



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 02:54 AM GMT

PDB ID : 4JRA
Title : CRYSTAL STRUCTURE OF THE BOTULINUM NEUROTOXIN A
RECEPTOR-BINDING DOMAIN IN COMPLEX WITH THE LUMINAL
DOMAIN Of SV2C
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G.; Kammerer, R.A.
Deposited on : 2013-03-21
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

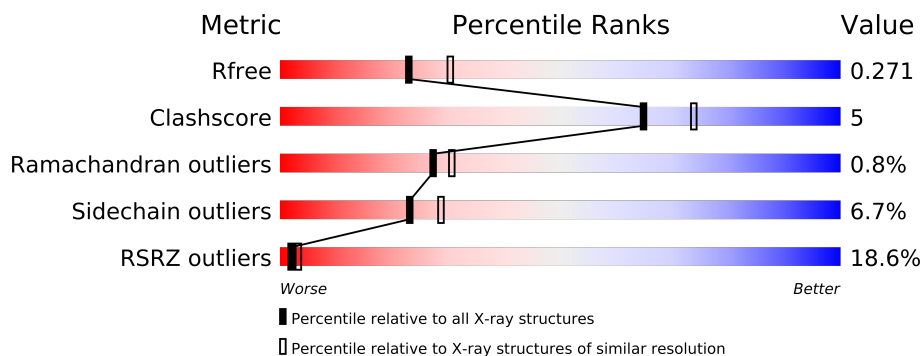
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	443	
1	B	443	
2	C	136	
2	D	136	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	CL	A	1301	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16539 atoms, of which 8131 are hydrogens and 0 are deuterium.

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.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	416	Total	C	H	N	O	S	0	3	0
			6854	2195	3412	593	641	13			
1	B	413	Total	C	H	N	O	S	0	0	0
			6778	2176	3367	585	637	13			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	854	MET	-	EXPRESSION TAG	UNP P10845
A	855	LYS	-	EXPRESSION TAG	UNP P10845
A	856	LYS	-	EXPRESSION TAG	UNP P10845
A	857	HIS	-	EXPRESSION TAG	UNP P10845
A	858	HIS	-	EXPRESSION TAG	UNP P10845
A	859	HIS	-	EXPRESSION TAG	UNP P10845
A	860	HIS	-	EXPRESSION TAG	UNP P10845
A	861	HIS	-	EXPRESSION TAG	UNP P10845
A	862	HIS	-	EXPRESSION TAG	UNP P10845
A	863	GLY	-	EXPRESSION TAG	UNP P10845
A	864	SER	-	EXPRESSION TAG	UNP P10845
A	865	LEU	-	EXPRESSION TAG	UNP P10845
A	866	VAL	-	EXPRESSION TAG	UNP P10845
A	867	PRO	-	EXPRESSION TAG	UNP P10845
A	868	ARG	-	EXPRESSION TAG	UNP P10845
A	869	GLY	-	EXPRESSION TAG	UNP P10845
A	870	SER	-	EXPRESSION TAG	UNP P10845
B	854	MET	-	EXPRESSION TAG	UNP P10845
B	855	LYS	-	EXPRESSION TAG	UNP P10845
B	856	LYS	-	EXPRESSION TAG	UNP P10845
B	857	HIS	-	EXPRESSION TAG	UNP P10845
B	858	HIS	-	EXPRESSION TAG	UNP P10845
B	859	HIS	-	EXPRESSION TAG	UNP P10845
B	860	HIS	-	EXPRESSION TAG	UNP P10845
B	861	HIS	-	EXPRESSION TAG	UNP P10845

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Chain	Residue	Modelled	Actual	Comment	Reference
B	862	HIS	-	EXPRESSION TAG	UNP P10845
B	863	GLY	-	EXPRESSION TAG	UNP P10845
B	864	SER	-	EXPRESSION TAG	UNP P10845
B	865	LEU	-	EXPRESSION TAG	UNP P10845
B	866	VAL	-	EXPRESSION TAG	UNP P10845
B	867	PRO	-	EXPRESSION TAG	UNP P10845
B	868	ARG	-	EXPRESSION TAG	UNP P10845
B	869	GLY	-	EXPRESSION TAG	UNP P10845
B	870	SER	-	EXPRESSION TAG	UNP P10845

