



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:50 PM UTC

PDB ID : 1AOR / pdb_00001aor
Title : STRUCTURE OF A HYPERTHERMOPHILIC TUNGSTOPTERIN ENZYME, ALDEHYDE FERREDOXIN OXIDOREDUCTASE
Authors : Chan, M.K.; Mukund, S.; Kletzin, A.; Adams, M.W.W.; Rees, D.C.
Deposited on : 1995-02-13
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

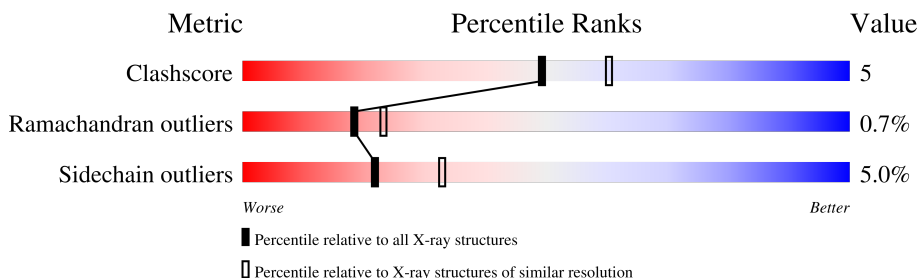
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	605	 82% 15% .
1	B	605	 84% 15% .

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9888 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 ALDEHYDE FERREDOXIN OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	605	Total	C	N	O	S	58	0	0
			4693	2993	791	888	21			
1	B	605	Total	C	N	O	S	63	0	0
			4693	2993	791	888	21			

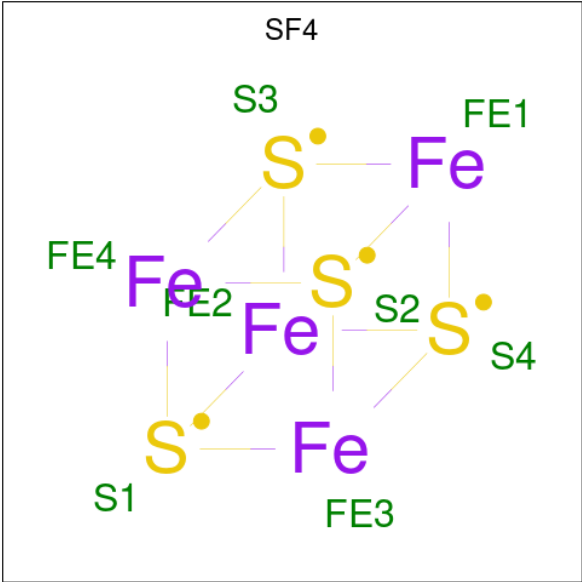
- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Fe	0	0
			1	1		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

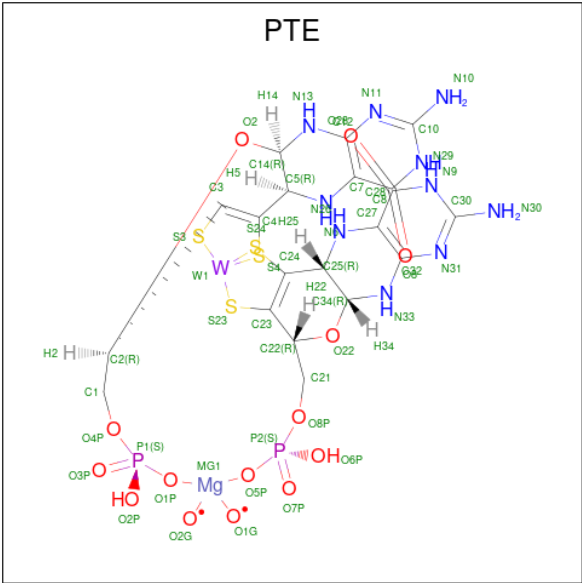
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		

- 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		

- Molecule 5 is TUNGSTOPTERIN COFACTOR (CCD ID: PTE) (formula: C₂₀H₂₂MgN₁₀O₁₄P₂S₄W).



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

- Molecule 6 is water.

