Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2021 – 10:39 AM EST

PDB ID	:	6X1O
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 following versions of software and data (see references ⓘ) were used in the production of this report:

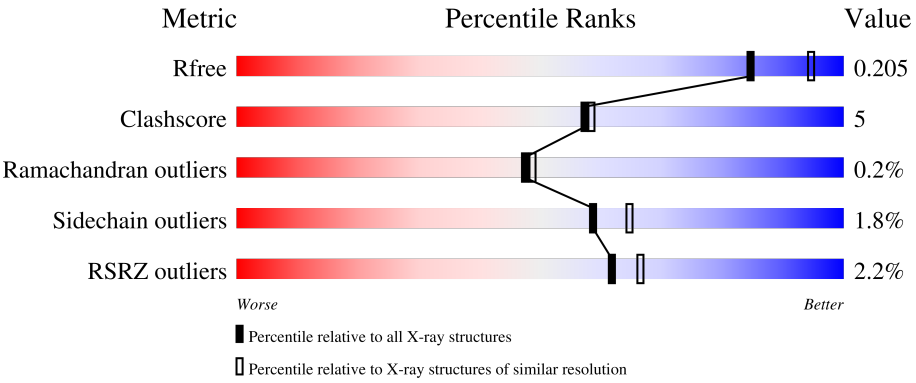
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.09 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}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 <=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% 15%
1	C	624	2% 88% 12%
2	B	166	% 94% 6%
2	D	166	% 96%

2 Entry composition (i)

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			

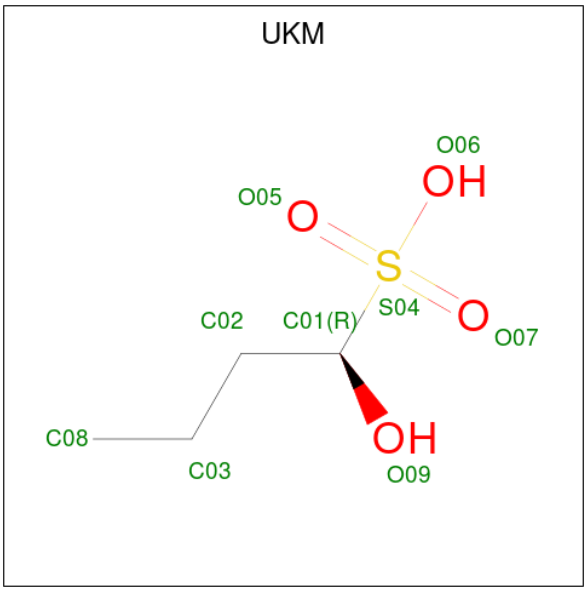
- Molecule 2 is a protein called Oxidoreductase, Fe-S subunit.

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:

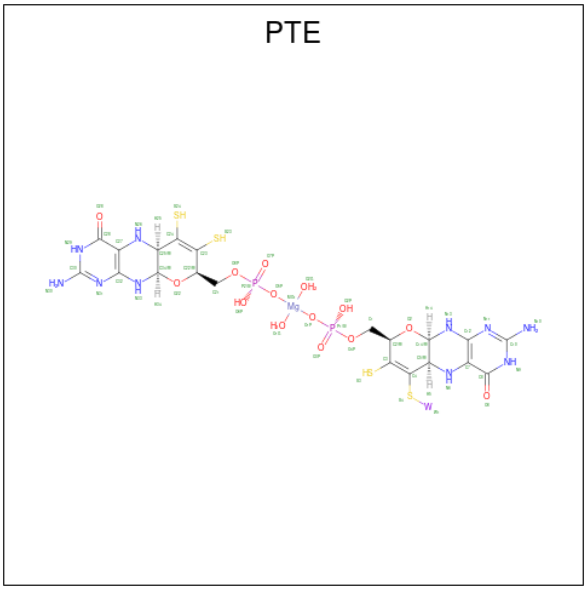
Chain	Residue	Modelled	Actual	Comment	Reference
B	8	ALA	-	expression tag	UNP I6U881
D	8	ALA	-	expression tag	UNP I6U881

- Molecule 3 is (1R)-1-hydroxybutane-1-sulfonic acid (three-letter code: UKM) (formula: $C_4H_{10}O_4S$).



