



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 10:38 AM UTC

PDB ID : 3ZDH / pdb_00003zdh
Title : Crystal structure of Ls-AChBP complexed with carbamoylcholine analogue N,N-dimethyl-4-(1-methyl-1H-imidazol-2-yloxy)butan-2-amine
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Deposited on : 2012-11-26
Resolution : 2.19 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

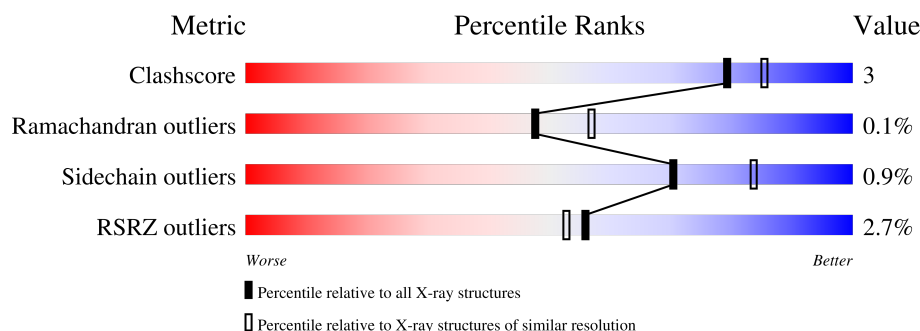
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	210	4% 86% 10% 5%
1	B	210	3% 90% 6% .
1	C	210	% 89% 7% .
1	D	210	2% 88% 7% 5%
1	E	210	% 87% 8% 5%
1	F	210	4% 89% 7% .

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Mol	Chain	Length	Quality of chain
1	G	210	2% 91% 5% 5%
1	H	210	3% 90% 5% 5%
1	I	210	2% 91% 5% 6%
1	J	210	3% 89% 5% 5%

2 Entry composition

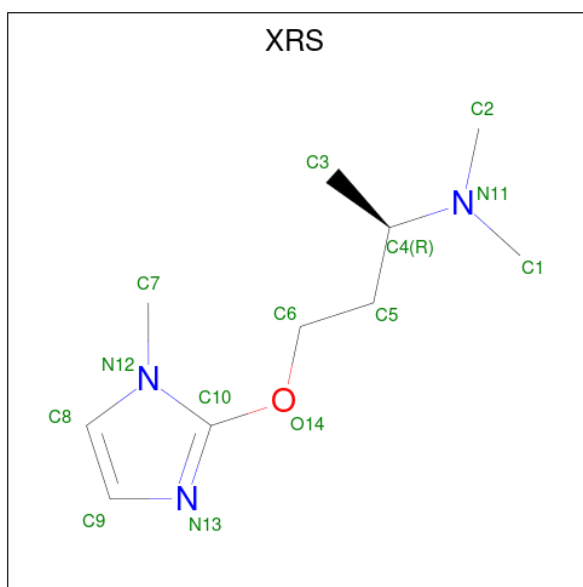
There are 5 unique types of molecules in this entry. The entry contains 17357 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYLCHOLINE BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	2	0
			1612	1013	274	320	5			
1	B	201	Total	C	N	O	S	0	3	0
			1633	1024	281	323	5			
1	C	201	Total	C	N	O	S	0	2	0
			1617	1014	275	322	6			
1	D	200	Total	C	N	O	S	0	2	0
			1610	1012	274	318	6			
1	E	200	Total	C	N	O	S	0	5	0
			1632	1026	277	324	5			
1	F	202	Total	C	N	O	S	0	2	0
			1622	1017	276	324	5			
1	G	201	Total	C	N	O	S	0	4	0
			1631	1023	281	321	6			
1	H	200	Total	C	N	O	S	0	0	0
			1602	1005	274	318	5			
1	I	198	Total	C	N	O	S	0	3	0
			1603	1008	275	314	6			
1	J	200	Total	C	N	O	S	0	1	0
			1608	1009	274	320	5			

- Molecule 2 is (2R)-N,N-dimethyl-4-(1-methylimidazol-2-yl)oxy-butan-2-amine (CCD ID: XRS) (formula: C₁₀H₁₉N₃O).



