



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:52 PM EDT

PDB ID : 3HN8 / pdb_00003hn8
Title : Crystal structure of synaptotagmin
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Deposited on : 2009-05-30
Resolution : 3.50 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

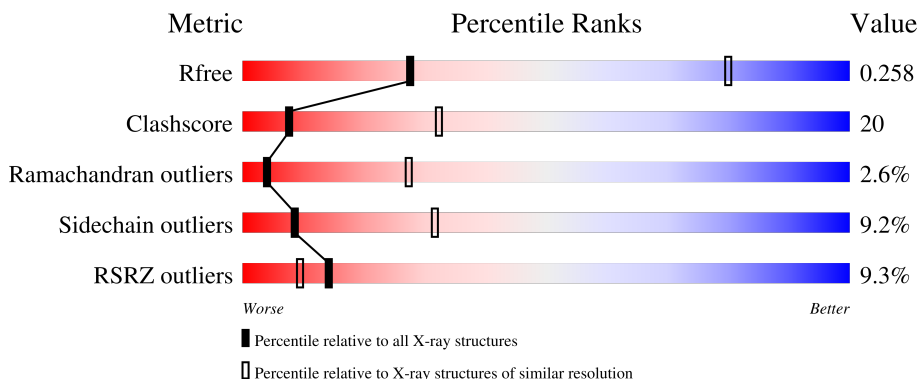
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	296	
1	B	296	
1	C	296	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6672 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-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2217	1417	385	409	6			
1	B	279	Total	C	N	O	S	0	0	0
			2217	1417	385	409	6			
1	C	279	Total	C	N	O	S	0	0	0
			2217	1417	385	409	6			

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

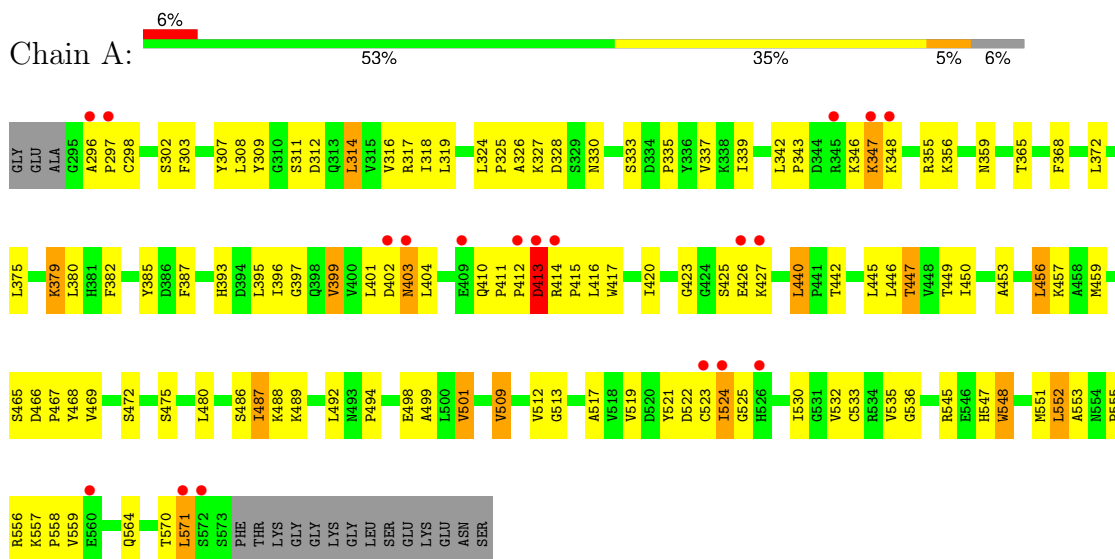
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

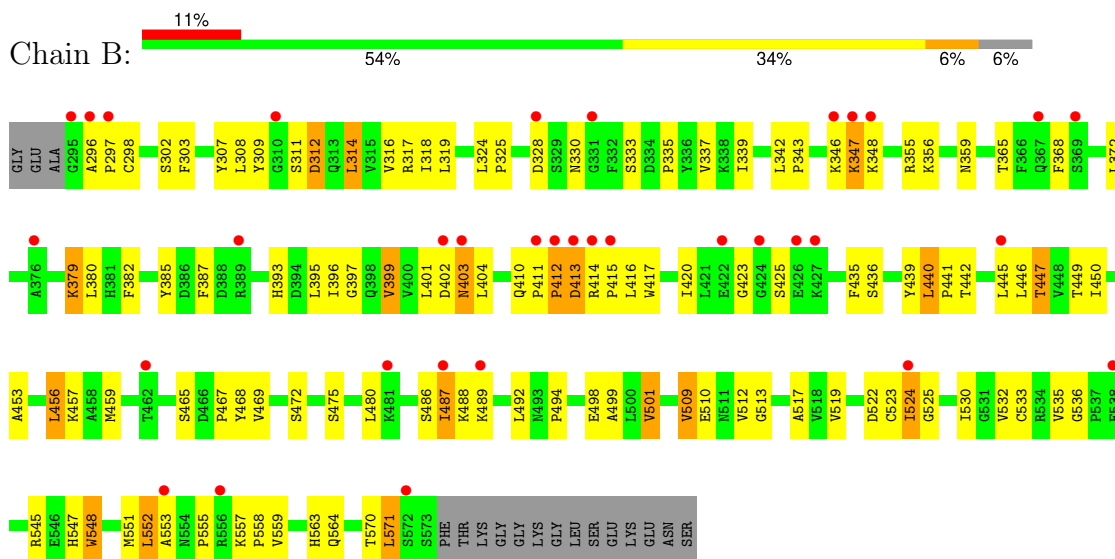
3 Residue-property plots [i](#)