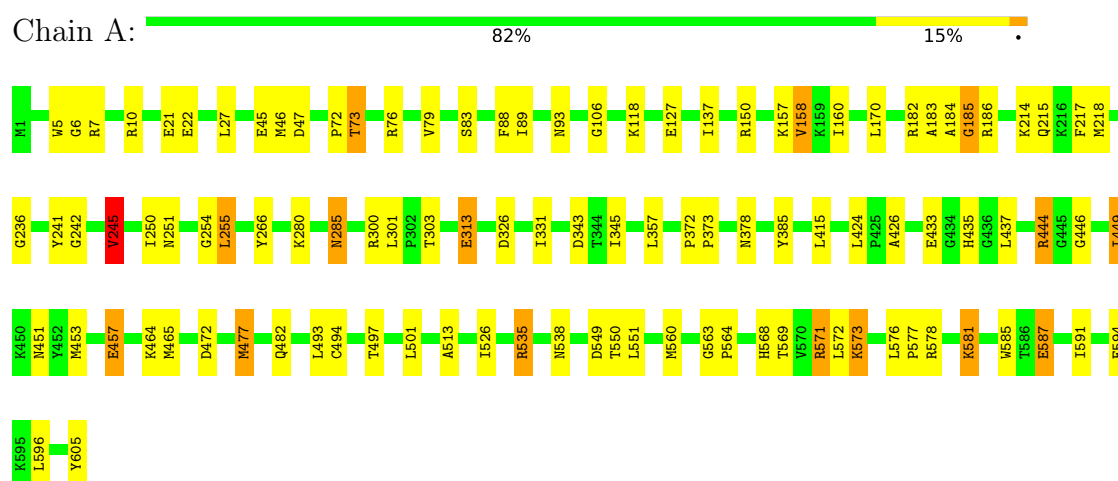
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	210	Total 210	O 210	0	0
6	B	169	Total 169	O 169	0	0

3 Residue-property plots

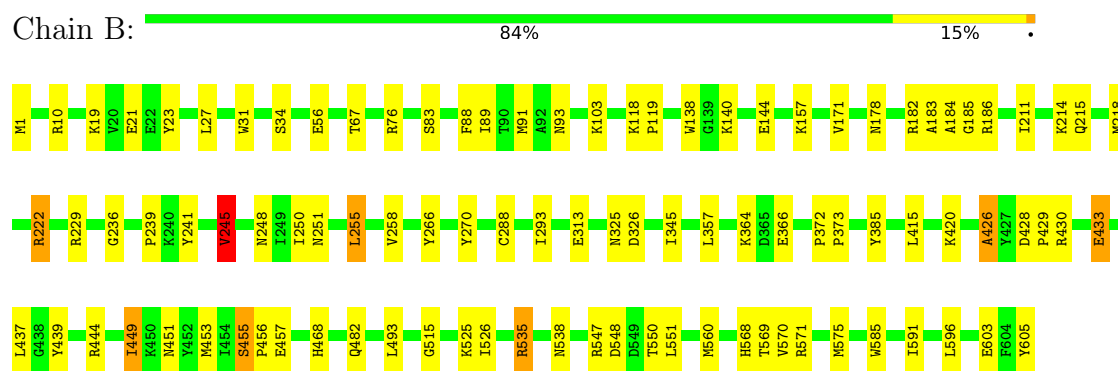
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

• Molecule 1: ALDEHYDE FERREDOXIN OXIDOREDUCTASE



• Molecule 1: ALDEHYDE FERREDOXIN OXIDOREDUCTASE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.94Å 108.33Å 159.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30	Depositor
% Data completeness (in resolution range)	89.0 (10.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.155 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9888	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PTE, NA, SF4, FE

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	0.48	0/4798	1.01	26/6488 (0.4%)
1	B	0.48	0/4798	0.97	18/6488 (0.3%)
All	All	0.48	0/9596	0.99	44/12976 (0.3%)

There are no bond length outliers.

