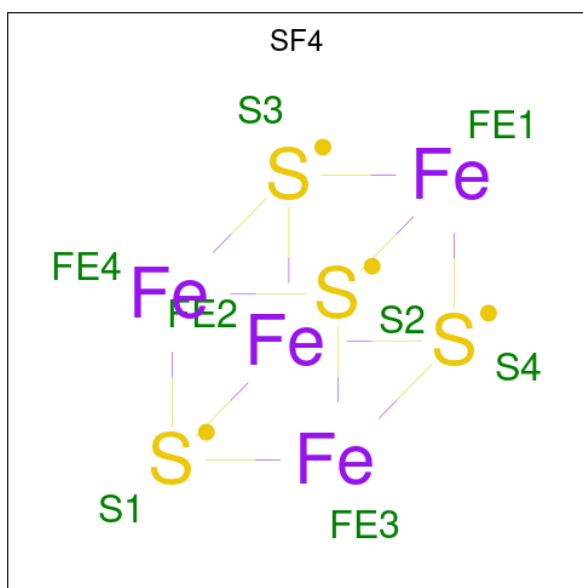
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			9	4	4	1		
3	C	1	Total	C	O	S	0	0
			9	4	4	1		

- Molecule 4 is TUNGSTOPTERIN COFACTOR (CCD ID: PTE) (formula: C₂₀H₂₂MgN₁₀O₁₄P₂S₄W).



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

- Molecule 5 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



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

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

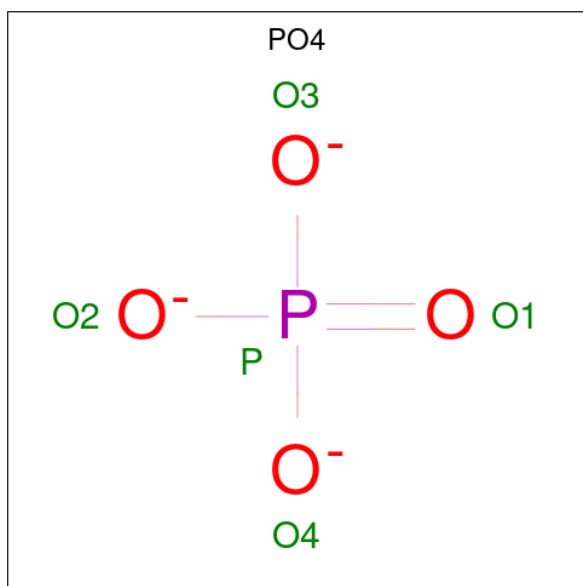
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total	Mg	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	2	Total	Mg	0	0
			2	2		

- 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	C	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	D	1	Total	Cl	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	98	Total	O	0	0
			98	98		
9	B	35	Total	O	0	0
			35	35		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	62	Total 62	O 62	0	0
9	D	20	Total 20	O 20	0	0

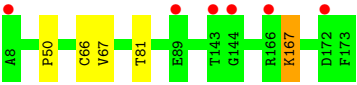
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- Molecule 1: Formaldehyde:ferredoxin oxidoreductase wor5





● 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	123.09Å 126.82Å 141.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.19 – 2.09 47.19 – 2.09	Depositor EDS
% Data completeness (in resolution range)	99.0 (47.19-2.09) 90.9 (47.19-2.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.178 , 0.205 0.179 , 0.203	Depositor DCC
R_{free} test set	2001 reflections (1.53%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.787	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 30.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.55$, $\langle L^2 \rangle = 0.39$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12790	wwPDB-VP
Average B, all atoms (Å ²)	39.0	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 46.02 % 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 1.2164e-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: PO4, PTE, MG, UKM, SF4, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	0/5046	0.67	4/6809 (0.1%)
1	C	0.50	0/5043	0.67	3/6805 (0.0%)
2	B	0.53	0/1279	0.67	1/1741 (0.1%)
2	D	0.55	0/1272	0.71	3/1732 (0.2%)
All	All	0.51	0/12640	0.67	11/17087 (0.1%)

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	C	0	3

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	185	ARG	N-CA-C	5.79	119.16	111.75
1	A	492	ALA	N-CA-C	5.77	118.04	111.11
2	D	81	THR	CA-C-N	-5.71	110.23	121.41
2	D	81	THR	C-N-CA	-5.71	110.23	121.41
1	C	185	ARG	N-CA-C	5.56	118.86	111.75
1	A	543	GLY	CA-C-N	-5.35	114.24	119.64
1	A	543	GLY	C-N-CA	-5.35	114.24	119.64
1	C	543	GLY	CA-C-N	-5.25	113.62	119.19
1	C	543	GLY	C-N-CA	-5.25	113.62	119.19
2	D	81	THR	O-C-N	-5.14	116.67	122.68
2	B	115	VAL	CB-CA-C	-5.02	104.76	111.13

There are no chirality outliers.

