



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:18 PM UTC

PDB ID : 2R83 / pdb_00002r83
Title : Crystal structure analysis of human synaptotagmin 1 C2A-C2B
Authors : Sutton, R.B.; Fuson, K.L.; Montes, M.; Robert, J.J.
Deposited on : 2007-09-10
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

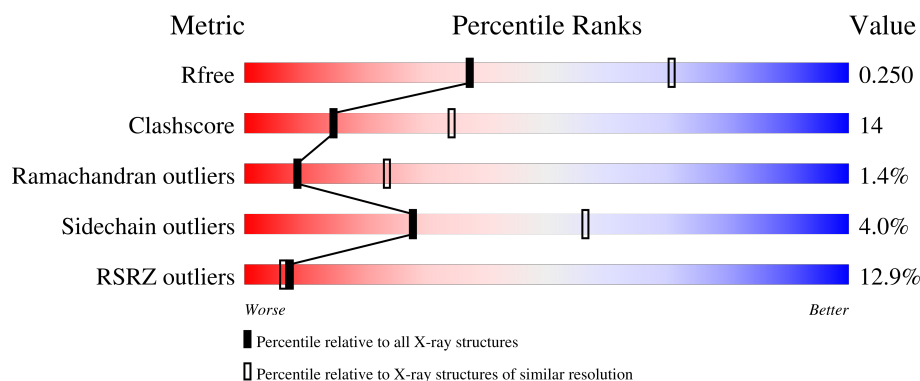
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	284	13% 70% 24% ...
1	B	284	13% 70% 25% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4563 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 Synaptotagmin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2256	1455	375	418	8			
1	B	279	Total	C	N	O	S	0	0	0
			2256	1455	375	418	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	138	GLY	-	expression tag	UNP P21579
A	139	SER	-	expression tag	UNP P21579
A	220	ALA	GLY	conflict	UNP P21579
B	138	GLY	-	expression tag	UNP P21579
B	139	SER	-	expression tag	UNP P21579
B	220	ALA	GLY	conflict	UNP P21579

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	6	Total	Cl	0	0
			6	6		
2	B	2	Total	Cl	0	0
			2	2		

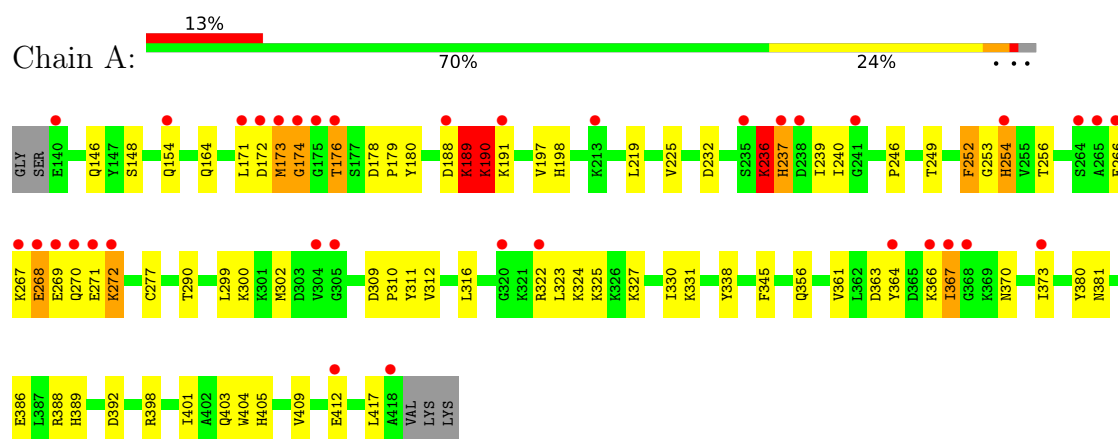
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		
3	B	24	Total	O	0	0
			24	24		

