WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

May 25, 2020 – 05:36 am BST

PDB ID	:	3ZUR
Title	:	Crystal structure of an engineered botulinum neurotoxin type A- SNARE23 derivative, LC0-A-SNAP25-Hn-A
Authors	:	Masuyer, G.; Stancombe, P.; Chaddock, J.A.; Acharya, K.R.
Deposited on	:	2011-07-19
Resolution	:	2.71 Å(reported)

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

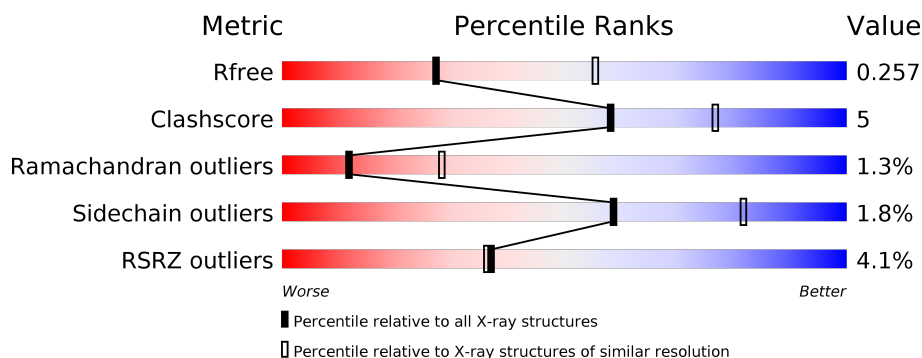|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.71 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	Percentile Ranks	Value
Rfree		0.257
Clashscore		5
Ramachandran outliers		1.3%
Sidechain outliers		1.8%
RSRZ outliers		4.1%

Worse ◼ Better

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

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 on 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 <=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	960	3% / 76% 11% • 12%
1	B	960	4% / 75% 12% • 12%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 13823 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 BOTULINUM NEUROTOXIN TYPE A, SYNAPTOSOMA L-ASSOCIATED PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	848	Total 6848	C 4401	N 1104	O 1324	S 19	0	0	1
1	B	844	Total 6801	C 4371	N 1097	O 1314	S 19	0	0	1

There are 122 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP P10845
A	-1	GLY	-	expression tag	UNP P10845
A	0	SER	-	expression tag	UNP P10845
A	1	MET	-	expression tag	UNP P10845
A	2	GLU	-	expression tag	UNP P10845
A	27	ALA	VAL	variant	UNP P10845
A	224	GLN	GLU	engineered mutation	UNP P10845
A	227	TYR	HIS	engineered mutation	UNP P10845
A	431	VAL	-	linker	UNP P10845
A	432	ASP	-	linker	UNP P10845
A	433	GLY	-	linker	UNP P10845
A	434	GLY	-	linker	UNP P10845
A	435	GLY	-	linker	UNP P10845
A	436	GLY	-	linker	UNP P10845
A	437	SER	-	linker	UNP P10845
A	438	GLY	-	linker	UNP P10845
A	439	GLY	-	linker	UNP P10845
A	440	GLY	-	linker	UNP P10845
A	441	GLY	-	linker	UNP P10845
A	442	SER	-	linker	UNP P10845
A	443	GLY	-	linker	UNP P10845
A	444	GLY	-	linker	UNP P10845
A	445	GLY	-	linker	UNP P10845
A	446	GLY	-	linker	UNP P10845

