



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:30 AM GMT

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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

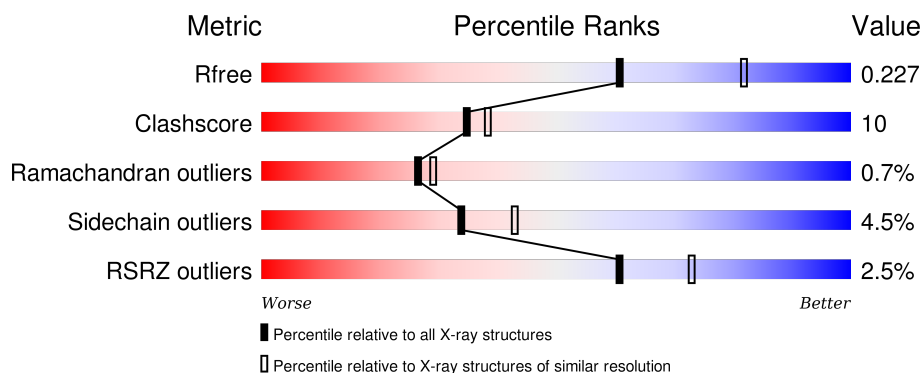
1 Overall quality at a glance

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}	91344	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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. 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	604	<div> <div>0%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>• •</div> </div> </div>
1	B	604	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>17%</div> <div>• • •</div> </div> </div>
1	C	604	<div> <div>3%</div> <div> <div></div> <div>77%</div> <div>17%</div> <div>• •</div> </div> </div>
1	D	604	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>• •</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

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

2 Entry composition

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

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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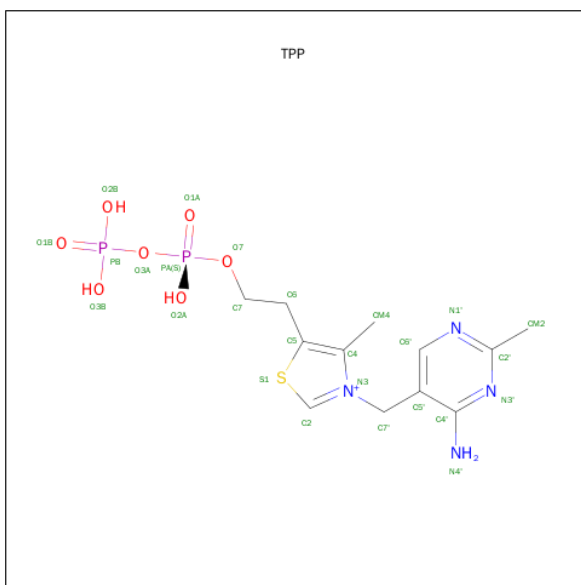
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	HIS	-	EXPRESSION TAG	UNP P23970
A	-2	MET	-	EXPRESSION TAG	UNP P23970
A	-1	LEU	-	EXPRESSION TAG	UNP P23970
A	0	GLU	-	EXPRESSION TAG	UNP P23970
B	-23	MET	-	EXPRESSION TAG	UNP P23970
B	-22	GLY	-	EXPRESSION TAG	UNP P23970
B	-21	SER	-	EXPRESSION TAG	UNP 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 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
2	C	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0
2	D	1	Total 26	C 12	N 4	O 7	P 2	S 1	0	0

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

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $\text{C}_2\text{H}_6\text{O}_2$).