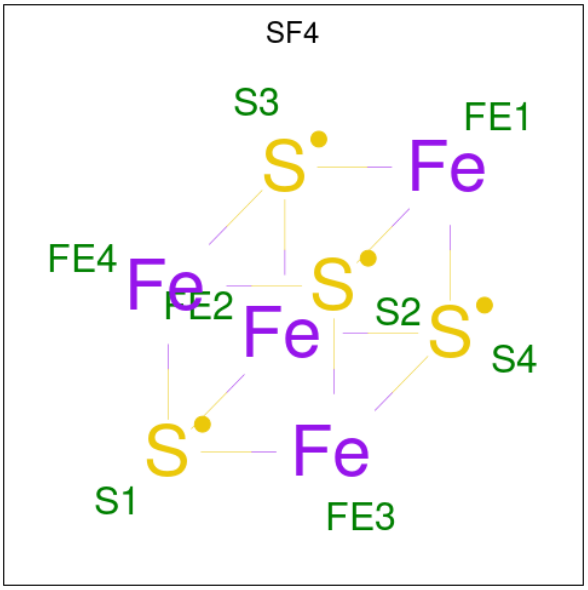
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			9	4	4	1		
3	C	1	Total	C	O	S	0	0
			9	4	4	1		

- Molecule 4 is TUNGSTOPTERIN COFACTOR (three-letter code: PTE) (formula: $C_{20}H_{29}MgN_{10}O_{14}P_2S$



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 (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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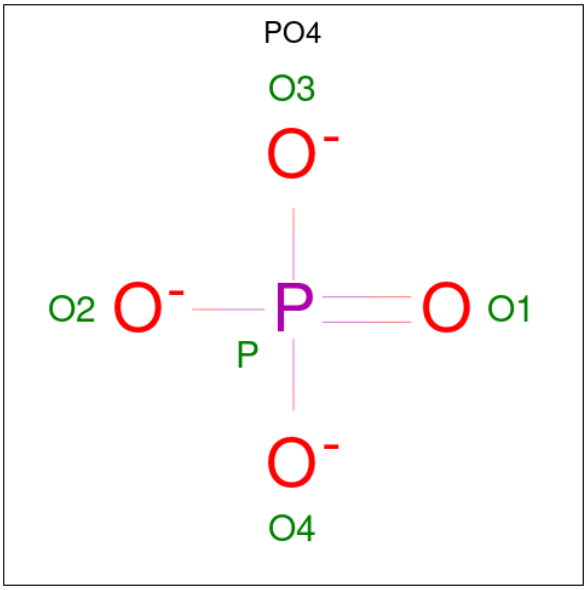
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	2	Total Mg 2 2	0	0

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 9 is water.

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

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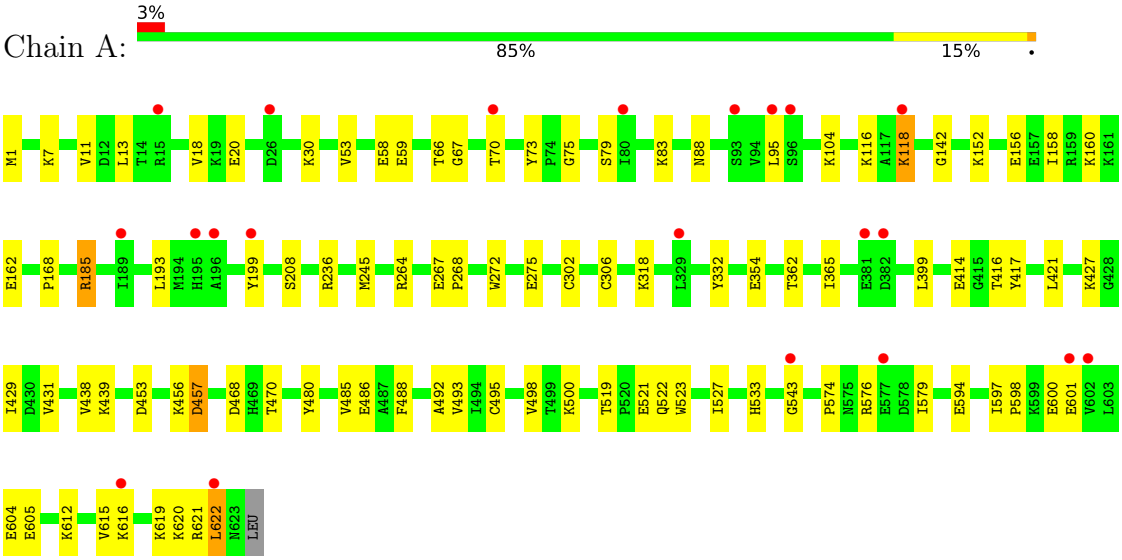
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	C	62	Total O 62 62	0	0
9	D	20	Total O 20 20	0	0

