



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2025 – 10:07 AM EDT

PDB ID : 9MSA / pdb_00009msa
Title : Alpha-ketoisovalerate decarboxylase (Kivd) from Synechocystis sp. PCC 6803
with substitution S286T
Authors : Begum, A.; Xie, H.; Gunn, L.H.
Deposited on : 2025-01-09
Resolution : 2.79 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

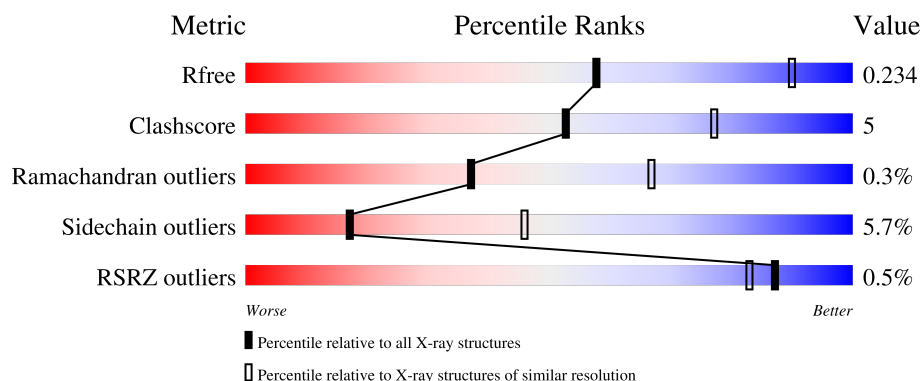
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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}	164625	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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	548	<div> <div style="width: 84%;"></div> <div style="width: 15%;"></div> <div style="width: 1%;"></div> </div> 84% 15% ..
1	B	548	<div> <div style="width: 84%;"></div> <div style="width: 13%;"></div> <div style="width: 3%;"></div> </div> 84% 13% ..
1	C	548	<div> <div style="width: 78%;"></div> <div style="width: 12%;"></div> <div style="width: 9%;"></div> <div style="width: 1%;"></div> </div> 78% 12% • 9%
1	D	548	<div> <div style="width: 77%;"></div> <div style="width: 13%;"></div> <div style="width: 9%;"></div> <div style="width: 1%;"></div> </div> 77% 13% • 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16412 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.

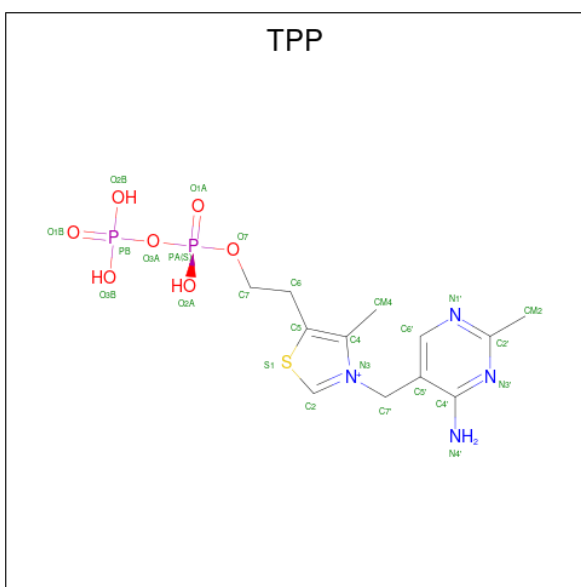
- Molecule 1 is a protein called Alpha-ketoisovalerate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	500	Total	C	N	O	S	0	0	0
			3909	2505	642	751	11			
1	D	500	Total	C	N	O	S	0	0	0
			3916	2508	644	753	11			
1	A	545	Total	C	N	O	S	0	2	0
			4258	2717	704	825	12			
1	B	542	Total	C	N	O	S	0	0	0
			4237	2709	699	817	12			

There are 4 discrepancies between the modelled and reference sequences:

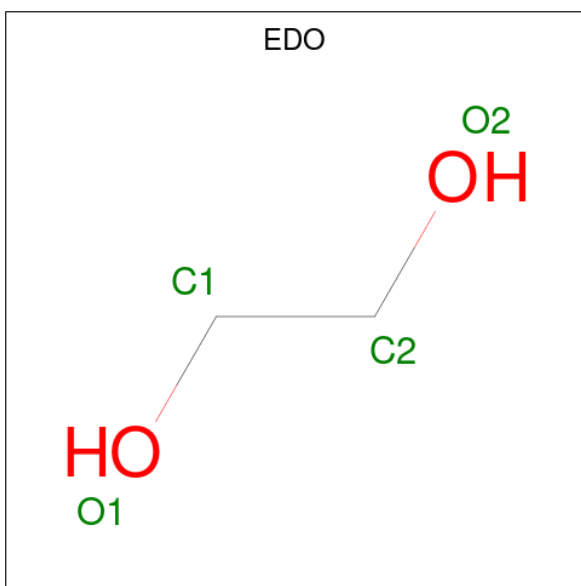
Chain	Residue	Modelled	Actual	Comment	Reference
C	286	THR	SER	engineered mutation	UNP Q684J7
D	286	THR	SER	engineered mutation	UNP Q684J7
A	286	THR	SER	engineered mutation	UNP Q684J7
B	286	THR	SER	engineered mutation	UNP Q684J7

- Molecule 2 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
2	A	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	B	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).