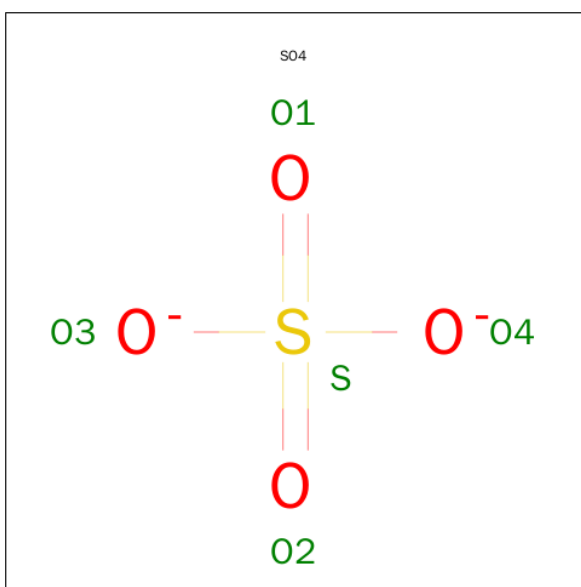


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		

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

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

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

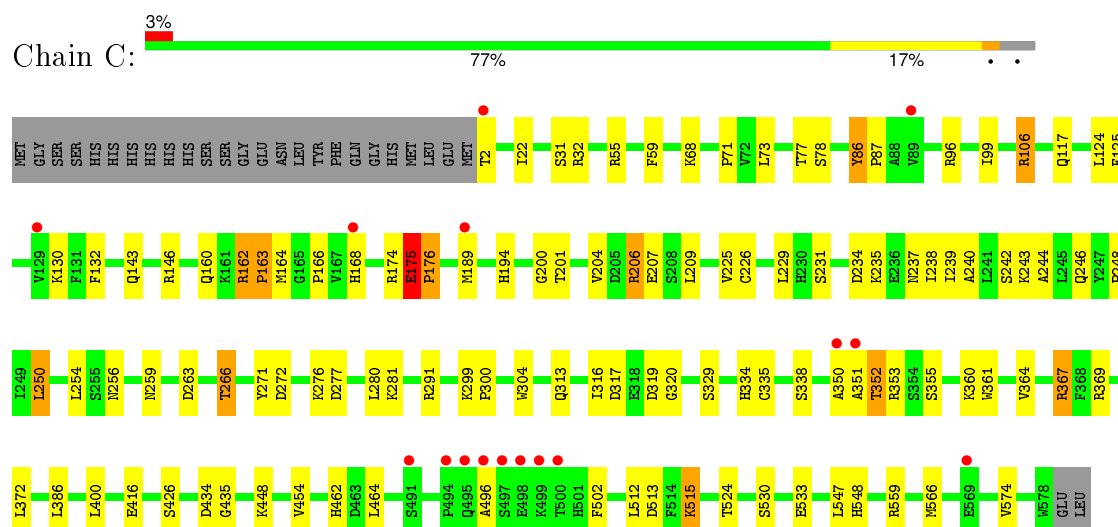


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	C	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

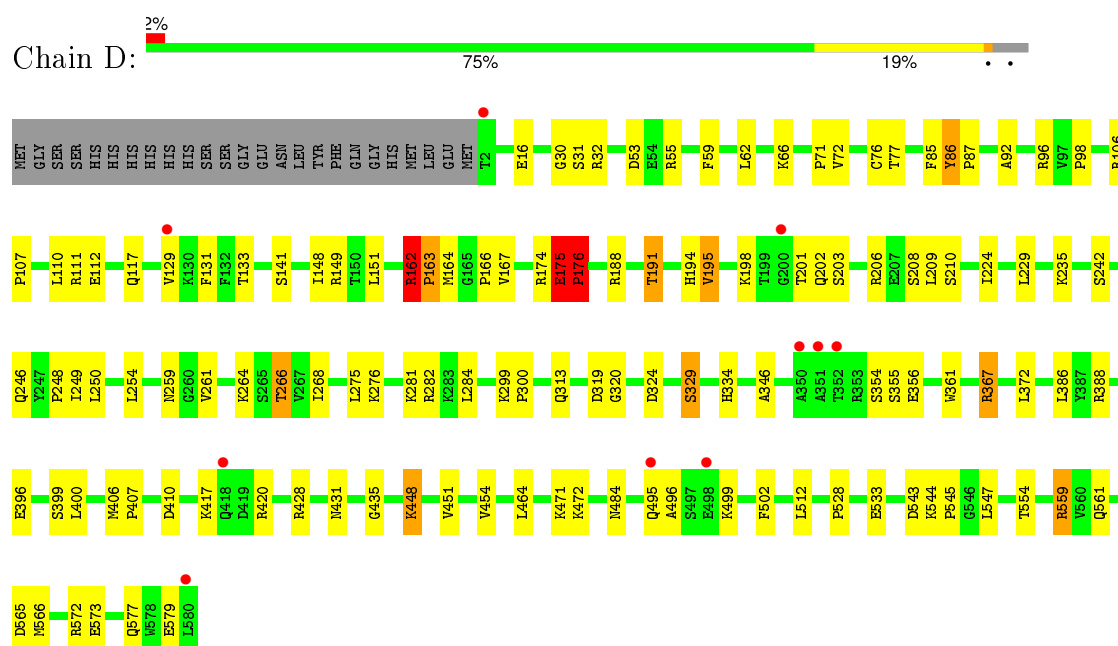
- Molecule 7 is water.

