



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:43 pm GMT

PDB ID : 1QON  
Title : ACHE FROM DROSOPHILA MELANOGASTER COMPLEX WITH  
TACRINE DERIVATIVE 9-(3-IODOBENZYLAMINO)-1,2,3,4-TETRA  
HYDROACRIDINE  
Authors : Harel, M.; Silman, I.; Sussman, J.L.  
Deposited on : 1999-11-15  
Resolution : 2.72 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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

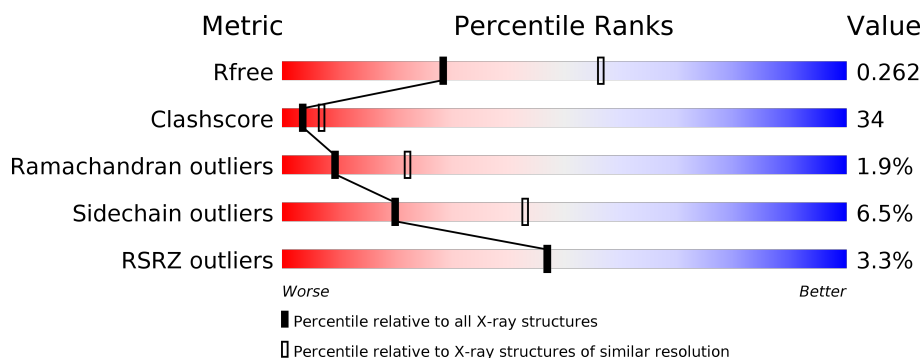
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.72 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))
$R_{free}$	100719	2649 (2.74-2.70)
Clashscore	112137	2993 (2.74-2.70)
Ramachandran outliers	110173	2946 (2.74-2.70)
Sidechain outliers	110143	2947 (2.74-2.70)
RSRZ outliers	101464	2665 (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 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	585	<div> <div>3%</div> <div>45%</div> <div>42%</div> <div>5%</div> <div>8%</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
2	SO4	A	593	-	-	X	-
3	BMA	A	994	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	BMA	A	995	X	-	-	-
3	BMA	A	996	X	-	-	-
4	I40	A	997	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 4486 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
1	A	540	Total	C	N	O	S	0	2	0
			4258	2718	712	803	25			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



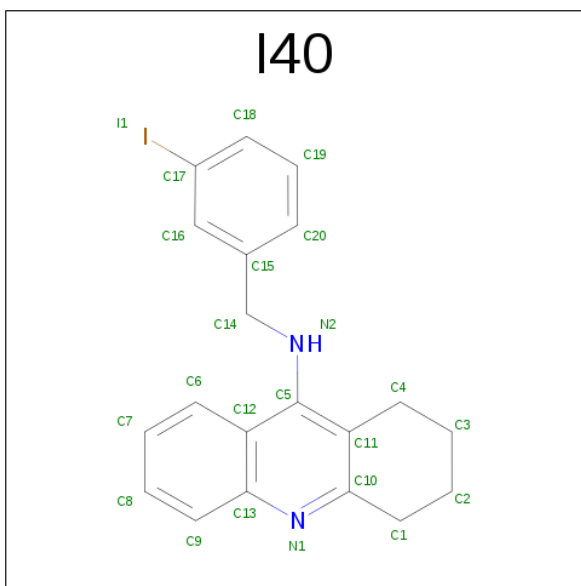
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 4 is 9-(3-IODOBENZYLAMINO)-1,2,3,4-TETRAHYDROACRIDINE (three-letter

code: I40) (formula: C<sub>20</sub>H<sub>19</sub>IN<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	I	N	0	0
			23	20	1	2		

