



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:17 AM UTC

PDB ID : 4HPE / pdb_00004hpe
Title : Crystal structure of a putative cell wall hydrolase (CD630_03720) from Clostridium difficile 630 at 2.38 Å resolution
Authors : Joint Center for Structural Genomics (JCSG)
Deposited on : 2012-10-23
Resolution : 2.38 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
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

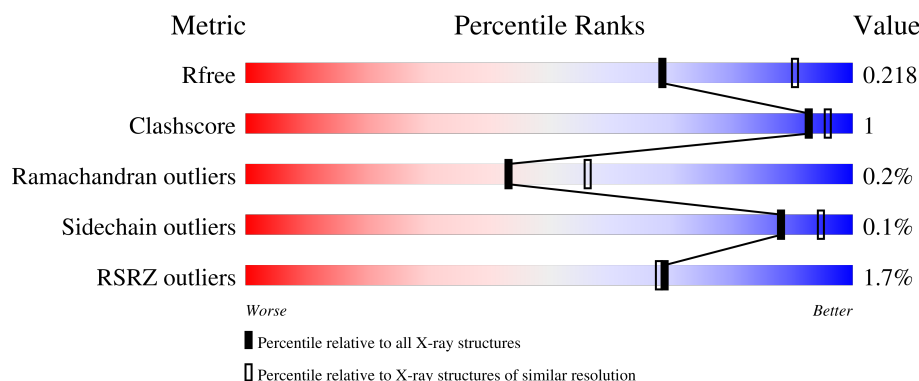
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

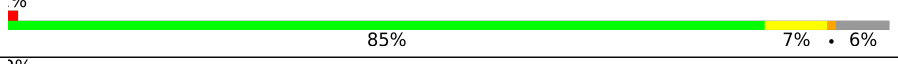
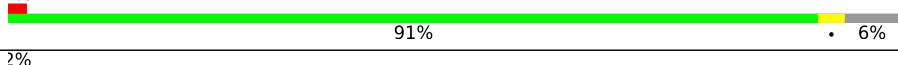
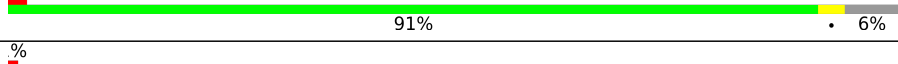
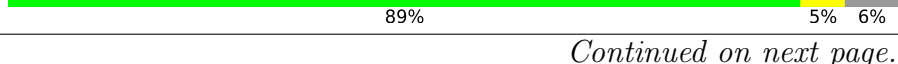
The reported resolution of this entry is 2.38 Å.

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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	308	 2% 88% 6% 6%
1	B	308	 % 85% 7% 6%
1	C	308	 2% 91% 6% 6%
1	D	308	 2% 91% 6% 6%
1	E	308	 % 89% 5% 6%

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Mol	Chain	Length	Quality of chain
1	F	308	3% 89% 5% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13970 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 Putative cell wall hydrolase Tn916-like,CTn1-Orf17.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	289	Total	C	N	O	S	Se	0	1	0
			2230	1408	378	435	3	6			
1	B	289	Total	C	N	O	S	Se	0	1	0
			2222	1403	377	433	3	6			
1	C	289	Total	C	N	O	S	Se	0	1	0
			2222	1403	377	433	3	6			
1	D	290	Total	C	N	O	S	Se	0	1	0
			2225	1406	376	434	3	6			
1	E	289	Total	C	N	O	S	Se	0	1	0
			2222	1403	375	435	3	6			
1	F	289	Total	C	N	O	S	Se	0	1	0
			2226	1405	377	435	3	6			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q18DB2
B	0	GLY	-	expression tag	UNP Q18DB2
C	0	GLY	-	expression tag	UNP Q18DB2
D	0	GLY	-	expression tag	UNP Q18DB2
E	0	GLY	-	expression tag	UNP Q18DB2
F	0	GLY	-	expression tag	UNP Q18DB2

