



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:14 PM UTC

PDB ID : 3FNK / pdb_00003fnk
Title : Crystal structure of the second type II cohesin module from the cellulosomal adaptor ScaA scaffoldin of *Acetivibrio cellulolyticus*
Authors : Noach, I.; Frolow, F.; Bayer, E.A.
Deposited on : 2008-12-25
Resolution : 1.99 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

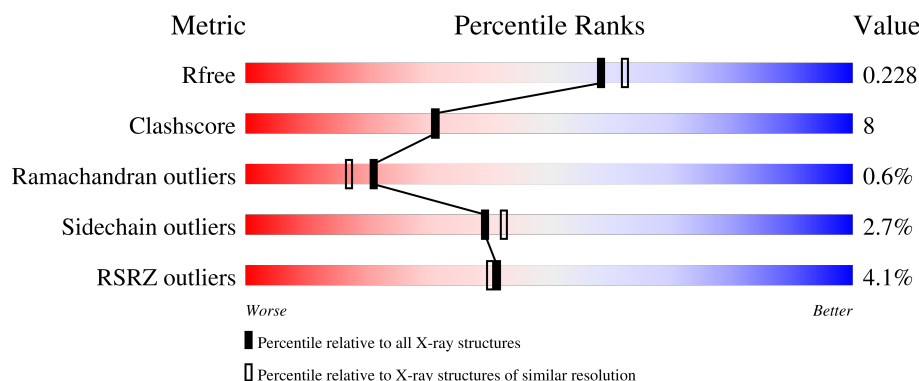
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	187	 7% 76% 14% • 7%
1	B	187	 2% 79% 11% • 9%
1	C	187	 2% 82% 9% • 8%

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	ACT	C	189	-	-	X	-
4	PDO	B	195	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4679 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 Cellulosomal scaffoldin adaptor protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	174	Total	C	N	O	S	0	8	0
			1373	877	219	274	3			
1	B	171	Total	C	N	O	S	0	6	0
			1355	861	218	272	4			
1	C	172	Total	C	N	O	S	0	4	0
			1341	853	216	269	3			

There are 24 discrepancies between the modelled and reference sequences:

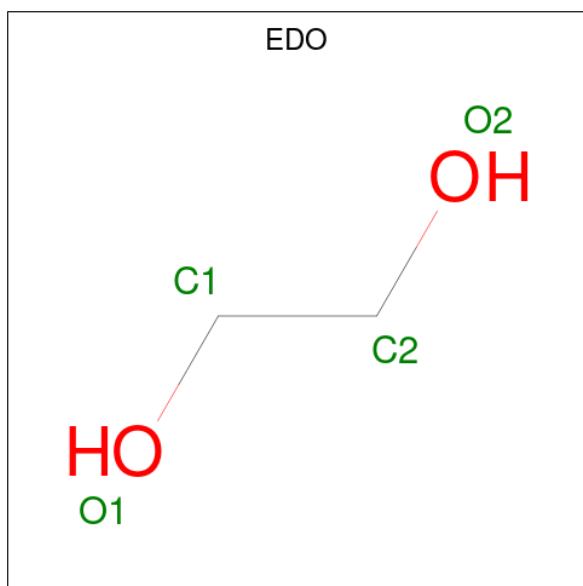
Chain	Residue	Modelled	Actual	Comment	Reference
A	180	LEU	-	expression tag	UNP Q7WYN3
A	181	GLU	-	expression tag	UNP Q7WYN3
A	182	HIS	-	expression tag	UNP Q7WYN3
A	183	HIS	-	expression tag	UNP Q7WYN3
A	184	HIS	-	expression tag	UNP Q7WYN3
A	185	HIS	-	expression tag	UNP Q7WYN3
A	186	HIS	-	expression tag	UNP Q7WYN3
A	187	HIS	-	expression tag	UNP Q7WYN3
B	180	LEU	-	expression tag	UNP Q7WYN3
B	181	GLU	-	expression tag	UNP Q7WYN3
B	182	HIS	-	expression tag	UNP Q7WYN3
B	183	HIS	-	expression tag	UNP Q7WYN3
B	184	HIS	-	expression tag	UNP Q7WYN3
B	185	HIS	-	expression tag	UNP Q7WYN3
B	186	HIS	-	expression tag	UNP Q7WYN3
B	187	HIS	-	expression tag	UNP Q7WYN3
C	180	LEU	-	expression tag	UNP Q7WYN3
C	181	GLU	-	expression tag	UNP Q7WYN3
C	182	HIS	-	expression tag	UNP Q7WYN3
C	183	HIS	-	expression tag	UNP Q7WYN3
C	184	HIS	-	expression tag	UNP Q7WYN3
C	185	HIS	-	expression tag	UNP Q7WYN3
C	186	HIS	-	expression tag	UNP Q7WYN3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	187	HIS	-	expression tag	UNP Q7WYN3