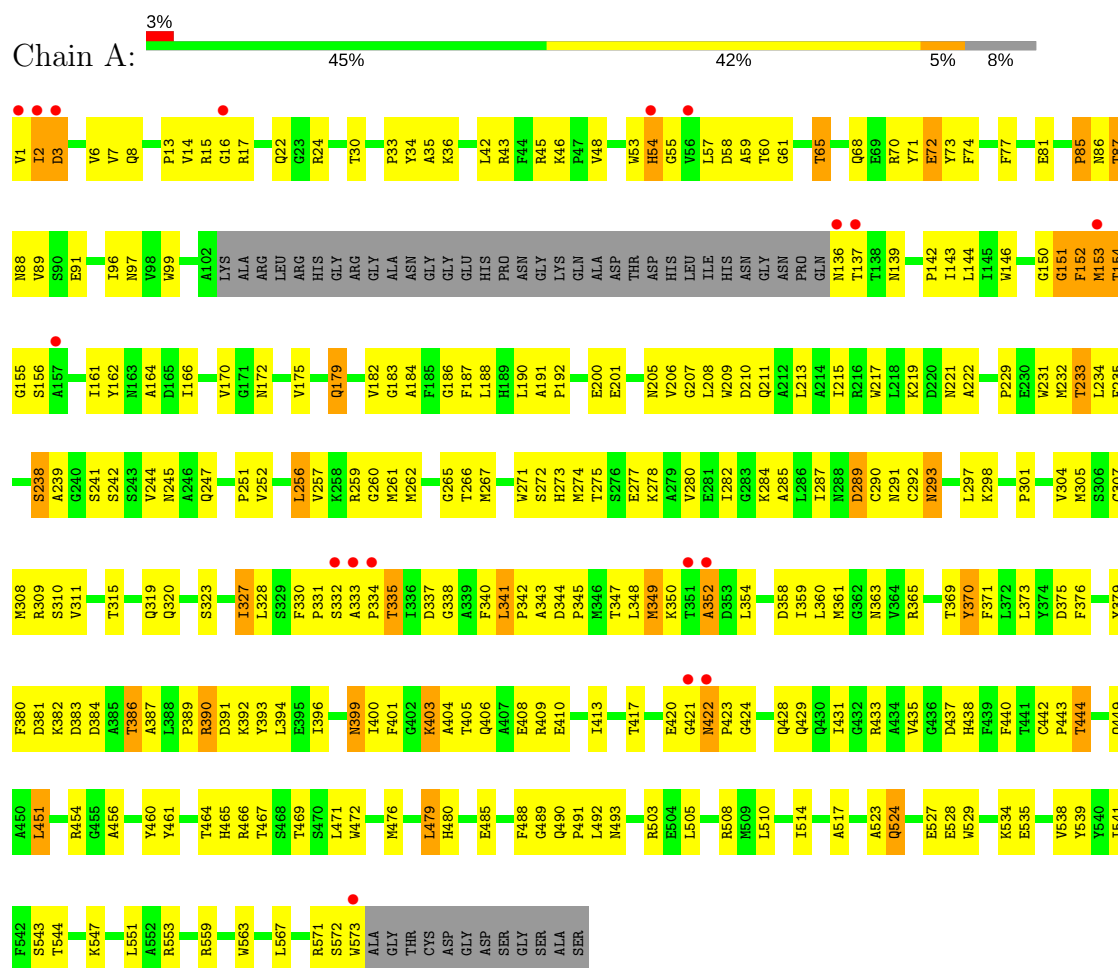
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	139	Total	O	0	0
			139	139		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.93Å 94.93Å 160.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.72 29.50 – 2.71	Depositor EDS
% Data completeness (in resolution range)	96.9 (30.00-2.72) 96.9 (29.50-2.71)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 2.72Å)	Xtriage
Refinement program	CNS 3.8	Depositor
R, $R_{free}$	0.220 , 0.265 0.234 , 0.262	Depositor DCC
$R_{free}$ test set	1698 reflections (9.44%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.2	Xtriage
Anisotropy	0.764	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 54.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	4486	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.29% 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, 0.333 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: BMA, NAG, I40, 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	0.53	4/4379 (0.1%)	0.72	4/5961 (0.1%)