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

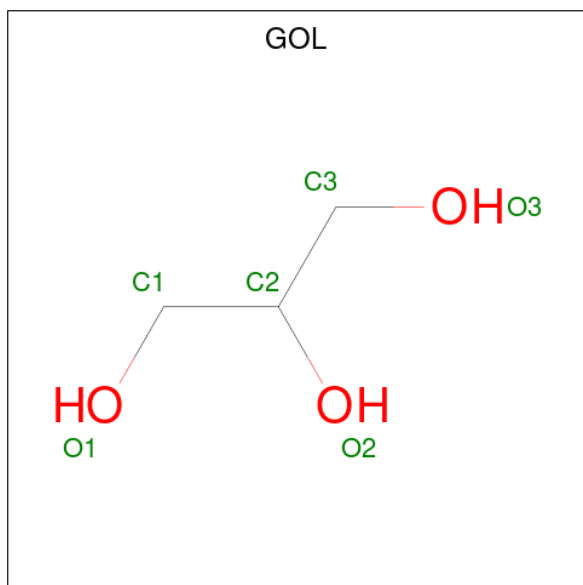
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Cl	0	0
			4	4		
2	B	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	F	1	Total Cl 1 1	0	0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	D	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

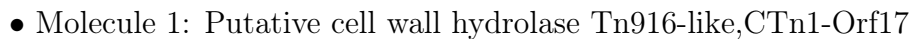
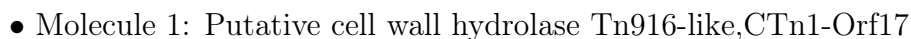
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	90	Total O 90 90	0	0
4	B	103	Total O 103 103	0	0

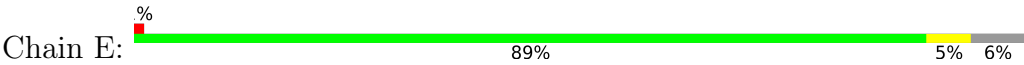
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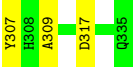
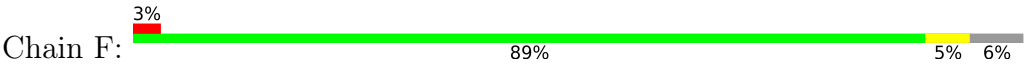
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	87	Total 87	O 87	0	0
4	D	108	Total 108	O 108	0	0
4	E	109	Total 109	O 109	0	0
4	F	93	Total 93	O 93	0	0

- Molecule 1: Putative cell wall hydrolase Tn916-like, CTn1-Orf17





● Molecule 1: Putative cell wall hydrolase Tn916-like,CTn1-Orf17



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.52Å 101.21Å 101.44Å 109.71° 108.86° 101.36°	Depositor
Resolution (Å)	49.40 – 2.38 49.40 – 2.38	Depositor EDS
% Data completeness (in resolution range)	87.6 (49.40-2.38) 87.6 (49.40-2.38)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.37Å)	Xtriage
Refinement program	BUSTER-TNT, BUSTER 2.10.0	Depositor
R, R_{free}	0.175 , 0.211 (Not available) , 0.218	Depositor DCC
R_{free} test set	3897 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	39.5	Xtriage
Anisotropy	0.600	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 61.6	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	0.95	EDS
Total number of atoms	13970	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: CL, GOL, OCS

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	0.87	0/2269	1.28	8/3060 (0.3%)
1	B	0.86	1/2261 (0.0%)	1.27	9/3051 (0.3%)
1	C	0.88	0/2261	1.28	1/3051 (0.0%)
1	D	0.87	0/2264	1.27	3/3055 (0.1%)
1	E	0.87	0/2261	1.29	2/3050 (0.1%)
1	F	0.86	0/2265	1.27	2/3056 (0.1%)
All	All	0.87	1/13581 (0.0%)	1.28	25/18323 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	299	ILE	CA-CB	5.17	1.60	1.54

