



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:10 AM UTC

PDB ID : 1RJN / pdb_00001rjn
Title : The Crystal Structure of MenB (Rv0548c) from Mycobacterium tuberculosis in Complex with the CoA Portion of Naphthoyl CoA
Authors : Johnston, J.M.; Arcus, V.L.; Baker, E.N.; TB Structural Genomics Consortium (TBSGC)
Deposited on : 2003-11-19
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

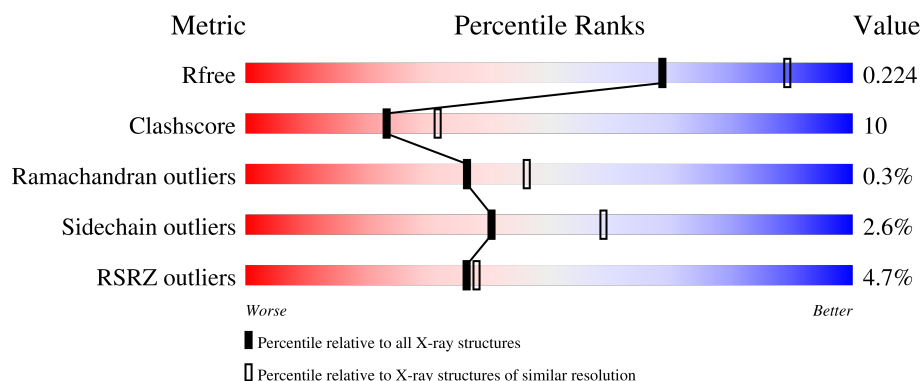
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	339	4% 60% 16% • 24%
1	B	339	2% 64% 15% • 19%
1	C	339	5% 58% 13% • 28%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6390 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 menB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	14	0	0
			2018	1269	368	372	9			
1	B	275	Total	C	N	O	S	0	0	0
			2167	1371	390	397	9			
1	C	245	Total	C	N	O	S	0	0	0
			1907	1205	344	350	8			

There are 75 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	expression tag	UNP O06414
A	-23	SER	-	expression tag	UNP O06414
A	-22	TYR	-	expression tag	UNP O06414
A	-21	TYR	-	expression tag	UNP O06414
A	-20	HIS	-	expression tag	UNP O06414
A	-19	HIS	-	expression tag	UNP O06414
A	-18	HIS	-	expression tag	UNP O06414
A	-17	HIS	-	expression tag	UNP O06414
A	-16	HIS	-	expression tag	UNP O06414
A	-15	HIS	-	expression tag	UNP O06414
A	-14	ASN	-	expression tag	UNP O06414
A	-13	TYR	-	expression tag	UNP O06414
A	-12	ASN	-	expression tag	UNP O06414
A	-11	ILE	-	expression tag	UNP O06414
A	-10	PRO	-	expression tag	UNP O06414
A	-9	THR	-	expression tag	UNP O06414
A	-8	THR	-	expression tag	UNP O06414
A	-7	GLU	-	expression tag	UNP O06414
A	-6	ASN	-	expression tag	UNP O06414
A	-5	LEU	-	expression tag	UNP O06414
A	-4	TYR	-	expression tag	UNP O06414
A	-3	PHE	-	expression tag	UNP O06414
A	-2	GLN	-	expression tag	UNP O06414

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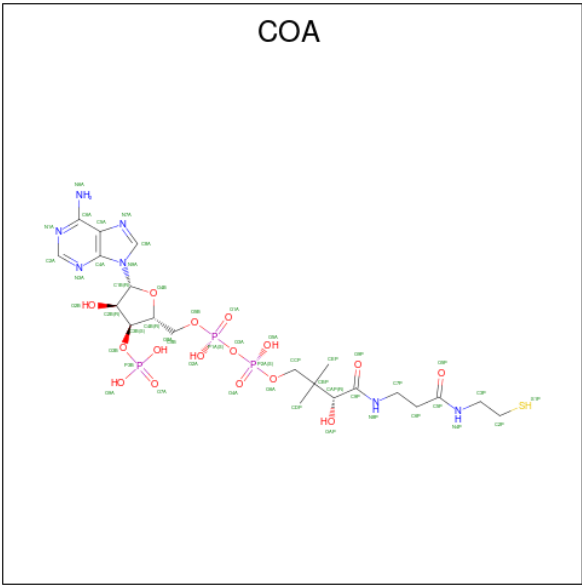
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP O06414
A	0	ALA	-	expression tag	UNP O06414
B	-24	MET	-	expression tag	UNP O06414
B	-23	SER	-	expression tag	UNP O06414
B	-22	TYR	-	expression tag	UNP O06414
B	-21	TYR	-	expression tag	UNP O06414
B	-20	HIS	-	expression tag	UNP O06414
B	-19	HIS	-	expression tag	UNP O06414
B	-18	HIS	-	expression tag	UNP O06414
B	-17	HIS	-	expression tag	UNP O06414
B	-16	HIS	-	expression tag	UNP O06414
B	-15	HIS	-	expression tag	UNP O06414
B	-14	ASN	-	expression tag	UNP O06414
B	-13	TYR	-	expression tag	UNP O06414
B	-12	ASN	-	expression tag	UNP O06414
B	-11	ILE	-	expression tag	UNP O06414
B	-10	PRO	-	expression tag	UNP O06414
B	-9	THR	-	expression tag	UNP O06414
B	-8	THR	-	expression tag	UNP O06414
B	-7	GLU	-	expression tag	UNP O06414
B	-6	ASN	-	expression tag	UNP O06414
B	-5	LEU	-	expression tag	UNP O06414
B	-4	TYR	-	expression tag	UNP O06414
B	-3	PHE	-	expression tag	UNP O06414
B	-2	GLN	-	expression tag	UNP O06414
B	-1	GLY	-	expression tag	UNP O06414
B	0	ALA	-	expression tag	UNP O06414
C	-24	MET	-	expression tag	UNP O06414
C	-23	SER	-	expression tag	UNP O06414
C	-22	TYR	-	expression tag	UNP O06414
C	-21	TYR	-	expression tag	UNP O06414
C	-20	HIS	-	expression tag	UNP O06414
C	-19	HIS	-	expression tag	UNP O06414
C	-18	HIS	-	expression tag	UNP O06414
C	-17	HIS	-	expression tag	UNP O06414
C	-16	HIS	-	expression tag	UNP O06414
C	-15	HIS	-	expression tag	UNP O06414
C	-14	ASN	-	expression tag	UNP O06414
C	-13	TYR	-	expression tag	UNP O06414
C	-12	ASN	-	expression tag	UNP O06414
C	-11	ILE	-	expression tag	UNP O06414
C	-10	PRO	-	expression tag	UNP O06414