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

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0

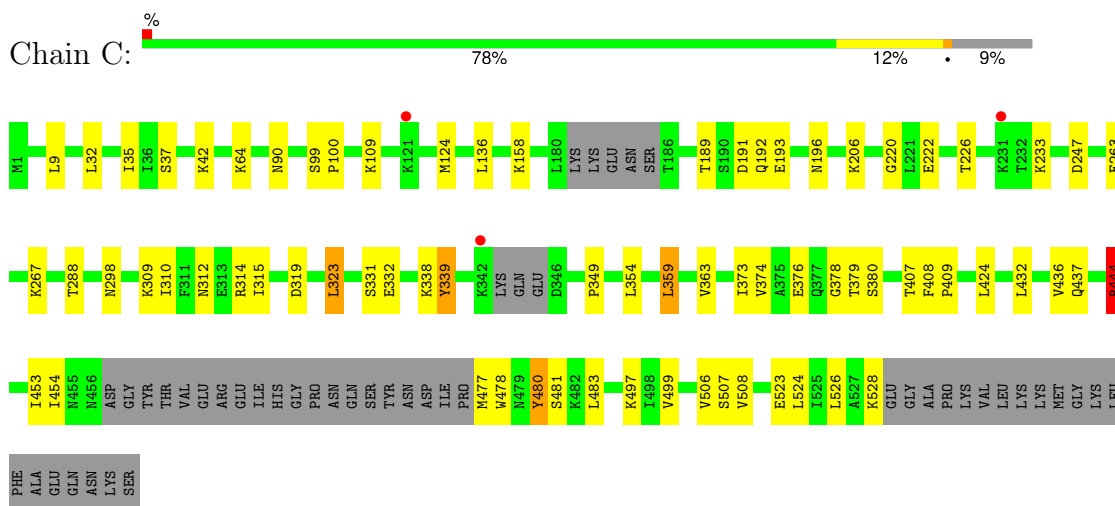
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total 1	O 1	0	0
5	D	2	Total 2	O 2	0	0
5	A	18	Total 19	O 19	0	1
5	B	8	Total 8	O 8	0	0

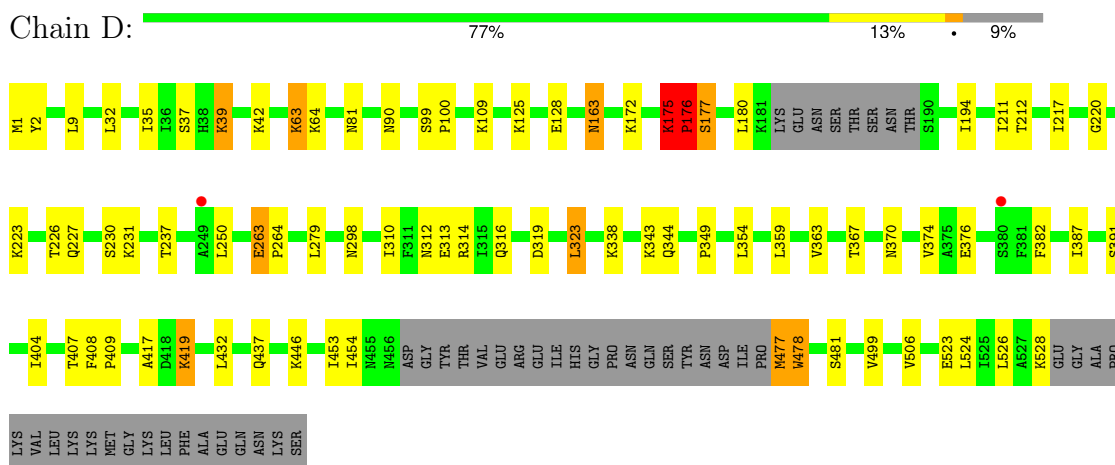
3 Residue-property plots

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 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.

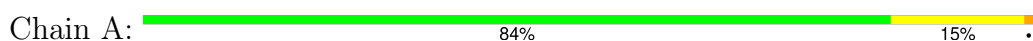
- Molecule 1: Alpha-ketoisovalerate decarboxylase

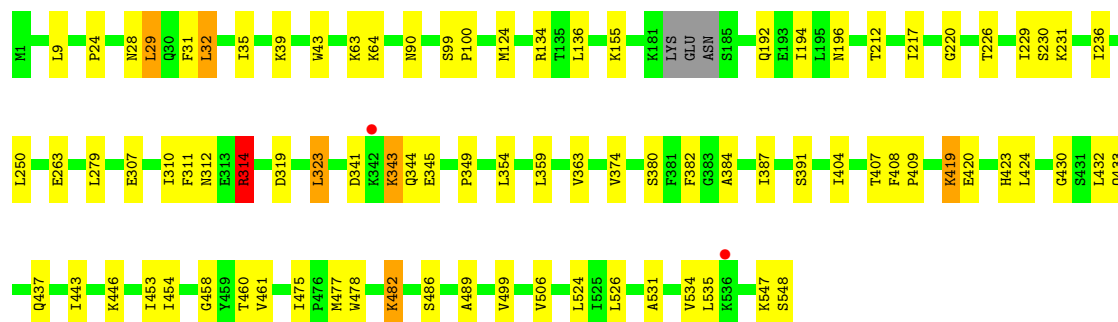


- Molecule 1: Alpha-ketoisovalerate decarboxylase

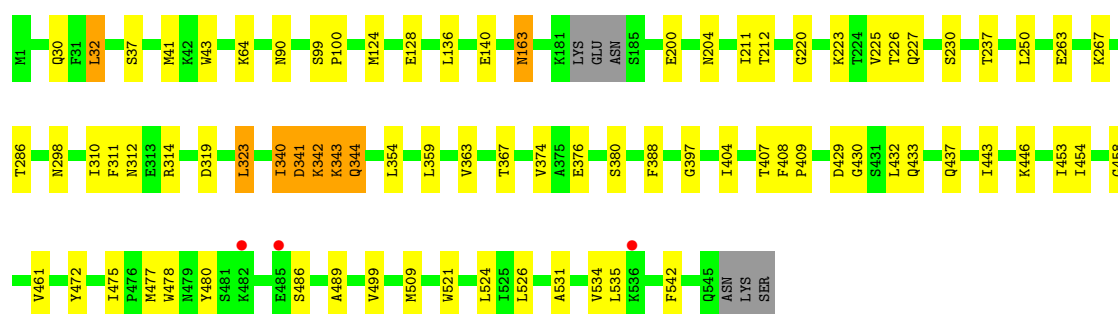
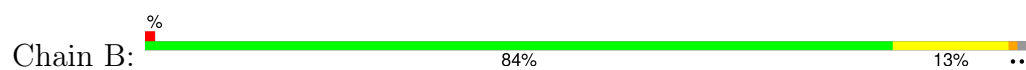


