



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:31 PM UTC

PDB ID : 3AHC / pdb_00003ahc
Title : Resting form of Phosphoketolase from Bifidobacterium Breve
Authors : Suzuki, R.; Katayama, T.; Kim, B.-J.; Wakagi, T.; Shoun, H.; Ashida, H.; Yamamoto, K.; Fushinobu, S.
Deposited on : 2010-04-22
Resolution : 1.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

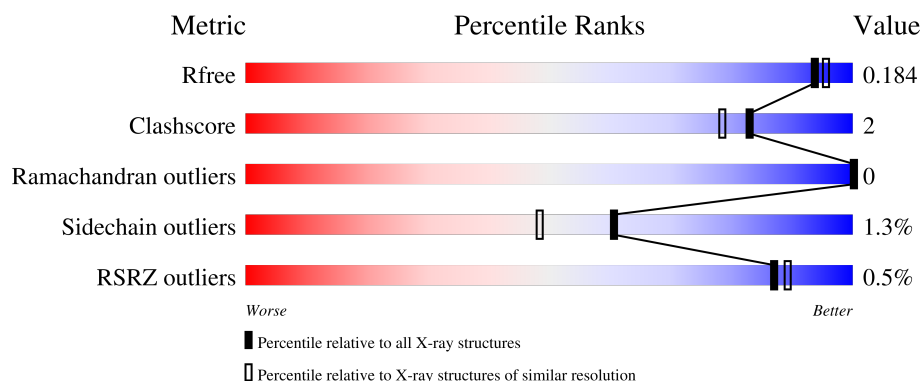
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	845	 72% 22% • 5%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7365 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 Xylulose 5-phosphate/fructose 6-phosphate phosphoketolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	802	Total	C	N	O	S	0	0	0
			6379	4053	1085	1217	24			

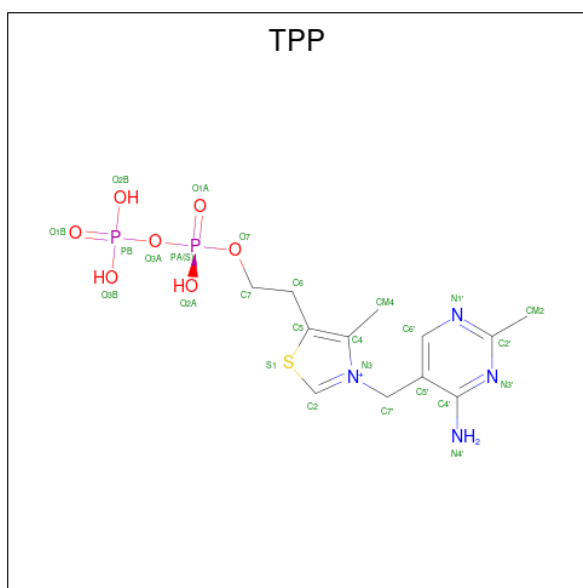
There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP D6PAH1
A	-18	GLY	-	expression tag	UNP D6PAH1
A	-17	SER	-	expression tag	UNP D6PAH1
A	-16	SER	-	expression tag	UNP D6PAH1
A	-15	HIS	-	expression tag	UNP D6PAH1
A	-14	HIS	-	expression tag	UNP D6PAH1
A	-13	HIS	-	expression tag	UNP D6PAH1
A	-12	HIS	-	expression tag	UNP D6PAH1
A	-11	HIS	-	expression tag	UNP D6PAH1
A	-10	HIS	-	expression tag	UNP D6PAH1
A	-9	SER	-	expression tag	UNP D6PAH1
A	-8	SER	-	expression tag	UNP D6PAH1
A	-7	GLY	-	expression tag	UNP D6PAH1
A	-6	LEU	-	expression tag	UNP D6PAH1
A	-5	VAL	-	expression tag	UNP D6PAH1
A	-4	PRO	-	expression tag	UNP D6PAH1
A	-3	ARG	-	expression tag	UNP D6PAH1
A	-2	GLY	-	expression tag	UNP D6PAH1
A	-1	SER	-	expression tag	UNP D6PAH1
A	0	HIS	-	expression tag	UNP D6PAH1

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is THIAMINE DIPHOSPHATE (CCD ID: TPP) (formula: $C_{12}H_{19}N_4O_7P_2S$).

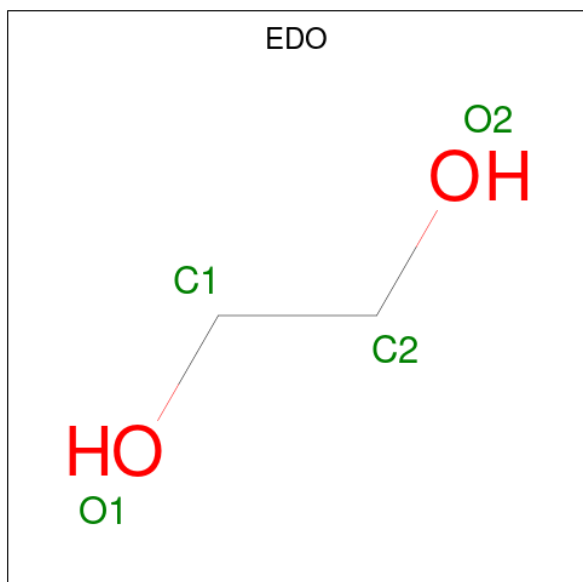


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

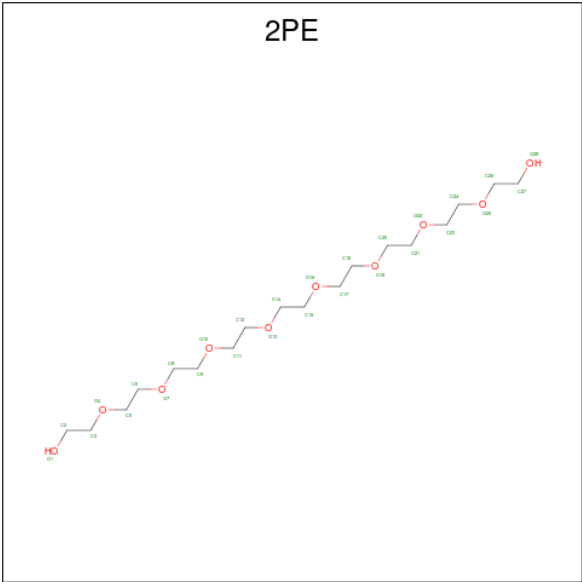
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0