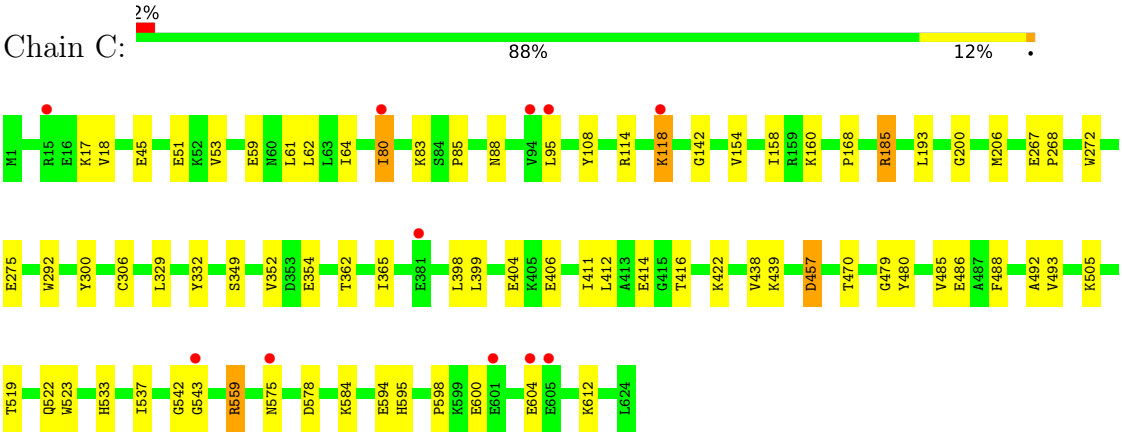
3 Residue-property plots (i)

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.

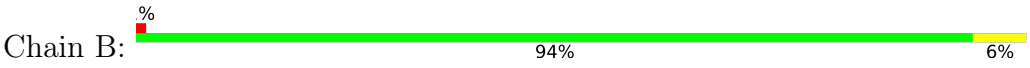
• Molecule 1: Formaldehyde:ferredoxin oxidoreductase wor5

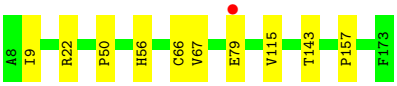


• Molecule 1: Formaldehyde:ferredoxin oxidoreductase wor5



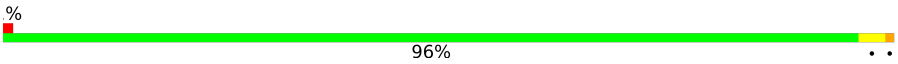
• Molecule 2: Oxidoreductase, Fe-S subunit

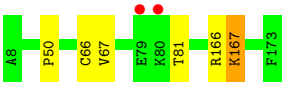




• Molecule 2: Oxidoreductase, Fe-S subunit

Chain D:





4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.26 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.178 , 0.205 0.180 , 0.205	Depositor DCC
R_{free} test set	2001 reflections (1.55%)	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 , 35.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.55$, $< L^2 > = 0.39$	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.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, CL, MG, UKM, SF4, PTE

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	0.58	0/5046	0.67	0/6809
1	C	0.58	0/5043	0.67	0/6805
2	B	0.57	0/1279	0.67	0/1741
2	D	0.56	0/1272	0.69	1/1732 (0.1%)
All	All	0.58	0/12640	0.67	1/17087 (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	C	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	81	THR	C-N-CA	-5.75	110.23	122.30

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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4931	0	4959	70	0
1	C	4931	0	4950	46	0
2	B	1251	0	1233	6	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	123	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 (123) 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: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:C:45:GLU:CD	1:C:114:ARG:HH22	1.79	0.86
1:A:162:GLU:OE1	9:A:801:HOH:O	2.00	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:67:GLY:H	1:A:70:THR:HG1	1.46	0.63
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
2:B:79:GLU:H	2:B:79:GLU:CD	2.05	0.59
1:A:67:GLY:O	1:A:70:THR:OG1	2.22	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: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: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
1:A:480:TYR:HA	1:A:485:VAL:HG21	1.91	0.53
1:C:83:LYS:HZ1	1:C:543:GLY:HA2	1.73	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:A:267:GLU:O	1:A:275:GLU:HA	2.10	0.51
1:C:537:ILE:HG13	1:C:598:PRO:HG2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:620:LYS:C	1:A:622:LEU:H	2.15	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:594:GLU:CD	1:A:594:GLU:H	2.15	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:A:612:LYS:O	1:A:616:LYS:HG2	2.13	0.48
1:C:62:LEU:HD21	1:C:206:MET:HE3	1.94	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:519:THR:HG22	1:A:522:GLN:CD	2.36	0.46
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:C:51:GLU:HA	1:C:542:GLY:O	2.15	0.46
1:A:519:THR:OG1	1:A:521:GLU:OE2	2.32	0.46
1:A:70:THR:HB	1:A:104:LYS:HZ3	1.80	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:88:ASN:CG	1:C:543:GLY:HA3	2.38	0.43
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:83:LYS:HZ3	1:A:543:GLY:HA2	1.83	0.42
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: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: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
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:A:88:ASN:CG	1:A:543:GLY:HA3	2.41	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
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%)	47 49
1	C	622/624 (100%)	594 (96%)	26 (4%)	2 (0%)	41 41
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%)	47 49