- Molecule 1: Alpha-ketoisovalerate decarboxylase





● Molecule 1: Alpha-ketoisovalerate decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	218.47Å 81.73Å 124.98Å 90.00° 105.52° 90.00°	Depositor
Resolution (Å)	40.00 – 2.79 40.00 – 2.79	Depositor EDS
% Data completeness (in resolution range)	99.7 (40.00-2.79) 99.7 (40.00-2.79)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0430	Depositor
R, R_{free}	0.189 , 0.234 0.189 , 0.234	Depositor DCC
R_{free} test set	2656 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	78.5	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 63.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16412	wwPDB-VP
Average B, all atoms (Å ²)	86.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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, MG, 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	0.53	0/4342	1.15	6/5880 (0.1%)
1	B	0.53	0/4321	1.13	4/5848 (0.1%)
1	C	0.51	0/3984	1.13	7/5390 (0.1%)
1	D	0.51	0/3992	1.15	7/5400 (0.1%)
All	All	0.52	0/16639	1.14	24/22518 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	C	0	1
All	All	0	3

There are no bond length outliers.

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	288	THR	N-CA-C	-9.02	96.96	109.95
1	A	29	LEU	N-CA-C	-8.12	100.13	110.19
1	C	339	TYR	N-CA-CB	8.01	124.02	110.49
1	D	81	ASN	CA-C-N	-7.45	106.81	121.41
1	D	81	ASN	C-N-CA	-7.45	106.81	121.41
1	D	176	PRO	CB-CA-C	6.88	122.92	111.56
1	A	155	LYS	CB-CG-CD	6.20	125.57	111.30
1	A	263	GLU	CB-CA-C	6.01	118.69	109.50
1	C	480	TYR	N-CA-CB	5.84	120.08	110.39
1	B	263	GLU	CB-CA-C	5.79	118.71	109.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	263	GLU	CB-CA-C	5.79	118.70	109.62
1	B	140	GLU	CB-CG-CD	5.75	122.38	112.60
1	D	109	LYS	CB-CG-CD	5.69	124.39	111.30
1	C	263	GLU	CB-CA-C	5.56	118.34	109.62
1	A	29	LEU	CA-C-O	-5.46	116.28	122.01
1	B	397	GLY	CA-C-N	-5.46	116.78	122.89
1	B	397	GLY	C-N-CA	-5.46	116.78	122.89
1	A	482	LYS	CB-CG-CD	5.42	123.77	111.30
1	D	175	LYS	CB-CA-C	5.41	119.53	109.51
1	C	158	LYS	CG-CD-CE	5.37	123.65	111.30
1	C	444	ARG	CD-NE-CZ	5.37	131.91	124.40
1	D	81	ASN	N-CA-C	-5.25	102.50	110.28
1	C	191	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	547	LYS	CB-CA-C	-5.09	102.63	110.26

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	134	ARG	Sidechain
1	A	314	ARG	Sidechain
1	C	444	ARG	Sidechain