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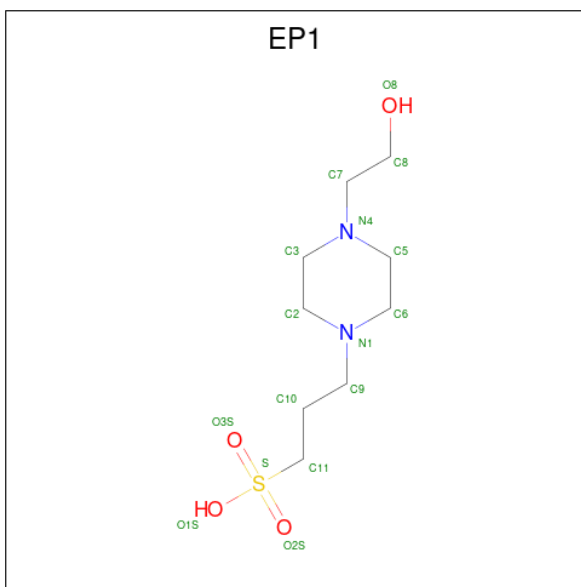
Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	THR	-	expression tag	UNP O06414
C	-8	THR	-	expression tag	UNP O06414
C	-7	GLU	-	expression tag	UNP O06414
C	-6	ASN	-	expression tag	UNP O06414
C	-5	LEU	-	expression tag	UNP O06414
C	-4	TYR	-	expression tag	UNP O06414
C	-3	PHE	-	expression tag	UNP O06414
C	-2	GLN	-	expression tag	UNP O06414
C	-1	GLY	-	expression tag	UNP O06414
C	0	ALA	-	expression tag	UNP O06414

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			39	16	5	15		

- Molecule 3 is 3-[4-(2-HYDROXYETHYL)PIPERAZIN-1-YL]PROPANE-1-SULFONIC ACID (CCD ID: EP1) (formula: C₉H₂₀N₂O₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	1
			48	27	6	12	3		

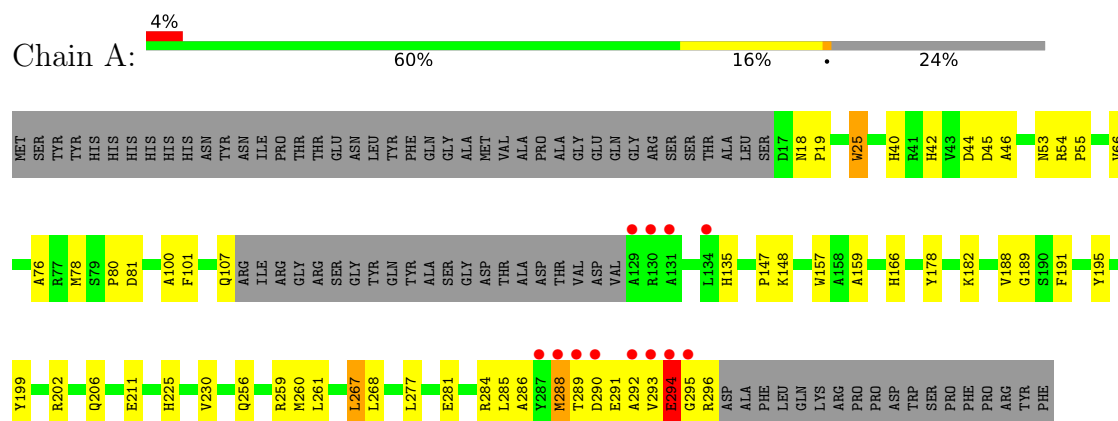
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	59	Total	O	0	0
			59	59		
4	B	74	Total	O	0	0
			74	74		
4	C	78	Total	O	0	0
			78	78		

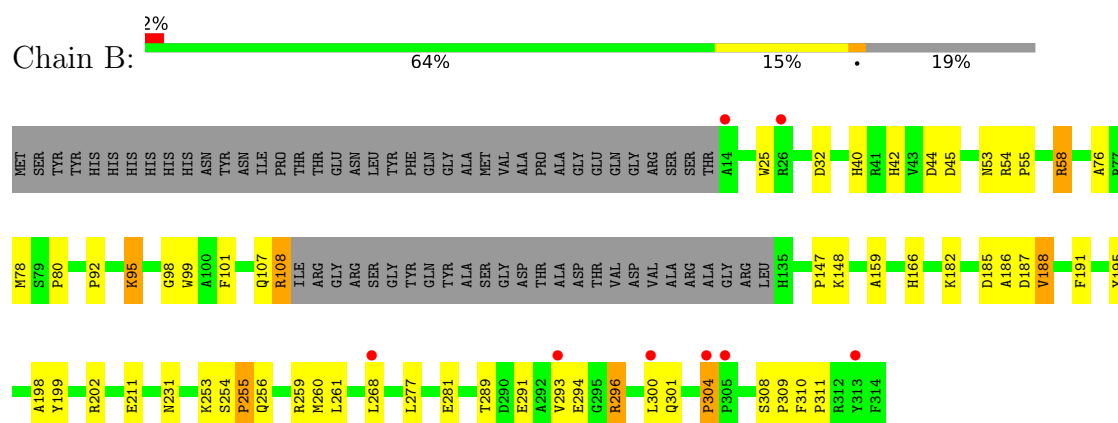
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

