



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:55 PM UTC

PDB ID : 2VQ6 / pdb_00002vq6
Title : Torpedo californica acetylcholinesterase complexed with 2-PAM
Authors : Harel, M.; Silman, I.; Sussman, J.L.
Deposited on : 2008-03-11
Resolution : 2.71 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

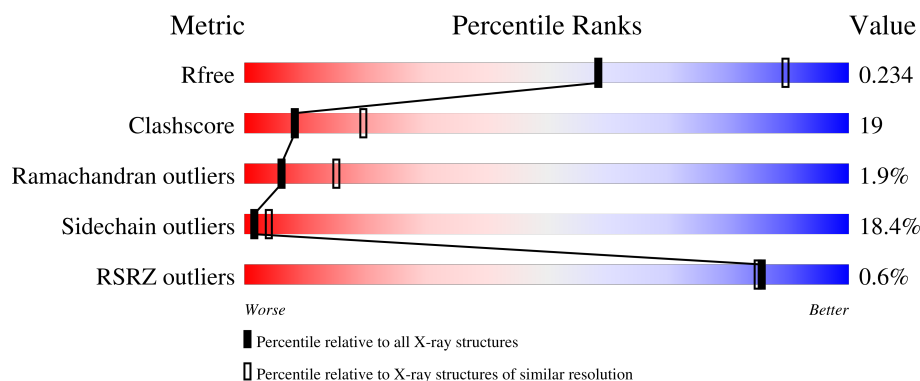
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	543	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FP1	A	1536	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	A	1538	X	-	-	-

2 Entry composition [i](#)

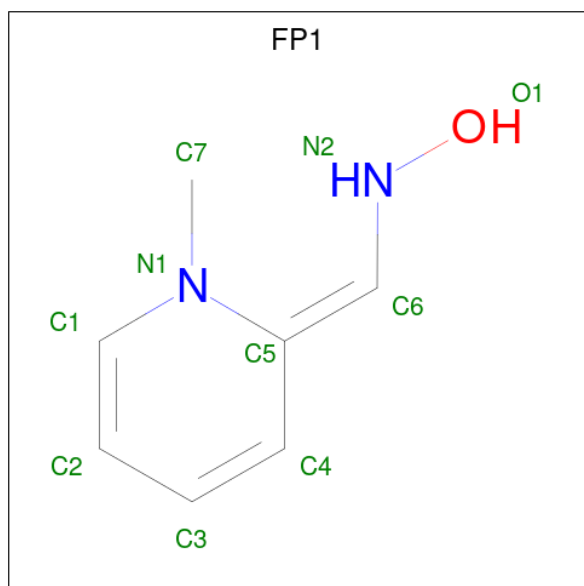
There are 5 unique types of molecules in this entry. The entry contains 4377 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYLCHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	529	4241	2723	722	774	22	0	5	0

- Molecule 2 is N-hydroxy-1-(1-methylpyridin-2(1H)-ylidene)methanamine (CCD ID: FP1) (formula: C₇H₁₀N₂O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	10	7	2	1	0	0

- 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		

- 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	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		