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	2
3	A	3	0
All	All	3	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	151	GLY	C-N	-13.27	1.03	1.34
1	A	352	ALA	C-N	12.00	1.61	1.34
1	A	349	MET	C-N	-9.45	1.12	1.34
1	A	154	THR	C-N	8.84	1.49	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	GLY	C-N-CA	14.46	157.86	121.70
1	A	151	GLY	O-C-N	-14.13	100.09	122.70
1	A	151	GLY	CA-C-N	9.63	138.39	117.20
1	A	153	MET	CG-SD-CE	5.97	109.76	100.20

All (3) chirality outliers are listed below:



Mol	Chain	Res	Type	Atom
3	A	994	BMA	C1
3	A	995	BMA	C1
3	A	996	BMA	C1

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	GLY	Mainchain,Peptide

## 5.2 Too-close contacts [i](#)

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	4258	0	4047	285	0
2	A	5	0	0	5	0
3	A	61	0	52	7	0
4	A	23	0	19	4	0
5	A	139	0	0	10	0
All	All	4486	0	4118	291	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 34.

All (291) 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:344:ASP:OD1	1:A:345:PRO:HD2	1.32	1.28
1:A:153:MET:SD	1:A:183:GLY:HA2	1.81	1.21
1:A:205:ASN:ND2	1:A:337:ASP:OD2	1.81	1.13
1:A:153:MET:CE	1:A:331:PRO:HG2	1.79	1.12
1:A:153:MET:HE2	1:A:331:PRO:HG2	1.28	1.09
1:A:272:SER:O	1:A:334:PRO:CG	2.02	1.08
1:A:344:ASP:OD1	1:A:345:PRO:CD	2.07	1.03
1:A:153:MET:SD	1:A:332:SER:OG	2.18	1.02
1:A:152:PHE:O	1:A:182:VAL:HB	1.63	0.98
1:A:347:THR:HA	1:A:350:LYS:HE2	1.45	0.97
4:A:997:I40:I1	5:A:2138:HOH:O	2.53	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ALA:HB1	1:A:334:PRO:HD2	1.45	0.97
1:A:403:LYS:HD3	1:A:403:LYS:H	1.28	0.96
1:A:485:GLU:HG3	5:A:2110:HOH:O	1.64	0.96
1:A:238:SER:OG	2:A:593:SO4:S	2.25	0.93
1:A:161:ILE:HD11	1:A:485:GLU:HG2	1.50	0.92
1:A:238:SER:HB3	2:A:593:SO4:O2	1.68	0.92
1:A:61:GLY:HA2	3:A:996:BMA:O4	1.72	0.90
1:A:272:SER:O	1:A:334:PRO:HG2	1.71	0.88
1:A:222:ALA:HB3	1:A:229:PRO:HG3	1.53	0.88
1:A:233:THR:HG21	1:A:517:ALA:HA	1.57	0.84
1:A:440:PHE:O	1:A:444:THR:HG23	1.78	0.83
1:A:413:ILE:O	1:A:417:THR:HG23	1.81	0.81
1:A:201:GLU:HG2	1:A:305:MET:HG3	1.65	0.78
1:A:245:ASN:HB2	1:A:262:MET:HE3	1.65	0.76
