



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:49 PM UTC

PDB ID : 8CIP / pdb_00008cip
Title : Crystal structure of transketolase from *Geobacillus stearothermophilus*
Authors : Leogrande, C.; Rabe von Pappenheim, F.; Tittmann, K.
Deposited on : 2023-02-10
Resolution : 2.10 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

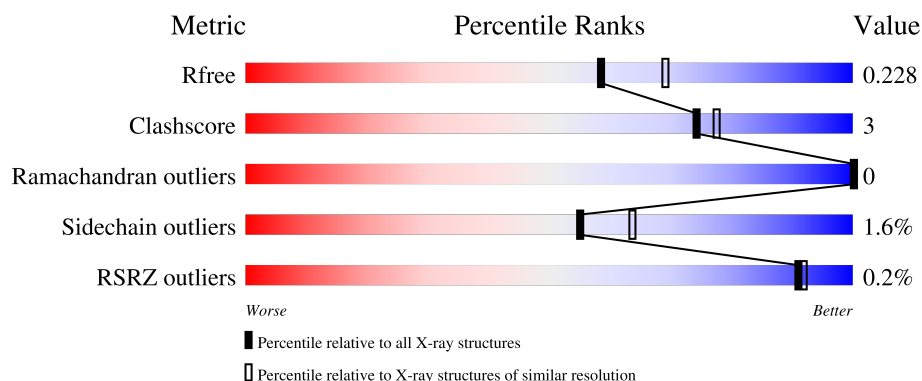
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

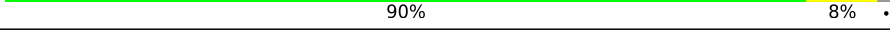
The reported resolution of this entry is 2.10 Å.

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	681	 91% 6% .
1	B	681	 90% 7% .
1	C	681	 89% 8% ..
1	D	681	 90% 8% .

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
2	EDO	A	801	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 41062 atoms, of which 20073 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 Transketolase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	665	Total	C	H	N	O	S	0	0	0
			10018	3204	4971	868	957	18			
1	B	665	Total	C	H	N	O	S	0	0	0
			10019	3204	4972	868	957	18			
1	C	665	Total	C	H	N	O	S	0	0	0
			10019	3204	4972	868	957	18			
1	D	665	Total	C	H	N	O	S	0	0	0
			10018	3204	4971	868	957	18			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP A0A0I9QGZ2
A	-11	ALA	-	expression tag	UNP A0A0I9QGZ2
A	-10	HIS	-	expression tag	UNP A0A0I9QGZ2
A	-9	HIS	-	expression tag	UNP A0A0I9QGZ2
A	-8	HIS	-	expression tag	UNP A0A0I9QGZ2
A	-7	HIS	-	expression tag	UNP A0A0I9QGZ2
A	-6	HIS	-	expression tag	UNP A0A0I9QGZ2
A	-5	HIS	-	expression tag	UNP A0A0I9QGZ2
A	-4	SER	-	expression tag	UNP A0A0I9QGZ2
A	-3	ALA	-	expression tag	UNP A0A0I9QGZ2
A	-2	ALA	-	expression tag	UNP A0A0I9QGZ2
A	-1	ARG	-	expression tag	UNP A0A0I9QGZ2
A	0	LEU	-	expression tag	UNP A0A0I9QGZ2
A	397	PHE	LEU	conflict	UNP A0A0I9QGZ2
A	399	GLY	ASP	conflict	UNP A0A0I9QGZ2
A	479	GLN	HIS	conflict	UNP A0A0I9QGZ2
B	-12	MET	-	initiating methionine	UNP A0A0I9QGZ2
B	-11	ALA	-	expression tag	UNP A0A0I9QGZ2
B	-10	HIS	-	expression tag	UNP A0A0I9QGZ2
B	-9	HIS	-	expression tag	UNP A0A0I9QGZ2
B	-8	HIS	-	expression tag	UNP A0A0I9QGZ2

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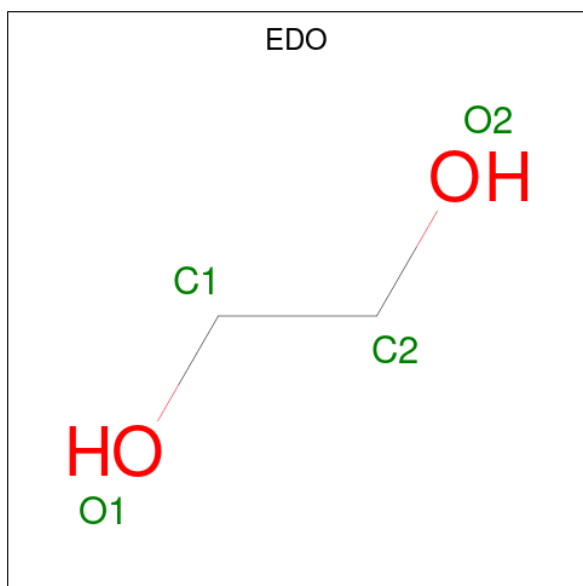
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP A0A0I9QGZ2
B	-6	HIS	-	expression tag	UNP A0A0I9QGZ2
B	-5	HIS	-	expression tag	UNP A0A0I9QGZ2
B	-4	SER	-	expression tag	UNP A0A0I9QGZ2
B	-3	ALA	-	expression tag	UNP A0A0I9QGZ2
B	-2	ALA	-	expression tag	UNP A0A0I9QGZ2
B	-1	ARG	-	expression tag	UNP A0A0I9QGZ2
B	0	LEU	-	expression tag	UNP A0A0I9QGZ2
B	397	PHE	LEU	conflict	UNP A0A0I9QGZ2
B	399	GLY	ASP	conflict	UNP A0A0I9QGZ2
B	479	GLN	HIS	conflict	UNP A0A0I9QGZ2
C	-12	MET	-	initiating methionine	UNP A0A0I9QGZ2
C	-11	ALA	-	expression tag	UNP A0A0I9QGZ2
C	-10	HIS	-	expression tag	UNP A0A0I9QGZ2
C	-9	HIS	-	expression tag	UNP A0A0I9QGZ2
C	-8	HIS	-	expression tag	UNP A0A0I9QGZ2
C	-7	HIS	-	expression tag	UNP A0A0I9QGZ2
C	-6	HIS	-	expression tag	UNP A0A0I9QGZ2
C	-5	HIS	-	expression tag	UNP A0A0I9QGZ2
C	-4	SER	-	expression tag	UNP A0A0I9QGZ2
C	-3	ALA	-	expression tag	UNP A0A0I9QGZ2
C	-2	ALA	-	expression tag	UNP A0A0I9QGZ2
C	-1	ARG	-	expression tag	UNP A0A0I9QGZ2
C	0	LEU	-	expression tag	UNP A0A0I9QGZ2
C	397	PHE	LEU	conflict	UNP A0A0I9QGZ2
C	399	GLY	ASP	conflict	UNP A0A0I9QGZ2
C	479	GLN	HIS	conflict	UNP A0A0I9QGZ2
D	-12	MET	-	initiating methionine	UNP A0A0I9QGZ2
D	-11	ALA	-	expression tag	UNP A0A0I9QGZ2
D	-10	HIS	-	expression tag	UNP A0A0I9QGZ2
D	-9	HIS	-	expression tag	UNP A0A0I9QGZ2
D	-8	HIS	-	expression tag	UNP A0A0I9QGZ2
D	-7	HIS	-	expression tag	UNP A0A0I9QGZ2
D	-6	HIS	-	expression tag	UNP A0A0I9QGZ2
D	-5	HIS	-	expression tag	UNP A0A0I9QGZ2
D	-4	SER	-	expression tag	UNP A0A0I9QGZ2
D	-3	ALA	-	expression tag	UNP A0A0I9QGZ2
D	-2	ALA	-	expression tag	UNP A0A0I9QGZ2
D	-1	ARG	-	expression tag	UNP A0A0I9QGZ2
D	0	LEU	-	expression tag	UNP A0A0I9QGZ2
D	397	PHE	LEU	conflict	UNP A0A0I9QGZ2
D	399	GLY	ASP	conflict	UNP A0A0I9QGZ2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	479	GLN	HIS	conflict	UNP A0A0I9QGZ2