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	4258	0	4205	47	0
1	B	4237	0	4217	49	0
1	C	3909	0	3906	28	0
1	D	3916	0	3914	36	0
2	A	26	0	16	4	0
2	B	26	0	16	4	0
3	A	4	0	6	0	0
3	B	4	0	6	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	19	0	0	0	0
5	B	8	0	0	2	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
All	All	16412	0	16286	161	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 (161) 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:D:1:MET:HE2	1:D:172:LYS:HE2	1.39	1.02
1:D:63:LYS:HE2	1:D:417:ALA:O	1.71	0.89
1:B:340:ILE:HG13	1:B:341:ASP:H	1.39	0.85
1:C:436:VAL:HG11	1:C:478:TRP:HH2	1.45	0.82
1:C:226:THR:HG22	1:C:247:ASP:H	1.45	0.80
1:B:286:THR:HG22	1:B:542:PHE:HZ	1.46	0.79
1:B:124:MET:HE1	1:B:136:LEU:HB2	1.68	0.76
1:B:286:THR:HG22	1:B:542:PHE:CZ	2.23	0.74
1:A:64:LYS:HE3	1:A:217:ILE:O	1.89	0.71
1:D:64:LYS:HE3	1:D:217:ILE:O	1.90	0.70
1:C:378:GLY:O	1:C:380:SER:N	2.23	0.70
1:C:124:MET:HE1	1:C:136:LEU:HB2	1.73	0.69
1:C:436:VAL:HG11	1:C:478:TRP:CH2	2.28	0.68
2:A:601:TPP:HN42	2:A:601:TPP:H2	1.57	0.68
1:B:340:ILE:HG13	1:B:341:ASP:N	2.09	0.68
2:B:601:TPP:HN42	2:B:601:TPP:H2	1.59	0.68
1:D:163:ASN:C	1:D:163:ASN:HD22	2.02	0.67
1:B:286:THR:CG2	1:B:542:PHE:HZ	2.10	0.65
1:B:163:ASN:HD22	1:B:163:ASN:C	2.04	0.65
1:D:2:TYR:HB3	1:D:175:LYS:HD3	1.78	0.64
1:B:408:PHE:HB3	1:B:409:PRO:HD3	1.79	0.64
1:C:432:LEU:HD22	1:C:453:ILE:HG12	1.79	0.64
1:D:432:LEU:HD22	1:D:453:ILE:HG12	1.79	0.64
1:C:331:SER:O	1:C:332:GLU:HG2	1.97	0.64
1:D:408:PHE:HB3	1:D:409:PRO:HD3	1.80	0.64
1:D:64:LYS:HE2	1:D:220:GLY:HA2	1.78	0.64
1:A:64:LYS:HE2	1:A:220:GLY:HA2	1.80	0.63
1:C:408:PHE:HB3	1:C:409:PRO:HD3	1.80	0.63
1:A:408:PHE:HB3	1:A:409:PRO:HD3	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:222:GLU:O	1:C:226:THR:HG23	2.00	0.62
1:C:64:LYS:HE3	1:C:220:GLY:HA2	1.81	0.60
1:B:64:LYS:HE3	1:B:220:GLY:HA2	1.82	0.60
1:A:486:SER:OG	1:B:486:SER:OG	2.20	0.59
1:C:332:GLU:O	1:C:332:GLU:HG3	2.02	0.59
1:B:41:MET:O	5:B:701:HOH:O	2.17	0.58
1:A:419:LYS:HD2	1:A:420:GLU:HG3	1.85	0.58
1:D:176:PRO:O	1:D:177:SER:OG	2.19	0.58
1:D:2:TYR:CB	1:D:175:LYS:HD3	2.34	0.57
1:A:461:VAL:HG23	1:A:535:LEU:HD11	1.86	0.57
2:A:601:TPP:HN42	2:A:601:TPP:C2	2.16	0.57
1:B:454:ILE:O	5:B:702:HOH:O	2.17	0.57
1:B:200:GLU:HA	1:B:200:GLU:OE1	2.06	0.56
1:B:298:ASN:OD1	1:B:312:ASN:ND2	2.39	0.56
1:D:419:LYS:HZ3	1:D:419:LYS:H	1.54	0.56
1:A:433:GLN:NE2	1:A:475:ILE:HD12	2.21	0.56
1:D:298:ASN:OD1	1:D:312:ASN:ND2	2.39	0.55
1:C:497:LYS:HE3	1:C:508:VAL:HG22	1.88	0.55
1:B:204:ASN:HB2	3:B:602:EDO:H12	1.89	0.55
1:B:433:GLN:NE2	1:B:475:ILE:HD12	2.21	0.54
1:C:298:ASN:OD1	1:C:312:ASN:ND2	2.41	0.54
2:B:601:TPP:HN42	2:B:601:TPP:C2	2.20	0.53
1:A:548:SER:HB3	1:B:30:GLN:HE22	1.75	0.52
1:D:454:ILE:HG23	1:D:526:LEU:HD23	1.92	0.52
1:B:458:GLY:HA2	1:B:475:ILE:HG12	1.92	0.52
1:C:454:ILE:HG23	1:C:526:LEU:HD23	1.91	0.52
1:D:64:LYS:HE2	1:D:220:GLY:CA	2.40	0.51
1:D:64:LYS:CE	1:D:220:GLY:HA2	2.40	0.51
1:A:341:ASP:HB3	1:A:343:LYS:HE3	1.91	0.51
1:D:481:SER:OG	1:D:523:GLU:OE1	2.27	0.50
1:B:433:GLN:HG2	1:B:478:TRP:CH2	2.46	0.50
1:A:384:ALA:HA	1:A:387:ILE:HD12	1.93	0.50
1:A:64:LYS:HE2	1:A:220:GLY:CA	2.41	0.50
1:C:332:GLU:O	1:C:332:GLU:CG	2.60	0.50
1:A:380:SER:OG	1:A:454:ILE:HD12	2.12	0.50
1:B:454:ILE:HG23	1:B:526:LEU:HD23	1.92	0.50
1:B:163:ASN:C	1:B:163:ASN:ND2	2.70	0.49
1:A:433:GLN:HG2	1:A:478:TRP:CH2	2.47	0.49
1:A:28:ASN:C	1:A:29:LEU:O	2.53	0.49
1:A:454:ILE:HG23	1:A:526:LEU:HD23	1.95	0.49
1:B:380:SER:OG	1:B:454:ILE:HD12	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:GLY:HA2	1:B:475:ILE:HD13	1.95	0.48
1:C:481:SER:OG	1:C:523:GLU:OE1	2.29	0.48
1:B:343:LYS:HB3	1:B:343:LYS:HE2	1.59	0.48
1:B:344:GLN:HE21	1:B:344:GLN:HB3	1.52	0.48
1:A:404:ILE:HG12	2:A:601:TPP:C2'	2.44	0.48
1:A:458:GLY:HA2	1:A:475:ILE:HG12	1.95	0.48
1:D:63:LYS:HD3	1:D:63:LYS:HA	1.63	0.47
1:D:9:LEU:HD21	1:D:35:ILE:HG12	1.96	0.47
1:B:359:LEU:O	1:B:363:VAL:HG23	2.15	0.47