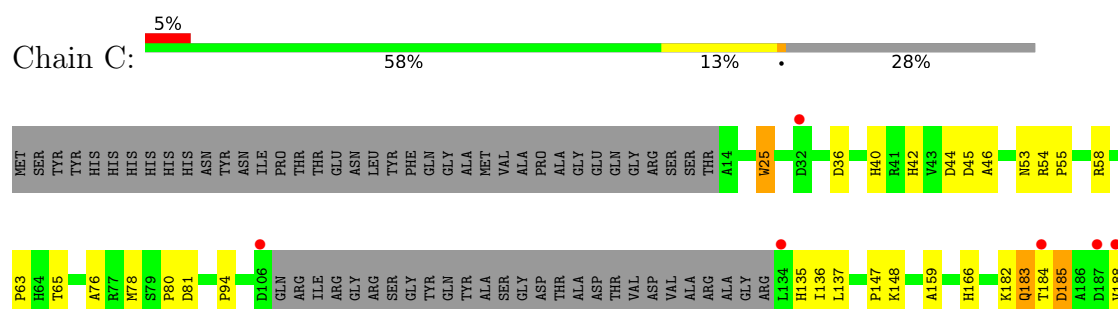
• Molecule 1: menB

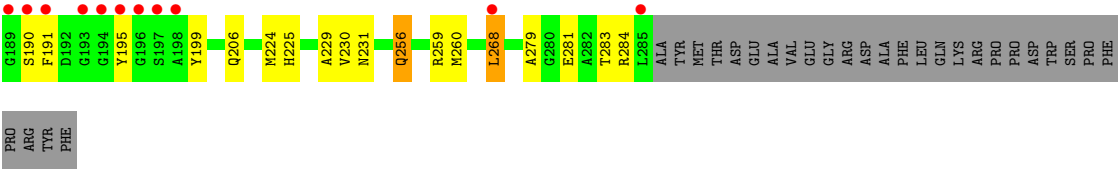


• Molecule 1: menB



• Molecule 1: menB





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	112.11Å 114.82Å 87.97Å 90.00° 123.36° 90.00°	Depositor
Resolution (Å)	24.49 – 2.30 24.49 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.6 (24.49-2.30) 96.5 (24.49-2.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.21 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.197 , 0.225 0.196 , 0.224	Depositor DCC
R_{free} test set	4001 reflections (9.67%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6390	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.31% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COA, EP1

