



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:37 AM GMT

PDB ID : 2XQF  
Title : X-RAY STRUCTURE OF HUMAN BUTYRYLCHOLINESTERASE INHIBITED BY RACEMIC VX  
Authors : Wandhammer, M.; Carletti, E.; Gillon, E.; Masson, P.; Goeldner, M.; Noort, D.; Nachon, F.  
Deposited on : 2010-09-02  
Resolution : 2.10 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

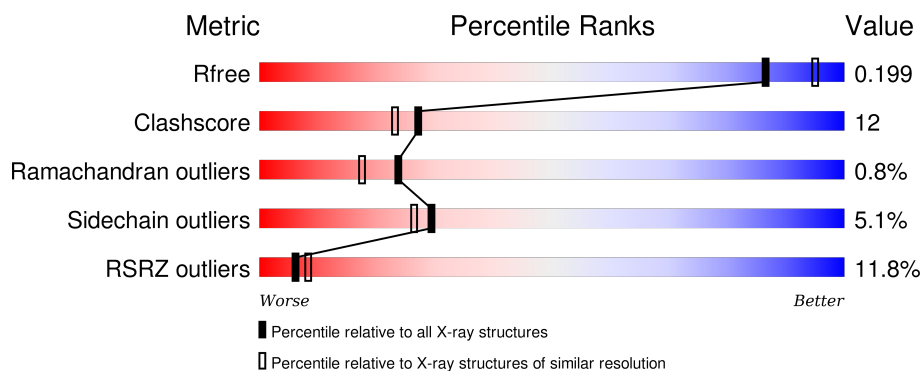
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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))
$R_{free}$	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	527	<div> <div>12%</div> <div>79%</div> <div>16%</div> <div>5%</div> </div>

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
10	NAG	A	1543	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UNX	A	1554	-	-	X	-
3	UNX	A	1562	-	-	-	X
3	UNX	A	1565	-	-	-	X
3	UNX	A	1567	-	-	-	X
3	UNX	A	1583	-	-	-	X
8	SO4	A	1537	-	-	-	X
9	NAG	A	1545	X	-	-	-
9	FUL	A	1547	-	-	-	X

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 4894 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.

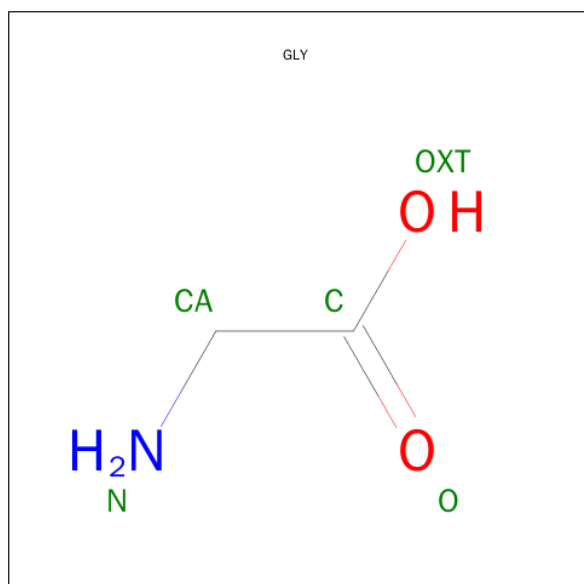
- Molecule 1 is a protein called CHOLINESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	11	0
			4269	2759	712	782	16			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	455	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	481	GLN	ASN	ENGINEERED MUTATION	UNP P06276
A	486	GLN	ASN	ENGINEERED MUTATION	UNP P06276

- Molecule 2 is GLYCINE (three-letter code: GLY) (formula: C<sub>2</sub>H<sub>5</sub>NO<sub>2</sub>).

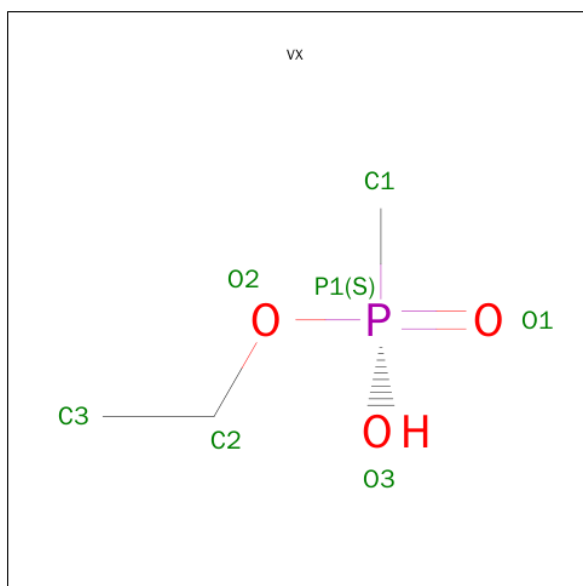


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			5	2	1	2		

- Molecule 3 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	36	Total X 36 36	0	0