- Molecule 6 is NONAETHYLENE GLYCOL (CCD ID: 2PE) (formula: C₁₈H₃₈O₁₀).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 28 18 10	0	0

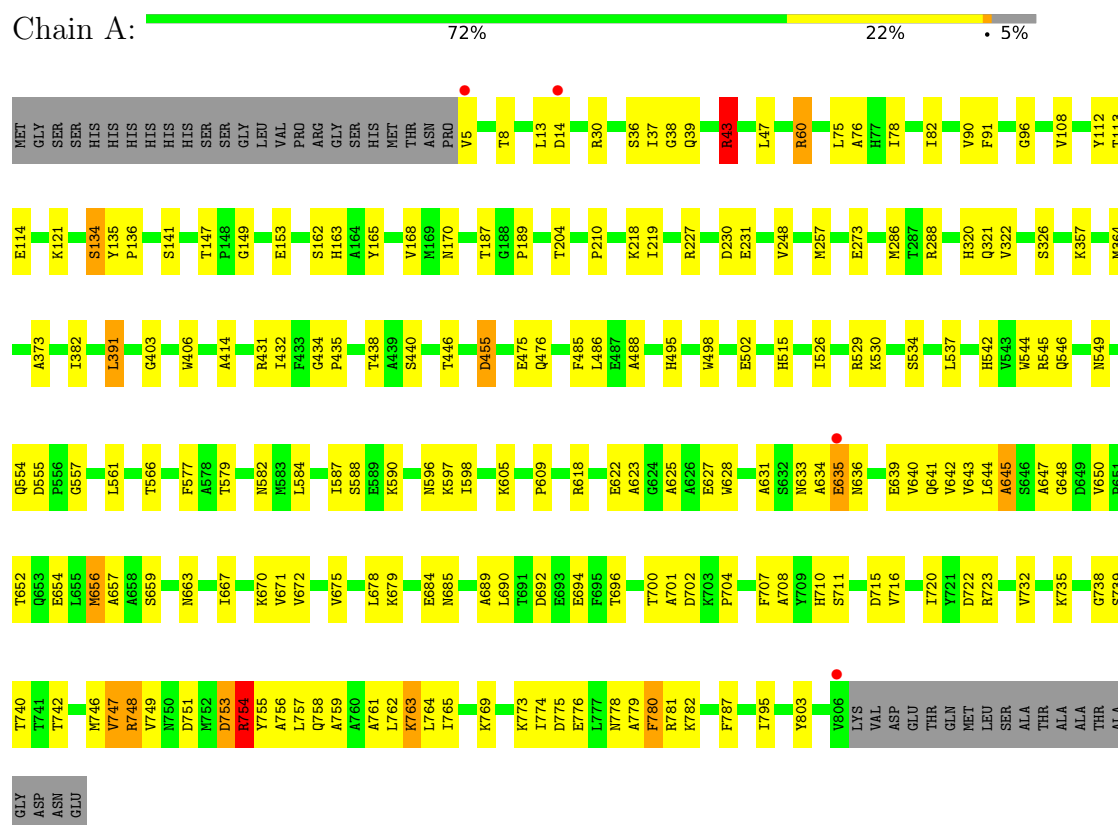
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	886	Total 886	O 886	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: Xylulose 5-phosphate/fructose 6-phosphate phosphoketolase



4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	174.77Å 174.77Å 163.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.18 – 1.70 34.18 – 1.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.18-1.70) 99.9 (34.18-1.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.37 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.150 , 0.181 0.154 , 0.184	Depositor DCC
R_{free} test set	6904 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	15.5	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7365	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% 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: NA, MG, 2PE, TPP, EDO

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	2.05	142/6553 (2.2%)	1.67	76/8909 (0.9%)