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	0.47	0/2062	0.96	10/2791 (0.4%)
1	B	0.49	0/2221	1.01	10/3009 (0.3%)
1	C	0.52	0/1950	0.98	6/2642 (0.2%)
All	All	0.49	0/6233	0.99	26/8442 (0.3%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	GLN	OE1-CD-NE2	-10.59	112.01	122.60
1	B	256	GLN	OE1-CD-NE2	-10.24	112.36	122.60
1	C	183	GLN	OE1-CD-NE2	-10.09	112.51	122.60
1	C	256	GLN	OE1-CD-NE2	-9.48	113.12	122.60
1	B	301	GLN	OE1-CD-NE2	-9.41	113.19	122.60
1	B	296	ARG	N-CA-C	-8.79	102.69	113.41
1	B	188	VAL	N-CA-C	-7.46	105.57	112.43
1	A	107	GLN	CG-CD-NE2	7.12	127.08	116.40
1	B	256	GLN	CG-CD-NE2	7.02	126.92	116.40
1	B	101	PHE	N-CA-C	-6.97	102.25	111.24
1	A	267	LEU	CA-C-N	6.88	129.49	120.28
1	A	267	LEU	C-N-CA	6.88	129.49	120.28
1	C	256	GLN	CG-CD-NE2	6.81	126.61	116.40
1	A	268	LEU	N-CA-C	6.62	118.49	111.28
1	C	183	GLN	CG-CD-NE2	6.44	126.05	116.40
1	B	301	GLN	CG-CD-NE2	6.26	125.79	116.40
1	B	294	GLU	N-CA-C	-6.17	102.38	110.53
1	A	101	PHE	N-CA-C	-6.09	103.39	111.24
1	B	186	ALA	N-CA-C	5.71	117.50	111.28
1	A	178	TYR	N-CA-C	5.64	121.06	113.72
1	B	304	PRO	N-CA-C	5.34	117.22	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	206	GLN	N-CA-C	5.32	117.08	111.28
1	C	25	TRP	N-CA-C	5.18	118.00	109.72
1	A	25	TRP	N-CA-C	5.10	117.87	109.72
1	A	291	GLU	N-CA-C	-5.07	105.20	111.33
1	A	206	GLN	N-CA-C	5.05	116.78	111.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2018	0	1948	44	0
1	B	2167	0	2082	42	0
1	C	1907	0	1846	46	0
2	B	39	0	21	2	0
3	B	48	0	58	6	0
4	A	59	0	0	1	0
4	B	74	0	0	2	0
4	C	78	0	0	3	0
All	All	6390	0	5955	125	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 (125) 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:268:LEU:O	4:C:377:HOH:O	1.72	1.06
1:C:259:ARG:HH21	1:C:284:ARG:NH2	1.60	0.99
1:A:285:LEU:HA	1:A:288:MET:HE3	1.41	0.98
1:C:259:ARG:NH2	1:C:284:ARG:NH2	2.12	0.97
1:B:32:ASP:OD2	4:B:1265:HOH:O	1.93	0.87
1:A:42:HIS:HD2	1:A:45:ASP:H	1.22	0.87
1:B:42:HIS:HD2	1:B:45:ASP:H	1.23	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:253:LYS:O	1:B:255:PRO:HD3	1.77	0.84
1:C:42:HIS:HD2	1:C:45:ASP:H	1.26	0.82
1:B:76:ALA:O	1:B:148:LYS:HE3	1.82	0.79
1:A:76:ALA:O	1:A:148:LYS:HE3	1.84	0.77
1:B:108:ARG:HE	1:B:108:ARG:HA	1.50	0.75
1:C:259:ARG:HH21	1:C:284:ARG:HH21	1.31	0.75
1:C:256:GLN:OE1	1:C:259:ARG:NH2	2.20	0.74
1:C:135:HIS:CD2	1:C:137:LEU:HG	2.22	0.74
1:B:42:HIS:CD2	1:B:45:ASP:H	2.06	0.73
1:C:76:ALA:O	1:C:148:LYS:HE3	1.87	0.73
1:C:147:PRO:HB2	1:C:259:ARG:HD2	1.71	0.72
1:C:259:ARG:NH2	1:C:284:ARG:HH22	1.85	0.72
1:C:42:HIS:CD2	1:C:45:ASP:H	2.08	0.71
1:B:308:SER:HB2	1:B:309:PRO:HD3	1.73	0.69
1:A:42:HIS:CD2	1:A:45:ASP:H	2.07	0.68
1:B:42:HIS:CD2	1:B:44:ASP:H	2.12	0.67
1:C:135:HIS:HD2	1:C:137:LEU:H	1.41	0.67
1:B:185:ASP:O	1:B:188:VAL:HG12	1.95	0.67
1:A:289:THR:O	1:A:293:VAL:HG23	1.94	0.66
1:A:42:HIS:CD2	1:A:44:ASP:H	2.14	0.66
1:C:42:HIS:CD2	1:C:44:ASP:H	2.14	0.66
1:A:289:THR:HG22	1:A:290:ASP:N	2.09	0.66
1:A:294:GLU:C	1:A:294:GLU:OE1	2.40	0.65
1:C:259:ARG:NH2	1:C:284:ARG:HH21	1.92	0.64
1:A:285:LEU:HA	1:A:288:MET:CE	2.24	0.63
1:A:285:LEU:O	1:A:288:MET:HG3	2.00	0.62
1:C:135:HIS:HD2	1:C:137:LEU:HG	1.65	0.62
1:C:147:PRO:HB2	1:C:259:ARG:CD	2.30	0.62
1:C:135:HIS:CD2	1:C:137:LEU:H	2.18	0.61
1:B:289:THR:O	1:B:293:VAL:HG23	2.00	0.60
1:A:294:GLU:OE1	1:A:295:GLY:N	2.34	0.60
1:C:260:MET:SD	1:C:281:GLU:HB3	2.42	0.60
1:C:185:ASP:HB3	1:C:191:PHE:HA	1.85	0.59
1:B:296:ARG:O	1:B:300:LEU:HD13	2.04	0.58
1:A:25:TRP:HB3	1:A:40:HIS:HB3	1.86	0.57
1:C:259:ARG:CZ	1:C:284:ARG:HH22	2.17	0.57
1:B:25:TRP:HB3	1:B:40:HIS:HB3	1.87	0.57
1:A:42:HIS:HD2	1:A:45:ASP:N	1.99	0.57
1:B:202:ARG:HD3	3:B:1211[A]:EP1:O1S	2.04	0.57
1:B:260:MET:SD	1:B:281:GLU:HB3	2.45	0.57
1:B:78:MET:O	1:B:80:PRO:HD3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:TRP:HB3	1:C:40:HIS:HB3	1.87	0.56
1:B:202:ARG:HA	3:B:1211[A]:EP1:O1S	2.06	0.56
1:A:260:MET:SD	1:A:281:GLU:HB3	2.46	0.55
1:A:225:HIS:HD2	1:A:230:VAL:O	1.90	0.55
1:C:147:PRO:HB2	1:C:259:ARG:CG	2.37	0.55
1:A:78:MET:O	1:A:80:PRO:HD3	2.06	0.55
1:C:78:MET:O	1:C:80:PRO:HD3	2.07	0.55
1:A:293:VAL:O	1:A:294:GLU:C	2.50	0.55
1:A:289:THR:HG22	1:A:290:ASP:H	1.72	0.53
1:C:225:HIS:HD2	1:C:230:VAL:O	1.91	0.53
1:A:147:PRO:HB2	1:A:259:ARG:CD	2.39	0.53
1:A:295:GLY:O	1:A:296:ARG:HB2	2.09	0.53
1:A:188:VAL:O	1:A:188:VAL:HG12	2.08	0.52
1:A:286:ALA:O	1:A:292:ALA:CB	2.58	0.52
1:C:54:ARG:N	1:C:55:PRO:HD3	2.25	0.51
1:A:256:GLN:O	1:A:260:MET:HG2	2.11	0.51
1:A:54:ARG:N	1:A:55:PRO:HD3	2.24	0.51
1:B:202:ARG:HD3	3:B:1211[B]:EP1:O1S	2.10	0.50
1:C:42:HIS:HD2	1:C:45:ASP:N	2.01	0.50
1:C:256:GLN:O	1:C:260:MET:HG2	2.12	0.49
1:A:53:ASN:C	1:A:55:PRO:HD3	2.37	0.49
1:A:189:GLY:HA2	1:B:254:SER:CB	2.43	0.49
1:B:54:ARG:N	1:B:55:PRO:HD3	2.27	0.49
1:C:185:ASP:O	1:C:188:VAL:O	2.32	0.48
1:C:195:TYR:O	1:C:199:TYR:HB3	2.14	0.48
1:C:190:SER:OG	1:C:191:PHE:N	2.46	0.48
1:B:147:PRO:HB2	1:B:259:ARG:CD	2.44	0.48
1:C:183:GLN:NE2	4:C:329:HOH:O	2.35	0.48
1:A:289:THR:CG2	1:A:290:ASP:N	2.76	0.48
1:B:291:GLU:HA	1:B:310:PHE:CZ	2.48	0.48
1:B:95:LYS:HE3	2:B:1210:COA:O7A	2.14	0.47
1:B:108:ARG:HA	1:B:108:ARG:NE	2.24	0.47
1:B:202:ARG:HD3	3:B:1211[C]:EP1:O3S	2.14	0.47
1:B:42:HIS:HD2	1:B:45:ASP:N	2.00	0.47
1:A:147:PRO:HB2	1:A:259:ARG:HD3	1.97	0.47
1:A:191:PHE:HB2	1:B:261:LEU:HD21	1.96	0.47
1:C:63:PRO:HA	4:C:367:HOH:O	2.15	0.47
1:B:195:TYR:O	1:B:199:TYR:HB3	2.14	0.46
1:A:211:GLU:HB2	1:B:231:ASN:ND2	2.31	0.46
1:B:198:ALA:HB1	1:C:268:LEU:CD1	2.46	0.46
1:A:284:ARG:HG2	1:A:284:ARG:HH11	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:HD3	3:B:1211[C]:EP1:O2S	2.15	0.45
1:A:277:LEU:HD12	4:A:320:HOH:O	2.15	0.45
1:A:66:VAL:HG11	1:A:135:HIS:HB3	1.98	0.45
1:B:53:ASN:C	1:B:55:PRO:HD3	2.41	0.45
1:C:147:PRO:HB2	1:C:259:ARG:HG3	1.99	0.45
1:B:198:ALA:HB1	1:C:268:LEU:HD11	1.98	0.45
1:C:36:ASP:HB3	1:C:65:THR:HG23	1.99	0.45
1:C:53:ASN:C	1:C:55:PRO:HD3	2.42	0.45
1:A:261:LEU:HD21	1:C:191:PHE:HB2	1.98	0.44
1:C:224:MET:HG3	1:C:229:ALA:HB3	1.99	0.44
1:C:279:ALA:O	1:C:283:THR:HG23	2.16	0.44
1:B:58:ARG:HH22	1:B:98:GLY:HA3	1.83	0.43
1:C:46:ALA:HB1	1:C:81:ASP:O	2.18	0.43
1:B:92:PRO:HD3	1:B:99:TRP:CH2	2.53	0.43
1:C:135:HIS:CD2	1:C:136:ILE:HG22	2.53	0.43
1:B:188:VAL:O	1:B:188:VAL:HG22	2.18	0.43
1:A:18:ASN:HA	1:A:19:PRO:HD3	1.90	0.43
1:B:92:PRO:HB3	1:B:99:TRP:CE2	2.54	0.43
1:A:284:ARG:HG2	1:A:284:ARG:NH1	2.34	0.43
1:A:159:ALA:HA	1:A:182:LYS:O	2.19	0.43
1:B:277:LEU:HD12	4:B:1243:HOH:O	2.20	0.42
1:C:185:ASP:CB	1:C:191:PHE:HA	2.46	0.42
1:A:286:ALA:O	1:A:292:ALA:HB2	2.20	0.42
1:C:159:ALA:HA	1:C:182:LYS:O	2.20	0.42
1:A:46:ALA:HB1	1:A:81:ASP:O	2.20	0.42
1:B:185:ASP:HB3	1:B:191:PHE:HA	2.01	0.42
1:A:100:ALA:HA	1:A:157:TRP:N	2.35	0.41
1:A:267:LEU:O	1:A:267:LEU:HD12	2.21	0.41
1:B:310:PHE:HA	1:B:311:PRO:HD3	1.74	0.41
1:A:195:TYR:O	1:A:199:TYR:HB3	2.21	0.41
1:B:159:ALA:HA	1:B:182:LYS:O	2.21	0.41
1:C:55:PRO:HB2	1:C:94:PRO:HD3	2.01	0.41
1:B:211:GLU:HB2	1:C:231:ASN:ND2	2.36	0.40
1:A:289:THR:CG2	1:A:290:ASP:H	2.33	0.40
1:B:202:ARG:HA	3:B:1211[B]:EP1:O1S	2.19	0.40
1:B:58:ARG:HG3	2:B:1210:COA:O4B	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	255/339 (75%)	243 (95%)	11 (4%)	1 (0%)	30	38
1	B	271/339 (80%)	258 (95%)	13 (5%)	0	100	100
1	C	241/339 (71%)	234 (97%)	6 (2%)	1 (0%)	30	38
All	All	767/1017 (75%)	735 (96%)	30 (4%)	2 (0%)	36	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	GLU
1	C	185	ASP

