



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:27 PM UTC

PDB ID : 4ISQ / pdb_00004isq
Title : Binding domain of Botulinum neurotoxin DC in complex with human synap-
totagmin I
Authors : Berntsson, R.P.-A.; Peng, L.; Svensson, L.M.; Dong, M.; Stenmark, P.
Deposited on : 2013-01-17
Resolution : 2.65 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:

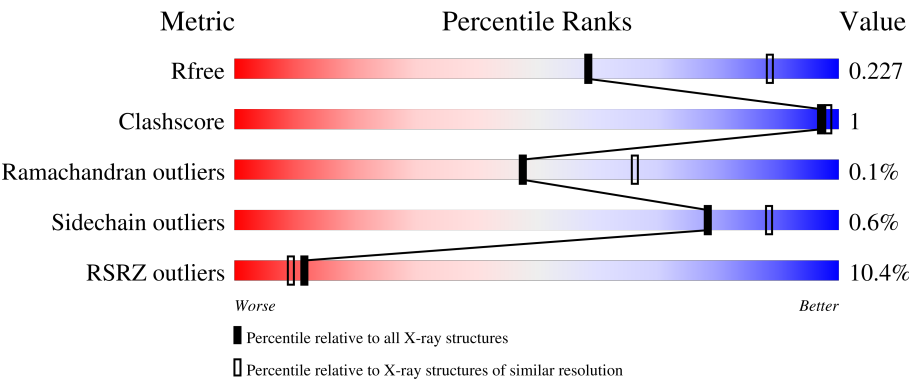
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

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	431	7% 94% ..
1	B	431	11% 95% ..
1	C	431	9% 94% ..
2	D	21	38% 71% 29%
2	E	21	19% 71% 29%

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Mol	Chain	Length	Quality of chain
2	F	21	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10970 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 Neurotoxin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3386	2172	560	640	14			
1	B	413	Total	C	N	O	S	0	0	0
			3378	2168	558	638	14			
1	C	414	Total	C	N	O	S	0	3	0
			3411	2185	566	646	14			

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	854	MET	-	expression tag	UNP Q9LBR1
A	855	HIS	-	expression tag	UNP Q9LBR1
A	856	HIS	-	expression tag	UNP Q9LBR1
A	857	HIS	-	expression tag	UNP Q9LBR1
A	858	HIS	-	expression tag	UNP Q9LBR1
A	859	HIS	-	expression tag	UNP Q9LBR1
A	860	HIS	-	expression tag	UNP Q9LBR1
A	861	TYR	-	expression tag	UNP Q9LBR1
A	862	PHE	-	expression tag	UNP Q9LBR1
B	854	MET	-	expression tag	UNP Q9LBR1
B	855	HIS	-	expression tag	UNP Q9LBR1
B	856	HIS	-	expression tag	UNP Q9LBR1
B	857	HIS	-	expression tag	UNP Q9LBR1
B	858	HIS	-	expression tag	UNP Q9LBR1
B	859	HIS	-	expression tag	UNP Q9LBR1
B	860	HIS	-	expression tag	UNP Q9LBR1
B	861	TYR	-	expression tag	UNP Q9LBR1
B	862	PHE	-	expression tag	UNP Q9LBR1
C	854	MET	-	expression tag	UNP Q9LBR1
C	855	HIS	-	expression tag	UNP Q9LBR1
C	856	HIS	-	expression tag	UNP Q9LBR1
C	857	HIS	-	expression tag	UNP Q9LBR1
C	858	HIS	-	expression tag	UNP Q9LBR1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	859	HIS	-	expression tag	UNP Q9LBR1
C	860	HIS	-	expression tag	UNP Q9LBR1
C	861	TYR	-	expression tag	UNP Q9LBR1
C	862	PHE	-	expression tag	UNP Q9LBR1

- Molecule 2 is a protein called Synaptotagmin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	15	Total	C	N	O	S	0	0	0
			128	82	20	25	1			
2	E	15	Total	C	N	O	S	0	0	0
			128	82	20	25	1			
2	F	15	Total	C	N	O	S	0	0	0
			128	82	20	25	1			

- 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	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