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Chain	Residue	Modelled	Actual	Comment	Reference
A	447	SER	-	linker	UNP P10845
A	510	ALA	-	linker	UNP P10845
A	511	ASN	-	linker	UNP P10845
A	512	SER	-	linker	UNP P10845
A	513	ALA	-	linker	UNP P10845
A	514	LEU	-	linker	UNP P10845
A	515	ALA	-	linker	UNP P10845
A	516	GLY	-	linker	UNP P10845
A	517	GLY	-	linker	UNP P10845
A	518	GLY	-	linker	UNP P10845
A	519	GLY	-	linker	UNP P10845
A	520	SER	-	linker	UNP P10845
A	521	GLY	-	linker	UNP P10845
A	522	GLY	-	linker	UNP P10845
A	523	GLY	-	linker	UNP P10845
A	524	GLY	-	linker	UNP P10845
A	525	SER	-	linker	UNP P10845
A	526	GLY	-	linker	UNP P10845
A	527	GLY	-	linker	UNP P10845
A	528	GLY	-	linker	UNP P10845
A	529	GLY	-	linker	UNP P10845
A	530	SER	-	linker	UNP P10845
A	531	LEU	-	linker	UNP P10845
A	532	GLN	-	linker	UNP P10845
A	945	LEU	-	expression tag	UNP P10845
A	946	GLU	-	expression tag	UNP P10845
A	947	ALA	-	expression tag	UNP P10845
A	948	HIS	-	expression tag	UNP P10845
A	949	HIS	-	expression tag	UNP P10845
A	950	HIS	-	expression tag	UNP P10845
A	951	HIS	-	expression tag	UNP P10845
A	952	HIS	-	expression tag	UNP P10845
A	953	HIS	-	expression tag	UNP P10845
A	954	HIS	-	expression tag	UNP P10845
A	955	HIS	-	expression tag	UNP P10845
A	956	HIS	-	expression tag	UNP P10845
A	957	HIS	-	expression tag	UNP P10845
B	-2	MET	-	expression tag	UNP P10845
B	-1	GLY	-	expression tag	UNP P10845
B	0	SER	-	expression tag	UNP P10845
B	1	MET	-	expression tag	UNP P10845
B	2	GLU	-	expression tag	UNP P10845

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Chain	Residue	Modelled	Actual	Comment	Reference
B	27	ALA	VAL	variant	UNP P10845
B	224	GLN	GLU	engineered mutation	UNP P10845
B	227	TYR	HIS	engineered mutation	UNP P10845
B	431	VAL	-	linker	UNP P10845
B	432	ASP	-	linker	UNP P10845
B	433	GLY	-	linker	UNP P10845
B	434	GLY	-	linker	UNP P10845
B	435	GLY	-	linker	UNP P10845
B	436	GLY	-	linker	UNP P10845
B	437	SER	-	linker	UNP P10845
B	438	GLY	-	linker	UNP P10845
B	439	GLY	-	linker	UNP P10845
B	440	GLY	-	linker	UNP P10845
B	441	GLY	-	linker	UNP P10845
B	442	SER	-	linker	UNP P10845
B	443	GLY	-	linker	UNP P10845
B	444	GLY	-	linker	UNP P10845
B	445	GLY	-	linker	UNP P10845
B	446	GLY	-	linker	UNP P10845
B	447	SER	-	linker	UNP P10845
B	510	ALA	-	linker	UNP P10845
B	511	ASN	-	linker	UNP P10845
B	512	SER	-	linker	UNP P10845
B	513	ALA	-	linker	UNP P10845
B	514	LEU	-	linker	UNP P10845
B	515	ALA	-	linker	UNP P10845
B	516	GLY	-	linker	UNP P10845
B	517	GLY	-	linker	UNP P10845
B	518	GLY	-	linker	UNP P10845
B	519	GLY	-	linker	UNP P10845
B	520	SER	-	linker	UNP P10845
B	521	GLY	-	linker	UNP P10845
B	522	GLY	-	linker	UNP P10845
B	523	GLY	-	linker	UNP P10845
B	524	GLY	-	linker	UNP P10845
B	525	SER	-	linker	UNP P10845
B	526	GLY	-	linker	UNP P10845
B	527	GLY	-	linker	UNP P10845
B	528	GLY	-	linker	UNP P10845
B	529	GLY	-	linker	UNP P10845
B	530	SER	-	linker	UNP P10845
B	531	LEU	-	linker	UNP P10845