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	241	ASP	CA-CB-CG	7.21	119.81	112.60
1	B	241	ASP	CA-CB-CG	7.00	119.60	112.60
1	A	241	ASP	CA-CB-CG	6.81	119.41	112.60
1	F	241	ASP	CA-CB-CG	6.61	119.21	112.60
1	D	241	ASP	CA-CB-CG	6.59	119.19	112.60
1	E	241	ASP	CA-CB-CG	6.41	119.01	112.60
1	B	198	GLU	CB-CG-CD	6.07	122.92	112.60
1	A	198	GLU	CB-CG-CD	5.99	122.79	112.60
1	A	104	ASP	CA-CB-CG	5.65	118.25	112.60
1	B	72	ASN	CA-CB-CG	5.54	118.14	112.60
1	B	297	VAL	CA-C-N	5.52	127.33	121.48
1	B	297	VAL	C-N-CA	5.52	127.33	121.48
1	B	146	GLY	CA-C-N	5.46	127.59	120.28
1	B	146	GLY	C-N-CA	5.46	127.59	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	328	ILE	N-CA-C	-5.41	106.42	111.45
1	E	198	GLU	CB-CG-CD	5.32	121.65	112.60
1	B	130	ASP	CA-CB-CG	5.17	117.77	112.60
1	D	328	ILE	N-CA-C	-5.14	106.78	111.67
1	F	46	ASN	CA-CB-CG	5.14	117.74	112.60
1	A	146	GLY	CA-C-N	5.08	127.05	120.44
1	A	146	GLY	C-N-CA	5.08	127.05	120.44
1	D	104	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	113	CYS	CA-C-N	5.02	127.01	120.28
1	A	113	CYS	C-N-CA	5.02	127.01	120.28
1	B	104	ASP	CA-CB-CG	5.01	117.61	112.60

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	2230	0	2126	7	0
1	B	2222	0	2111	11	0
1	C	2222	0	2111	5	0
1	D	2225	0	2112	2	0
1	E	2222	0	2107	7	0
1	F	2226	0	2115	7	0
2	A	4	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	12	0	16	0	0
3	B	6	0	8	0	0
3	D	6	0	8	0	0
4	A	90	0	0	1	0
4	B	103	0	0	2	0
4	C	87	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	108	0	0	0	0
4	E	109	0	0	1	0
4	F	93	0	0	1	0
All	All	13970	0	12714	38	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 1.

