



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:19 PM UTC

PDB ID : 8OTR / pdb_00008otr
Title : SARS-CoV-2 nsp10-16 methyltransferase in complex with SAM analog BDH
33959089
Authors : Kremling, V.; Sprenger, J.; Oberthuer, D.
Deposited on : 2023-04-21
Resolution : 1.77 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

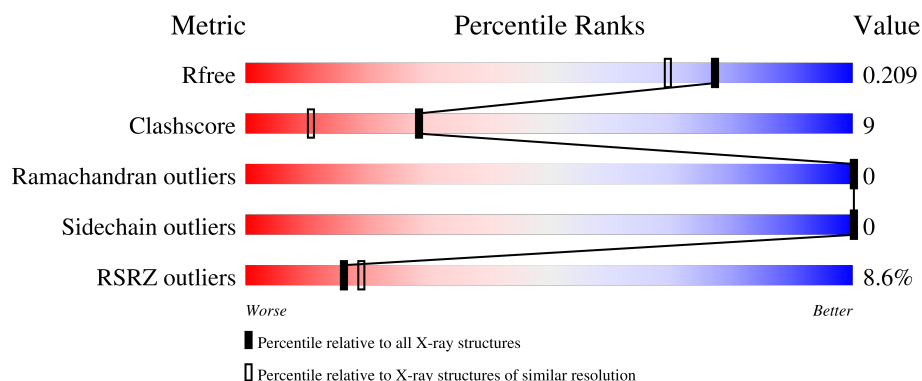
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.77 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	304	
2	B	140	

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
3	EDO	A	7209	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 3764 atoms, of which 12 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'-O-methyltransferase nsp16.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	301	Total	C	N	O	S	0	10	0
			2453	1557	416	463	17			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	7097	GLU	-	expression tag	UNP P0DTD1
A	7098	ASN	-	expression tag	UNP P0DTD1
A	7099	LEU	-	expression tag	UNP P0DTD1
A	7100	TYR	-	expression tag	UNP P0DTD1
A	7101	PHE	-	expression tag	UNP P0DTD1
A	7102	GLN	-	expression tag	UNP P0DTD1

- Molecule 2 is a protein called Non-structural protein 10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	116	Total	C	N	O	S	0	0	0
			856	533	144	164	15			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4253	GLY	-	expression tag	UNP P0DTD1

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



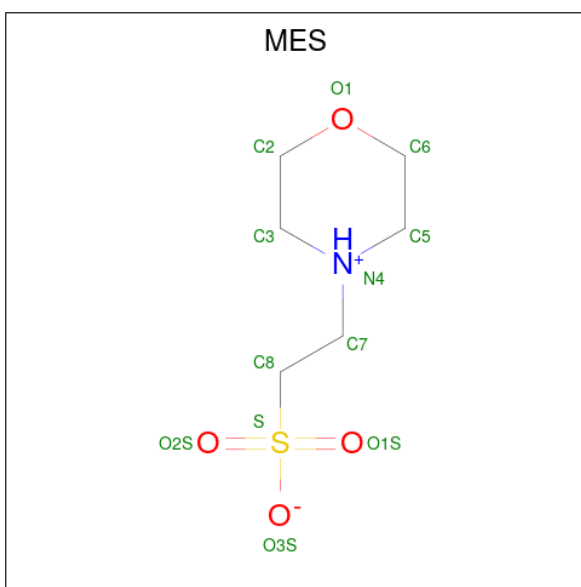
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total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

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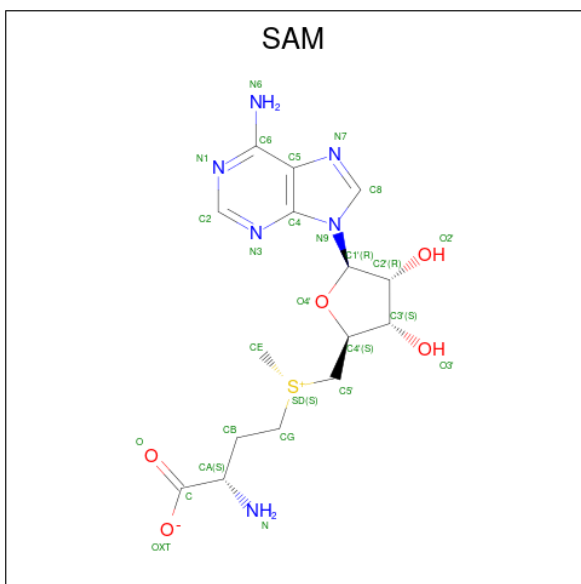
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			4	2	2			
3	A	1	Total	C	O		0	0
			4	2	2			
3	A	1	Total	C	O		0	1
			4	2	2			
3	A	1	Total	C	O		0	0
			4	2	2			
3	A	1	Total	C	O		0	0
			4	2	2			
3	A	1	Total	C	O		0	0
			4	2	2			
3	A	1	Total	C	O		0	0
			4	2	2			
3	A	1	Total	C	O		0	0
			4	2	2			
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	A	1	Total	C	H	O	0	0
			10	2	6	2		
3	B	1	Total	C	O		0	0
			4	2	2			
3	B	1	Total	C	O		0	0
			4	2	2			