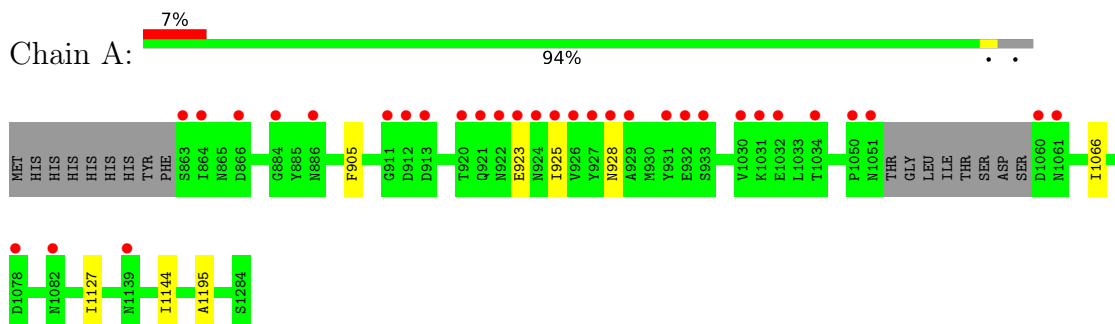
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total	O	0	0
			108	108		
5	B	85	Total	O	0	0
			85	85		
5	C	70	Total	O	0	0
			70	70		

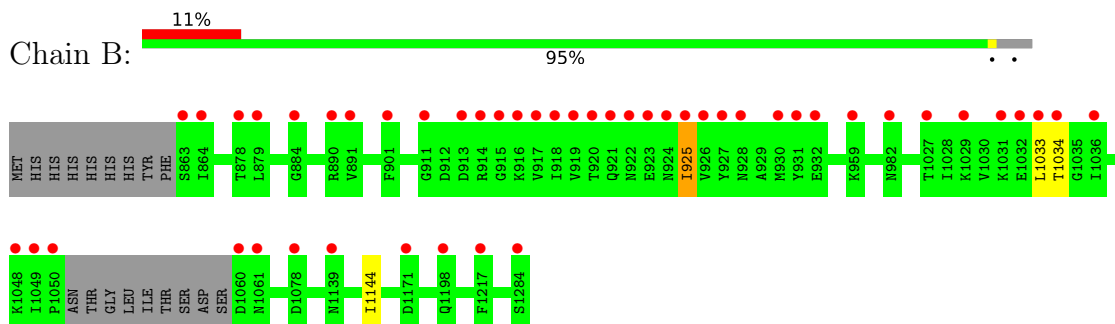
3 Residue-property plots [i](#)

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.