- Molecule 4 is O-ETHYLMETHYLPHOSPHONIC ACID ESTER GROUP (three-letter code: VX) (formula: C<sub>3</sub>H<sub>9</sub>O<sub>3</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O P 6 3 2 1	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total K 1 1	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

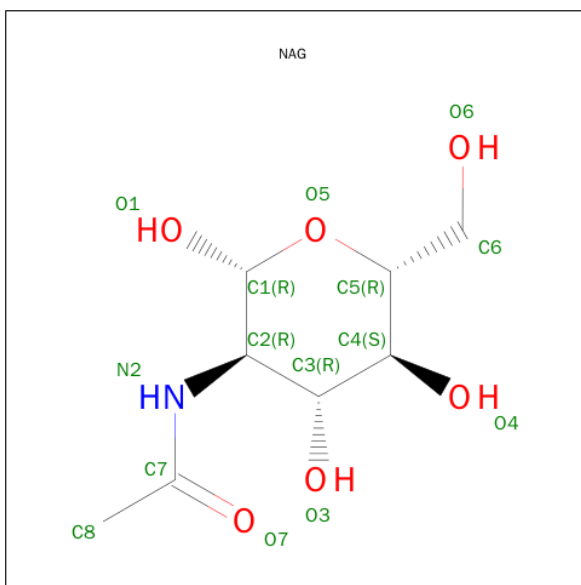


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total O S 5 4 1	0	0
8	A	1	Total O S 5 4 1	0	0

- Molecule 9 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	3	Total C N O 38 22 2 14	0	0
9	A	3	Total C N O 38 22 2 14	0	0

- Molecule 10 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	A	1	Total	C	N	O	0	0
			14	8	1	5		
10	A	1	Total	C	N	O	0	0
			14	8	1	5		

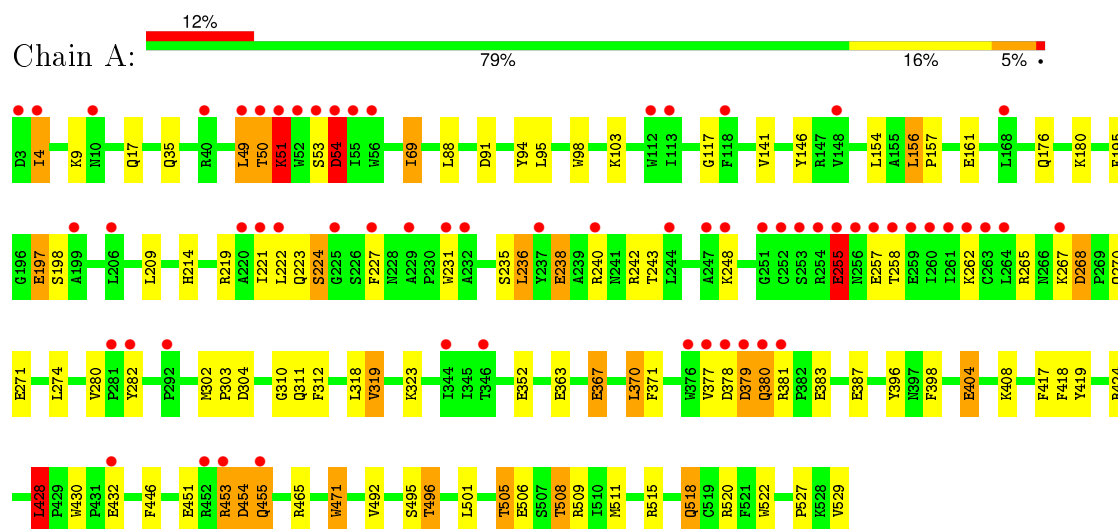
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	432	Total	O	0	0
			432	432		

### 3 Residue-property plots [i](#)

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

#### • Molecule 1: CHOLINESTERASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.11Å 155.11Å 128.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.00 – 2.10 47.95 – 2.39	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.00-2.10) 99.6 (47.95-2.39)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.12 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.149 , 0.189 0.199 , 0.199	Depositor DCC
$R_{free}$ test set	1242 reflections (4.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.4	Xtriage
Anisotropy	0.762	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 49.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 31041 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4894	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, CL, UNX, NA, K, SO4, VX, FUL

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	1.54	24/4419 (0.5%)	1.08	21/5997 (0.4%)