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



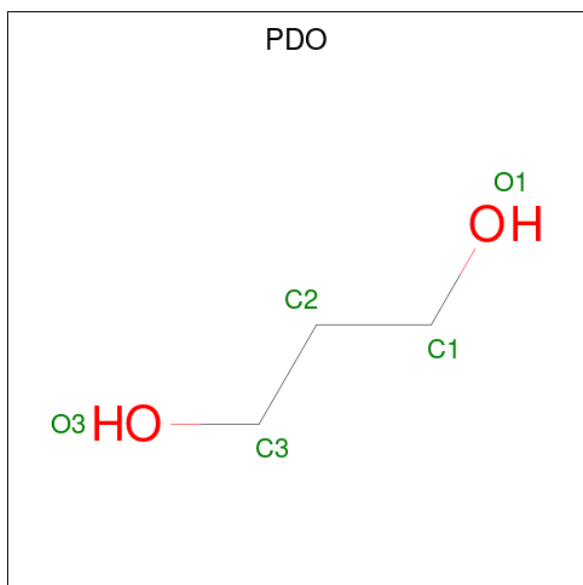
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



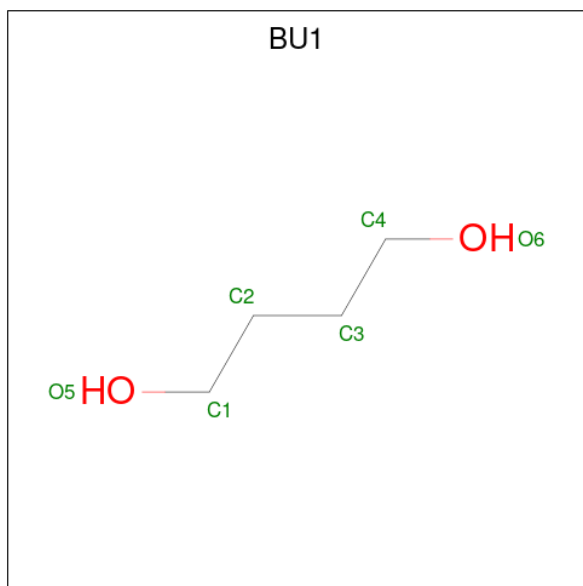
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 1,3-PROPANDIOL (CCD ID: PDO) (formula: C₃H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			5	3	2		
4	B	1	Total	C	O	0	0
			5	3	2		
4	C	1	Total	C	O	0	0
			5	3	2		

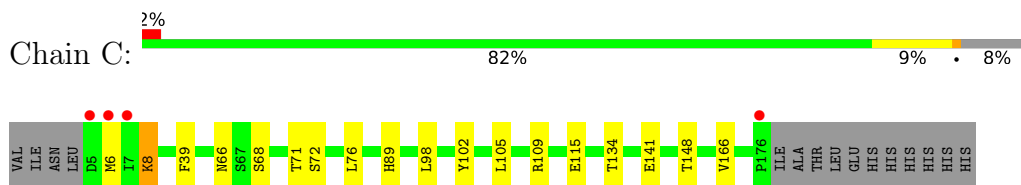
- Molecule 5 is 1,4-BUTANEDIOL (CCD ID: BU1) (formula: $C_4H_{10}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	4	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	160	Total	O	0	0
			160	160		
6	B	174	Total	O	0	0
			174	174		
6	C	207	Total	O	0	0
			207	207		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.36Å 68.64Å 111.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.07 – 1.99 29.07 – 1.99	Depositor EDS
% Data completeness (in resolution range)	95.1 (29.07-1.99) 95.1 (29.07-1.99)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.5.0044	Depositor
R, R_{free}	0.182 , 0.229 0.182 , 0.228	Depositor DCC
R_{free} test set	2305 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	24.7	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	4679	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% 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: EDO, PDO, ACT, BU1

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	0.93	1/1416 (0.1%)	0.94	0/1928
1	B	0.94	0/1380	0.92	1/1875 (0.1%)
1	C	1.00	0/1369	0.94	0/1862
All	All	0.96	1/4165 (0.0%)	0.94	1/5665 (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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	MET	N-CA	5.49	1.53	1.46

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	8	LYS	N-CA-C	6.70	121.83	112.72

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	6	MET	Peptide

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	1373	0	1383	20	0
1	B	1355	0	1346	28	0
1	C	1341	0	1336	18	0
2	A	4	0	6	0	0
2	B	20	0	30	3	1
2	C	8	0	12	1	0
3	A	4	0	3	0	0
3	B	4	0	3	1	0
3	C	8	0	6	9	0
4	A	5	0	8	0	1
4	B	5	0	8	4	0
4	C	5	0	8	0	0
5	B	6	0	10	1	0
6	A	160	0	0	3	0
6	B	174	0	0	3	1
6	C	207	0	0	5	0
All	All	4679	0	4159	68	2

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 8.