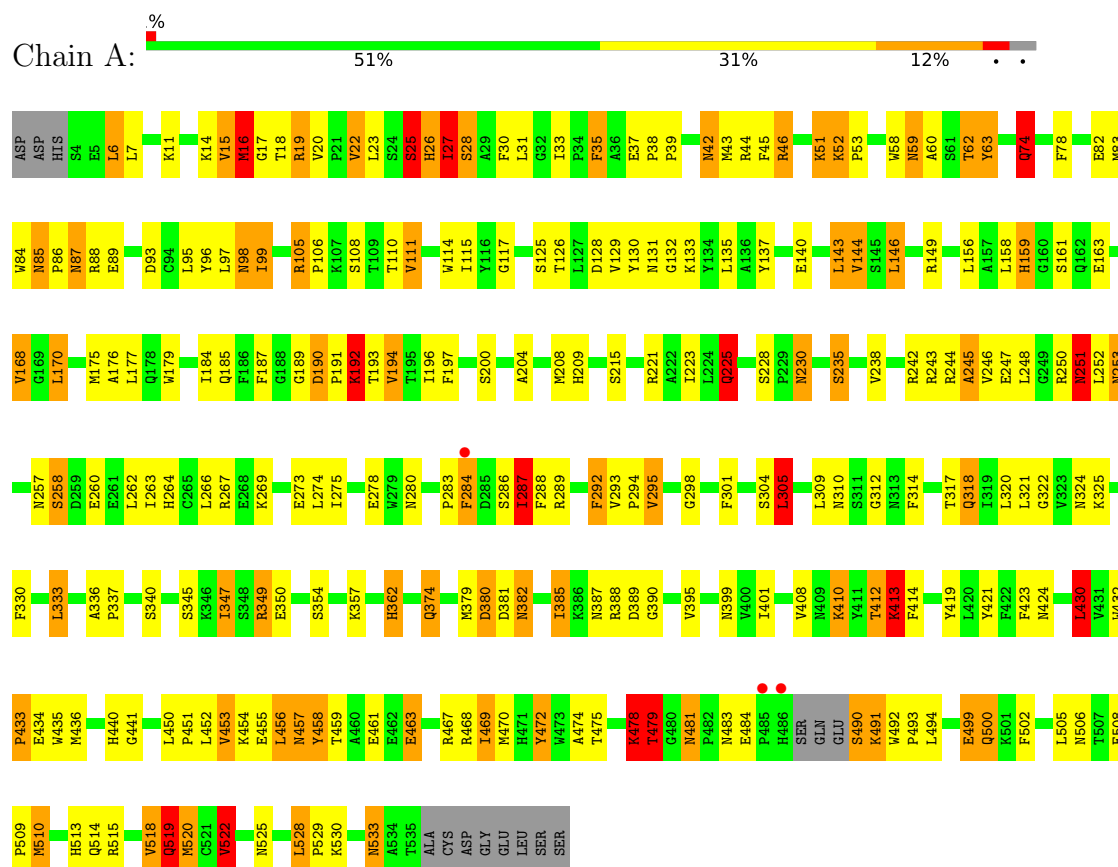
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	93	Total 93	O 93	0	0

3 Residue-property plots

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: ACETYLCHOLINESTERASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	113.95Å 113.95Å 138.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.66 – 2.71 15.66 – 2.71	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.66-2.71) 92.5 (15.66-2.71)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.171 , 0.234 0.173 , 0.234	Depositor DCC
R_{free} test set	1340 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	29.2	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4377	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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, FP1, 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	1.71	46/4373 (1.1%)	1.67	65/5934 (1.1%)

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	5

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	287	ILE	C-N	-14.89	1.12	1.33
1	A	283	PRO	C-N	14.35	1.52	1.33
1	A	114	TRP	C-N	-11.59	1.18	1.33
1	A	284	PHE	C-N	-9.43	1.20	1.33
1	A	52	LYS	CA-C	-9.37	1.45	1.52
1	A	196	ILE	CA-CB	-8.97	1.42	1.54
1	A	245	ALA	CA-CB	-8.76	1.39	1.53
1	A	287	ILE	C-O	8.44	1.32	1.23
1	A	111	VAL	CA-C	7.32	1.61	1.52
1	A	286	SER	C-N	-7.16	1.24	1.33
1	A	305	LEU	N-CA	-7.04	1.37	1.46
1	A	253	ASN	CA-C	-6.82	1.44	1.53
1	A	424	ASN	C-O	-6.82	1.15	1.23
1	A	385	ILE	CA-CB	-6.48	1.46	1.54
1	A	474	ALA	CA-CB	-6.46	1.43	1.53
1	A	525	ASN	C-O	-6.39	1.15	1.24
1	A	433	PRO	CA-C	-6.06	1.45	1.52
1	A	115	ILE	C-O	5.98	1.30	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	525	ASN	CA-C	-5.89	1.44	1.52
1	A	478	LYS	CD-CE	5.87	1.70	1.52
1	A	251	ASN	C-O	-5.86	1.16	1.24
1	A	292	PHE	C-O	5.72	1.30	1.24
1	A	458	TYR	N-CA	5.72	1.52	1.45
1	A	130	TYR	C-O	-5.52	1.16	1.24
1	A	74	GLN	CA-C	5.49	1.60	1.52
1	A	176	ALA	CA-CB	-5.40	1.44	1.53
1	A	117	GLY	N-CA	5.37	1.51	1.45
1	A	22	VAL	CA-CB	5.34	1.61	1.54
1	A	295	VAL	C-O	5.30	1.30	1.24
1	A	530	LYS	CG-CD	5.30	1.68	1.52
1	A	413[A]	LYS	C-O	-5.26	1.18	1.24
1	A	413[B]	LYS	C-O	-5.26	1.18	1.24
1	A	387	ASN	N-CA	-5.24	1.40	1.46
1	A	35	PHE	CA-CB	-5.23	1.45	1.53
1	A	481	ASN	C-N	5.19	1.39	1.34
1	A	96	TYR	CA-C	-5.18	1.46	1.52
1	A	478	LYS	C-O	-5.14	1.17	1.24
1	A	159	HIS	C-O	5.12	1.30	1.24
1	A	284	PHE	C-O	5.12	1.29	1.23
1	A	530	LYS	C-O	-5.12	1.18	1.24
1	A	63	TYR	CA-C	-5.10	1.48	1.53
1	A	26	HIS	N-CA	5.08	1.52	1.45
1	A	401	ILE	CA-C	-5.08	1.46	1.52
1	A	533	ASN	C-O	-5.07	1.18	1.24
1	A	522	VAL	CA-CB	5.06	1.60	1.54
1	A	273	GLU	CA-C	-5.02	1.45	1.52