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%)	507 (98%)	10 (2%)	57 63
1	C	516/517 (100%)	506 (98%)	10 (2%)	57 63
2	B	141/141 (100%)	140 (99%)	1 (1%)	84 88
2	D	139/141 (99%)	137 (99%)	2 (1%)	67 73
All	All	1313/1316 (100%)	1290 (98%)	23 (2%)	59 65

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	118	LYS
1	A	160	LYS
1	A	185	ARG
1	A	236	ARG
1	A	306	CYS
1	A	332	TYR
1	A	457	ASP
1	A	576	ARG
1	A	622	LEU
2	B	115	VAL
1	C	80	ILE
1	C	108	TYR
1	C	118	LYS
1	C	185	ARG
1	C	306	CYS
1	C	332	TYR
1	C	352	VAL
1	C	457	ASP
1	C	505	LYS
1	C	559	ARG
2	D	166	ARG
2	D	167	LYS

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 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	A	706	-	4,4,4	0.58	0	6,6,6	1.27	1 (16%)
3	UKM	A	701	4	6,8,8	4.18	3 (50%)	6,11,11	1.63	1 (16%)
5	SF4	C	703	1	0,12,12	-	-	-		
5	SF4	D	905	2	0,12,12	-	-	-		
5	SF4	B	904	2	0,12,12	-	-	-		
5	SF4	B	905	2	0,12,12	-	-	-		
7	PO4	C	706	-	4,4,4	1.36	1 (25%)	6,6,6	0.88	0
3	UKM	C	701	4	6,8,8	3.45	3 (50%)	6,11,11	3.05	1 (16%)
5	SF4	B	902	2	0,12,12	-	-	-		
5	SF4	D	904	2	0,12,12	-	-	-		
4	PTE	C	702	1,3,6	44,57,57	2.36	7 (15%)	35,89,89	2.19	14 (40%)
5	SF4	A	703	1	0,12,12	-	-	-		
4	PTE	A	702	1,3,6	44,57,57	2.39	7 (15%)	35,89,89	2.09	11 (31%)
5	SF4	B	903	2	0,12,12	-	-	-		
5	SF4	D	903	2	0,12,12	-	-	-		
5	SF4	D	902	2	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
3	UKM	A	701	4	-	0/5/9/9	-
5	SF4	C	703	1	-	-	0/6/5/5
5	SF4	D	905	2	-	-	0/6/5/5
5	SF4	B	904	2	-	-	0/6/5/5
5	SF4	B	905	2	-	-	0/6/5/5
3	UKM	C	701	4	-	0/5/9/9	-
5	SF4	B	902	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SF4	D	904	2	-	-	0/6/5/5
4	PTE	C	702	1,3,6	-	0/12/82/82	0/6/6/6
5	SF4	A	703	1	-	-	0/6/5/5
4	PTE	A	702	1,3,6	-	0/12/82/82	0/6/6/6
5	SF4	B	903	2	-	-	0/6/5/5
5	SF4	D	903	2	-	-	0/6/5/5
5	SF4	D	902	2	-	-	0/6/5/5

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	702	PTE	P1-O1P	9.00	1.64	1.50
4	C	702	PTE	P1-O1P	8.58	1.64	1.50
3	A	701	UKM	O07-S04	8.36	1.77	1.44
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	A	701	UKM	O05-S04	5.13	1.64	1.44
4	A	702	PTE	C4-S4	-5.06	1.70	1.75
3	C	701	UKM	O07-S04	4.98	1.63	1.44
4	C	702	PTE	C8-C7	4.96	1.48	1.41
4	A	702	PTE	C28-C27	4.95	1.48	1.41
3	C	701	UKM	O05-S04	4.76	1.62	1.44
3	C	701	UKM	O06-S04	4.42	1.76	1.48
4	C	702	PTE	C28-C27	4.38	1.47	1.41
4	C	702	PTE	C4-S4	-4.05	1.71	1.75
4	C	702	PTE	C7-C12	4.05	1.49	1.41
4	A	702	PTE	C8-C7	3.94	1.46	1.41
4	A	702	PTE	C7-C12	3.60	1.48	1.41
4	A	702	PTE	C27-C32	3.32	1.47	1.41
4	C	702	PTE	C27-C32	2.81	1.46	1.41
7	C	706	PO4	P-O1	2.54	1.56	1.50
3	A	701	UKM	O06-S04	2.49	1.63	1.48

