



Full wwPDB X-ray Structure Validation Report i

May 29, 2020 – 04:59 pm BST

PDB ID : 2X7J
Title : Structure of the menaquinone biosynthesis protein MenD from *Bacillus subtilis*
Authors : Dawson, A.; Chen, M.; Fyfe, P.K.; Guo, Z.; Hunter, W.N.
Deposited on : 2010-03-01
Resolution : 2.35 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 i symbol.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

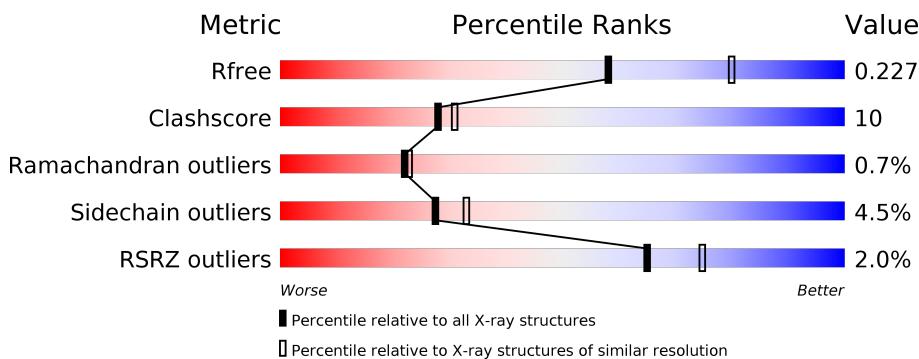
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

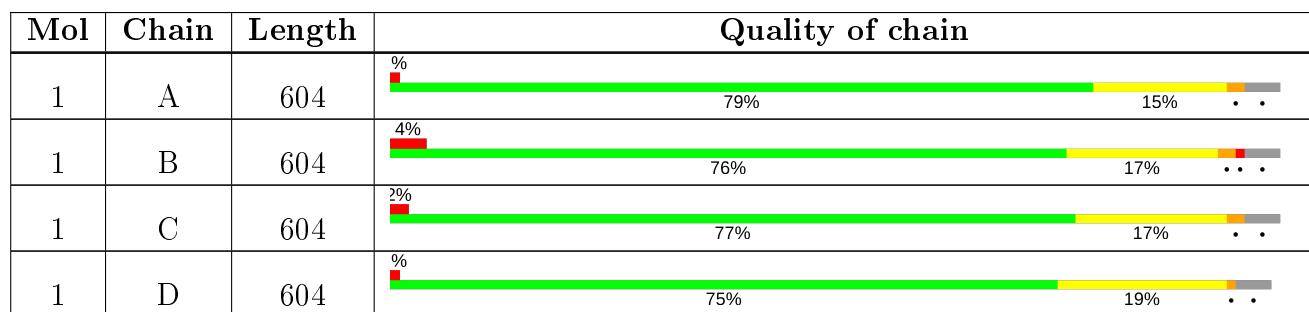
The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.



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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	A	603	-	-	X	-
4	EDO	B	603	-	-	X	-
4	EDO	C	603	-	-	X	-
4	EDO	D	603	-	-	X	-
6	SO4	A	1582	-	-	X	-
6	SO4	B	1582	-	-	X	-
6	SO4	C	1580	-	-	X	-
6	SO4	D	1582	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 19356 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 2-SUCCINYL-5-ENOLPYRUVYL-6-HYDROXY-3-CYCLOHEXENE -1-CARBOXYLATE SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	579	4544	2885	789	851	19	0	6	0
1	B	579	4520	2868	784	849	19	0	2	0
1	C	577	4502	2857	782	844	19	0	2	0
1	D	579	4548	2887	793	849	19	0	6	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-23	MET	-	expression tag	UNP P23970
A	-22	GLY	-	expression tag	UNP P23970
A	-21	SER	-	expression tag	UNP P23970
A	-20	SER	-	expression tag	UNP P23970
A	-19	HIS	-	expression tag	UNP P23970
A	-18	HIS	-	expression tag	UNP P23970
A	-17	HIS	-	expression tag	UNP P23970
A	-16	HIS	-	expression tag	UNP P23970
A	-15	HIS	-	expression tag	UNP P23970
A	-14	HIS	-	expression tag	UNP P23970
A	-13	SER	-	expression tag	UNP P23970
A	-12	SER	-	expression tag	UNP P23970
A	-11	GLY	-	expression tag	UNP P23970
A	-10	GLU	-	expression tag	UNP P23970
A	-9	ASN	-	expression tag	UNP P23970
A	-8	LEU	-	expression tag	UNP P23970
A	-7	TYR	-	expression tag	UNP P23970
A	-6	PHE	-	expression tag	UNP P23970
A	-5	GLN	-	expression tag	UNP P23970
A	-4	GLY	-	expression tag	UNP P23970

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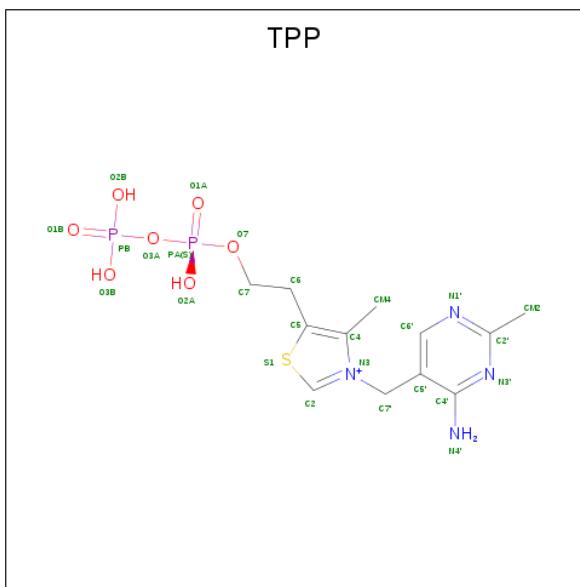
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	HIS	-	expression tag	UNP P23970
A	-2	MET	-	expression tag	UNP P23970
A	-1	LEU	-	expression tag	UNP P23970
A	0	GLU	-	expression tag	UNP P23970
B	-23	MET	-	expression tag	UNP P23970
B	-22	GLY	-	expression tag	UNP P23970
B	-21	SER	-	expression tag	UNP P23970
B	-20	SER	-	expression tag	UNP P23970
B	-19	HIS	-	expression tag	UNP P23970
B	-18	HIS	-	expression tag	UNP P23970
B	-17	HIS	-	expression tag	UNP P23970
B	-16	HIS	-	expression tag	UNP P23970
B	-15	HIS	-	expression tag	UNP P23970
B	-14	HIS	-	expression tag	UNP P23970
B	-13	SER	-	expression tag	UNP P23970
B	-12	SER	-	expression tag	UNP P23970
B	-11	GLY	-	expression tag	UNP P23970
B	-10	GLU	-	expression tag	UNP P23970
B	-9	ASN	-	expression tag	UNP P23970
B	-8	LEU	-	expression tag	UNP P23970
B	-7	TYR	-	expression tag	UNP P23970
B	-6	PHE	-	expression tag	UNP P23970
B	-5	GLN	-	expression tag	UNP P23970
B	-4	GLY	-	expression tag	UNP P23970
B	-3	HIS	-	expression tag	UNP P23970
B	-2	MET	-	expression tag	UNP P23970
B	-1	LEU	-	expression tag	UNP P23970
B	0	GLU	-	expression tag	UNP P23970
C	-23	MET	-	expression tag	UNP P23970
C	-22	GLY	-	expression tag	UNP P23970
C	-21	SER	-	expression tag	UNP P23970
C	-20	SER	-	expression tag	UNP P23970
C	-19	HIS	-	expression tag	UNP P23970
C	-18	HIS	-	expression tag	UNP P23970
C	-17	HIS	-	expression tag	UNP P23970
C	-16	HIS	-	expression tag	UNP P23970
C	-15	HIS	-	expression tag	UNP P23970
C	-14	HIS	-	expression tag	UNP P23970
C	-13	SER	-	expression tag	UNP P23970
C	-12	SER	-	expression tag	UNP P23970
C	-11	GLY	-	expression tag	UNP P23970
C	-10	GLU	-	expression tag	UNP P23970

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	ASN	-	expression tag	UNP P23970
C	-8	LEU	-	expression tag	UNP P23970
C	-7	TYR	-	expression tag	UNP P23970
C	-6	PHE	-	expression tag	UNP P23970
C	-5	GLN	-	expression tag	UNP P23970
C	-4	GLY	-	expression tag	UNP P23970
C	-3	HIS	-	expression tag	UNP P23970
C	-2	MET	-	expression tag	UNP P23970
C	-1	LEU	-	expression tag	UNP P23970
C	0	GLU	-	expression tag	UNP P23970
D	-23	MET	-	expression tag	UNP P23970
D	-22	GLY	-	expression tag	UNP P23970
D	-21	SER	-	expression tag	UNP P23970
D	-20	SER	-	expression tag	UNP P23970
D	-19	HIS	-	expression tag	UNP P23970
D	-18	HIS	-	expression tag	UNP P23970
D	-17	HIS	-	expression tag	UNP P23970
D	-16	HIS	-	expression tag	UNP P23970
D	-15	HIS	-	expression tag	UNP P23970
D	-14	HIS	-	expression tag	UNP P23970
D	-13	SER	-	expression tag	UNP P23970
D	-12	SER	-	expression tag	UNP P23970
D	-11	GLY	-	expression tag	UNP P23970
D	-10	GLU	-	expression tag	UNP P23970
D	-9	ASN	-	expression tag	UNP P23970
D	-8	LEU	-	expression tag	UNP P23970
D	-7	TYR	-	expression tag	UNP P23970
D	-6	PHE	-	expression tag	UNP P23970
D	-5	GLN	-	expression tag	UNP P23970
D	-4	GLY	-	expression tag	UNP P23970
D	-3	HIS	-	expression tag	UNP P23970
D	-2	MET	-	expression tag	UNP P23970
D	-1	LEU	-	expression tag	UNP P23970
D	0	GLU	-	expression tag	UNP P23970

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C₁₂H₁₉N₄O₇P₂S).

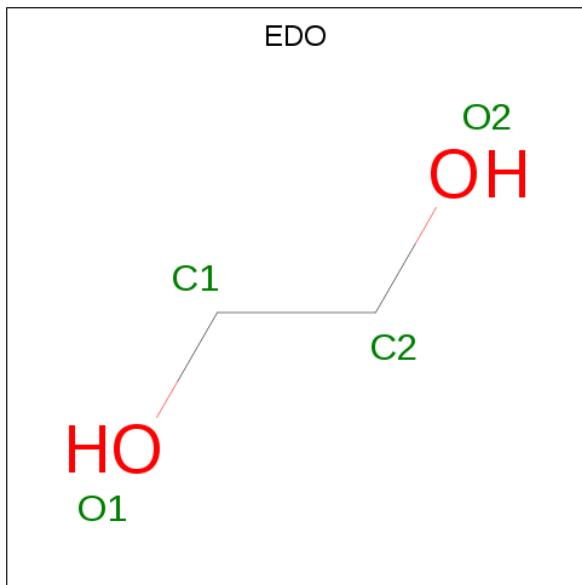


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	B	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	C	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		
2	D	1	Total	C	N	O	P	S	0	0
			26	12	4	7	2	1		

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mn	0	0
			1	1		
3	A	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).