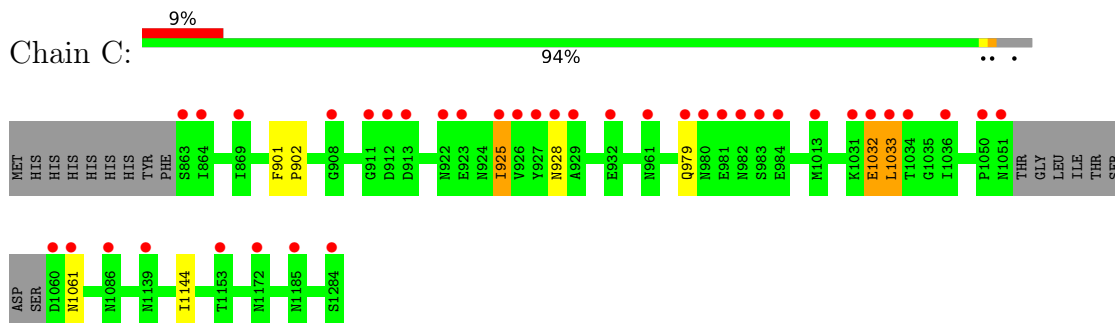
- Molecule 1: Neurotoxin



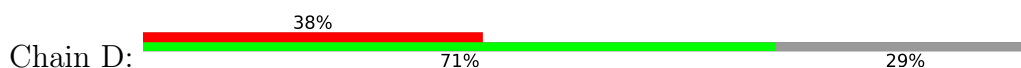
- Molecule 1: Neurotoxin

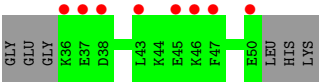


- Molecule 1: Neurotoxin

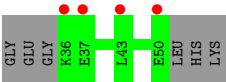


- Molecule 2: Synaptotagmin-1

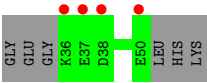




● Molecule 2: Synaptotagmin-1



● Molecule 2: Synaptotagmin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	164.23Å 57.55Å 165.27Å 90.00° 118.11° 90.00°	Depositor
Resolution (Å)	48.65 – 2.65 48.65 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.65-2.65) 99.9 (48.65-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.204 , 0.220 0.210 , 0.227	Depositor DCC
R_{free} test set	4003 reflections (4.52%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.521	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.016 for -h-l,k,h 0.016 for l,k,-h-l 0.022 for h,-k,-h-l 0.024 for -h-l,-k,l 0.021 for l,-k,h	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10970	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.39% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL

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	0/3463	0.57	0/4686
1	B	0.34	0/3455	0.57	0/4675
1	C	0.34	0/3488	0.58	0/4721
2	D	0.37	0/129	0.54	0/167
2	E	0.34	0/129	0.58	0/167
2	F	0.34	0/129	0.60	0/167
All	All	0.34	0/10793	0.58	0/14583

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 [i](#)

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	3386	0	3310	6	0
1	B	3378	0	3304	2	0
1	C	3411	0	3328	11	0
2	D	128	0	127	0	0
2	E	128	0	127	0	0
2	F	128	0	127	0	0
3	A	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	30	0	0	0	0
3	C	40	0	0	0	0
4	A	24	0	32	0	0
4	B	6	0	8	0	0
4	C	18	0	24	0	0
5	A	108	0	0	0	0
5	B	85	0	0	0	0
5	C	70	0	0	0	0
All	All	10970	0	10387	19	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 (19) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:925:ILE:HD13	1:C:925:ILE:H	1.50	0.75
1:C:925:ILE:HD13	1:C:925:ILE:N	2.04	0.72
1:A:923:GLU:HB2	1:A:925:ILE:HD12	1.78	0.65
1:C:1032:GLU:HB2	1:C:1033:LEU:HA	1.80	0.62
1:C:1061[B]:ASN:C	1:C:1061[B]:ASN:ND2	2.57	0.61
1:A:923:GLU:HB2	1:A:925:ILE:CD1	2.40	0.52
1:B:1144:ILE:HD12	1:B:1144:ILE:C	2.37	0.50
1:C:1032:GLU:CB	1:C:1033:LEU:HA	2.43	0.49
1:B:925:ILE:H	1:B:925:ILE:HG13	1.49	0.48
1:A:905:PHE:CZ	1:A:1066:ILE:HB	2.50	0.46
1:C:925:ILE:H	1:C:925:ILE:CD1	2.15	0.46
1:A:1127:ILE:HD11	1:A:1195:ALA:HB2	1.99	0.45
1:A:1144:ILE:C	1:A:1144:ILE:HD12	2.42	0.44
1:C:1032:GLU:CB	1:C:1033:LEU:CA	2.95	0.44
1:C:1061[B]:ASN:C	1:C:1061[B]:ASN:HD22	2.26	0.44
1:C:925:ILE:N	1:C:925:ILE:CD1	2.73	0.44
1:C:1144:ILE:C	1:C:1144:ILE:HD12	2.44	0.43
1:C:901:PHE:CG	1:C:902:PRO:HA	2.56	0.41
1:A:925:ILE:O	1:A:928:ASN:HB2	2.20	0.41

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	410/431 (95%)	394 (96%)	16 (4%)	0	100	100
1	B	409/431 (95%)	387 (95%)	22 (5%)	0	100	100
1	C	413/431 (96%)	394 (95%)	18 (4%)	1 (0%)	43	60
2	D	13/21 (62%)	13 (100%)	0	0	100	100
2	E	13/21 (62%)	13 (100%)	0	0	100	100
2	F	13/21 (62%)	13 (100%)	0	0	100	100
All	All	1271/1356 (94%)	1214 (96%)	56 (4%)	1 (0%)	48	66