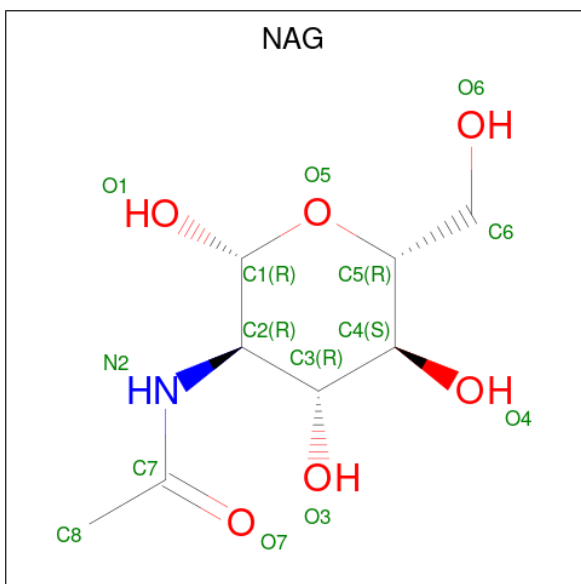
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	10	3	1		
2	B	1	Total	C	N	O	0	0
			14	10	3	1		
2	C	1	Total	C	N	O	0	0
			14	10	3	1		
2	D	1	Total	C	N	O	0	0
			14	10	3	1		
2	E	1	Total	C	N	O	0	0
			14	10	3	1		
2	F	1	Total	C	N	O	0	0
			14	10	3	1		
2	G	1	Total	C	N	O	0	0
			14	10	3	1		
2	H	1	Total	C	N	O	0	0
			14	10	3	1		
2	I	1	Total	C	N	O	0	0
			14	10	3	1		
2	J	1	Total	C	N	O	0	0
			14	10	3	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	G	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	108	Total	O	0	0
			108	108		
5	B	107	Total	O	0	0
			107	107		
5	C	101	Total	O	0	0
			101	101		
5	D	100	Total	O	0	0
			100	100		
5	E	93	Total	O	0	0
			93	93		
5	F	133	Total	O	0	0
			133	133		
5	G	112	Total	O	0	0
			112	112		
5	H	96	Total	O	0	0
			96	96		
5	I	92	Total	O	0	0
			92	92		
5	J	67	Total	O	0	0
			67	67		

3 Residue-property plots [i](#)

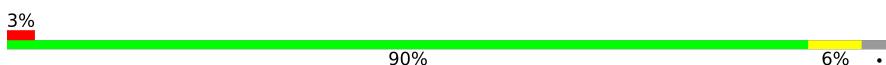
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ACETYLCHOLINE BINDING PROTEIN

Chain A: 



- Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain B: 

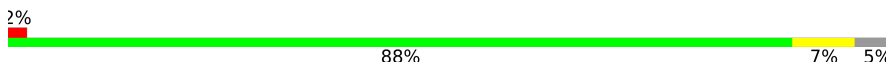


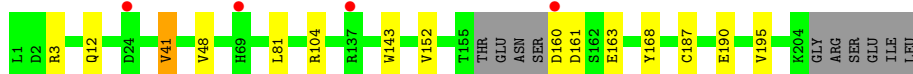
- Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain C: 



- Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain D: 

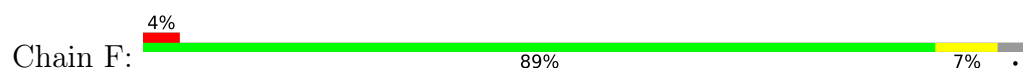


- Molecule 1: ACETYLCHOLINE BINDING PROTEIN

Chain E: 