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	284	PHE	CA-C-N	-10.73	105.79	121.24
1	A	284	PHE	C-N-CA	-10.73	105.79	121.24
1	A	286	SER	O-C-N	-9.42	111.90	122.92
1	A	105	ARG	CA-C-N	-8.92	108.69	119.84
1	A	105	ARG	C-N-CA	-8.92	108.69	119.84
1	A	287	ILE	CA-C-O	-8.07	113.20	121.67
1	A	434	GLU	N-CA-C	7.91	120.90	111.33
1	A	187	PHE	N-CA-C	-7.79	101.95	112.94
1	A	244	ARG	NE-CZ-NH2	7.69	126.12	119.20
1	A	283	PRO	CA-C-N	7.66	135.21	121.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	PRO	C-N-CA	7.66	135.21	121.89
1	A	499	GLU	N-CA-C	7.57	122.75	112.68
1	A	59	ASN	N-CA-C	7.50	120.64	108.63
1	A	18	THR	CA-C-N	-7.14	112.93	123.00
1	A	18	THR	C-N-CA	-7.14	112.93	123.00
1	A	374	GLN	N-CA-C	7.12	119.90	111.71
1	A	286	SER	CA-C-N	7.10	133.90	122.68
1	A	286	SER	C-N-CA	7.10	133.90	122.68
1	A	280	ASN	N-CA-C	6.96	121.03	112.54
1	A	253	ASN	CB-CA-C	-6.66	102.58	111.63
1	A	257	ASN	N-CA-C	6.62	121.49	112.68
1	A	244	ARG	NE-CZ-NH1	-6.53	114.97	121.50
1	A	450	LEU	CA-C-N	-6.48	113.47	119.82
1	A	450	LEU	C-N-CA	-6.48	113.47	119.82
1	A	250	ARG	N-CA-C	6.39	117.91	111.07
1	A	16	MET	N-CA-C	6.36	118.89	108.52
1	A	479	THR	CA-CB-OG1	-6.35	100.08	109.60
1	A	85	ASN	CA-C-N	-6.18	113.59	119.90
1	A	85	ASN	C-N-CA	-6.18	113.59	119.90
1	A	433	PRO	CA-C-N	6.11	128.76	120.38
1	A	433	PRO	C-N-CA	6.11	128.76	120.38
1	A	390	GLY	N-CA-C	-6.03	105.05	112.77
1	A	27	ILE	CA-C-N	-5.97	114.27	122.93
1	A	27	ILE	C-N-CA	-5.97	114.27	122.93
1	A	310	ASN	N-CA-C	5.97	117.79	111.28
1	A	441	GLY	CA-C-N	-5.83	113.46	122.49
1	A	441	GLY	C-N-CA	-5.83	113.46	122.49
1	A	159	HIS	N-CA-C	5.74	123.02	110.80
1	A	52	LYS	N-CA-C	-5.71	97.44	108.45
1	A	225	GLN	N-CA-C	5.70	117.81	108.52
1	A	62	THR	CB-CA-C	-5.70	98.95	109.37
1	A	192	LYS	N-CA-C	-5.64	106.38	113.20
1	A	467	ARG	N-CA-C	-5.64	105.22	111.36
1	A	179	TRP	N-CA-C	5.63	117.42	111.28
1	A	88	ARG	CG-CD-NE	-5.59	99.69	112.00
1	A	228	SER	N-CA-CB	-5.59	102.99	110.77
1	A	99	ILE	N-CA-C	5.58	116.52	108.48
1	A	312	GLY	CA-C-N	-5.51	113.90	122.16
1	A	312	GLY	C-N-CA	-5.51	113.90	122.16
1	A	414	PHE	N-CA-C	5.39	119.96	113.17
1	A	235	SER	CA-C-N	-5.37	115.73	123.03
1	A	235	SER	C-N-CA	-5.37	115.73	123.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	LEU	N-CA-C	-5.31	102.42	110.28
1	A	266	LEU	N-CA-C	-5.31	105.61	111.71
1	A	519	GLN	N-CA-CB	-5.22	101.66	110.49
1	A	52	LYS	CA-C-N	-5.20	114.59	119.90
1	A	52	LYS	C-N-CA	-5.20	114.59	119.90
1	A	190	ASP	CA-C-N	-5.20	114.35	120.12
1	A	190	ASP	C-N-CA	-5.20	114.35	120.12
1	A	115	ILE	O-C-N	-5.14	117.78	123.18
1	A	88	ARG	NE-CZ-NH1	-5.14	116.36	121.50
1	A	309	LEU	N-CA-C	-5.14	105.68	111.28
1	A	314	PHE	N-CA-C	5.12	116.31	108.42
1	A	350	GLU	N-CA-CB	-5.04	102.67	110.13
1	A	522	VAL	N-CA-CB	5.01	118.10	110.58