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

• 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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.18Å 152.99Å 158.50Å 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 2.34Å)	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 (5.29%)	DCC
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
Estimated twinning fraction	0.010 for -h,l,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	4 of 101872 reflections (0.004%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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, 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(°)	Ideal(°)
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(°)	Ideal(°)
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
6:C:1580:SO4:O4	7:C:2254:HOH:O	2.07	0.71
1:B:31:SER:H	4:B:603:EDO:H11	1.53	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:C:266:THR:HB	7:C:2131:HOH:O	2.02	0.58
1:A:400:LEU:HD11	1:A:454:VAL:CG2	2.34	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:D:59:PHE:CD1	1:D:435:GLY:HA3	2.39	0.57
1:C:250:LEU:N	1:C:250:LEU:HD23	2.20	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:C:434:ASP:HB3	1:C:462:HIS:CE1	2.40	0.57
1:A:78:SER:OG	1:A:106:ARG:NH1	2.38	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:D:174:ARG:HG3	6:D:1582:SO4:O2	2.07	0.55
1:A:249:ILE:HG13	1:A:266:THR:CG2	2.36	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:C:281:LYS:HG2	1:C:304:TRP:NE1	2.27	0.50
1:B:176:PRO:HD2	1:B:176:PRO:O	2.11	0.50
1:C:78:SER:OG	1:C:106:ARG:NH2	2.44	0.50
1:B:515:LYS:NZ	7:B:2205:HOH:O	2.44	0.50
1:B:162:ARG:HD3	1:B:319:ASP:OD1	2.11	0.50
1:A:372:LEU:HD23	1:A:375:ILE:HD12	1.92	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
4:C:603:EDO:H12	2:D:601:TPP:H7'2	1.94	0.49
1:C:320:GLY:HA2	1:C:334:HIS:CD2	2.47	0.49
1:C:277:ASP:OD2	1:C:280:LEU:N	2.36	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:D:117:GLN:NE2	4:D:603:EDO:C1	2.65	0.49
1:C:248:PRO:HG3	1:C:361:TRP:CD1	2.48	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:D:110:LEU:HD12	6:D:1582:SO4:O1	2.13	0.48
1:D:133:THR:HG21	1:D:151:LEU:HD11	1.95	0.48
1:A:86[B]:TYR:HD1	1:A:125:PHE:HD1	1.61	0.48
2:D:601:TPP:C2	2:D:601:TPP:HN42	2.27	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
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:D:471:LYS:HG3	1:D:472:LYS:N	2.28	0.48
1:B:299:LYS:HB3	1:B:300:PRO:HD3	1.94	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:32:ARG:H	4:A:603:EDO:H21	1.78	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:B:242:SER:OG	1:B:266:THR:HG21	2.13	0.48
1:A:242:SER:CB	1:A:266:THR:HG21	2.44	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:C:117:GLN:HE22	4:C:603:EDO:C2	2.27	0.47
1:B:445:GLU:O	1:B:448:LYS:HE2	2.13	0.47
1:D:248:PRO:CB	1:D:268:ILE:HD12	2.45	0.47
1:B:268:ILE:HG23	1:B:365:ASN:OD1	2.15	0.47
1:A:299:LYS:HB3	1:A:300:PRO:HD3	1.96	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:A:383:GLU:HB3	1:A:559[B]:ARG:HD2	1.96	0.47
1:D:141:SER:HB2	7:D:2077:HOH:O	2.15	0.47
1:B:203:SER:O	1:C:200:GLY:HA3	2.15	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:B:400:LEU:HD11	1:B:454:VAL:CG2	2.46	0.46
1:A:299:LYS:HE3	7:A:2159:HOH:O	2.14	0.46
1:D:428:ARG:HA	1:D:431:ASN:HD22	1.81	0.46
1:B:16:GLU:HG2	1:B:149:ARG:O	2.15	0.46
1:D:248:PRO:HB2	1:D:268:ILE:HD13	1.94	0.46
1:A:531:TRP:O	1:A:535:LYS:HG3	2.16	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:D:249:ILE:HG13	1:D:266:THR:HG23	1.98	0.46
1:B:249:ILE:HG13	1:B:266:THR:CG2	2.46	0.46
1:D:573:GLU:O	1:D:577:GLN:HG2	2.15	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:C:369:ARG:HD2	1:C:416:GLU:HG2	1.97	0.46
1:C:246:GLN:OE1	1:C:355:SER:HB3	2.15	0.46
1:D:96:ARG:HA	1:D:164:MET:O	2.16	0.46
1:B:86[B]:TYR:HB3	1:B:87:PRO:HD3	1.98	0.46
1:B:445:GLU:HG2	1:B:475:ILE:CD1	2.46	0.45
1:B:129:VAL:HG22	1:B:167:VAL:HA	1.98	0.45
1:D:250:LEU:N	1:D:250:LEU:HD23	2.31	0.45
1:D:284:LEU:HB3	1:D:361:TRP:CZ2	2.52	0.45
1:A:43:HIS:HA	1:A:44:PRO:HD3	1.78	0.45
1:C:524:THR:OG1	1:C:548:HIS:CD2	2.69	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: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:D:62:LEU:O	1:D:66:LYS:HB2	2.17	0.45
1:B:222:GLY:HA3	1:B:247:TYR:CZ	2.51	0.45
1:D:528:PRO:CB	1:D:533:GLU:HG3	2.47	0.45
1:D:92:ALA:HB3	1:D:166:PRO:HG3	1.99	0.45
1:A:112[B]:GLU:CD	7:A:2055:HOH:O	2.55	0.45
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:316:ILE:HD12	1:C:316:ILE:N	2.33	0.44
1:D:96:ARG:NH1	1:D:319:ASP:HB2	2.32	0.44
1:D:112[B]:GLU:OE1	7:D:2045:HOH:O	2.21	0.44
1:C:86[A]:TYR:CZ	1:C:125:PHE:HA	2.51	0.44
1:D:528:PRO:HB3	1:D:533:GLU:HG3	1.99	0.44
1:B:250:LEU:HD23	1:B:250:LEU:N	2.32	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:299:LYS:HB3	1:C:300:PRO:HD3	1.98	0.44
1:C:55:ARG:NH2	1:D:53:ASP:OD1	2.46	0.44
1:D:299:LYS:HB3	1:D:300:PRO:HD3	1.99	0.44
1:C:239:ILE:O	1:C:240:ALA:C	2.56	0.44
1:C:86[B]:TYR:CD1	1:D:86[B]:TYR:CD1	3.06	0.44
1:A:95:SER:O	1:A:96:ARG:HB2	2.17	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:C:515:LYS:HE3	1:C:515:LYS:HB3	1.48	0.44
1:A:193:ARG:NH1	7:A:2119:HOH:O	2.50	0.44