1:D:478:TRP:H	1:D:478:TRP:HE3	1.62	0.47
1:B:461:VAL:HG23	1:B:535:LEU:HD11	1.97	0.47
1:C:359:LEU:O	1:C:363:VAL:HG23	2.14	0.47
1:D:359:LEU:O	1:D:363:VAL:HG23	2.15	0.47
1:D:499:VAL:HB	1:D:524:LEU:HD23	1.97	0.47
1:A:359:LEU:O	1:A:363:VAL:HG23	2.15	0.47
1:B:499:VAL:HB	1:B:524:LEU:HD23	1.97	0.46
1:A:29:LEU:O	1:A:31:PHE:N	2.48	0.46
1:A:430:GLY:HA2	1:A:475:ILE:HD13	1.98	0.46
1:D:39:LYS:HD3	1:D:39:LYS:H	1.80	0.46
1:A:124:MET:HE1	1:A:136:LEU:HB2	1.96	0.46
1:A:374:VAL:HG12	1:A:407:THR:HB	1.97	0.46
1:B:404:ILE:HG12	2:B:601:TPP:C2'	2.46	0.46
1:B:374:VAL:HG12	1:B:407:THR:HB	1.98	0.46
1:D:163:ASN:C	1:D:163:ASN:ND2	2.68	0.46
1:D:99:SER:HB2	1:D:100:PRO:HD2	1.97	0.46
1:D:194:ILE:HG12	1:D:310:ILE:HD11	1.98	0.46
1:D:477:MET:HA	1:D:477:MET:HE2	1.96	0.45
1:C:374:VAL:HG12	1:C:407:THR:HB	1.97	0.45
1:C:499:VAL:HB	1:C:524:LEU:HD23	1.99	0.45
1:A:64:LYS:CE	1:A:220:GLY:HA2	2.45	0.45
1:B:342:LYS:HD3	1:B:388:PHE:CE2	2.52	0.45
1:D:263:GLU:HA	1:D:264:PRO:HD3	1.93	0.44
1:B:99:SER:HB2	1:B:100:PRO:HD2	1.99	0.44
1:B:226:THR:HG23	1:B:250:LEU:HD11	1.99	0.44
1:B:342:LYS:HD2	1:B:342:LYS:HA	1.78	0.44
1:A:29:LEU:HD22	1:B:472:TYR:CE1	2.53	0.44
1:C:99:SER:HB2	1:C:100:PRO:HD2	1.99	0.44
1:A:314:ARG:CB	1:A:314:ARG:CZ	2.96	0.44
1:B:32:LEU:HD21	1:B:43:TRP:CD2	2.53	0.44
1:C:478:TRP:CH2	1:C:483:LEU:HD11	2.52	0.43
1:D:226:THR:HG23	1:D:250:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:SER:HB2	1:A:100:PRO:HD2	2.00	0.43
1:D:223:LYS:HB2	1:D:223:LYS:HE2	1.67	0.43
1:A:32:LEU:HD21	1:A:43:TRP:CD2	2.53	0.43
1:A:343:LYS:HB3	1:A:343:LYS:HE2	1.70	0.43
1:B:531:ALA:HB1	1:B:535:LEU:HD23	2.01	0.43
1:C:9:LEU:HD21	1:C:35:ILE:HG12	2.01	0.43
1:D:374:VAL:HG12	1:D:407:THR:HB	2.01	0.43
1:B:343:LYS:HD2	1:B:343:LYS:H	1.82	0.43
1:A:499:VAL:HB	1:A:524:LEU:HD23	2.00	0.43
2:A:601:TPP:C2	2:A:601:TPP:N4'	2.80	0.43
1:D:376:GLU:HA	1:D:407:THR:HG21	2.00	0.43
1:C:373:ILE:HD13	1:C:424:LEU:HB2	2.01	0.42
1:A:432:LEU:HD22	1:A:453:ILE:HG12	2.01	0.42
1:D:319:ASP:O	1:D:323:LEU:HB2	2.20	0.42
1:A:319:ASP:O	1:A:323:LEU:HB2	2.20	0.42
1:B:453:ILE:HD11	1:B:521:TRP:CE2	2.54	0.42
1:B:319:ASP:O	1:B:323:LEU:HB2	2.20	0.42
1:A:192:GLN:O	1:A:196:ASN:OD1	2.37	0.42
1:A:531:ALA:HB1	1:A:535:LEU:HD23	2.01	0.42
1:A:548:SER:CB	1:B:30:GLN:HE22	2.32	0.42
1:A:226:THR:HG23	1:A:250:LEU:HD11	2.01	0.42
1:A:433:GLN:HA	1:A:478:TRP:CH2	2.55	0.42
1:A:443:ILE:HD13	1:A:489:ALA:HB2	2.02	0.42
1:D:176:PRO:O	1:D:177:SER:CB	2.68	0.42
1:C:444:ARG:HE	1:C:444:ARG:HB3	1.52	0.41
1:A:443:ILE:CD1	1:A:489:ALA:HB2	2.50	0.41
1:B:443:ILE:HD13	1:B:489:ALA:HB2	2.01	0.41
1:C:319:ASP:O	1:C:323:LEU:HB2	2.20	0.41
1:D:212:THR:HG22	1:D:279:LEU:HB2	2.03	0.41
1:A:194:ILE:HG12	1:A:310:ILE:HD11	2.00	0.41
1:B:311:PHE:O	1:B:312:ASN:HB2	2.20	0.41
1:A:229:ILE:HG13	1:A:236:ILE:HD12	2.02	0.41
1:A:311:PHE:O	1:A:312:ASN:HB2	2.20	0.41
1:B:376:GLU:HA	1:B:407:THR:HG21	2.02	0.41
1:A:349:PRO:HG3	1:A:506:VAL:HG21	2.01	0.41
1:C:349:PRO:HG3	1:C:506:VAL:HG21	2.03	0.41
1:C:376:GLU:HA	1:C:407:THR:HG21	2.03	0.41
1:B:212:THR:HG21	1:B:225:VAL:HG11	2.03	0.41
1:D:349:PRO:HG3	1:D:506:VAL:HG21	2.03	0.41
1:D:211:ILE:HA	1:D:237:THR:O	2.21	0.41
1:A:212:THR:HG22	1:A:279:LEU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:432:LEU:HD22	1:B:453:ILE:HG12	2.02	0.41
1:B:443:ILE:CD1	1:B:489:ALA:HB2	2.51	0.41
1:B:429:ASP:HB2	1:B:480:TYR:OH	2.21	0.41
1:A:9:LEU:HD21	1:A:35:ILE:HG12	2.03	0.40
1:A:382:PHE:CD2	1:A:535:LEU:HD13	2.56	0.40
1:A:423:HIS:C	1:A:424:LEU:HD12	2.46	0.40
1:B:211:ILE:HA	1:B:237:THR:O	2.21	0.40
1:C:192:GLN:O	1:C:196:ASN:OD1	2.39	0.40
1:A:24:PRO:O	2:B:601:TPP:H7'1	2.22	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	543/548 (99%)	524 (96%)	18 (3%)	1 (0%)	44	73
1	B	538/548 (98%)	517 (96%)	20 (4%)	1 (0%)	44	73
1	C	492/548 (90%)	475 (96%)	15 (3%)	2 (0%)	30	61
1	D	494/548 (90%)	477 (97%)	15 (3%)	2 (0%)	30	61
All	All	2067/2192 (94%)	1993 (96%)	68 (3%)	6 (0%)	37	67