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	ALA	N-CA-C	-10.38	87.43	107.57
1	A	184	ALA	N-CA-C	-9.39	91.24	108.24
1	A	385	TYR	N-CA-C	9.31	122.62	111.82
1	B	385	TYR	N-CA-C	9.26	121.46	111.36
1	A	185	GLY	N-CA-C	8.06	132.29	113.18
1	A	183	ALA	N-CA-C	7.66	121.88	109.40
1	B	183	ALA	N-CA-C	7.35	121.17	108.76
1	B	185	GLY	N-CA-C	7.11	130.03	113.18
1	A	214	LYS	N-CA-C	7.07	118.64	111.07
1	B	526	ILE	N-CA-C	-6.51	104.14	110.72
1	A	83	SER	N-CA-C	6.50	117.84	109.65
1	B	548	ASP	N-CA-C	6.47	120.39	112.23
1	A	563	GLY	CA-C-N	6.46	126.38	119.28
1	A	563	GLY	C-N-CA	6.46	126.38	119.28
1	B	186	ARG	N-CA-C	6.34	120.25	110.42
1	A	186	ARG	N-CA-C	6.34	120.03	109.95
1	A	245	VAL	CB-CA-C	-6.33	102.34	112.16
1	B	245	VAL	CB-CA-C	-6.29	102.42	112.16
1	B	449	ILE	N-CA-C	6.25	121.12	113.00
1	A	560	MET	CA-C-N	6.10	125.99	119.28
1	A	560	MET	C-N-CA	6.10	125.99	119.28
1	A	160	ILE	N-CA-C	6.07	117.22	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	560	MET	CA-C-N	6.00	125.88	119.28
1	B	560	MET	C-N-CA	6.00	125.88	119.28
1	A	457	GLU	N-CA-C	5.92	118.69	111.82
1	A	449	ILE	N-CA-C	5.92	120.69	113.00
1	B	426	ALA	N-CA-C	5.91	123.38	110.80
1	B	457	GLU	N-CA-C	5.70	118.26	111.71
1	A	526	ILE	N-CA-C	-5.67	104.99	110.72
1	A	46	MET	N-CA-C	5.64	118.60	109.40
1	B	288	CYS	N-CA-C	-5.58	102.64	110.35
1	A	424	LEU	CA-C-N	5.55	126.78	119.84
1	A	424	LEU	C-N-CA	5.55	126.78	119.84
1	B	83	SER	N-CA-C	5.54	117.64	109.50
1	A	433	GLU	N-CA-C	5.33	117.09	111.28
1	A	45	GLU	N-CA-C	5.26	120.70	113.97
1	A	280	LYS	N-CA-C	5.24	119.67	113.12
1	A	303	THR	N-CA-C	5.24	116.85	111.03
1	A	79	VAL	N-CA-C	-5.24	100.78	108.11
1	B	171	VAL	N-CA-C	-5.21	102.33	109.37
1	B	575	MET	N-CA-C	5.15	116.70	111.14
1	A	47	ASP	CA-C-N	5.10	124.82	119.82
1	A	47	ASP	C-N-CA	5.10	124.82	119.82
1	B	433	GLU	N-CA-C	5.07	117.54	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4693	0	4670	59	0
1	B	4693	0	4670	43	0
2	A	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	8	0	0	1	0
4	B	8	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	52	0	20	1	0
5	B	52	0	20	1	0
6	A	210	0	0	2	0
6	B	169	0	0	3	0
All	All	9888	0	9380	100	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 (100) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:TYR:HB2	1:A:245:VAL:HG13	1.42	1.00
1:B:241:TYR:HB2	1:B:245:VAL:HG13	1.51	0.92
1:A:251:ASN:HD21	1:A:266:TYR:H	1.23	0.86
1:B:251:ASN:HD21	1:B:266:TYR:H	1.26	0.84
1:A:73:THR:CG2	1:A:494:CYS:H	1.93	0.81
1:B:241:TYR:HB2	1:B:245:VAL:CG1	2.10	0.80
1:A:573:LYS:HD3	1:A:573:LYS:H	1.49	0.76
1:B:89:ILE:H	1:B:538:ASN:HD21	1.35	0.74
1:A:596:LEU:HD12	1:A:605:TYR:HD2	1.55	0.71
1:A:571:ARG:HA	1:A:573:LYS:HE2	1.74	0.67
1:A:89:ILE:H	1:A:538:ASN:HD21	1.40	0.67
1:A:285:ASN:H	1:A:285:ASN:HD22	1.42	0.66
1:A:73:THR:HG21	1:A:494:CYS:H	1.60	0.65
1:A:313:GLU:HG2	1:A:345:ILE:HD11	1.79	0.65
1:B:429:PRO:HG3	1:B:439:TYR:CE2	2.33	0.64
1:A:242:GLY:O	1:A:245:VAL:HG22	1.98	0.63
1:A:453:MET:HE1	1:A:477:MET:HB3	1.83	0.61
1:B:250:ILE:HG23	1:B:255:LEU:HD13	1.81	0.61
1:A:378:ASN:ND2	1:B:325:ASN:HD21	1.98	0.61
1:A:250:ILE:HG23	1:A:255:LEU:HD13	1.82	0.61
1:B:251:ASN:ND2	1:B:266:TYR:H	1.98	0.59
1:A:457:GLU:O	1:A:464:LYS:HE3	2.03	0.59
1:A:251:ASN:ND2	1:A:266:TYR:H	1.97	0.57
1:B:313:GLU:HG2	1:B:345:ILE:HD11	1.86	0.57
1:B:429:PRO:HG3	1:B:439:TYR:HE2	1.69	0.57
1:B:76:ARG:HD3	1:B:93:ASN:OD1	2.05	0.56
1:A:241:TYR:CB	1:A:245:VAL:HG13	2.24	0.56
1:B:89:ILE:H	1:B:538:ASN:ND2	2.04	0.55