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	B	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		

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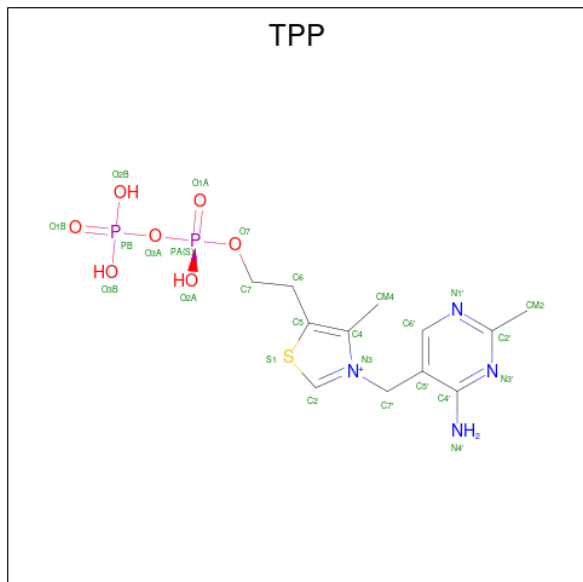
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	C	1	Total	C	H	O	0	0
			10	2	6	2		
2	D	1	Total	C	H	O	0	0
			10	2	6	2		
2	D	1	Total	C	H	O	0	0
			10	2	6	2		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			7	2	3	2		
3	C	1	Total	C	H	O	0	0
			7	2	3	2		
3	D	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 4 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		
4	B	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		
4	C	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		
4	D	1	Total	C	H	N	O	P	S	0	0
			42	12	16	4	7	2	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	B	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	3	Total 3	Cl 3	0	0
6	B	1	Total 1	Cl 1	0	0
6	C	1	Total 1	Cl 1	0	0

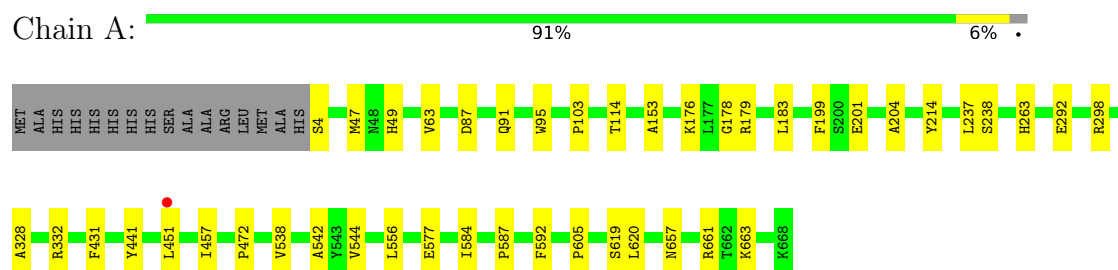
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	149	Total 149	O 149	0	0
7	B	148	Total 148	O 148	0	0
7	C	173	Total 173	O 173	0	0
7	D	130	Total 130	O 130	0	0

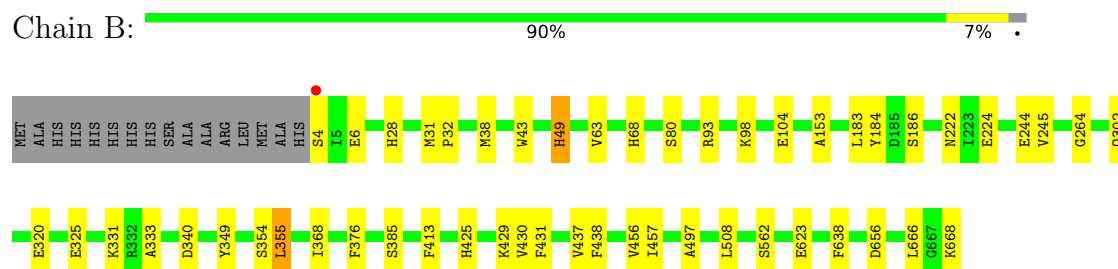
3 Residue-property plots [i](#)

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.