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1032	GLU

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	379/395 (96%)	379 (100%)	0	100	100
1	B	378/395 (96%)	375 (99%)	3 (1%)	73	85
1	C	382/395 (97%)	378 (99%)	4 (1%)	68	81
2	D	14/18 (78%)	14 (100%)	0	100	100
2	E	14/18 (78%)	14 (100%)	0	100	100
2	F	14/18 (78%)	14 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1181/1239 (95%)	1174 (99%)	7 (1%)	78	88

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	925	ILE
1	B	1033	LEU
1	B	1034	THR
1	C	925	ILE
1	C	928	ASN
1	C	979	GLN
1	C	1033	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	924	ASN
1	A	961	ASN
1	A	1082	ASN
1	A	1086	ASN
1	A	1089	GLN
1	B	922	ASN
1	B	979	GLN
1	B	1086	ASN
1	B	1089	GLN
1	B	1135	ASN
1	B	1198	GLN
1	B	1215	ASN
1	B	1223	GLN
1	C	928	ASN
1	C	1082	ASN
1	C	1089	GLN
1	C	1135	ASN
1	C	1198	GLN
1	C	1223	GLN
2	D	49	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](#)

28 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	B	1305	-	4,4,4	0.43	0	6,6,6	0.08	0
3	SO4	A	1306	-	4,4,4	0.43	0	6,6,6	0.08	0
4	GOL	C	1309	-	5,5,5	0.28	0	5,5,5	0.20	0
3	SO4	B	1304	-	4,4,4	0.42	0	6,6,6	0.06	0
4	GOL	A	1308	-	5,5,5	0.29	0	5,5,5	0.23	0
4	GOL	B	1307	-	5,5,5	0.30	0	5,5,5	0.17	0
4	GOL	A	1309	-	5,5,5	0.31	0	5,5,5	0.30	0
3	SO4	C	1303	-	4,4,4	0.43	0	6,6,6	0.09	0
3	SO4	C	1301	-	4,4,4	0.43	0	6,6,6	0.09	0
3	SO4	B	1306	-	4,4,4	0.44	0	6,6,6	0.06	0
3	SO4	B	1303	-	4,4,4	0.42	0	6,6,6	0.08	0
3	SO4	C	1307	-	4,4,4	0.43	0	6,6,6	0.09	0
4	GOL	C	1310	-	5,5,5	0.29	0	5,5,5	0.15	0
3	SO4	B	1302	-	4,4,4	0.43	0	6,6,6	0.09	0
3	SO4	A	1303	-	4,4,4	0.44	0	6,6,6	0.10	0
3	SO4	C	1304	-	4,4,4	0.44	0	6,6,6	0.08	0
3	SO4	C	1306	-	4,4,4	0.42	0	6,6,6	0.08	0
3	SO4	A	1302	-	4,4,4	0.42	0	6,6,6	0.07	0
4	GOL	A	1310	-	5,5,5	0.29	0	5,5,5	0.25	0
4	GOL	C	1311	-	5,5,5	0.31	0	5,5,5	0.20	0
3	SO4	A	1305	-	4,4,4	0.44	0	6,6,6	0.07	0
3	SO4	A	1304	-	4,4,4	0.43	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	1307	-	5,5,5	0.31	0	5,5,5	0.25	0
3	SO4	C	1308	-	4,4,4	0.44	0	6,6,6	0.08	0
3	SO4	B	1301	-	4,4,4	0.43	0	6,6,6	0.05	0
3	SO4	A	1301	-	4,4,4	0.41	0	6,6,6	0.07	0
3	SO4	C	1302	-	4,4,4	0.44	0	6,6,6	0.06	0
3	SO4	C	1305	-	4,4,4	0.43	0	6,6,6	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
4	GOL	A	1307	-	-	2/4/4/4	-
4	GOL	C	1309	-	-	0/4/4/4	-
4	GOL	A	1308	-	-	4/4/4/4	-
4	GOL	A	1310	-	-	3/4/4/4	-
4	GOL	B	1307	-	-	0/4/4/4	-
4	GOL	C	1311	-	-	3/4/4/4	-
4	GOL	C	1310	-	-	0/4/4/4	-
4	GOL	A	1309	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1307	GOL	C1-C2-C3-O3
4	A	1308	GOL	O1-C1-C2-C3
4	A	1308	GOL	C1-C2-C3-O3
4	A	1308	GOL	O2-C2-C3-O3
4	A	1309	GOL	O1-C1-C2-C3
4	C	1311	GOL	C1-C2-C3-O3
4	A	1307	GOL	O2-C2-C3-O3
4	A	1308	GOL	O1-C1-C2-O2
4	A	1309	GOL	O1-C1-C2-O2
4	A	1310	GOL	O2-C2-C3-O3
4	C	1311	GOL	O1-C1-C2-O2
4	C	1311	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	A	1310	GOL	O1-C1-C2-C3
4	A	1310	GOL	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