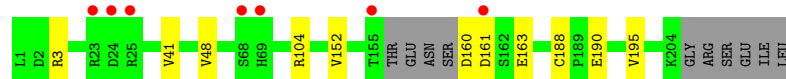
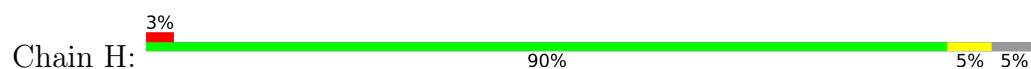
- Molecule 1: ACETYLCHOLINE BINDING PROTEIN



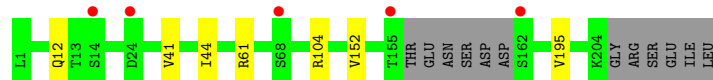
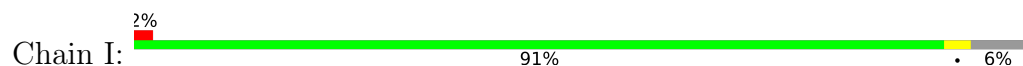
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN



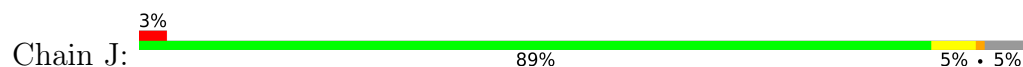
• Molecule 1: ACETYLCHOLINE BINDING PROTEIN



• Molecule 1: ACETYLCHOLINE BINDING PROTEIN



• Molecule 1: ACETYLCHOLINE BINDING PROTEIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.33Å 143.82Å 115.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.68 – 2.19 19.68 – 2.19	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.68-2.19) 98.6 (19.68-2.19)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.19Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8_1069)	Depositor
R, R_{free}	0.191 , 0.245 0.193 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	28.4	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17357	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: NAG, XRS, SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/1653	0.76	2/2255 (0.1%)
1	B	0.50	0/1680	0.73	0/2289
1	C	0.50	0/1658	0.73	0/2262
1	D	0.49	0/1651	0.72	0/2252
1	E	0.47	0/1682	0.72	0/2293
1	F	0.53	0/1663	0.78	0/2268
1	G	0.49	0/1678	0.72	0/2287
1	H	0.49	0/1637	0.72	0/2233
1	I	0.47	0/1647	0.73	0/2245
1	J	0.50	0/1646	0.74	0/2245
All	All	0.50	0/16595	0.74	2/22629 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	162	SER	CA-C-N	5.02	131.12	121.54
1	A	162	SER	C-N-CA	5.02	131.12	121.54

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	1612	0	1568	15	0
1	B	1633	0	1591	9	0
1	C	1617	0	1569	13	1
1	D	1610	0	1569	12	0
1	E	1632	0	1593	13	0
1	F	1622	0	1574	10	0
1	G	1631	0	1592	7	0
1	H	1602	0	1553	7	0
1	I	1603	0	1569	5	0
1	J	1608	0	1559	10	0
2	A	14	0	19	1	0
2	B	14	0	19	3	0
2	C	14	0	19	1	0
2	D	14	0	19	1	0
2	E	14	0	19	2	0
2	F	14	0	19	1	0
2	G	14	0	19	1	0
2	H	14	0	19	1	0
2	I	14	0	19	1	0
2	J	14	0	19	4	0
3	A	5	0	0	0	0
3	E	5	0	0	0	0
4	B	14	0	13	1	0
4	G	14	0	13	1	0
5	A	108	0	0	4	0
5	B	107	0	0	3	0
5	C	101	0	0	1	0
5	D	100	0	0	0	0
5	E	93	0	0	0	1
5	F	133	0	0	4	0
5	G	112	0	0	2	0
5	H	96	0	0	0	0
5	I	92	0	0	1	0
5	J	67	0	0	1	0
All	All	17357	0	15953	87	1

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 3.