All (142) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	754	ARG	CD-NE	-11.14	1.30	1.46
1	A	322	VAL	CA-CB	10.57	1.64	1.54
1	A	779	ALA	CA-CB	9.58	1.69	1.53
1	A	631	ALA	CA-CB	9.35	1.67	1.53
1	A	168	VAL	CA-CB	9.02	1.64	1.54
1	A	403	GLY	C-O	8.67	1.30	1.23
1	A	754	ARG	N-CA	8.46	1.56	1.46
1	A	701	ALA	CA-CB	8.44	1.67	1.53
1	A	554	GLN	N-CA	8.31	1.58	1.46
1	A	640	VAL	CA-CB	8.12	1.64	1.54
1	A	692	ASP	N-CA	8.07	1.56	1.46
1	A	679	LYS	N-CA	8.06	1.57	1.46
1	A	5	VAL	N-CA	8.02	1.61	1.46
1	A	656	MET	SD-CE	-7.91	1.59	1.79
1	A	555	ASP	C-N	7.86	1.39	1.33
1	A	675	VAL	N-CA	7.74	1.53	1.46
1	A	720	ILE	N-CA	7.70	1.56	1.46
1	A	732	VAL	CA-C	7.61	1.61	1.52
1	A	566	THR	CA-CB	7.60	1.63	1.53
1	A	659	SER	N-CA	7.43	1.55	1.46
1	A	787	PHE	N-CA	-7.30	1.37	1.46
1	A	438	THR	C-O	7.20	1.32	1.24
1	A	625	ALA	N-CA	7.20	1.54	1.45
1	A	753	ASP	CA-C	7.12	1.62	1.53
1	A	739	SER	CB-OG	7.05	1.56	1.42
1	A	230	ASP	CG-OD1	7.03	1.38	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	488	ALA	CA-CB	7.03	1.65	1.53
1	A	782	LYS	N-CA	7.02	1.54	1.46
1	A	671	VAL	CA-CB	-7.01	1.45	1.54
1	A	742	THR	CA-CB	6.88	1.63	1.53
1	A	685	ASN	N-CA	6.82	1.55	1.46
1	A	286	MET	SD-CE	-6.77	1.62	1.79
1	A	780	PHE	N-CA	-6.64	1.38	1.46
1	A	765	ILE	N-CA	6.62	1.54	1.46
1	A	696	THR	N-CA	6.60	1.54	1.46
1	A	732	VAL	CA-CB	-6.47	1.46	1.54
1	A	647	ALA	CA-C	6.46	1.60	1.52
1	A	663	ASN	C-O	6.46	1.31	1.24
1	A	781	ARG	N-CA	6.45	1.54	1.46
1	A	749	VAL	CA-CB	6.44	1.62	1.54
1	A	14	ASP	N-CA	6.43	1.56	1.46
1	A	39	GLN	CD-OE1	6.39	1.35	1.23
1	A	625	ALA	C-O	6.38	1.31	1.23
1	A	597	LYS	CB-CG	6.31	1.71	1.52
1	A	650	VAL	CA-C	6.30	1.59	1.52
1	A	671	VAL	N-CA	6.27	1.53	1.46
1	A	530	LYS	C-O	6.26	1.31	1.23
1	A	382	ILE	CA-CB	6.26	1.63	1.54
1	A	756	ALA	CA-CB	6.25	1.63	1.53
1	A	704	PRO	N-CA	6.21	1.54	1.47
1	A	257	MET	N-CA	6.20	1.53	1.46
1	A	748	ARG	C-N	6.18	1.40	1.34
1	A	210	PRO	C-O	6.17	1.30	1.23
1	A	755	TYR	CA-CB	6.14	1.63	1.53
1	A	545	ARG	CA-C	6.11	1.61	1.53
1	A	716	VAL	C-O	6.08	1.31	1.24
1	A	678	LEU	CA-C	6.04	1.61	1.52
1	A	644	LEU	N-CA	6.03	1.54	1.46
1	A	667	ILE	CA-CB	6.03	1.62	1.54
1	A	112	TYR	N-CA	6.02	1.53	1.46
1	A	689	ALA	N-CA	5.98	1.53	1.45
1	A	588	SER	N-CA	5.96	1.53	1.46
1	A	218	LYS	N-CA	5.92	1.53	1.46
1	A	710	HIS	ND1-CE1	5.92	1.38	1.32
1	A	43	ARG	CD-NE	-5.89	1.38	1.46
1	A	657	ALA	CA-CB	5.86	1.62	1.53
1	A	778	ASN	N-CA	5.84	1.53	1.46
1	A	544	TRP	N-CA	5.79	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	163	HIS	C-O	-5.78	1.17	1.24
1	A	775	ASP	CA-C	-5.77	1.45	1.52
1	A	762	LEU	N-CA	5.76	1.53	1.46
1	A	795	ILE	N-CA	5.74	1.54	1.47
1	A	373	ALA	CA-CB	5.74	1.63	1.53
1	A	90	VAL	N-CA	5.74	1.52	1.46
1	A	773	LYS	CA-C	5.73	1.60	1.52
1	A	406	TRP	CA-C	5.73	1.60	1.52
1	A	642	VAL	N-CA	5.72	1.53	1.46
1	A	639	GLU	CA-C	5.71	1.60	1.52
1	A	645	ALA	CA-C	5.71	1.59	1.52
1	A	577	PHE	CA-C	-5.71	1.45	1.52
1	A	529	ARG	C-O	5.69	1.30	1.23
1	A	735	LYS	C-O	5.65	1.30	1.24
1	A	627	GLU	C-O	5.64	1.30	1.23
1	A	781	ARG	CZ-NH2	5.60	1.40	1.33
1	A	326	SER	N-CA	5.59	1.52	1.46
1	A	670	LYS	CA-C	5.59	1.59	1.52
1	A	546	GLN	N-CA	5.56	1.53	1.46
1	A	587	ILE	CA-C	5.55	1.59	1.52
1	A	645	ALA	CA-CB	-5.54	1.40	1.53
1	A	8	THR	CA-CB	5.54	1.60	1.52
1	A	751	ASP	N-CA	5.52	1.54	1.46
1	A	187	THR	N-CA	5.52	1.52	1.45
1	A	38	GLY	N-CA	5.50	1.52	1.45
1	A	584	LEU	N-CA	5.48	1.52	1.46
1	A	640	VAL	N-CA	5.46	1.53	1.46
1	A	36	SER	C-O	5.43	1.30	1.24
1	A	711	SER	CA-CB	5.43	1.60	1.53
1	A	149	GLY	N-CA	5.43	1.52	1.45
1	A	582	ASN	CA-CB	5.42	1.61	1.53
1	A	248	VAL	C-O	5.42	1.29	1.24
1	A	579	THR	CA-CB	5.42	1.62	1.53
1	A	622	GLU	CG-CD	5.41	1.65	1.52
1	A	14	ASP	CA-C	5.41	1.60	1.53
1	A	747	VAL	CA-CB	5.38	1.61	1.54
1	A	91	PHE	C-O	5.38	1.30	1.23
1	A	82	ILE	CA-CB	5.37	1.60	1.54
1	A	738	GLY	CA-C	5.37	1.56	1.51
1	A	108	VAL	C-O	5.37	1.30	1.24
1	A	134	SER	CB-OG	-5.36	1.31	1.42
1	A	219	ILE	CA-CB	5.33	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	440	SER	CA-C	5.33	1.59	1.52
1	A	113	THR	N-CA	5.32	1.53	1.46
1	A	165	TYR	C-N	5.31	1.40	1.33
1	A	114	GLU	C-O	5.31	1.30	1.24
1	A	204	THR	N-CA	5.27	1.53	1.46
1	A	684	GLU	N-CA	-5.27	1.39	1.46
1	A	675	VAL	CA-CB	-5.26	1.47	1.55
1	A	486	LEU	N-CA	5.25	1.52	1.46
1	A	47	LEU	N-CA	5.25	1.52	1.46
1	A	648	GLY	C-O	5.25	1.30	1.24
1	A	75	LEU	CA-CB	5.23	1.61	1.53
1	A	596	ASN	CA-C	5.22	1.60	1.53
1	A	769	LYS	N-CA	-5.21	1.40	1.46
1	A	364	MET	C-O	5.19	1.30	1.23
1	A	542	HIS	CA-CB	5.18	1.60	1.53
1	A	644	LEU	CA-C	5.18	1.59	1.52
1	A	609	PRO	N-CA	5.16	1.53	1.47
1	A	690	LEU	N-CA	5.16	1.52	1.46
1	A	515	HIS	CA-C	5.14	1.59	1.52
1	A	780	PHE	CA-C	5.14	1.59	1.52
1	A	566	THR	C-O	5.13	1.31	1.23
1	A	700	THR	CA-CB	5.13	1.62	1.53
1	A	162	SER	CA-CB	5.12	1.61	1.53
1	A	39	GLN	CD-NE2	-5.10	1.22	1.33
1	A	675	VAL	C-O	5.06	1.30	1.24
1	A	414	ALA	CA-CB	5.06	1.61	1.53
1	A	590	LYS	N-CA	-5.05	1.40	1.46
1	A	633	ASN	N-CA	5.05	1.53	1.45
1	A	628	TRP	CA-C	5.02	1.59	1.53
1	A	776	GLU	N-CA	-5.02	1.40	1.46
1	A	765	ILE	C-O	5.01	1.29	1.24
1	A	710	HIS	CA-C	5.01	1.59	1.52