- Molecule 2 is a protein called Synaptic vesicle glycoprotein 2C.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	83	Total	C	H	N	O	S	0	0	0
			1320	444	634	103	134	5			
2	D	93	Total	C	H	N	O	S	0	0	0
			1497	502	718	121	151	5			

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	439	MET	-	EXPRESSION TAG	UNP Q496J9
C	440	LYS	-	EXPRESSION TAG	UNP Q496J9
C	441	LYS	-	EXPRESSION TAG	UNP Q496J9
C	442	HIS	-	EXPRESSION TAG	UNP Q496J9
C	443	HIS	-	EXPRESSION TAG	UNP Q496J9
C	444	HIS	-	EXPRESSION TAG	UNP Q496J9
C	445	HIS	-	EXPRESSION TAG	UNP Q496J9
C	446	HIS	-	EXPRESSION TAG	UNP Q496J9
C	447	HIS	-	EXPRESSION TAG	UNP Q496J9
C	448	GLY	-	EXPRESSION TAG	UNP Q496J9
C	449	SER	-	EXPRESSION TAG	UNP Q496J9
C	450	LEU	-	EXPRESSION TAG	UNP Q496J9
C	451	VAL	-	EXPRESSION TAG	UNP Q496J9
C	452	PRO	-	EXPRESSION TAG	UNP Q496J9
C	453	ARG	-	EXPRESSION TAG	UNP Q496J9
C	454	GLY	-	EXPRESSION TAG	UNP Q496J9
C	455	SER	-	EXPRESSION TAG	UNP Q496J9
D	439	MET	-	EXPRESSION TAG	UNP Q496J9
D	440	LYS	-	EXPRESSION TAG	UNP Q496J9
D	441	LYS	-	EXPRESSION TAG	UNP Q496J9
D	442	HIS	-	EXPRESSION TAG	UNP Q496J9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	443	HIS	-	EXPRESSION TAG	UNP Q496J9
D	444	HIS	-	EXPRESSION TAG	UNP Q496J9
D	445	HIS	-	EXPRESSION TAG	UNP Q496J9
D	446	HIS	-	EXPRESSION TAG	UNP Q496J9
D	447	HIS	-	EXPRESSION TAG	UNP Q496J9
D	448	GLY	-	EXPRESSION TAG	UNP Q496J9
D	449	SER	-	EXPRESSION TAG	UNP Q496J9
D	450	LEU	-	EXPRESSION TAG	UNP Q496J9
D	451	VAL	-	EXPRESSION TAG	UNP Q496J9
D	452	PRO	-	EXPRESSION TAG	UNP Q496J9
D	453	ARG	-	EXPRESSION TAG	UNP Q496J9
D	454	GLY	-	EXPRESSION TAG	UNP Q496J9
D	455	SER	-	EXPRESSION TAG	UNP Q496J9

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	6	Total Cl 6 6	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Na 2 2	0	0