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:GLN:NE2	4:C:603:EDO:H21	2.34	0.42
1:A:428:ARG:HA	1:A:428:ARG:HD2	1.88	0.42
1:A:559[A]:ARG:CG	1:A:560:VAL:N	2.78	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:B:431:ASN:HD22	1:B:431:ASN:N	2.18	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:B:69:GLN:OE1	1:B:164:MET:CE	2.68	0.42
1:A:476:PRO:HG3	1:A:542:ALA:HA	2.01	0.42
1:D:106:ARG:NH1	1:D:117:GLN:HB3	2.35	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:367:ARG:HA	1:A:367:ARG:HD3	1.81	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:86[B]:TYR:HB3	1:D:87:PRO:HD3	2.02	0.41
1:D:396:GLU:HG2	1:D:420:ARG:HB3	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:A:468:LEU:HD12	1:A:471:LYS:HD3	2.02	0.41
1:D:175:GLU:N	6:D:1582:SO4:O3	2.53	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:D:246:GLN:OE1	1:D:355:SER:HB3	2.21	0.41
1:B:406:MET:N	1:B:407:PRO:CD	2.83	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:A:394:VAL:HA	1:A:395:PRO:HD3	1.94	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: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:280:LEU:HD23	1:B:280:LEU:HA	1.90	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:576:LYS:C	1:B:578:TRP:N	2.75	0.40
1:B:428:ARG:HD2	1:B:428:ARG:HA	1.70	0.40
1:D:544:LYS:HB2	1:D:545:PRO:HD2	2.04	0.40
1:D:484:ASN:HB3	1:D:554:THR:OG1	2.21	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%)	26	29
1	B	579/604 (96%)	555 (96%)	17 (3%)	7 (1%)	16	15
1	C	577/604 (96%)	552 (96%)	22 (4%)	3 (0%)	34	39
1	D	583/604 (96%)	564 (97%)	17 (3%)	2 (0%)	46	55
All	All	2322/2416 (96%)	2226 (96%)	80 (3%)	16 (1%)	26	29