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	ARG	NE-CZ-NH2	-12.74	107.74	119.20
1	A	754	ARG	NE-CZ-NH2	-12.58	107.88	119.20
1	A	43	ARG	NE-CZ-NH1	11.01	132.50	121.50
1	A	43	ARG	CD-NE-CZ	9.54	137.76	124.40
1	A	754	ARG	CB-CG-CD	-9.07	90.45	111.30
1	A	774	ILE	N-CA-C	-8.87	102.19	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	618	ARG	NE-CZ-NH1	8.82	130.32	121.50
1	A	707	PHE	CA-C-O	-8.61	111.36	120.40
1	A	549	ASN	N-CA-C	8.37	123.97	113.43
1	A	618	ARG	NE-CZ-NH2	-8.23	111.79	119.20
1	A	60	ARG	NE-CZ-NH2	8.00	126.40	119.20
1	A	675	VAL	N-CA-C	-7.55	105.66	111.62
1	A	754	ARG	CG-CD-NE	-7.18	96.21	112.00
1	A	382	ILE	CB-CA-C	-6.87	101.97	111.65
1	A	759	ALA	N-CA-C	6.84	118.73	111.28
1	A	795	ILE	CB-CA-C	6.50	118.16	110.68
1	A	60	ARG	NE-CZ-NH1	-6.36	115.14	121.50
1	A	761	ALA	N-CA-C	-6.34	104.28	111.07
1	A	754	ARG	NE-CZ-NH1	6.34	127.84	121.50
1	A	641	GLN	CA-C-N	-6.32	113.49	121.96
1	A	641	GLN	C-N-CA	-6.32	113.49	121.96
1	A	618	ARG	CD-NE-CZ	6.29	133.21	124.40
1	A	779	ALA	N-CA-C	6.24	119.06	111.82
1	A	746	MET	CG-SD-CE	6.20	114.55	100.90
1	A	557	GLY	N-CA-C	6.20	122.99	115.31
1	A	780	PHE	O-C-N	6.18	129.20	122.15
1	A	526	ILE	CA-C-N	-6.18	113.37	120.04
1	A	526	ILE	C-N-CA	-6.18	113.37	120.04
1	A	678	LEU	O-C-N	6.14	130.66	122.43
1	A	643	VAL	CA-C-O	-6.11	113.80	120.71
1	A	134	SER	CB-CA-C	-6.06	102.95	111.80
1	A	707	PHE	O-C-N	5.98	131.02	123.12
1	A	757	LEU	N-CA-C	-5.96	104.86	111.36
1	A	708	ALA	N-CA-C	-5.95	98.03	108.20
1	A	740	THR	CA-CB-OG1	-5.94	100.69	109.60
1	A	694	GLU	N-CA-C	-5.82	105.07	111.82
1	A	623	ALA	CA-C-N	-5.77	116.57	123.44
1	A	623	ALA	C-N-CA	-5.77	116.57	123.44
1	A	753	ASP	O-C-N	5.76	129.36	122.79
1	A	757	LEU	O-C-N	5.76	128.72	122.15
1	A	764	LEU	O-C-N	5.68	129.26	122.27
1	A	485	PHE	CB-CA-C	-5.59	102.10	110.88
1	A	30	ARG	O-C-N	5.51	127.74	122.07
1	A	546	GLN	CB-CA-C	5.49	119.26	111.74
1	A	722	ASP	N-CA-C	-5.48	105.28	112.41
1	A	723	ARG	CA-C-N	-5.46	114.33	119.90
1	A	723	ARG	C-N-CA	-5.46	114.33	119.90
1	A	803	TYR	CA-C-N	-5.42	114.23	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	803	TYR	C-N-CA	-5.42	114.23	119.87
1	A	763	LYS	CD-CE-NZ	5.37	129.08	111.90
1	A	78	ILE	N-CA-C	-5.37	105.30	110.72
1	A	495	HIS	CA-C-N	-5.36	113.51	120.91
1	A	495	HIS	C-N-CA	-5.36	113.51	120.91
1	A	732	VAL	N-CA-C	-5.36	100.66	108.17
1	A	758	GLN	N-CA-C	-5.36	105.34	111.07
1	A	534	SER	CA-CB-OG	-5.35	100.39	111.10
1	A	598	ILE	O-C-N	5.31	128.76	123.18
1	A	414	ALA	N-CA-C	-5.31	105.66	111.82
1	A	715	ASP	N-CA-C	-5.31	105.19	110.97
1	A	286	MET	CG-SD-CE	-5.25	89.36	100.90
1	A	781	ARG	N-CA-C	-5.23	105.58	111.28
1	A	227	ARG	NE-CZ-NH2	-5.19	114.53	119.20
1	A	748	ARG	O-C-N	-5.19	116.69	122.09
1	A	502	GLU	CB-CG-CD	-5.18	103.80	112.60
1	A	162	SER	N-CA-C	-5.18	105.72	111.36
1	A	113	THR	N-CA-C	-5.13	105.77	112.23
1	A	37	ILE	N-CA-C	-5.13	105.54	110.72
1	A	320	HIS	O-C-N	5.12	127.34	122.07
1	A	391	LEU	CD1-CG-CD2	5.12	122.06	110.80
1	A	76	ALA	N-CA-C	-5.09	105.62	111.07
1	A	634	ALA	CA-C-N	5.07	127.03	120.44
1	A	634	ALA	C-N-CA	5.07	127.03	120.44
1	A	165	TYR	CA-C-N	-5.04	113.82	120.22
1	A	165	TYR	C-N-CA	-5.04	113.82	120.22
1	A	455	ASP	CA-CB-CG	-5.03	107.58	112.60
1	A	121	LYS	CB-CG-CD	-5.02	99.75	111.30