All (38) 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:E:317:ASP:HB2	4:E:547:HOH:O	1.90	0.70
1:F:242:OCS:HA	1:F:309:ALA:HB3	1.85	0.59
1:B:55:GLN:HG3	1:B:75:LEU:HD11	1.87	0.56
1:C:282:VAL:CG2	1:C:300:TYR:HB2	2.34	0.56
1:A:242:OCS:HA	1:A:309:ALA:HB3	1.88	0.55
1:B:242:OCS:HA	1:B:309:ALA:HB3	1.90	0.54
1:D:284:PHE:HB2	1:D:296:HIS:HB3	1.90	0.52
1:B:78:ILE:HG12	1:B:90:MSE:HG2	1.91	0.52
1:C:242:OCS:HA	1:C:309:ALA:HB3	1.92	0.52
1:C:282:VAL:HG23	1:C:300:TYR:HB2	1.93	0.50
1:B:282:VAL:HG22	1:B:300:TYR:HB2	1.93	0.49
1:B:213:LEU:HD13	1:B:255:ILE:HD12	1.94	0.49
1:F:317:ASP:HB2	4:F:556:HOH:O	2.13	0.49
1:E:260:THR:HG22	1:E:262:GLN:H	1.78	0.48
1:B:317:ASP:HB2	4:B:581:HOH:O	2.13	0.48
1:F:78:ILE:HG12	1:F:90:MSE:HG2	1.94	0.48
1:A:260:THR:HG22	1:A:262:GLN:H	1.79	0.46
1:E:284:PHE:HB2	1:E:296:HIS:HB3	1.97	0.46
1:C:284:PHE:HB2	1:C:296:HIS:HB3	1.98	0.45
1:E:242:OCS:HA	1:E:309:ALA:HB3	1.98	0.45
1:E:301:VAL:HG23	1:E:305:GLN:HG3	1.98	0.45
1:B:198:GLU:HB3	4:B:585:HOH:O	2.16	0.44
1:A:78:ILE:HG12	1:A:90:MSE:HG2	1.99	0.44
1:B:284:PHE:HB2	1:B:296:HIS:HB3	1.99	0.44
1:D:260:THR:HG22	1:D:262:GLN:H	1.83	0.44
1:A:202:GLN:NE2	4:A:558:HOH:O	2.52	0.43
1:E:73:VAL:HG21	1:E:131:LEU:HD21	2.02	0.42
1:F:188:ARG:HD2	1:F:193:ASN:HA	2.00	0.42
1:F:73:VAL:HG21	1:F:131:LEU:HD21	2.01	0.42
1:E:119:LEU:HD22	1:E:137:SER:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:284:PHE:HB2	1:F:296:HIS:HB3	2.02	0.42
1:A:192:GLY:HA2	1:B:289:ASN:OD1	2.20	0.41
1:F:218:MSE:HE1	1:F:307:TYR:CD2	2.56	0.41
1:B:128:ILE:HD11	1:B:149:ALA:HB2	2.02	0.41
1:B:273:LEU:HD13	1:B:282:VAL:HG13	2.03	0.41
1:A:218:MSE:HE1	1:A:307:TYR:CD2	2.57	0.40
1:A:284:PHE:HB2	1:A:296:HIS:HB3	2.03	0.40
1:C:301:VAL:HG23	1:C:305:GLN:HG3	2.03	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	285/308 (92%)	277 (97%)	8 (3%)	0	100	100
1	B	285/308 (92%)	277 (97%)	7 (2%)	1 (0%)	30	40
1	C	285/308 (92%)	277 (97%)	8 (3%)	0	100	100
1	D	286/308 (93%)	278 (97%)	7 (2%)	1 (0%)	36	48
1	E	285/308 (92%)	277 (97%)	8 (3%)	0	100	100
1	F	285/308 (92%)	279 (98%)	5 (2%)	1 (0%)	30	40
All	All	1711/1848 (93%)	1665 (97%)	43 (2%)	3 (0%)	43	56

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	190	ASN
1	D	190	ASN
1	F	190	ASN

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	230/242 (95%)	230 (100%)	0	100	100
1	B	228/242 (94%)	227 (100%)	1 (0%)	84	91
1	C	228/242 (94%)	228 (100%)	0	100	100
1	D	228/242 (94%)	228 (100%)	0	100	100
1	E	228/242 (94%)	227 (100%)	1 (0%)	84	91
1	F	229/242 (95%)	229 (100%)	0	100	100
All	All	1371/1452 (94%)	1369 (100%)	2 (0%)	88	95

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	282	VAL
1	E	46	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	132	ASN
1	B	158	ASN
1	B	303	ASN
1	B	305	GLN
1	B	325	GLN
1	C	46	ASN
1	C	101	ASN
1	C	225	GLN
1	C	305	GLN
1	C	325	GLN
1	D	46	ASN
1	D	91	GLN
1	D	101	ASN
1	D	132	ASN
1	D	158	ASN