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	284	PHE	Mainchain
1	A	287	ILE	Mainchain
1	A	292	PHE	Peptide
1	A	42	ASN	Peptide
1	A	490	SER	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	4241	0	4101	158	0
2	A	10	0	10	10	0
3	A	5	0	0	0	0
4	A	28	0	26	2	0
5	A	93	0	0	1	0
All	All	4377	0	4137	162	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 19.

All (162) 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:349[A]:ARG:HG2	1:A:349[A]:ARG:HH11	1.11	1.11
2:A:1536:FP1:H2	2:A:1536:FP1:H7C1	1.08	1.10
1:A:432:TRP:HB3	1:A:436:MET:HE3	1.31	1.08
1:A:432:TRP:HB3	1:A:436:MET:CE	1.95	0.96
2:A:1536:FP1:H2	2:A:1536:FP1:C7	1.80	0.95
1:A:251:ASN:HD22	1:A:251:ASN:H	1.15	0.94
2:A:1536:FP1:H7C1	2:A:1536:FP1:N2	1.85	0.89
1:A:204:ALA:O	1:A:208:MET:HG3	1.75	0.85
1:A:349[A]:ARG:HG2	1:A:349[A]:ARG:NH1	1.92	0.84
1:A:433:PRO:HD2	1:A:436:MET:CE	2.06	0.84
1:A:433:PRO:HD2	1:A:436:MET:HE2	1.59	0.84
1:A:374:GLN:HG3	1:A:520:MET:HE1	1.59	0.83
1:A:349[A]:ARG:HH11	1:A:349[A]:ARG:CG	1.92	0.80
1:A:479:THR:HG22	1:A:481:ASN:H	1.47	0.78
1:A:193:THR:HG22	1:A:193:THR:O	1.81	0.78
1:A:83:MET:HE2	1:A:84:TRP:CZ2	2.19	0.77
1:A:149:ARG:NH1	1:A:168:VAL:HG13	2.01	0.76
1:A:408:VAL:O	1:A:412:THR:HG23	1.85	0.76
1:A:230:ASN:H	1:A:230:ASN:HD22	1.34	0.75
1:A:508:GLU:HB2	1:A:509:PRO:HD3	1.68	0.75
1:A:87:ASN:HD22	1:A:87:ASN:H	1.31	0.75
1:A:208:MET:HE1	1:A:294:PRO:HG2	1.67	0.74
1:A:508:GLU:HB2	1:A:509:PRO:CD	2.17	0.74
1:A:132:GLY:HA3	1:A:143:LEU:HD12	1.69	0.74
1:A:518:VAL:HG13	1:A:519:GLN:H	1.53	0.74
1:A:432:TRP:CE3	1:A:436:MET:HE1	2.23	0.73
1:A:330:PHE:CD1	2:A:1536:FP1:HA	2.24	0.73
1:A:330:PHE:CE1	2:A:1536:FP1:HA	2.26	0.70
1:A:15:VAL:HG23	1:A:58:TRP:HB3	1.73	0.69
1:A:419:TYR:CZ	1:A:494:LEU:HD23	2.28	0.69
1:A:208:MET:HE1	1:A:294:PRO:CG	2.21	0.69
1:A:388:ARG:NH2	1:A:389:ASP:OD2	2.27	0.68
1:A:433:PRO:CD	1:A:436:MET:HE2	2.24	0.68
1:A:42:ASN:HB2	1:A:267:ARG:HH21	1.59	0.67
1:A:59:ASN:HB3	4:A:1539:NAG:H83	1.76	0.67
2:A:1536:FP1:C7	2:A:1536:FP1:N2	2.52	0.65
1:A:475:THR:O	1:A:479:THR:HB	1.98	0.64
1:A:479:THR:HG22	1:A:481:ASN:N	2.14	0.63
1:A:20:VAL:HG22	1:A:27:ILE:HG22	1.81	0.62
1:A:251:ASN:HD22	1:A:251:ASN:N	1.92	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:VAL:HG22	1:A:456:LEU:HG	1.82	0.61
1:A:251:ASN:H	1:A:251:ASN:ND2	1.90	0.61
1:A:193:THR:O	1:A:193:THR:CG2	2.47	0.61
1:A:44:ARG:HD3	1:A:45:PHE:CZ	2.36	0.60
1:A:111:VAL:HB	1:A:194:VAL:HG12	1.82	0.60
1:A:440:HIS:O	2:A:1536:FP1:H3	2.02	0.60
1:A:260:GLU:O	1:A:264[A]:HIS:CD2	2.55	0.60