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
9	A	1	0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	455[A]	GLN	CD-NE2	29.84	2.07	1.32
1	A	455[B]	GLN	CD-NE2	29.84	2.07	1.32
1	A	471	TRP	CB-CG	8.46	1.65	1.50
1	A	219	ARG	CG-CD	7.64	1.71	1.51
1	A	396	TYR	CD1-CE1	6.89	1.49	1.39
1	A	371	PHE	CE1-CZ	6.46	1.49	1.37
1	A	282	TYR	CE1-CZ	6.18	1.46	1.38
1	A	396	TYR	CD2-CE2	6.02	1.48	1.39
1	A	455[A]	GLN	CA-CB	6.00	1.67	1.53
1	A	455[B]	GLN	CA-CB	6.00	1.67	1.53
1	A	197	GLU	CB-CG	5.89	1.63	1.52
1	A	515	ARG	CZ-NH1	5.82	1.40	1.33
1	A	141	VAL	CB-CG2	5.61	1.64	1.52
1	A	146	TYR	CD2-CE2	5.60	1.47	1.39
1	A	465	ARG	CZ-NH1	5.58	1.40	1.33
1	A	398	PHE	CD1-CE1	5.42	1.50	1.39
1	A	419	TYR	CD1-CE1	5.34	1.47	1.39
1	A	404	GLU	CG-CD	5.33	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	TYR	CD1-CE1	5.32	1.47	1.39
1	A	319	VAL	CB-CG2	5.24	1.63	1.52
1	A	224	SER	CB-OG	5.18	1.49	1.42
1	A	255	GLU	CB-CG	5.11	1.61	1.52
1	A	446	PHE	CE1-CZ	5.06	1.47	1.37
1	A	221	ILE	CB-CG2	5.04	1.68	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	219	ARG	NE-CZ-NH1	-10.75	114.92	120.30
1	A	515	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	A	515	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	A	370	LEU	CA-CB-CG	6.99	131.38	115.30
1	A	465	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	A	154	LEU	CB-CG-CD1	-6.72	99.58	111.00
1	A	465	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	A	265	ARG	NE-CZ-NH1	-6.47	117.06	120.30
1	A	49	LEU	CB-CG-CD2	-6.45	100.04	111.00
1	A	508	THR	N-CA-CB	-6.42	98.10	110.30
1	A	455[A]	GLN	CG-CD-NE2	-6.07	102.12	116.70
1	A	455[B]	GLN	CG-CD-NE2	-6.07	102.12	116.70
1	A	219	ARG	CG-CD-NE	-5.97	99.27	111.80
1	A	103	LYS	CD-CE-NZ	-5.71	98.57	111.70
1	A	455[A]	GLN	OE1-CD-NE2	5.55	134.66	121.90
1	A	455[B]	GLN	OE1-CD-NE2	5.55	134.66	121.90
1	A	424	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	A	54	ASP	CB-CG-OD1	5.08	122.88	118.30
1	A	91	ASP	CB-CG-OD1	5.07	122.86	118.30
1	A	428	LEU	CA-CB-CG	5.05	126.92	115.30
1	A	302	MET	CG-SD-CE	-5.01	92.19	100.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	1545	NAG	C1

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	4269	0	4183	99	0
2	A	5	0	2	1	0
3	A	36	0	0	4	0
4	A	6	0	8	2	0
5	A	1	0	0	0	0
6	A	2	0	0	0	0
7	A	1	0	0	0	0
8	A	10	0	0	0	0
9	A	76	0	67	2	0
10	A	56	0	52	1	0
11	A	432	0	0	28	4
All	All	4894	0	4312	105	4

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 12.

