Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:34 PM GMT

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)

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

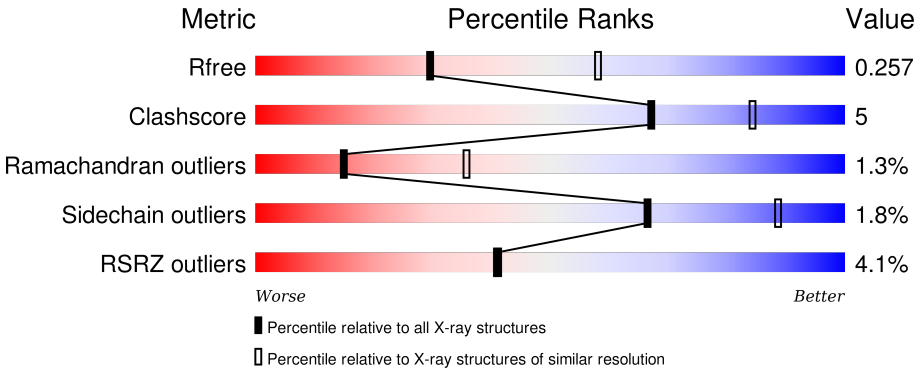
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.71 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (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. 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, SYNAPTOSOMAL-ASSOCIATED PROTEIN.

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

There are 42 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	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

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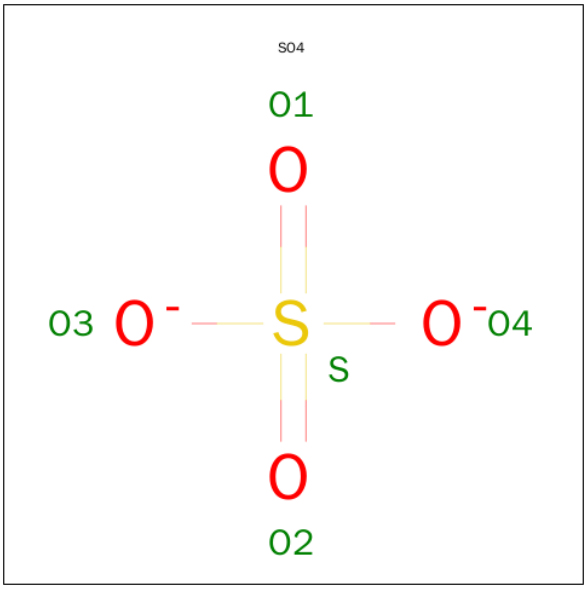
Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	EXPRESSION TAG	UNP P10845
B	2	GLU	-	EXPRESSION TAG	UNP P10845
B	27	ALA	VAL	VARIANT	UNP P10845
B	224	GLN	GLU	ENGINEERED MUTATION	UNP P10845
B	227	TYR	HIS	ENGINEERED MUTATION	UNP P10845
B	945	LEU	-	EXPRESSION TAG	UNP P10845
B	946	GLU	-	EXPRESSION 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 O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0

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

- Molecule 3 is water.