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 ⓘ

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%)	25	30
1	B	491/511 (96%)	466 (95%)	25 (5%)	29	36
1	C	489/511 (96%)	468 (96%)	21 (4%)	35	45
1	D	495/511 (97%)	473 (96%)	22 (4%)	35	44
All	All	1970/2044 (96%)	1874 (95%)	96 (5%)	34	39

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	$\# Z > 2$
6	SO4	A	1582	-	4,4,4	0.51	0	6,6,6	0.28	0
6	SO4	A	1583	-	4,4,4	0.34	0	6,6,6	0.12	0
2	TPP	A	601	3	20,27,27	1.47	2 (10%)	31,40,40	2.09	10 (32%)
4	EDO	A	603	-	3,3,3	0.46	0	2,2,2	0.44	0
6	SO4	B	1582	-	4,4,4	0.56	0	6,6,6	0.37	0
6	SO4	B	1583	-	4,4,4	0.14	0	6,6,6	0.14	0
2	TPP	B	601	3	20,27,27	1.49	3 (15%)	31,40,40	1.85	8 (25%)
4	EDO	B	603	-	3,3,3	0.54	0	2,2,2	0.54	0
6	SO4	C	1580	-	4,4,4	0.70	0	6,6,6	0.44	0
6	SO4	C	1581	-	4,4,4	0.26	0	6,6,6	0.18	0
2	TPP	C	601	3	20,27,27	1.32	4 (20%)	31,40,40	1.93	9 (29%)
4	EDO	C	603	-	3,3,3	0.54	0	2,2,2	0.42	0
6	SO4	D	1582	-	4,4,4	0.57	0	6,6,6	0.13	0
6	SO4	D	1583	-	4,4,4	0.37	0	6,6,6	0.27	0
2	TPP	D	601	3	20,27,27	1.56	4 (20%)	31,40,40	1.88	11 (35%)
4	EDO	D	603	-	3,3,3	0.56	0	2,2,2	0.36	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
6	SO4	A	1582	-	-	0/0/0/0	0/0/0/0
6	SO4	A	1583	-	-	0/0/0/0	0/0/0/0
2	TPP	A	601	3	-	0/16/17/17	0/2/2/2
4	EDO	A	603	-	-	0/1/1/1	0/0/0/0
6	SO4	B	1582	-	-	0/0/0/0	0/0/0/0
6	SO4	B	1583	-	-	0/0/0/0	0/0/0/0
2	TPP	B	601	3	-	0/16/17/17	0/2/2/2
4	EDO	B	603	-	-	0/1/1/1	0/0/0/0
6	SO4	C	1580	-	-	0/0/0/0	0/0/0/0
6	SO4	C	1581	-	-	0/0/0/0	0/0/0/0
2	TPP	C	601	3	-	0/16/17/17	0/2/2/2
4	EDO	C	603	-	-	0/1/1/1	0/0/0/0
6	SO4	D	1582	-	-	0/0/0/0	0/0/0/0
6	SO4	D	1583	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TPP	D	601	3	-	0/16/17/17	0/2/2/2
4	EDO	D	603	-	-	0/1/1/1	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	TPP	C4-N3	-4.21	1.36	1.39
2	B	601	TPP	C4-N3	-3.25	1.36	1.39
2	D	601	TPP	C4-N3	-2.92	1.37	1.39
2	C	601	TPP	C4-N3	-2.52	1.37	1.39
2	D	601	TPP	PB-O3B	-2.03	1.47	1.54
2	C	601	TPP	CM4-C4	2.02	1.54	1.49
2	C	601	TPP	PA-O1A	2.03	1.58	1.51
2	C	601	TPP	PB-O1B	2.37	1.59	1.51
2	B	601	TPP	PA-O1A	2.67	1.60	1.51
2	D	601	TPP	PA-O1A	2.72	1.61	1.51
2	A	601	TPP	PA-O1A	2.83	1.61	1.51
2	B	601	TPP	PB-O1B	3.50	1.62	1.51
2	D	601	TPP	PB-O1B	3.75	1.63	1.51