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Mol	Chain	Res	Type
1	D	237	ASN
1	D	325	GLN
1	E	91	GLN
1	E	101	ASN
1	E	132	ASN
1	E	177	ASN
1	E	190	ASN
1	E	237	ASN
1	E	275	GLN
1	E	325	GLN
1	F	111	GLN
1	F	158	ASN
1	F	177	ASN
1	F	190	ASN
1	F	325	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	OCS	B	242	1	6,8,9	0.94	0	7,11,13	3.48	3 (42%)
1	OCS	C	242	1	6,8,9	2.00	1 (16%)	7,11,13	2.64	4 (57%)
1	OCS	A	242	1	6,8,9	1.16	0	7,11,13	3.91	5 (71%)
1	OCS	D	242	1	6,8,9	0.91	0	7,11,13	4.19	2 (28%)
1	OCS	F	242	1	6,8,9	0.99	0	7,11,13	3.96	3 (42%)
1	OCS	E	242	1	6,8,9	1.07	0	7,11,13	6.19	5 (71%)

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
1	OCS	B	242	1	-	3/4/7/9	-
1	OCS	C	242	1	-	2/4/7/9	-
1	OCS	A	242	1	-	3/4/7/9	-
1	OCS	D	242	1	-	3/4/7/9	-
1	OCS	F	242	1	-	3/4/7/9	-
1	OCS	E	242	1	-	2/4/7/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	242	OCS	CB-CA	-4.36	1.50	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	242	OCS	OD3-SG-CB	12.26	125.07	106.76
1	F	242	OCS	OD3-SG-CB	9.49	120.93	106.76
1	D	242	OCS	OD3-SG-CB	8.18	118.97	106.76
1	B	242	OCS	OD3-SG-CB	7.44	117.86	106.76
1	A	242	OCS	OD3-SG-CB	7.10	117.36	106.76
1	E	242	OCS	OD1-SG-CB	-7.04	96.24	106.76
1	D	242	OCS	OD2-SG-OD1	-6.94	94.04	111.40
1	A	242	OCS	OD1-SG-CB	5.77	115.37	106.76
1	E	242	OCS	OD2-SG-OD3	-5.20	98.40	111.40
1	E	242	OCS	CA-CB-SG	-5.18	105.91	113.61
1	C	242	OCS	OD3-SG-CB	4.35	113.25	106.76
1	B	242	OCS	OD2-SG-CB	-3.71	98.81	105.97
1	F	242	OCS	OD2-SG-OD3	-3.45	102.77	111.40
1	E	242	OCS	OD2-SG-OD1	3.45	120.02	111.40
1	C	242	OCS	OD1-SG-CB	3.39	111.82	106.76
1	A	242	OCS	OD2-SG-OD3	-3.06	103.74	111.40
1	A	242	OCS	OD2-SG-CB	-3.02	100.15	105.97
1	B	242	OCS	OD2-SG-OD3	-2.96	103.99	111.40
1	C	242	OCS	OD2-SG-CB	-2.85	100.48	105.97
1	C	242	OCS	OD2-SG-OD1	-2.34	105.54	111.40
1	F	242	OCS	OD2-SG-OD1	-2.25	105.76	111.40
1	A	242	OCS	OD2-SG-OD1	-2.01	106.38	111.40

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	242	OCS	CA-CB-SG-OD1
1	A	242	OCS	CA-CB-SG-OD2
1	A	242	OCS	CA-CB-SG-OD3
1	B	242	OCS	CA-CB-SG-OD1
1	B	242	OCS	CA-CB-SG-OD2
1	B	242	OCS	CA-CB-SG-OD3
1	C	242	OCS	CA-CB-SG-OD2
1	D	242	OCS	CA-CB-SG-OD1
1	D	242	OCS	CA-CB-SG-OD2
1	D	242	OCS	CA-CB-SG-OD3
1	E	242	OCS	N-CA-CB-SG
1	F	242	OCS	CA-CB-SG-OD1
1	F	242	OCS	CA-CB-SG-OD2
1	F	242	OCS	CA-CB-SG-OD3
1	C	242	OCS	CA-CB-SG-OD3
1	E	242	OCS	CA-CB-SG-OD1

