



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:52 PM UTC

PDB ID : 4NN0 / pdb_00004nn0
Title : Crystal structure of the C1QTNF5 globular domain in space group P63
Authors : Tu, X.; Palczewski, K.
Deposited on : 2013-11-15
Resolution : 1.42 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

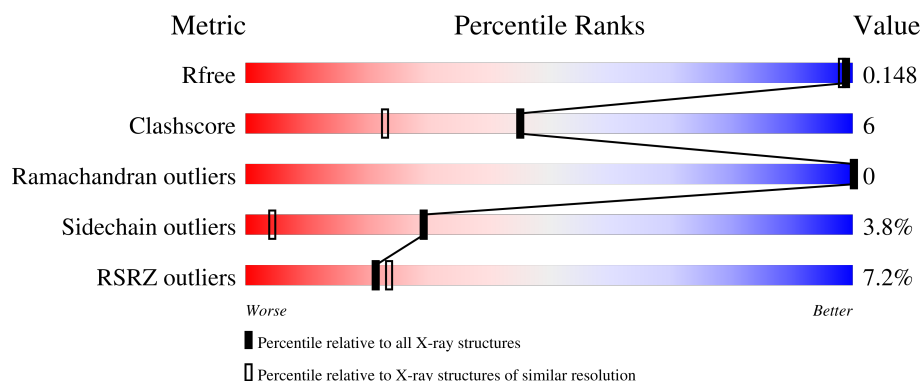
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.42 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	4041 (1.44-1.40)
Clashscore	190562	4154 (1.44-1.40)
Ramachandran outliers	187476	4083 (1.44-1.40)
Sidechain outliers	187428	4082 (1.44-1.40)
RSRZ outliers	180081	4039 (1.44-1.40)

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	148	87% 5% 7%
1	B	148	3% 83% 12% 5%
1	C	148	17% 75% 16% 7%

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
2	EDO	A	303	-	-	X	-
2	EDO	B	303	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3681 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 Complement C1q tumor necrosis factor-related protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	0	3	0
			1095	710	181	202	2			
1	B	141	Total	C	N	O	S	0	3	0
			1121	725	185	209	2			
1	C	138	Total	C	N	O	S	0	0	0
			1076	696	178	200	2			

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	102	ALA	-	expression tag	UNP Q9BXJ0
A	244	HIS	-	expression tag	UNP Q9BXJ0
A	245	HIS	-	expression tag	UNP Q9BXJ0
A	246	HIS	-	expression tag	UNP Q9BXJ0
A	247	HIS	-	expression tag	UNP Q9BXJ0
A	248	HIS	-	expression tag	UNP Q9BXJ0
A	249	HIS	-	expression tag	UNP Q9BXJ0
B	102	ALA	-	expression tag	UNP Q9BXJ0
B	244	HIS	-	expression tag	UNP Q9BXJ0
B	245	HIS	-	expression tag	UNP Q9BXJ0
B	246	HIS	-	expression tag	UNP Q9BXJ0
B	247	HIS	-	expression tag	UNP Q9BXJ0
B	248	HIS	-	expression tag	UNP Q9BXJ0
B	249	HIS	-	expression tag	UNP Q9BXJ0
C	102	ALA	-	expression tag	UNP Q9BXJ0
C	244	HIS	-	expression tag	UNP Q9BXJ0
C	245	HIS	-	expression tag	UNP Q9BXJ0
C	246	HIS	-	expression tag	UNP Q9BXJ0
C	247	HIS	-	expression tag	UNP Q9BXJ0
C	248	HIS	-	expression tag	UNP Q9BXJ0
C	249	HIS	-	expression tag	UNP Q9BXJ0

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



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 4 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

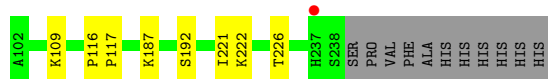
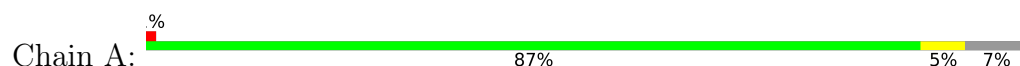
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	136	Total	O	0	0
			136	136		
5	B	131	Total	O	0	0
			131	131		
5	C	27	Total	O	0	0
			27	27		

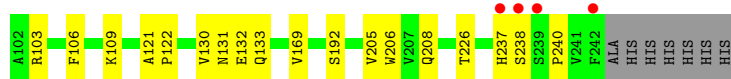
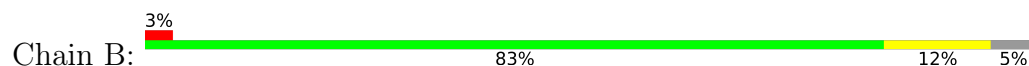
3 Residue-property plots [i](#)

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.