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	6379	0	6085	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1	0	0	0	0
3	A	26	0	16	3	0
4	A	1	0	0	0	0
5	A	44	0	66	4	0
6	A	28	0	38	1	0
7	A	886	0	0	6	0
All	All	7365	0	6205	31	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 2.

All (31) 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:654:GLU:OE1	1:A:754:ARG:HD3	1.66	0.94
1:A:60:ARG:NH1	7:A:1398:HOH:O	2.08	0.85
1:A:654:GLU:OE1	1:A:754:ARG:CD	2.28	0.81
1:A:273:GLU:OE1	7:A:1347:HOH:O	2.02	0.77
3:A:827:TPP:HN42	3:A:827:TPP:C2	2.00	0.75
1:A:635:GLU:OE1	1:A:635:GLU:HA	1.98	0.64
1:A:231:GLU:HA	5:A:832:EDO:H12	1.81	0.62
1:A:435:PRO:HA	1:A:476:GLN:O	2.05	0.56
6:A:840:2PE:H241	7:A:1531:HOH:O	2.07	0.55
1:A:170:ASN:HD21	1:A:431:ARG:HH11	1.55	0.54
1:A:432:ILE:CD1	1:A:446:THR:HG21	2.38	0.53
3:A:827:TPP:HN42	3:A:827:TPP:H2	1.71	0.53
1:A:43:ARG:HD3	7:A:1573:HOH:O	2.09	0.52
1:A:96:GLY:HA3	1:A:153:GLU:O	2.12	0.50
1:A:645:ALA:HA	1:A:672:VAL:O	2.13	0.49
1:A:134:SER:OG	1:A:141:SER:HB3	2.15	0.46
1:A:652:THR:O	1:A:656:MET:HG2	2.16	0.45
1:A:321:GLN:HB3	7:A:1306:HOH:O	2.16	0.45
1:A:780:PHE:CD1	5:A:837:EDO:H11	2.52	0.45
1:A:702:ASP:OD1	5:A:829:EDO:O1	2.29	0.45
1:A:357:LYS:NZ	7:A:1697:HOH:O	2.49	0.45
1:A:654:GLU:OE1	1:A:754:ARG:HD2	2.11	0.44
1:A:636:ASN:HA	5:A:830:EDO:H22	2.00	0.43
1:A:763:LYS:HE2	1:A:763:LYS:HB2	1.50	0.43
1:A:498:TRP:CE2	1:A:537:LEU:HD13	2.54	0.43
1:A:748:ARG:HA	1:A:753:ASP:OD2	2.19	0.42
1:A:288:ARG:HD3	1:A:455:ASP:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:TYR:CG	1:A:136:PRO:HD2	2.54	0.42
3:A:827:TPP:C2	3:A:827:TPP:N4'	2.77	0.41
1:A:13:LEU:HD23	1:A:13:LEU:HA	1.84	0.40
1:A:434:GLY:O	1:A:475:GLU:HA	2.21	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	800/845 (95%)	774 (97%)	26 (3%)	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	677/712 (95%)	668 (99%)	9 (1%)	61	48

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ARG
1	A	147	THR

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Mol	Chain	Res	Type
1	A	189	PRO
1	A	391	LEU
1	A	561	LEU
1	A	605	LYS
1	A	635	GLU
1	A	747	VAL
1	A	754	ARG