All (105) 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:453:ARG:HH11	1:A:453:ARG:CG	1.47	1.27
1:A:495:SER:HA	11:A:2385:HOH:O	1.51	1.10
1:A:453:ARG:HG2	1:A:453:ARG:NH1	1.33	1.09
1:A:455[A]:GLN:NE2	1:A:455[A]:GLN:CD	2.07	1.08
1:A:4:ILE:H	1:A:4:ILE:HD12	1.23	1.01
1:A:35:GLN:HG2	11:A:2025:HOH:O	1.59	0.99
1:A:496:THR:N	11:A:2385:HOH:O	1.75	0.99
1:A:495:SER:CA	11:A:2385:HOH:O	2.03	0.98
1:A:4:ILE:N	1:A:4:ILE:HD12	1.82	0.94
1:A:268:ASP:HB2	11:A:2199:HOH:O	1.66	0.94
1:A:518:GLN:H	1:A:518:GLN:HE21	1.18	0.92
1:A:255:GLU:CD	1:A:255:GLU:H	1.75	0.90
1:A:451:GLU:OE1	11:A:2345:HOH:O	1.92	0.87
1:A:176[B]:GLN:HE21	1:A:180:LYS:HG3	1.40	0.85
1:A:505:THR:HG21	11:A:2153:HOH:O	1.77	0.85
1:A:380:GLN:HA	1:A:380:GLN:NE2	1.97	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:LYS:HE3	11:A:2197:HOH:O	1.80	0.79
1:A:304:ASP:HB3	11:A:2091:HOH:O	1.84	0.78
1:A:156:LEU:HD13	1:A:243:THR:HG21	1.64	0.78
1:A:453:ARG:HH11	1:A:453:ARG:HG2	0.65	0.76
1:A:311:GLN:NE2	11:A:2238:HOH:O	1.91	0.75
1:A:453:ARG:NH1	1:A:453:ARG:CG	2.18	0.73
1:A:380:GLN:HA	1:A:380:GLN:HE21	1.54	0.73
1:A:379:ASP:O	1:A:380:GLN:NE2	2.23	0.72
1:A:408:LYS:HE3	11:A:2311:HOH:O	1.90	0.71
1:A:495:SER:O	1:A:496:THR:OG1	2.08	0.71
1:A:451:GLU:OE2	11:A:2343:HOH:O	2.10	0.69
1:A:404:GLU:HG2	11:A:2184:HOH:O	1.93	0.69
1:A:117:GLY:HA2	4:A:1530:VX:H22	1.73	0.69
1:A:4:ILE:CD1	1:A:4:ILE:H	2.03	0.68
1:A:98:TRP:HE1	2:A:1531:GLY:N	1.92	0.68
1:A:176[B]:GLN:NE2	1:A:180:LYS:HG3	2.08	0.67
1:A:323:LYS:HE2	11:A:2250:HOH:O	1.94	0.67
3:A:1580:UNX:UNK	3:A:1581:UNX:UNK	1.38	0.67
1:A:248:LYS:HD3	9:A:1547:FUL:H61	1.75	0.67
1:A:4:ILE:N	1:A:4:ILE:CD1	2.55	0.67
1:A:377:VAL:HA	1:A:378:ASP:HB2	1.77	0.65
1:A:311:GLN:HB3	11:A:2238:HOH:O	1.95	0.65
1:A:238[A]:GLU:OE1	1:A:242:ARG:NE	2.25	0.65
1:A:518:GLN:H	1:A:518:GLN:NE2	1.92	0.64
1:A:381:ARG:HB3	1:A:383:GLU:OE1	1.98	0.63
3:A:1554:UNX:UNK	3:A:1562:UNX:UNK	1.44	0.61
1:A:53:SER:O	1:A:54:ASP:OD1	2.18	0.61
1:A:408:LYS:HG3	11:A:2311:HOH:O	2.00	0.60
1:A:267:LYS:HE3	1:A:271:GLU:OE2	2.02	0.60
1:A:304:ASP:OD1	11:A:2232:HOH:O	2.16	0.59
1:A:176[B]:GLN:NE2	1:A:180:LYS:HE3	2.18	0.58
1:A:51:LYS:N	11:A:2044:HOH:O	2.36	0.58
1:A:270:GLN:OE1	1:A:274:LEU:CD1	2.53	0.57
1:A:255:GLU:CD	1:A:255:GLU:N	2.55	0.57
1:A:270:GLN:OE1	1:A:274:LEU:HD13	2.05	0.56
10:A:1542:NAG:H83	11:A:2047:HOH:O	2.05	0.56
1:A:227:PHE:CD1	1:A:227:PHE:C	2.79	0.55
1:A:209:LEU:HD12	1:A:312:PHE:HB3	1.88	0.54
1:A:522:TRP:O	1:A:527:PRO:HD3	2.07	0.54
1:A:227:PHE:CE1	1:A:303:PRO:HB2	2.42	0.54
1:A:235:SER:OG	1:A:238[B]:GLU:HG3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:509:ARG:NH1	11:A:2403:HOH:O	2.24	0.53
1:A:238[A]:GLU:CD	1:A:242:ARG:HE	2.12	0.53
1:A:363:GLU:O	1:A:367[B]:GLU:HG3	2.09	0.53
1:A:50:THR:O	1:A:51:LYS:HB3	2.09	0.53
1:A:53:SER:O	1:A:54:ASP:CG	2.48	0.52
1:A:432[B]:GLU:HG2	11:A:2334:HOH:O	2.08	0.52
1:A:198:SER:HA	1:A:224:SER:O	2.12	0.50
1:A:238[A]:GLU:OE1	1:A:242:ARG:HG3	2.12	0.49
1:A:383:GLU:O	1:A:387:GLU:HG3	2.13	0.48
1:A:69:ILE:HD11	1:A:88:LEU:HD11	1.95	0.48
1:A:50:THR:O	1:A:51:LYS:CB	2.63	0.47
1:A:161:GLU:HG3	1:A:258:THR:HG23	1.97	0.47
1:A:318:LEU:HD23	1:A:318:LEU:C	2.35	0.47
1:A:231:TRP:CE3	4:A:1530:VX:H21	2.50	0.47
1:A:511[B]:MET:CE	11:A:2320:HOH:O	2.63	0.46
1:A:236:LEU:HA	1:A:236:LEU:HD12	1.81	0.46
1:A:495:SER:O	1:A:496:THR:CB	2.63	0.46
1:A:352:GLU:HG3	11:A:2268:HOH:O	2.15	0.46
1:A:501:LEU:HD11	1:A:508:THR:HG22	1.97	0.45
1:A:176[B]:GLN:HE21	1:A:180:LYS:HE3	1.82	0.45
1:A:267:LYS:HE3	1:A:271:GLU:CD	2.37	0.45
1:A:267:LYS:CE	1:A:271:GLU:CD	2.85	0.45
1:A:319:VAL:O	1:A:418:PHE:HA	2.17	0.44
1:A:197:GLU:HA	1:A:223:GLN:O	2.17	0.44
1:A:255:GLU:N	1:A:255:GLU:OE1	2.44	0.44
1:A:455[A]:GLN:NE2	1:A:455[A]:GLN:CG	2.80	0.44
1:A:157:PRO:CD	1:A:240:ARG:HG2	2.47	0.44
1:A:17:GLN:HE21	1:A:17:GLN:HA	1.83	0.44
3:A:1577:UNX:UNK	3:A:1578:UNX:UNK	1.60	0.44
1:A:95:LEU:C	1:A:95:LEU:HD12	2.38	0.43
1:A:428:LEU:HD13	1:A:430:TRP:HB2	2.01	0.43
1:A:454:ASP:O	1:A:455[A]:GLN:HB2	2.18	0.43
1:A:214:HIS:HE1	11:A:2245:HOH:O	2.00	0.43
1:A:520:ARG:NH2	11:A:2416:HOH:O	2.52	0.42
1:A:157:PRO:HD3	1:A:240:ARG:HG2	2.01	0.42
1:A:240:ARG:NH1	1:A:257:GLU:OE2	2.53	0.42
1:A:417:PHE:CE2	1:A:492:VAL:HG12	2.54	0.42
1:A:451:GLU:OE1	11:A:2344:HOH:O	2.22	0.42
3:A:1554:UNX:UNK	3:A:1555:UNX:UNK	1.64	0.41
1:A:501:LEU:HD11	1:A:508:THR:CG2	2.50	0.41
1:A:505:THR:HG23	1:A:506[B]:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LEU:N	1:A:222:LEU:HD12	2.36	0.41
1:A:454:ASP:OD2	11:A:2348:HOH:O	2.22	0.40
1:A:378:ASP:O	1:A:379:ASP:O	2.39	0.40
9:A:1546:NAG:H5	9:A:1546:NAG:N2	2.36	0.40
1:A:453:ARG:HG3	11:A:2345:HOH:O	2.20	0.40
1:A:156:LEU:HA	1:A:156:LEU:HD12	1.76	0.40
1:A:310:GLY:HA2	1:A:312:PHE:CE2	2.56	0.40