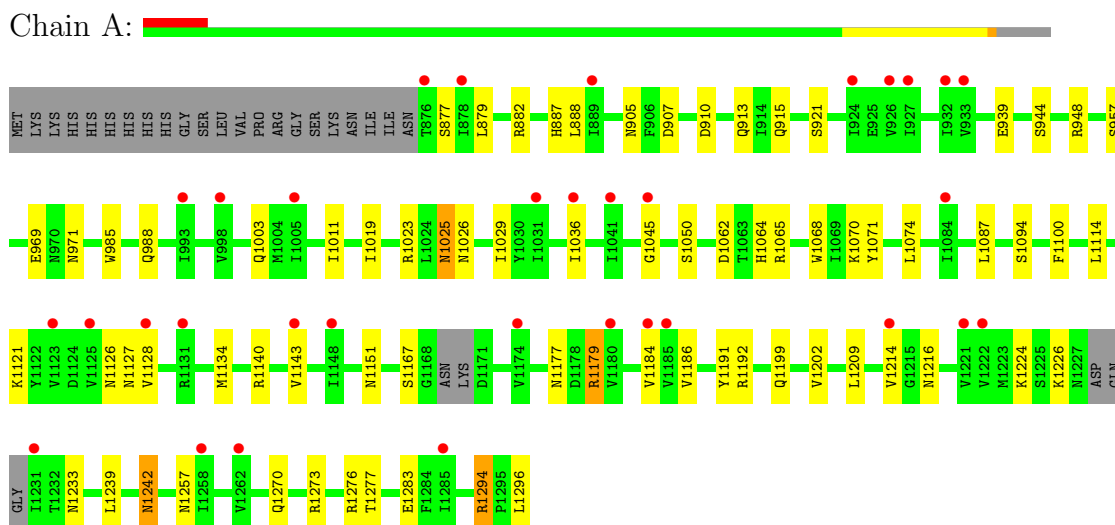
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	50	Total O 50 50	0	0
5	B	18	Total O 18 18	0	0
5	C	6	Total O 6 6	0	0
5	D	8	Total O 8 8	0	0

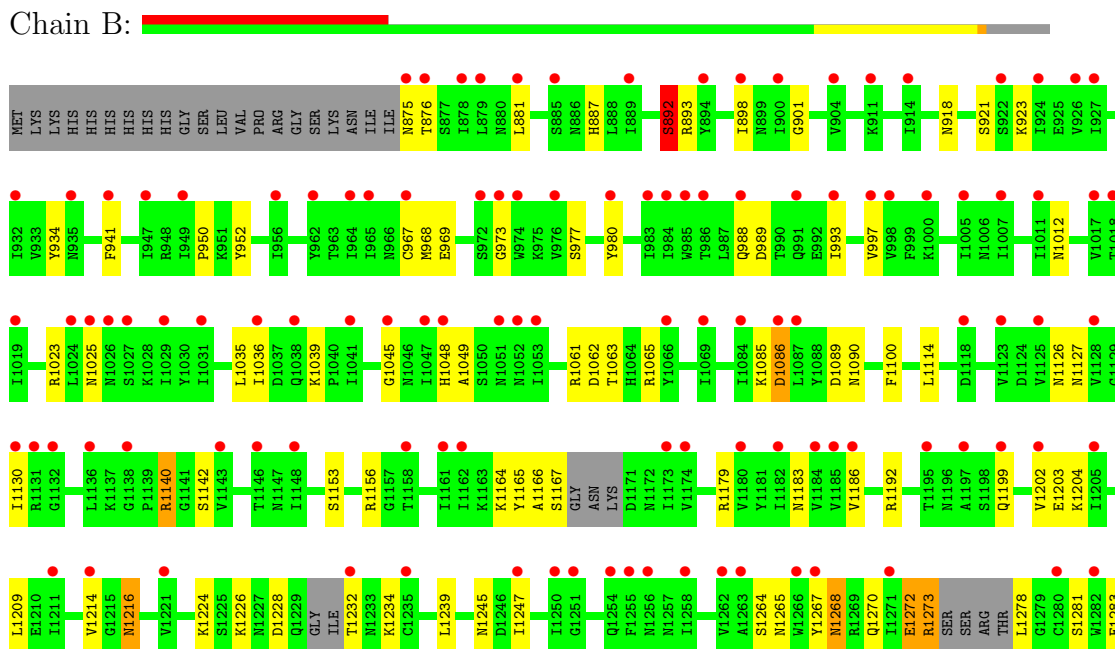
3 Residue-property plots

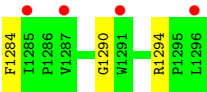
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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



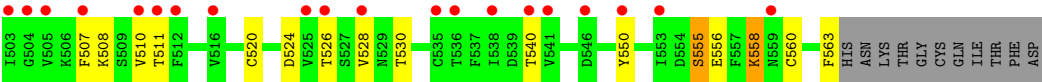
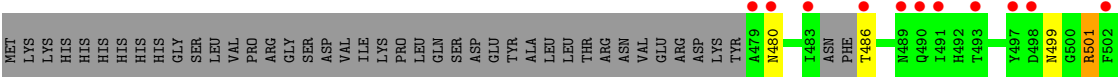
• Molecule 1: Botulinum neurotoxin type A





