



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 05:24 am BST

PDB ID : 4JRA
Title : CRYSTAL STRUCTURE OF THE BOTULINUM NEUROTOXIN A
RECEPTOR-BINDING DOMAIN IN COMPLEX WITH THE LUMINAL
DOMAIN Of SV2C
Authors : Benoit, R.M.; Frey, D.; Wieser, M.M.; Jaussi, R.; Schertler, G.F.X.; Capitani,
G.; Kammerer, R.A.
Deposited on : 2013-03-21
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
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

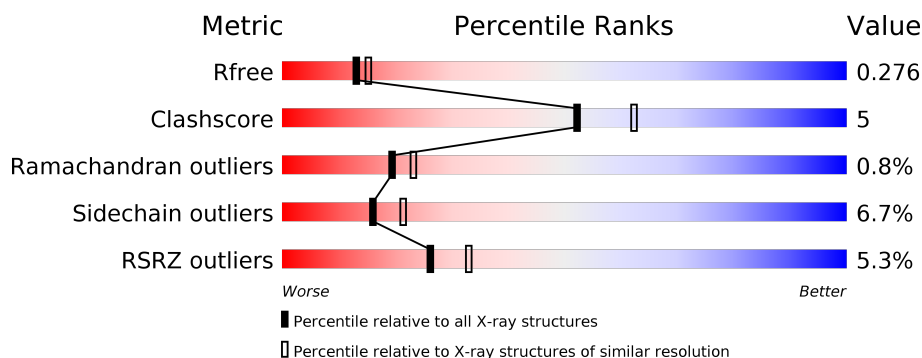
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 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	443	<div> <div>77%</div> <div>16%</div> <div>• 6%</div> </div>
1	B	443	<div> <div>9%</div> <div>72%</div> <div>20%</div> <div>• 7%</div> </div>
2	C	136	<div> <div>10%</div> <div>47%</div> <div>12%</div> <div>• 39%</div> </div>
2	D	136	<div> <div>57%</div> <div>11%</div> <div>• 32%</div> </div>

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 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.

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	443	HIS	-	EXPRESSION TAG	UNP Q496.J9
D	444	HIS	-	EXPRESSION TAG	UNP Q496.J9
D	445	HIS	-	EXPRESSION TAG	UNP Q496.J9
D	446	HIS	-	EXPRESSION TAG	UNP Q496.J9
D	447	HIS	-	EXPRESSION TAG	UNP Q496.J9
D	448	GLY	-	EXPRESSION TAG	UNP Q496.J9
D	449	SER	-	EXPRESSION TAG	UNP Q496.J9
D	450	LEU	-	EXPRESSION TAG	UNP Q496.J9
D	451	VAL	-	EXPRESSION TAG	UNP Q496.J9
D	452	PRO	-	EXPRESSION TAG	UNP Q496.J9
D	453	ARG	-	EXPRESSION TAG	UNP Q496.J9
D	454	GLY	-	EXPRESSION TAG	UNP Q496.J9
D	455	SER	-	EXPRESSION TAG	UNP Q496.J9

- 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

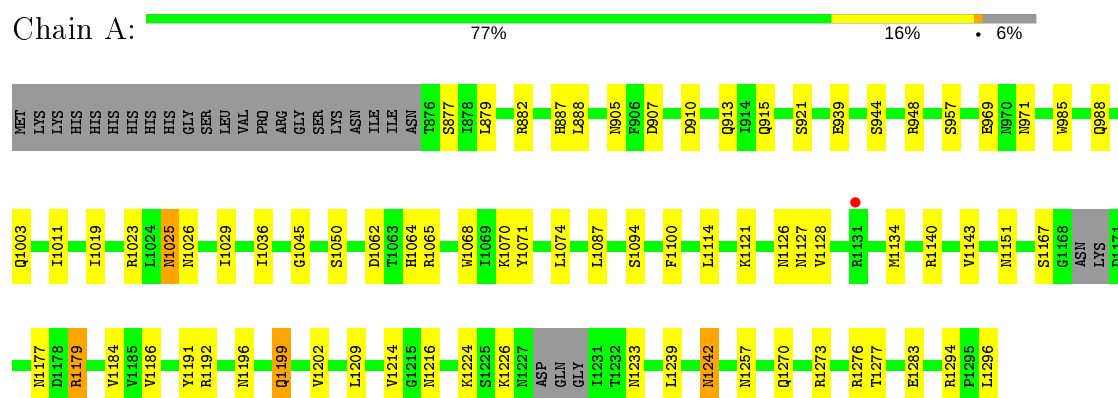
- Molecule 5 is water.