All (4) 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)
11:A:2240:HOH:O	11:A:2365:HOH:O[3_555]	1.86	0.34
11:A:2239:HOH:O	11:A:2365:HOH:O[3_555]	2.05	0.15
11:A:2179:HOH:O	11:A:2239:HOH:O[4_555]	2.14	0.06
11:A:2233:HOH:O	11:A:2368:HOH:O[3_555]	2.19	0.01

## 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	536/527 (102%)	516 (96%)	16 (3%)	4 (1%)	26 21

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	379	ASP
1	A	496	THR
1	A	51	LYS
1	A	54	ASP

### 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	463/452 (102%)	438 (95%)	25 (5%)	27	24

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	9	LYS
1	A	49	LEU
1	A	50	THR
1	A	51	LYS
1	A	69	ILE
1	A	156	LEU
1	A	195	PHE
1	A	236	LEU
1	A	238[A]	GLU
1	A	238[B]	GLU
1	A	255	GLU
1	A	268	ASP
1	A	280	VAL
1	A	367[A]	GLU
1	A	367[B]	GLU
1	A	370	LEU
1	A	380	GLN
1	A	428	LEU
1	A	453	ARG
1	A	454	ASP
1	A	471	TRP
1	A	505	THR
1	A	518	GLN
1	A	529	VAL

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



Mol	Chain	Res	Type
1	A	17	GLN
1	A	214	HIS
1	A	275	ASN
1	A	289	ASN
1	A	311	GLN
1	A	380	GLN
1	A	518	GLN