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	79	ASN
1	A	86	GLN
1	A	105	GLN
1	A	170	ASN
1	A	253	ASN
1	A	321	GLN
1	A	441	ASN
1	A	472	GLN
1	A	549	ASN
1	A	554	GLN
1	A	574	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	$\# Z > 2$
5	EDO	A	829	-	3,3,3	0.99	0	2,2,2	0.28	0
5	EDO	A	831	-	3,3,3	0.78	0	2,2,2	0.86	0
5	EDO	A	837	-	3,3,3	0.25	0	2,2,2	0.84	0
5	EDO	A	833	-	3,3,3	0.90	0	2,2,2	1.09	0
5	EDO	A	839	-	3,3,3	0.50	0	2,2,2	0.55	0
5	EDO	A	838	-	3,3,3	0.95	0	2,2,2	0.65	0
5	EDO	A	836	-	3,3,3	0.39	0	2,2,2	0.88	0
5	EDO	A	835	-	3,3,3	0.53	0	2,2,2	1.45	0
6	2PE	A	840	-	27,27,27	2.24	13 (48%)	26,26,26	1.50	4 (15%)
5	EDO	A	830	-	3,3,3	0.70	0	2,2,2	0.26	0
5	EDO	A	834	-	3,3,3	0.25	0	2,2,2	1.24	0
5	EDO	A	832	-	3,3,3	0.58	0	2,2,2	0.83	0
3	TPP	A	827	2	26,27,27	2.69	9 (34%)	38,40,40	2.07	8 (21%)

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	EDO	A	829	-	-	0/1/1/1	-
5	EDO	A	831	-	-	1/1/1/1	-
5	EDO	A	837	-	-	0/1/1/1	-
5	EDO	A	833	-	-	0/1/1/1	-
5	EDO	A	839	-	-	0/1/1/1	-
5	EDO	A	838	-	-	0/1/1/1	-
5	EDO	A	836	-	-	0/1/1/1	-
5	EDO	A	835	-	-	0/1/1/1	-
6	2PE	A	840	-	-	13/25/25/25	-
5	EDO	A	830	-	-	0/1/1/1	-
5	EDO	A	834	-	-	1/1/1/1	-
5	EDO	A	832	-	-	1/1/1/1	-
3	TPP	A	827	2	-	5/17/17/17	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	827	TPP	C2-S1	7.33	1.91	1.69
3	A	827	TPP	C2-N3	7.07	1.49	1.32
3	A	827	TPP	C5-C4	4.35	1.44	1.35
6	A	840	2PE	O7-C6	4.16	1.60	1.42
3	A	827	TPP	C5'-C4'	3.51	1.48	1.42
6	A	840	2PE	O10-C11	3.21	1.56	1.42
6	A	840	2PE	C15-C14	3.13	1.64	1.49
6	A	840	2PE	O13-C14	3.12	1.55	1.42
3	A	827	TPP	C5-S1	-3.06	1.64	1.72
6	A	840	2PE	O10-C9	2.90	1.54	1.42
6	A	840	2PE	O7-C8	2.90	1.54	1.42
6	A	840	2PE	C12-C11	2.89	1.63	1.49
6	A	840	2PE	O19-C18	2.87	1.54	1.42
3	A	827	TPP	C2'-N1'	2.76	1.38	1.34
6	A	840	2PE	C18-C17	2.75	1.62	1.49
3	A	827	TPP	C4'-N3'	2.37	1.38	1.35
6	A	840	2PE	O4-C3	2.30	1.52	1.42
3	A	827	TPP	C7'-C5'	2.27	1.55	1.51
6	A	840	2PE	C9-C8	2.23	1.60	1.49
3	A	827	TPP	CM4-C4	2.17	1.54	1.49
6	A	840	2PE	O13-C12	2.17	1.51	1.42
6	A	840	2PE	O4-C5	2.03	1.50	1.42

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	827	TPP	S1-C2-N3	-7.02	103.41	112.30
3	A	827	TPP	N4'-C4'-N3'	4.59	123.22	117.03
3	A	827	TPP	C4-C5-S1	4.43	117.47	110.56
6	A	840	2PE	O4-C5-C6	3.69	127.18	110.35
6	A	840	2PE	O4-C3-C2	-3.15	96.24	110.11
6	A	840	2PE	C17-O16-C15	2.82	125.59	113.26
6	A	840	2PE	O10-C11-C12	-2.72	97.96	110.35
3	A	827	TPP	C7-C6-C5	-2.62	104.51	112.73
3	A	827	TPP	C5'-C4'-N4'	-2.61	118.63	122.14
3	A	827	TPP	C5'-C4'-N3'	-2.33	117.89	121.31
3	A	827	TPP	O7-C7-C6	-2.07	100.30	108.63
3	A	827	TPP	C2-N3-C4	2.03	116.80	114.06

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	840	2PE	O19-C20-C21-O22
6	A	840	2PE	O4-C5-C6-O7
6	A	840	2PE	C11-C12-O13-C14
6	A	840	2PE	O7-C8-C9-O10
3	A	827	TPP	C4'-C5'-C7'-N3
3	A	827	TPP	C6'-C5'-C7'-N3
6	A	840	2PE	O13-C14-C15-O16
6	A	840	2PE	C14-C15-O16-C17
6	A	840	2PE	C2-C3-O4-C5
6	A	840	2PE	O25-C26-C27-O28
6	A	840	2PE	O10-C11-C12-O13
6	A	840	2PE	C6-C5-O4-C3
5	A	831	EDO	O1-C1-C2-O2
6	A	840	2PE	C20-C21-O22-C23
3	A	827	TPP	PA-O3A-PB-O1B
3	A	827	TPP	PA-O3A-PB-O2B
3	A	827	TPP	PA-O3A-PB-O3B
5	A	832	EDO	O1-C1-C2-O2
5	A	834	EDO	O1-C1-C2-O2
6	A	840	2PE	C9-C8-O7-C6
6	A	840	2PE	C27-C26-O25-C24