1:A:451:ASN:HD22	1:A:482:GLN:HE21	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:535:ARG:HG3	1:A:585:TRP:CH2	2.41	0.55
1:A:581:LYS:NZ	1:A:587:GLU:HA	2.22	0.54
1:B:1:MET:HE1	1:B:23:TYR:CE2	2.43	0.53
1:A:464:LYS:HE2	1:A:465:MET:O	2.09	0.53
1:B:214:LYS:O	1:B:218:MET:HG2	2.09	0.53
1:B:239:PRO:HB3	1:B:293:ILE:O	2.08	0.52
1:A:76:ARG:HD2	1:A:93:ASN:OD1	2.09	0.52
1:B:451:ASN:HB3	1:B:482:GLN:HG2	1.91	0.52
1:A:73:THR:HG23	1:A:73:THR:O	2.11	0.51
1:A:568:HIS:HE1	6:A:5211:HOH:O	1.93	0.51
1:B:535:ARG:HB3	1:B:591:ILE:HD11	1.92	0.51
1:B:568:HIS:HD2	6:B:5169:HOH:O	1.93	0.51
1:A:465:MET:SD	1:A:477:MET:HG3	2.52	0.50
1:A:254:GLY:HA3	1:A:564:PRO:HD2	1.93	0.49
1:B:222:ARG:HA	1:B:222:ARG:HE	1.76	0.49
1:A:472:ASP:OD1	1:A:578:ARG:HD2	2.12	0.49
1:A:215:GLN:HA	1:A:218:MET:HE3	1.95	0.49
1:A:535:ARG:HB3	1:A:591:ILE:HD11	1.95	0.49
1:B:596:LEU:HD12	1:B:605:TYR:HD1	1.77	0.49
1:A:378:ASN:HD21	1:B:325:ASN:HD21	1.61	0.49
1:B:88:PHE:HB3	1:B:538:ASN:ND2	2.28	0.48
1:B:27:LEU:HD23	1:B:31:TRP:HD1	1.77	0.48
1:B:140:LYS:HB3	1:B:144:GLU:HB2	1.95	0.48
1:A:72:PRO:O	1:A:73:THR:HB	2.13	0.48
1:A:451:ASN:HB3	1:A:482:GLN:HG2	1.95	0.48
1:A:313:GLU:HG2	1:A:345:ILE:CD1	2.41	0.48
1:A:73:THR:CG2	1:A:494:CYS:N	2.72	0.47
1:A:596:LEU:HD12	1:A:605:TYR:CD2	2.43	0.47
1:A:150:ARG:HG2	1:A:158:VAL:HG23	1.96	0.46
1:B:248:ASN:HD21	1:B:270:TYR:HA	1.79	0.46
1:B:430:ARG:O	1:B:468:HIS:HE1	1.98	0.46
1:A:451:ASN:ND2	1:A:482:GLN:HE21	2.13	0.46
1:B:182:ARG:HD3	5:B:608:PTE:O6P	2.16	0.46
1:A:185:GLY:O	1:A:343:ASP:HB2	2.16	0.45
1:B:258:VAL:CG2	1:B:266:TYR:HB2	2.47	0.45
1:B:515:GLY:HA2	6:B:5156:HOH:O	2.16	0.45
1:A:581:LYS:HZ2	1:A:587:GLU:HA	1.81	0.45
1:A:7:ARG:HA	1:A:21:GLU:O	2.18	0.44
1:A:301:LEU:HD11	1:A:331:ILE:HB	1.99	0.44
1:A:549:ASP:O	1:A:576:LEU:HD21	2.17	0.44
1:B:420:LYS:HE2	6:B:5079:HOH:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:GLY:O	1:A:22:GLU:HA	2.19	0.43
1:B:433:GLU:OE1	1:B:571:ARG:HD3	2.18	0.43
1:A:157:LYS:O	1:A:157:LYS:HG2	2.19	0.43
1:A:577:PRO:O	1:A:581:LYS:HE2	2.18	0.43
1:B:119:PRO:HB3	1:B:138:TRP:CE3	2.54	0.43
1:A:550:THR:HA	1:A:572:LEU:HD21	2.00	0.43
1:B:10:ARG:NH1	1:B:21:GLU:CD	2.77	0.43
1:B:357:LEU:HD23	1:B:415:LEU:HD12	2.00	0.43
1:A:73:THR:HG21	1:A:494:CYS:HB3	2.01	0.43
1:A:217:PHE:CE1	1:A:513:ALA:HB2	2.53	0.43
1:A:444:ARG:NH2	5:A:609:PTE:O2P	2.51	0.42
1:A:10:ARG:HH11	1:A:21:GLU:CD	2.28	0.42
1:A:76:ARG:NH2	4:A:608:SF4:S3	2.93	0.42
1:A:182:ARG:HD3	1:A:182:ARG:HA	1.76	0.41
1:B:364:LYS:HB2	1:B:364:LYS:HE2	1.77	0.41
1:B:455:SER:CB	1:B:456:PRO:HD3	2.50	0.41
1:A:5:TRP:CE2	1:A:106:GLY:HA2	2.56	0.41
1:B:429:PRO:HB2	1:B:570:VAL:HG21	2.02	0.41
1:B:372:PRO:HA	1:B:373:PRO:HD3	1.91	0.41
1:A:73:THR:CG2	1:A:73:THR:O	2.68	0.41
1:A:357:LEU:HD23	1:A:415:LEU:HD12	2.03	0.41
1:A:497:THR:HB	1:A:501:LEU:HD12	2.03	0.41
1:A:88:PHE:HB3	1:A:538:ASN:ND2	2.36	0.41
1:B:67:THR:O	1:B:103:LYS:HG3	2.22	0.40
1:B:453:MET:C	1:B:456:PRO:HD2	2.46	0.40
1:A:372:PRO:HA	1:A:373:PRO:HD3	1.90	0.40
1:B:178:ASN:O	1:B:182:ARG:HB2	2.21	0.40
1:A:435:HIS:CD2	6:A:5191:HOH:O	2.73	0.40
1:B:428:ASP:HA	1:B:429:PRO:HD3	1.97	0.40
1:B:535:ARG:HG3	1:B:585:TRP:CH2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	603/605 (100%)	577 (96%)	22 (4%)	4 (1%)	18	23
1	B	603/605 (100%)	581 (96%)	18 (3%)	4 (1%)	18	23
All	All	1206/1210 (100%)	1158 (96%)	40 (3%)	8 (1%)	18	23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	426	ALA
1	B	426	ALA
1	A	326	ASP
1	B	34	SER
1	B	326	ASP
1	A	446	GLY
1	A	236	GLY
1	B	236	GLY