All (68) 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:B:79:GLU:H	5:B:193:BU1:H31	1.30	0.94
1:C:72:SER:H	3:C:189:ACT:CH3	1.85	0.90
1:B:8:LYS:HG3	1:B:35:LYS:HE2	1.51	0.90
3:B:194:ACT:H1	6:B:297:HOH:O	1.80	0.80
1:C:72:SER:H	3:C:189:ACT:H3	1.50	0.77
1:B:8:LYS:HG3	1:B:35:LYS:CE	2.16	0.75
1:C:72:SER:H	3:C:189:ACT:H2	1.53	0.72
1:B:7:ILE:HG23	1:B:8:LYS:N	2.04	0.71
1:B:7:ILE:HG23	1:B:8:LYS:H	1.55	0.71
1:A:23:VAL:O	6:A:556:HOH:O	2.10	0.69
1:C:71:THR:HA	3:C:189:ACT:H2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3[B]:ASN:N	6:A:547:HOH:O	2.27	0.67
1:B:155:TRP:CH2	2:B:189:EDO:H22	2.30	0.67
1:B:155:TRP:HH2	2:B:189:EDO:H22	1.60	0.65
1:A:89:HIS:HE1	1:A:98:LEU:HD23	1.61	0.64
3:C:189:ACT:H1	6:C:467:HOH:O	1.98	0.63
1:C:141:GLU:HG2	6:C:276:HOH:O	1.99	0.63
1:C:8:LYS:HA	6:C:203:HOH:O	1.99	0.62
1:B:106[B]:GLU:HG2	1:B:109:ARG:NH2	2.14	0.62
1:C:68:SER:OG	3:C:188:ACT:H3	2.01	0.60
1:A:75:LEU:HD22	1:A:115:GLU:HB3	1.87	0.56
1:C:76:LEU:HA	1:C:102:TYR:CZ	2.41	0.56
1:C:66:ASN:HB2	2:C:191:EDO:O2	2.08	0.54
1:C:8:LYS:HG2	6:C:231:HOH:O	2.08	0.54
1:A:5:ASP:O	1:A:6:MET:HB2	2.08	0.52
1:B:109:ARG:HG2	1:B:155:TRP:CG	2.45	0.52
1:A:76:LEU:HA	1:A:102:TYR:CZ	2.45	0.51
1:A:25:GLU:HA	6:A:449:HOH:O	2.11	0.51
1:C:72:SER:N	3:C:189:ACT:H2	2.24	0.50
1:B:6[A]:MET:O	1:B:6[A]:MET:HG3	2.11	0.50
1:B:106[B]:GLU:HG3	4:B:195:PDO:H31	1.94	0.50
1:A:4:LEU:HD23	1:A:4:LEU:C	2.36	0.50
1:B:105:LEU:HB2	4:B:195:PDO:H11	1.92	0.50
1:B:75:LEU:HD22	1:B:115:GLU:HB3	1.93	0.49
1:A:60:THR:OG1	1:A:62[A]:VAL:HG12	2.13	0.49
1:B:6[A]:MET:O	1:B:6[A]:MET:CG	2.60	0.49
1:B:105:LEU:HB2	4:B:195:PDO:H32	1.95	0.49
1:A:20:ALA:HA	1:A:173[A]:ASN:OD1	2.12	0.48
1:A:4:LEU:C	1:A:4:LEU:CD2	2.87	0.48
1:B:6[B]:MET:SD	6:B:472:HOH:O	2.61	0.47
1:B:76:LEU:HA	1:B:102:TYR:CZ	2.50	0.47
1:B:7:ILE:CG2	1:B:8:LYS:N	2.76	0.46
1:A:28:LYS:HE2	1:A:28:LYS:HB3	1.67	0.46
1:A:134:THR:HG22	1:A:171:GLU:HA	1.98	0.46
1:A:142:THR:C	1:A:144:PRO:HD3	2.42	0.45
1:B:37:THR:OG1	2:B:191:EDO:H22	2.17	0.45
1:B:159:ARG:NH1	6:B:462:HOH:O	2.51	0.44
1:C:89:HIS:HE1	1:C:98:LEU:HD23	1.81	0.44
1:C:134:THR:HG23	6:C:297:HOH:O	2.16	0.43
1:C:39:PHE:HB3	1:C:115:GLU:O	2.18	0.43
1:B:7:ILE:HD12	1:B:7:ILE:HA	1.95	0.43
1:C:105:LEU:O	1:C:109:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:HIS:CE1	1:A:98:LEU:HD23	2.48	0.42
1:B:8:LYS:CG	1:B:35:LYS:HE2	2.36	0.42
1:B:106[A]:GLU:H	4:B:195:PDO:C3	2.32	0.42
1:B:70:PRO:HB3	1:B:98:LEU:HD22	2.03	0.41
1:A:174:SER:O	1:A:176:PRO:HD3	2.19	0.41
1:B:7:ILE:O	1:B:8:LYS:HD3	2.21	0.41
1:B:14:MET:HE1	1:B:46:ILE:HD13	2.03	0.41
1:C:71:THR:CA	3:C:189:ACT:H2	2.45	0.41
1:A:8:LYS:O	1:A:35:LYS:NZ	2.53	0.41
1:B:56:VAL:HG12	1:B:63:ALA:HA	2.03	0.41
1:C:72:SER:N	3:C:189:ACT:H3	2.28	0.40
1:C:148:THR:HB	1:C:166:VAL:HG21	2.03	0.40
1:A:14:MET:HB3	1:A:169:PRO:HB3	2.04	0.40
1:B:145:ASN:HB3	1:B:159:ARG:NH1	2.36	0.40
1:A:4:LEU:O	1:A:7:ILE:HD11	2.21	0.40