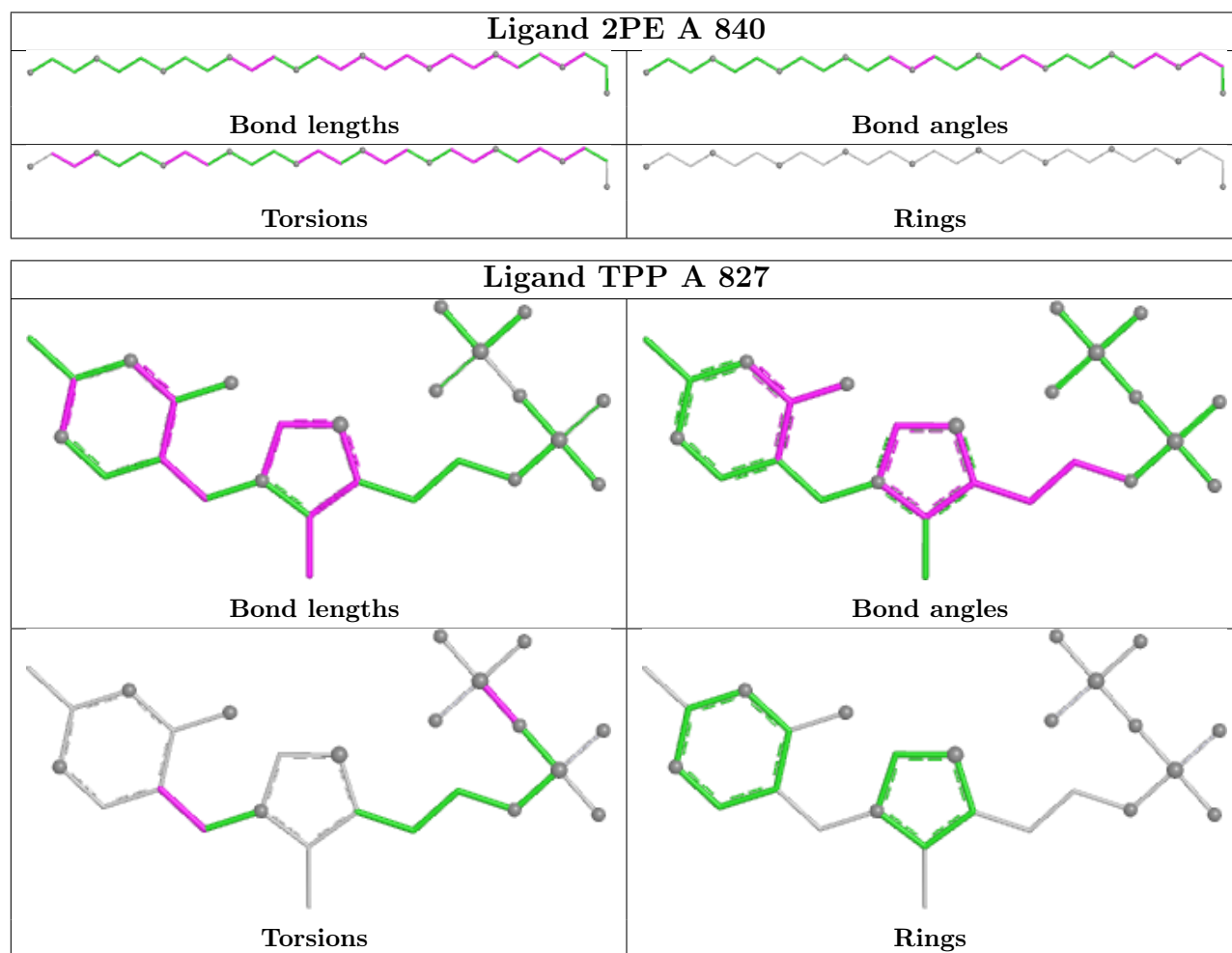
There are no ring outliers.

6 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	829	EDO	1	0
5	A	837	EDO	1	0
6	A	840	2PE	1	0
5	A	830	EDO	1	0
5	A	832	EDO	1	0
3	A	827	TPP	3	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 [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	802/845 (94%)	-0.48	4 (0%) 87 89	11, 17, 28, 46	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	ASP	2.7
1	A	5	VAL	2.6
1	A	635	GLU	2.3
1	A	806	VAL	2.1

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(Å ²)	Q<0.9
6	2PE	A	840	28/28	0.64	0.24	23,39,53,53	0
5	EDO	A	831	4/4	0.82	0.21	36,43,50,53	0
5	EDO	A	836	4/4	0.89	0.13	32,38,39,41	0