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	487/487 (100%)	462 (95%)	25 (5%)	21	32
1	B	487/487 (100%)	463 (95%)	24 (5%)	22	34
All	All	974/974 (100%)	925 (95%)	49 (5%)	22	33

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	73	THR
1	A	118	LYS
1	A	127	GLU
1	A	137	ILE

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Mol	Chain	Res	Type
1	A	158	VAL
1	A	170	LEU
1	A	245	VAL
1	A	255	LEU
1	A	285	ASN
1	A	300	ARG
1	A	313	GLU
1	A	437	LEU
1	A	444	ARG
1	A	449	ILE
1	A	477	MET
1	A	493	LEU
1	A	535	ARG
1	A	551	LEU
1	A	569	THR
1	A	571	ARG
1	A	573	LYS
1	A	581	LYS
1	A	587	GLU
1	A	594	GLU
1	B	19	LYS
1	B	56	GLU
1	B	91	MET
1	B	118	LYS
1	B	157	LYS
1	B	211	ILE
1	B	215	GLN
1	B	222	ARG
1	B	229	ARG
1	B	245	VAL
1	B	255	LEU
1	B	366	GLU
1	B	437	LEU
1	B	444	ARG
1	B	449	ILE
1	B	455	SER
1	B	493	LEU
1	B	525	LYS
1	B	535	ARG
1	B	547	ARG
1	B	550	THR
1	B	551	LEU

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Mol	Chain	Res	Type
1	B	569	THR
1	B	603	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	178	ASN
1	A	226	ASN
1	A	248	ASN
1	A	251	ASN
1	A	285	ASN
1	A	378	ASN
1	A	451	ASN
1	A	511	ASN
1	A	538	ASN
1	B	57	ASN
1	B	169	ASN
1	B	178	ASN
1	B	248	ASN
1	B	251	ASN
1	B	285	ASN
1	B	299	ASN
1	B	321	ASN
1	B	362	HIS
1	B	378	ASN
1	B	435	HIS
1	B	451	ASN
1	B	511	ASN
1	B	538	ASN
1	B	568	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 3 are monoatomic - leaving 4 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	A	608	1	0,12,12	-	-	-		
5	PTE	B	608	1,3	46,60,60	2.40	15 (32%)	42,98,98	4.62	23 (54%)
4	SF4	B	607	1	0,12,12	-	-	-		
5	PTE	A	609	1,3	46,60,60	2.49	15 (32%)	42,98,98	4.14	18 (42%)