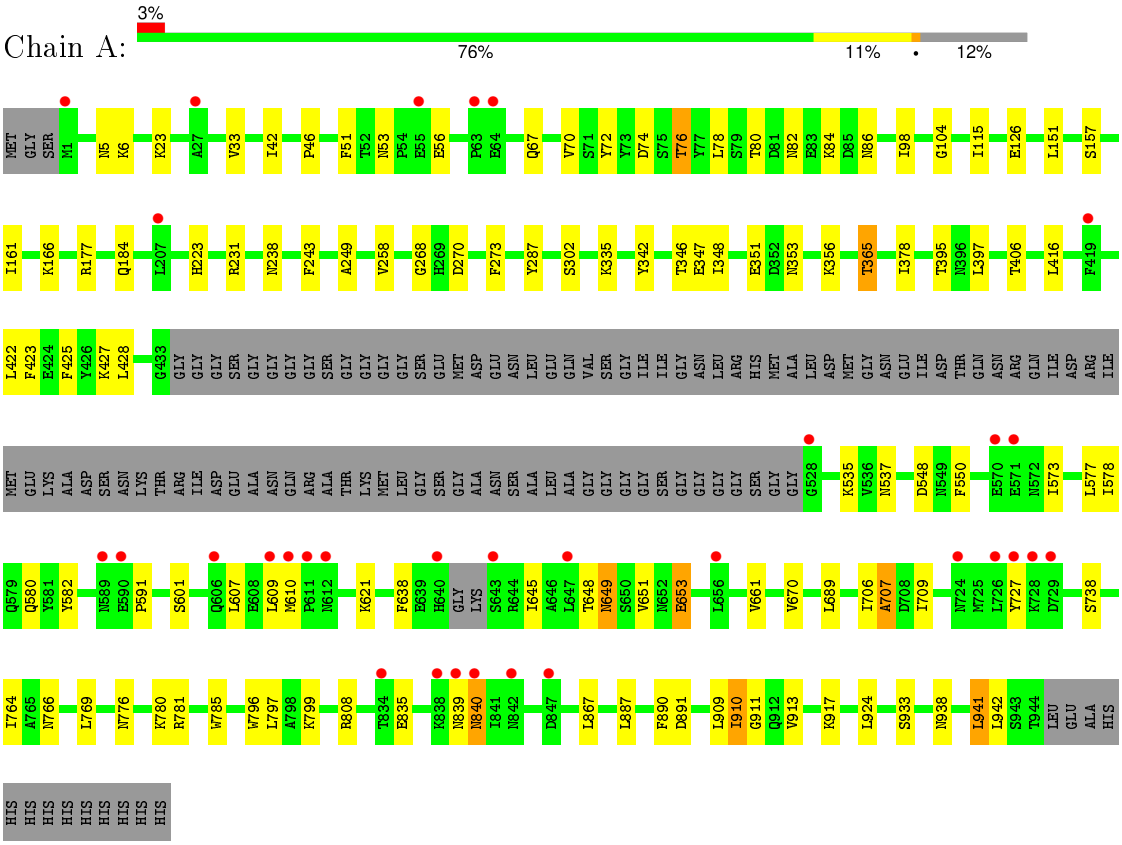
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	102	Total O 102 102	0	0
3	B	47	Total O 47 47	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

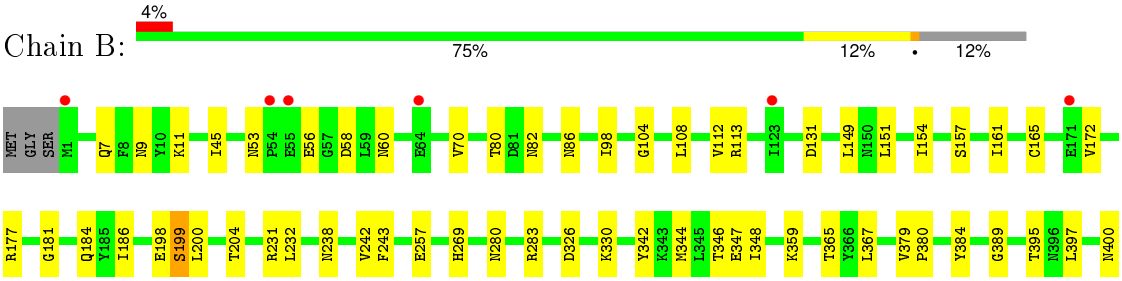
• Molecule 1: BOTULINUM NEUROTOXIN TYPE A, SYNAPTOSOMAL-ASSOCIATED PROTEIN

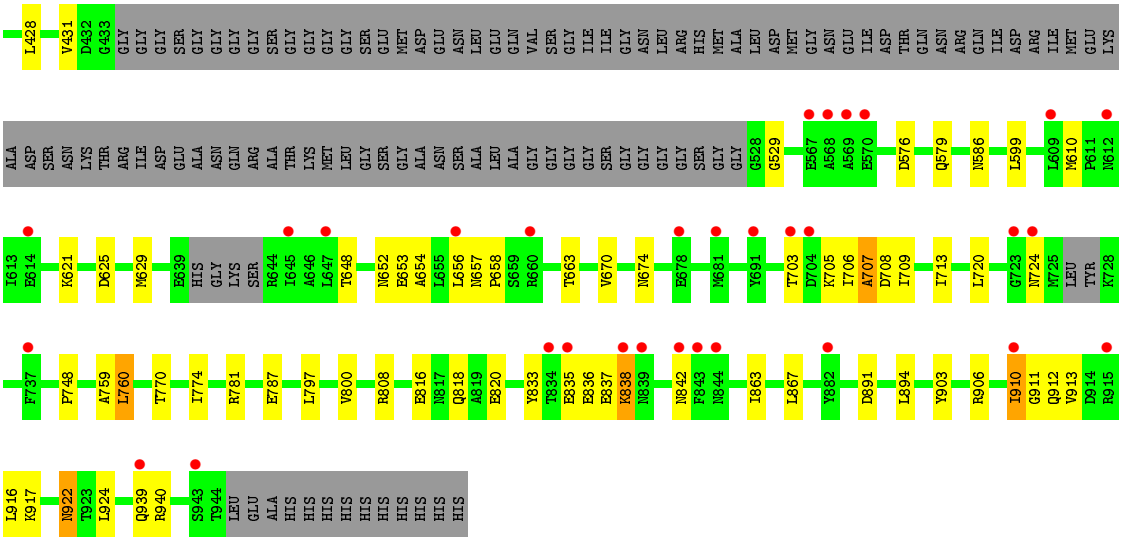
Chain A:



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

Chain B:




L428 V431 D432 G433 GLY GLY GLY SER GLY GLY GLY GLY SER GLY GLY GLY GLY SER GLU MET ASP GLU ASN LEU GLU GLN VAL SER GLY ILE ILE GLY ASN LEU ARG HIS MET ALA LEU ASP MET GLY ASN GLU ILE ASP THR GLN ASN ARG GLN ILE ASP ARG ILE MET GLU LYS
ALA ASP SER ASN LYS THR ARG ILE ASP GLU ALA ASN GLN ARG ALA THR LYS MET LEU GLY SER GLY ALA ASN SER ALA LEU ALA GLY GLY GLY GLY SER GLY GLY G528 G529 E567 A568 A569 E570 D576 Q579 N586 L599 L609 M610 P611 N612
I613 E614 K621 D625 M629 E639 HIS GLY LYS SER R644 I645 A646 L647 T648 N652 E653 A654 L655 L656 N657 P658 S659 R660 T663 V670 N674 E678 M681 Y691 T703 D704 K705 I706 A707 D708 I709 I713 L720 G723 N724 M725 LEU TYR K728
F737 P748 A759 L760 T770 I774 R781 E787 L797 V800 R808 E816 N817 Q818 A819 E820 Y833 T834 E835 E836 E837 R838 N839 N842 F843 N844 I863 L867 Y882 D891 L894 Y903 R906 I910 G911 Q912 V913 D914 R915
L916 K917 N922 T923 L924 Q939 R940 S943 T944 LEU GLU ALA HIS HIS HIS HIS HIS HIS HIS HIS HIS

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 (5.32%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 69387 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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

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:B:269:HIS:HE1	1:B:940:ARG:HE	1.25	0.82
1:A:651:VAL:HG13	1:A:653:GLU:HG3	1.60	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:707:ALA:O	1:B:708:ASP:HB2	2.01	0.59
1:B:184:GLN:OE1	1:B:231:ARG:HD3	2.02	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:629:MET:HG3	1:B:720:LEU:HB3	1.93	0.51
1:B:652:ASN:C	1:B:654:ALA:H	2.13	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:344:MET:HA	1:B:348:ILE:HB	2.01	0.42
1:B:280:ASN:OD1	1:B:283:ARG:NH2	2.53	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:B:198:GLU:CG	1:B:199:SER:H	2.32	0.41
1:A:638:PHE:HB3	1:A:661:VAL:CG2	2.50	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:72:TYR:CZ	1:A:416:LEU:HD13	2.56	0.41
1:A:423:PHE:HB3	1:A:535:LYS:HD2	2.02	0.41
1:B:625:ASP:OD1	1:B:625:ASP:N	2.48	0.41
1:A:910:ILE:HG23	1:A:911:GLY:H	1.85	0.41
1:A:428:LEU:HD23	1:A:621:LYS:HG3	2.02	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:913:VAL:O	1:A:917:LYS:HB2	2.21	0.41
1:A:115:ILE:HD11	1:A:591:PRO:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:911:GLY:C	1:B:913:VAL:H	2.24	0.40
1:A:796:TRP:CE3	1:A:797:LEU:HD13	2.56	0.40
1:A:249:ALA:O	1:A:427:LYS:NZ	2.54	0.40
1:B:838:LYS:HA	1:B:838:LYS:HD2	1.97	0.40
1:B:70:VAL:HG12	1:B:161:ILE:CD1	2.51	0.40
1:A:933:SER:HA	1:A:942:LEU:HD11	2.03	0.40
1:A:706:ILE:HG21	1:A:709:ILE:HD12	2.04	0.40
1:A:126:GLU:HG2	1:A:302:SER:OG	2.21	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%)	17	41
1	B	836/960 (87%)	780 (93%)	44 (5%)	12 (1%)	14	34
All	All	1678/1920 (87%)	1575 (94%)	82 (5%)	21 (1%)	15	36

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%)	63 87
1	B	755/840 (90%)	742 (98%)	13 (2%)	68 89
All	All	1517/1680 (90%)	1489 (98%)	28 (2%)	66 88

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

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 carbohydrates in this entry.