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.

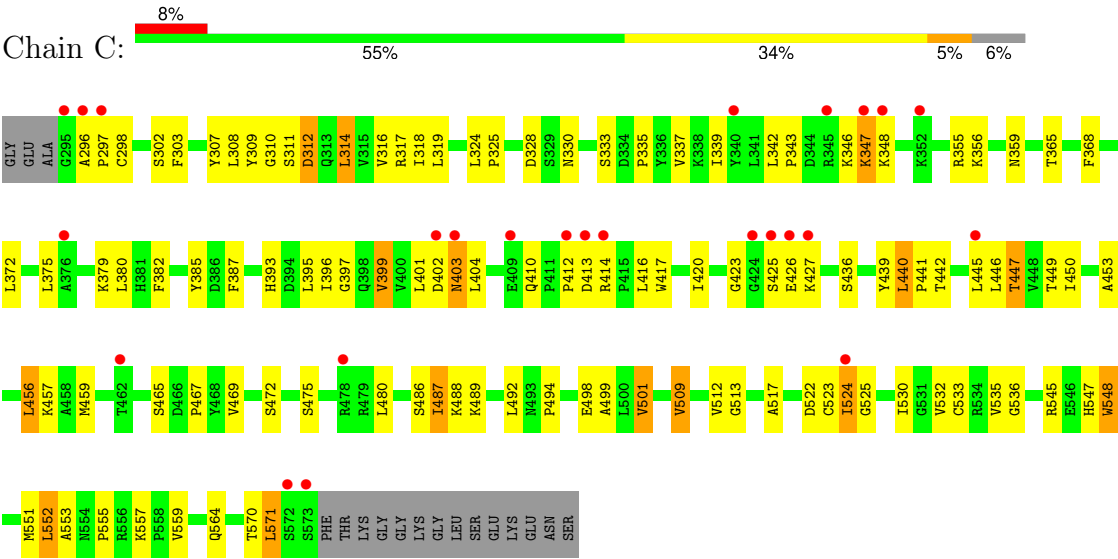
• Molecule 1: Synaptotagmin-3



• Molecule 1: Synaptotagmin-3



• Molecule 1: Synaptotagmin-3



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	205.68Å 205.68Å 143.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.82 – 3.50 29.82 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.82-3.50) 99.6 (29.82-3.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 3.47Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.238 , 0.259 0.233 , 0.258	Depositor DCC
R_{free} test set	3930 reflections (10.06%)	wwPDB-VP
Wilson B-factor (Å ²)	79.4	Xtriage
Anisotropy	0.706	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	6672	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.21% 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: CA, ZN

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	0.32	0/2268	0.81	2/3076 (0.1%)
1	B	0.31	0/2268	0.81	0/3076
1	C	0.33	0/2268	0.83	0/3076
All	All	0.32	0/6804	0.82	2/9228 (0.0%)

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
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	466	ASP	CA-C-N	5.19	124.95	119.76
1	A	466	ASP	C-N-CA	5.19	124.95	119.76

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	413	ASP	Peptide

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	2217	0	2228	97	0
1	B	2217	0	2228	89	0
1	C	2217	0	2228	92	0
2	A	6	0	0	0	0
2	B	6	0	0	0	0
2	C	6	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
All	All	6672	0	6684	268	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 20.