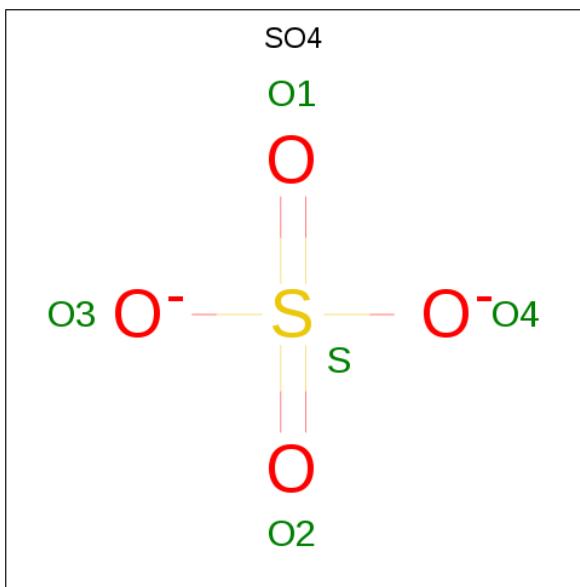


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

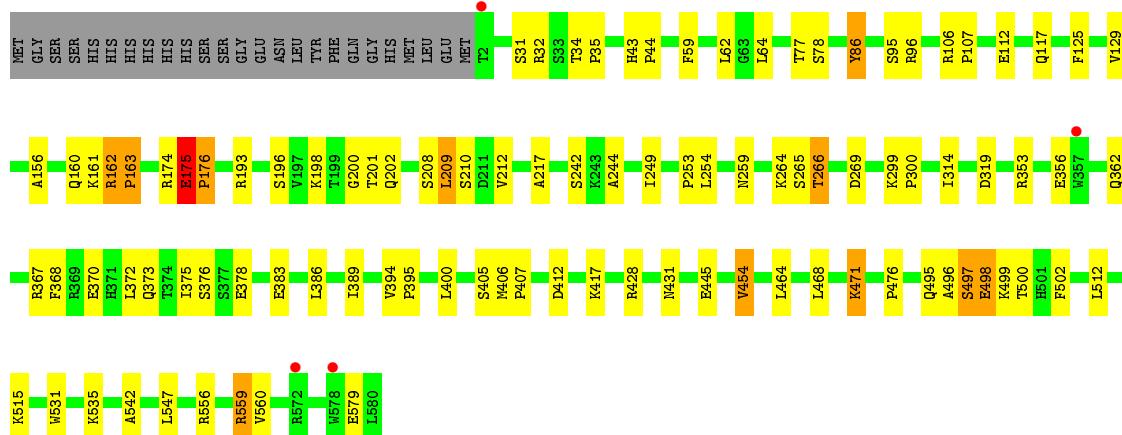
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	285	Total O 285 285	0	0
7	B	239	Total O 239 239	0	0
7	C	256	Total O 256 256	0	0
7	D	294	Total O 294 294	0	0

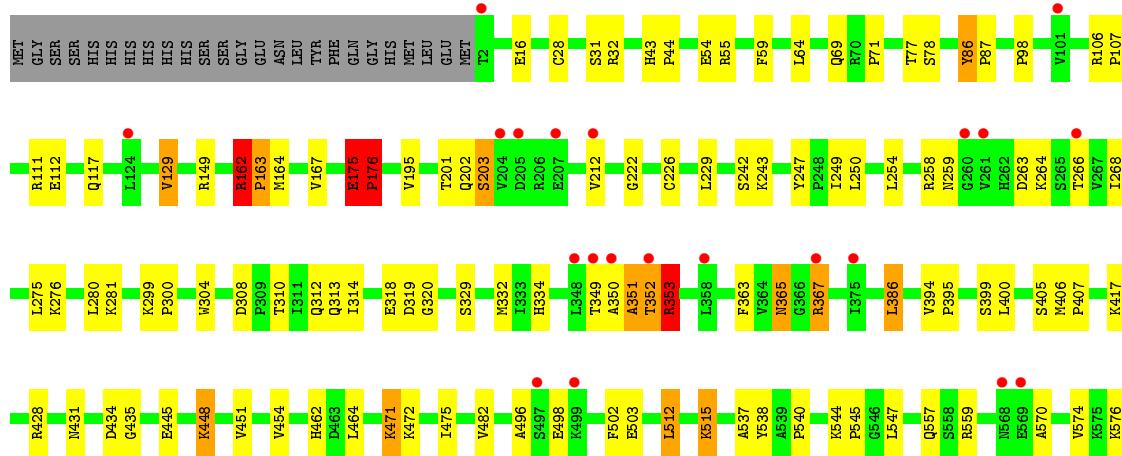
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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: 2-SUCCINYL-5-ENOLPYRUVYL-6-HYDROXY-3-CYCLOHEXENE -1-CARBOXYLATE SYNTHASE

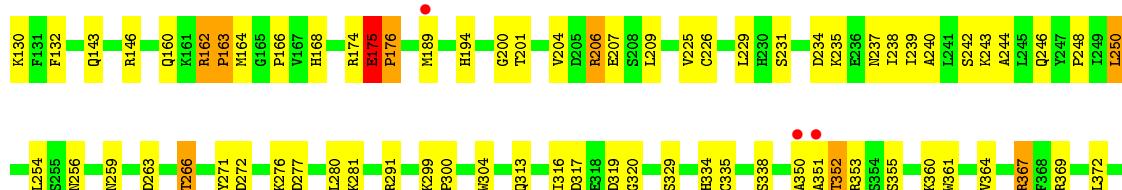
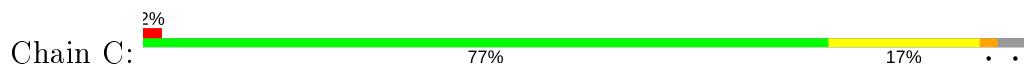


- Molecule 1: 2-SUCCINYL-5-ENOLPYRUVYL-6-HYDROXY-3-CYCLOHEXENE -1-CARBOXYLATE SYNTHASE

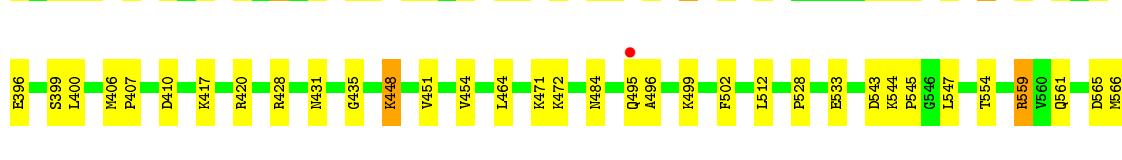
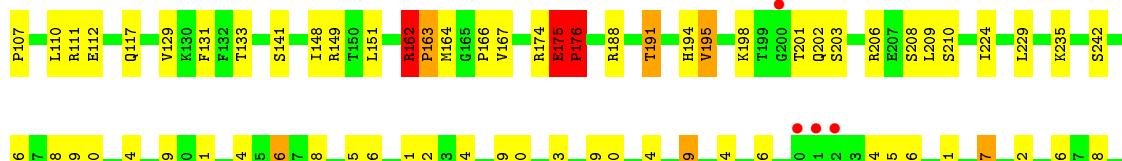
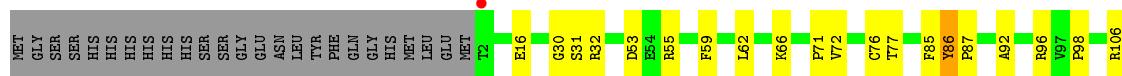
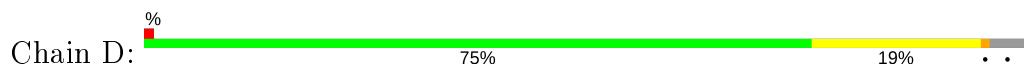




- Molecule 1: 2-SUCCINYL-5-ENOLPYRUVYL-6-HYDROXY-3-CYCLOHEXENE -1-CARBOXYLATE SYNTHASE



- Molecule 1: 2-SUCCINYL-5-ENOLPYRUVYL-6-HYDROXY-3-CYCLOHEXENE -1-CARBOXYLATE SYNTHASE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.18 Å 152.99 Å 158.50 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.14 – 2.35 62.15 – 2.35	Depositor EDS
% Data completeness (in resolution range)	100.0 (62.14-2.35) 100.0 (62.15-2.35)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle^1$	3.39 (at 2.34 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R , R_{free}	0.172 , 0.228 0.173 , 0.227	Depositor DCC
R_{free} test set	5118 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	19356	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.8341e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [\(i\)](#)

5.1 Standard geometry [\(i\)](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA, TPP, MN, EDO, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.48	0/4671	0.64	3/6342 (0.0%)
1	B	0.45	0/4635	0.61	3/6294 (0.0%)
1	C	0.45	0/4617	0.60	2/6271 (0.0%)
1	D	0.48	0/4675	0.64	3/6346 (0.0%)
All	All	0.46	0/18598	0.62	11/25253 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
All	All	0	8

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	175	GLU	C-N-CD	-11.48	95.34	120.60
1	C	162	ARG	C-N-CD	-11.36	95.60	120.60
1	A	175	GLU	C-N-CD	-11.26	95.83	120.60
1	A	162	ARG	C-N-CD	-10.23	98.08	120.60
1	B	162	ARG	C-N-CD	-10.04	98.52	120.60
1	D	162	ARG	C-N-CD	-9.91	98.79	120.60
1	C	175	GLU	C-N-CD	-9.86	98.90	120.60
1	A	176	PRO	N-CA-C	-7.56	92.44	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	175	GLU	C-N-CD	-7.45	104.20	120.60
1	D	176	PRO	N-CA-C	-7.41	92.83	112.10
1	B	176	PRO	N-CA-C	-7.33	93.03	112.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	162	ARG	Peptide
1	A	175	GLU	Peptide
1	B	162	ARG	Peptide
1	B	175	GLU	Peptide
1	C	162	ARG	Peptide
1	C	175	GLU	Peptide
1	D	162	ARG	Peptide
1	D	175	GLU	Peptide

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	4544	0	4503	74	0
1	B	4520	0	4465	91	0
1	C	4502	0	4448	82	0
1	D	4548	0	4513	111	0
2	A	26	0	16	2	0
2	B	26	0	16	0	0
2	C	26	0	16	1	0
2	D	26	0	16	2	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	4	0	6	13	0
4	B	4	0	6	6	0
4	C	4	0	6	8	0
4	D	4	0	6	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	10	0	0	5	0
6	B	10	0	0	6	0
6	C	10	0	0	6	0
6	D	10	0	0	9	0
7	A	285	0	0	11	0
7	B	239	0	0	9	0
7	C	256	0	0	10	0
7	D	294	0	0	17	0
All	All	19356	0	18017	359	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 10.