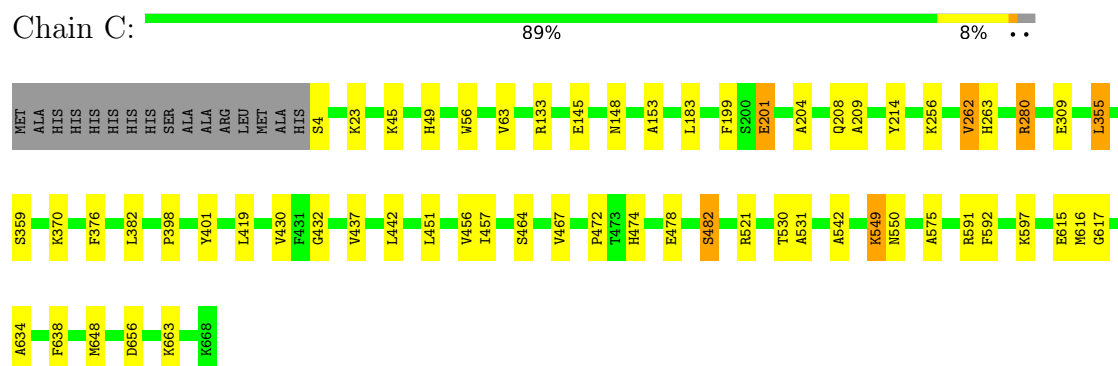
- Molecule 1: Transketolase



- Molecule 1: Transketolase

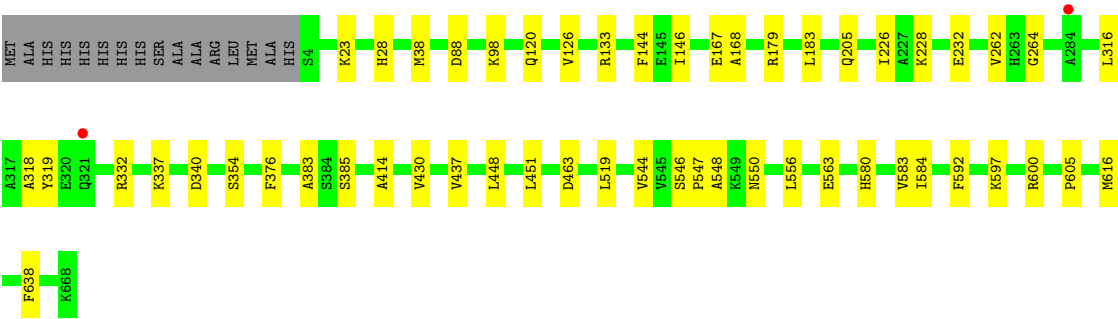


- Molecule 1: Transketolase



- Molecule 1: Transketolase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.44Å 82.71Å 106.14Å 80.89° 68.34° 69.99°	Depositor
Resolution (Å)	49.29 – 2.10 49.29 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.7 (49.29-2.10) 82.2 (49.29-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.96 (at 2.10Å)	Xtriage
Refinement program	PHENIX v1.20.1-4487	Depositor
R, R_{free}	0.168 , 0.228 0.168 , 0.228	Depositor DCC
R_{free} test set	6312 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtriage
Anisotropy	0.315	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 33.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,-h+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	41062	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TPP, CL, EDO, MG, ACT

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/5164	0.66	0/7010
1	B	0.49	0/5164	0.64	0/7010
1	C	0.51	0/5164	0.66	0/7010
1	D	0.49	0/5164	0.64	0/7010
All	All	0.50	0/20656	0.65	0/28040

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	B	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	179	ARG	Sidechain
1	B	93	ARG	Sidechain

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	5047	4971	4970	24	0
1	B	5047	4972	4970	35	0
1	C	5047	4972	4970	37	0
1	D	5047	4971	4970	31	0
2	A	28	42	42	4	0
2	B	12	18	18	4	0
2	C	28	42	42	4	0
2	D	8	12	12	2	0
3	A	4	3	3	0	0
3	C	4	3	3	0	0
3	D	4	3	3	0	0
4	A	26	16	16	1	0
4	B	26	16	16	0	0
4	C	26	16	16	2	0
4	D	26	16	16	5	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	3	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	149	0	0	2	0
7	B	148	0	0	3	0
7	C	173	0	0	2	0
7	D	130	0	0	2	0
All	All	20989	20073	20067	126	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 3.