All (268) 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:556:ARG:HG3	1:C:310:GLY:HA2	1.38	1.01
1:A:556:ARG:HB2	1:C:310:GLY:H	1.46	0.80
1:A:556:ARG:CG	1:C:310:GLY:HA2	2.10	0.80
1:B:303:PHE:HA	1:B:319:LEU:HG	1.65	0.79
1:A:303:PHE:HA	1:A:319:LEU:HG	1.65	0.78
1:C:303:PHE:HA	1:C:319:LEU:HG	1.66	0.77
1:B:412:PRO:O	1:B:413:ASP:HB2	1.85	0.77
1:B:413:ASP:O	1:B:415:PRO:HD3	1.85	0.76
1:A:557:LYS:HB2	1:C:309:TYR:CG	2.23	0.74
1:C:296:ALA:HB3	1:C:297:PRO:HD3	1.70	0.73
1:A:296:ALA:HB3	1:A:297:PRO:HD3	1.70	0.72
1:B:296:ALA:HB3	1:B:297:PRO:HD3	1.71	0.72
1:A:465:SER:O	1:A:467:PRO:HD3	1.90	0.72
1:B:465:SER:O	1:B:467:PRO:HD3	1.90	0.72
1:C:465:SER:O	1:C:467:PRO:HD3	1.90	0.71
1:A:395:LEU:CD2	1:A:425:SER:HB3	2.21	0.71
1:B:450:ILE:HG21	1:B:469:VAL:HG21	1.75	0.68
1:B:395:LEU:CD2	1:B:425:SER:HB3	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:ILE:HG21	1:C:469:VAL:HG21	1.76	0.67
1:C:395:LEU:CD2	1:C:425:SER:HB3	2.24	0.67
1:C:440:LEU:HD23	1:C:445:LEU:HB2	1.77	0.67
1:B:459:MET:HG3	1:B:530:ILE:HG12	1.77	0.67
1:A:453:ALA:HB3	1:A:494:PRO:HD2	1.77	0.66
1:C:453:ALA:HB3	1:C:494:PRO:HD2	1.77	0.66
1:A:395:LEU:HD22	1:A:425:SER:HB3	1.76	0.66
1:A:440:LEU:HD23	1:A:445:LEU:HB2	1.79	0.65
1:A:450:ILE:HG21	1:A:469:VAL:HG21	1.76	0.65
1:A:459:MET:HG3	1:A:530:ILE:HG12	1.77	0.65
1:C:570:THR:O	1:C:571:LEU:HD13	1.97	0.65
1:B:570:THR:O	1:B:571:LEU:HD13	1.96	0.65
1:B:395:LEU:HD22	1:B:425:SER:HB3	1.78	0.64
1:B:453:ALA:HB3	1:B:494:PRO:HD2	1.78	0.64
1:A:570:THR:O	1:A:571:LEU:HD13	1.96	0.64
1:A:302:SER:HB3	1:A:417:TRP:CD2	2.33	0.64
1:C:459:MET:HG3	1:C:530:ILE:HG12	1.78	0.64
1:B:440:LEU:HD23	1:B:445:LEU:HB2	1.78	0.63
1:B:302:SER:HB3	1:B:417:TRP:CD2	2.33	0.63
1:C:302:SER:HB3	1:C:417:TRP:CD2	2.33	0.63
1:A:557:LYS:HB2	1:C:309:TYR:CD1	2.34	0.63
1:A:302:SER:HB3	1:A:417:TRP:CE3	2.34	0.62
1:C:486:SER:HB3	1:C:498:GLU:OE2	1.98	0.62
1:A:486:SER:HB3	1:A:498:GLU:OE2	2.00	0.62
1:B:486:SER:HB3	1:B:498:GLU:OE2	2.00	0.62
1:C:302:SER:HB3	1:C:417:TRP:CE3	2.35	0.62
1:C:395:LEU:HD22	1:C:425:SER:HB3	1.81	0.61
1:C:413:ASP:C	1:C:414:ARG:HG3	2.25	0.61
1:B:302:SER:HB3	1:B:417:TRP:CE3	2.36	0.61
1:C:512:VAL:HG22	1:C:513:GLY:H	1.65	0.61
1:A:475:SER:HB2	1:A:512:VAL:HG23	1.83	0.61
1:B:512:VAL:HG22	1:B:513:GLY:H	1.66	0.61
1:A:447:THR:HG23	1:A:501:VAL:HG22	1.82	0.60
1:B:447:THR:HG23	1:B:501:VAL:HG22	1.84	0.60
1:C:447:THR:HG23	1:C:501:VAL:HG22	1.84	0.59
1:B:402:ASP:O	1:B:403:ASN:C	2.46	0.59
1:A:316:VAL:HG21	1:A:380:LEU:HD11	1.83	0.59
1:A:512:VAL:HG22	1:A:513:GLY:H	1.68	0.59
1:B:475:SER:HB2	1:B:512:VAL:HG23	1.83	0.59
1:C:402:ASP:O	1:C:403:ASN:C	2.46	0.59
1:A:552:LEU:O	1:A:553:ALA:HB3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ASP:O	1:A:403:ASN:C	2.46	0.58
1:A:475:SER:HB3	1:A:480:LEU:HD11	1.85	0.58
1:A:524:ILE:H	1:A:524:ILE:HD12	1.69	0.58
1:B:524:ILE:HD12	1:B:524:ILE:H	1.69	0.58
1:B:412:PRO:O	1:B:413:ASP:CB	2.51	0.58
1:B:523:CYS:O	1:B:525:GLY:N	2.37	0.58
1:C:475:SER:HB3	1:C:480:LEU:HD11	1.86	0.58
1:B:316:VAL:HG21	1:B:380:LEU:HD11	1.86	0.57