All (359) 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:31:SER:H	4:C:603:EDO:H11	1.04	1.20
1:D:31:SER:H	4:D:603:EDO:H22	1.00	1.17
1:D:163:PRO:HD3	1:D:319:ASP:HB3	1.34	1.08
1:C:206:ARG:HH11	1:C:206:ARG:HG3	0.89	1.06
1:B:163:PRO:CD	1:B:319:ASP:HB3	1.85	1.06
1:B:163:PRO:HD3	1:B:319:ASP:HB3	1.05	1.04
1:C:206:ARG:CG	1:C:206:ARG:HH11	1.75	1.00
1:D:559[A]:ARG:HH11	1:D:559[A]:ARG:HG2	1.28	0.99
1:C:206:ARG:HG3	1:C:206:ARG:NH1	1.65	0.98
1:A:406:MET:HG3	1:A:559[B]:ARG:HH22	1.27	0.98
1:D:31:SER:N	4:D:603:EDO:H22	1.80	0.95
1:B:163:PRO:HD3	1:B:319:ASP:CB	1.98	0.93
1:B:352:THR:O	1:B:353:ARG:HB2	1.69	0.92
1:D:242:SER:OG	1:D:266:THR:HG21	1.70	0.91
1:D:31:SER:H	4:D:603:EDO:C2	1.84	0.91
1:B:349:THR:O	1:B:351:ALA:N	2.04	0.90
1:C:31:SER:N	4:C:603:EDO:H11	1.85	0.90
1:B:32:ARG:NH1	6:B:1582:SO4:O2	2.04	0.89
1:D:117:GLN:HE22	4:D:603:EDO:C1	1.87	0.87
1:D:107:PRO:HG3	6:D:1582:SO4:O2	1.76	0.86
1:C:242:SER:OG	1:C:266:THR:HG21	1.77	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:SER:H	4:A:603:EDO:H21	1.45	0.81
1:A:163:PRO:HD3	1:A:319:ASP:HB3	1.62	0.81
1:C:31:SER:H	4:C:603:EDO:C1	1.92	0.80
6:C:1580:SO4:O3	7:C:2255:HOH:O	2.00	0.80
6:A:1582:SO4:O2	7:A:2283:HOH:O	2.00	0.80
1:A:406:MET:CG	1:A:559[B]:ARG:HH22	1.94	0.80
1:D:410:ASP:OD2	1:D:559[B]:ARG:NH2	2.15	0.79
1:A:356:GLU:OE2	7:A:2189:HOH:O	2.00	0.78
1:D:276:LYS:NZ	7:D:2145:HOH:O	2.17	0.78
1:C:163:PRO:HD3	1:C:319:ASP:HB3	1.66	0.77
1:D:162:ARG:HD3	1:D:319:ASP:OD1	1.84	0.77
1:C:31:SER:HB3	4:C:603:EDO:H22	1.65	0.77
1:B:276:LYS:NZ	7:B:2120:HOH:O	2.14	0.76
1:D:559[A]:ARG:NH1	1:D:559[A]:ARG:HG2	1.94	0.76
1:D:117:GLN:HE22	4:D:603:EDO:H12	1.48	0.76
1:C:176:PRO:HD3	7:C:2095:HOH:O	1.86	0.75
1:D:282:ARG:HD3	7:D:2148:HOH:O	1.86	0.74
1:A:31:SER:N	4:A:603:EDO:H21	2.03	0.73
1:A:378:GLU:OE1	7:A:2195:HOH:O	2.05	0.73
1:D:175:GLU:HB2	6:D:1582:SO4:O4	1.87	0.73
1:D:471:LYS:HG2	7:D:2237:HOH:O	1.89	0.72
1:C:367:ARG:HB3	1:C:574:VAL:HG22	1.72	0.72
1:A:175:GLU:N	6:A:1582:SO4:O3	2.23	0.72
1:D:31:SER:HB3	4:D:603:EDO:H11	1.71	0.72
1:B:31:SER:H	4:B:603:EDO:H11	1.53	0.71
6:C:1580:SO4:O4	7:C:2254:HOH:O	2.07	0.71
1:C:130:LYS:NZ	1:C:163:PRO:O	2.22	0.71
1:C:276:LYS:NZ	6:C:1581:SO4:O2	2.24	0.71
1:D:261:VAL:HG22	7:D:2137:HOH:O	1.91	0.70
1:B:175:GLU:CB	6:B:1582:SO4:O4	2.40	0.70
1:C:513:ASP:OD2	1:C:515:LYS:HD2	1.92	0.69
1:B:363:PHE:HZ	1:B:577:GLN:HG3	1.57	0.69
1:B:78:SER:OG	1:B:106:ARG:NH2	2.25	0.69
1:B:226:CYS:SG	1:B:229:LEU:HD11	2.32	0.69
1:C:175:GLU:N	6:C:1580:SO4:O2	2.27	0.68
1:A:244:ALA:O	1:A:353:ARG:HG3	1.94	0.68
1:D:129[A]:VAL:HG13	1:D:167:VAL:HA	1.76	0.67
1:A:31:SER:H	4:A:603:EDO:C2	2.06	0.67
1:B:503:GLU:HG3	7:B:2196:HOH:O	1.95	0.67
1:D:248:PRO:HB2	1:D:268:ILE:CD1	2.24	0.66
1:D:261:VAL:O	7:D:2138:HOH:O	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:543:ASP:HB3	7:D:2272:HOH:O	1.96	0.66
1:D:410:ASP:CG	1:D:559[B]:ARG:HH22	2.00	0.66
1:D:117:GLN:NE2	4:D:603:EDO:H12	2.10	0.66
1:B:363:PHE:CZ	1:B:577:GLN:HG3	2.31	0.65
1:A:497:SER:O	1:A:499:LYS:N	2.30	0.65
1:D:499:LYS:O	7:D:2251:HOH:O	2.15	0.65
1:A:556:ARG:HG2	7:A:2276:HOH:O	1.96	0.64
1:B:242:SER:CB	1:B:266:THR:HG21	2.27	0.64
1:C:2:THR:HG23	1:C:2:THR:O	1.98	0.64
1:B:107:PRO:HG3	6:B:1582:SO4:O1	1.97	0.64
1:A:156:ALA:O	1:A:160:GLN:HG3	1.97	0.64
1:D:559[A]:ARG:HH11	1:D:559[A]:ARG:CG	2.07	0.63
1:C:130:LYS:HE2	7:C:2090:HOH:O	1.97	0.63
1:C:189:MET:HE3	7:C:2106:HOH:O	1.99	0.63
1:C:400:LEU:HD11	1:C:454:VAL:CG2	2.29	0.63
1:B:242:SER:HB2	1:B:266:THR:HG21	1.80	0.62
1:D:324:ASP:OD2	1:D:329:SER:HB3	1.99	0.62
1:B:471:LYS:HG2	1:B:472:LYS:N	2.13	0.62
2:A:601:TPP:H7'2	4:B:603:EDO:H12	1.81	0.62
1:A:370:GLU:O	1:A:373:GLN:HB2	2.00	0.62
1:D:206:ARG:HH22	1:D:346:ALA:HB3	1.65	0.61
1:A:265:SER:O	1:A:362[B]:GLN:NE2	2.33	0.61
1:B:243:LYS:NZ	1:B:263:ASP:OD2	2.34	0.60
1:D:194:HIS:CD2	1:D:195:VAL:HG22	2.36	0.60
1:C:281:LYS:HG2	1:C:304:TRP:CE2	2.37	0.60
1:D:106:ARG:NE	7:D:2039:HOH:O	2.34	0.60
1:D:112[A]:GLU:OE1	7:D:2048:HOH:O	2.16	0.59
1:B:31:SER:HB3	4:B:603:EDO:H22	1.83	0.59
1:C:32:ARG:NH1	6:C:1580:SO4:O1	2.34	0.59
1:D:354:SER:OG	1:D:356:GLU:HG3	2.02	0.59
1:D:163:PRO:CD	1:D:319:ASP:HB3	2.22	0.59
1:D:229:LEU:HD13	1:D:235:LYS:HG2	1.85	0.59
1:A:579:GLU:OE2	1:A:579:GLU:HA	2.03	0.59
1:D:194:HIS:HD2	1:D:195:VAL:HG22	1.68	0.58
1:B:363:PHE:HD1	1:B:367:ARG:NH1	2.02	0.58
1:C:400:LEU:HD11	1:C:454:VAL:HG23	1.85	0.58
1:B:31:SER:H	4:B:603:EDO:C1	2.16	0.58
1:A:400:LEU:HD11	1:A:454:VAL:CG2	2.34	0.58
1:C:266:THR:HB	7:C:2131:HOH:O	2.02	0.58
1:B:363:PHE:CD1	1:B:367:ARG:NH1	2.71	0.58
1:D:248:PRO:HB2	1:D:268:ILE:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:SER:HB3	4:A:603:EDO:H21	1.86	0.57
1:C:250:LEU:N	1:C:250:LEU:HD23	2.20	0.57
1:D:59:PHE:CD1	1:D:435:GLY:HA3	2.39	0.57
1:D:275:LEU:O	1:D:281:LYS:HD2	2.03	0.57
1:B:243:LYS:HE3	1:B:263:ASP:OD2	2.04	0.57
1:D:248:PRO:CB	1:D:268:ILE:CD1	2.83	0.57
1:A:78:SER:OG	1:A:106:ARG:NH1	2.38	0.57
1:C:434:ASP:HB3	1:C:462:HIS:CE1	2.40	0.57
1:C:174:ARG:HA	6:C:1580:SO4:O1	2.05	0.56
1:A:242:SER:OG	1:A:266:THR:HG21	2.05	0.56
1:B:400:LEU:HD11	1:B:454:VAL:HG23	1.87	0.56
1:A:431:ASN:N	1:A:431:ASN:HD22	2.04	0.56
1:B:320:GLY:HA2	1:B:334:HIS:CD2	2.40	0.56
1:D:163:PRO:HD3	1:D:319:ASP:CB	2.24	0.55
1:C:234:ASP:O	1:C:238:ILE:HG13	2.06	0.55
1:B:175:GLU:HB3	6:B:1582:SO4:O4	2.05	0.55
1:B:496:ALA:HA	1:B:502:PHE:CD1	2.42	0.55
1:A:217:ALA:O	1:A:353:ARG:NH2	2.39	0.55
1:B:243:LYS:CE	1:B:263:ASP:OD2	2.55	0.55
1:B:117:GLN:HE22	4:B:603:EDO:C2	2.19	0.55
1:A:249:ILE:HG13	1:A:266:THR:CG2	2.36	0.55
1:D:174:ARG:HG3	6:D:1582:SO4:O2	2.07	0.55
1:C:86[B]:TYR:HB3	1:C:87:PRO:HD3	1.89	0.54
1:B:503:GLU:CG	7:B:2196:HOH:O	2.52	0.54
1:C:71:PRO:HD3	1:C:160:GLN:HG3	1.88	0.54
1:D:110:LEU:CD1	6:D:1582:SO4:O1	2.55	0.54
1:C:68:LYS:HD2	7:C:2028:HOH:O	2.08	0.54
1:D:210:SER:HB3	7:D:2120:HOH:O	2.08	0.54
1:C:231:SER:HB3	1:C:234:ASP:HB2	1.90	0.54
1:A:210:SER:HB2	7:A:2124:HOH:O	2.08	0.53
1:D:107:PRO:O	1:D:111:ARG:HG3	2.08	0.53
1:D:188[B]:ARG:NH2	1:D:191:THR:O	2.41	0.53
1:D:313:GLN:HB2	1:D:329:SER:HA	1.91	0.53
1:C:143:GLN:OE1	1:C:146:ARG:NH1	2.42	0.53
1:D:32:ARG:NH1	6:D:1582:SO4:O3	2.42	0.52
1:B:281:LYS:HG2	1:B:304:TRP:CE2	2.45	0.52
1:B:212:VAL:HG13	1:B:314:ILE:HD13	1.92	0.52
1:A:406:MET:HG3	1:A:559[B]:ARG:NH2	2.11	0.52
1:B:162:ARG:O	1:B:163:PRO:HG2	2.10	0.52
1:D:282:ARG:CD	7:D:2148:HOH:O	2.50	0.52
1:C:86[A]:TYR:HE1	1:C:124:LEU:O	1.93	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:175:GLU:HB2	6:B:1582:SO4:O4	2.08	0.51
1:D:388:ARG:HD2	1:D:566:MET:HE1	1.93	0.51
1:A:496:ALA:HA	1:A:502:PHE:CD1	2.46	0.51
1:A:117:GLN:HE22	4:A:603:EDO:H11	1.75	0.51
1:C:317:ASP:O	1:C:334:HIS:HA	2.11	0.51
1:B:580:LEU:OXT	7:B:2237:HOH:O	2.19	0.51
1:B:77:THR:OG1	4:B:603:EDO:O2	2.19	0.50
1:D:224:ILE:HD12	1:D:242:SER:HB3	1.94	0.50
1:B:176:PRO:HD2	1:B:176:PRO:O	2.11	0.50
1:B:515:LYS:NZ	7:B:2205:HOH:O	2.44	0.50
1:C:78:SER:OG	1:C:106:ARG:NH2	2.44	0.50
1:C:281:LYS:HG2	1:C:304:TRP:NE1	2.27	0.50
1:A:372:LEU:HD23	1:A:375:ILE:HD12	1.92	0.50
1:B:162:ARG:HD3	1:B:319:ASP:OD1	2.11	0.50
1:D:399:SER:HB2	1:D:451:VAL:HG22	1.94	0.50
1:B:264:LYS:HD2	1:B:417:LYS:HB2	1.93	0.50
1:C:277:ASP:OD2	1:C:280:LEU:N	2.36	0.49
1:C:320:GLY:HA2	1:C:334:HIS:CD2	2.47	0.49
4:C:603:EDO:H12	2:D:601:TPP:H7'2	1.94	0.49
1:A:406:MET:N	1:A:407:PRO:CD	2.75	0.49
1:A:200:GLY:HA3	1:D:203:SER:O	2.12	0.49
1:C:320:GLY:HA2	1:C:334:HIS:CG	2.47	0.49
1:C:248:PRO:HG3	1:C:361:TRP:CD1	2.48	0.49
1:D:117:GLN:NE2	4:D:603:EDO:C1	2.65	0.49
1:A:368:PHE:CE2	1:A:372:LEU:HD12	2.48	0.49
1:D:367:ARG:HG2	1:D:577:GLN:HG3	1.95	0.49
1:C:226:CYS:SG	1:C:229:LEU:HD11	2.53	0.49
1:B:544:LYS:HB2	1:B:545:PRO:HD2	1.95	0.49
1:A:559[B]:ARG:HD3	7:A:2199:HOH:O	2.11	0.49
1:A:86[B]:TYR:HD1	1:A:125:PHE:HD1	1.61	0.48
1:D:133:THR:HG21	1:D:151:LEU:HD11	1.95	0.48
1:D:110:LEU:HD12	6:D:1582:SO4:O1	2.13	0.48
1:D:129[B]:VAL:HG12	1:D:166:PRO:HB2	1.94	0.48
1:D:194:HIS:HD2	1:D:195:VAL:CG2	2.26	0.48
1:D:400:LEU:HD11	1:D:454:VAL:CG2	2.43	0.48
2:D:601:TPP:C2	2:D:601:TPP:HN42	2.27	0.48
1:A:174:ARG:HA	6:A:1582:SO4:O4	2.13	0.48
1:D:496:ALA:HA	1:D:502:PHE:CD1	2.48	0.48