All (3) planarity outliers are listed below:

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

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	4931	0	4959	72	0
1	C	4931	0	4950	48	0
2	B	1251	0	1233	7	0
2	D	1244	0	1227	3	0
3	A	9	0	0	1	0
3	C	9	0	0	1	0
4	A	52	0	20	2	0
4	C	52	0	20	2	0
5	A	8	0	0	0	0
5	B	32	0	0	0	0
5	C	8	0	0	0	0
5	D	32	0	0	0	0
6	A	2	0	0	0	0
6	C	2	0	0	0	0
7	A	5	0	0	0	0
7	C	5	0	0	0	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	A	98	0	0	1	0
9	B	35	0	0	0	0
9	C	62	0	0	0	0
9	D	20	0	0	0	0
All	All	12790	0	12409	127	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 5.

All (127) 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:C:45:GLU:CD	1:C:114:ARG:HH22	1.79	0.91
1:C:45:GLU:OE1	1:C:114:ARG:NH2	2.06	0.89
1:A:597:ILE:HD11	1:A:622:LEU:HD12	1.55	0.88
1:A:519:THR:HG23	1:A:522:GLN:H	1.37	0.87
1:A:162:GLU:OE1	9:A:801:HOH:O	2.00	0.80
1:A:7:LYS:HD2	1:A:20:GLU:OE2	1.83	0.78
1:A:597:ILE:HD11	1:A:622:LEU:CD1	2.17	0.73
1:A:73:TYR:HE2	1:A:498:VAL:HG13	1.52	0.73
1:A:600:GLU:HB3	1:A:612:LYS:HG2	1.76	0.67
1:A:118:LYS:HE2	1:A:118:LYS:H	1.60	0.66
3:C:701:UKM:O05	4:C:702:PTE:S4	2.54	0.66
1:A:67:GLY:N	1:A:70:THR:OG1	2.21	0.65
1:C:53:VAL:HG13	1:C:59:GLU:HG2	1.77	0.65
2:B:79:GLU:H	2:B:79:GLU:CD	2.05	0.64
1:C:185:ARG:HG3	1:C:414:GLU:HA	1.81	0.62
1:A:600:GLU:O	1:A:604:GLU:HG3	2.00	0.62
1:C:600:GLU:O	1:C:604:GLU:HG3	2.00	0.61
1:A:601:GLU:O	1:A:605:GLU:HG3	2.00	0.60
1:A:53:VAL:HG13	1:A:59:GLU:HG2	1.82	0.60
1:C:142:GLY:HA3	1:C:354:GLU:OE2	2.02	0.59
1:A:495:CYS:O	1:A:498:VAL:HG12	2.01	0.59
1:A:621:ARG:O	1:A:621:ARG:HG2	2.02	0.59
1:A:67:GLY:H	1:A:70:THR:HG1	1.49	0.58
1:A:67:GLY:O	1:A:70:THR:OG1	2.22	0.58
1:C:62:LEU:HD21	1:C:206:MET:HE3	1.85	0.58
1:C:83:LYS:NZ	1:C:543:GLY:HA2	2.18	0.58
1:C:365:ILE:HD13	1:C:416:THR:HA	1.85	0.58
1:A:66:THR:HB	1:A:70:THR:OG1	2.04	0.57
1:C:154:VAL:O	1:C:158:ILE:HG12	2.03	0.57
1:C:268:PRO:HB3	1:C:272:TRP:CE2	2.41	0.56
1:A:620:LYS:C	1:A:622:LEU:H	2.15	0.55
1:A:118:LYS:H	1:A:118:LYS:CE	2.19	0.55
1:A:264:ARG:HH11	1:A:453:ASP:HA	1.72	0.55
3:A:701:UKM:O05	4:A:702:PTE:S4	2.64	0.55
1:A:66:THR:HB	1:A:70:THR:HG21	1.89	0.55
1:A:594:GLU:CD	1:A:594:GLU:H	2.15	0.54
1:C:88:ASN:HB3	1:C:543:GLY:N	2.23	0.54
1:A:268:PRO:HB3	1:A:272:TRP:CE2	2.42	0.54
1:C:95:LEU:HA	4:C:702:PTE:O1P	2.08	0.53
1:C:404:GLU:HB2	1:C:406:GLU:HG3	1.90	0.53
1:A:152:LYS:O	1:A:156:GLU:HG3	2.07	0.53
1:A:67:GLY:O	1:A:70:THR:CB	2.56	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:TYR:HA	1:A:485:VAL:HG21	1.91	0.53
1:C:470:THR:O	1:C:486:GLU:HG3	2.09	0.53
1:C:329:LEU:HD23	1:C:349:SER:HB3	1.91	0.52
1:A:83:LYS:NZ	1:A:543:GLY:HA2	2.24	0.52
1:C:83:LYS:HZ3	1:C:543:GLY:HA2	1.75	0.52
1:A:267:GLU:O	1:A:275:GLU:HA	2.10	0.51
1:A:519:THR:HG22	1:A:522:GLN:CD	2.36	0.51
2:B:39:GLU:OE2	1:C:217:LYS:NZ	2.41	0.51
1:C:537:ILE:HG13	1:C:598:PRO:HG2	1.92	0.51
1:A:58:GLU:HG3	1:A:116:LYS:HB3	1.93	0.51
1:A:79:SER:HB2	1:A:493:VAL:HG21	1.92	0.51
1:C:61:LEU:HD21	1:C:114:ARG:NH1	2.26	0.51
1:C:267:GLU:O	1:C:275:GLU:HA	2.11	0.50
1:C:584:LYS:HE3	1:C:594:GLU:O	2.11	0.50
1:A:66:THR:CG2	1:A:70:THR:HG21	2.41	0.50
1:A:318:LYS:HB3	1:A:318:LYS:NZ	2.25	0.50
1:A:95:LEU:HA	4:A:702:PTE:O1P	2.11	0.50
1:A:193:LEU:HB2	1:A:194:MET:HE3	1.93	0.50