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	414/431 (96%)	0.19	32 (7%) 19 14	27, 38, 72, 102	0
1	B	413/431 (95%)	0.49	48 (11%) 9 8	28, 44, 92, 105	0
1	C	414/431 (96%)	0.37	38 (9%) 14 11	18, 43, 74, 100	3 (0%)
2	D	15/21 (71%)	2.27	8 (53%) 0 0	46, 65, 85, 86	0
2	E	15/21 (71%)	1.60	4 (26%) 1 1	45, 54, 72, 74	0
2	F	15/21 (71%)	1.26	4 (26%) 1 1	40, 50, 69, 69	0
All	All	1286/1356 (94%)	0.40	134 (10%) 11 9	18, 42, 84, 105	3 (0%)

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1050	PRO	6.6
1	C	1033	LEU	5.6
1	C	1034	THR	5.2
1	A	931	TYR	5.0
1	C	980	ASN	4.6
1	B	927	TYR	4.6
1	A	929	ALA	4.5
1	B	925	ILE	4.5
2	D	36	LYS	4.3
1	B	917	VAL	4.2
1	C	1050	PRO	4.2
1	A	925	ILE	4.2
1	A	913	ASP	4.1
1	A	921	GLN	3.9
1	C	925	ILE	3.9
1	A	1051	ASN	3.8
1	C	923	GLU	3.7
1	A	926	VAL	3.7
2	E	37	GLU	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	45	GLU	3.7
1	B	1033	LEU	3.7
1	B	959	LYS	3.7
2	D	37	GLU	3.7
1	C	1061[A]	ASN	3.7
1	B	926	VAL	3.7
1	A	928	ASN	3.6
1	B	1060	ASP	3.6
1	B	913	ASP	3.5
1	C	1051	ASN	3.5
1	C	1032	GLU	3.5
1	B	1139	ASN	3.4
1	C	983	SER	3.3
1	B	1284	SER	3.3
1	B	863	SER	3.3
1	C	979	GLN	3.3
1	A	924	ASN	3.2
2	D	38	ASP	3.2
2	E	36	LYS	3.1
2	E	50	GLU	3.1
1	B	1027	THR	3.1
2	D	46	LYS	3.1
2	D	50	GLU	3.1
1	C	1284	SER	3.1
1	B	932	GLU	3.0
1	A	863	SER	3.0
1	A	1061	ASN	3.0
2	D	43	LEU	3.0
1	A	1078	ASP	3.0
1	C	981	GLU	3.0
1	A	927	TYR	3.0
1	C	1013	MET	3.0
1	A	1034	THR	3.0
1	B	1171	ASP	2.9
1	B	1034	THR	2.9
1	B	1032	GLU	2.9
1	B	928	ASN	2.9
1	B	878	THR	2.8
1	B	921	GLN	2.8
2	E	43	LEU	2.8
1	A	923	GLU	2.8
1	B	891	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	1060	ASP	2.7
1	A	1050	PRO	2.7
1	C	927	TYR	2.7
2	F	36	LYS	2.7
1	A	1139	ASN	2.7
1	C	912	ASP	2.7
1	C	864	ILE	2.7
1	C	863	SER	2.6
1	C	913	ASP	2.6
2	D	47	PHE	2.6
1	C	1060	ASP	2.6
1	B	884	GLY	2.6
1	A	912	ASP	2.6
1	B	931	TYR	2.6
1	B	901	PHE	2.6
1	B	1078	ASP	2.5
2	F	37	GLU	2.5
1	A	1030	VAL	2.5
1	B	1061	ASN	2.5
1	A	933	SER	2.5
1	A	866	ASP	2.5
1	B	982	ASN	2.5
1	B	919	VAL	2.5
1	C	1086	ASN	2.5
1	C	926	VAL	2.5
1	B	1031	LYS	2.4
1	B	864	ILE	2.4
1	C	932	GLU	2.4
1	A	884	GLY	2.4
1	B	930	MET	2.4
1	C	1031	LYS	2.4
1	C	922	ASN	2.4
1	A	1082	ASN	2.4
1	A	911	GLY	2.4
1	C	1185[A]	ASN	2.4
1	B	916	LYS	2.4
1	B	923	GLU	2.3
1	A	1031	LYS	2.3
1	B	1029	LYS	2.3
1	B	890	ARG	2.3
1	B	1217	PHE	2.3
1	B	1049	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	922	ASN	2.3
1	B	879	LEU	2.3
1	A	864	ILE	2.3
1	A	886	ASN	2.3
1	B	922	ASN	2.3
1	C	984	GLU	2.3
1	B	914	ARG	2.3
1	C	1153	THR	2.3
1	C	929	ALA	2.2
1	C	1036	ILE	2.2
1	A	1032	GLU	2.2
1	B	924	ASN	2.2
1	A	932	GLU	2.2
1	C	982	ASN	2.2
1	B	911	GLY	2.2
1	A	920	THR	2.2
1	C	928	ASN	2.2
1	C	961	ASN	2.2
1	B	1048	LYS	2.2
1	B	920	THR	2.1
1	B	1198	GLN	2.1
1	C	1139	ASN	2.1
1	B	915	GLY	2.1
1	B	918	ILE	2.1
1	C	1172	ASN	2.1
1	B	1036	ILE	2.1
2	F	38	ASP	2.1
1	C	908	GLY	2.1
1	C	911	GLY	2.1
2	F	50	GLU	2.0
1	C	869	ILE	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 ⓘ