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	203/270 (75%)	200 (98%)	3 (2%)	57	75
1	B	220/270 (82%)	211 (96%)	9 (4%)	27	41
1	C	194/270 (72%)	190 (98%)	4 (2%)	47	66
All	All	617/810 (76%)	601 (97%)	16 (3%)	40	59

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	166	HIS

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Mol	Chain	Res	Type
1	A	288	MET
1	A	294	GLU
1	B	58	ARG
1	B	95	LYS
1	B	107	GLN
1	B	108	ARG
1	B	166	HIS
1	B	187	ASP
1	B	255	PRO
1	B	268	LEU
1	B	304	PRO
1	C	58	ARG
1	C	166	HIS
1	C	184	THR
1	C	268	LEU

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

Mol	Chain	Res	Type
1	A	42	HIS
1	A	64	HIS
1	A	140	GLN
1	A	225	HIS
1	B	42	HIS
1	B	64	HIS
1	B	226	GLN
1	B	301	GLN
1	C	42	HIS
1	C	64	HIS
1	C	135	HIS
1	C	140	GLN
1	C	225	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EP1	B	1211[A]	-	16,16,16	1.90	1 (6%)	21,21,21	3.01	9 (42%)
3	EP1	B	1211[B]	-	16,16,16	1.98	1 (6%)	21,21,21	3.04	8 (38%)
2	COA	B	1210	-	40,41,50	3.11	18 (45%)	59,64,75	2.50	19 (32%)
3	EP1	B	1211[C]	-	16,16,16	1.93	1 (6%)	21,21,21	3.01	8 (38%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EP1	B	1211[A]	-	-	5/10/20/20	0/1/1/1
3	EP1	B	1211[B]	-	-	8/10/20/20	0/1/1/1
2	COA	B	1210	-	-	16/33/52/64	0/3/3/3
3	EP1	B	1211[C]	-	-	4/10/20/20	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1210	COA	CBP-CAP	12.17	1.70	1.55
3	B	1211[B]	EP1	C11-S	-7.50	1.67	1.77
3	B	1211[C]	EP1	C11-S	-7.12	1.67	1.77
3	B	1211[A]	EP1	C11-S	-7.01	1.67	1.77
2	B	1210	COA	CCP-CBP	5.68	1.61	1.52
2	B	1210	COA	P1A-O3A	-5.27	1.53	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1210	COA	O4B-C1B	4.38	1.52	1.42
2	B	1210	COA	P3B-O3B	4.09	1.66	1.59
2	B	1210	COA	C2A-N1A	4.07	1.41	1.33
2	B	1210	COA	C5A-C4A	4.02	1.46	1.39
2	B	1210	COA	P2A-O3A	3.74	1.63	1.59
2	B	1210	COA	OAP-CAP	3.70	1.48	1.43
2	B	1210	COA	C2A-N3A	3.60	1.40	1.33
2	B	1210	COA	C6A-N6A	2.71	1.41	1.34
2	B	1210	COA	C4A-N3A	2.47	1.39	1.34
2	B	1210	COA	CDP-CBP	2.31	1.58	1.53
2	B	1210	COA	C8A-N9A	2.29	1.41	1.37
2	B	1210	COA	C5B-C4B	2.24	1.58	1.51
2	B	1210	COA	O4B-C4B	-2.22	1.40	1.45
2	B	1210	COA	O9P-C9P	2.17	1.28	1.20
2	B	1210	COA	C5A-C6A	2.06	1.46	1.41