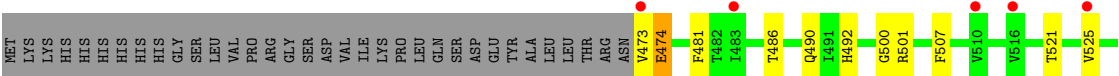
• Molecule 2: Synaptic vesicle glycoprotein 2C

Chain C:



• Molecule 2: Synaptic vesicle glycoprotein 2C

Chain D:



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	115.44Å 105.26Å 127.96Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	19.93 – 2.30 19.93 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.93-2.30) 99.9 (19.93-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.81 (at 2.30Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1389)	Depositor
R, R_{free}	0.235 , 0.269 0.238 , 0.271	Depositor DCC
R_{free} test set	2035 reflections (3.00%)	DCC
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.47 , 33.9	EDS
Estimated twinning fraction	0.430 for -h,-k,l	Xtriage
L-test for twinning	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 67843 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16539	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	0/3524	0.60	0/4761
1	B	0.33	0/3481	0.52	0/4703
2	C	0.31	0/703	0.48	0/945
2	D	0.46	0/800	0.58	0/1077
All	All	0.39	0/8508	0.56	0/11486

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	563	PHE	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the

Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3442	3412	0	36	0
1	B	3411	3367	0	34	0
2	C	686	634	0	13	0
2	D	779	718	0	6	0
3	A	6	0	0	0	0
4	A	2	0	0	0	0
5	A	50	0	0	7	0
5	B	18	0	0	0	0
5	C	6	0	0	1	0
5	D	8	0	0	1	0
All	All	8408	8131	0	87	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 5.