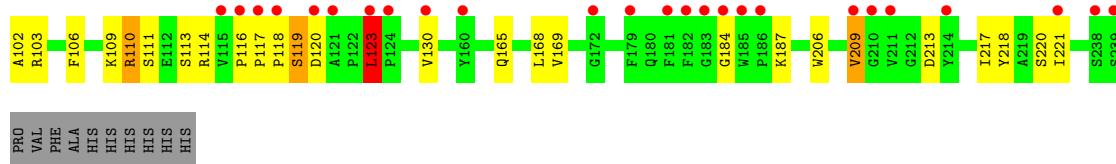
- Molecule 1: Complement C1q tumor necrosis factor-related protein 5



- Molecule 1: Complement C1q tumor necrosis factor-related protein 5



- Molecule 1: Complement C1q tumor necrosis factor-related protein 5



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	50.60Å 50.60Å 268.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	134.26 – 1.42 134.26 – 1.42	Depositor EDS
% Data completeness (in resolution range)	99.0 (134.26-1.42) 99.1 (134.26-1.42)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 1.42Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.104 , 0.142 0.114 , 0.148	Depositor DCC
R_{free} test set	3646 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	11.5	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 46.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.175 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	3681	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% 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, ACT, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.82	0/1130	0.90	0/1539
1	B	0.87	4/1157 (0.3%)	0.90	0/1577
1	C	0.65	0/1111	1.00	3/1513 (0.2%)
All	All	0.79	4/3398 (0.1%)	0.93	3/4629 (0.1%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	131	ASN	CA-CB	5.62	1.62	1.53
1	B	133	GLN	C-O	-5.19	1.17	1.24
1	B	131	ASN	C-O	-5.19	1.17	1.24
1	B	132	GLU	CA-CB	-5.13	1.44	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	116	PRO	CA-C-N	7.54	128.15	120.38
1	C	116	PRO	C-N-CA	7.54	128.15	120.38
1	C	123	LEU	CD1-CG-CD2	-5.81	98.01	110.80

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	1095	0	1043	8	0
1	B	1121	0	1061	16	0
1	C	1076	0	1021	14	0
2	A	48	0	72	8	0
2	B	20	0	30	8	0
2	C	4	0	6	1	0
3	A	5	0	0	0	0
3	B	10	0	0	0	0
4	A	4	0	3	0	0
4	B	4	0	3	1	0
5	A	136	0	0	0	0
5	B	131	0	0	2	0
5	C	27	0	0	0	0
All	All	3681	0	3239	39	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 6.

All (39) 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:192:SER:OG	2:A:301:EDO:H11	1.73	0.87
1:B:103:ARG:H	2:B:302:EDO:H11	1.45	0.79
1:B:192:SER:O	2:B:303:EDO:H21	1.83	0.79
2:A:303:EDO:H11	2:A:305:EDO:H22	1.65	0.78
1:C:123:LEU:HD21	1:C:217:ILE:HG21	1.65	0.78
1:B:238:SER:HA	1:C:218:TYR:OH	1.88	0.74
1:A:192:SER:OG	2:A:301:EDO:C1	2.42	0.68
1:C:119:SER:HA	1:C:209:VAL:HG23	1.75	0.67
4:B:308:ACT:H2	5:B:526:HOH:O	1.99	0.62
1:A:187:LYS:HE2	2:A:303:EDO:H22	1.84	0.59
1:B:192:SER:H	2:B:303:EDO:H21	1.67	0.59
2:A:303:EDO:C1	2:A:305:EDO:H22	2.34	0.55
1:C:165:GLN:O	1:C:209:VAL:HG12	2.06	0.55
1:B:240:PRO:HB2	1:C:187:LYS:HG2	1.90	0.53
2:A:302:EDO:O1	2:A:309:EDO:H22	2.10	0.52
1:B:238:SER:O	1:C:220:SER:HB2	2.11	0.51
1:B:106:PHE:HA	1:B:130:VAL:O	2.10	0.51
1:B:121:ALA:HB3	2:B:304:EDO:H21	1.93	0.51
1:B:122:PRO:O	2:B:304:EDO:H22	2.11	0.50
1:B:206:TRP:HE1	1:B:208[A]:GLN:HE21	1.60	0.50
1:C:123:LEU:HD23	1:C:217:ILE:HD13	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:LYS:HG2	1:A:226:THR:HG22	1.93	0.49
1:B:109:LYS:HG2	1:B:226:THR:HG22	1.95	0.48
1:C:169:VAL:HG21	1:C:206:TRP:CE2	2.48	0.48
1:A:221[B]:ILE:HG22	1:A:222:LYS:HG2	1.96	0.48
1:B:192:SER:H	2:B:303:EDO:C2	2.27	0.47
1:A:187:LYS:HE2	2:A:303:EDO:C2	2.44	0.47
5:B:498:HOH:O	1:C:184:GLY:HA2	2.15	0.46
1:B:192:SER:N	2:B:303:EDO:H21	2.30	0.46
1:C:117:PRO:HA	1:C:118:PRO:HD3	1.80	0.46
1:C:110:ARG:HH22	1:C:117:PRO:HB3	1.81	0.45
1:C:106:PHE:HA	1:C:130:VAL:O	2.18	0.43
1:C:102:ALA:N	2:C:301:EDO:HO1	2.17	0.42
1:A:187:LYS:NZ	2:A:303:EDO:H21	2.34	0.42
1:B:192:SER:C	2:B:303:EDO:H21	2.45	0.42
1:A:116:PRO:HA	1:A:117:PRO:HD3	1.98	0.41
1:B:206:TRP:HE1	1:B:208[A]:GLN:NE2	2.18	0.40
1:B:169:VAL:O	1:B:205:VAL:HA	2.21	0.40
1:C:114:ARG:HG2	1:C:114:ARG:NH1	2.37	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	138/148 (93%)	132 (96%)	6 (4%)	0	100	100
1	B	142/148 (96%)	134 (94%)	8 (6%)	0	100	100
1	C	136/148 (92%)	130 (96%)	6 (4%)	0	100	100
All	All	416/444 (94%)	396 (95%)	20 (5%)	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	116/123 (94%)	116 (100%)	0	100	100
1	B	119/123 (97%)	118 (99%)	1 (1%)	73	47
1	C	114/123 (93%)	102 (90%)	12 (10%)	6	0
All	All	349/369 (95%)	336 (96%)	13 (4%)	29	5