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Chain	Residue	Modelled	Actual	Comment	Reference
B	532	GLN	-	linker	UNP P10845
B	945	LEU	-	expression tag	UNP P10845
B	946	GLU	-	expression tag	UNP P10845
B	947	ALA	-	expression tag	UNP P10845
B	948	HIS	-	expression tag	UNP P10845
B	949	HIS	-	expression tag	UNP P10845
B	950	HIS	-	expression tag	UNP P10845
B	951	HIS	-	expression tag	UNP P10845
B	952	HIS	-	expression tag	UNP P10845
B	953	HIS	-	expression tag	UNP P10845
B	954	HIS	-	expression tag	UNP P10845
B	955	HIS	-	expression tag	UNP P10845
B	956	HIS	-	expression tag	UNP P10845
B	957	HIS	-	expression tag	UNP P10845

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).

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

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total 102	O 102	0	0
3	B	47	Total 47	O 47	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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: BOTULINUM NEUROTOXIN TYPE A, SYNAPTOSOMAL-ASSOCIATED PROTEIN

• Molecule 1: BOTULINUM NEUROTOXIN TYPE A, SYNAPTOSOMAL-ASSOCIATED PROTEIN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	78.96Å 157.50Å 209.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	125.86 – 2.71 29.58 – 2.71	Depositor EDS
% Data completeness (in resolution range)	96.5 (125.86-2.71) 96.6 (29.58-2.71)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.212 , 0.266 0.207 , 0.257	Depositor DCC
R_{free} test set	3503 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	50.5	Xtriage
Anisotropy	0.194	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 48.0	EDS
L-test for twinning[2]	$< |L| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13823	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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

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	0.44	0/6991	0.56	0/9471
1	B	0.43	0/6941	0.55	0/9403
All	All	0.44	0/13932	0.55	0/18874

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	6848	0	6742	63	0
1	B	6801	0	6692	71	0
2	A	20	0	0	0	0
2	B	5	0	0	0	0
3	A	102	0	0	1	0
3	B	47	0	0	0	0
All	All	13823	0	13434	131	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 5.