1:A:179:GLN:HA	1:A:179:GLN:HE21	1.48	0.76
1:A:153:MET:HE3	1:A:331:PRO:HG2	1.67	0.76
1:A:74:PHE:CE2	1:A:382:LYS:HB2	2.21	0.75
1:A:333:ALA:HB1	1:A:334:PRO:CD	2.16	0.75
1:A:403:LYS:CD	1:A:403:LYS:H	2.00	0.74
1:A:297:LEU:HD23	1:A:304:VAL:HG21	1.69	0.74
1:A:152:PHE:O	1:A:182:VAL:CB	2.34	0.73
1:A:272:SER:O	1:A:334:PRO:CD	2.37	0.73
1:A:390:ARG:O	1:A:390:ARG:HD3	1.89	0.72
1:A:262:MET:HE2	1:A:266:THR:HG22	1.70	0.72
1:A:245:ASN:HD22	1:A:267:MET:H	1.37	0.71
1:A:272:SER:O	1:A:334:PRO:HG3	1.92	0.70
1:A:70:ARG:HG2	1:A:85:PRO:HD2	1.73	0.70
1:A:161:ILE:HD11	1:A:485:GLU:CG	2.20	0.69
1:A:347:THR:CA	1:A:350:LYS:HE2	2.20	0.69
1:A:308:MET:HE2	1:A:308:MET:HA	1.74	0.69
1:A:390:ARG:HH21	1:A:417:THR:HG21	1.57	0.68
1:A:376:PHE:HB3	1:A:379:TYR:HD2	1.59	0.68
1:A:74:PHE:HZ	1:A:373:LEU:HD21	1.57	0.68
1:A:280:VAL:HG12	1:A:284:LYS:HE3	1.78	0.66
1:A:343:ALA:H	1:A:348:LEU:HD21	1.60	0.66
1:A:68:GLN:HE22	1:A:155:GLY:H	1.42	0.66
1:A:347:THR:HG22	1:A:350:LYS:HE2	1.78	0.66
1:A:309:ARG:HG2	1:A:309:ARG:HH11	1.62	0.65
1:A:143:ILE:HB	1:A:232:MET:HG2	1.78	0.65
1:A:161:ILE:CD1	1:A:485:GLU:HG2	2.26	0.65
1:A:365:ARG:HB2	1:A:464:THR:HG22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:VAL:HG13	5:A:2001:HOH:O	1.97	0.65
1:A:523:ALA:HB2	1:A:529:TRP:HB3	1.79	0.64
1:A:363:ASN:ND2	1:A:460:TYR:OH	2.30	0.64
1:A:479:LEU:HD23	1:A:479:LEU:H	1.62	0.64
1:A:405:THR:OG1	1:A:408:GLU:HG2	1.98	0.64
4:A:997:I40:H6	4:A:997:I40:H141	1.80	0.64
1:A:238:SER:CB	2:A:593:SO4:O2	2.46	0.63
1:A:8:GLN:NE2	1:A:13:PRO:HB3	2.13	0.63
1:A:488:PHE:HB3	1:A:490:GLN:HE21	1.63	0.63
1:A:161:ILE:HG23	1:A:162:TYR:CD1	2.32	0.63
1:A:390:ARG:NH2	1:A:417:THR:HG21	2.13	0.63
1:A:297:LEU:O	1:A:301:PRO:HG3	1.99	0.62
1:A:1:VAL:O	1:A:2:ILE:HB	1.99	0.62
1:A:238:SER:CB	2:A:593:SO4:S	2.88	0.62
1:A:16:GLY:HA2	1:A:59:ALA:O	2.01	0.61
1:A:373:LEU:C	1:A:373:LEU:HD23	2.21	0.61
1:A:330:PHE:CZ	4:A:997:I40:I1	3.23	0.61
1:A:304:VAL:O	1:A:307:CYS:HB3	2.00	0.61
1:A:505:LEU:HD13	1:A:508:ARG:HH21	1.66	0.61
1:A:1:VAL:HG11	5:A:2002:HOH:O	2.00	0.61
1:A:535:GLU:H	1:A:535:GLU:CD	2.03	0.60
1:A:201:GLU:CG	1:A:305:MET:HG3	2.31	0.60