All (87) 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)
2:C:301:XRS:H8	1:D:104:ARG:HB2	1.65	0.77
1:B:41:VAL:HG22	1:B:48:VAL:HG23	1.69	0.74
1:D:187[B]:CYS:SG	1:E:114:MET:HE1	2.29	0.72
2:H:301:XRS:H8	1:I:104:ARG:HB2	1.73	0.70
1:A:104:ARG:HB2	2:E:301:XRS:H8	1.75	0.69
2:I:301:XRS:H8	1:J:104:ARG:HB2	1.73	0.69
2:A:301:XRS:H8	1:B:104:ARG:HB2	1.76	0.67
2:B:301:XRS:H8	1:C:104:ARG:HB2	1.77	0.67
1:B:17[B]:ASP:OD2	5:B:2017:HOH:O	2.12	0.66
1:A:196:GLU:OE1	5:A:2107:HOH:O	2.15	0.65
2:D:301:XRS:H8	1:E:104:ARG:HB2	1.79	0.65
1:F:161:ASP:OD2	1:F:178:GLN:NE2	2.30	0.64
2:G:301:XRS:H8	1:H:104:ARG:HB2	1.81	0.64
1:C:146:HIS:HB3	1:C:190[B]:GLU:HG3	1.80	0.63
1:F:104:ARG:HB2	2:J:301:XRS:H8	1.81	0.63
1:E:160:ASP:HB3	1:E:163:GLU:HB2	1.80	0.63
1:D:160:ASP:HB3	1:D:163:GLU:HB2	1.80	0.62
2:F:301:XRS:H8	1:G:104:ARG:HB2	1.81	0.62
1:H:160:ASP:OD1	1:H:161:ASP:N	2.33	0.61
1:C:41:VAL:HG22	1:C:48:VAL:HG23	1.83	0.61
1:B:66:ASN:HA	4:B:401:NAG:H82	1.82	0.60
1:A:12:GLN:HB3	1:G:12:GLN:HB3	1.85	0.59
1:B:160:ASP:O	5:B:2089:HOH:O	2.17	0.58
1:G:5:ASP:OD1	5:G:2003:HOH:O	2.17	0.57
1:G:41:VAL:HG22	1:G:48:VAL:HG23	1.85	0.57
1:D:12:GLN:HB3	1:I:12:GLN:HB3	1.87	0.56
1:D:160:ASP:OD1	1:D:161:ASP:N	2.39	0.55
1:B:12:GLN:HB3	1:F:12:GLN:HB3	1.89	0.55
1:A:41:VAL:HG22	1:A:48:VAL:HG23	1.88	0.53
1:H:160:ASP:HB3	1:H:163:GLU:HB2	1.91	0.53
1:H:41:VAL:HG22	1:H:48:VAL:HG23	1.89	0.52
5:A:2054:HOH:O	1:E:190[A]:GLU:OE2	2.19	0.51
1:A:170:ARG:HD3	1:E:44:ILE:HG22	1.91	0.51
1:H:152:VAL:HG22	1:H:195:VAL:HG23	1.93	0.51
1:I:61:ARG:NH2	5:I:2039:HOH:O	2.44	0.51
1:J:76:VAL:HG11	1:J:81:LEU:HD21	1.93	0.51
5:C:2087:HOH:O	1:D:3:ARG:HD3	2.09	0.50
1:J:152:VAL:HG22	1:J:195:VAL:HG23	1.94	0.50
1:J:160:ASP:HB3	1:J:163:GLU:HB2	1.93	0.50
1:E:152:VAL:HG22	1:E:195:VAL:HG23	1.94	0.50
1:A:61:ARG:NH1	4:G:401:NAG:H4	2.28	0.48
1:B:152:VAL:HG22	1:B:195:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:178:GLN:NE2	5:J:2017:HOH:O	2.45	0.48
1:C:188[B]:CYS:HB3	1:C:190[B]:GLU:OE2	2.13	0.48