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	TPP	CM4-C4-C5	-4.11	119.66	128.90
2	D	601	TPP	CM4-C4-C5	-3.66	120.67	128.90
2	A	601	TPP	PA-O3A-PB	-3.48	121.01	132.67
2	C	601	TPP	CM4-C4-C5	-3.44	121.17	128.90
2	A	601	TPP	CM4-C4-C5	-3.40	121.27	128.90
2	A	601	TPP	O2B-PB-O1B	-3.29	100.00	110.58
2	B	601	TPP	N1'-C2'-N3'	-3.28	119.52	125.60
2	D	601	TPP	N1'-C2'-N3'	-3.05	119.96	125.60
2	C	601	TPP	N1'-C2'-N3'	-3.01	120.03	125.60
2	A	601	TPP	C5'-C6'-N1'	-3.00	118.65	123.86
2	A	601	TPP	N1'-C2'-N3'	-2.98	120.08	125.60
2	D	601	TPP	PA-O3A-PB	-2.88	123.02	132.67
2	C	601	TPP	PA-O3A-PB	-2.64	123.80	132.67
2	A	601	TPP	C5'-C4'-N4'	-2.17	119.06	122.25
2	C	601	TPP	C5'-C6'-N1'	-2.11	120.20	123.86
2	D	601	TPP	C5'-C4'-N4'	-2.10	119.17	122.25
2	B	601	TPP	PA-O3A-PB	-2.05	125.81	132.67
2	C	601	TPP	C5'-C4'-N4'	-2.04	119.26	122.25
2	D	601	TPP	N4'-C4'-N3'	2.06	119.93	116.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	601	TPP	O3A-PA-O7	2.10	108.52	102.94
2	B	601	TPP	O3A-PA-O7	2.13	108.58	102.94
2	D	601	TPP	O3B-PB-O3A	2.29	115.47	105.09
2	B	601	TPP	C6-C5-S1	2.77	124.11	120.24
2	D	601	TPP	C6-C5-C4	2.80	130.07	127.56
2	D	601	TPP	CM2-C2'-N1'	2.91	120.53	117.03
2	C	601	TPP	C6'-N1'-C2'	3.08	121.16	115.77
2	B	601	TPP	CM2-C2'-N1'	3.09	120.74	117.03
2	D	601	TPP	C6'-N1'-C2'	3.21	121.37	115.77
2	C	601	TPP	C6-C5-C4	3.32	130.54	127.56
2	A	601	TPP	CM2-C2'-N1'	3.34	121.03	117.03
2	A	601	TPP	C5-C4-N3	3.34	115.04	107.69
2	B	601	TPP	C6'-N1'-C2'	3.34	121.61	115.77
2	B	601	TPP	C5-C4-N3	3.39	115.15	107.69
2	D	601	TPP	C5-C4-N3	3.45	115.28	107.69
2	A	601	TPP	C6-C5-C4	3.57	130.76	127.56
2	C	601	TPP	C5-C4-N3	3.75	115.94	107.69
2	A	601	TPP	C6'-N1'-C2'	4.10	122.93	115.77
2	C	601	TPP	CM2-C2'-N1'	4.13	121.99	117.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1582	SO4	5	0
2	A	601	TPP	2	0
4	A	603	EDO	13	0
6	B	1582	SO4	6	0
4	B	603	EDO	6	0
6	C	1580	SO4	5	0
6	C	1581	SO4	1	0
2	C	601	TPP	1	0
4	C	603	EDO	8	0
6	D	1582	SO4	9	0
2	D	601	TPP	2	0
4	D	603	EDO	8	0