1:A:234:LEU:HG	1:A:257:VAL:HG11	1.83	0.60
1:A:382:LYS:HE3	1:A:383:ASP:OD1	2.01	0.60
3:A:993:NAG:H61	3:A:994:BMA:O2	2.01	0.60
1:A:87:THR:HG22	1:A:88:ASN:H	1.65	0.60
1:A:390:ARG:NH1	1:A:394:LEU:HD11	2.17	0.60
1:A:349:MET:O	1:A:350:LYS:C	2.34	0.60
1:A:327:ILE:HB	1:A:375:ASP:CG	2.22	0.60
1:A:400:ILE:O	1:A:403:LYS:HE3	2.02	0.59
1:A:406:GLN:O	1:A:410:GLU:HG3	2.03	0.59
1:A:251:PRO:HG3	1:A:342:PRO:HG2	1.85	0.58
1:A:338:GLY:HA2	1:A:342:PRO:HA	1.84	0.58
1:A:380:PHE:HD2	1:A:428:GLN:HE21	1.50	0.58
1:A:251:PRO:HG3	1:A:342:PRO:CG	2.34	0.58
1:A:390:ARG:HH11	1:A:394:LEU:HD11	1.68	0.58
1:A:238:SER:OG	1:A:480:HIS:NE2	2.36	0.58
1:A:205:ASN:OD1	1:A:334:PRO:O	2.22	0.57
1:A:449:GLN:NE2	1:A:534:LYS:HG3	2.18	0.57
1:A:273:HIS:HA	1:A:334:PRO:HD2	1.86	0.57
1:A:179:GLN:HA	1:A:179:GLN:NE2	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:191:ALA:HB3	1:A:192:PRO:HD3	1.87	0.57
1:A:143:ILE:HD11	1:A:222:ALA:HB1	1.86	0.57
1:A:36:LYS:HD3	1:A:48:VAL:HG21	1.86	0.57
1:A:42:LEU:HA	1:A:45:ARG:HD2	1.86	0.57
1:A:22:GLN:HG3	1:A:170:VAL:CG2	2.35	0.56
1:A:406:GLN:HG3	1:A:409:ARG:NH1	2.20	0.56
1:A:6:VAL:HA	1:A:14:VAL:O	2.06	0.56
1:A:245:ASN:ND2	1:A:267:MET:H	2.02	0.56
1:A:347:THR:HA	1:A:350:LYS:CE	2.26	0.56
1:A:96:ILE:CG2	1:A:97:ASN:N	2.68	0.56
1:A:380:PHE:HA	1:A:386:THR:HG21	1.87	0.56
1:A:505:LEU:HD13	1:A:508:ARG:NH2	2.19	0.56
1:A:77:PHE:HZ	1:A:471:LEU:O	1.89	0.56
1:A:422:ASN:C	1:A:422:ASN:OD1	2.43	0.56
1:A:289:ASP:HB3	1:A:319:GLN:HB3	1.88	0.56
1:A:323:SER:HB2	1:A:331:PRO:HB3	1.87	0.56
1:A:547:LYS:HE3	5:A:2129:HOH:O	2.06	0.56
1:A:330:PHE:CE1	4:A:997:I40:I1	3.29	0.55
1:A:205:ASN:OD1	1:A:335:THR:HB	2.06	0.55
1:A:6:VAL:HG22	1:A:15:ARG:HB3	1.87	0.55
1:A:154:THR:HG22	1:A:155:GLY:N	2.21	0.55
1:A:57:LEU:HD23	1:A:58:ASP:N	2.22	0.55
1:A:403:LYS:HD3	1:A:403:LYS:N	2.08	0.55
1:A:137:THR:HG22	1:A:231:TRP:CZ2	2.42	0.55
1:A:309:ARG:NH1	1:A:309:ARG:HG2	2.20	0.55
1:A:71:TYR:HD2	1:A:73:TYR:HE1	1.53	0.55
1:A:219:LYS:HD3	1:A:256:LEU:HD23	1.89	0.54
1:A:245:ASN:HB2	1:A:262:MET:CE	2.36	0.54
1:A:390:ARG:HH21	1:A:417:THR:CG2	2.20	0.54
1:A:54:HIS:CD2	1:A:55:GLY:H	2.26	0.54