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	PTE	A	609	1,3	-	0/12/100/100	-
5	PTE	B	608	1,3	-	0/12/100/100	-
4	SF4	B	607	1	-	-	0/6/5/5
4	SF4	A	608	1	-	-	0/6/5/5

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	608	PTE	O8-C8	7.84	1.38	1.23
5	A	609	PTE	O28-C28	7.70	1.38	1.23
5	A	609	PTE	O8-C8	7.62	1.38	1.23
5	B	608	PTE	O28-C28	6.90	1.36	1.23
5	A	609	PTE	P1-O1P	6.13	1.60	1.50
5	B	608	PTE	P1-O1P	6.10	1.60	1.50
5	B	608	PTE	P2-O5P	4.62	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	609	PTE	P2-O5P	4.44	1.57	1.50
5	A	609	PTE	C14-C5	3.64	1.56	1.53
5	A	609	PTE	O2-C14	-3.47	1.38	1.43
5	A	609	PTE	C7-C12	3.34	1.44	1.38
5	B	608	PTE	C27-C32	3.24	1.44	1.38
5	B	608	PTE	C14-C5	3.10	1.56	1.53
5	A	609	PTE	C34-C25	2.98	1.56	1.53
5	A	609	PTE	C27-C32	2.96	1.43	1.38
5	B	608	PTE	P2-O8P	-2.90	1.48	1.59
5	A	609	PTE	O22-C34	-2.87	1.39	1.43
5	B	608	PTE	O22-C34	-2.68	1.39	1.43
5	A	609	PTE	O22-C22	-2.64	1.38	1.43
5	B	608	PTE	C7-C12	2.58	1.43	1.38
5	B	608	PTE	C8-N9	-2.54	1.34	1.38
5	B	608	PTE	O2-C14	-2.36	1.40	1.43
5	A	609	PTE	C8-N9	-2.34	1.34	1.38
5	B	608	PTE	C28-N29	-2.32	1.34	1.38
5	A	609	PTE	C21-C22	2.30	1.55	1.51
5	A	609	PTE	C28-N29	-2.13	1.34	1.38
5	B	608	PTE	O22-C22	-2.06	1.39	1.43
5	A	609	PTE	C1-C2	2.05	1.54	1.51
5	B	608	PTE	C34-C25	2.02	1.55	1.53
5	B	608	PTE	O2-C2	-2.02	1.39	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	609	PTE	O22-C34-C25	-19.35	96.06	108.96
5	B	608	PTE	O22-C34-C25	-16.99	97.63	108.96
5	B	608	PTE	O2-C14-N13	16.90	123.94	108.61
5	A	609	PTE	O2-C14-C5	-8.21	103.49	108.96
5	B	608	PTE	C34-C25-N26	7.85	115.58	107.87
5	A	609	PTE	O2-C14-N13	7.13	115.07	108.61
5	B	608	PTE	O2-C14-C5	-5.96	104.99	108.96
5	A	609	PTE	C14-C5-N6	5.58	113.35	107.87
5	A	609	PTE	O22-C22-C23	-5.46	101.38	109.09
5	B	608	PTE	C10-N11-C12	5.02	122.23	113.36
5	B	608	PTE	C30-N31-C32	5.02	122.21	113.36
5	A	609	PTE	C10-N11-C12	4.86	121.94	113.36
5	A	609	PTE	C34-C25-N26	4.45	112.24	107.87
5	A	609	PTE	C30-N31-C32	4.43	121.19	113.36
5	B	608	PTE	O2P-P1-O1P	-4.09	95.60	108.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	608	PTE	O22-C22-C23	-3.74	103.81	109.09
5	B	608	PTE	C4-C3-S3	-3.68	114.28	119.62
5	B	608	PTE	C27-C28-N29	3.61	122.03	112.13
5	B	608	PTE	N30-C30-N29	3.46	124.07	116.76
5	B	608	PTE	O4P-C1-C2	-3.41	100.15	108.58
5	A	609	PTE	N30-C30-N29	3.18	123.48	116.76
5	B	608	PTE	C7-C8-N9	3.17	120.85	112.13
5	A	609	PTE	C7-C8-N9	2.92	120.14	112.13
5	A	609	PTE	O28-C28-C27	-2.88	120.33	127.26
5	B	608	PTE	C10-N9-C8	-2.86	119.92	125.11
5	B	608	PTE	C8-C7-N6	2.83	123.97	116.27
5	B	608	PTE	N10-C10-N9	2.77	122.61	116.76
5	B	608	PTE	C28-C27-N26	2.66	123.53	116.27
5	A	609	PTE	C27-C28-N29	2.65	119.39	112.13
5	A	609	PTE	O8-C8-C7	-2.59	121.01	127.26
5	A	609	PTE	C23-C24-S24	2.50	123.25	119.62
5	A	609	PTE	O8P-C21-C22	2.46	114.64	108.58
5	A	609	PTE	N10-C10-N9	2.40	121.83	116.76
5	B	608	PTE	O28-C28-N29	-2.34	115.72	120.11
5	A	609	PTE	C8-C7-N6	2.33	122.62	116.27
5	B	608	PTE	C30-N29-C28	-2.29	120.97	125.11
5	B	608	PTE	O8-C8-N9	-2.21	115.95	120.11
5	A	609	PTE	C28-C27-N26	2.18	122.21	116.27
5	B	608	PTE	N29-C30-N31	-2.16	119.36	123.32
5	B	608	PTE	O28-C28-C27	-2.11	122.18	127.26
5	B	608	PTE	C14-C5-N6	2.06	109.89	107.87