### 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 ⓘ

6 carbohydrates 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	$\# Z  > 2$
9	NAG	A	1538	1,9	14,14,15	1.66	3 (21%)	15,19,21	1.92	4 (26%)
9	NAG	A	1539	9	14,14,15	0.58	0	15,19,21	2.38	5 (33%)
9	FUL	A	1540	9	10,10,11	1.14	1 (10%)	14,14,16	3.96	5 (35%)
9	NAG	A	1545	1,9	14,14,15	0.78	0	15,19,21	2.13	5 (33%)
9	NAG	A	1546	9	14,14,15	1.50	2 (14%)	15,19,21	2.59	5 (33%)
9	FUL	A	1547	9	10,10,11	0.78	0	14,14,16	3.00	5 (35%)

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
9	NAG	A	1538	1,9	-	0/6/23/26	0/1/1/1
9	NAG	A	1539	9	-	0/6/23/26	0/1/1/1
9	FUL	A	1540	9	-	0/0/17/20	0/1/1/1
9	NAG	A	1545	1,9	1/1/5/7	0/6/23/26	0/1/1/1
9	NAG	A	1546	9	-	0/6/23/26	0/1/1/1
9	FUL	A	1547	9	-	0/0/17/20	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1538	NAG	C2-N2	-3.31	1.40	1.46
9	A	1538	NAG	O5-C1	-3.16	1.38	1.43
9	A	1540	FUL	C4-C5	2.17	1.57	1.52
9	A	1546	NAG	C2-N2	2.69	1.51	1.46
9	A	1538	NAG	C1-C2	3.05	1.56	1.52
9	A	1546	NAG	C1-C2	4.37	1.58	1.52

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1540	FUL	C1-C2-C3	-11.48	95.96	109.54
9	A	1547	FUL	C1-C2-C3	-7.00	101.26	109.54
9	A	1540	FUL	C1-O5-C5	-6.34	102.59	112.38
9	A	1539	NAG	C3-C4-C5	-6.05	99.65	110.20
9	A	1547	FUL	C1-O5-C5	-5.76	103.48	112.38
9	A	1538	NAG	C3-C4-C5	-4.24	102.80	110.20
9	A	1539	NAG	C2-N2-C7	-3.24	118.87	123.04
9	A	1540	FUL	O5-C1-C2	-2.63	106.60	110.86
9	A	1545	NAG	O3-C3-C4	-2.18	105.43	110.34
9	A	1546	NAG	C4-C3-C2	-2.18	107.84	111.23
9	A	1545	NAG	C8-C7-N2	2.09	120.10	116.11
9	A	1546	NAG	O7-C7-N2	2.13	126.21	121.86
9	A	1538	NAG	C6-C5-C4	2.24	118.54	113.02
9	A	1539	NAG	O4-C4-C3	2.31	115.55	110.34
9	A	1539	NAG	O3-C3-C2	2.35	113.76	109.11
9	A	1538	NAG	C2-N2-C7	2.49	126.24	123.04
9	A	1540	FUL	C6-C5-C4	2.50	118.00	113.08
9	A	1546	NAG	O5-C5-C6	2.75	113.30	107.35
9	A	1546	NAG	O3-C3-C4	2.87	116.80	110.34
9	A	1545	NAG	C2-N2-C7	3.05	126.95	123.04
9	A	1539	NAG	O5-C5-C6	3.14	114.16	107.35
9	A	1545	NAG	C3-C2-N2	3.17	118.14	110.56
9	A	1538	NAG	C1-O5-C5	3.20	116.31	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	1547	FUL	C3-C4-C5	3.22	115.14	109.72
9	A	1547	FUL	O5-C5-C6	3.25	111.51	106.13
9	A	1547	FUL	O2-C2-C1	3.58	116.39	109.21
9	A	1540	FUL	O5-C5-C6	4.95	114.32	106.13
9	A	1545	NAG	C1-O5-C5	5.78	119.58	112.25
9	A	1546	NAG	C2-N2-C7	7.86	133.13	123.04

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	A	1545	NAG	C1

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1546	NAG	1	0
9	A	1547	FUL	1	0

## 5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 36 are unknown and 4 are monoatomic - leaving 8 for Mogul analysis.

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	VX	A	1530	1	1,5,6	0.71	0	1,5,8	0.14	0
2	GLY	A	1531	-	1,4,4	0.61	0	0,4,4	0.00	-
8	SO4	A	1536	-	4,4,4	1.37	0	6,6,6	0.52	0
8	SO4	A	1537	-	4,4,4	0.41	0	6,6,6	0.38	0
10	NAG	A	1541	1	14,14,15	1.46	2 (14%)	15,19,21	2.19	5 (33%)
10	NAG	A	1542	1	14,14,15	0.87	0	15,19,21	3.17	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	NAG	A	1543	1	14,14,15	1.15	1 (7%)	15,19,21	2.20	4 (26%)
10	NAG	A	1544	1	14,14,15	0.83	1 (7%)	15,19,21	1.82	3 (20%)