1:C:475:SER:HB2	1:C:512:VAL:HG23	1.86	0.57
1:C:524:ILE:HD12	1:C:524:ILE:H	1.69	0.57
1:A:523:CYS:O	1:A:525:GLY:N	2.37	0.57
1:B:475:SER:HB3	1:B:480:LEU:HD11	1.86	0.57
1:A:413:ASP:O	1:A:415:PRO:HD3	2.04	0.57
1:C:523:CYS:O	1:C:525:GLY:N	2.37	0.57
1:A:522:ASP:O	1:A:523:CYS:HB3	2.04	0.56
1:B:387:PHE:HA	1:B:393:HIS:CD2	2.41	0.56
1:B:552:LEU:O	1:B:553:ALA:HB3	2.04	0.56
1:A:387:PHE:HA	1:A:393:HIS:CD2	2.40	0.56
1:A:325:PRO:HD2	1:A:396:ILE:HG23	1.88	0.56
1:C:387:PHE:HA	1:C:393:HIS:CD2	2.41	0.56
1:A:318:ILE:HD11	1:A:339:ILE:HD11	1.88	0.55
1:C:318:ILE:HD11	1:C:339:ILE:HD11	1.88	0.55
1:C:325:PRO:HD2	1:C:396:ILE:HG23	1.87	0.55
1:C:316:VAL:HG21	1:C:380:LEU:HD11	1.87	0.55
1:A:347:LYS:HE3	1:A:368:PHE:HD2	1.72	0.54
1:C:339:ILE:O	1:C:348:LYS:HA	2.07	0.54
1:B:347:LYS:HE3	1:B:368:PHE:HD2	1.73	0.54
1:B:325:PRO:HD2	1:B:396:ILE:HG23	1.87	0.54
1:A:423:GLY:HA3	1:A:564:GLN:HG2	1.90	0.54
1:B:423:GLY:HA3	1:B:564:GLN:HG2	1.90	0.54
1:C:347:LYS:HE3	1:C:368:PHE:HD2	1.72	0.54
1:C:382:PHE:HB2	1:C:399:VAL:HG22	1.89	0.54
1:C:552:LEU:O	1:C:553:ALA:HB3	2.08	0.53
1:A:339:ILE:O	1:A:348:LYS:HA	2.08	0.53
1:B:318:ILE:HD11	1:B:339:ILE:HD11	1.90	0.53
1:A:382:PHE:HB2	1:A:399:VAL:HG22	1.90	0.53
1:A:509:VAL:O	1:A:548:TRP:CH2	2.62	0.53
1:C:423:GLY:HA3	1:C:564:GLN:HG2	1.90	0.53
1:C:509:VAL:O	1:C:548:TRP:CH2	2.61	0.53
1:B:382:PHE:HB2	1:B:399:VAL:HG22	1.90	0.53
1:B:339:ILE:O	1:B:348:LYS:HA	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:509:VAL:O	1:B:548:TRP:CH2	2.62	0.52
1:A:347:LYS:HE3	1:A:368:PHE:CD2	2.45	0.52
1:C:347:LYS:HE3	1:C:368:PHE:CD2	2.45	0.52
1:A:330:ASN:HB3	1:B:510:GLU:HB3	1.92	0.51
1:A:465:SER:C	1:A:467:PRO:HD3	2.36	0.51
1:A:307:TYR:CE1	1:A:372:LEU:HD13	2.46	0.51
1:C:317:ARG:HG3	1:C:365:THR:HG23	1.93	0.51
1:C:465:SER:C	1:C:467:PRO:HD3	2.36	0.51
1:C:522:ASP:O	1:C:523:CYS:HB3	2.10	0.51
1:B:317:ARG:HG3	1:B:365:THR:HG23	1.93	0.51
1:C:536:GLY:O	1:C:545:ARG:HB3	2.11	0.50
1:B:347:LYS:HE3	1:B:368:PHE:CD2	2.45	0.50
1:A:317:ARG:HG3	1:A:365:THR:HG23	1.94	0.50
1:B:307:TYR:CE1	1:B:372:LEU:HD13	2.46	0.50
1:B:536:GLY:O	1:B:545:ARG:HB3	2.12	0.50
1:A:536:GLY:O	1:A:545:ARG:HB3	2.11	0.50
1:B:532:VAL:HG12	1:B:533:CYS:N	2.27	0.50
1:B:465:SER:C	1:B:467:PRO:HD3	2.37	0.49
1:B:536:GLY:HA2	1:B:548:TRP:CG	2.46	0.49
1:A:536:GLY:HA2	1:A:548:TRP:CG	2.47	0.49
1:C:307:TYR:CE1	1:C:372:LEU:HD13	2.47	0.49
1:B:524:ILE:HD12	1:B:524:ILE:N	2.28	0.48
1:C:413:ASP:C	1:C:414:ARG:CG	2.85	0.48
1:B:522:ASP:O	1:B:523:CYS:HB3	2.11	0.48
1:B:449:THR:HA	1:B:499:ALA:HA	1.95	0.48
1:B:467:PRO:HD2	1:B:488:LYS:O	2.13	0.48
1:C:449:THR:HA	1:C:499:ALA:HA	1.96	0.48
1:A:314:LEU:HD11	1:A:404:LEU:HD13	1.96	0.48
1:A:467:PRO:HD2	1:A:488:LYS:O	2.14	0.48
1:C:380:LEU:HB2	1:C:401:LEU:HB2	1.95	0.48
1:C:524:ILE:HD12	1:C:524:ILE:N	2.28	0.47
1:C:467:PRO:HD2	1:C:488:LYS:O	2.14	0.47
1:C:536:GLY:HA2	1:C:548:TRP:CG	2.48	0.47
1:A:380:LEU:HB2	1:A:401:LEU:HB2	1.96	0.47
1:A:449:THR:HA	1:A:499:ALA:HA	1.94	0.47
1:A:532:VAL:HG12	1:A:533:CYS:N	2.30	0.47