All (2) 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)
4:A:190:PDO:O3	2:B:192:EDO:O2[2_574]	2.03	0.17
6:B:214:HOH:O	6:B:494:HOH:O[3_555]	2.04	0.16

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	179/187 (96%)	172 (96%)	4 (2%)	3 (2%)	7	3
1	B	174/187 (93%)	170 (98%)	3 (2%)	1 (1%)	21	17
1	C	174/187 (93%)	171 (98%)	3 (2%)	0	100	100
All	All	527/561 (94%)	513 (97%)	10 (2%)	4 (1%)	21	11

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	6	MET
1	B	7	ILE
1	A	173[A]	ASN
1	A	173[B]	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	156/160 (98%)	148 (95%)	8 (5%)	21	19
1	B	151/160 (94%)	148 (98%)	3 (2%)	48	54
1	C	150/160 (94%)	148 (99%)	2 (1%)	61	68
All	All	457/480 (95%)	444 (97%)	13 (3%)	39	41

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	19	ASN
1	A	90	LYS
1	A	91	ILE
1	A	139[A]	ASP
1	A	139[B]	ASP
1	A	142	THR
1	A	174	SER
1	B	7	ILE
1	B	8	LYS
1	B	28	LYS
1	C	6	MET
1	C	8	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	GLN
1	A	145	ASN
1	B	38	ASN
1	B	86	GLN
1	B	129	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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	$\# Z > 2$
4	PDO	A	190	-	4,4,4	0.32	0	3,3,3	0.88	0
2	EDO	B	190	-	3,3,3	0.65	0	2,2,2	0.15	0
4	PDO	B	195	-	4,4,4	0.55	0	3,3,3	0.53	0
2	EDO	B	188	-	3,3,3	0.61	0	2,2,2	0.24	0
3	ACT	B	194	-	3,3,3	0.92	0	3,3,3	2.07	2 (66%)
2	EDO	C	191	-	3,3,3	0.46	0	2,2,2	0.36	0
3	ACT	A	189	-	3,3,3	0.93	0	3,3,3	1.91	1 (33%)
3	ACT	C	189	-	3,3,3	1.24	1 (33%)	3,3,3	1.55	1 (33%)
2	EDO	A	188	-	3,3,3	0.32	0	2,2,2	0.50	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	B	191	-	3,3,3	0.51	0	2,2,2	0.36	0
5	BU1	B	193	-	5,5,5	0.47	0	4,4,4	0.42	0
4	PDO	C	192	-	4,4,4	0.47	0	3,3,3	0.32	0
3	ACT	C	188	-	3,3,3	0.68	0	3,3,3	2.11	2 (66%)
2	EDO	B	192	-	3,3,3	0.77	0	2,2,2	0.43	0
2	EDO	C	190	-	3,3,3	0.48	0	2,2,2	0.42	0
2	EDO	B	189	-	3,3,3	0.52	0	2,2,2	0.14	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PDO	A	190	-	-	2/2/2/2	-
2	EDO	B	190	-	-	0/1/1/1	-
4	PDO	B	195	-	-	0/2/2/2	-
2	EDO	B	188	-	-	0/1/1/1	-
2	EDO	C	191	-	-	1/1/1/1	-
2	EDO	A	188	-	-	0/1/1/1	-
2	EDO	B	191	-	-	0/1/1/1	-
5	BU1	B	193	-	-	1/3/3/3	-
4	PDO	C	192	-	-	2/2/2/2	-
2	EDO	B	192	-	-	1/1/1/1	-
2	EDO	C	190	-	-	1/1/1/1	-
2	EDO	B	189	-	-	1/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	189	ACT	OXT-C	-2.02	1.21	1.30