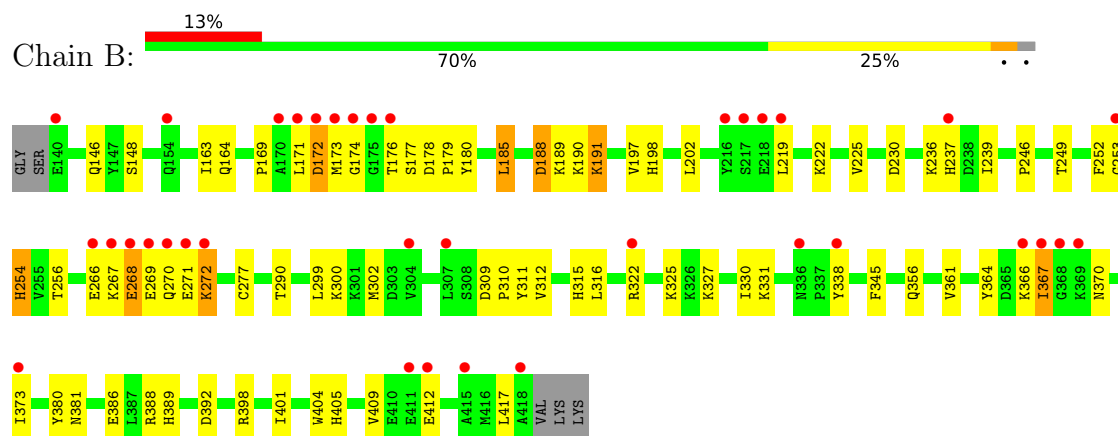
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Synaptotagmin-1



• Molecule 1: Synaptotagmin-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.37Å 86.31Å 147.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.31 – 2.70 46.31 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.31-2.70) 99.2 (46.31-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.253 0.228 , 0.250	Depositor DCC
R_{free} test set	2921 reflections (9.97%)	wwPDB-VP
Wilson B-factor (Å ²)	48.3	Xtriage
Anisotropy	0.411	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.033 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4563	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.35% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.43	0/2305	0.94	7/3111 (0.2%)
1	B	0.44	0/2305	0.92	8/3111 (0.3%)
All	All	0.44	0/4610	0.93	15/6222 (0.2%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	309	ASP	CA-C-N	6.51	126.27	119.76
1	B	309	ASP	C-N-CA	6.51	126.27	119.76
1	A	272	LYS	N-CA-C	6.37	118.55	108.67
1	A	309	ASP	CA-C-N	6.19	125.95	119.76
1	A	309	ASP	C-N-CA	6.19	125.95	119.76
1	B	272	LYS	N-CA-C	6.14	118.18	108.67
1	B	310	PRO	N-CA-C	5.67	120.09	111.19
1	A	310	PRO	N-CA-C	5.52	119.85	111.19
1	A	179	PRO	N-CA-C	5.34	119.88	111.38
1	A	236	LYS	N-CA-C	5.24	121.95	110.80
1	A	190	LYS	N-CA-C	-5.20	105.26	111.03
1	B	188	ASP	N-CA-C	-5.18	105.32	110.97
1	B	179	PRO	N-CA-C	5.18	119.61	111.38
1	B	163	ILE	N-CA-C	5.17	115.44	110.74
1	B	174	GLY	N-CA-C	5.10	118.84	111.24

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	2256	0	2279	61	0
1	B	2256	0	2279	65	0
2	A	6	0	0	0	0
2	B	2	0	0	0	0
3	A	19	0	0	2	0
3	B	24	0	0	0	0
All	All	4563	0	4558	126	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 14.