1:B:380:LEU:HB2	1:B:401:LEU:HB2	1.96	0.47
1:B:314:LEU:HD11	1:B:404:LEU:HD13	1.97	0.47
1:C:314:LEU:HD11	1:C:404:LEU:HD13	1.97	0.47
1:A:296:ALA:C	1:A:298:CYS:H	2.23	0.47
1:C:532:VAL:HG12	1:C:533:CYS:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:PRO:HA	1:A:385:TYR:O	2.16	0.46
1:A:524:ILE:HD12	1:A:524:ILE:N	2.30	0.46
1:B:296:ALA:C	1:B:298:CYS:H	2.24	0.46
1:B:413:ASP:C	1:B:415:PRO:HD3	2.39	0.46
1:A:551:MET:HE3	1:A:552:LEU:HD13	1.98	0.46
1:C:397:GLY:HA3	1:C:420:ILE:HG22	1.98	0.46
1:C:296:ALA:C	1:C:298:CYS:H	2.23	0.45
1:C:335:PRO:HA	1:C:385:TYR:O	2.16	0.45
1:B:335:PRO:HA	1:B:385:TYR:O	2.17	0.45
1:C:551:MET:HE3	1:C:552:LEU:HD13	1.99	0.45
1:A:399:VAL:HG12	1:A:420:ILE:HA	1.98	0.45
1:C:456:LEU:O	1:C:492:LEU:HD22	2.17	0.45
1:A:413:ASP:C	1:A:415:PRO:HD3	2.42	0.45
1:B:411:PRO:HG2	1:B:414:ARG:HB2	1.99	0.45
1:A:387:PHE:CD1	1:A:393:HIS:NE2	2.83	0.45
1:A:456:LEU:O	1:A:492:LEU:HD22	2.17	0.44
1:A:489:LYS:HB3	1:A:489:LYS:HE2	1.71	0.44
1:A:318:ILE:CD1	1:A:339:ILE:HD11	2.47	0.44
1:C:489:LYS:HB3	1:C:489:LYS:HE2	1.71	0.44
1:B:489:LYS:HE2	1:B:489:LYS:HB3	1.70	0.44
1:B:551:MET:HE3	1:B:552:LEU:HD13	1.98	0.44
1:C:399:VAL:HG12	1:C:420:ILE:HA	1.99	0.44
1:B:302:SER:HB3	1:B:417:TRP:CE2	2.53	0.44
1:B:324:LEU:HD22	1:B:396:ILE:HG21	1.99	0.44
1:C:303:PHE:CE2	1:C:382:PHE:HE1	2.36	0.44
1:C:318:ILE:CD1	1:C:339:ILE:HD11	2.47	0.44
1:A:548:TRP:O	1:A:552:LEU:HD22	2.17	0.44
1:B:399:VAL:HG12	1:B:420:ILE:HA	2.00	0.44
1:B:303:PHE:HB2	1:B:317:ARG:O	2.18	0.44
1:C:401:LEU:HD23	1:C:401:LEU:HA	1.81	0.44
1:A:328:ASP:HB2	1:A:330:ASN:OD1	2.18	0.44
1:A:467:PRO:HG2	1:A:494:PRO:HG3	1.99	0.44
1:B:457:LYS:HD3	1:B:459:MET:SD	2.58	0.44
1:B:571:LEU:HD22	1:B:571:LEU:N	2.33	0.44
1:B:487:ILE:O	1:B:488:LYS:C	2.61	0.43
1:A:411:PRO:HB2	1:C:414:ARG:HH12	1.84	0.43
1:C:302:SER:HB3	1:C:417:TRP:CE2	2.53	0.43
1:A:551:MET:HE2	1:A:551:MET:HB3	1.96	0.43
1:B:303:PHE:CE2	1:B:382:PHE:HE1	2.36	0.43
1:C:309:TYR:C	1:C:311:SER:H	2.27	0.43
1:A:302:SER:HB3	1:A:417:TRP:CZ3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:LEU:HB3	1:A:343:PRO:HA	2.00	0.43
1:A:571:LEU:N	1:A:571:LEU:HD22	2.33	0.43
1:A:303:PHE:CE2	1:A:382:PHE:HE1	2.36	0.43
1:C:439:TYR:O	1:C:441:PRO:HD3	2.19	0.43
1:C:547:HIS:HE2	1:C:559:VAL:HG23	1.84	0.43
1:A:309:TYR:C	1:A:311:SER:H	2.27	0.43
1:B:397:GLY:HA3	1:B:420:ILE:HG22	1.99	0.43
1:A:302:SER:HB3	1:A:417:TRP:CE2	2.53	0.43
1:A:375:LEU:HD23	1:A:375:LEU:HA	1.81	0.43
1:A:457:LYS:HD3	1:A:459:MET:SD	2.59	0.43
1:B:346:LYS:O	1:B:348:LYS:N	2.52	0.43
1:A:346:LYS:O	1:A:348:LYS:N	2.52	0.42
1:A:547:HIS:HE2	1:A:559:VAL:HG23	1.84	0.42
1:B:309:TYR:C	1:B:311:SER:H	2.27	0.42
1:C:324:LEU:HD22	1:C:396:ILE:HG21	2.00	0.42
1:C:457:LYS:HD3	1:C:459:MET:SD	2.58	0.42
1:A:379:LYS:HB2	1:A:379:LYS:HE3	1.76	0.42
1:A:468:TYR:CE2	1:A:519:VAL:HB	2.54	0.42
1:B:548:TRP:O	1:B:552:LEU:HD22	2.19	0.42
1:A:324:LEU:HD22	1:A:396:ILE:HG21	2.01	0.42
1:A:557:LYS:HA	1:A:558:PRO:HD2	1.94	0.42
1:C:328:ASP:HB2	1:C:330:ASN:OD1	2.19	0.42
1:C:342:LEU:HB3	1:C:343:PRO:HA	2.00	0.42