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	379	THR
1	D	176	PRO
1	C	339	TYR
1	D	177	SER
1	A	343	LYS
1	B	340	ILE

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	463/474 (98%)	443 (96%)	20 (4%)	25	57
1	B	463/474 (98%)	440 (95%)	23 (5%)	20	51
1	C	429/474 (90%)	406 (95%)	23 (5%)	18	48
1	D	430/474 (91%)	395 (92%)	35 (8%)	9	29
All	All	1785/1896 (94%)	1684 (94%)	101 (6%)	17	46

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	32	LEU
1	C	37	SER
1	C	42	LYS
1	C	90	ASN
1	C	109	LYS
1	C	189	THR
1	C	193	GLU
1	C	206	LYS
1	C	233	LYS
1	C	267	LYS
1	C	309	LYS
1	C	310	ILE
1	C	314	ARG
1	C	315	ILE
1	C	323	LEU
1	C	338	LYS
1	C	354	LEU
1	C	359	LEU
1	C	437	GLN
1	C	477	MET
1	C	480	TYR
1	C	507	SER
1	C	528	LYS
1	D	32	LEU

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Mol	Chain	Res	Type
1	D	37	SER
1	D	39	LYS
1	D	42	LYS
1	D	63	LYS
1	D	90	ASN
1	D	125	LYS
1	D	128	GLU
1	D	163	ASN
1	D	175	LYS
1	D	176	PRO
1	D	180	LEU
1	D	227	GLN
1	D	230	SER
1	D	231	LYS
1	D	313	GLU
1	D	314	ARG
1	D	316	GLN
1	D	323	LEU
1	D	338	LYS
1	D	343	LYS
1	D	344	GLN
1	D	354	LEU
1	D	367	THR
1	D	370	ASN
1	D	382	PHE
1	D	387	ILE
1	D	391	SER
1	D	404	ILE
1	D	419	LYS
1	D	437	GLN
1	D	446	LYS
1	D	477	MET
1	D	478	TRP
1	D	528	LYS
1	A	32	LEU
1	A	39	LYS
1	A	63	LYS
1	A	90	ASN
1	A	230	SER
1	A	231	LYS
1	A	307	GLU
1	A	314	ARG

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Mol	Chain	Res	Type
1	A	323	LEU
1	A	344	GLN
1	A	345	GLU
1	A	354	LEU
1	A	391	SER
1	A	419	LYS
1	A	437	GLN
1	A	446	LYS
1	A	460	THR
1	A	477	MET
1	A	482	LYS
1	A	534	VAL
1	B	32	LEU
1	B	37	SER
1	B	90	ASN
1	B	128	GLU
1	B	163	ASN
1	B	223	LYS
1	B	227	GLN
1	B	230	SER
1	B	267	LYS
1	B	310	ILE
1	B	314	ARG
1	B	323	LEU
1	B	341	ASP
1	B	342	LYS
1	B	343	LYS
1	B	344	GLN
1	B	354	LEU
1	B	367	THR
1	B	437	GLN
1	B	446	LYS
1	B	477	MET
1	B	509	MET
1	B	534	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	30	GLN
1	C	34	GLN
1	C	370	ASN

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Mol	Chain	Res	Type
1	C	437	GLN
1	C	479	ASN
1	D	34	GLN
1	D	163	ASN
1	D	196	ASN
1	D	437	GLN
1	D	479	ASN
1	A	34	GLN
1	A	192	GLN
1	A	196	ASN
1	A	312	ASN
1	A	437	GLN
1	B	30	GLN
1	B	163	ASN
1	B	192	GLN
1	B	344	GLN
1	B	437	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 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
3	EDO	A	602	-	3,3,3	0.25	0	2,2,2	0.34	0
2	TPP	A	601	4	23,27,27	1.07	2 (8%)	30,40,40	1.00	1 (3%)
3	EDO	B	602	-	3,3,3	0.25	0	2,2,2	0.46	0
2	TPP	B	601	4	23,27,27	1.08	2 (8%)	30,40,40	0.99	1 (3%)

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	EDO	A	602	-	-	1/1/1/1	-
2	TPP	A	601	4	-	4/16/17/17	0/2/2/2
3	EDO	B	602	-	-	1/1/1/1	-
2	TPP	B	601	4	-	6/16/17/17	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	TPP	C6-C5	-3.69	1.48	1.51
2	B	601	TPP	C6-C5	-3.36	1.49	1.51
2	B	601	TPP	C4-N3	2.62	1.42	1.39
2	A	601	TPP	C4-N3	2.40	1.41	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	TPP	C5-C4-N3	3.26	114.09	107.57
2	A	601	TPP	C5-C4-N3	2.68	112.93	107.57

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	TPP	C4-C5-C6-C7
2	A	601	TPP	PA-O3A-PB-O3B
2	B	601	TPP	C7-O7-PA-O1A
2	B	601	TPP	C7-O7-PA-O3A
2	B	601	TPP	PA-O3A-PB-O2B
2	B	601	TPP	C7-O7-PA-O2A