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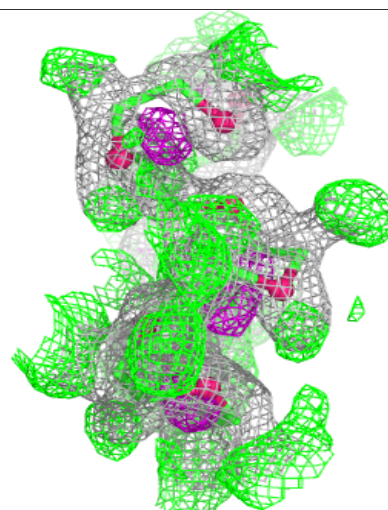
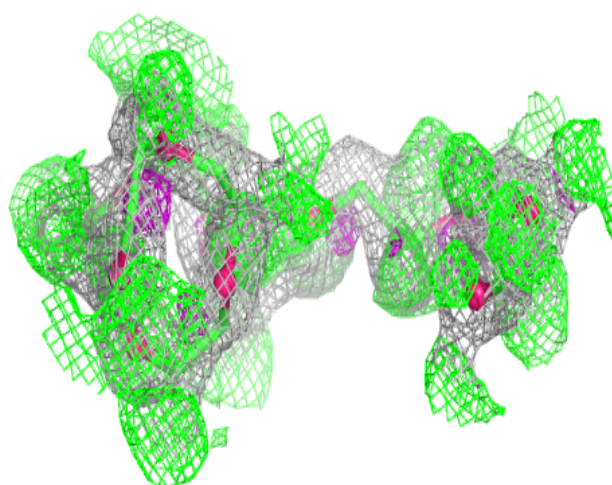
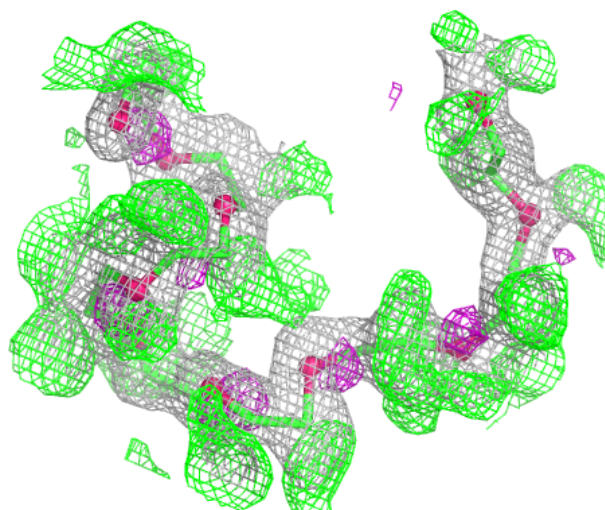
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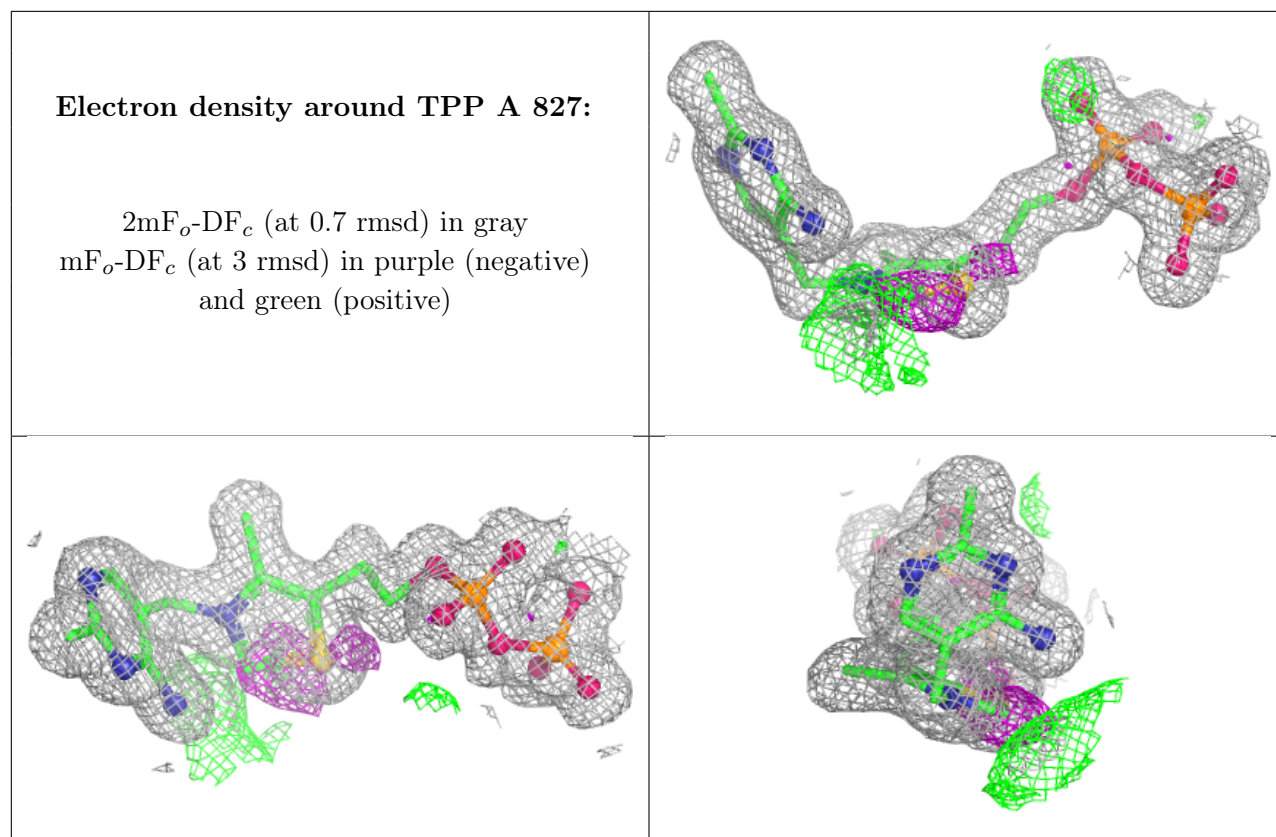
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	A	830	4/4	0.91	0.12	41,42,45,46	0
5	EDO	A	837	4/4	0.91	0.14	30,33,37,37	0
5	EDO	A	832	4/4	0.91	0.13	37,42,42,43	0
5	EDO	A	835	4/4	0.92	0.12	27,28,33,38	0
5	EDO	A	829	4/4	0.93	0.11	26,28,30,33	0
4	NA	A	828	1/1	0.93	0.12	32,32,32,32	1
5	EDO	A	833	4/4	0.94	0.10	25,27,28,33	0
5	EDO	A	834	4/4	0.94	0.11	25,30,32,32	0
5	EDO	A	839	4/4	0.97	0.08	23,23,25,26	0
5	EDO	A	838	4/4	0.98	0.05	14,15,17,19	0
3	TPP	A	827	26/26	0.99	0.04	11,15,20,34	0
2	MG	A	826	1/1	0.99	0.02	13,13,13,13	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 2PE A 840:

$2mF_o-DF_c$ (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.