1:A:303:PHE:HB2	1:A:317:ARG:O	2.19	0.42
1:A:487:ILE:O	1:A:488:LYS:C	2.62	0.42
1:A:426:GLU:O	1:A:427:LYS:C	2.63	0.42
1:B:318:ILE:CD1	1:B:339:ILE:HD11	2.49	0.42
1:C:346:LYS:O	1:C:348:LYS:N	2.52	0.42
1:C:387:PHE:CD1	1:C:393:HIS:NE2	2.83	0.42
1:C:487:ILE:O	1:C:488:LYS:C	2.61	0.42
1:C:509:VAL:O	1:C:548:TRP:CZ3	2.73	0.42
1:A:411:PRO:HG2	1:A:414:ARG:HB2	2.01	0.42
1:A:517:ALA:HB2	1:A:532:VAL:HG13	2.02	0.42
1:A:556:ARG:NH1	1:C:312:ASP:CG	2.77	0.42
1:A:570:THR:C	1:A:571:LEU:HD13	2.44	0.42
1:C:303:PHE:HB2	1:C:317:ARG:O	2.20	0.42
1:B:536:GLY:HA2	1:B:548:TRP:CB	2.50	0.42
1:B:570:THR:C	1:B:571:LEU:HD13	2.44	0.42
1:C:375:LEU:HD23	1:C:375:LEU:HA	1.80	0.42
1:C:548:TRP:O	1:C:552:LEU:HD22	2.20	0.42
1:A:411:PRO:HB2	1:C:414:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ARG:HG2	1:B:365:THR:OG1	2.20	0.42
1:B:328:ASP:HB2	1:B:330:ASN:OD1	2.20	0.42
1:B:439:TYR:O	1:B:441:PRO:HD3	2.20	0.42
1:B:467:PRO:HG2	1:B:494:PRO:HG3	2.02	0.42
1:B:492:LEU:C	1:B:494:PRO:HD3	2.44	0.42
1:B:436:SER:OG	1:B:449:THR:HB	2.20	0.41
1:B:342:LEU:HB3	1:B:343:PRO:HA	2.01	0.41
1:B:456:LEU:O	1:B:492:LEU:HD22	2.20	0.41
1:C:302:SER:HB3	1:C:417:TRP:CZ3	2.55	0.41
1:A:492:LEU:C	1:A:494:PRO:HD3	2.45	0.41
1:B:547:HIS:HE2	1:B:559:VAL:HG23	1.85	0.41
1:B:557:LYS:HA	1:B:558:PRO:HD2	1.94	0.41
1:B:302:SER:HB3	1:B:417:TRP:CZ3	2.56	0.41
1:B:551:MET:HE2	1:B:551:MET:HB3	1.95	0.41
1:C:426:GLU:O	1:C:427:LYS:C	2.64	0.41
1:C:517:ALA:HB2	1:C:532:VAL:HG13	2.03	0.41
1:A:521:TYR:CD2	1:A:522:ASP:N	2.88	0.41
1:B:311:SER:O	1:B:312:ASP:C	2.64	0.41
1:B:435:PHE:CZ	1:B:563:HIS:CD2	3.09	0.41
1:C:436:SER:OG	1:C:449:THR:HB	2.21	0.41
1:A:380:LEU:HD23	1:A:380:LEU:HA	1.94	0.41
1:C:324:LEU:HA	1:C:325:PRO:HD3	1.91	0.41
1:C:456:LEU:HB2	1:C:492:LEU:O	2.21	0.41
1:C:571:LEU:N	1:C:571:LEU:HD22	2.36	0.41
1:A:559:VAL:HG23	1:A:559:VAL:O	2.21	0.41
1:B:333:SER:C	1:B:335:PRO:HD3	2.47	0.40
1:C:547:HIS:NE2	1:C:559:VAL:HG23	2.36	0.40
1:A:333:SER:C	1:A:335:PRO:HD3	2.46	0.40
1:A:509:VAL:O	1:A:548:TRP:CZ3	2.74	0.40
1:A:536:GLY:HA2	1:A:548:TRP:CB	2.52	0.40
1:C:570:THR:C	1:C:571:LEU:HD13	2.46	0.40
1:A:397:GLY:HA3	1:A:420:ILE:HG22	2.03	0.40
1:A:456:LEU:HB2	1:A:492:LEU:O	2.21	0.40
1:B:379:LYS:HE3	1:B:379:LYS:HB2	1.77	0.40
1:B:559:VAL:HG23	1:B:559:VAL:O	2.21	0.40
1:C:317:ARG:HG2	1:C:365:THR:OG1	2.21	0.40
1:B:325:PRO:HD2	1:B:396:ILE:CG2	2.51	0.40
1:B:456:LEU:HB2	1:B:492:LEU:O	2.22	0.40
1:B:468:TYR:CE2	1:B:519:VAL:HB	2.56	0.40
1:B:517:ALA:HB2	1:B:532:VAL:HG13	2.02	0.40
1:C:333:SER:C	1:C:335:PRO:HD3	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:492:LEU:C	1:C:494:PRO:HD3	2.45	0.40
1:A:309:TYR:CG	1:C:557:LYS:HB2	2.56	0.40
1:A:326:ALA:O	1:A:327:LYS:HD3	2.21	0.40
1:C:551:MET:HE2	1:C:551:MET:HB3	1.93	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	277/296 (94%)	234 (84%)	36 (13%)	7 (2%)	4	28
1	B	277/296 (94%)	231 (83%)	38 (14%)	8 (3%)	3	26
1	C	277/296 (94%)	234 (84%)	36 (13%)	7 (2%)	4	28
All	All	831/888 (94%)	699 (84%)	110 (13%)	22 (3%)	4	27