All (126) 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:299:LEU:HD22	1:A:373:ILE:HD11	1.50	0.91
1:B:299:LEU:HD22	1:B:373:ILE:HD11	1.52	0.89
1:B:169:PRO:HG2	1:B:171:LEU:HD22	1.60	0.82
1:A:266:GLU:HG3	1:A:267:LYS:H	1.42	0.82
1:B:266:GLU:HG3	1:B:267:LYS:H	1.44	0.82
1:A:191:LYS:HA	1:A:412:GLU:OE2	1.79	0.81
1:A:271:GLU:O	1:A:271:GLU:HG3	1.81	0.80
1:B:271:GLU:OE2	1:B:409:VAL:HG13	1.82	0.80
1:A:389:HIS:CD2	1:A:405:HIS:HE1	2.03	0.77
1:B:389:HIS:CD2	1:B:405:HIS:HE1	2.03	0.77
1:B:271:GLU:HG3	1:B:271:GLU:O	1.82	0.77
1:B:169:PRO:HG2	1:B:171:LEU:CD2	2.16	0.76
1:A:271:GLU:OE2	1:A:409:VAL:HG13	1.91	0.70
1:B:191:LYS:HA	1:B:412:GLU:OE2	1.91	0.70
1:B:146:GLN:HE21	1:B:164:GLN:HG2	1.57	0.70
1:B:169:PRO:O	1:B:171:LEU:HD23	1.91	0.70
1:A:299:LEU:HD22	1:A:373:ILE:CD1	2.23	0.69
1:A:146:GLN:HE21	1:A:164:GLN:HG2	1.57	0.67
1:B:409:VAL:HG23	1:B:412:GLU:HG2	1.77	0.67
1:B:239:ILE:HD13	1:B:268:GLU:HG2	1.76	0.66
1:A:268:GLU:HA	1:A:268:GLU:OE1	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:299:LEU:HD22	1:B:373:ILE:CD1	2.24	0.65
1:A:409:VAL:HG23	1:A:412:GLU:HG2	1.79	0.64
1:B:266:GLU:HG3	1:B:267:LYS:N	2.13	0.64
1:A:266:GLU:HG3	1:A:267:LYS:N	2.12	0.62
1:B:268:GLU:HA	1:B:268:GLU:OE1	1.98	0.62
1:B:171:LEU:HG	1:B:172:ASP:OD1	2.01	0.61
1:B:185:LEU:HD22	1:B:222:LYS:HB3	1.83	0.61
1:B:176:THR:HG22	1:B:202:LEU:HG	1.82	0.60
1:B:389:HIS:CD2	1:B:405:HIS:CE1	2.88	0.60
1:A:171:LEU:HD21	3:A:436:HOH:O	2.00	0.60
1:B:189:LYS:HE2	1:B:269:GLU:HG3	1.84	0.59
1:A:389:HIS:CD2	1:A:405:HIS:CE1	2.89	0.59
1:B:409:VAL:CG2	1:B:412:GLU:HG2	2.31	0.59
1:A:232:ASP:OD1	1:A:232:ASP:C	2.46	0.58
1:B:322:ARG:HD2	1:B:325:LYS:NZ	2.19	0.58
1:A:409:VAL:CG2	1:A:412:GLU:HG2	2.33	0.58
1:A:322:ARG:HD2	1:A:325:LYS:NZ	2.19	0.57
1:A:311:TYR:CD2	1:A:327:LYS:HE3	2.40	0.57
1:A:300:LYS:HG2	1:A:302:MET:HE3	1.87	0.56
1:B:300:LYS:HG2	1:B:302:MET:HE3	1.86	0.56
1:B:311:TYR:CD2	1:B:327:LYS:HE3	2.41	0.56