All (126) 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:256:LYS:HB3	1:C:262:VAL:HG13	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:ARG:NH1	7:A:902:HOH:O	2.22	0.72
1:A:95:TRP:O	7:A:901:HOH:O	2.13	0.66
1:A:263:HIS:ND1	4:A:809:TPP:O1B	2.27	0.66
1:D:383:ALA:HB2	2:D:801:EDO:H12	1.78	0.65
1:C:663:LYS:NZ	7:C:901:HOH:O	2.30	0.64
1:C:542:ALA:HB3	1:C:592:PHE:CD1	2.34	0.62
1:A:441:TYR:O	2:A:801:EDO:H21	2.00	0.61
1:B:302:GLN:O	7:B:901:HOH:O	2.16	0.60
1:A:556:LEU:HD11	1:A:605:PRO:HD2	1.82	0.60
1:C:597:LYS:NZ	7:C:904:HOH:O	2.34	0.59
4:D:804:TPP:HN42	4:D:804:TPP:H2	1.68	0.58
1:B:222:ASN:OD1	1:B:224:GLU:HG2	2.03	0.58
1:A:176:LYS:HE3	1:A:238:SER:O	2.04	0.57
1:A:199:PHE:CZ	1:A:201:GLU:HG3	2.41	0.56
1:D:556:LEU:HD11	1:D:605:PRO:HD2	1.88	0.55
1:B:183:LEU:HD12	1:B:183:LEU:N	2.22	0.55
4:D:804:TPP:H2	7:D:1013:HOH:O	2.07	0.54
1:B:320:GLU:OE2	1:B:331:LYS:NZ	2.34	0.54
1:C:617:GLY:O	1:C:634:ALA:HB1	2.07	0.54
1:C:376:PHE:O	1:C:430:VAL:HA	2.08	0.53
1:A:542:ALA:HB3	1:A:592:PHE:CD1	2.44	0.52
1:B:562:SER:HB2	2:B:803:EDO:C2	2.40	0.52
4:D:804:TPP:HN42	4:D:804:TPP:C2	2.22	0.52
1:D:167:GLU:HB2	1:D:414:ALA:HB2	1.92	0.52
1:D:376:PHE:O	1:D:430:VAL:HA	2.09	0.51
1:C:199:PHE:CZ	1:C:201:GLU:HG3	2.45	0.51
1:C:382:LEU:HD21	4:D:804:TPP:H7'1	1.92	0.51
1:C:549:LYS:HE3	1:C:575:ALA:HB2	1.93	0.51
1:C:419:LEU:HD11	1:C:432:GLY:HA3	1.93	0.51
1:D:183:LEU:HD12	1:D:183:LEU:N	2.26	0.51
1:B:43:TRP:NE1	1:B:80:SER:OG	2.40	0.51
7:B:904:HOH:O	1:C:280:ARG:HD3	2.11	0.50
1:A:87:ASP:O	1:A:91:GLN:HG2	2.12	0.50
1:B:437:VAL:HG13	1:B:438:PHE:CD1	2.47	0.49
1:D:120:GLN:OE1	1:D:448:LEU:HD12	2.11	0.49
1:A:451:LEU:HD12	1:B:638:PHE:CD2	2.47	0.49
1:B:562:SER:HB2	2:B:803:EDO:H22	1.95	0.49
4:C:809:TPP:H2	4:C:809:TPP:HN42	1.78	0.49
1:A:183:LEU:N	1:A:183:LEU:HD12	2.29	0.48
1:A:204:ALA:HB2	1:A:214:TYR:CZ	2.49	0.48
1:A:538:VAL:HG22	1:A:587:PRO:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:801:EDO:H22	1:B:413:PHE:CE2	2.49	0.48
1:C:456:VAL:HG12	1:C:457:ILE:N	2.29	0.48
1:D:332:ARG:CG	1:D:337:LYS:HB2	2.44	0.48
1:B:376:PHE:O	1:B:430:VAL:HA	2.15	0.47
1:B:456:VAL:HG12	1:B:457:ILE:N	2.29	0.47
1:A:63:VAL:O	1:A:153:ALA:HA	2.14	0.47
1:C:204:ALA:HB2	1:C:214:TYR:CZ	2.49	0.47
1:C:204:ALA:O	1:C:208:GLN:HG3	2.15	0.47
1:C:437:VAL:HG11	1:C:474:HIS:HA	1.95	0.47
1:A:103:PRO:O	1:A:114:THR:HA	2.15	0.47
1:D:592:PHE:O	1:D:600:ARG:HD3	2.15	0.47
1:C:263:HIS:ND1	4:C:809:TPP:O2B	2.47	0.47
1:D:228:LYS:HE3	1:D:232:GLU:OE2	2.14	0.46
2:A:801:EDO:H11	1:B:413:PHE:CD2	2.50	0.46
1:B:38:MET:HE2	1:B:245:VAL:HG11	1.98	0.46
1:D:23:LYS:NZ	7:D:903:HOH:O	2.39	0.46
1:D:332:ARG:HG3	1:D:337:LYS:HB2	1.96	0.46
1:B:31:MET:HB3	1:B:32:PRO:HD3	1.98	0.46
1:C:56:TRP:CD1	1:C:309:GLU:HG3	2.50	0.46
1:C:472:PRO:HB2	1:D:451:LEU:HD11	1.97	0.45
1:C:183:LEU:HD12	1:C:183:LEU:N	2.30	0.45
1:C:451:LEU:HD13	1:D:638:PHE:CG	2.52	0.45
1:C:549:LYS:HD3	1:C:549:LYS:N	2.31	0.45
1:A:657:ASN:O	1:A:661:ARG:HG3	2.16	0.45
1:B:431:PHE:HA	1:B:457:ILE:O	2.17	0.45
1:A:431:PHE:HA	1:A:457:ILE:O	2.17	0.45
1:C:615:GLU:O	1:C:634:ALA:HA	2.17	0.44
1:D:133:ARG:CZ	1:D:179:ARG:HE	2.29	0.44
1:C:355:LEU:HD12	1:C:359:SER:HB2	1.99	0.44
1:D:146:ILE:HG13	1:D:319:TYR:CD1	2.52	0.44
1:D:550:ASN:HB2	1:D:580:HIS:CG	2.52	0.44
1:C:398:PRO:HA	1:C:401:TYR:CZ	2.52	0.44
1:A:619:SER:O	1:A:620:LEU:C	2.60	0.44
1:B:456:VAL:CG1	1:B:457:ILE:N	2.80	0.44
1:B:28:HIS:CG	1:B:68:HIS:HB2	2.52	0.44
1:B:623:GLU:H	1:B:623:GLU:CD	2.26	0.44
1:C:63:VAL:O	1:C:153:ALA:HA	2.18	0.43
1:C:23:LYS:NZ	2:C:802:EDO:H21	2.33	0.43
1:D:126:VAL:HG21	1:D:168:ALA:HB1	2.00	0.43
1:D:144:PHE:CZ	1:D:318:ALA:O	2.72	0.43
1:B:333:ALA:HA	2:B:802:EDO:O1	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:383:ALA:HB2	2:D:801:EDO:C1	2.48	0.43
1:B:49:HIS:CD2	1:B:49:HIS:N	2.87	0.43
1:A:328:ALA:O	1:A:332:ARG:HG3	2.19	0.43
1:B:186:SER:OG	1:B:244:GLU:OE2	2.32	0.43
1:D:463:ASP:HB3	1:D:519:LEU:O	2.19	0.43
1:B:425:HIS:HA	7:B:982:HOH:O	2.18	0.43
1:D:547:PRO:O	1:D:548:ALA:C	2.61	0.42
1:B:63:VAL:O	1:B:153:ALA:HA	2.19	0.42
1:B:429:LYS:HZ1	2:B:801:EDO:H12	1.84	0.42
1:C:263:HIS:NE2	2:C:801:EDO:O2	2.46	0.42
1:A:472:PRO:HD2	1:B:104:GLU:OE2	2.19	0.42
1:D:38:MET:HA	1:D:226:ILE:HD13	2.01	0.42
1:C:209:ALA:HB2	1:D:205:GLN:HB3	2.01	0.42
1:C:521:ARG:HE	2:C:805:EDO:C1	2.33	0.42
1:D:88:ASP:OD2	1:D:98:LYS:HD2	2.20	0.42
1:C:145:GLU:OE2	1:C:148:ASN:ND2	2.52	0.42
1:C:478:GLU:O	1:C:482:SER:HB3	2.19	0.42
1:D:133:ARG:NH1	1:D:179:ARG:HH21	2.18	0.42
1:D:316:LEU:O	1:D:319:TYR:HB3	2.19	0.42
2:A:801:EDO:H22	1:B:413:PHE:HE2	1.85	0.41
1:C:464:SER:O	1:C:467:VAL:HG23	2.20	0.41
1:C:616:MET:SD	1:C:648:MET:HG2	2.59	0.41
1:B:355:LEU:HD12	1:B:355:LEU:N	2.35	0.41
1:D:546:SER:HB3	1:D:583:VAL:HB	2.02	0.41
1:D:28:HIS:CD2	1:D:264:GLY:HA2	2.55	0.41
1:C:638:PHE:CG	1:D:451:LEU:HD13	2.55	0.41
1:D:544:VAL:HG22	1:D:584:ILE:CD1	2.50	0.41
1:B:349:TYR:CD1	1:B:497:ALA:HB1	2.56	0.41
1:B:184:TYR:CD1	1:B:184:TYR:C	2.99	0.40
1:A:199:PHE:CZ	1:A:201:GLU:CG	3.04	0.40
1:B:6:GLU:OE1	1:B:6:GLU:N	2.53	0.40
1:B:28:HIS:CD2	1:B:264:GLY:HA2	2.56	0.40
1:B:222:ASN:OD1	1:B:222:ASN:C	2.64	0.40
1:C:591:ARG:HD2	2:C:803:EDO:O2	2.22	0.40
4:D:804:TPP:C2	4:D:804:TPP:N4'	2.85	0.40
1:A:577:GLU:OE1	1:A:663:LYS:NZ	2.48	0.40
1:B:368:ILE:HD13	1:B:508:LEU:CD1	2.52	0.40
1:B:666:LEU:HB2	1:B:668:LYS:HG3	2.03	0.40
1:C:133:ARG:NE	1:C:133:ARG:HA	2.37	0.40
1:C:530:THR:O	1:C:531:ALA:C	2.65	0.40
1:A:178:GLY:HA3	1:A:237:LEU:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:544:VAL:HG22	1:A:584:ILE:CD1	2.51	0.40
1:D:563:GLU:CD	1:D:616:MET:HG3	2.46	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	663/681 (97%)	644 (97%)	19 (3%)	0	100	100
1	B	663/681 (97%)	637 (96%)	26 (4%)	0	100	100
1	C	663/681 (97%)	639 (96%)	24 (4%)	0	100	100
1	D	663/681 (97%)	635 (96%)	28 (4%)	0	100	100
All	All	2652/2724 (97%)	2555 (96%)	97 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	508/520 (98%)	504 (99%)	4 (1%)	73	81
1	B	508/520 (98%)	499 (98%)	9 (2%)	51	60
1	C	508/520 (98%)	495 (97%)	13 (3%)	40	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	508/520 (98%)	502 (99%)	6 (1%)	63	72
All	All	2032/2080 (98%)	2000 (98%)	32 (2%)	55	64