There are no chirality outliers.

There are no torsion outliers.

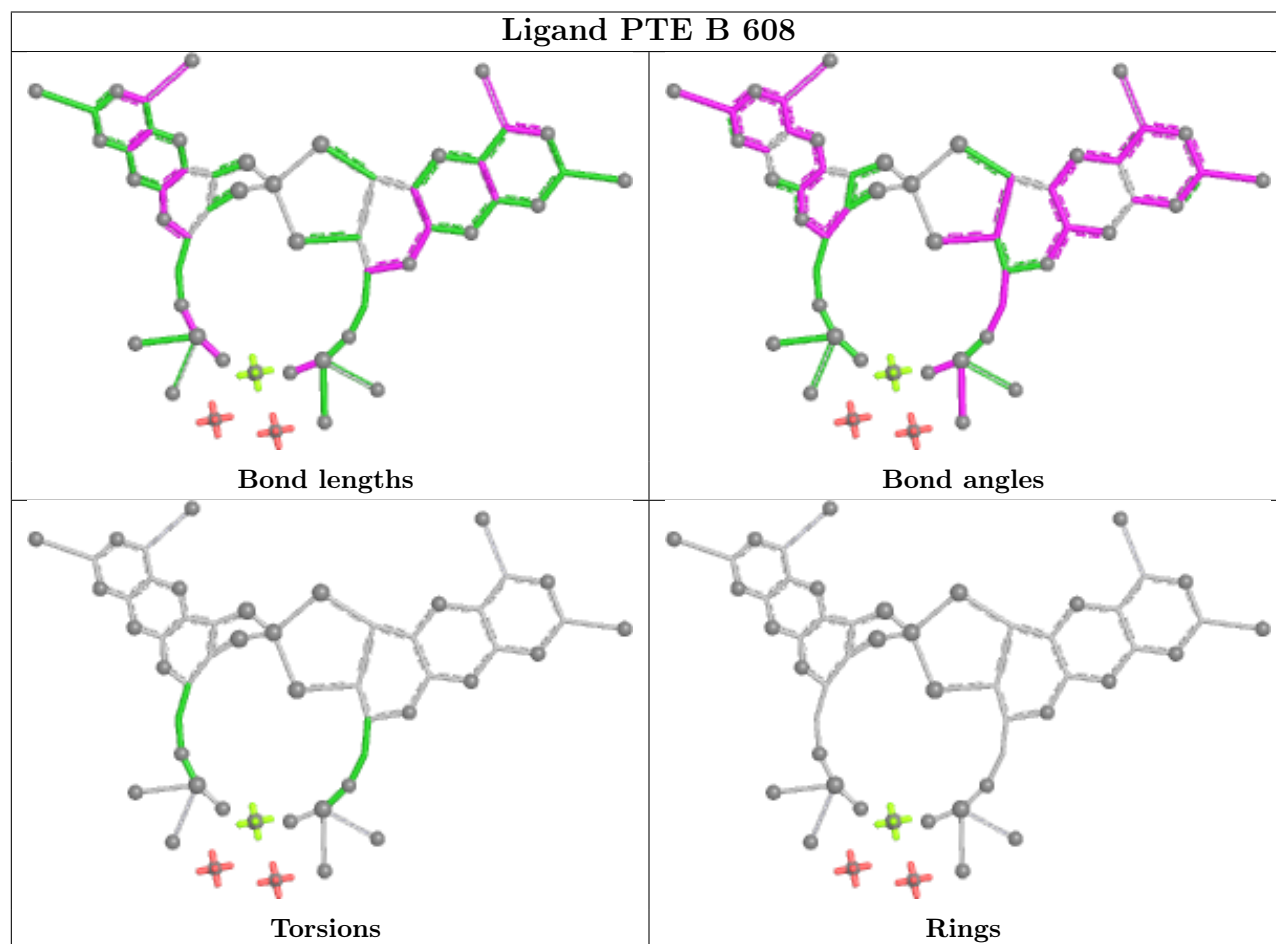
There are no ring outliers.