1:A:389:HIS:HD2	1:A:405:HIS:HE1	1.53	0.55
1:A:312:VAL:HG22	1:A:361:VAL:HG22	1.87	0.55
1:B:380:TYR:O	1:B:381:ASN:HB2	2.06	0.55
1:B:312:VAL:HG22	1:B:361:VAL:HG22	1.89	0.55
1:B:389:HIS:HD2	1:B:405:HIS:CE1	2.25	0.54
1:A:386:GLU:OE1	1:A:405:HIS:HD2	1.91	0.54
1:A:302:MET:HA	1:A:302:MET:HE2	1.89	0.54
1:A:380:TYR:O	1:A:381:ASN:HB2	2.06	0.54
1:B:188:ASP:O	1:B:189:LYS:HB3	2.07	0.54
1:B:302:MET:HA	1:B:302:MET:HE2	1.90	0.53
1:A:389:HIS:HD2	1:A:405:HIS:CE1	2.25	0.53
1:A:277:CYS:HB2	1:A:404:TRP:CD2	2.44	0.53
1:B:386:GLU:OE1	1:B:405:HIS:HD2	1.92	0.53
1:B:190:LYS:HG2	1:B:271:GLU:OE2	2.09	0.52
1:B:271:GLU:OE2	1:B:409:VAL:CG1	2.56	0.52
1:B:277:CYS:HB2	1:B:404:TRP:CD2	2.44	0.52
1:B:271:GLU:CD	1:B:409:VAL:HG13	2.33	0.52
1:A:225:VAL:HG11	1:A:268:GLU:OE2	2.10	0.51
1:A:236:LYS:O	1:A:237:HIS:HB2	2.10	0.51
1:A:271:GLU:CD	1:A:409:VAL:HG13	2.35	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:VAL:HG11	1:B:268:GLU:OE2	2.11	0.51
1:B:277:CYS:HB2	1:B:404:TRP:CE3	2.46	0.51
1:A:188:ASP:C	1:A:190:LYS:H	2.19	0.50
1:B:172:ASP:C	1:B:173:MET:HG2	2.36	0.50
1:A:189:LYS:HG2	1:A:269:GLU:HG3	1.93	0.50
1:A:277:CYS:HB2	1:A:404:TRP:CE3	2.46	0.50
1:B:386:GLU:N	1:B:386:GLU:OE2	2.44	0.50
1:B:188:ASP:C	1:B:190:LYS:H	2.20	0.49
1:B:398:ARG:NH2	1:B:398:ARG:HB2	2.27	0.49
1:A:331:LYS:HE2	1:A:338:TYR:O	2.13	0.48
1:B:300:LYS:HE2	1:B:302:MET:HE1	1.95	0.48
1:A:236:LYS:O	1:A:237:HIS:CB	2.62	0.48
1:A:403:GLN:NE2	3:A:423:HOH:O	2.47	0.48
1:A:154:GLN:HE21	1:A:154:GLN:HB3	1.55	0.47
1:A:398:ARG:NH2	1:A:398:ARG:HB2	2.29	0.47
1:B:180:TYR:HB3	1:B:197:VAL:HA	1.96	0.47
1:A:146:GLN:NE2	1:A:164:GLN:HG2	2.29	0.47
1:B:331:LYS:HE2	1:B:338:TYR:O	2.15	0.47
1:B:389:HIS:HE1	1:B:401:ILE:O	1.98	0.47
1:A:180:TYR:HB3	1:A:197:VAL:HA	1.97	0.46
1:B:252:PHE:O	1:B:253:GLY:C	2.55	0.46
1:A:311:TYR:CE2	1:A:327:LYS:HE3	2.51	0.46
1:B:148:SER:HA	1:B:256:THR:O	2.16	0.46
1:A:367:ILE:O	1:A:367:ILE:HG12	2.16	0.46
1:B:246:PRO:HB2	1:B:249:THR:HG23	1.98	0.46