All (131) 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:200:LEU:HD21	1:B:940:ARG:NH1	1.80	0.96
1:B:200:LEU:HD21	1:B:940:ARG:HH11	1.39	0.87
1:A:651:VAL:HG13	1:A:653:GLU:HG3	1.60	0.82
1:B:269:HIS:HE1	1:B:940:ARG:HE	1.25	0.82
1:A:346:THR:HG22	1:A:347:GLU:HG3	1.66	0.78
1:B:113:ARG:NH2	1:B:586:ASN:O	2.21	0.72
1:B:346:THR:HG22	1:B:347:GLU:HG3	1.70	0.72
1:A:781:ARG:HD2	1:A:891:ASP:OD1	1.89	0.71
1:B:703:THR:HG22	1:B:705:LYS:H	1.56	0.70
1:A:80:THR:HG22	1:A:82:ASN:H	1.55	0.70
1:B:200:LEU:CD2	1:B:940:ARG:HH11	2.07	0.68
1:A:395:THR:HG22	1:A:397:LEU:H	1.60	0.67
1:B:269:HIS:CE1	1:B:940:ARG:HE	2.11	0.65
1:A:582:TYR:CD2	1:B:359:LYS:HD2	2.31	0.65
1:B:198:GLU:HG3	1:B:199:SER:H	1.62	0.65
1:B:916:LEU:O	1:B:917:LYS:HB3	1.96	0.64
1:A:342:TYR:O	1:A:346:THR:HB	1.98	0.64
1:A:651:VAL:CG1	1:A:653:GLU:HG3	2.28	0.63
1:A:5:ASN:O	1:A:6:LYS:HG3	1.98	0.63
1:A:184:GLN:OE1	1:A:231:ARG:HD3	2.00	0.62
1:A:651:VAL:HG13	1:A:653:GLU:CG	2.30	0.61
1:B:80:THR:HG22	1:B:82:ASN:H	1.65	0.61
1:B:326:ASP:HB2	1:B:330:LYS:H	1.67	0.60
1:B:184:GLN:OE1	1:B:231:ARG:HD3	2.02	0.59
1:B:707:ALA:O	1:B:708:ASP:HB2	2.01	0.59
1:A:706:ILE:O	1:A:707:ALA:HB3	2.03	0.59
1:B:781:ARG:HD2	1:B:891:ASP:OD1	2.02	0.58
1:A:23:LYS:HE3	1:A:601:SER:O	2.02	0.58
1:A:781:ARG:HG3	1:A:890:PHE:HE2	1.69	0.57
1:B:198:GLU:HG3	1:B:199:SER:N	2.20	0.57
1:B:395:THR:HG22	1:B:397:LEU:H	1.70	0.56
1:A:70:VAL:HG12	1:A:161:ILE:HD11	1.88	0.56
1:B:903:TYR:O	1:B:906:ARG:HG2	2.06	0.55
1:A:67:GLN:HG2	1:A:425:PHE:CE1	2.42	0.55
1:B:748:PRO:HG3	1:B:800:VAL:HG22	1.89	0.55
1:B:165:CYS:SG	1:B:186:ILE:HG12	2.47	0.55
1:B:833:TYR:HB3	1:B:836:GLU:CG	2.38	0.54
1:B:108:LEU:O	1:B:112:VAL:HG23	2.08	0.54
1:A:74:ASP:OD1	1:A:76:THR:HG22	2.08	0.54
1:B:80:THR:HG22	1:B:82:ASN:N	2.22	0.53
1:B:808:ARG:HB3	1:B:867:LEU:HD12	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:GLY:HA2	1:A:938:ASN:HD21	1.74	0.53
1:A:582:TYR:CE2	1:B:359:LYS:HD2	2.43	0.53
1:A:70:VAL:HG12	1:A:161:ILE:CD1	2.39	0.53
1:B:833:TYR:HB3	1:B:836:GLU:HG3	1.90	0.52
1:B:151:LEU:HD11	1:B:186:ILE:HD12	1.91	0.52
1:A:53:ASN:HB3	1:A:56:GLU:HB2	1.91	0.52
1:B:663:THR:HG22	1:B:818:GLN:OE1	2.10	0.51
1:B:200:LEU:CD2	1:B:940:ARG:NH1	2.60	0.51
1:A:909:LEU:O	1:A:911:GLY:N	2.44	0.51
1:A:785:TRP:CE3	1:A:887:LEU:HD13	2.46	0.51
1:A:651:VAL:CG1	1:A:653:GLU:CG	2.88	0.51
1:B:652:ASN:C	1:B:654:ALA:H	2.13	0.51
1:B:629:MET:HG3	1:B:720:LEU:HB3	1.93	0.51
1:A:33:VAL:HG11	1:A:51:PHE:CZ	2.46	0.50
1:B:58:ASP:OD2	1:B:60:ASN:HB2	2.10	0.50
1:A:243:PHE:CZ	1:A:273:PHE:HB3	2.46	0.50
1:B:365:THR:HG22	1:B:367:LEU:H	1.77	0.50
1:B:45:ILE:HB	1:B:154:ILE:HG22	1.94	0.50
1:A:840:ASN:HD22	1:A:840:ASN:N	2.09	0.49
1:B:428:LEU:HD23	1:B:621:LYS:HG3	1.94	0.49
1:B:131:ASP:HB2	1:B:599:LEU:HD13	1.95	0.49
1:B:922:ASN:HD22	1:B:922:ASN:N	2.10	0.49
1:A:573:ILE:HD13	1:A:577:LEU:HD23	1.95	0.49
1:B:53:ASN:HB3	1:B:56:GLU:HB2	1.94	0.49