1:C:152:VAL:HG22	1:C:195:VAL:HG23	1.95	0.47
1:A:168:TYR:CE1	1:E:124:ASP:HB2	2.49	0.47
1:J:143:TRP:CE2	2:J:301:XRS:H62C	2.49	0.47
1:F:44:ILE:O	1:G:170:ARG:HD3	2.15	0.47
1:A:152:VAL:HG22	1:A:195:VAL:HG23	1.98	0.46
1:C:160:ASP:HB3	1:C:163:GLU:HB2	1.98	0.46
1:G:152:VAL:HG22	1:G:195:VAL:HG23	1.97	0.46
1:D:152:VAL:HG22	1:D:195:VAL:HG23	1.98	0.46
1:I:152:VAL:HG22	1:I:195:VAL:HG23	1.98	0.46
1:J:41:VAL:HG22	1:J:48:VAL:HG23	1.99	0.45
1:C:190[B]:GLU:HG2	1:C:192:TYR:CE1	2.52	0.45
1:F:59:SER:O	5:F:2017:HOH:O	2.21	0.45
1:D:143:TRP:CE2	1:E:99:THR:HG21	2.52	0.45
5:G:2096:HOH:O	1:H:3:ARG:HD3	2.15	0.45
1:A:168:TYR:HB3	1:E:46:ASN:HB3	1.99	0.44
1:J:143:TRP:NE1	2:J:301:XRS:H62C	2.32	0.44
1:C:190[B]:GLU:CD	1:C:190[B]:GLU:H	2.26	0.44
1:F:61:ARG:NH1	5:F:2019:HOH:O	2.50	0.44
1:F:114:MET:HB3	2:J:301:XRS:H61C	2.00	0.44
1:A:14:SER:OG	1:A:80:SER:O	2.27	0.43
2:B:301:XRS:H8	1:C:104:ARG:CB	2.47	0.43
1:F:137:ARG:NH1	5:F:2095:HOH:O	2.50	0.43
5:F:2107:HOH:O	1:G:3:ARG:HD3	2.18	0.43
1:C:124:ASP:HB2	1:D:168:TYR:CE1	2.53	0.43
1:D:143:TRP:CZ2	1:E:99:THR:HG21	2.53	0.43
2:B:301:XRS:H61C	1:C:114:MET:HB3	2.00	0.42
1:D:41:VAL:CG2	1:D:48:VAL:HG23	2.49	0.42
1:H:161:ASP:C	1:H:163:GLU:H	2.27	0.42
1:C:146:HIS:CB	1:C:190[B]:GLU:HG3	2.49	0.42
1:A:160:ASP:OD1	1:A:160:ASP:N	2.52	0.42
5:B:2088:HOH:O	1:C:3:ARG:HD3	2.20	0.42
1:D:41:VAL:HG22	1:D:48:VAL:HG23	2.01	0.42
1:E:14:SER:OG	1:E:80:SER:O	2.32	0.42
1:A:104:ARG:CB	2:E:301:XRS:H8	2.46	0.42
1:F:152:VAL:HG22	1:F:195:VAL:HG23	2.01	0.41
1:A:3:ARG:HD3	5:A:2003:HOH:O	2.19	0.41
1:I:44:ILE:HG22	1:J:170:ARG:HD3	2.01	0.41
1:F:41:VAL:HG22	1:F:48:VAL:HG23	2.03	0.41
1:A:124:ASP:HB2	1:B:168:TYR:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:41:VAL:HG22	1:E:48:VAL:HG23	2.03	0.41
1:A:143:TRP:CE2	1:B:99:THR:HG21	2.55	0.41
1:J:41:VAL:HG13	1:J:125:VAL:HG11	2.03	0.40
5:A:2099:HOH:O	1:E:137:ARG:NH1	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:ASN:OD1	5:E:2087:HOH:O[4_444]	2.15	0.05