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	347	LYS
1	A	524	ILE
1	B	347	LYS
1	B	524	ILE
1	C	347	LYS
1	C	524	ILE
1	A	412	PRO
1	B	412	PRO
1	B	413	ASP
1	C	412	PRO
1	A	555	PRO
1	B	555	PRO
1	C	555	PRO

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Mol	Chain	Res	Type
1	A	403	ASN
1	B	403	ASN
1	C	403	ASN
1	C	312	ASP
1	C	356	LYS
1	A	312	ASP
1	A	356	LYS
1	B	312	ASP
1	B	356	LYS

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	244/256 (95%)	221 (91%)	23 (9%)	8	31
1	B	244/256 (95%)	222 (91%)	22 (9%)	9	32
1	C	244/256 (95%)	222 (91%)	22 (9%)	9	32
All	All	732/768 (95%)	665 (91%)	67 (9%)	8	32

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	308	LEU
1	A	314	LEU
1	A	337	VAL
1	A	355	ARG
1	A	359	ASN
1	A	379	LYS
1	A	399	VAL
1	A	410	GLN
1	A	413	ASP
1	A	416	LEU
1	A	440	LEU
1	A	442	THR
1	A	446	LEU

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Mol	Chain	Res	Type
1	A	447	THR
1	A	456	LEU
1	A	472	SER
1	A	487	ILE
1	A	501	VAL
1	A	509	VAL
1	A	535	VAL
1	A	548	TRP
1	A	552	LEU
1	A	571	LEU
1	B	308	LEU
1	B	314	LEU
1	B	337	VAL
1	B	355	ARG
1	B	359	ASN
1	B	379	LYS
1	B	399	VAL
1	B	410	GLN
1	B	416	LEU
1	B	440	LEU
1	B	442	THR
1	B	446	LEU
1	B	447	THR
1	B	456	LEU
1	B	472	SER
1	B	487	ILE
1	B	501	VAL
1	B	509	VAL
1	B	535	VAL
1	B	548	TRP
1	B	552	LEU
1	B	571	LEU
1	C	308	LEU
1	C	314	LEU
1	C	337	VAL
1	C	355	ARG
1	C	359	ASN
1	C	379	LYS
1	C	399	VAL
1	C	410	GLN
1	C	416	LEU
1	C	440	LEU