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

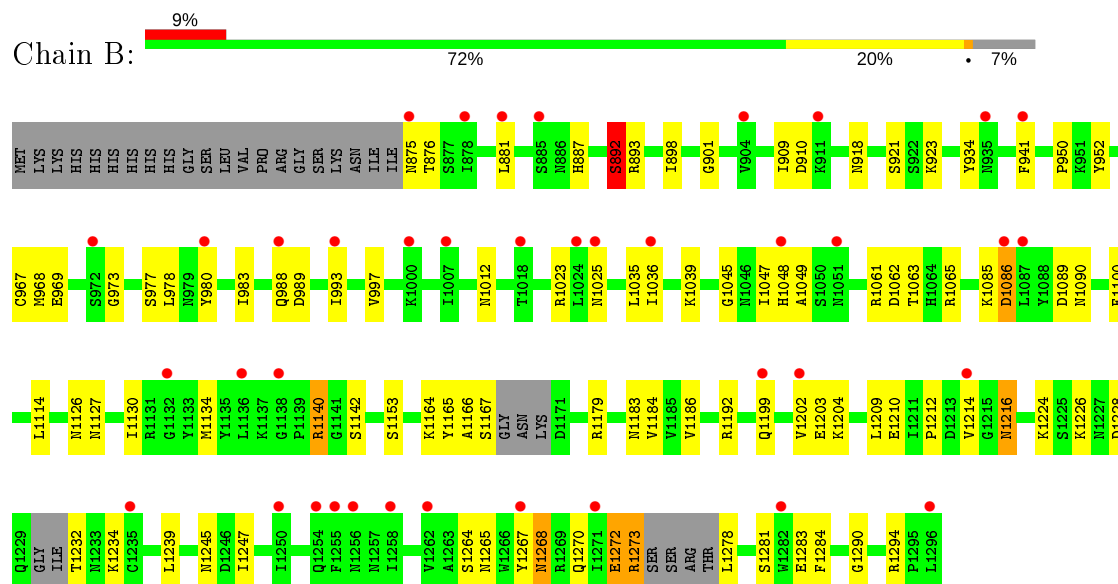
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ($\text{RSRZ} > 2$). 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

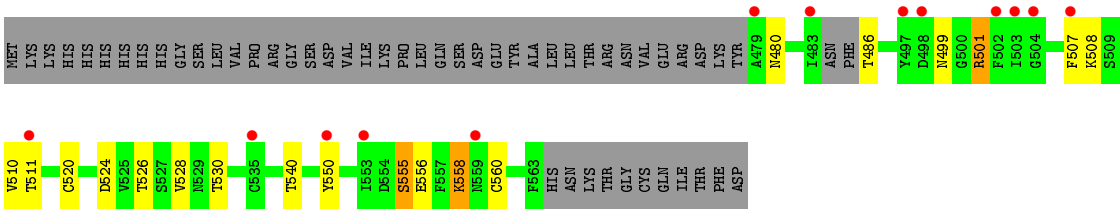


• Molecule 1: Botulinum neurotoxin type A

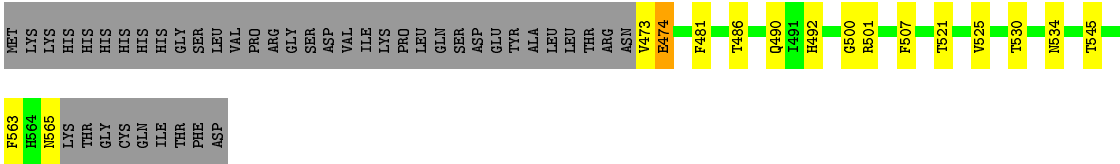


• Molecule 2: Synaptic vesicle glycoprotein 2C





● Molecule 2: Synaptic vesicle glycoprotein 2C



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: 1.8.2_1309)	Depositor
R, R_{free}	0.235 , 0.269 0.242 , 0.276	Depositor DCC
R_{free} test set	2032 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å ²)	29.6	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.430 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	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.