1:A:190:ASP:OD2	1:A:192:LYS:HB2	2.03	0.59
1:A:19:ARG:HD3	1:A:19:ARG:C	2.27	0.58
1:A:345:SER:O	1:A:388:ARG:HG3	2.02	0.58
1:A:63:TYR:CD2	1:A:126:THR:HG22	2.39	0.58
1:A:483:ASN:HD21	1:A:492:TRP:H	1.50	0.58
1:A:432:TRP:HE3	1:A:436:MET:HE1	1.66	0.58
1:A:110:THR:OG1	1:A:478:LYS:HE2	2.03	0.58
1:A:78:PHE:O	1:A:82:GLU:HG2	2.04	0.58
1:A:324:ASN:HD22	1:A:423:PHE:HB3	1.69	0.57
1:A:225:GLN:HB3	1:A:421:TYR:OH	2.04	0.57
1:A:499:GLU:O	1:A:500:GLN:HB2	2.03	0.57
1:A:200:SER:HB3	1:A:440:HIS:CE1	2.40	0.56
1:A:258:SER:HB2	1:A:260:GLU:HB2	1.87	0.56
1:A:260:GLU:O	1:A:264[A]:HIS:HD2	1.88	0.56
1:A:223:ILE:HA	1:A:320:LEU:O	2.05	0.56
1:A:317:THR:OG1	1:A:318:GLN:N	2.39	0.55
1:A:518:VAL:O	1:A:522:VAL:HG12	2.05	0.55
1:A:221:ARG:NH1	1:A:318:GLN:OE1	2.37	0.55
1:A:74:GLN:NE2	5:A:2017:HOH:O	2.39	0.55
1:A:158:LEU:HD12	1:A:263:ILE:HD11	1.89	0.55
1:A:209:HIS:HD2	1:A:215:SER:OG	1.90	0.55
1:A:87:ASN:HD22	1:A:87:ASN:N	1.97	0.54
1:A:433:PRO:CG	1:A:436:MET:HE2	2.37	0.54
1:A:85:ASN:O	1:A:86:PRO:C	2.47	0.54
1:A:345:SER:O	1:A:347:ILE:HD12	2.07	0.54
1:A:469:ILE:O	1:A:472:TYR:HB2	2.08	0.54
1:A:379:MET:O	1:A:380:ASP:HB2	2.07	0.54
1:A:87:ASN:H	1:A:87:ASN:ND2	2.05	0.53
1:A:170:LEU:HD21	1:A:208:MET:HE3	1.90	0.53
1:A:105:ARG:HG2	1:A:106:PRO:O	2.09	0.53
1:A:433:PRO:HG2	1:A:436:MET:HE2	1.90	0.53
1:A:456:LEU:O	1:A:457:ASN:HB2	2.08	0.53
1:A:330:PHE:CZ	2:A:1536:FP1:HB	2.44	0.52
1:A:374:GLN:CG	1:A:520:MET:HE1	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ASP:OD1	1:A:93:ASP:C	2.53	0.52
1:A:502:PHE:CZ	1:A:513:HIS:HB2	2.45	0.52
1:A:6:LEU:CD1	1:A:28:SER:HB3	2.39	0.52
1:A:98:ASN:O	1:A:144:VAL:HA	2.08	0.52
1:A:362:HIS:H	1:A:362:HIS:CD2	2.27	0.52
1:A:131:ASN:ND2	1:A:133:LYS:HD3	2.26	0.51
1:A:156:LEU:HD11	1:A:245:ALA:HB1	1.93	0.51
1:A:247:GLU:O	1:A:251:ASN:ND2	2.44	0.50
1:A:380:ASP:C	1:A:382:ASN:H	2.19	0.50
1:A:506:ASN:OD1	1:A:506:ASN:C	2.54	0.50
1:A:324:ASN:ND2	1:A:423:PHE:HB3	2.27	0.50
1:A:251:ASN:N	1:A:251:ASN:ND2	2.52	0.49
1:A:528:LEU:HB3	1:A:529:PRO:HD3	1.94	0.49
1:A:46:ARG:HD2	1:A:163:GLU:OE1	2.13	0.49
1:A:520:MET:HE2	1:A:520:MET:HA	1.94	0.48
1:A:459:THR:HG22	1:A:461:GLU:H	1.78	0.48
1:A:287:ILE:HG13	1:A:287:ILE:O	2.13	0.48
1:A:508:GLU:CB	1:A:509:PRO:CD	2.87	0.48
1:A:349[A]:ARG:NH1	1:A:349[A]:ARG:CG	2.60	0.48
1:A:146:LEU:C	1:A:146:LEU:HD12	2.39	0.48
1:A:230:ASN:HD22	1:A:230:ASN:N	2.06	0.48
1:A:451:PRO:HA	1:A:458:TYR:CD2	2.50	0.47
1:A:288:PHE:C	1:A:289:ARG:HG2	2.38	0.47
1:A:35:PHE:CD2	1:A:97:LEU:HD23	2.49	0.47
1:A:248:LEU:HD21	1:A:274:LEU:HD12	1.95	0.47