1:A:142:GLY:HA3	1:A:354:GLU:OE2	2.12	0.49
1:A:70:THR:HB	1:A:104:LYS:NZ	2.28	0.49
1:A:470:THR:O	1:A:486:GLU:HG2	2.13	0.49
1:C:88:ASN:CG	1:C:543:GLY:HA3	2.38	0.49
1:A:612:LYS:O	1:A:616:LYS:HG2	2.13	0.48
1:C:17:LYS:HE3	1:C:18:VAL:H	1.79	0.48
1:C:488:PHE:HA	1:C:523:TRP:CZ2	2.49	0.47
1:A:11:VAL:HG22	1:A:18:VAL:HG13	1.97	0.47
1:A:88:ASN:HB3	1:A:543:GLY:N	2.29	0.47
1:A:574:PRO:HB2	1:A:579:ILE:HD11	1.96	0.47
1:C:62:LEU:HD21	1:C:206:MET:CE	2.44	0.47
2:B:66:CYS:SG	2:B:67:VAL:N	2.88	0.47
1:A:116:LYS:HD2	1:A:208:SER:O	2.14	0.47
1:A:67:GLY:O	1:A:70:THR:HB	2.15	0.46
1:C:519:THR:OG1	1:C:522:GLN:HG2	2.14	0.46
1:A:519:THR:OG1	1:A:521:GLU:OE2	2.32	0.46
1:C:51:GLU:HA	1:C:542:GLY:O	2.15	0.46
1:A:75:GLY:HA2	1:A:302:CYS:HB2	1.97	0.46
1:C:292:TRP:O	2:D:167:LYS:HE2	2.16	0.46
1:A:533:HIS:ND1	1:A:598:PRO:HB3	2.31	0.46
1:A:73:TYR:CE2	1:A:498:VAL:HG13	2.42	0.46
1:A:438:VAL:HG12	1:A:439:LYS:HG2	1.96	0.46
1:A:30:LYS:O	1:A:527:ILE:HG23	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ASN:CG	1:A:543:GLY:HA3	2.41	0.45
1:A:456:LYS:HE2	1:A:456:LYS:HB3	1.73	0.45
1:C:160:LYS:NZ	1:C:160:LYS:HB3	2.32	0.45
1:A:96:SER:HB3	1:A:299:ASP:CG	2.43	0.44
1:C:575:ASN:HB3	1:C:578:ASP:OD2	2.17	0.44
1:C:85:PRO:HD2	1:C:200:GLY:O	2.17	0.44
1:C:438:VAL:HG12	1:C:439:LYS:HG2	2.00	0.44
2:B:56:HIS:CD2	2:B:157:PRO:HG3	2.53	0.44
1:A:427:LYS:HB2	1:A:429:ILE:HG22	1.99	0.44
2:B:50:PRO:HG2	1:C:193:LEU:HG	1.99	0.44
1:C:118:LYS:H	1:C:118:LYS:HE2	1.83	0.44
1:C:411:ILE:HG12	1:C:422:LYS:HE2	2.01	0.43
1:C:64:ILE:HD12	1:C:80:ILE:HD13	2.01	0.43
1:C:600:GLU:HB3	1:C:612:LYS:HE2	2.00	0.43
1:A:199:TYR:CZ	1:A:468:ASP:HA	2.53	0.42
1:A:362:THR:HG21	1:A:399:LEU:HD21	1.99	0.42
2:B:22:ARG:HD2	1:C:300:TYR:CD2	2.54	0.42
1:C:96:SER:HB3	1:C:299:ASP:CG	2.45	0.42
1:A:365:ILE:HD13	1:A:416:THR:HA	2.01	0.42
1:C:533:HIS:ND1	1:C:598:PRO:HB3	2.35	0.42
1:C:594:GLU:HG3	1:C:595:HIS:CD2	2.54	0.42
1:A:70:THR:HB	1:A:104:LYS:HZ2	1.83	0.42
1:A:59:GLU:OE2	1:A:59:GLU:N	2.40	0.42
1:A:158:ILE:HG22	1:A:168:PRO:HG2	2.01	0.42
1:A:488:PHE:HA	1:A:523:TRP:CZ2	2.55	0.42
1:C:480:TYR:HA	1:C:485:VAL:HG21	2.01	0.41
1:A:13:LEU:O	1:A:118:LYS:NZ	2.53	0.41
1:A:83:LYS:HZ3	1:A:543:GLY:HA2	1.85	0.41
2:D:66:CYS:SG	2:D:67:VAL:N	2.94	0.41
1:A:66:THR:HB	1:A:70:THR:CG2	2.50	0.41
1:C:118:LYS:HE2	1:C:118:LYS:HB2	1.67	0.41
1:C:158:ILE:HG22	1:C:168:PRO:HG2	2.02	0.41
2:B:9:ILE:HG22	2:B:143:THR:HG22	2.02	0.41
1:C:362:THR:CG2	1:C:399:LEU:HD21	2.51	0.41
1:C:398:LEU:HD11	1:C:412:LEU:HD12	2.03	0.41
1:A:245:MET:SD	1:A:500:LYS:HD3	2.60	0.40
1:A:429:ILE:HG23	1:A:431:VAL:HG13	2.02	0.40
1:C:559:ARG:O	1:C:559:ARG:HG3	2.21	0.40
1:A:67:GLY:HA3	1:A:492:ALA:O	2.20	0.40
1:A:615:VAL:O	1:A:619:LYS:HG3	2.20	0.40
1:A:417:TYR:CZ	1:A:421:LEU:HD11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:THR:CB	1:A:70:THR:HG21	2.51	0.40
1:A:185:ARG:HG3	1:A:414:GLU:HA	2.03	0.40
1:A:193:LEU:HG	2:D:50:PRO:HG2	2.03	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	622/624 (100%)	594 (96%)	27 (4%)	1 (0%)	43	44
1	C	622/624 (100%)	594 (96%)	26 (4%)	2 (0%)	36	36
2	B	164/166 (99%)	159 (97%)	5 (3%)	0	100	100
2	D	164/166 (99%)	158 (96%)	6 (4%)	0	100	100
All	All	1572/1580 (100%)	1505 (96%)	64 (4%)	3 (0%)	43	44