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: 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 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	3442	3412	3401	35	0
1	B	3411	3367	3363	38	0
2	C	686	634	633	12	0
2	D	779	718	716	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	8113	90	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 (90) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A: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: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:1224:LYS:NZ	1:B:1226:LYS:O	2.32	0.55
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:A:1100:PHE:HD1	1:A:1283:GLU:HG2	1.74	0.52
2:D:507:PHE:HB3	2:D:530:THR:HG21	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:507:PHE:HB3	2:C:530:THR:HG21	1.92	0.51
1:A:1029:ILE:HG23	1:A:1036:ILE:HB	1.92	0.51
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
1:A:1003:GLN:HA	1:A:1011:ILE:HD11	1.93	0.49
1:A:1094:SER:O	5:A:1409:HOH:O	2.20	0.49
1:B:1100:PHE:HD1	1:B:1283:GLU:HG2	1.78	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:1121:LYS:O	5:A:1405:HOH:O	2.20	0.48
1:A:1179:ARG:H	1:A:1179:ARG:HE	1.60	0.48
1:B:989:ASP:OD1	1:B:993:ILE:N	2.40	0.48
1:A:1128:VAL:HG11	1:A:1191:TYR:CE1	2.48	0.48
1:A:905:ASN:ND2	1:A:915:GLN:OE1	2.43	0.48
1:A:948:ARG:HB3	1:A:1068:TRP:HB2	1.96	0.48
1:A:1134:MET:CE	1:A:1184:VAL:HG21	2.44	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
1:B:1134:MET:HE1	1:B:1184:VAL:HG21	1.95	0.47
1:A:1126:ASN:OD1	1:A:1127:ASN:N	2.48	0.47
2:C:510:VAL:HG12	2:C:511:THR:N	2.30	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
1:B:1183:ASN:OD1	1:B:1192:ARG:NE	2.48	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: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:A:1196:ASN:O	1:A:1199:GLN:NE2	2.41	0.45
1:A:1192:ARG:HG2	1:A:1214:VAL:HG11	1.97	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:957:SER:OG	1:A:1062:ASP:OD2	2.32	0.44
1:A:913:GLN:HG2	1:A:1070:LYS:HD3	1.99	0.44
2:D:525:VAL:HG22	2:D:545:THR:HG22	1.99	0.44
1:A:907:ASP:HB3	1:A:910:ASP:O	2.18	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:879:LEU:HB3	1:A:1074:LEU:HB2	2.01	0.42
1:B:978:LEU:HD23	1:B:983:ILE:HA	2.00	0.42
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:501:ARG:HE	2:C:501:ARG:HA	1.84	0.42
2:C:520:CYS:H	2:C:540:THR:HG22	1.84	0.42
2:D:481:PHE:CE1	2:D:500:GLY:HA3	2.55	0.42
1:B:967:CYS:SG	1:B:1049:ALA:HB1	2.59	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:1140:ARG:NH2	1:B:1153:SER:O	2.50	0.42
1:B:1203:GLU:HG3	1:B:1264:SER:HB2	2.02	0.42
1:B:881:LEU:HD21	1:B:898:ILE:HG12	2.02	0.42
1:A:1023:ARG:NH1	1:A:1045:GLY:O	2.48	0.41
1:B:1272:GLU:OE1	1:B:1273:ARG:NH1	2.50	0.41
1:A:882:ARG:NH2	1:A:1071:TYR:HA	2.36	0.41
1:B:1012:ASN:ND2	1:B:1290:GLY:O	2.54	0.41
1:A:1114:LEU:HD13	1:A:1140:ARG:NH1	2.35	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
1:B:1210:GLU:HG3	1:B:1212:PRO:HD2	2.03	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:B:909:ILE:HG13	1:B:910:ASP:N	2.36	0.40
1:B:934:TYR:HE1	1:B:1047:ILE:HB	1.87	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