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

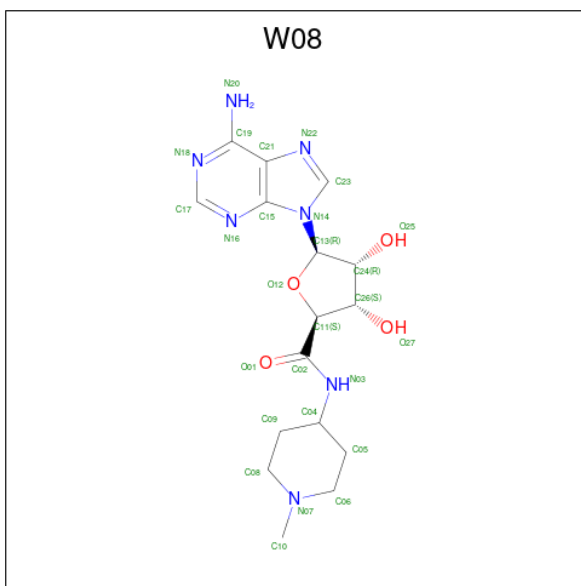
- Molecule 5 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	1
			27	15	6	5	1		

- Molecule 6 is (2S,3S,4R,5R)-5-(6-aminopurin-9-yl)-N-(1-methylpiperidin-4-yl)-3,4-bis(oxadanyl)oxolane-2-carboxamide (CCD ID: W08) (formula: $C_{16}H_{23}N_7O_4$) (labeled as "Ligand of

Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	1
			27	16	7	4		

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Cl	0	0
			1	1		

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	2	Total	Zn	0	0
			2	2		

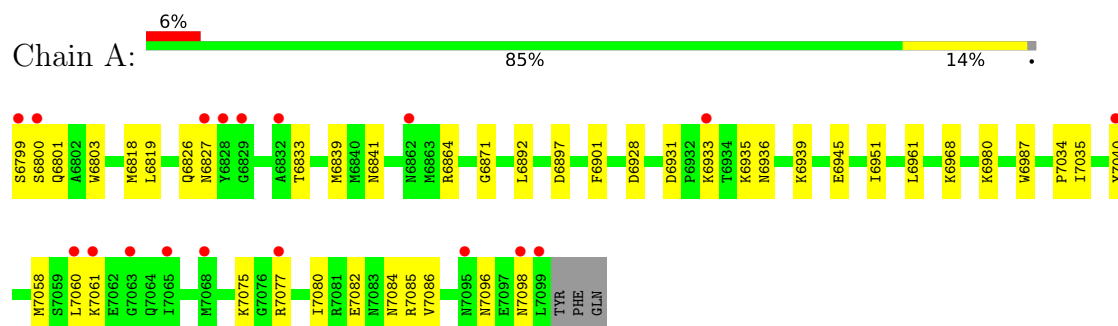
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	199	Total	O	0	0
			199	199		
9	B	63	Total	O	0	0
			63	63		

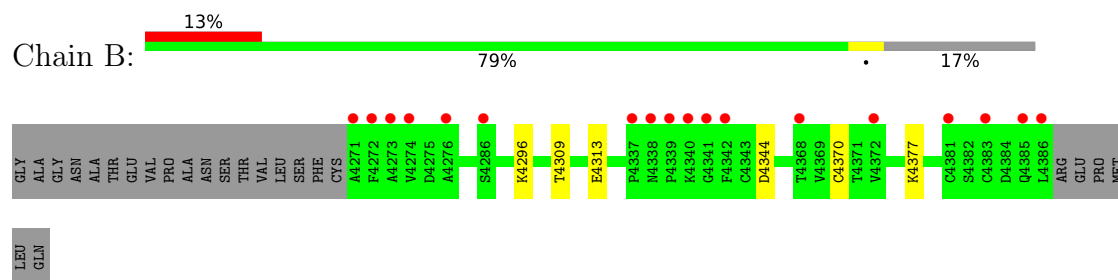
3 Residue-property plots

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: 2'-O-methyltransferase nsp16



• Molecule 2: Non-structural protein 10



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	167.60Å 167.60Å 51.48Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.99 – 1.77 41.99 – 1.77	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.99-1.77) 99.8 (41.99-1.77)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 1.50Å)	Xtriage
Refinement program	PHENIX 1.07	Depositor
R, R_{free}	0.188 , 0.209 0.188 , 0.209	Depositor DCC
R_{free} test set	825 reflections (0.86%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.019 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	3764	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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: SAM, CL, ZN, EDO, MES, W08

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	0.34	0/2505	0.55	0/3397
2	B	0.27	0/875	0.48	0/1187
All	All	0.32	0/3380	0.53	0/4584

There are no bond length outliers.

There are no bond angle outliers.

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	2453	0	2415	51	0
2	B	856	0	816	7	0
3	A	104	12	156	23	0
3	B	8	0	12	2	0
4	A	12	0	12	1	0
5	A	27	0	22	4	0
6	A	27	0	0	1	0
7	A	1	0	0	0	0
8	B	2	0	0	0	0
9	A	199	0	0	4	1
9	B	63	0	0	0	0
All	All	3752	12	3433	61	1

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 9.