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	457	ASP
1	C	457	ASP
1	C	493	VAL

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	517/517 (100%)	514 (99%)	3 (1%)	78	86
1	C	516/517 (100%)	514 (100%)	2 (0%)	84	89
2	B	141/141 (100%)	140 (99%)	1 (1%)	76	83
2	D	139/141 (99%)	138 (99%)	1 (1%)	76	83
All	All	1313/1316 (100%)	1306 (100%)	7 (0%)	81	88

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42[A]	LEU
1	A	42[B]	LEU
1	A	622	LEU
2	B	115	VAL
1	C	80	ILE
1	C	352	VAL
2	D	167	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	68	ASN
2	B	73	ASN
1	C	182	ASN
2	D	32	HIS
2	D	53	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 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 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
7	PO4	C	706	-	4,4,4	1.43	1 (25%)	6,6,6	0.91	0
5	SF4	B	903	2	0,12,12	-	-	-		
5	SF4	D	904	2	0,12,12	-	-	-		
3	UKM	A	701	4	6,8,8	4.72	3 (50%)	6,11,11	1.95	1 (16%)
5	SF4	B	905	2	0,12,12	-	-	-		
5	SF4	B	902	2	0,12,12	-	-	-		
5	SF4	B	904	2	0,12,12	-	-	-		
7	PO4	A	706	-	4,4,4	0.61	0	6,6,6	1.32	1 (16%)
5	SF4	D	903	2	0,12,12	-	-	-		
5	SF4	D	902	2	0,12,12	-	-	-		
5	SF4	D	905	2	0,12,12	-	-	-		
4	PTE	C	702	6,3,1	46,60,60	2.38	8 (17%)	42,98,98	1.93	16 (38%)
5	SF4	C	703	1	0,12,12	-	-	-		
4	PTE	A	702	6,3,1	46,60,60	2.38	9 (19%)	42,98,98	2.01	15 (35%)
3	UKM	C	701	4	6,8,8	4.14	4 (66%)	6,11,11	2.72	2 (33%)
5	SF4	A	703	1	0,12,12	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SF4	B	903	2	-	-	0/6/5/5
5	SF4	D	904	2	-	-	0/6/5/5
3	UKM	A	701	4	-	0/5/9/9	-
5	SF4	B	905	2	-	-	0/6/5/5
5	SF4	B	902	2	-	-	0/6/5/5
5	SF4	B	904	2	-	-	0/6/5/5
5	SF4	D	903	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SF4	D	902	2	-	-	0/6/5/5
5	SF4	D	905	2	-	-	0/6/5/5
4	PTE	C	702	6,3,1	-	0/12/100/100	-
5	SF4	C	703	1	-	-	0/6/5/5
4	PTE	A	702	6,3,1	-	0/12/100/100	-
3	UKM	C	701	4	-	0/5/9/9	-
5	SF4	A	703	1	-	-	0/6/5/5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	UKM	O07-S04	9.28	1.77	1.44
4	A	702	PTE	P1-O1P	9.00	1.64	1.50
4	C	702	PTE	P1-O1P	8.58	1.64	1.50
4	C	702	PTE	P2-O5P	8.22	1.63	1.50
4	A	702	PTE	P2-O5P	7.91	1.63	1.50
3	C	701	UKM	O06-S04	6.32	1.76	1.48
4	C	702	PTE	C7-C12	6.11	1.49	1.38
3	A	701	UKM	O05-S04	5.67	1.64	1.44
4	A	702	PTE	C7-C12	5.61	1.48	1.38
3	C	701	UKM	O07-S04	5.50	1.63	1.44
4	A	702	PTE	C27-C32	5.31	1.47	1.38
3	C	701	UKM	O05-S04	5.25	1.62	1.44
4	C	702	PTE	C27-C32	4.74	1.46	1.38
3	A	701	UKM	O06-S04	3.52	1.63	1.48
4	C	702	PTE	C28-N29	-2.91	1.33	1.38
4	A	702	PTE	C28-N29	-2.77	1.33	1.38
7	C	706	PO4	P-O1	2.66	1.56	1.50
4	C	702	PTE	C24-S24	-2.39	1.67	1.74
4	A	702	PTE	C24-S24	-2.38	1.67	1.74
4	A	702	PTE	C8-N9	-2.29	1.34	1.38
4	C	702	PTE	C8-N9	-2.18	1.34	1.38
4	A	702	PTE	C23-S23	-2.14	1.67	1.74
3	C	701	UKM	C01-S04	-2.13	1.77	1.81
4	C	702	PTE	C7-C8	2.13	1.48	1.41
4	A	702	PTE	C27-C28	2.12	1.48	1.41