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	198/210 (94%)	195 (98%)	2 (1%)	1 (0%)	24	27
1	B	201/210 (96%)	199 (99%)	2 (1%)	0	100	100
1	C	199/210 (95%)	197 (99%)	2 (1%)	0	100	100
1	D	198/210 (94%)	195 (98%)	3 (2%)	0	100	100
1	E	201/210 (96%)	199 (99%)	2 (1%)	0	100	100
1	F	200/210 (95%)	198 (99%)	1 (0%)	1 (0%)	24	27
1	G	201/210 (96%)	198 (98%)	3 (2%)	0	100	100
1	H	196/210 (93%)	192 (98%)	4 (2%)	0	100	100
1	I	197/210 (94%)	196 (100%)	1 (0%)	0	100	100
1	J	197/210 (94%)	195 (99%)	2 (1%)	0	100	100
All	All	1988/2100 (95%)	1964 (99%)	22 (1%)	2 (0%)	48	57

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	163	GLU
1	A	163	GLU

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	189/196 (96%)	186 (98%)	3 (2%)	55	71
1	B	191/196 (97%)	189 (99%)	2 (1%)	68	81
1	C	190/196 (97%)	190 (100%)	0	100	100
1	D	189/196 (96%)	185 (98%)	4 (2%)	47	63
1	E	192/196 (98%)	188 (98%)	4 (2%)	47	63
1	F	190/196 (97%)	189 (100%)	1 (0%)	81	90
1	G	191/196 (97%)	191 (100%)	0	100	100
1	H	187/196 (95%)	185 (99%)	2 (1%)	65	79
1	I	188/196 (96%)	187 (100%)	1 (0%)	81	90
1	J	188/196 (96%)	186 (99%)	2 (1%)	65	79
All	All	1895/1960 (97%)	1876 (99%)	19 (1%)	70	81

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	81[A]	LEU
1	A	81[B]	LEU
1	A	190	GLU
1	B	188	CYS
1	B	190	GLU
1	D	41	VAL
1	D	81[A]	LEU
1	D	81[B]	LEU
1	D	190	GLU
1	E	41	VAL
1	E	81[A]	LEU
1	E	81[B]	LEU