All (61) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7082:GLU:HB2	3:A:7209:EDO:H21	1.47	0.95
1:A:6980:LYS:HD3	3:A:7207:EDO:H22	1.59	0.84
1:A:6819:LEU:H	3:A:7227:EDO:H11	1.44	0.83
1:A:6839:MET:HB3	3:A:7225:EDO:H21	1.62	0.80
1:A:7082:GLU:HB2	3:A:7209:EDO:C2	2.18	0.73
1:A:6801:GLN:HG3	3:A:7222:EDO:O1	1.88	0.73
1:A:6897:ASP:OD1	5:A:7213[C]:SAM:H1'	1.89	0.72
1:A:6901:PHE:O	3:A:7216:EDO:H11	1.91	0.70
1:A:7058:MET:CE	1:A:7060:LEU:HD11	2.23	0.68
1:A:6936:ASN:ND2	1:A:6939:LYS:HD2	2.10	0.66
1:A:6892:LEU:HD12	1:A:7086:VAL:HG21	1.78	0.65
2:B:4370:CYS:HB2	2:B:4377:LYS:HE2	1.78	0.65
1:A:7061:LYS:N	1:A:7061:LYS:HD3	2.13	0.63
1:A:6799:SER:OG	1:A:6800:SER:N	2.31	0.62
1:A:7077[B]:ARG:HA	3:A:7220:EDO:H21	1.82	0.61
1:A:7058:MET:HE1	1:A:7060:LEU:HD11	1.83	0.60
1:A:7077[A]:ARG:HA	3:A:7220:EDO:H21	1.83	0.59
1:A:6871:GLY:O	5:A:7213[C]:SAM:HG2	2.02	0.59
1:A:7085:ARG:HG3	9:A:7455:HOH:O	2.06	0.56
1:A:7096:ASN:HD21	1:A:7098:ASN:HD22	1.54	0.55
1:A:7058:MET:HE2	1:A:7060:LEU:HD11	1.88	0.55
1:A:7082:GLU:HB2	3:A:7209:EDO:C1	2.37	0.55
1:A:6935:LYS:O	1:A:6935:LYS:HG3	2.06	0.54
1:A:6833:THR:H	3:A:7205:EDO:H22	1.74	0.53
1:A:6818:MET:HE1	3:A:7227:EDO:H22	1.90	0.52
3:A:7218:EDO:H22	2:B:4296:LYS:NZ	2.24	0.52
1:A:6827[A]:ASN:ND2	1:A:7035:ILE:O	2.44	0.51
1:A:6818:MET:CE	3:A:7227:EDO:H22	2.41	0.51
1:A:7075:LYS:HD3	1:A:7077[B]:ARG:NH1	2.26	0.50
1:A:7077[B]:ARG:CA	3:A:7220:EDO:H21	2.42	0.49
1:A:7060:LEU:C	1:A:7061:LYS:HD3	2.38	0.49
2:B:4344:ASP:H	3:B:4404:EDO:H21	1.77	0.48
2:B:4370:CYS:CB	2:B:4377:LYS:HE2	2.42	0.48
3:A:7218:EDO:H22	2:B:4296:LYS:HZ3	1.79	0.47
3:A:7224:EDO:O2	3:A:7225:EDO:H11	2.15	0.47
1:A:6928:ASP:OD2	1:A:6968:LYS:CE	2.63	0.46
1:A:7034:PRO:O	3:A:7222:EDO:H21	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4344:ASP:H	3:B:4404:EDO:C2	2.29	0.46
1:A:6987:TRP:CD2	4:A:7202:MES:H32	2.51	0.46
1:A:6839:MET:HG3	9:A:7349:HOH:O	2.15	0.46
1:A:6931:ASP:OD2	6:A:7228[B]:W08:O27	2.34	0.46
1:A:6841:ASN:ND2	5:A:7213[C]:SAM:OXT	2.50	0.45
1:A:6945[A]:GLU:OE2	3:A:7221:EDO:O1	2.19	0.45
1:A:6961:LEU:HB2	1:A:7080:ILE:HB	1.98	0.45
1:A:6803:TRP:HD1	1:A:7040[A]:TYR:CZ	2.35	0.45
1:A:6968:LYS:NZ	3:A:7219[D]:EDO:O1	2.51	0.44
1:A:6833:THR:H	3:A:7205:EDO:C2	2.29	0.44
1:A:7096:ASN:HD21	1:A:7098:ASN:HB2	1.83	0.43
1:A:6864:ARG:NH2	1:A:7084[A]:ASN:O	2.52	0.43
1:A:6951:ILE:HD13	1:A:6951:ILE:HA	1.89	0.43
1:A:6864:ARG:NH2	1:A:7084[B]:ASN:O	2.52	0.42
1:A:6933:LYS:HE2	1:A:6933:LYS:HB2	1.83	0.42
1:A:7082:GLU:HB2	3:A:7209:EDO:H11	2.02	0.41
2:B:4309:THR:HG21	2:B:4313:GLU:HG3	2.01	0.41
1:A:6928:ASP:OD2	1:A:6968:LYS:HE3	2.19	0.41
3:A:7222:EDO:H12	9:A:7462:HOH:O	2.20	0.41
1:A:7058:MET:HE2	1:A:7060:LEU:CD1	2.50	0.41
5:A:7213[C]:SAM:H2	9:A:7336:HOH:O	2.20	0.41
1:A:6892:LEU:HD12	1:A:7086:VAL:CG2	2.50	0.40
1:A:6803:TRP:HA	1:A:7040[A]:TYR:CD2	2.57	0.40
1:A:6826:GLN:HG2	1:A:6827[B]:ASN:OD1	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:7399:HOH:O	9:A:7399:HOH:O[5_554]	2.09	0.11