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	701	UKM	O07-S04-O05	-7.05	88.72	116.52
4	C	702	PTE	C28-C27-N26	5.05	123.36	119.12
4	A	702	PTE	C8-C7-N6	4.55	122.94	119.12
4	A	702	PTE	C28-C27-N26	4.51	122.90	119.12
4	C	702	PTE	C8-C7-N6	4.42	122.83	119.12
4	C	702	PTE	C8-N9-C10	4.04	122.35	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	702	PTE	O22-C34-C25	-3.70	106.50	108.96
4	A	702	PTE	C8-N9-C10	3.66	121.75	115.93
4	A	702	PTE	C28-N29-C30	3.40	121.33	115.93
4	A	702	PTE	C27-C32-N33	3.25	121.10	118.13
4	C	702	PTE	C28-N29-C30	3.24	121.07	115.93
3	A	701	UKM	O06-S04-O05	-3.12	92.15	110.37
4	A	702	PTE	C30-N31-C32	2.96	121.18	114.54
4	A	702	PTE	C8-C7-C12	2.88	117.12	114.57
4	C	702	PTE	C30-N31-C32	2.83	120.88	114.54
4	A	702	PTE	C28-C27-C32	2.71	116.97	114.57
4	A	702	PTE	C27-N26-C25	-2.69	110.24	120.00
4	A	702	PTE	C32-N33-C34	-2.62	118.53	123.67
4	C	702	PTE	C28-C27-C32	2.57	116.86	114.57
4	C	702	PTE	C27-N26-C25	-2.54	110.78	120.00
4	C	702	PTE	C10-N11-C12	2.52	120.18	114.54
4	A	702	PTE	C10-N11-C12	2.48	120.09	114.54
4	C	702	PTE	C8-C7-C12	2.31	116.62	114.57
4	C	702	PTE	C32-N33-C34	-2.24	119.29	123.67
4	C	702	PTE	C27-C32-N33	2.20	120.14	118.13
4	C	702	PTE	O2-C14-C5	2.14	110.39	108.96
4	C	702	PTE	O22-C34-N33	2.03	110.66	108.57
7	A	706	PO4	O4-P-O3	2.01	114.42	107.97

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

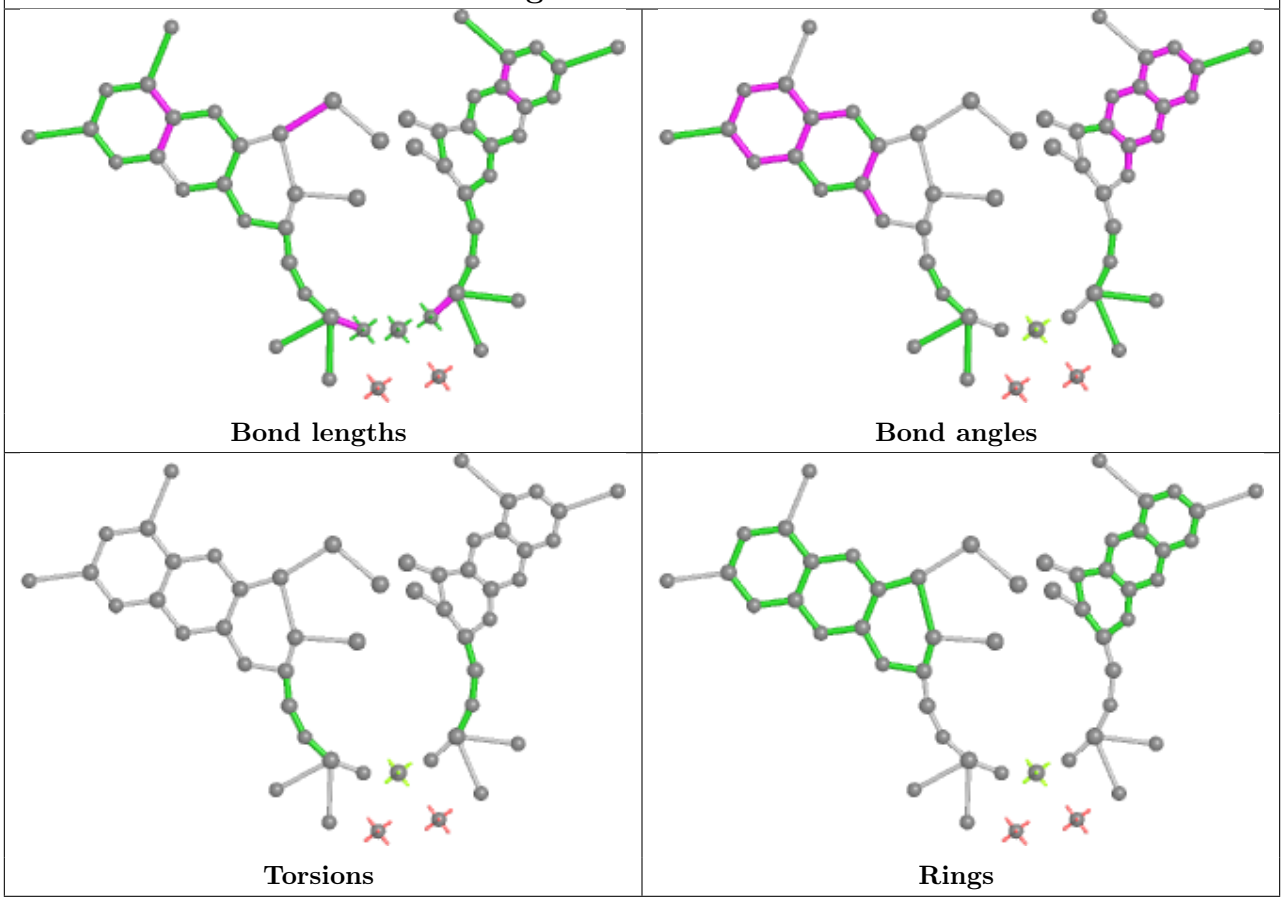
4 monomers are involved in 4 short contacts:

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

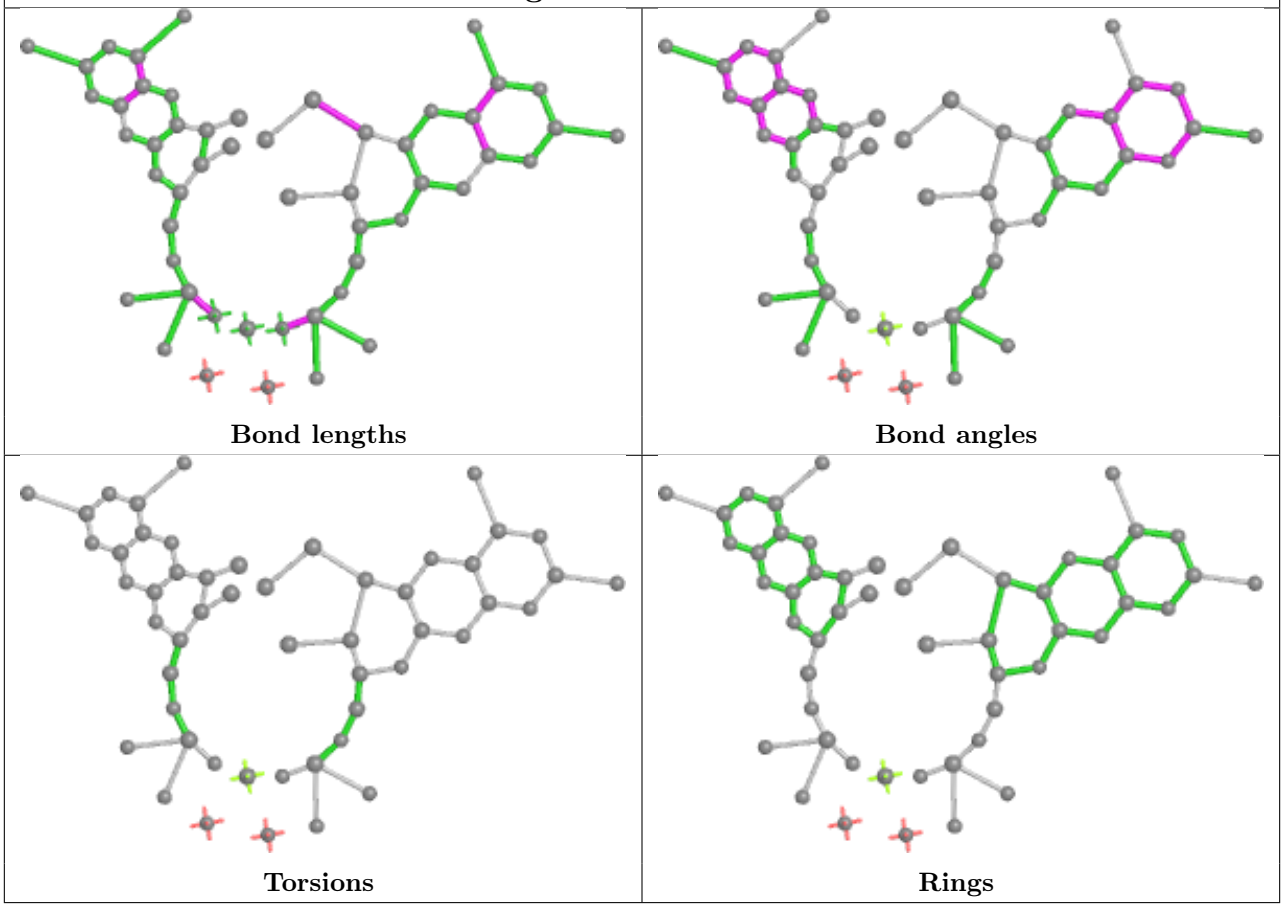
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand PTE C 702