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Mol	Chain	Res	Type
1	E	188	CYS
1	F	188	CYS
1	H	188	CYS
1	H	190	GLU
1	I	41	VAL
1	J	41	VAL
1	J	81	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	GLN
1	D	9	ASN
1	D	101	GLN
1	F	9	ASN
1	F	69	HIS
1	H	101	GLN
1	I	9	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	401	1	14,14,15	0.71	0	17,19,21	1.34	3 (17%)
2	XRS	F	301	-	13,14,14	0.92	0	13,18,18	1.58	3 (23%)
2	XRS	G	301	-	13,14,14	1.02	0	13,18,18	1.18	2 (15%)
3	SO4	A	1205	-	4,4,4	0.29	0	6,6,6	0.16	0
2	XRS	C	301	-	13,14,14	1.21	0	13,18,18	1.33	1 (7%)
2	XRS	A	301	-	13,14,14	0.96	0	13,18,18	1.14	0
2	XRS	B	301	-	13,14,14	0.94	0	13,18,18	1.42	2 (15%)
3	SO4	E	1205	-	4,4,4	0.28	0	6,6,6	0.14	0
2	XRS	I	301	-	13,14,14	0.92	0	13,18,18	1.57	2 (15%)
2	XRS	H	301	-	13,14,14	0.98	0	13,18,18	1.14	1 (7%)
2	XRS	J	301	-	13,14,14	0.95	0	13,18,18	1.37	2 (15%)
2	XRS	D	301	-	13,14,14	0.87	0	13,18,18	1.11	1 (7%)
4	NAG	G	401	1	14,14,15	0.57	0	17,19,21	1.39	3 (17%)
2	XRS	E	301	-	13,14,14	0.98	0	13,18,18	1.20	2 (15%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	401	1	-	0/6/23/26	0/1/1/1
2	XRS	F	301	-	-	0/10/10/10	0/1/1/1
2	XRS	G	301	-	-	0/10/10/10	0/1/1/1
2	XRS	C	301	-	-	0/10/10/10	0/1/1/1
2	XRS	A	301	-	-	0/10/10/10	0/1/1/1
2	XRS	B	301	-	-	0/10/10/10	0/1/1/1
2	XRS	I	301	-	-	0/10/10/10	0/1/1/1
2	XRS	H	301	-	-	0/10/10/10	0/1/1/1
2	XRS	J	301	-	-	2/10/10/10	0/1/1/1
2	XRS	D	301	-	-	0/10/10/10	0/1/1/1
4	NAG	G	401	1	-	2/6/23/26	0/1/1/1
2	XRS	E	301	-	-	0/10/10/10	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	401	NAG	C1-O5-C5	-3.97	106.86	112.19
2	I	301	XRS	O14-C10-N13	3.96	130.69	127.66
2	F	301	XRS	O14-C10-N13	3.35	130.22	127.66
2	B	301	XRS	O14-C10-N12	3.27	119.10	116.89
2	J	301	XRS	O14-C10-N12	2.82	118.80	116.89
4	B	401	NAG	C1-O5-C5	-2.69	108.59	112.19
2	G	301	XRS	O14-C10-N13	2.68	129.71	127.66
2	D	301	XRS	O14-C10-N12	2.65	118.68	116.89
2	C	301	XRS	O14-C10-N13	2.60	129.65	127.66
2	J	301	XRS	C6-C5-C4	2.47	117.43	113.69
2	E	301	XRS	C3-C4-N11	-2.46	109.84	114.28
2	H	301	XRS	O14-C10-N12	2.29	118.44	116.89
2	F	301	XRS	C6-C5-C4	2.23	117.06	113.69
4	B	401	NAG	O5-C5-C6	2.16	111.86	107.66
2	F	301	XRS	C3-C4-N11	-2.11	110.48	114.28
4	B	401	NAG	O5-C1-C2	2.10	114.54	111.29
4	G	401	NAG	O5-C5-C6	2.07	111.68	107.66
2	B	301	XRS	C3-C4-N11	-2.06	110.57	114.28
4	G	401	NAG	C8-C7-N2	2.03	119.48	116.12
2	E	301	XRS	C6-C5-C4	2.02	116.76	113.69
2	I	301	XRS	C7-N12-C8	2.01	128.45	125.11
2	G	301	XRS	C7-N12-C8	2.01	128.45	125.11

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	401	NAG	C4-C5-C6-O6
4	G	401	NAG	O5-C5-C6-O6
2	J	301	XRS	C5-C6-O14-C10
2	J	301	XRS	N13-C10-O14-C6

There are no ring outliers.

12 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	401	NAG	1	0
2	F	301	XRS	1	0
2	G	301	XRS	1	0
2	C	301	XRS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	XRS	1	0
2	B	301	XRS	3	0
2	I	301	XRS	1	0
2	H	301	XRS	1	0
2	J	301	XRS	4	0
2	D	301	XRS	1	0
4	G	401	NAG	1	0
2	E	301	XRS	2	0