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	VX	A	1530	1	-	0/1/3/4	0/0/0/0
2	GLY	A	1531	-	-	0/0/2/2	0/0/0/0
8	SO4	A	1536	-	-	0/0/0/0	0/0/0/0
8	SO4	A	1537	-	-	0/0/0/0	0/0/0/0
10	NAG	A	1541	1	-	0/6/23/26	0/1/1/1
10	NAG	A	1542	1	-	0/6/23/26	0/1/1/1
10	NAG	A	1543	1	-	0/6/23/26	0/1/1/1
10	NAG	A	1544	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	A	1544	NAG	C1-C2	2.16	1.55	1.52
10	A	1541	NAG	C2-N2	2.34	1.50	1.46
10	A	1543	NAG	C1-C2	2.40	1.55	1.52
10	A	1541	NAG	C1-C2	3.40	1.57	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1541	NAG	O7-C7-C8	-4.13	114.49	122.06
10	A	1542	NAG	O7-C7-C8	-2.35	117.75	122.06
10	A	1542	NAG	C3-C4-C5	2.07	113.81	110.20
10	A	1542	NAG	O4-C4-C5	2.08	114.74	109.24
10	A	1544	NAG	O3-C3-C2	2.13	113.33	109.11
10	A	1543	NAG	C4-C3-C2	2.23	114.70	111.23
10	A	1543	NAG	O7-C7-N2	2.68	127.33	121.86
10	A	1541	NAG	C6-C5-C4	2.71	119.70	113.02
10	A	1541	NAG	C3-C2-N2	2.83	117.33	110.56
10	A	1542	NAG	C8-C7-N2	3.04	121.93	116.11
10	A	1541	NAG	C2-N2-C7	3.53	127.58	123.04
10	A	1543	NAG	O5-C5-C6	3.73	115.42	107.35
10	A	1544	NAG	C2-N2-C7	3.79	127.91	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	A	1544	NAG	C1-O5-C5	3.81	117.08	112.25
10	A	1541	NAG	C8-C7-N2	4.31	124.34	116.11
10	A	1543	NAG	C1-O5-C5	5.03	118.64	112.25
10	A	1542	NAG	C1-O5-C5	10.96	126.16	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1530	VX	2	0
2	A	1531	GLY	1	0
10	A	1542	NAG	1	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	527/527 (100%)	0.86	62 (11%) 6 8	19, 32, 59, 92	14 (2%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	377	VAL	6.8
1	A	255	GLU	6.3
1	A	50	THR	5.8
1	A	378	ASP	5.7
1	A	54	ASP	5.3
1	A	3	ASP	5.2
1	A	51	LYS	4.8
1	A	379	ASP	4.7
1	A	455[A]	GLN	4.4
1	A	260	ILE	4.3
1	A	55	ILE	4.1
1	A	452	ARG	4.1
1	A	261	ILE	4.0
1	A	262	LYS	3.9
1	A	4	ILE	3.9
1	A	40	ARG	3.6
1	A	253	SER	3.6
1	A	53	SER	3.5
1	A	453	ARG	3.5
1	A	376	TRP	3.4
1	A	282	TYR	3.4
1	A	237	TYR	3.3
1	A	113	ILE	3.3
1	A	52	TRP	3.2
1	A	252	CYS	3.2
1	A	257	GLU	3.1
1	A	259	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	380	GLN	3.1
1	A	240	ARG	3.1
1	A	251	GLY	2.9
1	A	49	LEU	2.9
1	A	263	CYS	2.8
1	A	344	ILE	2.8
1	A	247	ALA	2.8
1	A	281	PRO	2.7
1	A	244	LEU	2.7
1	A	256	ASN	2.7
1	A	10	ASN	2.6
1	A	254	ARG	2.6
1	A	225	GLY	2.5
1	A	168	LEU	2.4
1	A	229	ALA	2.4
1	A	292	PRO	2.4
1	A	227	PHE	2.4
1	A	112	TRP	2.4
1	A	206	LEU	2.3
1	A	56	TRP	2.3
1	A	267	LYS	2.3
1	A	148	VAL	2.3
1	A	248	LYS	2.3
1	A	258	THR	2.2
1	A	381	ARG	2.2
1	A	231	TRP	2.2
1	A	220	ALA	2.2
1	A	221	ILE	2.2
1	A	199	ALA	2.1
1	A	432[A]	GLU	2.1
1	A	346	THR	2.1
1	A	264	LEU	2.1
1	A	232	ALA	2.1
1	A	222	LEU	2.1
1	A	118	PHE	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
9	FUL	A	1547	10/11	0.87	0.46	4.38	73,76,77,80	0
9	NAG	A	1538	14/15	0.94	0.16	-0.19	36,49,55,64	0
9	NAG	A	1546	14/15	0.64	0.55	-	91,95,99,100	0
9	NAG	A	1545	14/15	0.84	0.33	-	65,76,85,86	0
9	NAG	A	1539	14/15	0.87	0.30	-	63,71,75,78	0
9	FUL	A	1540	10/11	0.85	0.30	-	67,72,74,74	0