1:A:148:SER:HA	1:A:256:THR:O	2.16	0.46
1:A:252:PHE:O	1:A:253:GLY:C	2.57	0.46
1:A:190:LYS:HE2	1:A:271:GLU:OE2	2.15	0.46
1:A:386:GLU:OE2	1:A:386:GLU:N	2.49	0.45
1:B:176:THR:HB	1:B:177:SER:H	1.56	0.45
1:A:171:LEU:HD22	1:A:176:THR:O	2.16	0.45
1:B:367:ILE:HG12	1:B:367:ILE:O	2.15	0.45
1:B:172:ASP:O	1:B:173:MET:CB	2.65	0.45
1:B:356:GLN:NE2	1:B:417:LEU:HD22	2.32	0.45
1:B:311:TYR:CE2	1:B:327:LYS:HE3	2.53	0.44
1:A:173:MET:HE3	1:A:174:GLY:HA3	1.98	0.44
1:B:146:GLN:NE2	1:B:164:GLN:HG2	2.29	0.44
1:A:246:PRO:HB2	1:A:249:THR:HG23	2.00	0.44
1:B:185:LEU:CD2	1:B:222:LYS:HB3	2.46	0.44
1:A:300:LYS:HE2	1:A:302:MET:HE1	1.99	0.44
1:A:330:ILE:HD13	1:A:364:TYR:CG	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ASP:OD1	1:B:230:ASP:OD2	2.36	0.44
1:A:389:HIS:HE1	1:A:401:ILE:O	2.00	0.43
1:A:271:GLU:OE2	1:A:409:VAL:CG1	2.64	0.43
1:A:356:GLN:NE2	1:A:417:LEU:HD22	2.34	0.43
1:B:388:ARG:HD2	1:B:392:ASP:OD2	2.19	0.43
1:A:239:ILE:O	1:A:240:ILE:C	2.61	0.43
1:B:316:LEU:HD22	1:B:345:PHE:CD2	2.53	0.42
1:A:364:TYR:CE2	1:A:366:LYS:HG2	2.55	0.42
1:B:330:ILE:HD13	1:B:364:TYR:CG	2.54	0.42
1:A:370:ASN:N	1:A:370:ASN:HD22	2.17	0.42
1:B:239:ILE:CD1	1:B:268:GLU:HG2	2.47	0.42
1:B:364:TYR:CE2	1:B:366:LYS:HG2	2.54	0.42
1:A:302:MET:HG3	1:A:363:ASP:HB2	2.02	0.42
1:B:370:ASN:HD22	1:B:370:ASN:N	2.17	0.41
1:A:316:LEU:HD22	1:A:345:PHE:CD2	2.55	0.41
1:A:172:ASP:OD2	1:A:172:ASP:N	2.47	0.41
1:A:178:ASP:HA	1:A:198:HIS:O	2.20	0.41
1:A:388:ARG:HD2	1:A:392:ASP:OD2	2.19	0.41
1:B:315:HIS:CG	1:B:322:ARG:NH1	2.89	0.41
1:B:236:LYS:O	1:B:237:HIS:C	2.63	0.41
1:A:323:LEU:O	1:A:324:LYS:HG2	2.21	0.40
1:B:178:ASP:HA	1:B:198:HIS:O	2.21	0.40
1:B:364:TYR:CZ	1:B:366:LYS:HG2	2.55	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	277/284 (98%)	250 (90%)	21 (8%)	6 (2%)	5	14
1	B	277/284 (98%)	252 (91%)	23 (8%)	2 (1%)	18	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	554/568 (98%)	502 (91%)	44 (8%)	8 (1%)	9	23