All (87) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1216:ASN:ND2	5:A:1432:HOH:O	2.14	0.78
1:A:1186:VAL:O	5:A:1425:HOH:O	2.07	0.71
1:B:1265:ASN:OD1	1:B:1268:ASN:ND2	2.23	0.71
2:D:565:ASN:OD1	5:D:608:HOH:O	2.09	0.70
1:A:1179:ARG:NH2	5:A:1413:HOH:O	2.25	0.68
1:A:1177:ASN:OD1	1:A:1224:LYS:NZ	2.25	0.68
1:A:1226:LYS:NZ	5:A:1409:HOH:O	2.27	0.66
1:A:1134:MET:HE2	1:A:1184:VAL:HG21	1.77	0.66
1:B:934:TYR:OH	1:B:1023:ARG:NH2	2.29	0.65
1:B:1023:ARG:NH1	1:B:1045:GLY:O	2.32	0.63
1:B:1216:ASN:ND2	1:B:1216:ASN:O	2.33	0.62
1:B:950:PRO:O	1:B:1065:ARG:NH2	2.31	0.62
1:A:1025:ASN:N	1:A:1025:ASN:OD1	2.32	0.61
1:B:892:SER:OG	1:B:893:ARG:N	2.32	0.60
1:B:1086:ASP:O	1:B:1090:ASN:ND2	2.34	0.59
1:B:1278:LEU:N	1:B:1281:SER:HG	2.00	0.59
2:C:555:SER:OG	2:C:556:GLU:N	2.35	0.58
2:C:480:ASN:OD1	2:C:499:ASN:ND2	2.35	0.58
1:B:1165:TYR:O	1:B:1167:SER:N	2.41	0.54
2:C:486:THR:OG1	2:C:508:LYS:NZ	2.40	0.54
2:C:510:VAL:O	2:C:511:THR:OG1	2.24	0.53
1:A:1242:ASN:N	1:A:1242:ASN:OD1	2.42	0.53
1:B:968:MET:SD	1:B:973:GLY:N	2.83	0.51
1:A:971:ASN:O	1:A:988:GLN:NE2	2.43	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1029:ILE:HG23	1:A:1036:ILE:HB	1.93	0.51
1:A:1100:PHE:HD1	1:A:1283:GLU:HG2	1.76	0.50
2:C:507:PHE:HB3	2:C:530:THR:HG21	1.94	0.50
2:D:507:PHE:HB3	2:D:530:THR:HG21	1.94	0.49
1:A:1094:SER:O	5:A:1409:HOH:O	2.20	0.49
1:B:1114:LEU:O	1:B:1283:GLU:N	2.45	0.49
2:C:480:ASN:HA	2:C:499:ASN:HB3	1.95	0.49
2:C:558:LYS:N	2:C:560:CYS:SG	2.82	0.49
1:A:1179:ARG:H	1:A:1179:ARG:HE	1.60	0.48
1:A:1003:GLN:HA	1:A:1011:ILE:HD11	1.94	0.48
1:A:1121:LYS:O	5:A:1405:HOH:O	2.20	0.48
1:B:989:ASP:OD1	1:B:993:ILE:N	2.40	0.48
1:A:905:ASN:ND2	1:A:915:GLN:OE1	2.43	0.48
1:A:1128:VAL:HG11	1:A:1191:TYR:CE1	2.48	0.48
1:A:1100:PHE:HD1	1:A:1283:GLU:CG	2.26	0.48
1:A:1270:GLN:OE1	1:A:1276:ARG:NH1	2.47	0.48
2:C:510:VAL:HG12	2:C:511:THR:N	2.29	0.47
1:B:1100:PHE:HD1	1:B:1283:GLU:HG2	1.80	0.47
1:A:1126:ASN:OD1	1:A:1127:ASN:N	2.48	0.47
2:C:507:PHE:O	2:C:528:VAL:N	2.41	0.47
1:A:969:GLU:HB2	1:A:1050:SER:HA	1.96	0.47
2:D:473:VAL:HG13	2:D:474:GLU:H	1.80	0.47
2:D:490:GLN:OE1	2:D:492:HIS:NE2	2.43	0.47
1:B:1183:ASN:OD1	1:B:1192:ARG:NE	2.48	0.47
1:A:948:ARG:HB3	1:A:1068:TRP:HB2	1.98	0.46
1:A:957:SER:OG	1:A:1062:ASP:OD2	2.32	0.46
1:B:875:ASN:O	1:B:893:ARG:NH1	2.48	0.46
1:B:1085:LYS:NZ	1:B:1089:ASP:OD2	2.38	0.46
1:B:918:ASN:ND2	1:B:1062:ASP:O	2.38	0.46
1:B:1224:LYS:NZ	1:B:1226:LYS:O	2.32	0.45
1:B:1164:LYS:O	1:B:1167:SER:OG	2.34	0.45
2:C:550:TYR:O	5:C:601:HOH:O	2.21	0.45
1:B:901:GLY:N	1:B:923:LYS:O	2.50	0.45
1:A:1134:MET:CE	1:A:1184:VAL:HG21	2.44	0.44
1:A:1192:ARG:HG2	1:A:1214:VAL:HG11	1.99	0.43
2:D:525:VAL:HG22	2:D:545:THR:HG22	2.00	0.43
1:A:1167:SER:O	1:B:1245:ASN:ND2	2.50	0.43
1:B:1126:ASN:OD1	1:B:1127:ASN:N	2.52	0.43
1:A:907:ASP:HB3	1:A:910:ASP:O	2.19	0.43
1:A:882:ARG:NH2	1:A:1071:TYR:HA	2.35	0.42
1:A:913:GLN:HG2	1:A:1070:LYS:HD3	2.00	0.42
2:C:501:ARG:HE	2:C:501:ARG:HA	1.84	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:1199:GLN:O	1:B:1204:LYS:NZ	2.45	0.42
1:B:989:ASP:N	1:B:993:ILE:O	2.50	0.42
2:C:520:CYS:H	2:C:540:THR:HG22	1.84	0.42
1:A:1026:ASN:O	5:A:1450:HOH:O	2.21	0.42
1:B:952:TYR:HA	1:B:1065:ARG:NH1	2.35	0.42
1:B:967:CYS:SG	1:B:1049:ALA:HB1	2.59	0.42
1:B:1140:ARG:NH2	1:B:1153:SER:O	2.50	0.42
1:A:1023:ARG:NH1	1:A:1045:GLY:O	2.48	0.41
1:A:879:LEU:HB3	1:A:1074:LEU:HB2	2.03	0.41
1:B:1272:GLU:OE1	1:B:1273:ARG:NH1	2.50	0.41
1:B:881:LEU:HD21	1:B:898:ILE:HG12	2.03	0.41
1:A:1294:ARG:HA	1:A:1294:ARG:HE	1.85	0.41
1:B:1203:GLU:HG3	1:B:1264:SER:HB2	2.02	0.41
1:B:1012:ASN:ND2	1:B:1290:GLY:O	2.54	0.41
1:A:985:TRP:CD2	1:A:1019:ILE:HG21	2.56	0.41
1:A:1003:GLN:O	1:A:1151:ASN:ND2	2.48	0.40
2:D:481:PHE:CE1	2:D:500:GLY:HA3	2.56	0.40
1:B:1156:ARG:HD3	2:C:563:PHE:CZ	2.56	0.40
1:B:1267:TYR:O	1:B:1270:GLN:N	2.53	0.40
1:B:1100:PHE:N	1:B:1284:PHE:O	2.53	0.40
1:A:1114:LEU:HD13	1:A:1140:ARG:NH1	2.36	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	413/443 (93%)	385 (93%)	28 (7%)	0	100	100
1	B	405/443 (91%)	349 (86%)	49 (12%)	7 (2%)	14	11
2	C	79/136 (58%)	71 (90%)	8 (10%)	0	100	100
2	D	91/136 (67%)	87 (96%)	3 (3%)	1 (1%)	21	21
All	All	988/1158 (85%)	892 (90%)	88 (9%)	8 (1%)	27	30