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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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%)	-0.06	6 (1%) 84 92	15, 29, 46, 61	1 (0%)
1	B	579/604 (95%)	0.22	25 (4%) 39 53	16, 34, 57, 67	3 (0%)
1	C	577/604 (95%)	0.13	16 (2%) 56 69	15, 33, 55, 68	6 (1%)
1	D	579/604 (95%)	-0.16	10 (1%) 73 83	17, 28, 44, 60	2 (0%)
All	All	2314/2416 (95%)	0.03	57 (2%) 61 73	15, 30, 52, 68	12 (0%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	2	THR	6.7
1	B	352	THR	5.1
1	C	351	ALA	4.8
1	D	2	THR	4.8
1	B	2	THR	4.6
1	C	496	ALA	4.3
1	A	2	THR	3.9
1	D	350	ALA	3.9
1	B	348	LEU	3.9
1	C	350	ALA	3.9
1	D	351	ALA	3.3
1	C	495	GLN	3.2
1	B	349	THR	3.1
1	B	261	VAL	3.0
1	C	189	MET	3.0
1	B	578	TRP	2.9
1	B	260	GLY	2.9
1	C	494	PRO	2.8
1	B	569	GLU	2.8
1	D	580	LEU	2.8
1	B	266	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	101	VAL	2.7
1	B	497	SER	2.6
1	B	568	ASN	2.6
1	D	495	GLN	2.6
1	B	367	ARG	2.6
1	B	499	LYS	2.6
1	C	129	VAL	2.5
1	B	580	LEU	2.5
1	B	212	VAL	2.5
1	D	352	THR	2.4
1	C	491	SER	2.4
1	B	350	ALA	2.4
1	B	375	ILE	2.4
1	C	498	GLU	2.4
1	A	357	TRP	2.4
1	B	204	VAL	2.3
1	B	358	LEU	2.3
1	C	497	SER	2.3
1	B	124	LEU	2.3
1	A	578	TRP	2.2
1	D	200	GLY	2.2
1	C	569	GLU	2.2
1	B	205	ASP	2.2
1	B	207	GLU	2.2
1	A	572	ARG	2.1
1	C	499	LYS	2.1
1	B	245	LEU	2.1
1	C	168	HIS	2.1
1	D	129[A]	VAL	2.1
1	C	89	VAL	2.1
1	D	418	GLN	2.0
1	D	498	GLU	2.0
1	B	353	ARG	2.0
1	A	101	VAL	2.0
1	C	500	THR	2.0
1	A	494	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
6	SO4	A	1582	5/5	0.96	0.18	9.10	10,10,11,11	5
6	SO4	D	1582	5/5	0.98	0.28	8.07	16,16,17,17	5
4	EDO	A	603	4/4	0.94	0.20	6.88	25,27,28,29	0
4	EDO	D	603	4/4	0.90	0.20	4.78	26,27,29,29	0
6	SO4	B	1582	5/5	0.94	0.22	4.39	13,14,15,15	5
6	SO4	C	1580	5/5	0.98	0.20	4.19	10,12,12,12	5
4	EDO	C	603	4/4	0.93	0.18	3.03	27,27,27,28	0
5	NA	D	1581	1/1	0.96	0.14	1.81	33,33,33,33	0
4	EDO	B	603	4/4	0.94	0.15	1.58	23,24,25,25	0
2	TPP	C	601	26/26	0.98	0.10	-0.45	22,23,24,24	0
5	NA	A	1581	1/1	0.91	0.10	-0.45	35,35,35,35	0
3	MN	D	602	1/1	1.00	0.09	-0.59	23,23,23,23	0
2	TPP	A	601	26/26	0.98	0.10	-0.64	20,23,25,25	0
2	TPP	B	601	26/26	0.98	0.10	-0.70	21,24,26,27	0
2	TPP	D	601	26/26	0.99	0.09	-0.76	19,21,23,24	0
5	NA	C	1579	1/1	0.96	0.10	-0.99	36,36,36,36	0
5	NA	B	1581	1/1	0.96	0.10	-1.49	33,33,33,33	0
3	MN	A	602	1/1	0.99	0.07	-2.13	24,24,24,24	0
3	MN	B	602	1/1	0.99	0.08	-2.24	29,29,29,29	0
3	MN	C	602	1/1	1.00	0.04	-3.89	24,24,24,24	0
6	SO4	A	1583	5/5	0.97	0.14	-	24,24,24,24	5
6	SO4	D	1583	5/5	0.97	0.24	-	21,22,22,22	5
6	SO4	C	1581	5/5	0.94	0.15	-	26,27,27,27	5
6	SO4	B	1583	5/5	0.93	0.13	-	31,31,31,31	5

6.5 Other polymers ⓘ

There are no such residues in this entry.