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	189	ACT	OXT-C-O	-2.69	112.06	122.03
3	C	188	ACT	OXT-C-CH3	2.64	126.10	115.05
3	B	194	ACT	OXT-C-O	-2.57	112.48	122.03
3	C	188	ACT	OXT-C-O	-2.51	112.72	122.03
3	B	194	ACT	OXT-C-CH3	2.50	125.53	115.05
3	C	189	ACT	OXT-C-O	-2.24	113.73	122.03

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	190	PDO	O1-C1-C2-C3
4	A	190	PDO	C1-C2-C3-O3
4	C	192	PDO	C1-C2-C3-O3
2	B	189	EDO	O1-C1-C2-O2
5	B	193	BU1	O5-C1-C2-C3
2	C	191	EDO	O1-C1-C2-O2
4	C	192	PDO	O1-C1-C2-C3
2	B	192	EDO	O1-C1-C2-O2
2	C	190	EDO	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	190	PDO	0	1
4	B	195	PDO	4	0
3	B	194	ACT	1	0
2	C	191	EDO	1	0
3	C	189	ACT	8	0
2	B	191	EDO	1	0
5	B	193	BU1	1	0
3	C	188	ACT	1	0
2	B	192	EDO	0	1
2	B	189	EDO	2	0

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	174/187 (93%)	0.41	14 (8%)	18 17	14, 31, 55, 65	8 (4%)
1	B	171/187 (91%)	-0.25	3 (1%)	67 67	12, 25, 40, 54	6 (3%)
1	C	172/187 (91%)	-0.44	4 (2%)	61 60	9, 22, 35, 65	4 (2%)
All	All	517/561 (92%)	-0.09	21 (4%)	41 40	9, 25, 50, 65	18 (3%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3[A]	ASN	6.1
1	B	6[A]	MET	5.9
1	A	176	PRO	3.8
1	A	6	MET	3.6
1	A	173[A]	ASN	3.3
1	B	7	ILE	3.2
1	A	128	LEU	2.9
1	C	176	PRO	2.9
1	A	170	GLY	2.9
1	A	144	PRO	2.8
1	A	145	ASN	2.6
1	B	176	PRO	2.5
1	C	6	MET	2.4
1	A	142	THR	2.4
1	A	172	ILE	2.4
1	A	20	ALA	2.4
1	C	5	ASP	2.4
1	A	23	VAL	2.3
1	C	7	ILE	2.3
1	A	7	ILE	2.2
1	A	21	ALA	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($\text{\AA}^2$)	Q<0.9
2	EDO	B	192	4/4	0.64	0.34	79,82,82,83	0
3	ACT	C	188	4/4	0.70	0.21	48,49,49,49	0
3	ACT	A	189	4/4	0.72	0.17	34,34,35,38	0
4	PDO	A	190	5/5	0.79	0.21	66,68,72,73	0
5	BU1	B	193	6/6	0.79	0.16	42,44,48,49	0
4	PDO	B	195	5/5	0.84	0.14	43,45,46,46	0
4	PDO	C	192	5/5	0.85	0.14	40,46,49,50	0
3	ACT	C	189	4/4	0.85	0.12	35,36,38,39	0
2	EDO	B	189	4/4	0.88	0.19	38,38,41,41	0
2	EDO	B	191	4/4	0.89	0.12	44,45,45,46	0
2	EDO	C	191	4/4	0.90	0.11	55,55,56,56	0
3	ACT	B	194	4/4	0.90	0.14	35,36,36,37	0
2	EDO	A	188	4/4	0.92	0.09	29,33,35,37	0
2	EDO	C	190	4/4	0.96	0.10	20,30,34,36	0
2	EDO	B	188	4/4	0.96	0.07	36,38,39,41	0
2	EDO	B	190	4/4	0.97	0.06	23,25,26,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.