1:B:299:LYS:HB3	1:B:300:PRO:HD3	1.94	0.48
1:D:471:LYS:HG3	1:D:472:LYS:N	2.28	0.48
1:D:30:GLY:HA3	1:D:77:THR:HB	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:SER:CB	1:A:266:THR:HG21	2.44	0.48
1:A:32:ARG:H	4:A:603:EDO:H21	1.78	0.48
1:B:242:SER:OG	1:B:266:THR:HG21	2.13	0.48
1:C:360:LYS:NZ	7:C:2172:HOH:O	2.30	0.48
1:D:129[A]:VAL:CG1	1:D:131:PHE:O	2.62	0.48
1:C:256:ASN:HA	7:C:2129:HOH:O	2.13	0.48
1:C:59:PHE:CD1	1:C:435:GLY:HA3	2.48	0.48
1:B:175:GLU:HB2	6:B:1582:SO4:S	2.54	0.48
1:C:22:ILE:HG21	1:C:73:LEU:HG	1.96	0.48
1:D:561:GLN:NE2	1:D:565:ASP:OD1	2.47	0.48
1:B:557:GLN:OE1	1:B:557:GLN:HA	2.14	0.47
1:C:204:VAL:HG23	1:C:335:CYS:HB2	1.96	0.47
1:B:445:GLU:O	1:B:448:LYS:HE2	2.13	0.47
1:C:117:GLN:HE22	4:C:603:EDO:C2	2.27	0.47
1:A:299:LYS:HB3	1:A:300:PRO:HD3	1.96	0.47
1:B:268:ILE:HG23	1:B:365:ASN:OD1	2.15	0.47
1:D:248:PRO:CB	1:D:268:ILE:HD12	2.45	0.47
1:C:237:ASN:HD22	1:C:338:SER:CB	2.27	0.47
1:D:428:ARG:HA	1:D:431:ASN:ND2	2.29	0.47
1:A:32:ARG:H	4:A:603:EDO:C2	2.28	0.47
1:B:78:SER:HB2	7:B:2063:HOH:O	2.13	0.47
1:B:203:SER:O	1:C:200:GLY:HA3	2.15	0.47
1:D:141:SER:HB2	7:D:2077:HOH:O	2.15	0.47
1:A:383:GLU:HB3	1:A:559[B]:ARG:HD2	1.96	0.47
1:A:212:VAL:HG13	1:A:314:ILE:HD13	1.97	0.47
1:D:266:THR:HB	7:D:2140:HOH:O	2.14	0.47
1:D:264:LYS:HD2	1:D:417:LYS:HB2	1.97	0.47
1:A:86[B]:TYR:CD1	1:A:125:PHE:HD1	2.32	0.46
1:D:448:LYS:HA	1:D:448:LYS:HD2	1.61	0.46
1:C:86[A]:TYR:CE1	1:C:124:LEU:O	2.69	0.46
1:A:299:LYS:HE3	7:A:2159:HOH:O	2.14	0.46
1:B:16:GLU:HG2	1:B:149:ARG:O	2.15	0.46
1:B:400:LEU:HD11	1:B:454:VAL:CG2	2.46	0.46
1:D:428:ARG:HA	1:D:431:ASN:HD22	1.81	0.46
1:A:531:TRP:O	1:A:535:LYS:HG3	2.16	0.46
1:D:248:PRO:HB2	1:D:268:ILE:HD13	1.94	0.46
1:B:275:LEU:O	1:B:281:LYS:HD3	2.16	0.46
1:A:198:LYS:HE3	1:D:208:SER:O	2.15	0.46
1:B:249:ILE:HG13	1:B:266:THR:CG2	2.46	0.46
1:C:369:ARG:HD2	1:C:416:GLU:HG2	1.97	0.46
1:D:249:ILE:HG13	1:D:266:THR:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:572[B]:ARG:NH1	7:D:2289:HOH:O	2.48	0.46
1:D:573:GLU:O	1:D:577:GLN:HG2	2.15	0.46
1:C:246:GLN:OE1	1:C:355:SER:HB3	2.15	0.46
1:B:86[B]:TYR:HB3	1:B:87:PRO:HD3	1.98	0.46
1:D:96:ARG:HA	1:D:164:MET:O	2.16	0.46
1:B:129:VAL:HG22	1:B:167:VAL:HA	1.98	0.45
1:B:445:GLU:HG2	1:B:475:ILE:CD1	2.46	0.45
1:D:250:LEU:N	1:D:250:LEU:HD23	2.31	0.45
1:A:43:HIS:HA	1:A:44:PRO:HD3	1.78	0.45
1:B:332:MET:HE1	7:B:2135:HOH:O	2.15	0.45
1:B:434:ASP:HB3	1:B:462:HIS:CE1	2.51	0.45
1:C:524:THR:OG1	1:C:548:HIS:CD2	2.69	0.45
1:D:284:LEU:HB3	1:D:361:TRP:CZ2	2.52	0.45
1:A:117:GLN:OE1	4:A:603:EDO:H11	2.16	0.45
1:B:576:LYS:C	1:B:578:TRP:H	2.19	0.45
2:C:601:TPP:C2	2:C:601:TPP:HN42	2.30	0.45
1:B:222:GLY:HA3	1:B:247:TYR:CZ	2.51	0.45
1:D:62:LEU:O	1:D:66:LYS:HB2	2.17	0.45
1:D:528:PRO:CB	1:D:533:GLU:HG3	2.47	0.45
1:A:112[B]:GLU:CD	7:A:2055:HOH:O	2.55	0.45
1:D:92:ALA:HB3	1:D:166:PRO:HG3	1.99	0.45
1:C:316:ILE:HD12	1:C:316:ILE:N	2.33	0.44
1:C:360:LYS:O	1:C:364:VAL:HG23	2.17	0.44
1:D:248:PRO:HG3	1:D:361:TRP:CD1	2.52	0.44
1:C:86[A]:TYR:CZ	1:C:125:PHE:HA	2.51	0.44
1:D:112[B]:GLU:OE1	7:D:2045:HOH:O	2.21	0.44
1:D:96:ARG:NH1	1:D:319:ASP:HB2	2.32	0.44
1:B:250:LEU:HD23	1:B:250:LEU:N	2.32	0.44
1:D:528:PRO:HB3	1:D:533:GLU:HG3	1.99	0.44
1:D:198:LYS:HD3	1:D:198:LYS:HA	1.68	0.44
1:B:176:PRO:O	1:B:176:PRO:CD	2.64	0.44
1:C:239:ILE:O	1:C:240:ALA:C	2.56	0.44
1:C:299:LYS:HB3	1:C:300:PRO:HD3	1.98	0.44
1:D:299:LYS:HB3	1:D:300:PRO:HD3	1.99	0.44
1:C:55:ARG:NH2	1:D:53:ASP:OD1	2.46	0.44
1:A:95:SER:O	1:A:96:ARG:HB2	2.17	0.44
1:C:86[B]:TYR:CD1	1:D:86[B]:TYR:CD1	3.06	0.44
1:C:513:ASP:CG	1:C:515:LYS:HD2	2.37	0.44
1:A:193:ARG:HD3	1:A:196:SER:HB3	1.99	0.44
1:A:193:ARG:NH1	7:A:2119:HOH:O	2.50	0.44
1:C:515:LYS:HE3	1:C:515:LYS:HB3	1.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:LYS:HD2	1:A:417:LYS:HB2	2.00	0.43
1:B:43:HIS:HA	1:B:44:PRO:HD3	1.78	0.43
1:B:162:ARG:O	1:B:163:PRO:CG	2.59	0.43
1:B:176:PRO:HD2	7:B:2004:HOH:O	2.17	0.43
1:C:55:ARG:HH21	1:D:55:ARG:HB2	1.83	0.43
1:D:282:ARG:NE	7:D:2148:HOH:O	2.51	0.43
1:D:71:PRO:HA	1:D:98:PRO:O	2.19	0.43
1:A:163:PRO:CD	1:A:319:ASP:HB3	2.39	0.43
1:C:496:ALA:HA	1:C:502:PHE:CD1	2.53	0.43
1:C:78:SER:HB2	7:C:2061:HOH:O	2.19	0.43
1:D:406:MET:N	1:D:407:PRO:CD	2.81	0.43
1:A:498:GLU:HA	7:A:2244:HOH:O	2.18	0.43
1:A:579:GLU:OE2	1:A:579:GLU:CA	2.67	0.43
1:D:372:LEU:HA	1:D:372:LEU:HD23	1.86	0.43
1:A:175:GLU:HB2	6:A:1582:SO4:O3	2.17	0.43
1:A:269:ASP:OD2	1:A:417:LYS:HG2	2.18	0.43
2:A:601:TPP:N1'	1:B:54:GLU:OE2	2.52	0.43
1:C:244:ALA:O	1:C:353:ARG:HD2	2.19	0.43
1:C:243:LYS:NZ	1:C:263:ASP:OD2	2.31	0.43
1:C:225:VAL:HB	1:C:291:ARG:HG2	1.99	0.43
1:C:530:SER:OG	1:C:533:GLU:HG2	2.19	0.43
1:A:209:LEU:HA	1:A:209:LEU:HD12	1.88	0.43
1:A:34:THR:HB	1:A:35:PRO:CD	2.48	0.43
1:A:31:SER:CB	4:A:603:EDO:H21	2.48	0.43
1:B:202:GLN:NE2	1:B:318:GLU:O	2.52	0.43
1:C:364:VAL:HG13	1:C:574:VAL:HG11	2.00	0.43
1:D:148:ILE:HD12	1:D:148:ILE:HA	1.77	0.43
1:D:320:GLY:HA2	1:D:334:HIIS:CD2	2.54	0.43
1:A:253:PRO:HG3	1:A:412:ASP:HA	2.01	0.43
1:B:399:SER:HB2	1:B:451:VAL:HG22	2.01	0.43
1:D:175:GLU:HB2	6:D:1582:SO4:S	2.58	0.43
1:B:313:GLN:HB2	1:B:329:SER:HA	2.01	0.42
1:B:363:PHE:HZ	1:B:577:GLN:CG	2.27	0.42
1:C:99:ILE:O	1:C:166:PRO:HA	2.18	0.42
1:C:132:PHE:HA	1:C:168:HIS:O	2.19	0.42
1:D:107:PRO:CG	6:D:1582:SO4:O2	2.57	0.42
1:A:117:GLN:HE22	4:A:603:EDO:C1	2.32	0.42
1:C:313:GLN:HB2	1:C:329:SER:HA	2.01	0.42
1:D:76:CYS:HB3	1:D:85:PHE:CZ	2.54	0.42
1:B:308:ASP:OD1	1:B:310:THR:OG1	2.37	0.42
1:C:254:LEU:HD21	1:C:426:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:ARG:HA	1:A:428:ARG:HD2	1.88	0.42
1:C:117:GLN:NE2	4:C:603:EDO:H21	2.34	0.42
1:A:559[A]:ARG:CG	1:A:560:VAL:N	2.78	0.42
1:B:431:ASN:HD22	1:B:431:ASN:N	2.18	0.42
1:B:537:ALA:O	7:B:2221:HOH:O	2.21	0.42
1:C:271:TYR:CD2	1:C:272:ASP:N	2.88	0.42
1:A:117:GLN:HE22	4:A:603:EDO:C2	2.32	0.42
1:B:59:PHE:CD1	1:B:435:GLY:HA3	2.54	0.42
1:C:96:ARG:HA	1:C:164:MET:O	2.19	0.42
1:A:31:SER:CA	4:A:603:EDO:H21	2.50	0.42
1:B:129:VAL:HG22	1:B:167:VAL:CA	2.50	0.42
1:C:350:ALA:O	1:C:352:THR:N	2.52	0.42
1:D:176:PRO:HD2	7:D:2002:HOH:O	2.18	0.42
1:A:476:PRO:HG3	1:A:542:ALA:HA	2.01	0.42
1:B:69:GLN:OE1	1:B:164:MET:CE	2.68	0.42
1:D:106:ARG:NH1	1:D:117:GLN:HB3	2.35	0.41
1:A:367:ARG:HA	1:A:367:ARG:HD3	1.81	0.41
1:A:406:MET:CE	1:A:559[B]:ARG:NH2	2.83	0.41
1:C:231:SER:O	1:C:235:LYS:HG3	2.20	0.41
1:A:78:SER:HB2	7:A:2068:HOH:O	2.21	0.41
1:B:258:ARG:O	1:B:417:LYS:HA	2.21	0.41
1:B:386:LEU:O	1:B:386:LEU:HD22	2.20	0.41
1:B:386:LEU:HD12	1:B:482:VAL:HG22	2.02	0.41
1:B:107:PRO:O	1:B:111:ARG:HG3	2.21	0.41
1:D:129[A]:VAL:HG22	1:D:166:PRO:HB2	2.03	0.41
1:D:396:GLU:HG2	1:D:420:ARG:HB3	2.02	0.41
1:D:86[B]:TYR:HB3	1:D:87:PRO:HD3	2.02	0.41
1:A:468:LEU:HD12	1:A:471:LYS:HD3	2.02	0.41
1:B:28:CYS:SG	1:B:54:GLU:HG3	2.61	0.41
1:C:146:ARG:HG2	1:C:194:HIS:HE1	1.86	0.41
1:B:538:TYR:CE1	1:B:540:PRO:HG3	2.56	0.41
1:B:71:PRO:HA	1:B:98:PRO:O	2.21	0.41
1:A:59:PHE:O	1:A:62:LEU:HB3	2.21	0.41
1:B:406:MET:N	1:B:407:PRO:CD	2.83	0.41
1:D:175:GLU:N	6:D:1582:SO4:O3	2.53	0.41
1:D:246:GLN:OE1	1:D:355:SER:HB3	2.21	0.41
1:A:394:VAL:HA	1:A:395:PRO:HD3	1.94	0.41
1:C:77:THR:OG1	4:C:603:EDO:O2	2.29	0.41
1:D:16:GLU:HG2	1:D:149:ARG:O	2.21	0.41
1:D:400:LEU:HD11	1:D:454:VAL:HG23	2.03	0.40
1:A:107:PRO:HD3	6:A:1582:SO4:O4	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:LEU:HD23	1:B:280:LEU:HA	1.90	0.40
1:B:394:VAL:HA	1:B:395:PRO:HD3	1.97	0.40
1:B:512:LEU:HA	1:B:512:LEU:HD12	1.92	0.40
1:B:570:ALA:O	1:B:574:VAL:HG23	2.21	0.40
1:A:77:THR:OG1	4:A:603:EDO:H22	2.21	0.40
1:B:428:ARG:HD2	1:B:428:ARG:HA	1.70	0.40
1:B:576:LYS:C	1:B:578:TRP:N	2.75	0.40
1:D:484:ASN:HB3	1:D:554:THR:OG1	2.21	0.40
1:D:544:LYS:HB2	1:D:545:PRO:HD2	2.04	0.40
1:C:2:THR:O	1:C:2:THR:CG2	2.68	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	583/604 (96%)	555 (95%)	24 (4%)	4 (1%)	22 23
1	B	579/604 (96%)	555 (96%)	17 (3%)	7 (1%)	13 11
1	C	577/604 (96%)	552 (96%)	22 (4%)	3 (0%)	29 32
1	D	583/604 (96%)	564 (97%)	17 (3%)	2 (0%)	41 47
All	All	2322/2416 (96%)	2226 (96%)	80 (3%)	16 (1%)	22 23