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1166	ALA
2	D	474	GLU
1	B	1140	ARG
1	B	892	SER
1	B	980	TYR
1	B	1025	ASN
1	B	1130	ILE
1	B	1247	ILE

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	387/408 (95%)	364 (94%)	23 (6%)	28	35
1	B	382/408 (94%)	351 (92%)	31 (8%)	17	20
2	C	79/128 (62%)	74 (94%)	5 (6%)	25	32
2	D	89/128 (70%)	85 (96%)	4 (4%)	38	50
All	All	937/1072 (87%)	874 (93%)	63 (7%)	23	29

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	877	SER
1	A	887	HIS
1	A	888	LEU
1	A	921	SER
1	A	939	GLU
1	A	944	SER
1	A	1025	ASN
1	A	1064	HIS
1	A	1065	ARG
1	A	1087	LEU
1	A	1143	VAL
1	A	1179	ARG
1	A	1199	GLN

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Mol	Chain	Res	Type
1	A	1202	VAL
1	A	1209	LEU
1	A	1233	ASN
1	A	1239	LEU
1	A	1242	ASN
1	A	1257	ASN
1	A	1273	ARG
1	A	1277	THR
1	A	1294	ARG
1	A	1296	LEU
1	B	876	THR
1	B	887	HIS
1	B	892	SER
1	B	921	SER
1	B	941	PHE
1	B	969	GLU
1	B	977	SER
1	B	988	GLN
1	B	997	VAL
1	B	1035	LEU
1	B	1036	ILE
1	B	1039	LYS
1	B	1048	HIS
1	B	1061	ARG
1	B	1063	THR
1	B	1086	ASP
1	B	1142	SER
1	B	1179	ARG
1	B	1186	VAL
1	B	1202	VAL
1	B	1209	LEU
1	B	1214	VAL
1	B	1216	ASN
1	B	1228	ASP
1	B	1232	THR
1	B	1234	LYS
1	B	1239	LEU
1	B	1268	ASN
1	B	1272	GLU
1	B	1273	ARG
1	B	1294	ARG
2	C	501	ARG

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Mol	Chain	Res	Type
2	C	524	ASP
2	C	526	THR
2	C	555	SER
2	C	558	LYS
2	D	486	THR
2	D	501	ARG
2	D	521	THR
2	D	534	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	913	GLN
1	A	988	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

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.