1:A:776:ASN:O	1:A:780:LYS:HB2	2.13	0.48
1:A:649:ASN:ND2	1:A:651:VAL:H	2.12	0.48
1:B:342:TYR:O	1:B:346:THR:HB	2.14	0.48
1:A:422:LEU:O	1:A:537:ASN:ND2	2.46	0.48
1:B:781:ARG:HD3	1:B:924:LEU:CD2	2.44	0.47
1:A:98:ILE:O	1:A:104:GLY:HA3	2.14	0.47
1:B:910:ILE:HG22	1:B:911:GLY:H	1.79	0.47
1:B:653:GLU:HG3	1:B:656:LEU:HD22	1.97	0.46
1:A:287:TYR:OH	1:A:335:LYS:HG2	2.15	0.46
1:A:223:HIS:ND1	1:A:351:GLU:OE1	2.48	0.46
1:B:9:ASN:HD22	1:B:11:LYS:H	1.64	0.46
1:B:70:VAL:HG12	1:B:161:ILE:HD11	1.99	0.46
1:B:816:GLU:O	1:B:820:GLU:HG2	2.16	0.46
1:A:177:ARG:HD3	1:A:238:ASN:HA	1.97	0.45
1:A:781:ARG:HG3	1:A:890:PHE:CE2	2.51	0.45
1:B:384:TYR:HA	1:B:389:GLY:O	2.17	0.45
1:B:576:ASP:O	1:B:579:GLN:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:796:TRP:CE3	1:A:797:LEU:CD1	3.00	0.45
1:A:808:ARG:HB3	1:A:867:LEU:HD12	2.00	0.44
1:A:270:ASP:OD1	1:A:365:THR:HG23	2.16	0.44
1:B:835:GLU:C	1:B:837:GLU:H	2.20	0.44
1:B:770:THR:O	1:B:774:ILE:HD12	2.17	0.44
1:A:166:LYS:HB3	1:A:607:LEU:HD22	2.00	0.44
1:A:46:PRO:O	1:A:84:LYS:HG2	2.17	0.44
1:B:759:ALA:O	1:B:760:LEU:HB2	2.18	0.44
1:A:580:GLN:OE1	1:B:939:GLN:CD	2.56	0.43
1:B:808:ARG:HB3	1:B:867:LEU:CD1	2.48	0.43
1:B:713:ILE:HD12	1:B:863:ILE:HA	2.00	0.43
1:A:766:ASN:HD21	1:A:769:LEU:HD13	1.83	0.43
1:A:781:ARG:HD3	1:A:924:LEU:HD22	2.01	0.43
1:B:379:VAL:HB	1:B:380:PRO:HD3	2.01	0.43
1:B:200:LEU:HD21	1:B:940:ARG:HH12	1.74	0.43
1:B:748:PRO:HG3	1:B:800:VAL:CG2	2.48	0.43
1:A:42:ILE:HG12	1:A:151:LEU:HB3	2.00	0.42
1:B:706:ILE:HG21	1:B:709:ILE:HD12	2.01	0.42
1:B:181:GLY:HA3	1:B:232:LEU:O	2.19	0.42
1:B:280:ASN:OD1	1:B:283:ARG:NH2	2.53	0.42
1:B:344:MET:HA	1:B:348:ILE:HB	2.01	0.42
1:A:348:ILE:HG23	1:A:578:ILE:HG12	2.01	0.42
1:B:98:ILE:O	1:B:104:GLY:HA3	2.19	0.42
1:B:657:ASN:HA	1:B:658:PRO:HD2	1.91	0.42
1:B:7:GLN:H	1:B:7:GLN:NE2	2.17	0.42
1:A:689:LEU:HD23	1:A:689:LEU:HA	1.93	0.42
1:A:638:PHE:HB3	1:A:661:VAL:CG2	2.50	0.41
1:B:198:GLU:CG	1:B:199:SER:H	2.32	0.41
1:B:177:ARG:HD3	1:B:238:ASN:HA	2.02	0.41
1:A:764:ILE:HG13	1:A:764:ILE:H	1.68	0.41
1:B:670:VAL:O	1:B:674:ASN:ND2	2.52	0.41
1:A:423:PHE:HB3	1:A:535:LYS:HD2	2.02	0.41
1:A:72:TYR:CZ	1:A:416:LEU:HD13	2.56	0.41
1:B:625:ASP:OD1	1:B:625:ASP:N	2.48	0.41
1:A:428:LEU:HD23	1:A:621:LYS:HG3	2.02	0.41
1:A:910:ILE:HG23	1:A:911:GLY:H	1.85	0.41
1:A:550:PHE:CE2	1:A:799:LYS:HE3	2.56	0.41
1:A:353:ASN:HA	1:A:356:LYS:HD2	2.03	0.41
1:A:378:ILE:HG12	3:A:2032:HOH:O	2.19	0.41
1:A:115:ILE:HD11	1:A:591:PRO:HB2	2.01	0.41
1:A:913:VAL:O	1:A:917:LYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249:ALA:O	1:A:427:LYS:NZ	2.54	0.40
1:A:796:TRP:CE3	1:A:797:LEU:HD13	2.56	0.40
1:B:911:GLY:C	1:B:913:VAL:H	2.24	0.40
1:B:838:LYS:HA	1:B:838:LYS:HD2	1.97	0.40
1:A:933:SER:HA	1:A:942:LEU:HD11	2.03	0.40
1:B:70:VAL:HG12	1:B:161:ILE:CD1	2.51	0.40
1:A:126:GLU:HG2	1:A:302:SER:OG	2.21	0.40
1:A:706:ILE:HG21	1:A:709:ILE:HD12	2.04	0.40