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	701	UKM	O07-S04-O05	-5.95	88.72	114.67
4	A	702	PTE	C30-N31-C32	4.43	121.18	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	702	PTE	C30-N31-C32	4.26	120.88	113.36
4	A	702	PTE	C14-C5-N6	4.13	111.92	107.87
4	C	702	PTE	C10-N11-C12	3.86	120.18	113.36
3	A	701	UKM	O06-S04-O05	-3.85	92.15	110.15
4	A	702	PTE	C10-N11-C12	3.82	120.09	113.36
4	C	702	PTE	O22-C34-C25	-3.70	106.50	108.96
4	A	702	PTE	C3-C4-S4	3.51	124.72	119.62
4	A	702	PTE	O8-C8-C7	-3.31	119.28	127.26
4	A	702	PTE	C34-C25-N26	3.25	111.06	107.87
4	C	702	PTE	O28-C28-C27	-3.16	119.64	127.26
4	A	702	PTE	O28-C28-C27	-3.02	119.99	127.26
4	C	702	PTE	C3-C4-S4	2.96	123.92	119.62
4	C	702	PTE	C14-C5-N6	2.93	110.75	107.87
4	C	702	PTE	O8-C8-C7	-2.86	120.36	127.26
4	A	702	PTE	O2-C2-C3	2.72	112.94	109.09
4	C	702	PTE	C28-C27-N26	2.60	123.36	116.27
4	A	702	PTE	O22-C22-C23	2.60	112.76	109.09
4	C	702	PTE	O2-C2-C3	2.55	112.68	109.09
4	A	702	PTE	C23-C24-S24	2.52	123.28	119.62
4	C	702	PTE	C23-C24-S24	2.46	123.20	119.62
4	A	702	PTE	C8-C7-N6	2.45	122.94	116.27
4	A	702	PTE	C28-C27-N26	2.43	122.90	116.27
4	A	702	PTE	C7-C8-N9	2.41	118.75	112.13
4	C	702	PTE	C8-C7-N6	2.41	122.83	116.27
4	C	702	PTE	C27-C28-N29	2.39	118.70	112.13
4	A	702	PTE	C27-C28-N29	2.38	118.66	112.13
4	C	702	PTE	C7-C8-N9	2.28	118.40	112.13
4	C	702	PTE	O22-C34-N33	2.26	110.66	108.61
4	C	702	PTE	C30-N29-C28	-2.23	121.07	125.11
4	C	702	PTE	O2-C14-C5	2.14	110.39	108.96
3	C	701	UKM	O09-C01-C02	2.13	117.15	109.45
7	A	706	PO4	O4-P-O3	2.09	114.42	107.91
4	A	702	PTE	C30-N29-C28	-2.09	121.33	125.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