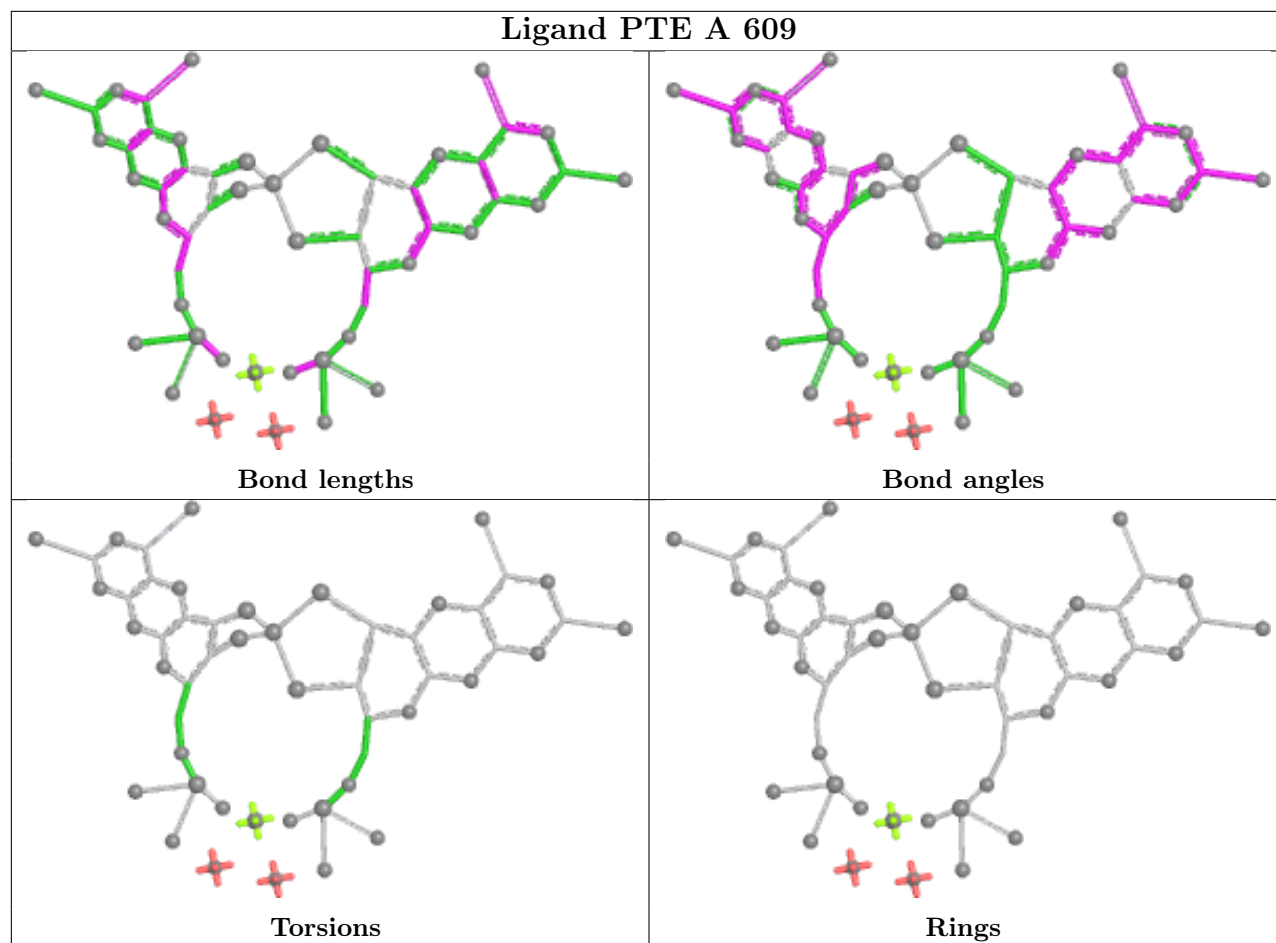
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	608	SF4	1	0
5	B	608	PTE	1	0
5	A	609	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.