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, 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	416/443 (93%)	0.56	33 (7%) 13 19	12, 22, 45, 64	0
1	B	413/443 (93%)	1.44	118 (28%) 1 1	26, 51, 76, 103	0
2	C	83/136 (61%)	1.89	31 (37%) 1 1	26, 56, 73, 82	0
2	D	93/136 (68%)	0.58	6 (6%) 18 26	14, 27, 46, 66	0
All	All	1005/1158 (86%)	1.04	188 (18%) 2 3	12, 37, 71, 103	0

All (188) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	483	ILE	9.9
1	B	1202	VAL	7.9
1	B	875	ASN	6.8
1	B	878	ILE	6.8
2	C	511	THR	6.4
1	B	1271	ILE	6.1
2	C	510	VAL	6.1
2	C	525	VAL	6.1
1	B	904	VAL	6.0
1	B	1258	ILE	5.9
1	B	1250	ILE	5.8
1	B	1138	GLY	5.8
1	B	1262	VAL	5.7
1	B	1018	THR	5.7
1	B	1214	VAL	5.7
2	C	505	VAL	5.6
1	B	926	VAL	5.5
1	B	993	ILE	5.4
2	C	503	ILE	5.3
1	B	1128	VAL	5.0
1	B	1036	ILE	4.9