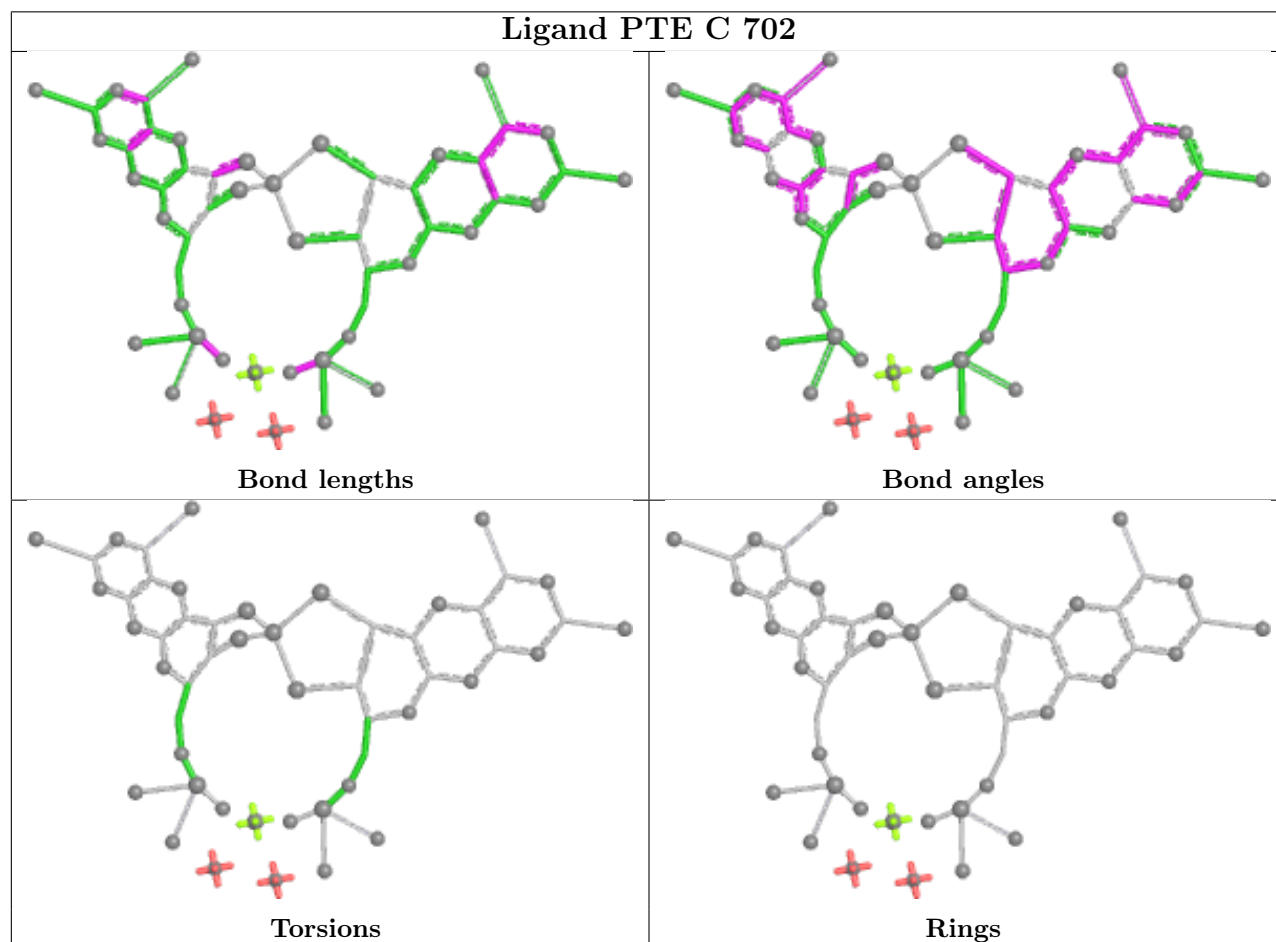
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	UKM	1	0

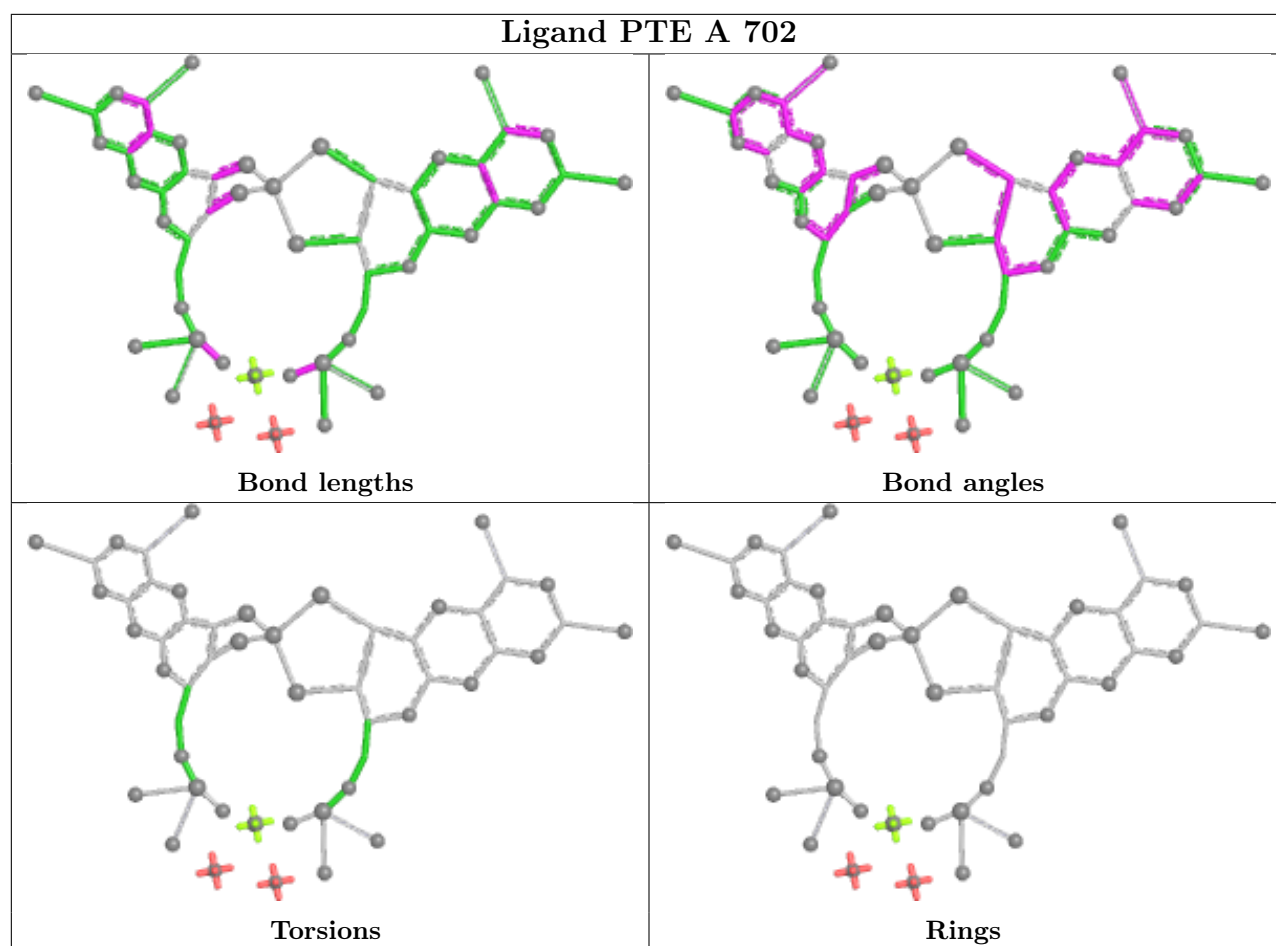
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	702	PTE	2	0
4	A	702	PTE	2	0
3	C	701	UKM	1	0