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1210	COA	O5B-C5B-C4B	10.83	145.86	108.99
3	B	1211[B]	EP1	C6-N1-C2	8.54	127.23	108.84
3	B	1211[C]	EP1	C6-N1-C2	8.41	126.96	108.84
3	B	1211[A]	EP1	C6-N1-C2	8.38	126.90	108.84
2	B	1210	COA	N3A-C4A-N9A	5.53	136.58	127.17
3	B	1211[C]	EP1	C2-C3-N4	5.16	121.06	110.65
3	B	1211[B]	EP1	C2-C3-N4	5.06	120.85	110.65
3	B	1211[A]	EP1	C6-C5-N4	5.05	120.84	110.65
3	B	1211[B]	EP1	C5-N4-C3	5.01	119.62	108.84
2	B	1210	COA	P1A-O5B-C5B	5.00	150.02	121.35
3	B	1211[A]	EP1	C5-N4-C3	5.00	119.60	108.84
3	B	1211[A]	EP1	C2-C3-N4	4.99	120.72	110.65
3	B	1211[B]	EP1	C6-C5-N4	4.99	120.71	110.65
3	B	1211[C]	EP1	C6-C5-N4	4.99	120.71	110.65
3	B	1211[C]	EP1	C5-N4-C3	4.96	119.53	108.84
2	B	1210	COA	C5A-C4A-N9A	-4.74	100.64	105.81
2	B	1210	COA	C4A-N9A-C8A	4.59	110.56	105.74
2	B	1210	COA	O4B-C1B-N9A	4.36	116.46	108.09
2	B	1210	COA	O4B-C1B-C2B	-3.64	98.84	106.62
2	B	1210	COA	O2A-P1A-O3A	3.41	116.50	107.27
2	B	1210	COA	CEP-CBP-CCP	-3.31	102.75	108.22
2	B	1210	COA	O6A-CCP-CBP	3.13	115.58	110.55
2	B	1210	COA	CDP-CBP-CAP	-2.91	104.05	109.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1210	COA	C5A-C4A-N3A	-2.86	122.78	126.72
3	B	1211[C]	EP1	C5-C6-N1	2.67	116.03	110.65
3	B	1211[A]	EP1	C5-C6-N1	2.66	116.02	110.65
3	B	1211[A]	EP1	C3-C2-N1	2.62	115.92	110.65
3	B	1211[B]	EP1	C5-C6-N1	2.61	115.91	110.65
3	B	1211[C]	EP1	C3-C2-N1	2.51	115.71	110.65
3	B	1211[B]	EP1	C3-C2-N1	2.49	115.67	110.65
2	B	1210	COA	CEP-CBP-CDP	2.48	114.15	109.20
2	B	1210	COA	N3A-C2A-N1A	-2.36	125.02	128.58
3	B	1211[C]	EP1	O3S-S-C11	2.34	110.27	106.73
2	B	1210	COA	N6A-C6A-N1A	2.32	123.54	118.38
3	B	1211[B]	EP1	C10-C9-N1	-2.29	107.49	113.93
2	B	1210	COA	C5A-C6A-N6A	-2.24	117.74	123.29
3	B	1211[A]	EP1	O1S-S-C11	2.18	110.27	106.00
2	B	1210	COA	O6A-P2A-O4A	2.17	117.53	108.94
2	B	1210	COA	CEP-CBP-CAP	2.14	113.52	109.51
3	B	1211[A]	EP1	C10-C9-N1	-2.13	107.93	113.93
3	B	1211[C]	EP1	C9-N1-C6	2.13	116.91	111.24
3	B	1211[A]	EP1	C9-N1-C2	2.12	116.88	111.24
2	B	1210	COA	N9A-C8A-N7A	-2.12	110.93	113.94
3	B	1211[B]	EP1	C9-N1-C2	2.00	116.57	111.24

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1210	COA	CCP-O6A-P2A-O3A
2	B	1210	COA	CCP-O6A-P2A-O4A
2	B	1210	COA	CCP-O6A-P2A-O5A
2	B	1210	COA	CDP-CBP-CCP-O6A
2	B	1210	COA	CEP-CBP-CCP-O6A
2	B	1210	COA	CAP-CBP-CCP-O6A
2	B	1210	COA	OAP-CAP-CBP-CEP
2	B	1210	COA	C9P-CAP-CBP-CEP
3	B	1211[A]	EP1	C11-C10-C9-N1
3	B	1211[C]	EP1	C11-C10-C9-N1
2	B	1210	COA	C3B-C4B-C5B-O5B
2	B	1210	COA	O4B-C4B-C5B-O5B
3	B	1211[B]	EP1	C10-C11-S-O1S
3	B	1211[A]	EP1	C9-C10-C11-S
3	B	1211[B]	EP1	C11-C10-C9-N1
3	B	1211[A]	EP1	C10-C9-N1-C6

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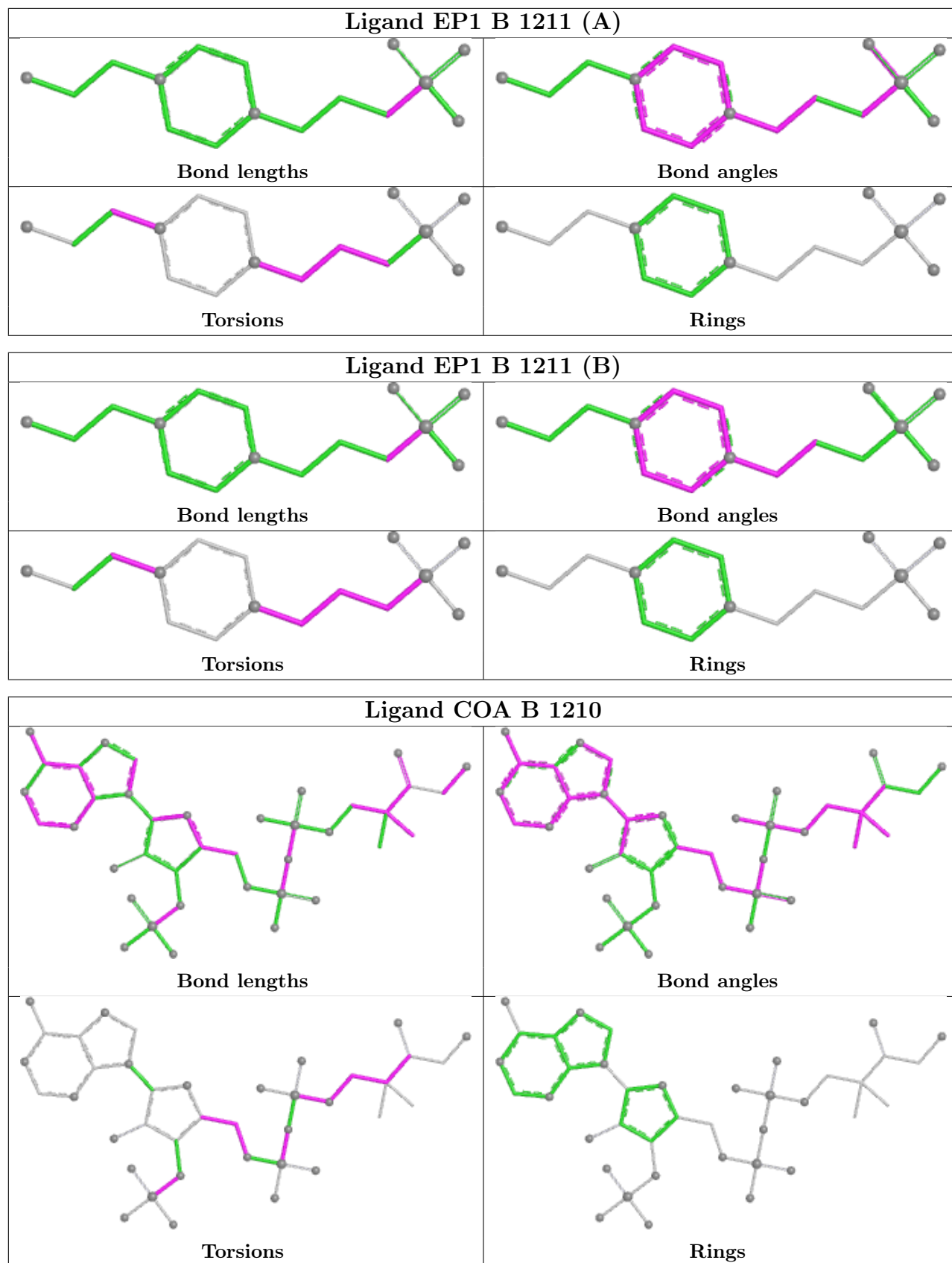
Mol	Chain	Res	Type	Atoms
3	B	1211[C]	EP1	C10-C9-N1-C2
3	B	1211[B]	EP1	C10-C9-N1-C6
3	B	1211[B]	EP1	C8-C7-N4-C5
3	B	1211[C]	EP1	C9-C10-C11-S
3	B	1211[B]	EP1	C10-C11-S-O2S
3	B	1211[B]	EP1	C10-C11-S-O3S
3	B	1211[B]	EP1	C9-C10-C11-S
3	B	1211[B]	EP1	C8-C7-N4-C3
2	B	1210	COA	P2A-O3A-P1A-O2A
3	B	1211[A]	EP1	C8-C7-N4-C5
2	B	1210	COA	C4B-C5B-O5B-P1A
2	B	1210	COA	C3B-O3B-P3B-O9A
3	B	1211[C]	EP1	C8-C7-N4-C5
2	B	1210	COA	P2A-O3A-P1A-O1A
2	B	1210	COA	CBP-CCP-O6A-P2A
2	B	1210	COA	C3B-O3B-P3B-O7A
3	B	1211[A]	EP1	C8-C7-N4-C3