There are no symmetry-related clashes.

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	842/960 (88%)	795 (94%)	38 (4%)	9 (1%)	14	32
1	B	836/960 (87%)	780 (93%)	44 (5%)	12 (1%)	11	26
All	All	1678/1920 (87%)	1575 (94%)	82 (5%)	21 (1%)	12	28

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	910	ILE
1	A	609	LEU
1	A	645	ILE
1	B	199	SER
1	B	529	GLY
1	B	842	ASN
1	B	910	ILE
1	A	941	LEU
1	B	707	ALA
1	B	724	ASN

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Mol	Chain	Res	Type
1	B	838	LYS
1	A	727	TYR
1	A	835	GLU
1	B	157	SER
1	B	610	MET
1	A	157	SER
1	A	610	MET
1	B	257	GLU
1	B	760	LEU
1	A	707	ALA
1	B	912	GLN

5.3.2 Protein sidechains (i)

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	762/840 (91%)	747 (98%)	15 (2%)	55	80
1	B	755/840 (90%)	742 (98%)	13 (2%)	60	83
All	All	1517/1680 (90%)	1489 (98%)	28 (2%)	59	82

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	THR
1	A	78	LEU
1	A	86	ASN
1	A	258	VAL
1	A	365	THR
1	A	406	THR
1	A	548	ASP
1	A	648	THR
1	A	649	ASN
1	A	653	GLU
1	A	670	VAL
1	A	738	SER

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Mol	Chain	Res	Type
1	A	839	ASN
1	A	840	ASN
1	A	941	LEU
1	B	86	ASN
1	B	149	LEU
1	B	172	VAL
1	B	204	THR
1	B	242	VAL
1	B	243	PHE
1	B	400	ASN
1	B	431	VAL
1	B	648	THR
1	B	787	GLU
1	B	797	LEU
1	B	894	LEU
1	B	922	ASN