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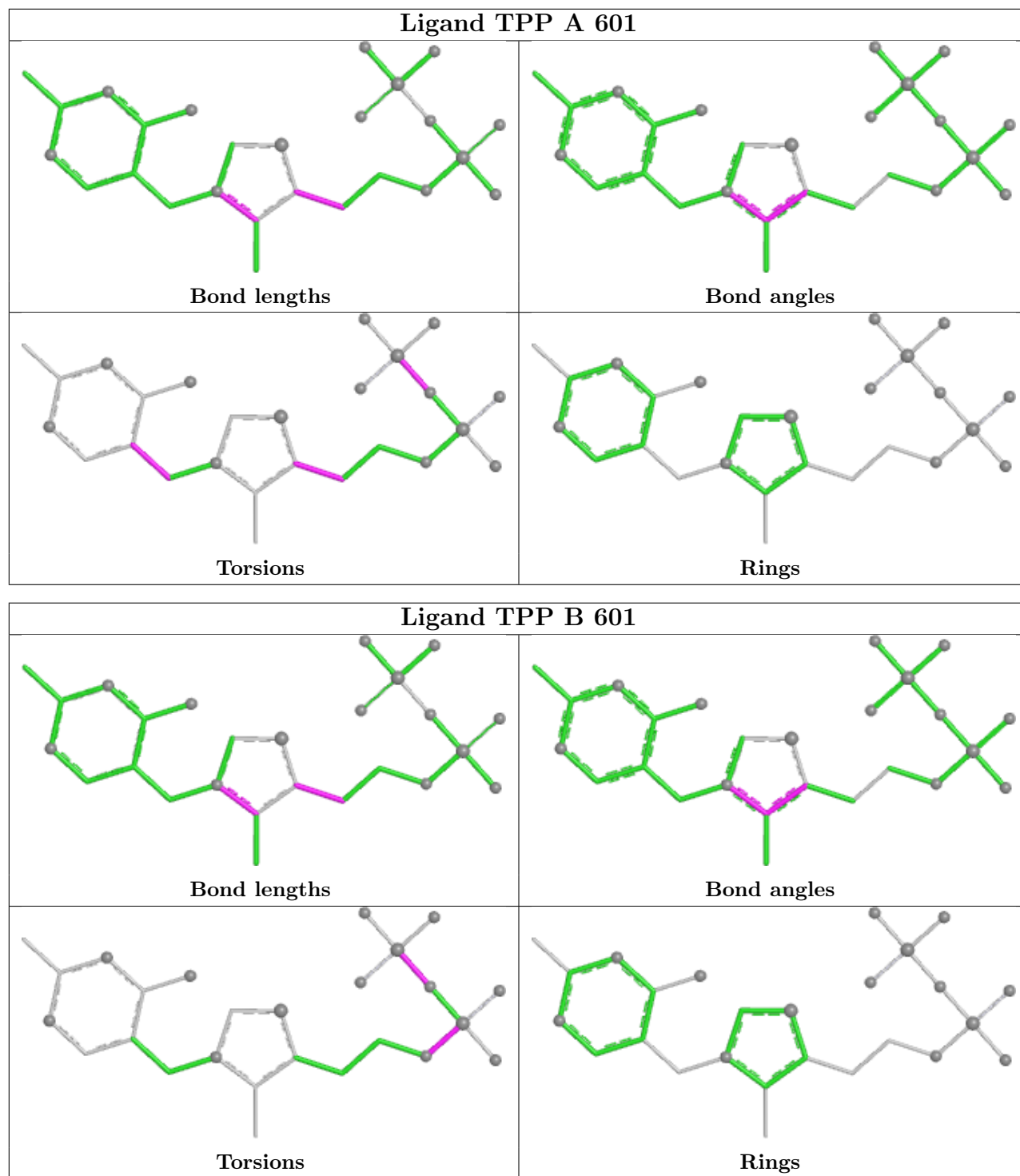
Mol	Chain	Res	Type	Atoms
3	A	602	EDO	O1-C1-C2-O2
2	A	601	TPP	C4'-C5'-C7'-N3
2	B	601	TPP	PA-O3A-PB-O3B
3	B	602	EDO	O1-C1-C2-O2
2	A	601	TPP	PA-O3A-PB-O1B
2	B	601	TPP	PA-O3A-PB-O1B

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	TPP	4	0
3	B	602	EDO	1	0
2	B	601	TPP	4	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 ⓘ

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	545/548 (99%)	-0.78	2 (0%) 89 85	34, 71, 111, 162	11 (2%)
1	B	542/548 (98%)	-0.85	3 (0%) 85 81	42, 69, 103, 134	5 (0%)
1	C	500/548 (91%)	-0.47	3 (0%) 85 81	49, 89, 136, 173	20 (4%)
1	D	500/548 (91%)	-0.40	2 (0%) 89 85	67, 98, 145, 190	1 (0%)
All	All	2087/2192 (95%)	-0.63	10 (0%) 87 83	34, 81, 131, 190	37 (1%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	342	LYS	4.7
1	B	536	LYS	3.9
1	B	482	LYS	3.4
1	A	342	LYS	2.7
1	C	121	LYS	2.5
1	D	380	SER	2.4
1	C	231	LYS	2.4
1	B	485	GLU	2.3
1	D	249	ALA	2.1
1	A	536	LYS	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](#)