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	PRO
1	A	176	PRO
1	A	498	GLU
1	B	163	PRO
1	B	176	PRO

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Mol	Chain	Res	Type
1	B	350	ALA
1	B	352	THR
1	C	163	PRO
1	C	176	PRO
1	C	351	ALA
1	D	163	PRO
1	D	176	PRO
1	B	353	ARG
1	A	405	SER
1	B	351	ALA
1	B	405	SER

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	495/511 (97%)	467 (94%)	28 (6%)	20 22
1	B	491/511 (96%)	466 (95%)	25 (5%)	24 27
1	C	489/511 (96%)	468 (96%)	21 (4%)	29 35
1	D	495/511 (97%)	473 (96%)	22 (4%)	28 34
All	All	1970/2044 (96%)	1874 (95%)	96 (5%)	27 29

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	LEU
1	A	86[A]	TYR
1	A	86[B]	TYR
1	A	129[A]	VAL
1	A	129[B]	VAL
1	A	161	LYS
1	A	201	THR
1	A	202	GLN
1	A	208	SER
1	A	209	LEU

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Mol	Chain	Res	Type
1	A	254	LEU
1	A	259	ASN
1	A	266	THR
1	A	376	SER
1	A	386	LEU
1	A	389	ILE
1	A	445	GLU
1	A	454	VAL
1	A	464	LEU
1	A	471	LYS
1	A	495	GLN
1	A	497	SER
1	A	500	THR
1	A	512	LEU
1	A	515	LYS
1	A	547	LEU
1	A	559[A]	ARG
1	A	559[B]	ARG
1	B	55	ARG
1	B	64	LEU
1	B	86[A]	TYR
1	B	86[B]	TYR
1	B	112[A]	GLU
1	B	112[B]	GLU
1	B	129	VAL
1	B	195	VAL
1	B	201	THR
1	B	203	SER
1	B	254	LEU
1	B	259	ASN
1	B	312	GLN
1	B	353	ARG
1	B	365	ASN
1	B	367	ARG
1	B	386	LEU
1	B	448	LYS
1	B	464	LEU
1	B	471	LYS
1	B	498	GLU
1	B	512	LEU
1	B	515	LYS
1	B	547	LEU