Ligand PTE A 702



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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	623/624 (99%)	0.15	21 (3%) 45 51	28, 39, 55, 63	0
1	C	624/624 (100%)	0.02	11 (1%) 68 72	27, 38, 53, 66	0
2	B	166/166 (100%)	-0.28	1 (0%) 89 91	28, 35, 47, 61	0
2	D	166/166 (100%)	-0.20	2 (1%) 79 82	28, 35, 47, 65	0
All	All	1579/1580 (99%)	0.02	35 (2%) 62 66	27, 38, 53, 66	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	THR	5.4
1	C	15	ARG	3.5
1	C	118	LYS	3.3
1	A	15	ARG	3.3
2	D	79	GLU	3.2
1	A	26	ASP	3.2
1	A	622	LEU	3.1
1	A	601	GLU	3.1
1	C	604	GLU	3.0
2	B	79	GLU	3.0
1	C	543	GLY	3.0
1	A	602	VAL	2.9
2	D	80	LYS	2.9
1	A	543	GLY	2.9
1	C	94	VAL	2.8
1	A	118	LYS	2.7
1	C	605	GLU	2.6
1	A	95	LEU	2.6
1	A	189	ILE	2.5
1	A	196	ALA	2.5
1	C	95	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	381	GLU	2.4
1	C	601	GLU	2.4
1	C	80	ILE	2.4
1	A	80	ILE	2.3
1	A	96	SER	2.3
1	A	195	HIS	2.2
1	A	199	TYR	2.2
1	A	577	GLU	2.2
1	A	616	LYS	2.2
1	A	382	ASP	2.2
1	C	575	ASN	2.2
1	A	93	SER	2.0
1	C	381	GLU	2.0
1	A	329	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	PO4	C	706	5/5	0.92	0.32	40,49,56,65	0
8	CL	D	901	1/1	0.92	0.19	52,52,52,52	0
8	CL	B	901	1/1	0.93	0.05	48,48,48,48	0
7	PO4	A	706	5/5	0.93	0.31	42,46,56,65	0
3	UKM	C	701	9/9	0.96	0.19	23,35,43,45	0
6	MG	A	704	1/1	0.96	0.15	35,35,35,35	0
3	UKM	A	701	9/9	0.97	0.21	24,37,43,46	0
5	SF4	D	904	8/8	0.98	0.06	33,35,37,38	0
5	SF4	D	905	8/8	0.98	0.06	32,33,34,34	0

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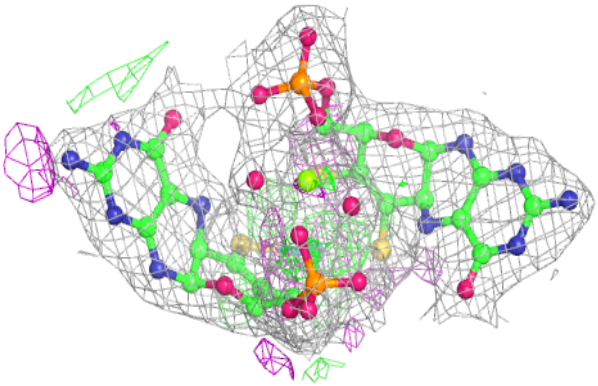
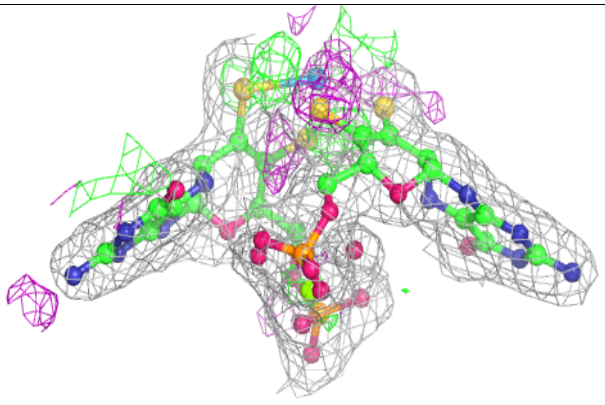
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SF4	A	703	8/8	0.98	0.13	29,31,34,35	0
6	MG	A	705	1/1	0.98	0.13	37,37,37,37	0
6	MG	C	705	1/1	0.98	0.13	38,38,38,38	0
5	SF4	B	903	8/8	0.98	0.07	29,31,32,32	0
5	SF4	B	904	8/8	0.98	0.06	34,35,37,40	0
5	SF4	B	905	8/8	0.98	0.06	31,33,35,35	0
5	SF4	D	903	8/8	0.98	0.07	29,30,32,33	0
6	MG	C	704	1/1	0.99	0.09	33,33,33,33	0
4	PTE	C	702	52/52	0.99	0.15	29,33,36,37	0
4	PTE	A	702	52/52	0.99	0.18	30,33,37,37	0
5	SF4	B	902	8/8	0.99	0.11	28,29,30,31	0
5	SF4	C	703	8/8	0.99	0.11	28,30,32,32	0
5	SF4	D	902	8/8	0.99	0.10	28,30,30,31	0