1:A:16:MET:HE3	1:A:16:MET:HB3	1.84	0.47
1:A:235:SER:HA	1:A:294:PRO:O	2.15	0.47
1:A:333:LEU:HD22	1:A:333:LEU:O	2.15	0.47
1:A:46:ARG:CZ	1:A:46:ARG:HB3	2.44	0.46
1:A:430:LEU:HD23	1:A:430:LEU:HA	1.73	0.46
1:A:491:LYS:O	1:A:493:PRO:HD3	2.15	0.46
1:A:452:LEU:CD2	1:A:463:GLU:HG2	2.45	0.46
1:A:110:THR:HG23	1:A:193:THR:HG22	1.96	0.46
1:A:304:SER:O	1:A:305:LEU:C	2.58	0.46
1:A:27:ILE:HG23	1:A:28:SER:N	2.31	0.46
1:A:38:PRO:HA	1:A:39:PRO:HD3	1.78	0.46
1:A:505:LEU:HD12	1:A:505:LEU:HA	1.63	0.45
1:A:410:LYS:HA	1:A:413[A]:LYS:HZ3	1.81	0.45
1:A:349[A]:ARG:HG3	1:A:381:ASP:O	2.17	0.45
1:A:388:ARG:HD3	1:A:435:TRP:CE3	2.51	0.45
1:A:110:THR:OG1	1:A:478:LYS:CE	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:HA	1:A:170:LEU:HD12	1.66	0.45
1:A:191:PRO:C	1:A:193:THR:H	2.25	0.45
1:A:330:PHE:CZ	2:A:1536:FP1:C1	2.99	0.44
1:A:42:ASN:HB2	1:A:267:ARG:HD3	1.99	0.44
1:A:499:GLU:O	1:A:500:GLN:CB	2.65	0.44
1:A:330:PHE:CE1	2:A:1536:FP1:C2	2.99	0.44
1:A:37:GLU:OE2	1:A:51:LYS:HD2	2.17	0.44
1:A:137:TYR:CD1	1:A:137:TYR:C	2.95	0.44
1:A:490:SER:O	1:A:510:MET:HE3	2.18	0.43
1:A:197:PHE:HB2	1:A:223:ILE:HB	2.00	0.43
1:A:223:ILE:HD13	1:A:223:ILE:HG21	1.74	0.43
1:A:322:GLY:HA3	1:A:421:TYR:CZ	2.53	0.43
1:A:25:SER:HB3	1:A:26:HIS:H	1.54	0.43
1:A:410:LYS:HA	1:A:410:LYS:HD2	1.81	0.43
1:A:135:LEU:HD12	1:A:135:LEU:HA	1.87	0.43
1:A:252:LEU:O	1:A:253:ASN:HB2	2.19	0.42
1:A:380:ASP:C	1:A:382:ASN:N	2.78	0.42
1:A:481:ASN:OD1	1:A:483:ASN:HB2	2.19	0.42
1:A:30:PHE:HB3	1:A:33:ILE:HD11	2.00	0.42
1:A:59:ASN:CB	4:A:1539:NAG:H83	2.48	0.42
1:A:336:ALA:HA	1:A:337:PRO:HD2	1.74	0.42
1:A:184:ILE:HD12	1:A:184:ILE:HA	1.77	0.42
1:A:478:LYS:HB2	1:A:478:LYS:HE3	1.15	0.42
1:A:320:LEU:C	1:A:320:LEU:HD23	2.43	0.42
1:A:432:TRP:HB3	1:A:436:MET:HE1	1.94	0.42
1:A:345:SER:O	1:A:347:ILE:CD1	2.67	0.42
1:A:17:GLY:HA2	1:A:60:ALA:HB3	2.02	0.41
1:A:87:ASN:ND2	1:A:87:ASN:C	2.76	0.41
1:A:197:PHE:CB	1:A:223:ILE:HB	2.50	0.41
1:A:185:GLN:HA	1:A:189:GLY:O	2.21	0.41
1:A:419:TYR:CZ	1:A:494:LEU:CD2	2.99	0.41
1:A:44:ARG:HB3	1:A:267:ARG:HG2	2.02	0.41
1:A:298:GLY:HA2	1:A:301:PHE:O	2.20	0.41
1:A:395:VAL:O	1:A:399:ASN:HB2	2.20	0.41
1:A:468:ARG:HH11	1:A:468:ARG:HD3	1.73	0.41
1:A:518:VAL:CG1	1:A:519:GLN:H	2.30	0.40
1:A:52:LYS:O	1:A:53:PRO:C	2.61	0.40
1:A:95:LEU:HA	1:A:95:LEU:HD23	1.70	0.40
1:A:200:SER:HB3	1:A:440:HIS:HE1	1.83	0.40
1:A:225:GLN:HB3	1:A:225:GLN:HE21	1.56	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	528/543 (97%)	473 (90%)	45 (8%)	10 (2%)	6	15