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Mol	Chain	Res	Type
1	B	559	ARG
1	C	86[A]	TYR
1	C	86[B]	TYR
1	C	106	ARG
1	C	201	THR
1	C	206	ARG
1	C	207	GLU
1	C	209	LEU
1	C	250	LEU
1	C	259	ASN
1	C	266	THR
1	C	352	THR
1	C	367	ARG
1	C	372	LEU
1	C	386	LEU
1	C	448	LYS
1	C	464	LEU
1	C	512	LEU
1	C	515	LYS
1	C	547	LEU
1	C	559	ARG
1	C	566	MET
1	D	72	VAL
1	D	86[A]	TYR
1	D	86[B]	TYR
1	D	191	THR
1	D	195	VAL
1	D	201	THR
1	D	202	GLN
1	D	209	LEU
1	D	254	LEU
1	D	259	ASN
1	D	266	THR
1	D	329	SER
1	D	367	ARG
1	D	386	LEU
1	D	448	LYS
1	D	464	LEU
1	D	495	GLN
1	D	512	LEU
1	D	547	LEU
1	D	559[A]	ARG

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Mol	Chain	Res	Type
1	D	559[B]	ARG
1	D	579	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	431	ASN
1	B	127	ASN
1	B	202	GLN
1	B	334	HIS
1	B	431	ASN
1	C	117	GLN
1	C	127	ASN
1	C	431	ASN
1	D	117	GLN
1	D	127	ASN
1	D	194	HIS
1	D	431	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [\(i\)](#)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	EDO	C	603	-	3,3,3	0.53	0	2,2,2	0.33	0
4	EDO	A	603	-	3,3,3	0.46	0	2,2,2	0.35	0
6	SO4	B	1583	-	4,4,4	0.14	0	6,6,6	0.16	0
6	SO4	A	1583	-	4,4,4	0.15	0	6,6,6	0.14	0
6	SO4	D	1583	-	4,4,4	0.17	0	6,6,6	0.27	0
4	EDO	D	603	-	3,3,3	0.55	0	2,2,2	0.28	0
2	TPP	B	601	3	22,27,27	1.70	4 (18%)	29,40,40	1.97	10 (34%)
6	SO4	C	1580	-	4,4,4	0.31	0	6,6,6	0.50	0
4	EDO	B	603	-	3,3,3	0.54	0	2,2,2	0.45	0
2	TPP	D	601	3	22,27,27	2.19	5 (22%)	29,40,40	2.05	11 (37%)
6	SO4	C	1581	-	4,4,4	0.13	0	6,6,6	0.17	0
2	TPP	C	601	3	22,27,27	1.93	6 (27%)	29,40,40	2.12	10 (34%)
6	SO4	B	1582	-	4,4,4	0.23	0	6,6,6	0.58	0
2	TPP	A	601	3	22,27,27	1.99	3 (13%)	29,40,40	2.23	12 (41%)
6	SO4	A	1582	-	4,4,4	0.28	0	6,6,6	0.20	0
6	SO4	D	1582	-	4,4,4	0.24	0	6,6,6	0.11	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	EDO	C	603	-	-	0/1/1/1	-
4	EDO	A	603	-	-	0/1/1/1	-
4	EDO	D	603	-	-	1/1/1/1	-
4	EDO	B	603	-	-	0/1/1/1	-
2	TPP	D	601	3	-	1/16/17/17	0/2/2/2
2	TPP	B	601	3	-	1/16/17/17	0/2/2/2
2	TPP	C	601	3	-	0/16/17/17	0/2/2/2
2	TPP	A	601	3	-	1/16/17/17	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	TPP	C6-C5	7.20	1.54	1.50
2	C	601	TPP	C6-C5	6.44	1.53	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	TPP	C6-C5	6.35	1.53	1.50
2	A	601	TPP	C4-N3	-4.21	1.36	1.39
2	D	601	TPP	PB-O1B	4.02	1.63	1.50
2	B	601	TPP	C6-C5	3.84	1.52	1.50
2	B	601	TPP	PB-O1B	3.76	1.62	1.50
2	B	601	TPP	C4-N3	-3.25	1.36	1.39
2	A	601	TPP	PA-O1A	2.99	1.61	1.50
2	D	601	TPP	C4-N3	-2.92	1.37	1.39
2	D	601	TPP	PA-O1A	2.88	1.61	1.50
2	B	601	TPP	PA-O1A	2.82	1.60	1.50
2	C	601	TPP	PB-O1B	2.61	1.59	1.50
2	C	601	TPP	C5'-C4'	-2.57	1.38	1.42
2	C	601	TPP	C4-N3	-2.52	1.37	1.39
2	D	601	TPP	C5'-C4'	-2.25	1.39	1.42
2	C	601	TPP	PA-O1A	2.17	1.58	1.50
2	C	601	TPP	CM4-C4	2.14	1.54	1.49

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	TPP	CM2-C2'-N1'	4.41	121.99	117.14
2	C	601	TPP	C5-C4-N3	4.18	115.94	107.57
2	A	601	TPP	C6-C5-C4	4.15	130.76	127.43
2	A	601	TPP	C6'-N1'-C2'	4.10	122.93	115.96
2	C	601	TPP	C6-C5-C4	3.87	130.54	127.43
2	D	601	TPP	C5-C4-N3	3.85	115.28	107.57
2	B	601	TPP	C5-C4-N3	3.79	115.15	107.57
2	A	601	TPP	C5-C4-N3	3.73	115.04	107.57
2	B	601	TPP	CM4-C4-C5	-3.63	119.66	127.60
2	A	601	TPP	CM2-C2'-N1'	3.54	121.03	117.14
2	B	601	TPP	N1'-C2'-N3'	-3.50	119.52	125.54
2	A	601	TPP	PA-O3A-PB	-3.44	121.01	132.83
2	B	601	TPP	C6'-N1'-C2'	3.32	121.61	115.96
2	D	601	TPP	C6-C5-C4	3.29	130.07	127.43
2	B	601	TPP	CM2-C2'-N1'	3.27	120.74	117.14
2	D	601	TPP	N1'-C2'-N3'	-3.24	119.96	125.54
2	D	601	TPP	O3B-PB-O3A	3.23	115.47	104.64
2	C	601	TPP	N1'-C2'-N3'	-3.20	120.03	125.54
2	D	601	TPP	C6'-N1'-C2'	3.18	121.37	115.96
2	D	601	TPP	CM4-C4-C5	-3.17	120.67	127.60
2	A	601	TPP	N1'-C2'-N3'	-3.17	120.08	125.54
2	A	601	TPP	C5'-C6'-N1'	-3.10	118.65	123.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	TPP	CM2-C2'-N1'	3.08	120.53	117.14
2	C	601	TPP	C6'-N1'-C2'	3.05	121.16	115.96
2	C	601	TPP	CM4-C4-C5	-2.94	121.17	127.60
2	B	601	TPP	C7'-N3-C2	-2.93	120.05	125.35
2	A	601	TPP	CM4-C4-C5	-2.90	121.27	127.60
2	D	601	TPP	PA-O3A-PB	-2.86	123.02	132.83
2	A	601	TPP	O2B-PB-O1B	-2.73	100.00	110.68
2	C	601	TPP	PA-O3A-PB	-2.63	123.80	132.83
2	D	601	TPP	C7'-N3-C2	-2.63	120.60	125.35
2	B	601	TPP	O3B-PB-O3A	2.61	113.40	104.64
2	A	601	TPP	O3B-PB-O3A	2.58	113.30	104.64
2	C	601	TPP	O3B-PB-O3A	2.52	113.10	104.64
2	A	601	TPP	C7'-N3-C2	-2.33	121.14	125.35
2	A	601	TPP	C5'-C4'-N4'	-2.20	119.06	122.19
2	C	601	TPP	C5'-C6'-N1'	-2.17	120.20	123.82
2	D	601	TPP	C5'-C4'-N4'	-2.12	119.17	122.19
2	B	601	TPP	CM4-C4-N3	2.08	125.19	122.53
2	B	601	TPP	C2'-N3'-C4'	2.08	121.32	118.08
2	C	601	TPP	C5'-C4'-N4'	-2.06	119.26	122.19
2	D	601	TPP	N4'-C4'-N3'	2.05	119.93	117.03
2	B	601	TPP	PA-O3A-PB	-2.05	125.81	132.83

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	601	TPP	PB-O3A-PA-O7
2	B	601	TPP	PB-O3A-PA-O7
2	A	601	TPP	PB-O3A-PA-O7
4	D	603	EDO	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 64 short contacts:

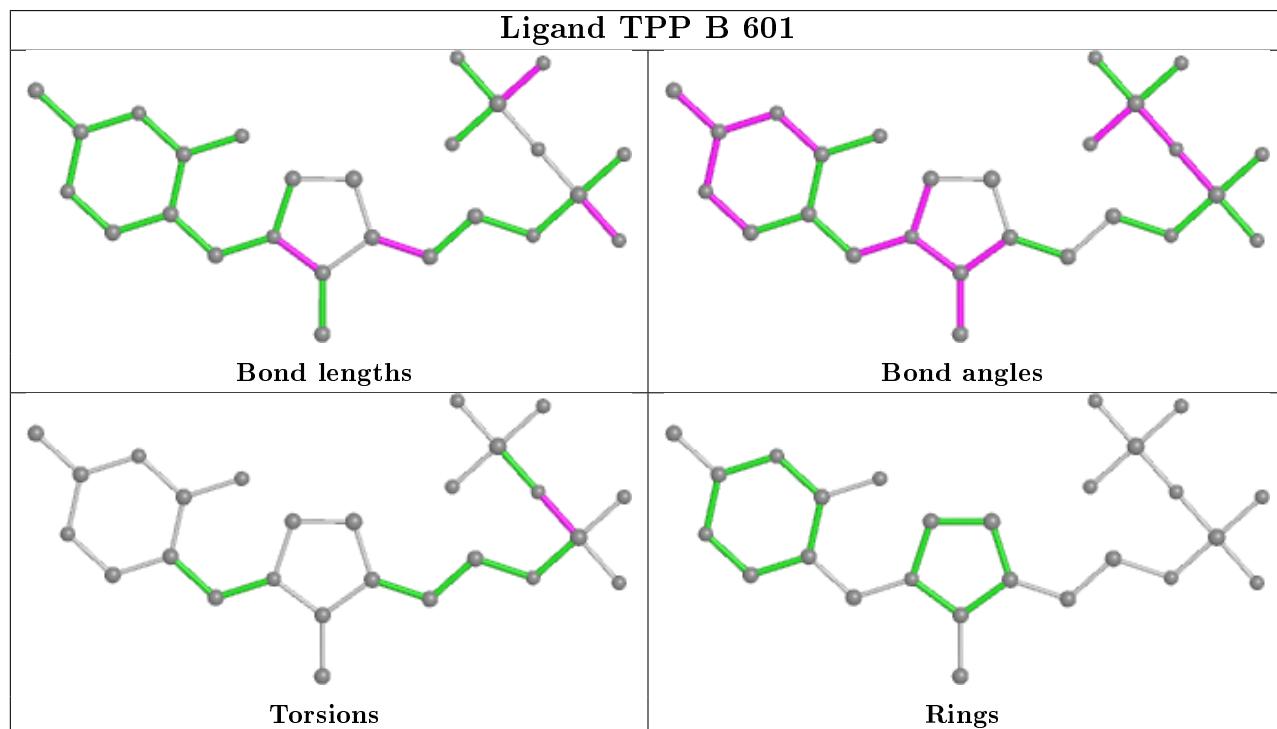
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	603	EDO	8	0
4	A	603	EDO	13	0
4	D	603	EDO	8	0
6	C	1580	SO4	5	0
4	B	603	EDO	6	0
2	D	601	TPP	2	0