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	309/304 (102%)	296 (96%)	13 (4%)	0	100	100
2	B	114/140 (81%)	110 (96%)	4 (4%)	0	100	100
All	All	423/444 (95%)	406 (96%)	17 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	271/264 (103%)	271 (100%)	0	100	100
2	B	94/113 (83%)	94 (100%)	0	100	100
All	All	365/377 (97%)	365 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6804	GLN
1	A	6841	ASN
1	A	6862	ASN
1	A	6917	HIS
1	A	7096	ASN
2	B	4293	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 34 ligands modelled in this entry, 3 are monoatomic - leaving 31 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EDO	A	7217	-	3,3,3	0.52	0	2,2,2	0.14	0
3	EDO	A	7222	-	3,3,3	0.49	0	2,2,2	0.30	0
3	EDO	B	4403	-	3,3,3	0.57	0	2,2,2	0.19	0
3	EDO	A	7216	-	3,3,3	0.61	0	2,2,2	0.12	0
3	EDO	A	7206	-	3,3,3	0.44	0	2,2,2	0.42	0
3	EDO	A	7215	-	3,3,3	0.55	0	2,2,2	0.25	0
3	EDO	A	7226	-	3,3,3	0.45	0	2,2,2	0.47	0
3	EDO	A	7205	-	3,3,3	0.45	0	2,2,2	0.38	0
3	EDO	A	7207	-	3,3,3	0.43	0	2,2,2	0.51	0
3	EDO	A	7212	-	3,3,3	0.42	0	2,2,2	0.35	0
3	EDO	A	7225	-	3,3,3	0.48	0	2,2,2	0.43	0
3	EDO	A	7211	-	3,3,3	0.51	0	2,2,2	0.22	0
3	EDO	A	7219[D]	-	3,3,3	0.57	0	2,2,2	0.26	0
3	EDO	A	7224	-	3,3,3	0.46	0	2,2,2	0.36	0
3	EDO	A	7227	-	3,3,3	0.55	0	2,2,2	0.20	0
5	SAM	A	7213[C]	-	27,29,29	3.54	12 (44%)	34,42,42	2.12	12 (35%)
3	EDO	A	7203	-	3,3,3	0.44	0	2,2,2	0.95	0
3	EDO	B	4404	-	3,3,3	0.57	0	2,2,2	0.21	0
3	EDO	A	7218	-	3,3,3	0.45	0	2,2,2	0.50	0
3	EDO	A	7223	-	3,3,3	0.50	0	2,2,2	0.24	0
3	EDO	A	7208	-	3,3,3	0.42	0	2,2,2	0.51	0
3	EDO	A	7201	-	3,3,3	0.45	0	2,2,2	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MES	A	7202	-	12,12,12	2.01	1 (8%)	15,16,16	2.05	2 (13%)
3	EDO	A	7210	-	3,3,3	0.48	0	2,2,2	0.43	0
3	EDO	A	7214	-	3,3,3	0.43	0	2,2,2	0.73	0
6	W08	A	7228[B]	-	30,30,30	4.30	16 (53%)	44,44,44	2.34	18 (40%)
3	EDO	A	7220	-	3,3,3	0.47	0	2,2,2	0.38	0
3	EDO	A	7209	-	3,3,3	0.43	0	2,2,2	0.64	0
3	EDO	A	7221	-	3,3,3	0.49	0	2,2,2	0.35	0
3	EDO	A	7204	-	3,3,3	0.47	0	2,2,2	0.51	0
3	EDO	A	7229	-	3,3,3	0.51	0	2,2,2	0.27	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
3	EDO	A	7217	-	-	0/1/1/1	-
3	EDO	A	7222	-	-	0/1/1/1	-
3	EDO	B	4403	-	-	0/1/1/1	-
3	EDO	A	7216	-	-	0/1/1/1	-
3	EDO	A	7206	-	-	0/1/1/1	-
3	EDO	A	7215	-	-	0/1/1/1	-
3	EDO	A	7226	-	-	1/1/1/1	-
3	EDO	A	7205	-	-	0/1/1/1	-
3	EDO	A	7207	-	-	1/1/1/1	-
3	EDO	A	7212	-	-	1/1/1/1	-
3	EDO	A	7225	-	-	1/1/1/1	-
3	EDO	A	7211	-	-	0/1/1/1	-
3	EDO	A	7219[D]	-	-	0/1/1/1	-
3	EDO	A	7224	-	-	0/1/1/1	-
3	EDO	A	7227	-	-	0/1/1/1	-
5	SAM	A	7213[C]	-	-	6/17/33/33	0/3/3/3
3	EDO	A	7203	-	-	1/1/1/1	-
3	EDO	B	4404	-	-	0/1/1/1	-
3	EDO	A	7218	-	-	1/1/1/1	-
3	EDO	A	7223	-	-	1/1/1/1	-
3	EDO	A	7208	-	-	1/1/1/1	-
3	EDO	A	7201	-	-	0/1/1/1	-
4	MES	A	7202	-	-	4/6/14/14	0/1/1/1
3	EDO	A	7210	-	-	0/1/1/1	-
3	EDO	A	7214	-	-	1/1/1/1	-
6	W08	A	7228[B]	-	-	1/12/47/47	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	A	7220	-	-	0/1/1/1	-