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

Mol	Chain	Res	Type
1	A	162	GLN
1	A	396	ASN
1	A	410	ASN
1	A	586	ASN
1	A	649	ASN
1	A	652	ASN
1	A	840	ASN
1	A	868	ASN
1	A	922	ASN
1	A	931	GLN
1	A	938	ASN
1	B	7	GLN
1	B	9	ASN
1	B	31	GLN
1	B	40	ASN
1	B	82	ASN
1	B	832	GLN
1	B	842	ASN
1	B	868	ASN
1	B	922	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

5 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	SO4	A	1944	-	4,4,4	0.15	0	6,6,6	0.27	0
2	SO4	A	1946	-	4,4,4	0.14	0	6,6,6	0.09	0
2	SO4	B	1939	-	4,4,4	0.19	0	6,6,6	0.18	0
2	SO4	A	1943	-	4,4,4	0.11	0	6,6,6	0.18	0
2	SO4	A	1945	-	4,4,4	0.14	0	6,6,6	0.22	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	848/960 (88%)	-0.05	32 (3%)	40	40	25, 43, 71, 88	0
1	B	844/960 (87%)	0.06	37 (4%)	34	33	28, 51, 87, 108	0
All	All	1692/1920 (88%)	0.00	69 (4%)	37	36	25, 47, 80, 108	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	727	TYR	6.4
1	B	839	ASN	6.3
1	A	726	LEU	6.0
1	B	609	LEU	5.8
1	B	1	MET	5.2
1	A	643	SER	4.9
1	A	839	ASN	4.8
1	A	589	ASN	4.7
1	A	724	ASN	4.5
1	B	844	ASN	4.4
1	B	569	ALA	4.4
1	B	939	GLN	4.2
1	B	703	THR	4.0
1	A	838	LYS	3.8
1	B	910	ILE	3.7
1	B	568	ALA	3.5
1	A	571	GLU	3.4
1	A	729	ASP	3.4
1	B	843	PHE	3.4
1	B	724	ASN	3.3
1	A	609	LEU	3.3
1	B	915	ARG	3.3
1	B	737	PHE	3.2
1	B	656	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	612	ASN	3.2
1	B	834	THR	3.1
1	B	882	TYR	3.1
1	B	645	ILE	3.1
1	B	943	SER	3.1
1	B	704	ASP	3.1
1	B	647	LEU	3.0
1	A	528	GLY	3.0
1	A	640	HIS	2.9
1	A	656	LEU	2.9
1	A	647	LEU	2.8
1	B	64	GLU	2.8
1	A	847	ASP	2.7
1	B	842	ASN	2.7
1	B	835	GLU	2.7
1	A	834	THR	2.7
1	A	64	GLU	2.6
1	B	614	GLU	2.6
1	B	681	MET	2.6
1	B	570	GLU	2.5
1	A	63	PRO	2.5
1	A	570	GLU	2.5
1	A	590	GLU	2.4
1	A	55	GLU	2.4
1	B	838	LYS	2.4
1	A	611	PRO	2.4
1	A	610	MET	2.3
1	B	660	ARG	2.3
1	A	1	MET	2.3
1	A	725	MET	2.3
1	A	207	LEU	2.3
1	A	840	ASN	2.3
1	B	55	GLU	2.3
1	B	710	THR	2.2
1	A	842	ASN	2.2
1	B	612	ASN	2.2
1	B	567	GLU	2.2
1	B	907	GLY	2.2
1	A	419	PHE	2.1
1	A	903	TYR	2.1
1	B	54	PRO	2.1
1	B	725	MET	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	27	ALA	2.1
1	B	678	GLU	2.1
1	B	691	TYR	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 carbohydrates 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	SO4	B	1939	5/5	0.94	0.15	62,63,63,63	0
2	SO4	A	1945	5/5	0.94	0.17	68,68,69,69	0
2	SO4	A	1944	5/5	0.95	0.15	64,65,66,67	0
2	SO4	A	1946	5/5	0.96	0.14	79,79,79,79	0
2	SO4	A	1943	5/5	0.98	0.09	47,48,48,49	0

6.5 Other polymers (i)

There are no such residues in this entry.