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

Mol	Chain	Res	Type
1	B	237	HIS
1	C	103	ARG
1	C	109	LYS
1	C	110	ARG
1	C	111	SER
1	C	113	SER
1	C	119	SER
1	C	120	ASP
1	C	123	LEU
1	C	168	LEU
1	C	209	VAL
1	C	213	ASP
1	C	221	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	GLN
1	A	237	HIS
1	B	204	GLN
1	C	204	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

23 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	$\# Z > 2$
2	EDO	A	310	-	3,3,3	0.43	0	2,2,2	0.35	0
2	EDO	B	304	-	3,3,3	0.72	0	2,2,2	0.89	0
2	EDO	B	302	-	3,3,3	0.51	0	2,2,2	0.26	0
2	EDO	B	305	-	3,3,3	0.28	0	2,2,2	0.50	0
2	EDO	A	306	-	3,3,3	0.43	0	2,2,2	0.36	0
3	SO4	A	313	-	4,4,4	0.43	0	6,6,6	0.07	0
2	EDO	A	305	-	3,3,3	0.54	0	2,2,2	0.62	0
2	EDO	A	308	-	3,3,3	0.34	0	2,2,2	0.55	0
3	SO4	B	306	-	4,4,4	0.43	0	6,6,6	0.08	0
4	ACT	A	314	-	3,3,3	1.16	0	3,3,3	0.70	0
3	SO4	B	307	-	4,4,4	0.38	0	6,6,6	0.08	0
2	EDO	A	307	-	3,3,3	0.62	0	2,2,2	0.31	0
2	EDO	A	302	-	3,3,3	0.16	0	2,2,2	0.65	0
2	EDO	A	312	-	3,3,3	0.31	0	2,2,2	0.85	0
2	EDO	C	301	-	3,3,3	0.46	0	2,2,2	0.27	0
2	EDO	A	301	-	3,3,3	0.97	0	2,2,2	1.80	0
2	EDO	A	303	-	3,3,3	0.57	0	2,2,2	0.42	0
2	EDO	B	301	-	3,3,3	0.25	0	2,2,2	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	B	303	-	3,3,3	0.99	0	2,2,2	1.44	0
2	EDO	A	309	-	3,3,3	0.50	0	2,2,2	0.31	0
4	ACT	B	308	-	3,3,3	0.48	0	3,3,3	1.00	0
2	EDO	A	311	-	3,3,3	0.49	0	2,2,2	0.24	0
2	EDO	A	304	-	3,3,3	0.80	0	2,2,2	0.07	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
2	EDO	A	312	-	-	1/1/1/1	-
2	EDO	A	303	-	-	1/1/1/1	-
2	EDO	A	306	-	-	1/1/1/1	-
2	EDO	A	305	-	-	0/1/1/1	-
2	EDO	A	308	-	-	1/1/1/1	-
2	EDO	A	310	-	-	0/1/1/1	-
2	EDO	C	301	-	-	1/1/1/1	-
2	EDO	B	304	-	-	0/1/1/1	-
2	EDO	A	309	-	-	1/1/1/1	-
2	EDO	B	301	-	-	0/1/1/1	-
2	EDO	A	301	-	-	0/1/1/1	-
2	EDO	B	303	-	-	0/1/1/1	-
2	EDO	A	307	-	-	1/1/1/1	-
2	EDO	B	302	-	-	0/1/1/1	-
2	EDO	B	305	-	-	1/1/1/1	-
2	EDO	A	311	-	-	1/1/1/1	-
2	EDO	A	304	-	-	0/1/1/1	-
2	EDO	A	302	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	306	EDO	O1-C1-C2-O2
2	A	309	EDO	O1-C1-C2-O2
2	C	301	EDO	O1-C1-C2-O2
2	A	308	EDO	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
2	A	311	EDO	O1-C1-C2-O2
2	B	305	EDO	O1-C1-C2-O2
2	A	307	EDO	O1-C1-C2-O2