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	SER
1	A	380	ASP
1	A	519	GLN
1	A	74	GLN
1	A	457	ASN
1	A	500	GLN
1	A	11	LYS
1	A	472	TYR
1	A	159	HIS
1	A	470	MET

5.3.2 Protein sidechains [i](#)

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	465/474 (98%)	378 (81%)	87 (19%)	1	4

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU

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Mol	Chain	Res	Type
1	A	7	LEU
1	A	14	LYS
1	A	15	VAL
1	A	16	MET
1	A	19	ARG
1	A	22	VAL
1	A	23	LEU
1	A	25	SER
1	A	27	ILE
1	A	28	SER
1	A	31	LEU
1	A	43	MET
1	A	46	ARG
1	A	51	LYS
1	A	62	THR
1	A	87	ASN
1	A	89	GLU
1	A	98	ASN
1	A	99	ILE
1	A	108	SER
1	A	125	SER
1	A	128	ASP
1	A	129	VAL
1	A	140	GLU
1	A	143	LEU
1	A	144	VAL
1	A	146	LEU
1	A	161	SER
1	A	168	VAL
1	A	170	LEU
1	A	175	MET
1	A	177	LEU
1	A	192	LYS
1	A	194	VAL
1	A	225	GLN
1	A	230	ASN
1	A	238	VAL
1	A	242	ARG
1	A	243	ARG
1	A	246	VAL
1	A	251	ASN
1	A	258	SER

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Mol	Chain	Res	Type
1	A	262	LEU
1	A	269	LYS
1	A	275	ILE
1	A	278	GLU
1	A	293	VAL
1	A	295	VAL
1	A	305	LEU
1	A	318	GLN
1	A	321	LEU
1	A	325	LYS
1	A	333	LEU
1	A	340	SER
1	A	347	ILE
1	A	349[A]	ARG
1	A	349[B]	ARG
1	A	354	SER
1	A	357	LYS
1	A	362	HIS
1	A	382	ASN
1	A	385	ILE
1	A	410	LYS
1	A	412	THR
1	A	413[A]	LYS
1	A	413[B]	LYS
1	A	430	LEU
1	A	453	VAL
1	A	454	LYS
1	A	455	GLU
1	A	456	LEU
1	A	463	GLU
1	A	469	ILE
1	A	478	LYS
1	A	479	THR
1	A	484	GLU
1	A	491	LYS
1	A	510	MET
1	A	514	GLN
1	A	515	ARG
1	A	518	VAL
1	A	519	GLN
1	A	520	MET
1	A	522	VAL