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	LYS
1	A	237	HIS
1	B	172	ASP
1	A	254	HIS
1	B	254	HIS
1	A	189	LYS
1	A	252	PHE
1	A	174	GLY

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	249/253 (98%)	238 (96%)	11 (4%)	25	53
1	B	249/253 (98%)	240 (96%)	9 (4%)	31	60
All	All	498/506 (98%)	478 (96%)	20 (4%)	28	56

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	173	MET
1	A	176	THR
1	A	189	LYS
1	A	190	LYS
1	A	219	LEU
1	A	254	HIS
1	A	268	GLU
1	A	270	GLN
1	A	272	LYS
1	A	290	THR

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Mol	Chain	Res	Type
1	A	367	ILE
1	B	185	LEU
1	B	191	LYS
1	B	219	LEU
1	B	254	HIS
1	B	268	GLU
1	B	270	GLN
1	B	272	LYS
1	B	290	THR
1	B	367	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	GLN
1	A	154	GLN
1	A	156	ASN
1	A	157	GLN
1	A	164	GLN
1	A	270	GLN
1	A	318	GLN
1	A	319	ASN
1	A	340	ASN
1	A	356	GLN
1	A	370	ASN
1	A	381	ASN
1	A	389	HIS
1	A	396	ASN
1	A	403	GLN
1	A	405	HIS
1	B	146	GLN
1	B	154	GLN
1	B	157	GLN
1	B	164	GLN
1	B	207	ASN
1	B	270	GLN
1	B	318	GLN
1	B	319	ASN
1	B	340	ASN
1	B	356	GLN
1	B	370	ASN
1	B	381	ASN

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Mol	Chain	Res	Type
1	B	389	HIS
1	B	403	GLN
1	B	405	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	279/284 (98%)	0.54	36 (12%) 7 6	22, 44, 77, 97	0
1	B	279/284 (98%)	0.60	36 (12%) 7 6	21, 43, 81, 97	0
All	All	558/568 (98%)	0.57	72 (12%) 7 6	21, 44, 81, 97	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	171	LEU	7.6
1	A	271	GLU	6.4
1	B	172	ASP	6.0
1	B	237	HIS	5.6
1	B	271	GLU	5.4
1	B	217	SER	4.8
1	B	173	MET	4.6
1	B	175	GLY	4.6
1	A	265	ALA	4.5
1	B	369	LYS	4.5
1	A	173	MET	4.4
1	B	304	VAL	4.4
1	A	267	LYS	4.3
1	A	171	LEU	4.2
1	B	268	GLU	4.0
1	B	174	GLY	4.0
1	A	367	ILE	3.7
1	A	175	GLY	3.7
1	A	172	ASP	3.7
1	B	218	GLU	3.6
1	A	268	GLU	3.6
1	A	266	GLU	3.3
1	B	367	ILE	3.3
1	B	366	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	235	SER	3.2
1	B	338	TYR	3.2
1	A	412	GLU	3.1
1	B	270	GLN	3.0
1	B	322	ARG	2.9
1	B	219	LEU	2.8
1	B	269	GLU	2.8
1	B	266	GLU	2.8
1	A	237	HIS	2.8
1	A	304	VAL	2.8
1	A	373	ILE	2.7
1	A	188	ASP	2.7
1	B	170	ALA	2.7
1	B	216	TYR	2.7
1	A	264	SER	2.7
1	B	253	GLY	2.7
1	B	412	GLU	2.7
1	A	269	GLU	2.7
1	A	368	GLY	2.6
1	B	267	LYS	2.6
1	B	140	GLU	2.6
1	A	305	GLY	2.6
1	B	373	ILE	2.5
1	A	270	GLN	2.5
1	B	411	GLU	2.5
1	A	176	THR	2.4
1	A	174	GLY	2.4
1	A	364	TYR	2.3
1	A	418	ALA	2.3
1	A	140	GLU	2.3
1	A	241	GLY	2.3
1	B	368	GLY	2.3
1	A	254	HIS	2.2
1	A	154	GLN	2.2
1	B	154	GLN	2.2
1	B	272	LYS	2.2
1	A	272	LYS	2.2
1	A	366	LYS	2.2
1	B	418	ALA	2.2
1	A	238	ASP	2.2
1	A	322	ARG	2.1
1	B	307	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	336	ASN	2.1
1	A	191	LYS	2.1
1	A	213	LYS	2.1
1	A	320	GLY	2.1
1	B	415	ALA	2.0
1	B	176	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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	CL	A	108	1/1	0.95	0.10	55,55,55,55	0
2	CL	A	104	1/1	0.97	0.06	36,36,36,36	0
2	CL	A	101	1/1	0.97	0.07	37,37,37,37	0
2	CL	B	107	1/1	0.97	0.06	45,45,45,45	0
2	CL	A	105	1/1	0.98	0.07	39,39,39,39	0
2	CL	A	102	1/1	0.99	0.07	38,38,38,38	0
2	CL	B	106	1/1	0.99	0.04	34,34,34,34	0
2	CL	A	103	1/1	0.99	0.09	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.