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	47	MET
1	A	49	HIS
1	A	292	GLU
1	B	4	SER
1	B	49	HIS
1	B	98	LYS
1	B	325	GLU
1	B	340	ASP
1	B	354	SER
1	B	355	LEU
1	B	385	SER
1	B	656	ASP
1	C	4	SER
1	C	45	LYS
1	C	49	HIS
1	C	201	GLU
1	C	262	VAL
1	C	280	ARG
1	C	355	LEU
1	C	370	LYS
1	C	442	LEU
1	C	482	SER
1	C	549	LYS
1	C	550	ASN
1	C	656	ASP
1	D	262	VAL
1	D	340	ASP
1	D	354	SER
1	D	385	SER
1	D	437	VAL
1	D	597	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	196	ASN
1	A	321	GLN
1	A	329	GLN
1	B	94	GLN
1	B	329	GLN
1	B	550	ASN
1	B	595	GLN
1	C	329	GLN
1	D	208	GLN
1	D	315	GLN
1	D	595	GLN

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 35 ligands modelled in this entry, 9 are monoatomic - leaving 26 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	TPP	C	809	5	26,27,27	0.98	2 (7%)	38,40,40	0.49	0
2	EDO	D	802	-	3,3,3	0.29	0	2,2,2	0.82	0
2	EDO	A	801	-	3,3,3	0.61	0	2,2,2	0.27	0
2	EDO	A	803	-	3,3,3	0.56	0	2,2,2	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	805	-	3,3,3	0.75	0	2,2,2	0.18	0
2	EDO	B	801	-	3,3,3	0.42	0	2,2,2	0.72	0
2	EDO	C	804	-	3,3,3	0.35	0	2,2,2	0.96	0
2	EDO	B	802	-	3,3,3	0.29	0	2,2,2	0.80	0
3	ACT	D	803	-	3,3,3	1.46	0	3,3,3	1.30	0
2	EDO	C	801	-	3,3,3	0.41	0	2,2,2	0.62	0
2	EDO	C	805	-	3,3,3	0.24	0	2,2,2	0.60	0
2	EDO	A	802	-	3,3,3	0.47	0	2,2,2	0.25	0
2	EDO	A	807	-	3,3,3	0.46	0	2,2,2	0.43	0
2	EDO	D	801	-	3,3,3	0.47	0	2,2,2	0.32	0
3	ACT	A	808	-	3,3,3	1.79	1 (33%)	3,3,3	1.37	0
4	TPP	B	804	5	26,27,27	1.27	1 (3%)	38,40,40	0.58	0
2	EDO	A	806	-	3,3,3	0.70	0	2,2,2	0.11	0
2	EDO	C	803	-	3,3,3	0.45	0	2,2,2	0.32	0
4	TPP	A	809	5	26,27,27	0.84	1 (3%)	38,40,40	0.70	1 (2%)
2	EDO	C	802	-	3,3,3	0.93	0	2,2,2	0.83	0
3	ACT	C	807	-	3,3,3	1.94	1 (33%)	3,3,3	1.13	0
4	TPP	D	804	5	26,27,27	1.69	2 (7%)	38,40,40	0.67	1 (2%)
2	EDO	B	803	-	3,3,3	0.47	0	2,2,2	0.45	0
2	EDO	C	808	-	3,3,3	0.43	0	2,2,2	0.49	0
2	EDO	C	806	-	3,3,3	0.55	0	2,2,2	0.40	0
2	EDO	A	804	-	3,3,3	0.57	0	2,2,2	0.22	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TPP	C	809	5	-	5/17/17/17	0/2/2/2
2	EDO	D	802	-	-	0/1/1/1	-
2	EDO	A	801	-	-	1/1/1/1	-
2	EDO	A	803	-	-	0/1/1/1	-
2	EDO	A	805	-	-	1/1/1/1	-
2	EDO	B	801	-	-	0/1/1/1	-
2	EDO	C	804	-	-	0/1/1/1	-
2	EDO	B	802	-	-	0/1/1/1	-
2	EDO	C	801	-	-	0/1/1/1	-
2	EDO	C	805	-	-	0/1/1/1	-
2	EDO	A	802	-	-	1/1/1/1	-
2	EDO	A	807	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	D	801	-	-	1/1/1/1	-
4	TPP	B	804	5	-	1/17/17/17	0/2/2/2
2	EDO	A	806	-	-	1/1/1/1	-
2	EDO	C	803	-	-	0/1/1/1	-
4	TPP	A	809	5	-	1/17/17/17	0/2/2/2
2	EDO	C	802	-	-	1/1/1/1	-
4	TPP	D	804	5	-	1/17/17/17	0/2/2/2
2	EDO	B	803	-	-	0/1/1/1	-
2	EDO	C	808	-	-	1/1/1/1	-
2	EDO	C	806	-	-	1/1/1/1	-
2	EDO	A	804	-	-	1/1/1/1	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	804	TPP	PA-O3A	-7.93	1.50	1.59
4	B	804	TPP	PA-O3A	-6.00	1.53	1.59
4	A	809	TPP	PA-O3A	3.41	1.63	1.59
3	C	807	ACT	CH3-C	2.92	1.60	1.49
3	A	808	ACT	CH3-C	2.82	1.60	1.49
4	C	809	TPP	PA-O3A	-2.62	1.56	1.59
4	C	809	TPP	C5-C4	-2.50	1.29	1.35
4	D	804	TPP	PB-O2B	-2.23	1.46	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	804	TPP	O2A-PA-O1A	2.54	124.26	112.44
4	A	809	TPP	O3B-PB-O2B	2.52	117.23	107.80