3	EDO	A	7209	-	-	1/1/1/1	-
3	EDO	A	7221	-	-	0/1/1/1	-
3	EDO	A	7204	-	-	0/1/1/1	-
3	EDO	A	7229	-	-	1/1/1/1	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	7228[B]	W08	C10-N07	-10.68	1.20	1.46
6	A	7228[B]	W08	C26-C24	-10.62	1.24	1.53
6	A	7228[B]	W08	O12-C11	-10.23	1.29	1.43
5	A	7213[C]	SAM	C2'-C3'	-9.28	1.28	1.53
6	A	7228[B]	W08	C26-C11	8.04	1.64	1.53
5	A	7213[C]	SAM	O4'-C4'	-7.82	1.27	1.45
4	A	7202	MES	C8-S	-6.52	1.68	1.77
5	A	7213[C]	SAM	C3'-C4'	6.19	1.68	1.53
5	A	7213[C]	SAM	C6-N6	6.05	1.49	1.34
5	A	7213[C]	SAM	O4'-C1'	5.84	1.55	1.42
6	A	7228[B]	W08	C02-N03	5.43	1.45	1.34
6	A	7228[B]	W08	C19-N20	4.79	1.46	1.34
5	A	7213[C]	SAM	C1'-N9	-4.78	1.33	1.46
6	A	7228[B]	W08	O12-C13	3.88	1.51	1.42
6	A	7228[B]	W08	C13-N14	-3.87	1.35	1.46
6	A	7228[B]	W08	O25-C24	3.65	1.52	1.43
6	A	7228[B]	W08	C09-C04	-3.55	1.43	1.52
5	A	7213[C]	SAM	C8-N9	-3.31	1.31	1.37
5	A	7213[C]	SAM	O3'-C3'	3.20	1.50	1.43
6	A	7228[B]	W08	C05-C04	-3.19	1.44	1.52
6	A	7228[B]	W08	C23-N22	3.12	1.37	1.31
5	A	7213[C]	SAM	C4-N3	2.84	1.39	1.34
6	A	7228[B]	W08	O27-C26	2.49	1.49	1.43
5	A	7213[C]	SAM	O-C	2.32	1.29	1.22
5	A	7213[C]	SAM	OXT-C	-2.26	1.23	1.30
6	A	7228[B]	W08	C21-C15	-2.25	1.35	1.39
6	A	7228[B]	W08	C15-N16	2.23	1.38	1.34
6	A	7228[B]	W08	O01-C02	-2.21	1.19	1.23
5	A	7213[C]	SAM	O2'-C2'	2.19	1.48	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	7202	MES	C5-N4-C3	5.96	121.68	108.84
5	A	7213[C]	SAM	C5-C4-N3	-5.64	118.95	126.72
6	A	7228[B]	W08	C21-C15-N16	-5.54	119.09	126.72
6	A	7228[B]	W08	C05-C06-N07	4.37	116.83	111.20
6	A	7228[B]	W08	C06-C05-C04	4.26	117.39	110.67
6	A	7228[B]	W08	N14-C23-N22	-4.13	108.07	113.94
6	A	7228[B]	W08	C04-N03-C02	-4.09	116.71	123.29
6	A	7228[B]	W08	N18-C17-N16	-4.05	122.45	128.58
5	A	7213[C]	SAM	N3-C2-N1	-3.93	122.63	128.58
5	A	7213[C]	SAM	N3-C4-N9	3.81	133.65	127.17
5	A	7213[C]	SAM	C4-C5-N7	-3.60	106.47	110.58
6	A	7228[B]	W08	C06-N07-C08	3.58	115.23	109.54
6	A	7228[B]	W08	C17-N16-C15	3.54	120.48	111.83
5	A	7213[C]	SAM	C2-N3-C4	3.54	120.48	111.83
5	A	7213[C]	SAM	C5-N7-C8	3.34	108.70	103.45
6	A	7228[B]	W08	C26-C11-C02	-3.32	106.15	113.07
6	A	7228[B]	W08	N16-C15-N14	3.30	132.78	127.17
4	A	7202	MES	O3S-S-C8	3.25	112.36	106.00
5	A	7213[C]	SAM	N9-C8-N7	-3.17	109.44	113.94
6	A	7228[B]	W08	C24-C26-C11	3.11	105.36	101.69
6	A	7228[B]	W08	O12-C13-N14	2.88	113.62	108.09
6	A	7228[B]	W08	O12-C13-C24	-2.87	100.47	106.62
5	A	7213[C]	SAM	O4'-C1'-C2'	-2.71	100.81	106.62
6	A	7228[B]	W08	C13-O12-C11	-2.50	104.18	108.78
6	A	7228[B]	W08	C21-N22-C23	2.47	107.34	103.45
5	A	7213[C]	SAM	CG-SD-C5'	2.45	109.42	103.43
5	A	7213[C]	SAM	C4'-O4'-C1'	-2.33	104.32	109.47
6	A	7228[B]	W08	C09-C04-C05	2.25	114.69	110.80
6	A	7228[B]	W08	C09-C04-N03	-2.20	106.18	110.57
6	A	7228[B]	W08	C21-C15-N14	2.13	108.14	105.81
5	A	7213[C]	SAM	C4-N9-C8	2.13	107.98	105.74
5	A	7213[C]	SAM	C2'-C3'-C4'	2.03	106.53	102.61