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Mol	Chain	Res	Type
1	C	442	THR
1	C	446	LEU
1	C	447	THR
1	C	456	LEU
1	C	472	SER
1	C	487	ILE
1	C	501	VAL
1	C	509	VAL
1	C	535	VAL
1	C	548	TRP
1	C	552	LEU
1	C	571	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 21 ligands modelled in this entry, 21 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	279/296 (94%)	0.39	19 (6%) 23 14	54, 79, 141, 221	0
1	B	279/296 (94%)	0.69	34 (12%) 8 6	54, 89, 160, 218	0
1	C	279/296 (94%)	0.43	25 (8%) 15 10	53, 78, 147, 230	0
All	All	837/888 (94%)	0.50	78 (9%) 14 9	53, 82, 148, 230	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	297	PRO	8.3
1	B	402	ASP	6.1
1	C	524	ILE	5.6
1	C	413	ASP	5.3
1	A	524	ILE	5.0
1	B	524	ILE	4.4
1	A	297	PRO	4.4
1	A	402	ASP	4.1
1	B	347	LYS	4.1
1	B	296	ALA	4.1
1	B	348	LYS	4.0
1	C	572	SER	4.0
1	B	403	ASN	3.9
1	B	411	PRO	3.9
1	B	412	PRO	3.9
1	A	413	ASP	3.9
1	A	409	GLU	3.8
1	C	412	PRO	3.8
1	B	462	THR	3.6
1	B	427	LYS	3.5
1	B	295	GLY	3.4
1	B	556	ARG	3.4
1	A	347	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	348	LYS	3.3
1	C	424	GLY	3.3
1	B	481	LYS	3.3
1	A	348	LYS	3.3
1	C	462	THR	3.3
1	A	427	LYS	3.3
1	A	296	ALA	3.2
1	A	526	HIS	3.2
1	C	296	ALA	3.1
1	A	414	ARG	3.0
1	B	413	ASP	3.0
1	B	489	LYS	2.9
1	C	347	LYS	2.9
1	C	426	GLU	2.9
1	B	424	GLY	2.9
1	C	295	GLY	2.9
1	A	572	SER	2.8
1	C	345	ARG	2.8
1	B	331	GLY	2.8
1	B	367	GLN	2.8
1	C	376	ALA	2.8
1	C	402	ASP	2.8
1	B	376	ALA	2.7
1	B	297	PRO	2.7
1	B	414	ARG	2.7
1	B	369	SER	2.7
1	C	409	GLU	2.7
1	A	426	GLU	2.6
1	B	445	LEU	2.6
1	C	414	ARG	2.6
1	B	426	GLU	2.6
1	B	572	SER	2.6
1	C	427	LYS	2.5
1	C	425	SER	2.5
1	C	445	LEU	2.5
1	C	340	TYR	2.5
1	A	523	CYS	2.4
1	B	310	GLY	2.4
1	B	538	GLU	2.4
1	A	412	PRO	2.3
1	C	478	ARG	2.3
1	A	571	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	403	ASN	2.2
1	B	553	ALA	2.1
1	C	573	SER	2.1
1	B	328	ASP	2.1
1	B	415	PRO	2.1
1	A	560	GLU	2.1
1	A	403	ASN	2.1
1	B	389	ARG	2.1
1	C	352	LYS	2.0
1	A	345	ARG	2.0
1	B	346	LYS	2.0
1	B	487	ILE	2.0
1	B	422	GLU	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($\text{\AA}^2$)	Q<0.9
2	CA	B	603	1/1	0.88	0.08	76,76,76,76	0
2	CA	C	603	1/1	0.91	0.17	98,98,98,98	0
2	CA	C	602	1/1	0.92	0.10	64,64,64,64	0
2	CA	C	601	1/1	0.94	0.08	50,50,50,50	0
2	CA	A	603	1/1	0.94	0.10	79,79,79,79	0
2	CA	B	605	1/1	0.94	0.05	51,51,51,51	0
2	CA	B	606	1/1	0.95	0.05	57,57,57,57	0
2	CA	B	601	1/1	0.95	0.04	50,50,50,50	0
2	CA	C	605	1/1	0.96	0.12	65,65,65,65	0
2	CA	C	606	1/1	0.97	0.04	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CA	A	600	1/1	0.98	0.04	58,58,58,58	0
2	CA	B	600	1/1	0.98	0.05	53,53,53,53	0
2	CA	A	602	1/1	0.98	0.06	51,51,51,51	0
2	CA	B	602	1/1	0.98	0.07	52,52,52,52	0
2	CA	A	605	1/1	0.99	0.10	55,55,55,55	0
2	CA	A	606	1/1	0.99	0.07	57,57,57,57	0
2	CA	C	600	1/1	0.99	0.02	51,51,51,51	0
2	CA	A	601	1/1	0.99	0.04	50,50,50,50	0
3	ZN	B	700	1/1	0.99	0.04	74,74,74,74	0
3	ZN	A	700	1/1	1.00	0.02	65,65,65,65	0
3	ZN	C	700	1/1	1.00	0.01	58,58,58,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.