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Mol	Chain	Res	Type
1	A	528	LEU
1	A	533	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	66	ASN
1	A	74	GLN
1	A	87	ASN
1	A	209	HIS
1	A	225	GLN
1	A	230	ASN
1	A	251	ASN
1	A	324	ASN
1	A	362	HIS
1	A	483	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
2	FP1	A	1536	-	9,10,10	5.68	5 (55%)	8,12,12	3.23	3 (37%)
3	SO4	A	1537	-	4,4,4	0.48	0	6,6,6	1.21	1 (16%)
4	NAG	A	1538	1	14,14,15	1.43	1 (7%)	17,19,21	3.47	10 (58%)
4	NAG	A	1539	1	14,14,15	1.17	2 (14%)	17,19,21	2.90	11 (64%)

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
2	FP1	A	1536	-	-	0/0/3/3	0/1/1/1
4	NAG	A	1539	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1538	1	1/1/5/7	2/6/23/26	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1536	FP1	C6-N2	13.07	1.47	1.30
2	A	1536	FP1	C6-C5	9.14	1.54	1.40
2	A	1536	FP1	C5-N1	4.11	1.43	1.38
4	A	1538	NAG	C4-C5	3.24	1.59	1.53
4	A	1539	NAG	C1-C2	2.96	1.56	1.52
2	A	1536	FP1	C1-C2	2.65	1.40	1.35
2	A	1536	FP1	C1-N1	2.54	1.42	1.36
4	A	1539	NAG	C4-C5	2.06	1.57	1.53

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1536	FP1	C5-C6-N2	-8.39	109.89	126.83
4	A	1538	NAG	C1-O5-C5	8.06	122.99	112.19
4	A	1538	NAG	C3-C4-C5	-6.11	99.16	110.23
4	A	1539	NAG	C2-N2-C7	5.51	130.28	122.90
4	A	1538	NAG	O4-C4-C5	5.13	121.96	109.32
4	A	1538	NAG	C6-C5-C4	4.68	124.52	113.02
4	A	1539	NAG	C3-C4-C5	4.01	117.49	110.23
4	A	1539	NAG	C4-C3-C2	3.87	116.69	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1539	NAG	C8-C7-N2	3.54	122.00	116.12
4	A	1538	NAG	C2-N2-C7	3.53	127.64	122.90
4	A	1539	NAG	O3-C3-C4	-3.40	102.36	110.38
4	A	1538	NAG	O3-C3-C2	3.23	116.11	109.40
4	A	1539	NAG	C1-O5-C5	3.17	116.44	112.19
4	A	1539	NAG	O4-C4-C5	3.17	117.13	109.32
4	A	1539	NAG	O4-C4-C3	-2.89	103.57	110.38
4	A	1539	NAG	O7-C7-C8	-2.57	117.48	122.05
4	A	1539	NAG	O5-C5-C4	2.56	117.06	110.83
4	A	1538	NAG	O3-C3-C4	2.51	116.30	110.38
4	A	1539	NAG	C1-C2-N2	2.49	114.36	110.43
4	A	1538	NAG	O5-C1-C2	2.47	115.12	111.29
4	A	1538	NAG	C8-C7-N2	-2.24	112.41	116.12
4	A	1538	NAG	C1-C2-N2	2.19	113.88	110.43
3	A	1537	SO4	O3-S-O1	2.17	120.89	109.56
2	A	1536	FP1	C7-N1-C1	-2.05	116.56	120.41
2	A	1536	FP1	C2-C1-N1	-2.05	119.08	121.45

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1538	NAG	C1

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1539	NAG	O5-C5-C6-O6
4	A	1538	NAG	C8-C7-N2-C2
4	A	1539	NAG	C8-C7-N2-C2
4	A	1539	NAG	O7-C7-N2-C2
4	A	1538	NAG	O7-C7-N2-C2
4	A	1539	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1536	FP1	10	0
4	A	1539	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	284:PHE	C	285:ASP	N	1.19
1	A	114:TRP	C	115:ILE	N	1.18
1	A	287:ILE	C	288:PHE	N	1.12

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	529/543 (97%)	-0.96	3 (0%) 85 85	7, 23, 48, 70	4 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	485[A]	PRO	6.9
1	A	486[A]	HIS	4.0
1	A	284	PHE	2.4

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
4	NAG	A	1539	14/15	0.71	0.21	94,100,101,101	0
2	FP1	A	1536	10/10	0.78	0.20	20,20,20,20	10
4	NAG	A	1538	14/15	0.85	0.11	57,61,64,65	0
3	SO4	A	1537	5/5	0.99	0.08	28,29,31,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.