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Mol	Chain	Res	Type	RSRZ
1	B	1087	LEU	4.8
1	B	1255	PHE	4.7
1	B	1186	VAL	4.5
1	B	898	ILE	4.5
2	C	507	PHE	4.5
1	B	1007	ILE	4.5
1	B	941	PHE	4.5
1	B	927	ILE	4.4
1	B	900	ILE	4.2
1	B	1051	ASN	4.2
1	B	1084	ILE	4.1
2	C	541	VAL	4.1
1	B	1162	ILE	4.1
2	C	479	ALA	4.1
1	B	1125	VAL	4.0
2	C	528	VAL	4.0
1	B	881	LEU	4.0
2	C	553	ILE	3.9
1	B	1235	CYS	3.9
1	B	1024	LEU	3.9
1	B	1256	ASN	3.9
2	C	535	CYS	3.8
1	B	1205	ILE	3.8
1	B	1287	VAL	3.7
1	B	980	TYR	3.7
1	B	1199	GLN	3.6
1	B	1086	ASP	3.6
1	B	956	ILE	3.6
1	B	986	THR	3.6
1	B	1031	ILE	3.5
1	B	1047	ILE	3.5
1	B	1148	ILE	3.5
1	B	1185	VAL	3.5
1	B	1025	ASN	3.5
2	C	486	THR	3.4
2	C	526	THR	3.4
1	B	1069	ILE	3.4
2	C	536	THR	3.4
1	B	1041	ILE	3.4
2	C	493	THR	3.4
1	B	1282	TRP	3.4
2	C	491	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
2	C	504	GLY	3.3
1	B	972	SER	3.3
1	B	1254	GLN	3.3
1	B	1132	GLY	3.3
2	C	516	VAL	3.2
1	B	1048	HIS	3.1
1	B	1005	ILE	3.1
1	A	876	THR	3.1
1	B	965	ILE	3.1
1	B	998	VAL	3.1
1	B	1136	LEU	3.0
1	A	1123	VAL	3.0
2	D	525	VAL	3.0
1	A	1148	ILE	3.0
1	B	932	ILE	3.0
1	B	922	SER	3.0
1	B	1174	VAL	3.0
1	B	1019	ILE	3.0
1	A	998	VAL	3.0
1	B	935	ASN	3.0
1	B	1017	VAL	2.9
1	B	1184	VAL	2.9
1	B	1011	ILE	2.9
1	B	997	VAL	2.9
1	B	1267	TYR	2.9
1	B	885	SER	2.9
2	C	502	PHE	2.8
1	B	1029	ILE	2.8
1	B	1280	CYS	2.8
1	A	1128	VAL	2.8
2	C	538	ILE	2.8
1	B	1158	THR	2.8
2	C	559	ASN	2.7
1	A	1125	VAL	2.7
1	B	1285	ILE	2.7
1	B	1232	THR	2.7
2	C	497	TYR	2.7
2	C	550	TYR	2.7
1	B	1180	VAL	2.7
2	C	498	ASP	2.7
2	D	528	VAL	2.7
1	B	967	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	984	ILE	2.7
1	B	1052	ASN	2.7
1	B	876	THR	2.6
1	B	1247	ILE	2.6
1	B	1123	VAL	2.6
1	A	1084	ILE	2.6
1	B	1130	ILE	2.6
1	A	1214	VAL	2.6
1	B	976	VAL	2.6
1	A	1180	VAL	2.6
1	B	1197	ALA	2.5
2	C	490	GLN	2.5
2	C	546	ASP	2.5
1	B	1195	THR	2.5
1	A	926	VAL	2.5
1	A	1005	ILE	2.5
1	B	911	LYS	2.5
1	B	947	ILE	2.5
1	A	1184	VAL	2.5
2	D	510	VAL	2.5
1	A	889	ILE	2.5
1	B	1161	ILE	2.5
1	B	1146	THR	2.4
2	C	480	ASN	2.4
2	D	483	ILE	2.4
1	B	879	LEU	2.4
1	B	1000	LYS	2.4
1	B	1296	LEU	2.4
1	A	1262	VAL	2.4
1	A	878	ILE	2.4
1	A	927	ILE	2.4
2	C	540	THR	2.4
1	B	988	GLN	2.4
1	A	1231	ILE	2.4
1	B	983	ILE	2.3
1	A	1143	VAL	2.3
1	A	924	ILE	2.3
1	A	993	ILE	2.3
1	A	1045	GLY	2.3
1	B	1066	TYR	2.3
1	B	1027	SER	2.3
1	B	985	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	962	TYR	2.3
1	A	1258	ILE	2.3
1	B	889	ILE	2.3
1	B	1263	ALA	2.3
1	B	1221	VAL	2.2
1	B	924	ILE	2.2
1	A	1174	VAL	2.2
1	A	1221	VAL	2.2
1	B	1251	GLY	2.2
1	A	1185	VAL	2.2
1	A	1131	ARG	2.2
1	A	1285	ILE	2.2
1	B	1211	ILE	2.2
2	D	516	VAL	2.2
2	C	489	ASN	2.2
2	C	512	PHE	2.1
1	A	933	VAL	2.1
1	A	1031	ILE	2.1
1	B	1118	ASP	2.1
1	B	1291	TRP	2.1
1	B	1026	ASN	2.1
1	B	973	GLY	2.1
1	A	1041	ILE	2.1
1	B	964	ILE	2.1
1	B	1038	GLN	2.1
1	B	914	ILE	2.1
1	B	1173	ILE	2.1
1	A	1222	VAL	2.1
1	B	1143	VAL	2.1
1	A	932	ILE	2.1
1	B	1182	ILE	2.1
1	B	1131	ARG	2.0
1	B	991	GLN	2.0
1	B	1266	TRP	2.0
1	B	894	TYR	2.0
1	B	1045	GLY	2.0
1	B	974	TRP	2.0
1	A	1036	ILE	2.0
1	B	949	ILE	2.0
1	B	1053	ILE	2.0
2	D	473	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. 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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CL	A	1301	1/1	0.18	3.15	37,37,37,37	0
3	CL	A	1308	1/1	0.18	0.04	24,24,24,24	0
3	CL	A	1305	1/1	0.15	-0.35	32,32,32,32	0
4	NA	A	1306	1/1	0.14	-0.60	22,22,22,22	0
3	CL	A	1303	1/1	0.11	-1.59	30,30,30,30	0
3	CL	A	1302	1/1	0.10	-1.95	45,45,45,45	0
3	CL	A	1304	1/1	0.11	-2.12	24,24,24,24	0
4	NA	A	1307	1/1	0.12	-3.24	15,15,15,15	0

6.5 Other polymers ⓘ

There are no such residues in this entry.