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	7213[C]	SAM	C4'-C5'-SD-CG
5	A	7213[C]	SAM	C4'-C5'-SD-CE
4	A	7202	MES	C7-C8-S-O3S
3	A	7203	EDO	O1-C1-C2-O2
3	A	7207	EDO	O1-C1-C2-O2
3	A	7226	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	A	7202	MES	C8-C7-N4-C5
4	A	7202	MES	C7-C8-S-O1S
4	A	7202	MES	C7-C8-S-O2S
3	A	7208	EDO	O1-C1-C2-O2
5	A	7213[C]	SAM	OXT-C-CA-CB
5	A	7213[C]	SAM	O-C-CA-CB
3	A	7209	EDO	O1-C1-C2-O2
5	A	7213[C]	SAM	CB-CG-SD-CE
3	A	7214	EDO	O1-C1-C2-O2
3	A	7218	EDO	O1-C1-C2-O2
3	A	7223	EDO	O1-C1-C2-O2
3	A	7225	EDO	O1-C1-C2-O2
3	A	7229	EDO	O1-C1-C2-O2
6	A	7228[B]	W08	O12-C13-N14-C23
3	A	7212	EDO	O1-C1-C2-O2
5	A	7213[C]	SAM	CB-CG-SD-C5'

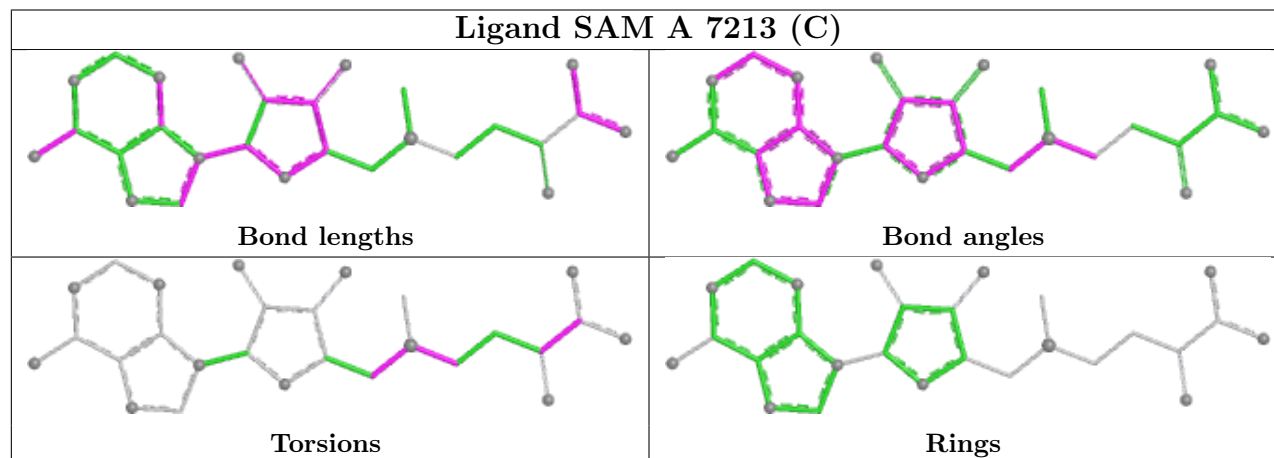
There are no ring outliers.