2	A	312	EDO	O1-C1-C2-O2
2	A	303	EDO	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	304	EDO	2	0
2	B	302	EDO	1	0
2	A	305	EDO	2	0
2	A	302	EDO	1	0
2	C	301	EDO	1	0
2	A	301	EDO	2	0
2	A	303	EDO	5	0
2	B	303	EDO	5	0
2	A	309	EDO	1	0
4	B	308	ACT	1	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	137/148 (92%)	-0.68	1 (0%) 84 87	6, 11, 22, 62	3 (2%)
1	B	141/148 (95%)	-0.51	4 (2%) 55 58	6, 12, 31, 99	3 (2%)
1	C	138/148 (93%)	1.15	25 (18%) 3 4	27, 44, 98, 139	0
All	All	416/444 (93%)	-0.02	30 (7%) 21 23	6, 15, 73, 139	6 (1%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	209	VAL	5.1
1	C	116	PRO	4.9
1	C	210	GLY	4.7
1	C	123	LEU	4.7
1	C	238	SER	4.5
1	C	118	PRO	4.5
1	C	117	PRO	4.1
1	C	211	VAL	4.0
1	C	115	VAL	3.8
1	C	121	ALA	3.7
1	B	237	HIS	3.7
1	C	221	ILE	3.6
1	C	124	PRO	3.6
1	C	179	PHE	3.4
1	C	214	TYR	3.4
1	B	242	PHE	3.4
1	C	181	PHE	3.1
1	C	120	ASP	3.1
1	C	185	TRP	2.9
1	C	239	SER	2.6
1	C	182	PHE	2.6
1	C	160	TYR	2.6
1	C	184	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	172	GLY	2.4
1	C	183	GLY	2.3
1	B	238	SER	2.2
1	C	186	PRO	2.1
1	A	237	HIS	2.1
1	B	239	SER	2.1
1	C	130	VAL	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	EDO	A	305	4/4	0.79	0.17	34,35,37,64	0
2	EDO	A	308	4/4	0.82	0.21	45,51,53,113	0
2	EDO	A	310	4/4	0.82	0.16	38,44,47,53	0
2	EDO	A	303	4/4	0.85	0.14	21,38,48,56	0
2	EDO	B	305	4/4	0.87	0.17	28,29,30,33	4
4	ACT	B	308	4/4	0.87	0.16	17,20,24,51	4
2	EDO	C	301	4/4	0.89	0.11	48,53,53,58	0
2	EDO	A	306	4/4	0.89	0.13	40,44,54,67	0
2	EDO	A	309	4/4	0.91	0.10	26,29,35,49	0
2	EDO	A	307	4/4	0.91	0.12	30,36,37,61	0
4	ACT	A	314	4/4	0.91	0.13	15,18,26,57	4
2	EDO	A	312	4/4	0.91	0.13	20,24,44,57	0
2	EDO	A	311	4/4	0.93	0.10	25,30,33,62	0
3	SO4	B	307	5/5	0.94	0.07	35,38,55,58	5
2	EDO	B	301	4/4	0.94	0.08	22,25,26,32	0
2	EDO	B	302	4/4	0.94	0.11	33,33,59,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	EDO	A	302	4/4	0.95	0.08	21,28,30,35	0
2	EDO	B	304	4/4	0.96	0.13	17,18,23,32	4
2	EDO	A	304	4/4	0.96	0.11	19,21,23,25	0
2	EDO	B	303	4/4	0.97	0.09	12,17,17,24	4
2	EDO	A	301	4/4	0.97	0.09	13,15,16,19	4
3	SO4	B	306	5/5	0.97	0.09	12,12,24,30	5
3	SO4	A	313	5/5	0.98	0.08	15,19,33,37	5

6.5 Other polymers [i](#)

There are no such residues in this entry.