5.6 Ligand geometry

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	1943	-	4,4,4	0.22	0	6,6,6	0.19	0
2	SO4	A	1944	-	4,4,4	0.23	0	6,6,6	0.25	0
2	SO4	A	1945	-	4,4,4	0.26	0	6,6,6	0.22	0
2	SO4	A	1946	-	4,4,4	0.17	0	6,6,6	0.09	0
2	SO4	B	1939	-	4,4,4	0.22	0	6,6,6	0.13	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	SO4	A	1943	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1944	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1945	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1946	-	-	0/0/0/0	0/0/0/0
2	SO4	B	1939	-	-	0/0/0/0	0/0/0/0

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.03	32 (3%)	44	44	25, 43, 71, 88	0
1	B	844/960 (87%)	0.10	37 (4%)	38	37	28, 51, 87, 108	0
All	All	1692/1920 (88%)	0.03	69 (4%)	41	41	25, 47, 80, 108	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	727	TYR	6.3
1	B	839	ASN	6.3
1	B	609	LEU	6.0
1	A	726	LEU	5.6
1	B	1	MET	5.6
1	A	839	ASN	5.2
1	B	844	ASN	4.9
1	A	643	SER	4.6
1	B	569	ALA	4.4
1	A	589	ASN	4.3
1	A	724	ASN	4.2
1	A	838	LYS	4.2
1	B	939	GLN	4.1
1	B	703	THR	4.1
1	B	568	ALA	3.9
1	B	915	ARG	3.7
1	B	910	ILE	3.7
1	B	843	PHE	3.7
1	A	729	ASP	3.6
1	A	612	ASN	3.5
1	B	943	SER	3.5
1	A	647	LEU	3.3
1	B	882	TYR	3.2
1	B	704	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	737	PHE	3.1
1	B	647	LEU	3.1
1	A	571	GLU	3.1
1	A	609	LEU	3.1
1	A	640	HIS	3.1
1	B	656	LEU	3.0
1	B	834	THR	3.0
1	B	724	ASN	3.0
1	A	656	LEU	2.9
1	B	64	GLU	2.9
1	B	614	GLU	2.8
1	A	842	ASN	2.8
1	B	838	LYS	2.7
1	B	645	ILE	2.7
1	A	63	PRO	2.7
1	B	567	GLU	2.6
1	A	528	GLY	2.6
1	B	660	ARG	2.6
1	B	570	GLU	2.6
1	B	835	GLU	2.5
1	A	64	GLU	2.5
1	A	847	ASP	2.5
1	B	842	ASN	2.5
1	A	590	GLU	2.5
1	B	681	MET	2.5
1	A	840	ASN	2.5
1	A	207	LEU	2.4
1	B	55	GLU	2.3
1	A	834	THR	2.3
1	A	55	GLU	2.3
1	A	611	PRO	2.3
1	B	612	ASN	2.3
1	A	728	LYS	2.2
1	A	1	MET	2.2
1	A	606	GLN	2.2
1	B	691	TYR	2.2
1	A	419	PHE	2.1
1	B	678	GLU	2.1
1	A	610	MET	2.1
1	B	723	GLY	2.1
1	A	570	GLU	2.1
1	B	54	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	123	ILE	2.1
1	B	171	GLU	2.0
1	A	27	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	B	1939	5/5	0.95	0.14	0.00	62,63,63,63	0
2	SO4	A	1944	5/5	0.95	0.16	-0.48	64,65,66,67	0
2	SO4	A	1945	5/5	0.94	0.17	-0.61	68,68,69,69	0
2	SO4	A	1943	5/5	0.98	0.08	-	47,48,48,49	0
2	SO4	A	1946	5/5	0.97	0.15	-	79,79,79,79	0

6.5 Other polymers (i)

There are no such residues in this entry.