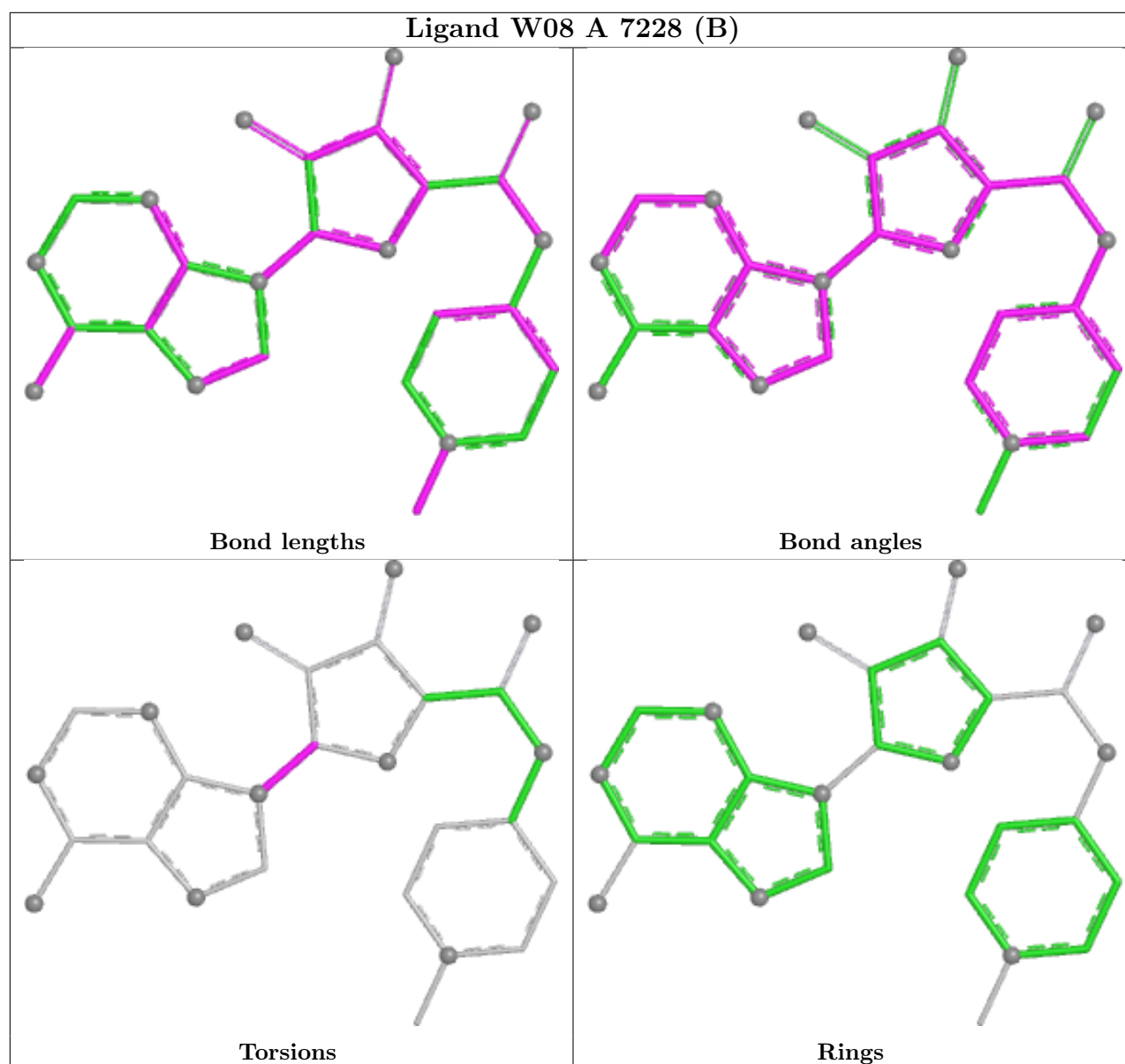
16 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	7222	EDO	3	0
3	A	7216	EDO	1	0
3	A	7205	EDO	2	0
3	A	7207	EDO	1	0
3	A	7225	EDO	2	0
3	A	7219[D]	EDO	1	0
3	A	7224	EDO	1	0
3	A	7227	EDO	3	0
5	A	7213[C]	SAM	4	0
3	B	4404	EDO	2	0
3	A	7218	EDO	2	0
4	A	7202	MES	1	0
6	A	7228[B]	W08	1	0
3	A	7220	EDO	3	0
3	A	7209	EDO	4	0
3	A	7221	EDO	1	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	301/304 (99%)	0.24	18 (5%) 27 33	15, 33, 62, 98	10 (3%)
2	B	116/140 (82%)	0.90	18 (15%) 5 5	29, 45, 78, 109	0
All	All	417/444 (93%)	0.43	36 (8%) 16 19	15, 36, 68, 109	10 (2%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	4386	LEU	13.0
1	A	7099	LEU	10.8
2	B	4271	ALA	7.6
2	B	4342	PHE	6.0
2	B	4339	PRO	5.1
1	A	6828	TYR	4.8
1	A	6799	SER	4.5
1	A	6800	SER	4.5
1	A	6832	ALA	3.3
2	B	4341	GLY	3.2
1	A	7040[A]	TYR	3.2
1	A	6829	GLY	3.2
2	B	4286	SER	3.2
2	B	4273	ALA	2.8
2	B	4337	PRO	2.8
1	A	7068	MET	2.7
1	A	7063	GLY	2.7
1	A	6862	ASN	2.7
1	A	7095	ASN	2.7
2	B	4368	THR	2.6
2	B	4383	CYS	2.6
1	A	6827[A]	ASN	2.6
1	A	7098	ASN	2.6
2	B	4338	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	7060	LEU	2.4
2	B	4340	LYS	2.4
1	A	7061	LYS	2.3
1	A	7065	ILE	2.3
1	A	7077[A]	ARG	2.3
2	B	4272	PHE	2.3
2	B	4276	ALA	2.2
2	B	4385	GLN	2.2
1	A	6933	LYS	2.2
2	B	4274	VAL	2.1
2	B	4372	VAL	2.1
2	B	4381	CYS	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
3	EDO	A	7227	4/4	0.75	0.20	57,69,92,92	0
3	EDO	A	7215	4/4	0.76	0.26	39,54,56,58	0
3	EDO	A	7210	4/4	0.78	0.23	51,60,64,70	0
3	EDO	B	4404	4/4	0.78	0.25	55,58,59,68	0
5	SAM	A	7213[C]	27/27	0.78	0.24	31,35,40,45	27
6	W08	A	7228[B]	27/27	0.79	0.24	33,36,41,46	27
3	EDO	A	7220	4/4	0.81	0.17	46,48,50,58	0
4	MES	A	7202	12/12	0.82	0.18	41,54,78,97	0
3	EDO	B	4403	4/4	0.82	0.21	52,53,59,64	0
3	EDO	A	7217	4/4	0.82	0.23	56,64,71,72	0
3	EDO	A	7216	4/4	0.83	0.21	50,53,60,62	0