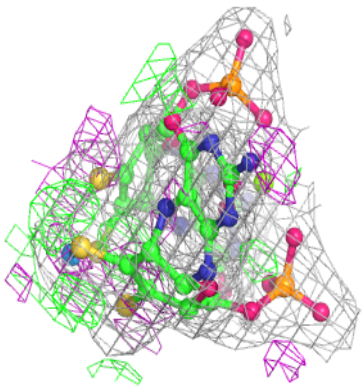
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around PTE C 702:

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

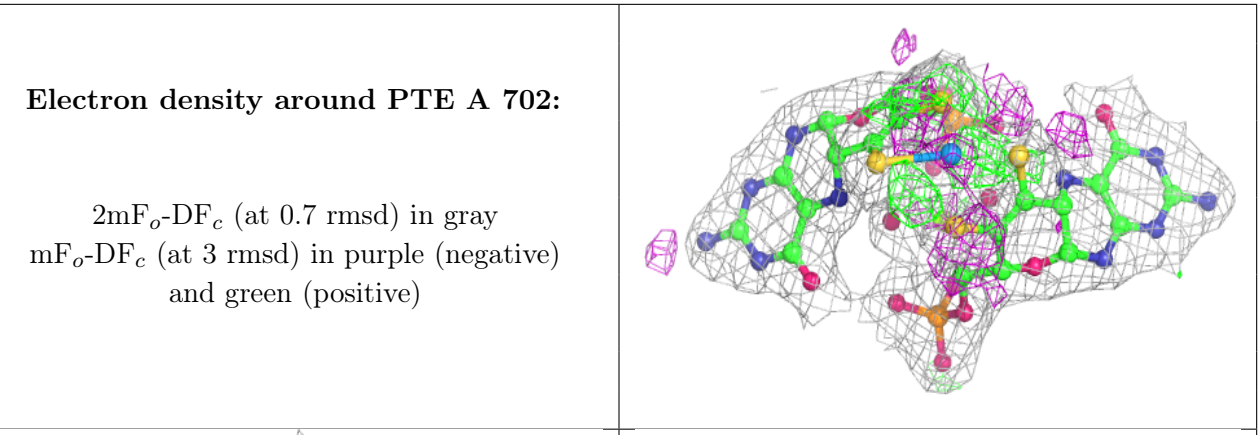


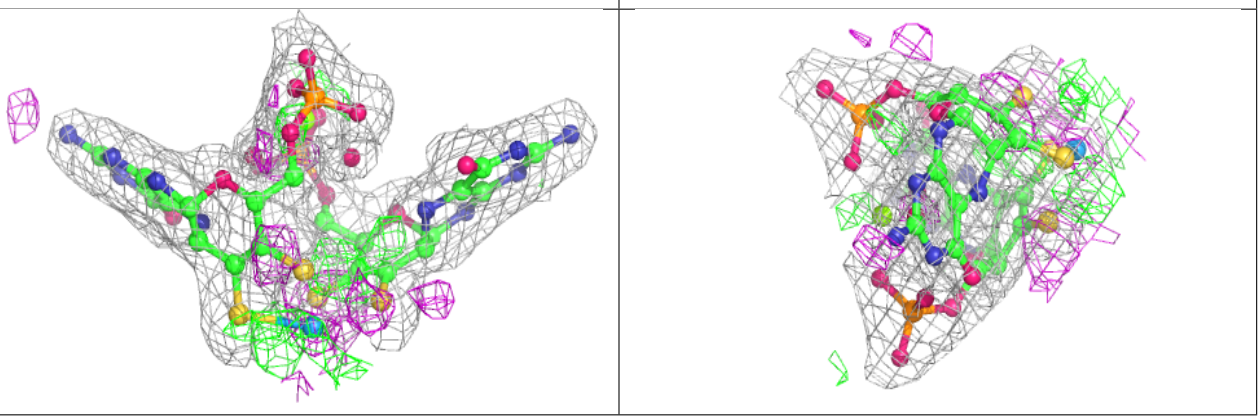




Electron density around PTE A 702:

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





6.5 Other polymers (i)

There are no such residues in this entry.