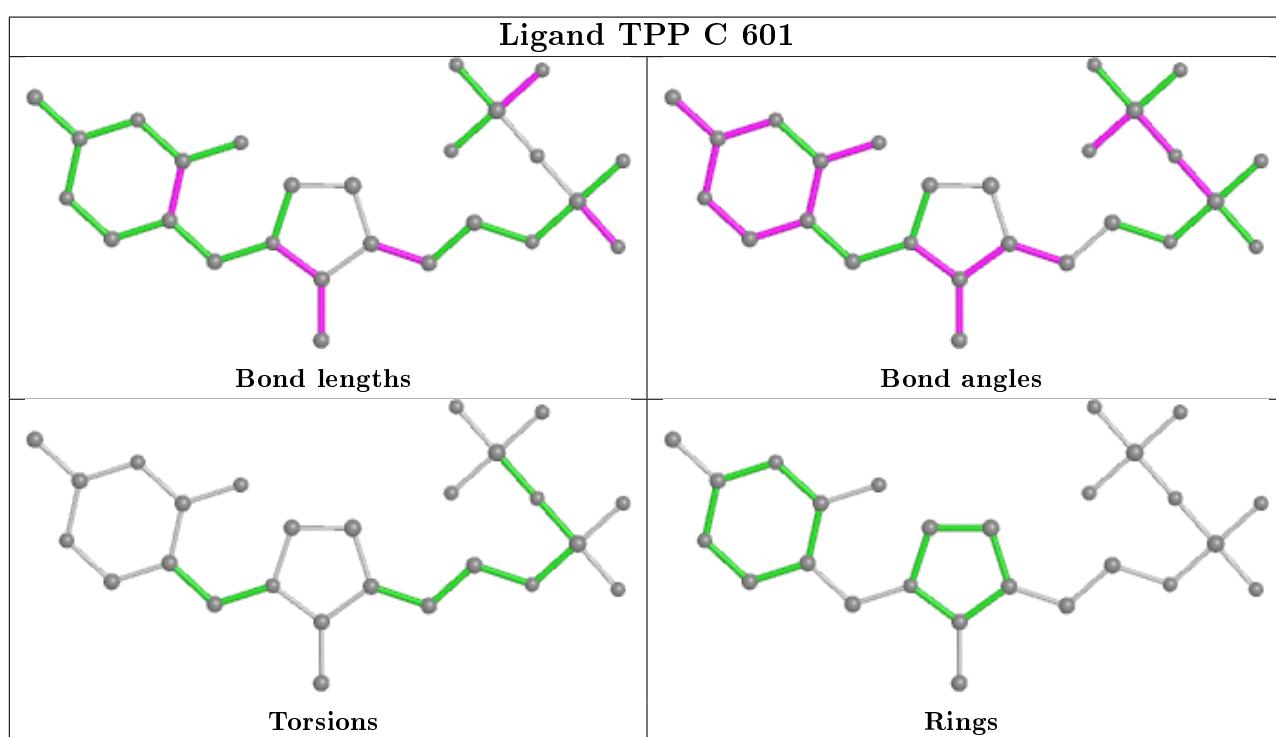
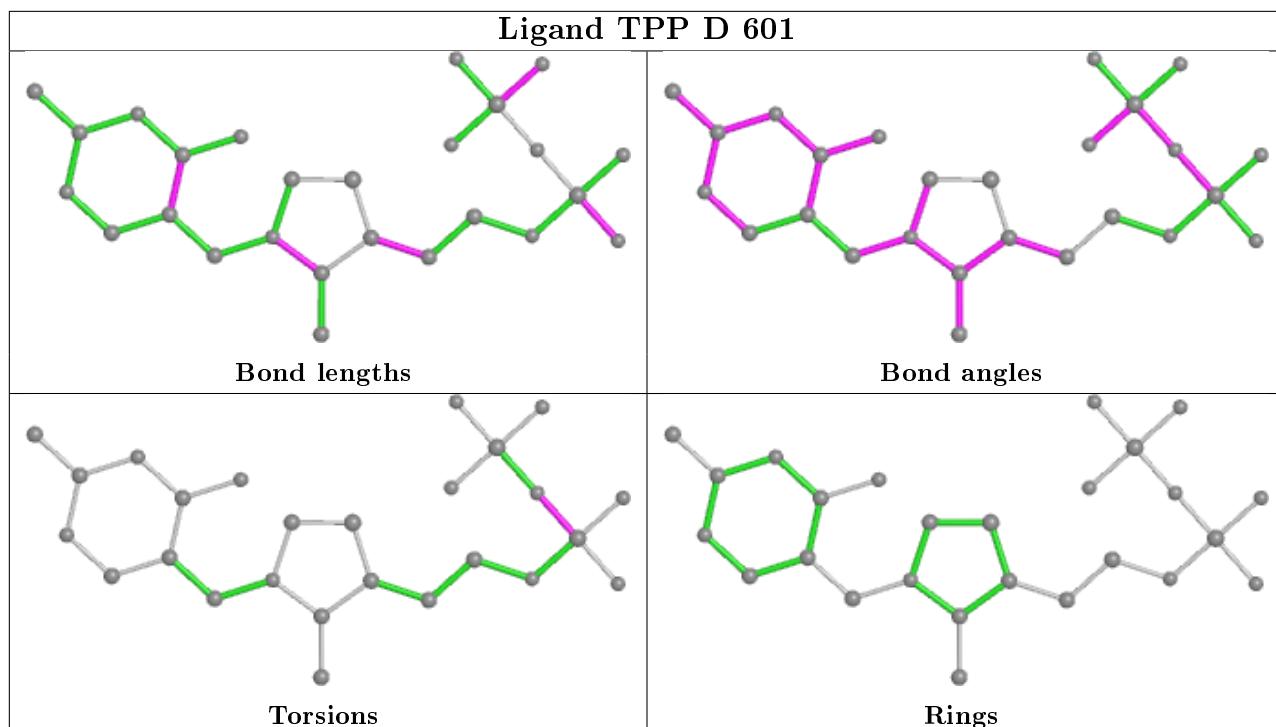
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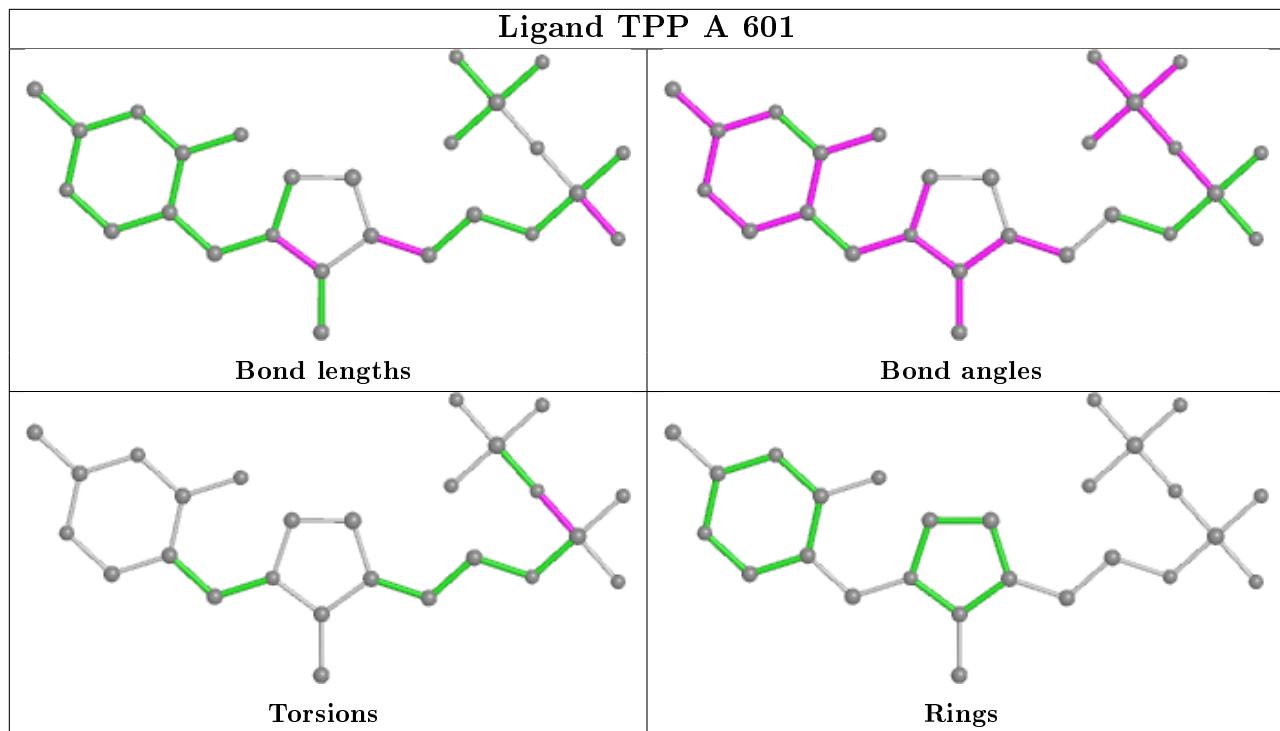
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1581	SO4	1	0
2	C	601	TPP	1	0
6	B	1582	SO4	6	0
2	A	601	TPP	2	0
6	A	1582	SO4	5	0
6	D	1582	SO4	9	0

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	579/604 (95%)	-0.11	4 (0%) 87 92	15, 29, 46, 61	1 (0%)
1	B	579/604 (95%)	0.16	23 (3%) 38 51	16, 34, 57, 67	3 (0%)
1	C	577/604 (95%)	0.07	13 (2%) 60 70	15, 33, 55, 68	6 (1%)
1	D	579/604 (95%)	-0.21	7 (1%) 79 86	17, 28, 44, 60	2 (0%)
All	All	2314/2416 (95%)	-0.02	47 (2%) 65 75	15, 30, 52, 68	12 (0%)