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	200/210 (95%)	-0.05	8 (4%)	42	39	8, 21, 46, 87	2 (1%)
1	B	201/210 (95%)	-0.14	6 (2%)	52	49	9, 20, 42, 68	3 (1%)
1	C	201/210 (95%)	-0.15	2 (0%)	79	77	11, 20, 43, 82	2 (0%)
1	D	200/210 (95%)	-0.15	4 (2%)	65	62	10, 21, 45, 74	2 (1%)
1	E	200/210 (95%)	-0.19	3 (1%)	72	69	9, 20, 46, 75	5 (2%)
1	F	202/210 (96%)	-0.14	9 (4%)	38	35	8, 20, 43, 75	2 (0%)
1	G	201/210 (95%)	-0.20	4 (1%)	65	62	9, 19, 43, 74	4 (1%)
1	H	200/210 (95%)	-0.10	7 (3%)	47	44	12, 22, 47, 80	0
1	I	198/210 (94%)	-0.13	5 (2%)	58	55	14, 24, 45, 74	3 (1%)
1	J	200/210 (95%)	-0.02	7 (3%)	47	44	13, 24, 48, 76	1 (0%)
All	All	2003/2100 (95%)	-0.12	55 (2%)	56	53	8, 21, 46, 87	24 (1%)

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	205	GLY	3.8
1	G	23	ARG	3.6
1	B	25	ARG	3.5
1	C	24	ASP	3.1
1	E	67	SER	3.1
1	H	68	SER	3.1
1	A	182	SER	3.1
1	A	168	TYR	3.0
1	F	23	ARG	2.9
1	A	163	GLU	2.9
1	B	69	HIS	2.9
1	B	160	ASP	2.7
1	H	155	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	24	ASP	2.6
1	E	68	SER	2.6
1	F	66	ASN	2.5
1	J	186	SER	2.5
1	G	25	ARG	2.5
1	H	25	ARG	2.4
1	H	23	ARG	2.4
1	J	69	HIS	2.4
1	A	24	ASP	2.4
1	J	185	TYR	2.4
1	G	69	HIS	2.4
1	F	67	SER	2.4
1	A	25	ARG	2.3
1	I	14	SER	2.3
1	A	160	ASP	2.3
1	I	24	ASP	2.3
1	E	69	HIS	2.3
1	A	23	ARG	2.3
1	G	24	ASP	2.3
1	A	69	HIS	2.2
1	J	184	THR	2.2
1	D	137	ARG	2.2
1	F	69	HIS	2.2
1	I	68	SER	2.2
1	I	162	SER	2.2
1	J	187	CYS	2.2
1	H	161	ASP	2.2
1	B	68	SER	2.2
1	D	160	ASP	2.2
1	B	61	ARG	2.1
1	F	155	THR	2.1
1	D	69	HIS	2.1
1	F	68	SER	2.1
1	C	69	HIS	2.1
1	B	24	ASP	2.1
1	F	24	ASP	2.0
1	H	24	ASP	2.0
1	J	23	ARG	2.0
1	H	69	HIS	2.0
1	I	155	THR	2.0
1	F	168	TYR	2.0
1	J	160	ASP	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
4	NAG	B	401	14/15	0.50	0.17	55,74,82,87	0
4	NAG	G	401	14/15	0.57	0.16	57,66,72,74	0
3	SO4	A	1205	5/5	0.72	0.17	42,52,72,73	0
3	SO4	E	1205	5/5	0.80	0.13	53,54,68,75	0
2	XRS	H	301	14/14	0.95	0.07	10,15,21,24	0
2	XRS	J	301	14/14	0.95	0.06	9,16,18,21	0
2	XRS	C	301	14/14	0.95	0.06	10,12,16,16	0
2	XRS	A	301	14/14	0.96	0.07	12,16,20,21	0
2	XRS	D	301	14/14	0.96	0.06	13,17,21,22	0
2	XRS	F	301	14/14	0.96	0.05	10,13,16,16	0
2	XRS	G	301	14/14	0.96	0.05	12,15,20,21	0
2	XRS	B	301	14/14	0.96	0.05	14,17,21,22	0
2	XRS	I	301	14/14	0.97	0.05	15,19,23,23	0
2	XRS	E	301	14/14	0.97	0.05	10,13,16,22	0

6.5 Other polymers [i](#)

There are no such residues in this entry.