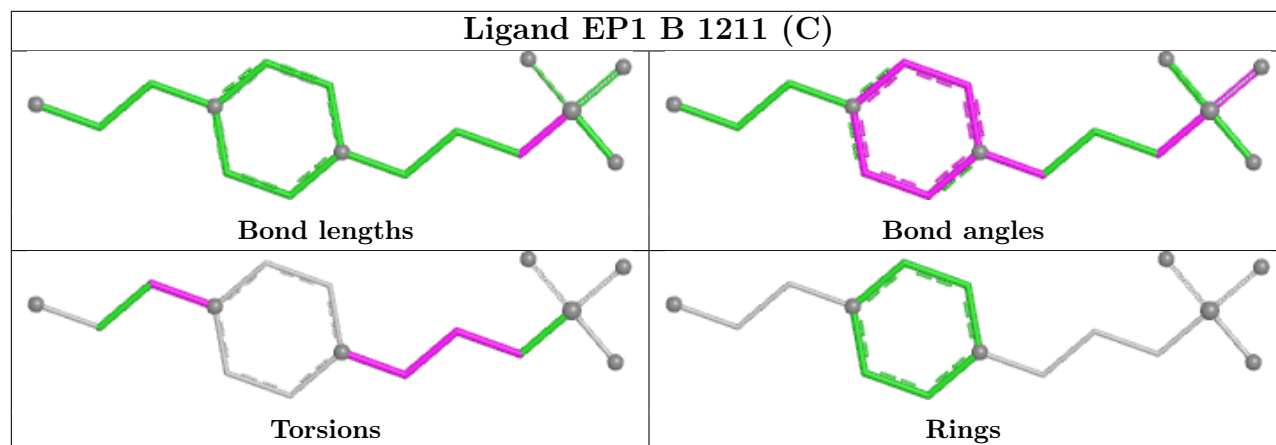
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1211[A]	EP1	2	0
3	B	1211[B]	EP1	2	0
2	B	1210	COA	2	0
3	B	1211[C]	EP1	2	0

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





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

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	259/339 (76%)	0.16	12 (4%) 37 39	18, 29, 61, 94	4 (1%)
1	B	275/339 (81%)	0.03	8 (2%) 53 56	16, 28, 61, 77	1 (0%)
1	C	245/339 (72%)	0.09	17 (6%) 23 25	17, 27, 55, 78	0
All	All	779/1017 (76%)	0.09	37 (4%) 36 38	16, 28, 61, 94	5 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	188	VAL	5.2
1	C	195	TYR	4.8
1	A	129	ALA	4.7
1	A	287	TYR	4.6
1	C	189	GLY	4.6
1	B	14	ALA	4.3
1	A	293	VAL	4.1
1	C	194	GLY	3.9
1	B	305	PRO	3.8
1	A	292	ALA	3.6
1	A	289	THR	3.5
1	A	288	MET	3.4
1	C	190	SER	3.4
1	C	184	THR	3.2
1	A	130	ARG	3.2
1	C	134	LEU	3.2
1	C	196	GLY	3.1
1	C	285	LEU	3.0
1	C	197	SER	2.9
1	A	134	LEU	2.8
1	C	193	GLY	2.7
1	B	293	VAL	2.7
1	A	294	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	313	TYR	2.6
1	C	191	PHE	2.6
1	A	295	GLY	2.6
1	C	268	LEU	2.6
1	C	187	ASP	2.5
1	B	268	LEU	2.4
1	C	198	ALA	2.3
1	A	131	ALA	2.3
1	C	106	ASP	2.2
1	B	304	PRO	2.2
1	C	32	ASP	2.2
1	A	290	ASP	2.1
1	B	300	LEU	2.0
1	B	26	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