### 6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	UNX	A	1567	1/1	0.88	0.84	16.60	33,33,33,33	0
3	UNX	A	1583	1/1	0.81	0.41	16.38	45,45,45,45	0
3	UNX	A	1565	1/1	0.89	0.78	13.75	30,30,30,30	0
3	UNX	A	1562	1/1	0.93	0.30	3.24	40,40,40,40	0
10	NAG	A	1543	14/15	0.66	0.27	3.16	48,63,72,73	0
8	SO4	A	1537	5/5	0.89	0.27	2.95	67,70,73,73	5
4	VX	A	1530	6/7	0.89	0.23	1.58	24,30,42,43	0
3	UNX	A	1566	1/1	0.89	0.23	1.34	40,40,40,40	0
2	GLY	A	1531	5/5	0.87	0.16	1.03	32,38,43,47	0
8	SO4	A	1536	5/5	0.95	0.18	0.78	25,29,34,37	5
3	UNX	A	1558	1/1	0.78	0.20	-0.00	47,47,47,47	0
3	UNX	A	1568	1/1	0.83	0.36	-	28,28,28,28	0
3	UNX	A	1574	1/1	0.95	0.16	-	53,53,53,53	0
6	CL	A	1534	1/1	0.96	0.10	-	69,69,69,69	0
3	UNX	A	1577	1/1	0.61	0.45	-	53,53,53,53	0
3	UNX	A	1569	1/1	0.52	0.41	-	35,35,35,35	0
6	CL	A	1533	1/1	0.94	0.08	-	72,72,72,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	UNX	A	1555	1/1	0.97	0.20	-	37,37,37,37	0
10	NAG	A	1542	14/15	0.73	0.41	-	59,69,73,75	0
3	UNX	A	1570	1/1	0.96	0.31	-	37,37,37,37	0
3	UNX	A	1556	1/1	0.86	0.53	-	59,59,59,59	0
3	UNX	A	1586	1/1	0.90	0.30	-	41,41,41,41	0
3	UNX	A	1571	1/1	0.95	0.34	-	39,39,39,39	0
3	UNX	A	1552	1/1	0.60	0.50	-	37,37,37,37	0
3	UNX	A	1572	1/1	0.92	0.29	-	36,36,36,36	0
3	UNX	A	1559	1/1	0.04	0.42	-	27,27,27,27	0
3	UNX	A	1553	1/1	0.82	0.92	-	47,47,47,47	0
3	UNX	A	1584	1/1	0.86	0.17	-	31,31,31,31	0
3	UNX	A	1554	1/1	0.96	0.34	-	41,41,41,41	0
3	UNX	A	1580	1/1	0.89	0.37	-	26,26,26,26	0
3	UNX	A	1573	1/1	0.78	0.84	-	60,60,60,60	0
10	NAG	A	1544	14/15	0.75	0.46	-	78,87,93,94	0
3	UNX	A	1563	1/1	0.75	0.93	-	44,44,44,44	0
3	UNX	A	1561	1/1	0.69	0.47	-	31,31,31,31	0
3	UNX	A	1557	1/1	0.80	0.35	-	61,61,61,61	0
3	UNX	A	1582	1/1	0.88	0.44	-	39,39,39,39	0
3	UNX	A	1585	1/1	0.92	0.27	-	43,43,43,43	0
3	UNX	A	1581	1/1	0.85	0.27	-	35,35,35,35	0
3	UNX	A	1560	1/1	0.32	0.74	-	56,56,56,56	0
3	UNX	A	1564	1/1	0.88	1.36	-	54,54,54,54	0
5	NA	A	1532	1/1	0.90	0.29	-	57,57,57,57	1
3	UNX	A	1578	1/1	0.89	0.31	-	46,46,46,46	0
3	UNX	A	1579	1/1	0.80	0.94	-	54,54,54,54	0
3	UNX	A	1551	1/1	0.53	0.74	-	47,47,47,47	0
3	UNX	A	1575	1/1	0.85	0.20	-	46,46,46,46	0
7	K	A	1535	1/1	0.87	0.14	-	89,89,89,89	1
10	NAG	A	1541	14/15	0.84	0.25	-	57,65,69,71	0
3	UNX	A	1576	1/1	0.96	0.23	-	47,47,47,47	0

## 6.5 Other polymers

There are no such residues in this entry.