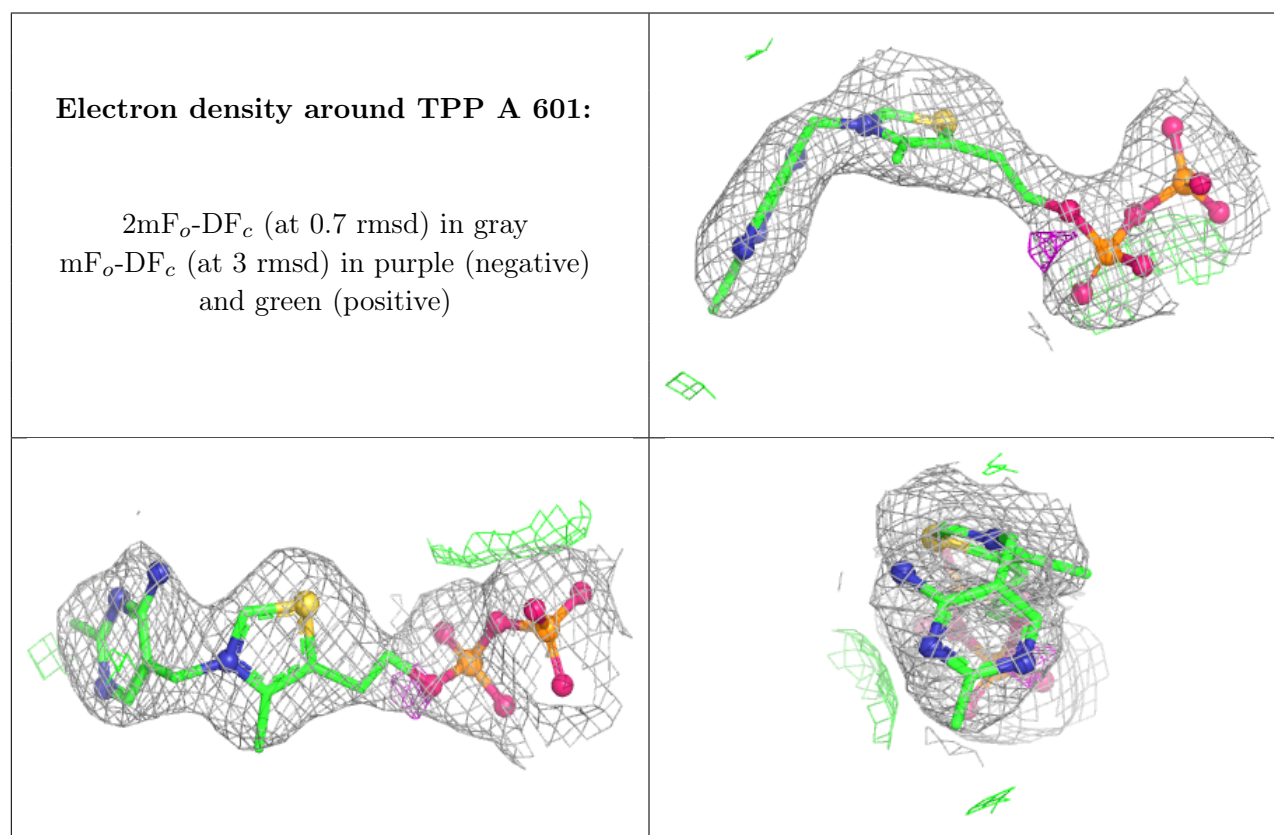
There are no oligosaccharides in this entry.

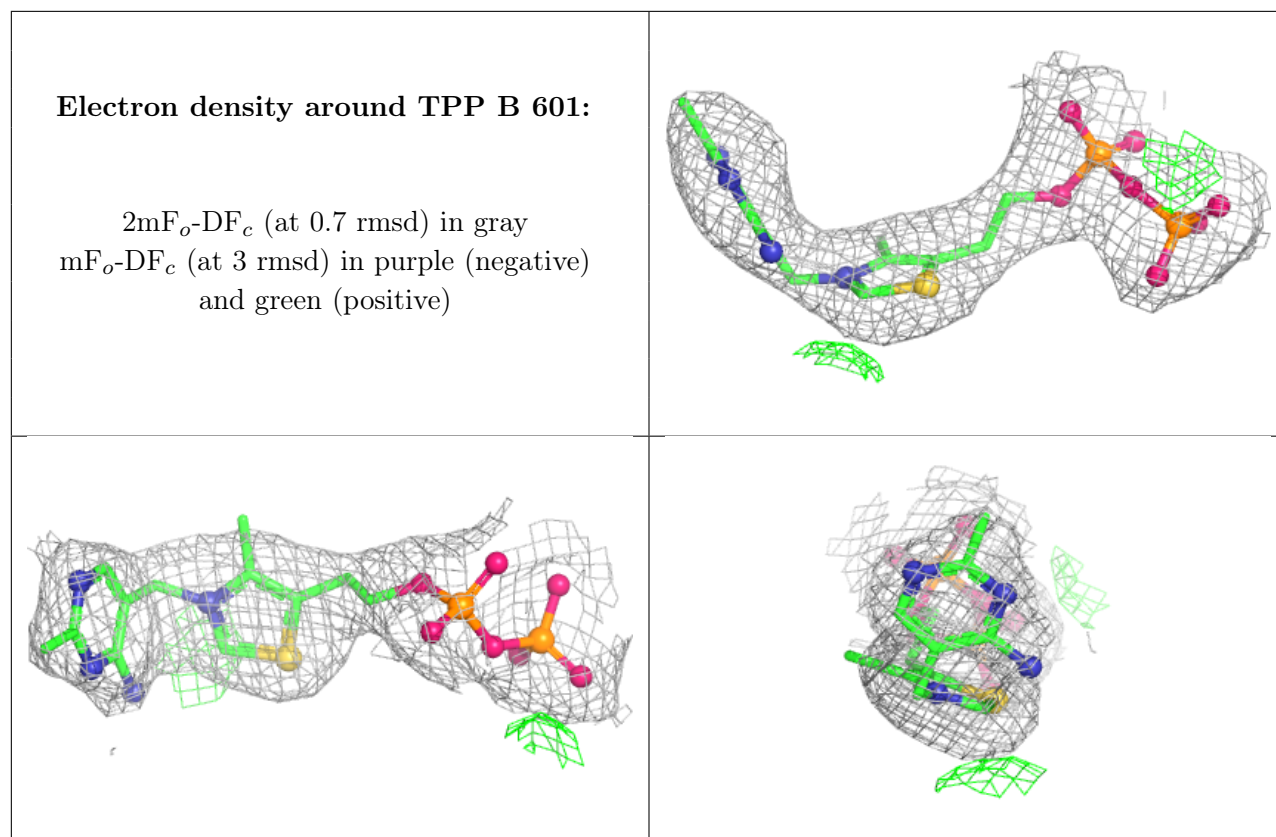
6.4 Ligands ⓘ

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
3	EDO	B	602	4/4	0.57	0.21	102,110,113,113	0
3	EDO	A	602	4/4	0.80	0.14	93,97,101,104	0
2	TPP	A	601	26/26	0.97	0.06	54,61,68,70	0
4	MG	A	603	1/1	0.97	0.03	61,61,61,61	0
2	TPP	B	601	26/26	0.98	0.05	55,65,70,71	0
4	MG	B	603	1/1	1.00	0.01	71,71,71,71	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.