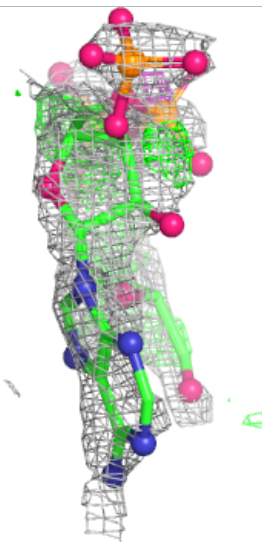
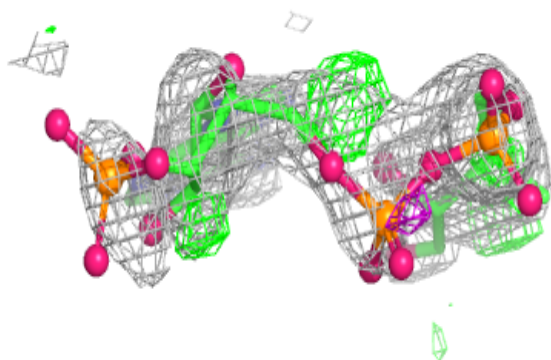
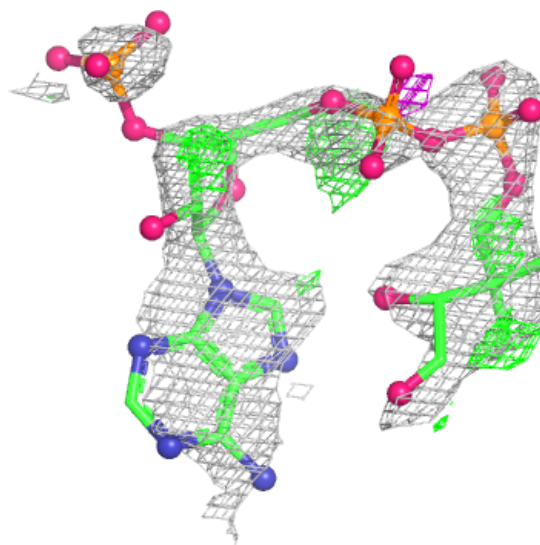
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	COA	B	1210	39/48	0.71	0.27	53,57,62,62	39
3	EP1	B	1211[A]	16/16	0.79	0.23	27,29,36,36	16
3	EP1	B	1211[B]	16/16	0.79	0.23	32,34,38,38	16
3	EP1	B	1211[C]	16/16	0.79	0.23	16,19,20,21	16

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

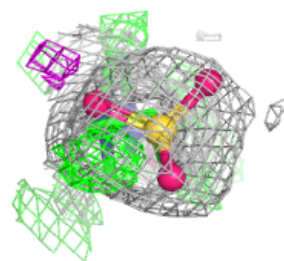
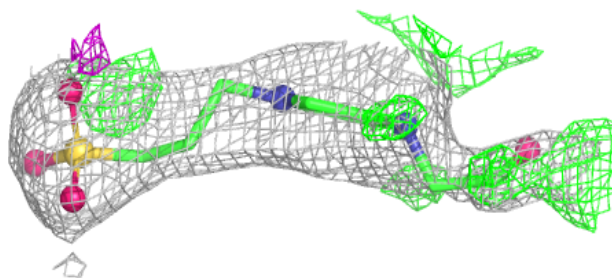
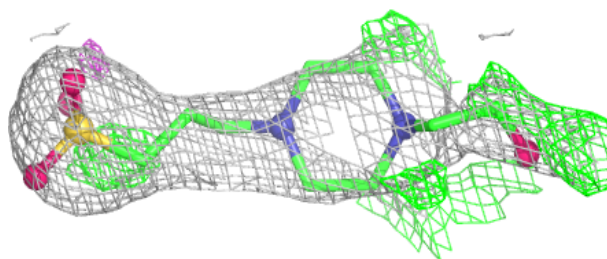
Electron density around COA B 1210:

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

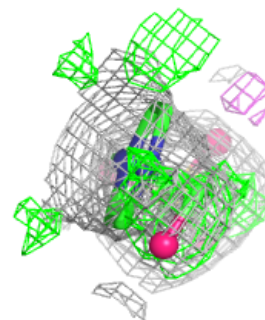
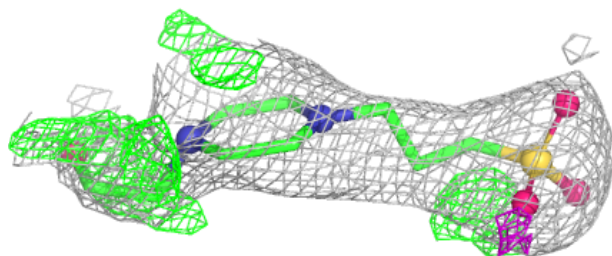
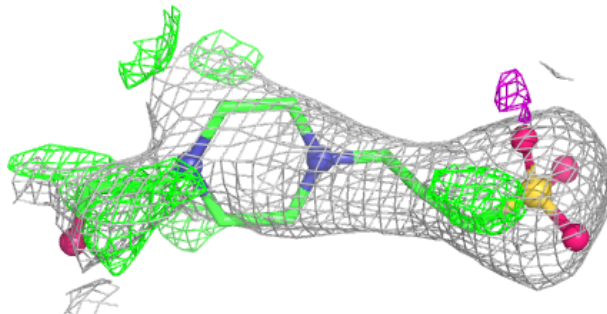


Electron density around EP1 B 1211 (A):

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

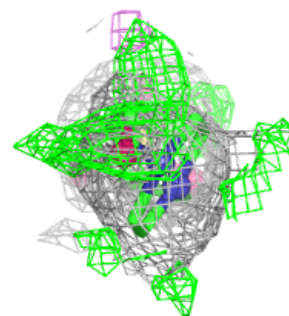
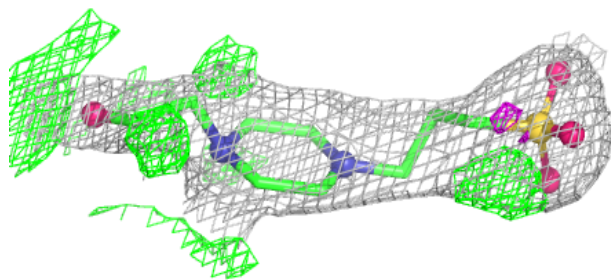
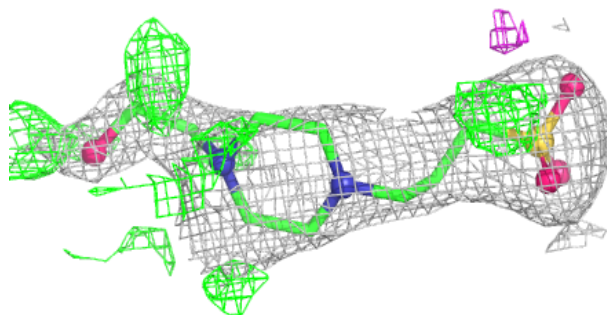
**Electron density around EP1 B 1211 (B):**

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



Electron density around EP1 B 1211 (C):

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



6.5 Other polymers ⓘ

There are no such residues in this entry.