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	SO4	B	1306	5/5	0.73	0.28	80,81,82,82	0
4	GOL	A	1310	6/6	0.73	0.19	41,42,42,43	0
4	GOL	C	1311	6/6	0.79	0.20	49,50,50,51	0
4	GOL	B	1307	6/6	0.82	0.20	47,47,48,48	0
3	SO4	C	1304	5/5	0.84	0.27	88,88,88,89	0
3	SO4	A	1306	5/5	0.84	0.27	94,95,96,96	0
3	SO4	C	1307	5/5	0.87	0.27	92,92,92,92	0
3	SO4	C	1301	5/5	0.87	0.14	62,63,64,65	0
4	GOL	A	1308	6/6	0.88	0.17	43,44,44,44	0
4	GOL	A	1309	6/6	0.89	0.16	38,38,38,38	0
3	SO4	A	1304	5/5	0.89	0.17	75,75,76,76	0
3	SO4	B	1303	5/5	0.90	0.14	75,75,75,75	0
3	SO4	A	1305	5/5	0.91	0.20	85,86,87,87	0
3	SO4	C	1306	5/5	0.91	0.25	89,90,90,90	0
3	SO4	B	1305	5/5	0.91	0.22	89,90,91,92	0
3	SO4	C	1303	5/5	0.91	0.18	72,73,74,74	0
4	GOL	A	1307	6/6	0.93	0.13	45,45,45,46	0
3	SO4	A	1303	5/5	0.93	0.26	66,66,67,67	0
3	SO4	C	1305	5/5	0.93	0.23	78,79,79,79	0
3	SO4	B	1302	5/5	0.94	0.14	65,65,66,67	0
3	SO4	A	1302	5/5	0.94	0.12	54,54,55,55	0
4	GOL	C	1310	6/6	0.94	0.11	40,40,41,41	0
3	SO4	C	1308	5/5	0.94	0.24	87,88,88,89	0
3	SO4	C	1302	5/5	0.95	0.11	62,62,63,63	0
3	SO4	B	1301	5/5	0.96	0.09	50,50,51,51	0
4	GOL	C	1309	6/6	0.96	0.08	34,35,35,35	0
3	SO4	A	1301	5/5	0.98	0.06	33,33,34,34	0
3	SO4	B	1304	5/5	0.99	0.06	38,39,39,39	0

6.5 Other polymers ⓘ

There are no such residues in this entry.