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	242	OCS	1	0
1	C	242	OCS	1	0
1	A	242	OCS	1	0
1	F	242	OCS	1	0
1	E	242	OCS	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	A	405	-	5,5,5	0.08	0	5,5,5	0.30	0
3	GOL	B	402	-	5,5,5	0.16	0	5,5,5	0.41	0
3	GOL	D	402	-	5,5,5	0.14	0	5,5,5	0.33	0
3	GOL	A	406	-	5,5,5	0.14	0	5,5,5	0.39	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	GOL	A	405	-	-	1/4/4/4	-
3	GOL	B	402	-	-	0/4/4/4	-
3	GOL	D	402	-	-	2/4/4/4	-
3	GOL	A	406	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	405	GOL	O2-C2-C3-O3
3	D	402	GOL	C1-C2-C3-O3
3	D	402	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

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	282/308 (91%)	0.09	5 (1%) 67 66	31, 46, 71, 104	1 (0%)
1	B	282/308 (91%)	0.06	2 (0%) 84 83	30, 47, 71, 99	1 (0%)
1	C	282/308 (91%)	0.06	5 (1%) 67 66	24, 46, 75, 113	1 (0%)
1	D	283/308 (91%)	0.05	6 (2%) 63 62	25, 46, 72, 98	1 (0%)
1	E	282/308 (91%)	0.15	2 (0%) 84 83	27, 47, 77, 97	1 (0%)
1	F	282/308 (91%)	0.28	8 (2%) 55 54	31, 52, 89, 106	1 (0%)
All	All	1693/1848 (91%)	0.12	28 (1%) 69 68	24, 47, 78, 113	6 (0%)

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	206	VAL	4.9
1	C	43	THR	3.9
1	A	205	THR	3.7
1	A	43	THR	3.6
1	B	43	THR	3.6
1	D	43	THR	3.4
1	E	43	THR	3.3
1	E	205	THR	3.0
1	D	44	GLY	3.0
1	F	205	THR	2.8
1	F	43	THR	2.8
1	A	210	SER	2.7
1	F	44	GLY	2.7
1	D	210	SER	2.7
1	F	215	GLN	2.4
1	C	205	THR	2.4
1	D	46	ASN	2.3
1	A	46	ASN	2.3
1	A	211	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	179	ILE	2.1
1	D	205	THR	2.1
1	C	44	GLY	2.1
1	C	211	GLY	2.1
1	C	46	ASN	2.1
1	B	205	THR	2.1
1	F	121	SER	2.0
1	F	70	TYR	2.0
1	F	146	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	OCS	C	242	9/10	0.90	0.12	56,57,66,69	0
1	OCS	A	242	9/10	0.91	0.12	51,51,65,65	0
1	OCS	B	242	9/10	0.94	0.10	47,50,67,67	0
1	OCS	E	242	9/10	0.95	0.14	38,40,51,53	0
1	OCS	F	242	9/10	0.95	0.11	33,40,55,56	0
1	OCS	D	242	9/10	0.97	0.08	44,46,60,61	0

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	CL	E	401	1/1	0.87	0.14	62,62,62,62	0
2	CL	D	401	1/1	0.88	0.10	60,60,60,60	0
3	GOL	A	405	6/6	0.91	0.13	53,56,57,57	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	A	406	6/6	0.91	0.13	39,48,50,52	0
3	GOL	B	402	6/6	0.91	0.13	49,54,55,59	0
3	GOL	D	402	6/6	0.91	0.10	50,52,53,54	0
2	CL	B	401	1/1	0.92	0.23	81,81,81,81	0
2	CL	A	402	1/1	0.93	0.11	75,75,75,75	0
2	CL	C	401	1/1	0.94	0.12	70,70,70,70	0
2	CL	F	401	1/1	0.94	0.14	69,69,69,69	0
2	CL	A	403	1/1	0.94	0.10	87,87,87,87	0
2	CL	A	404	1/1	0.95	0.10	75,75,75,75	0
2	CL	A	401	1/1	0.97	0.12	41,41,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.