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	623/624 (99%)	0.27	21 (3%)	48 50	23, 39, 55, 63	1 (0%)
1	C	624/624 (100%)	0.20	11 (1%)	67 70	27, 38, 53, 66	0
2	B	166/166 (100%)	0.06	2 (1%)	76 78	28, 35, 47, 61	0
2	D	166/166 (100%)	0.16	6 (3%)	46 48	28, 35, 47, 65	0
All	All	1579/1580 (99%)	0.21	40 (2%)	58 61	23, 38, 53, 66	1 (0%)

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	THR	7.1
1	C	543	GLY	6.2
1	A	543	GLY	5.8
1	A	622	LEU	5.4
1	C	162	GLU	3.4
2	D	144	GLY	3.4
1	C	624	LEU	3.4
1	A	278	ASP	3.4
2	D	143	THR	3.2
1	A	71	GLY	3.2
1	A	577	GLU	3.1
2	B	8	ALA	3.0
1	C	479	GLY	2.9
1	A	621	ARG	2.7
1	C	575	ASN	2.7
1	A	623	ASN	2.7
1	A	479	GLY	2.7
2	B	79	GLU	2.6
1	A	594	GLU	2.4
1	A	595	HIS	2.4
1	A	481	THR	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	8	ALA	2.3
1	A	160	LYS	2.3
2	D	89	GLU	2.2
2	D	172	ASP	2.2
1	A	620	LYS	2.2
1	C	517	ASN	2.2
1	A	584	LYS	2.2
1	A	519	THR	2.2
1	C	477	ALA	2.2
1	A	575	ASN	2.2
1	C	604	GLU	2.1
1	A	118	LYS	2.1
1	A	492	ALA	2.1
1	A	604	GLU	2.1
2	D	166	ARG	2.1
1	C	578	ASP	2.1
1	C	562	GLU	2.0
1	A	588	GLU	2.0
1	C	601	GLU	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
7	PO4	A	706	5/5	0.87	0.33	42,46,56,65	0
7	PO4	C	706	5/5	0.87	0.35	40,49,56,65	0
3	UKM	C	701	9/9	0.94	0.14	23,35,43,45	0
3	UKM	A	701	9/9	0.95	0.13	24,37,43,46	0