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	809	TPP	C5-C6-C7-O7
4	C	809	TPP	C7-O7-PA-O1A
4	C	809	TPP	C7-O7-PA-O2A
4	C	809	TPP	C7-O7-PA-O3A
2	C	808	EDO	O1-C1-C2-O2
2	A	804	EDO	O1-C1-C2-O2
2	C	802	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	D	801	EDO	O1-C1-C2-O2
2	A	806	EDO	O1-C1-C2-O2
2	C	806	EDO	O1-C1-C2-O2
4	A	809	TPP	C5-C6-C7-O7
4	B	804	TPP	C5-C6-C7-O7
2	A	801	EDO	O1-C1-C2-O2
2	A	805	EDO	O1-C1-C2-O2
2	A	802	EDO	O1-C1-C2-O2
4	C	809	TPP	C5'-C7'-N3-C2
4	D	804	TPP	C5'-C7'-N3-C2

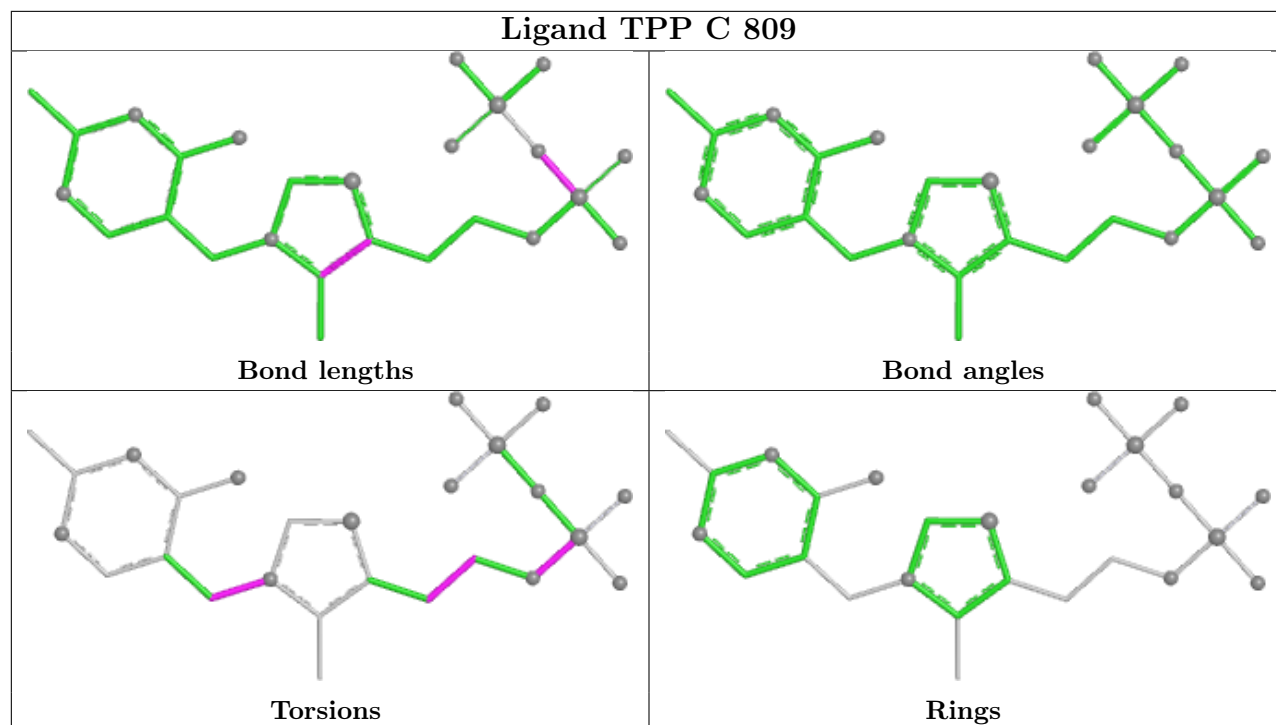
There are no ring outliers.

12 monomers are involved in 22 short contacts:

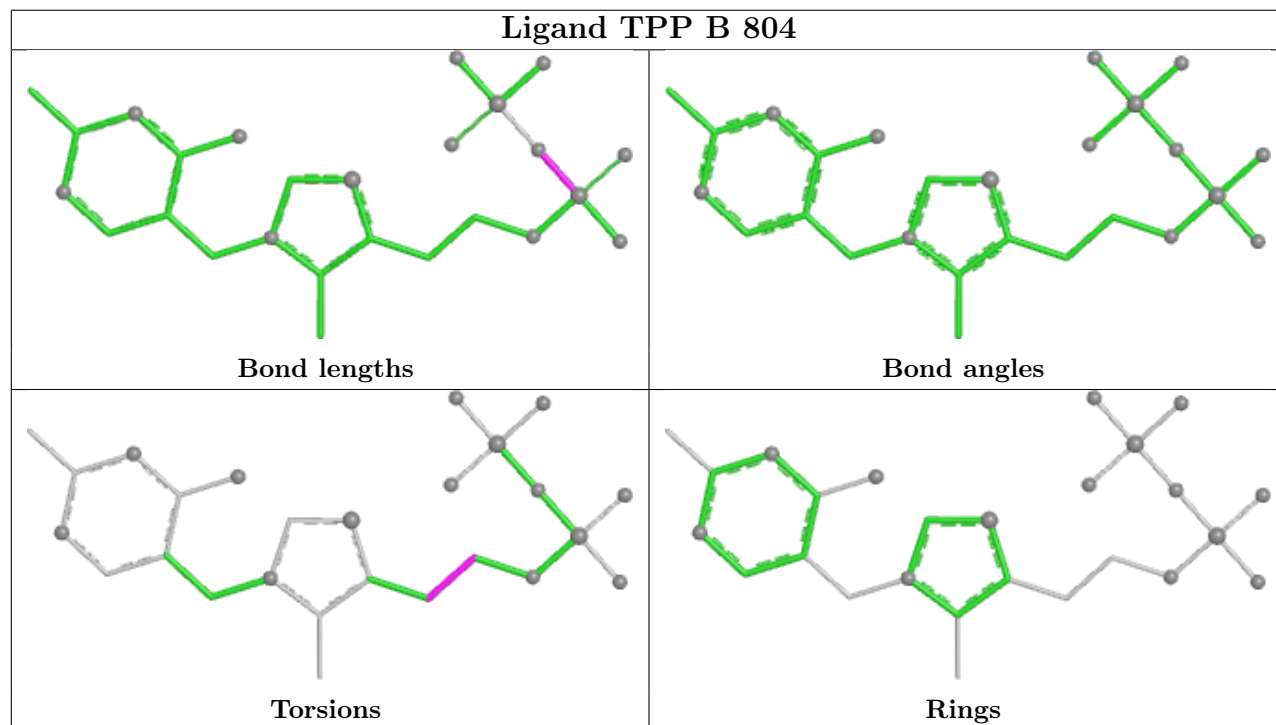
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	809	TPP	2	0
2	A	801	EDO	4	0
2	B	801	EDO	1	0
2	B	802	EDO	1	0
2	C	801	EDO	1	0
2	C	805	EDO	1	0
2	D	801	EDO	2	0
2	C	803	EDO	1	0
4	A	809	TPP	1	0
2	C	802	EDO	1	0
4	D	804	TPP	5	0
2	B	803	EDO	2	0