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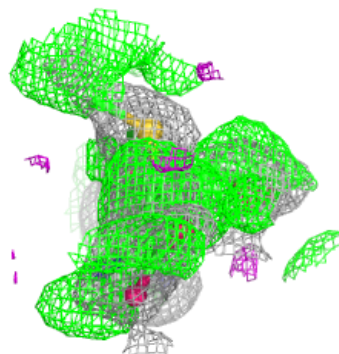
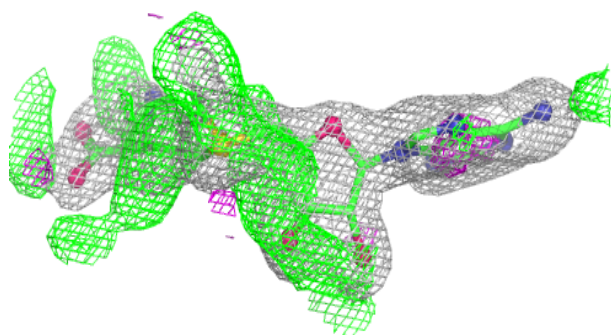
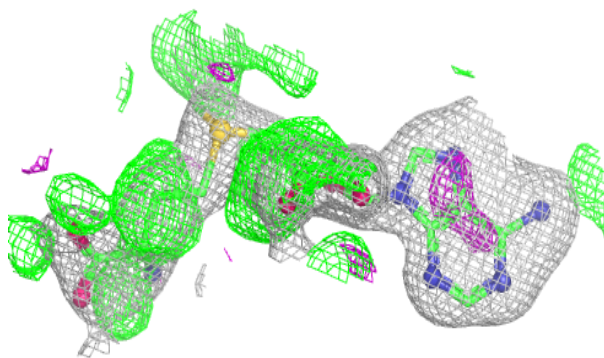
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	7222	4/4	0.84	0.19	56,58,62,66	0
3	EDO	A	7225	4/4	0.84	0.16	47,61,62,66	0
3	EDO	A	7223	4/4	0.85	0.20	53,60,60,61	0
3	EDO	A	7207	4/4	0.86	0.18	46,59,64,65	0
3	EDO	A	7209	4/4	0.87	0.15	44,48,52,56	0
3	EDO	A	7221	4/4	0.88	0.17	39,46,59,61	0
3	EDO	A	7219[D]	4/4	0.88	0.17	44,47,49,61	0
3	EDO	A	7208	4/4	0.89	0.17	43,54,54,67	0
3	EDO	A	7205	4/4	0.89	0.15	47,49,50,69	0
3	EDO	A	7218	4/4	0.91	0.16	50,58,58,63	0
3	EDO	A	7226	4/4	0.91	0.14	51,53,54,59	0
3	EDO	A	7211	4/4	0.91	0.13	42,46,51,55	0
3	EDO	A	7224	4/4	0.91	0.14	53,59,65,75	0
3	EDO	A	7229	4/4	0.92	0.11	41,58,65,69	0
3	EDO	A	7214	4/4	0.92	0.12	38,41,48,50	0
3	EDO	A	7203	4/4	0.94	0.12	47,51,52,56	0
7	CL	A	7230	1/1	0.94	0.12	64,64,64,64	0
3	EDO	A	7204	4/4	0.95	0.10	36,39,41,46	0
3	EDO	A	7206	4/4	0.95	0.11	40,50,52,57	0
3	EDO	A	7212	4/4	0.96	0.08	45,47,48,54	0
3	EDO	A	7201	4/4	0.96	0.09	34,38,41,44	0
8	ZN	B	4402	1/1	0.97	0.06	58,58,58,58	0
8	ZN	B	4401	1/1	1.00	0.02	39,39,39,39	0

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

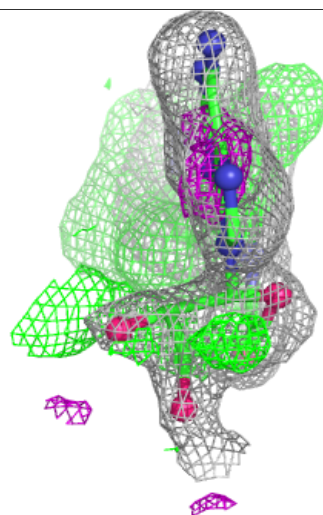
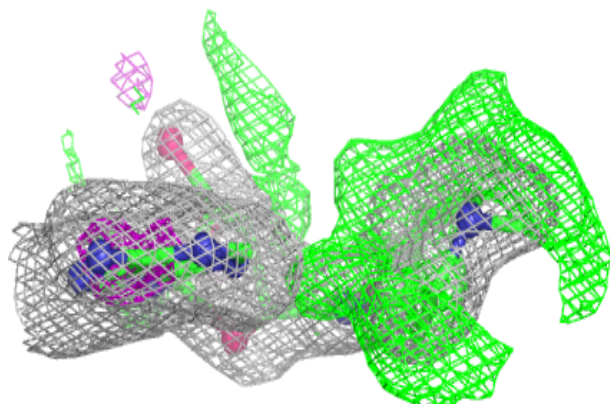
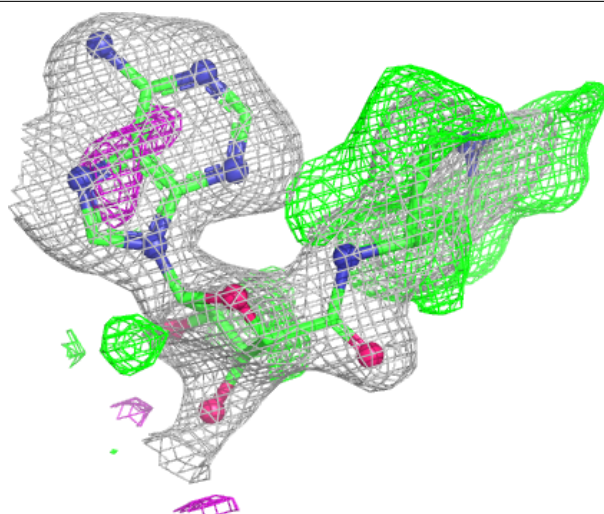
Electron density around SAM A 7213 (C):

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



Electron density around W08 A 7228 (B):

$2mF_o-DF_c$ (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.