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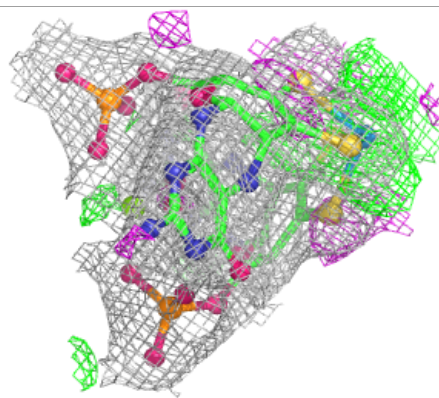
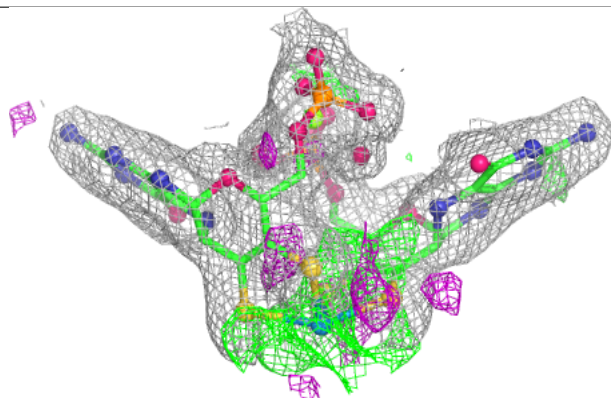
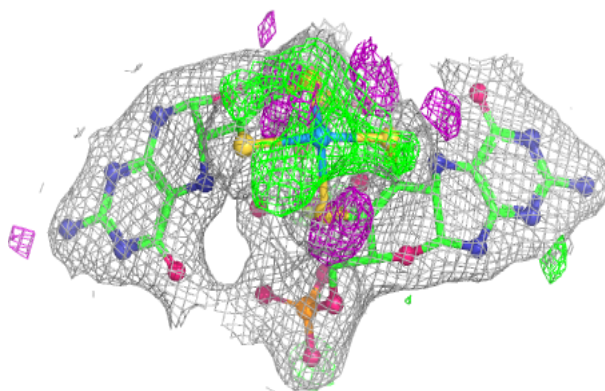
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	CL	B	901	1/1	0.96	0.08	48,48,48,48	0
5	SF4	D	904	8/8	0.98	0.04	33,35,37,38	0
6	MG	A	705	1/1	0.98	0.03	37,37,37,37	0
6	MG	C	705	1/1	0.98	0.03	38,38,38,38	0
8	CL	D	901	1/1	0.98	0.14	52,52,52,52	0
5	SF4	C	703	8/8	0.99	0.04	28,30,32,32	0
5	SF4	D	902	8/8	0.99	0.03	28,30,30,31	0
5	SF4	D	903	8/8	0.99	0.04	29,30,32,33	0
4	PTE	A	702	52/52	0.99	0.06	30,33,37,37	0
5	SF4	D	905	8/8	0.99	0.04	32,33,34,34	0
6	MG	A	704	1/1	0.99	0.04	35,35,35,35	0
4	PTE	C	702	52/52	0.99	0.06	29,33,36,37	0
5	SF4	A	703	8/8	0.99	0.04	29,31,34,35	0
5	SF4	B	902	8/8	0.99	0.03	28,29,30,31	0
5	SF4	B	903	8/8	0.99	0.03	29,31,32,32	0
5	SF4	B	904	8/8	0.99	0.04	34,35,37,40	0
5	SF4	B	905	8/8	0.99	0.03	31,33,35,35	0
6	MG	C	704	1/1	1.00	0.05	33,33,33,33	0

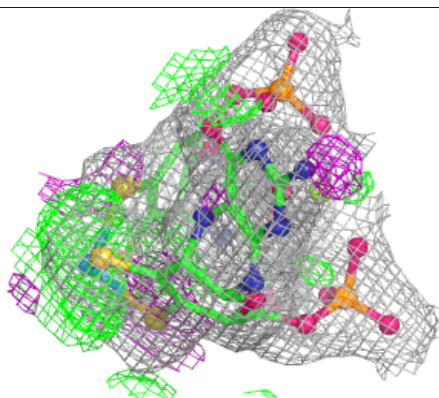
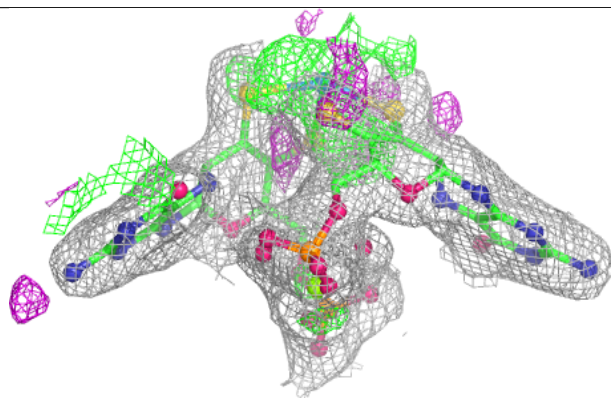
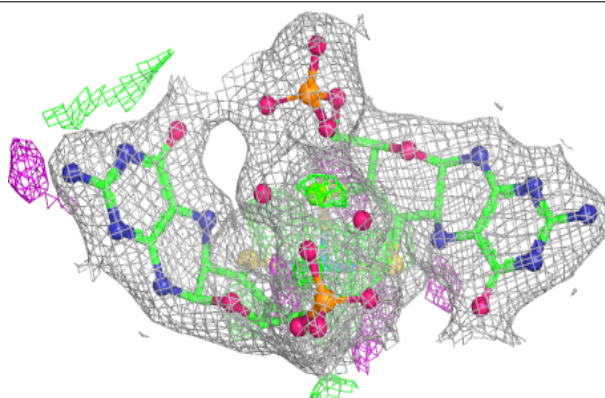
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PTE A 702:

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

**Electron density around PTE C 702:**

$2mF_o-DF_c$ (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.