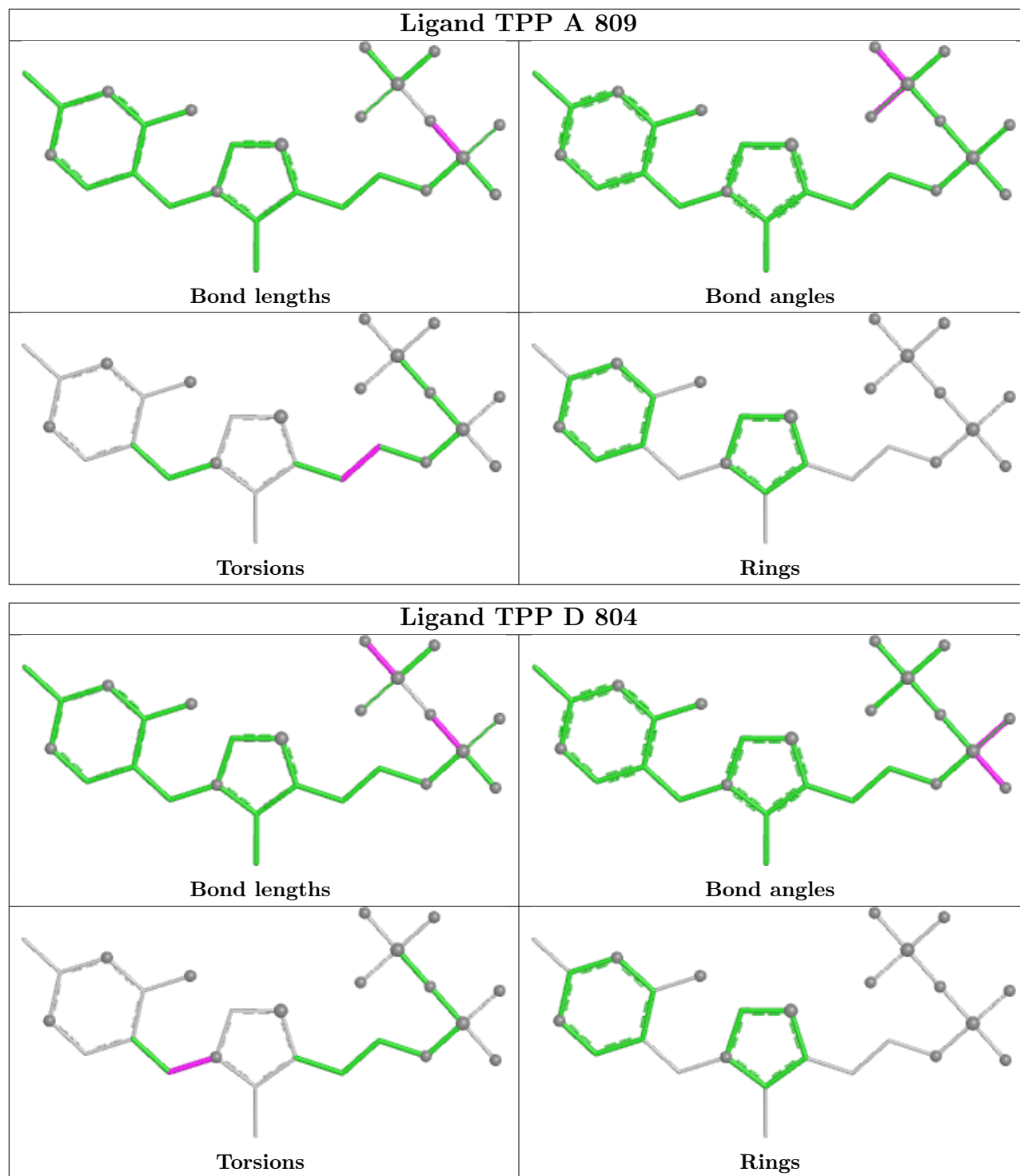
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand TPP C 809



Ligand TPP B 804





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	665/681 (97%)	-0.33	1 (0%) 91 92	24, 38, 55, 84	0
1	B	665/681 (97%)	-0.33	1 (0%) 91 92	25, 38, 59, 82	0
1	C	665/681 (97%)	-0.38	0 100 100	24, 36, 56, 79	0
1	D	665/681 (97%)	-0.23	2 (0%) 90 91	23, 40, 67, 112	0
All	All	2660/2724 (97%)	-0.32	4 (0%) 91 92	23, 38, 59, 112	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	4	SER	2.4
1	D	321	GLN	2.2
1	D	284	ALA	2.1
1	A	451	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

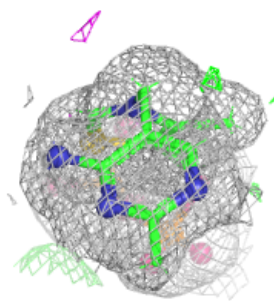
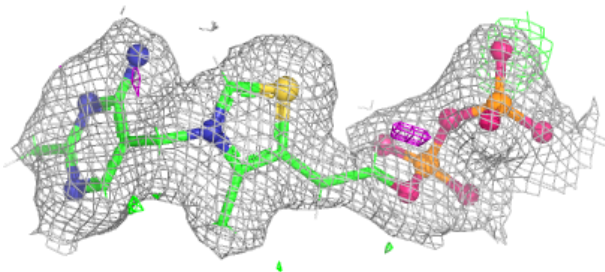
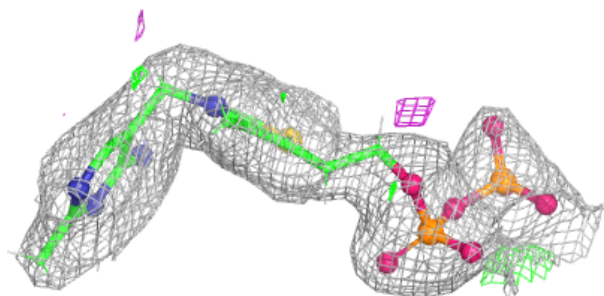
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists 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
3	ACT	A	808	4/4	0.62	0.15	48,52,60,60	0
3	ACT	D	803	4/4	0.70	0.19	41,45,55,59	0
2	EDO	A	802	4/4	0.80	0.15	54,65,75,75	0
2	EDO	C	805	4/4	0.81	0.16	35,44,57,58	0
2	EDO	A	806	4/4	0.82	0.14	40,49,54,54	0
2	EDO	B	803	4/4	0.82	0.12	62,75,82,82	0
2	EDO	C	802	4/4	0.82	0.11	27,38,53,53	0
2	EDO	C	804	4/4	0.83	0.11	41,49,56,65	0
2	EDO	C	808	4/4	0.83	0.16	53,64,75,75	0
2	EDO	A	805	4/4	0.84	0.15	49,59,67,67	0
3	ACT	C	807	4/4	0.86	0.13	52,55,62,62	0
2	EDO	A	803	4/4	0.87	0.14	43,59,72,72	0
2	EDO	C	806	4/4	0.87	0.15	45,54,56,62	0
2	EDO	C	801	4/4	0.88	0.11	42,50,59,59	0
2	EDO	C	803	4/4	0.89	0.11	38,46,56,66	0
6	CL	C	811	1/1	0.90	0.13	68,68,68,68	0
2	EDO	B	801	4/4	0.92	0.12	43,51,58,68	0
2	EDO	A	801	4/4	0.92	0.16	30,37,50,60	0
2	EDO	A	804	4/4	0.92	0.09	33,44,51,53	0
6	CL	A	813	1/1	0.92	0.12	60,60,60,60	0
2	EDO	D	802	4/4	0.92	0.08	36,44,48,50	0
2	EDO	A	807	4/4	0.94	0.12	41,49,51,54	0
6	CL	B	806	1/1	0.94	0.21	58,58,58,58	0
2	EDO	D	801	4/4	0.94	0.07	34,41,42,47	0
5	MG	A	810	1/1	0.95	0.04	27,27,27,27	0
2	EDO	B	802	4/4	0.95	0.07	38,45,49,55	0
6	CL	A	812	1/1	0.96	0.09	67,67,67,67	0
4	TPP	D	804	26/26	0.96	0.06	26,32,39,44	0
5	MG	D	805	1/1	0.97	0.03	23,23,23,23	0
6	CL	A	811	1/1	0.97	0.06	36,36,36,36	0
4	TPP	C	809	26/26	0.97	0.06	28,36,46,52	0
4	TPP	A	809	26/26	0.97	0.06	23,34,42,45	0
4	TPP	B	804	26/26	0.97	0.06	25,35,44,48	0
5	MG	B	805	1/1	0.97	0.05	27,27,27,27	0
5	MG	C	810	1/1	0.98	0.03	32,32,32,32	0