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	405/443 (91%)	349 (86%)	49 (12%)	7 (2%)	9	8
2	C	79/136 (58%)	71 (90%)	8 (10%)	0	100	100
2	D	91/136 (67%)	87 (96%)	3 (3%)	1 (1%)	14	15
All	All	988/1158 (85%)	892 (90%)	88 (9%)	8 (1%)	19	23

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%)	19	27
1	B	382/408 (94%)	351 (92%)	31 (8%)	11	15
2	C	79/128 (62%)	74 (94%)	5 (6%)	18	24
2	D	89/128 (70%)	85 (96%)	4 (4%)	27	39
All	All	937/1072 (87%)	874 (93%)	63 (7%)	16	21

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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 (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	988	GLN
2	C	480	ASN
2	C	499	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

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.

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, 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%)	-0.01	1 (0%) 95 96	12, 22, 43, 59	0
1	B	413/443 (93%)	0.73	39 (9%) 8 11	26, 51, 75, 103	0
2	C	83/136 (61%)	1.00	13 (15%) 2 2	26, 56, 73, 78	0
2	D	93/136 (68%)	-0.01	0 100 100	14, 27, 44, 66	0
All	All	1005/1158 (86%)	0.38	53 (5%) 26 33	12, 37, 71, 103	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	483	ILE	6.2
1	B	875	ASN	5.9
1	B	1202	VAL	5.0
1	B	1087	LEU	4.9
1	B	1138	GLY	4.9
1	B	1271	ILE	4.4
1	B	878	ILE	4.0
1	B	1255	PHE	4.0
2	C	507	PHE	4.0
1	B	941	PHE	3.8
1	B	1051	ASN	3.8
1	B	1024	LEU	3.7
2	C	511	THR	3.6
2	C	479	ALA	3.4
1	B	1256	ASN	3.3
1	B	1199	GLN	3.2
1	B	1086	ASP	3.2
1	B	1025	ASN	3.2
1	B	980	TYR	3.1
1	B	881	LEU	3.1
2	C	504	GLY	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	C	503	ILE	3.0
1	B	1282	TRP	3.0
1	B	1258	ILE	2.9
1	B	1250	ILE	2.9
1	B	1048	HIS	2.9
1	B	1132	GLY	2.8
1	B	1018	THR	2.8
1	B	1235	CYS	2.8
1	B	1254	GLN	2.7
1	B	1136	LEU	2.6
1	B	993	ILE	2.6
2	C	550	TYR	2.6
1	B	935	ASN	2.6
1	B	904	VAL	2.5
1	B	885	SER	2.5
2	C	535	CYS	2.5
2	C	559	ASN	2.4
1	B	1267	TYR	2.4
1	B	1036	ILE	2.3
1	B	972	SER	2.3
1	B	911	LYS	2.3
1	B	1007	ILE	2.2
2	C	502	PHE	2.2
1	B	1000	LYS	2.2
1	B	1214	VAL	2.2
2	C	553	ILE	2.2
2	C	498	ASP	2.2
2	C	497	TYR	2.1
1	B	988	GLN	2.1
1	B	1296	LEU	2.1
1	B	1262	VAL	2.1
1	A	1131	ARG	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(\AA^2)	Q<0.9
3	CL	A	1301	1/1	0.93	0.14	37,37,37,37	0
3	CL	A	1302	1/1	0.94	0.07	45,45,45,45	0
3	CL	A	1305	1/1	0.97	0.12	32,32,32,32	0
4	NA	A	1307	1/1	0.98	0.10	15,15,15,15	0
3	CL	A	1303	1/1	0.99	0.08	30,30,30,30	0
4	NA	A	1306	1/1	0.99	0.13	22,22,22,22	0
3	CL	A	1308	1/1	0.99	0.15	24,24,24,24	0
3	CL	A	1304	1/1	0.99	0.08	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.