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	THR	6.4
1	B	352	THR	4.9
1	C	351	ALA	4.6
1	D	2	THR	4.6
1	B	2	THR	4.5
1	C	496	ALA	4.2
1	D	350	ALA	3.8
1	B	348	LEU	3.8
1	A	2	THR	3.8
1	C	350	ALA	3.7
1	D	351	ALA	3.1
1	C	495	GLN	3.1
1	B	349	THR	3.0
1	B	261	VAL	2.9
1	C	189	MET	2.8
1	B	578	TRP	2.8
1	B	260	GLY	2.7
1	B	569	GLU	2.7
1	C	494	PRO	2.7
1	D	580	LEU	2.6
1	B	266	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	101	VAL	2.5
1	B	497	SER	2.5
1	D	495	GLN	2.5
1	B	568	ASN	2.5
1	B	367	ARG	2.5
1	B	499	LYS	2.5
1	C	129	VAL	2.4
1	B	580	LEU	2.4
1	C	491	SER	2.3
1	D	352	THR	2.3
1	B	212	VAL	2.3
1	B	350	ALA	2.3
1	B	375	ILE	2.3
1	C	498	GLU	2.2
1	A	357	TRP	2.2
1	B	358	LEU	2.2
1	B	204	VAL	2.2
1	B	124	LEU	2.2
1	C	497	SER	2.1
1	D	200	GLY	2.1
1	C	569	GLU	2.1
1	A	578	TRP	2.1
1	A	572	ARG	2.1
1	B	207	GLU	2.1
1	C	499	LYS	2.1
1	B	205	ASP	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 [\(i\)](#)

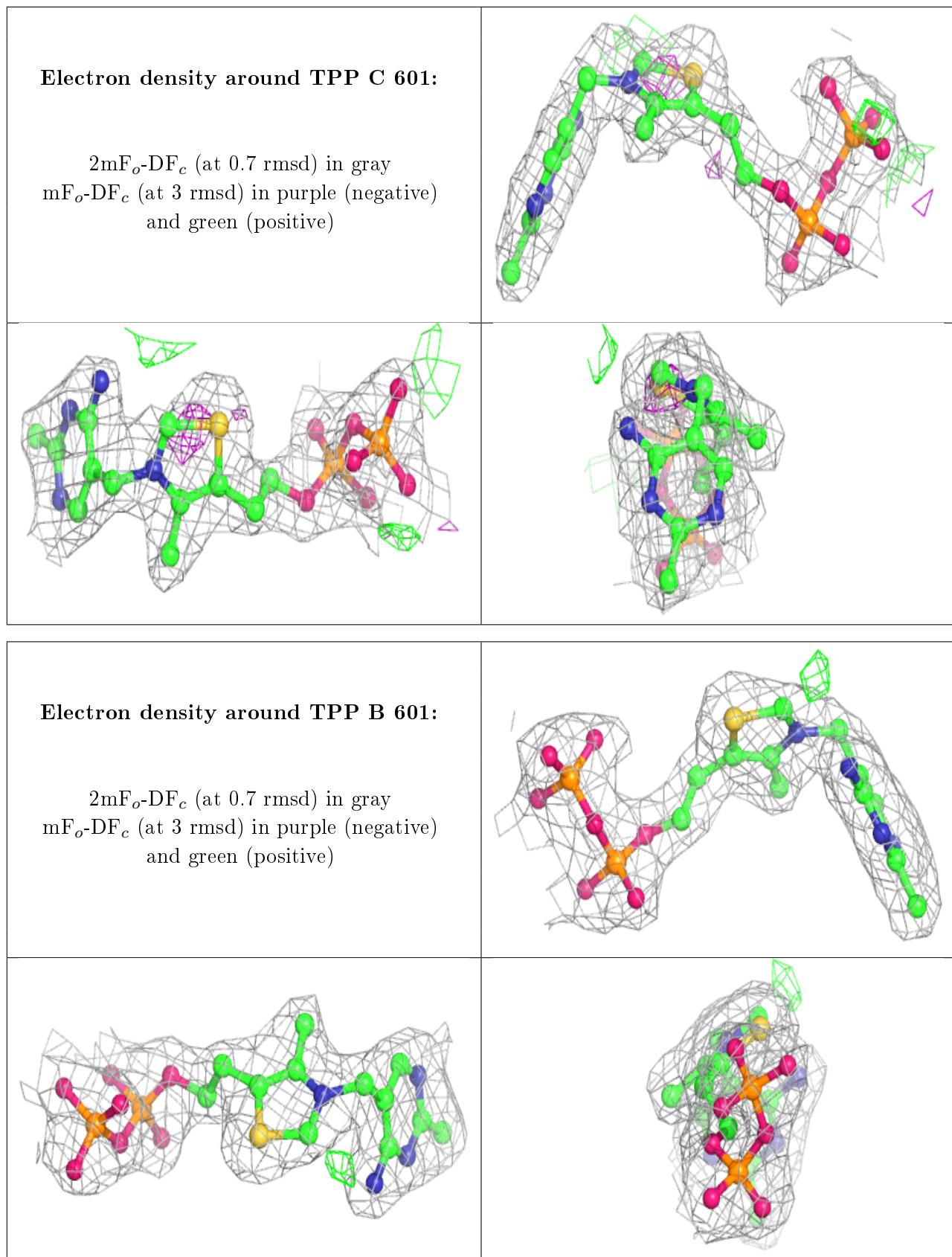
There are no carbohydrates in this entry.

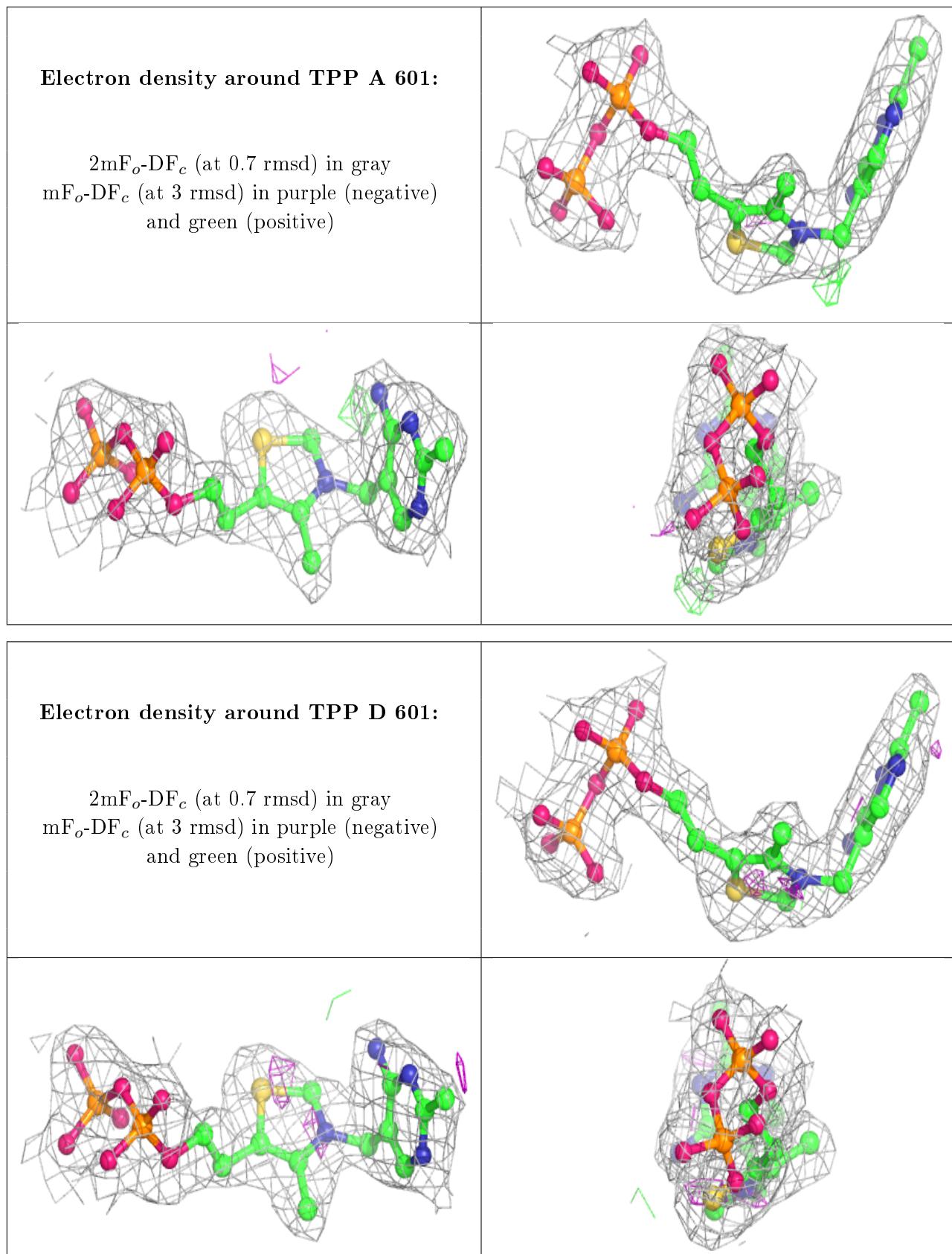
6.4 Ligands [\(i\)](#)

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
4	EDO	D	603	4/4	0.90	0.20	26,27,29,29	0
5	NA	A	1581	1/1	0.91	0.10	35,35,35,35	0
4	EDO	C	603	4/4	0.93	0.18	27,27,27,28	0
6	SO4	B	1583	5/5	0.93	0.13	31,31,31,31	5
4	EDO	A	603	4/4	0.94	0.20	25,27,28,29	0
6	SO4	B	1582	5/5	0.94	0.22	13,14,15,15	5
4	EDO	B	603	4/4	0.94	0.15	23,24,25,25	0
6	SO4	C	1581	5/5	0.94	0.15	26,27,27,27	5
6	SO4	A	1582	5/5	0.96	0.18	10,10,11,11	5
5	NA	C	1579	1/1	0.96	0.10	36,36,36,36	0
5	NA	B	1581	1/1	0.96	0.10	33,33,33,33	0
5	NA	D	1581	1/1	0.96	0.14	33,33,33,33	0
6	SO4	D	1583	5/5	0.97	0.24	21,22,22,22	5
6	SO4	A	1583	5/5	0.97	0.14	24,24,24,24	5
6	SO4	D	1582	5/5	0.98	0.28	16,16,17,17	5
2	TPP	C	601	26/26	0.98	0.10	22,23,24,24	0
2	TPP	B	601	26/26	0.98	0.10	21,24,26,27	0
6	SO4	C	1580	5/5	0.98	0.20	10,12,12,12	5
2	TPP	A	601	26/26	0.98	0.10	20,23,25,25	0
3	MN	B	602	1/1	0.99	0.08	29,29,29,29	0
2	TPP	D	601	26/26	0.99	0.09	19,21,23,24	0
3	MN	A	602	1/1	0.99	0.07	24,24,24,24	0
3	MN	C	602	1/1	1.00	0.04	24,24,24,24	0
3	MN	D	602	1/1	1.00	0.09	23,23,23,23	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.