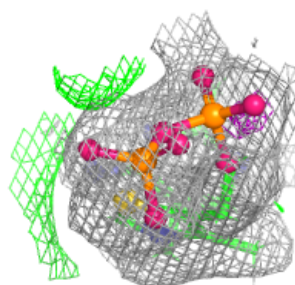
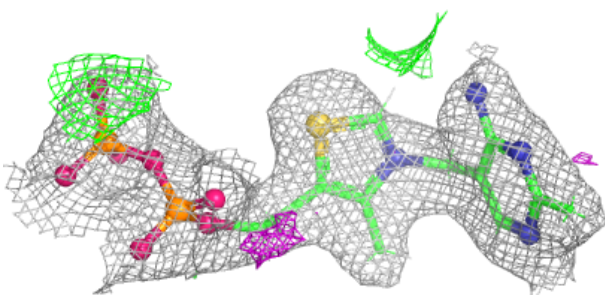
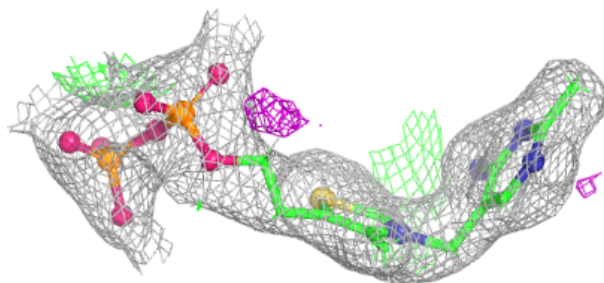
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TPP D 804:

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

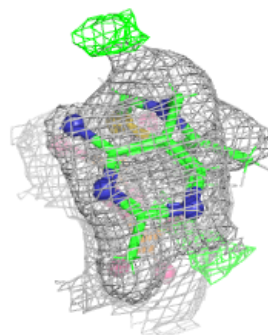
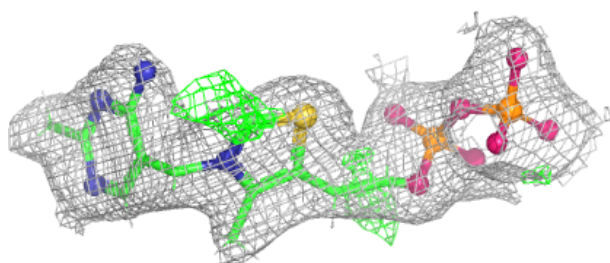
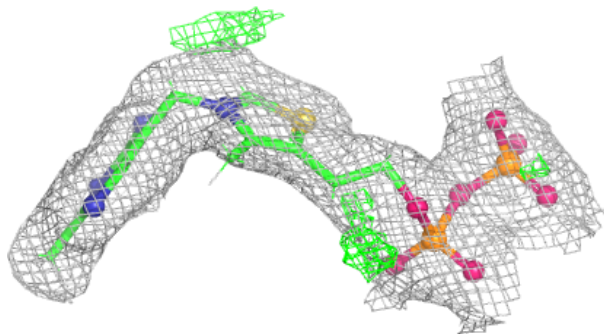
**Electron density around TPP C 809:**

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

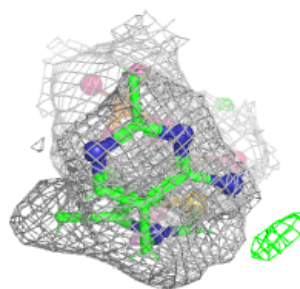
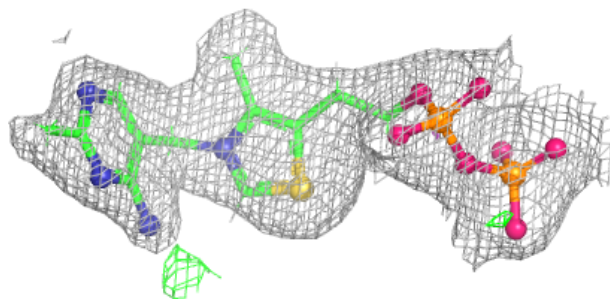
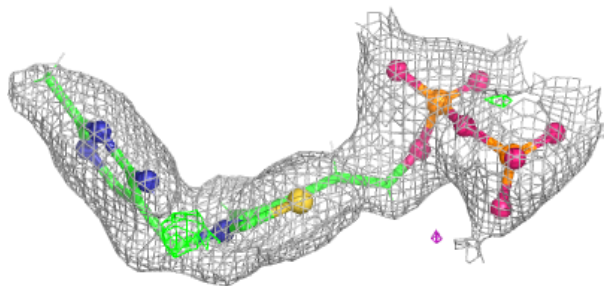


Electron density around TPP A 809:

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

**Electron density around TPP B 804:**

$2mF_o-DF_c$ (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.