1:A:74:PHE:CZ	1:A:373:LEU:HD21	2.40	0.53
1:A:184:ALA:H	1:A:320:GLN:NE2	2.06	0.53
1:A:36:LYS:HB2	1:A:48:VAL:HG23	1.89	0.53
1:A:68:GLN:NE2	1:A:155:GLY:H	2.06	0.53
3:A:993:NAG:H61	3:A:994:BMA:C2	2.38	0.53
1:A:233:THR:HB	1:A:259:ARG:HG2	1.89	0.53
1:A:261:MET:HA	1:A:360:LEU:O	2.09	0.53
1:A:280:VAL:CG1	1:A:284:LYS:HE3	2.38	0.53
1:A:404:ALA:HB1	1:A:408:GLU:HG3	1.90	0.53
1:A:421:GLY:O	1:A:422:ASN:CG	2.46	0.53
1:A:381:ASP:OD1	1:A:383:ASP:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:401:PHE:HA	1:A:403:LYS:HE3	1.89	0.53
1:A:304:VAL:HG23	1:A:305:MET:N	2.24	0.53
1:A:437:ASP:O	1:A:442:CYS:HB2	2.09	0.52
1:A:559:ARG:NH2	5:A:2135:HOH:O	2.41	0.52
1:A:344:ASP:OD1	1:A:345:PRO:N	2.43	0.52
1:A:547:LYS:HE3	5:A:2128:HOH:O	2.08	0.52
1:A:156:SER:HA	1:A:179:GLN:HE22	1.76	0.52
1:A:30:THR:HA	1:A:97:ASN:HD22	1.74	0.52
1:A:301:PRO:O	1:A:304:VAL:HG22	2.11	0.51
1:A:166:ILE:HG13	3:A:991:NAG:H83	1.93	0.51
1:A:35:ALA:HB2	1:A:213:LEU:HD23	1.91	0.51
1:A:349:MET:HE2	1:A:451:LEU:HD12	1.93	0.51
1:A:137:THR:HG22	1:A:231:TRP:CH2	2.46	0.50
1:A:333:ALA:CB	1:A:334:PRO:HD2	2.32	0.50
1:A:187:PHE:CD1	1:A:333:ALA:O	2.65	0.50
1:A:334:PRO:HB2	1:A:341:LEU:HD12	1.93	0.50
1:A:34:TYR:OH	1:A:210:ASP:HB3	2.12	0.50
1:A:461:TYR:CD1	1:A:461:TYR:C	2.85	0.49
1:A:68:GLN:NE2	1:A:154:THR:HG23	2.27	0.49
1:A:3:ASP:OD2	1:A:6:VAL:HG23	2.12	0.49
1:A:290:CYS:O	1:A:291:ASN:HB2	2.13	0.49
1:A:422:ASN:OD1	1:A:422:ASN:O	2.31	0.49
1:A:510:LEU:O	1:A:514:ILE:HG12	2.12	0.49
1:A:1:VAL:O	1:A:2:ILE:CB	2.60	0.48
1:A:373:LEU:HD11	1:A:382:LYS:HA	1.94	0.48
1:A:153:MET:SD	1:A:332:SER:CB	3.01	0.48
1:A:74:PHE:CD2	1:A:382:LYS:HD3	2.48	0.48
1:A:46:LYS:HE3	1:A:200:GLU:OE2	2.13	0.48
1:A:60:THR:O	3:A:996:BMA:O4	2.28	0.48
1:A:347:THR:CB	1:A:350:LYS:HE2	2.43	0.48
1:A:508:ARG:NH2	1:A:543:SER:O	2.45	0.48
1:A:347:THR:HG22	1:A:350:LYS:CE	2.43	0.48
1:A:352:ALA:O	1:A:454:ARG:CD	2.62	0.48
1:A:440:PHE:O	1:A:443:PRO:HD2	2.14	0.48
1:A:467:THR:HG22	1:A:469:THR:H	1.79	0.48
1:A:349:MET:CE	1:A:451:LEU:HD12	2.44	0.48
1:A:238:SER:HB3	1:A:239:ALA:H	1.31	0.48
1:A:211:GLN:HE21	1:A:247:GLN:NE2	2.12	0.47
1:A:241:SER:HB3	1:A:265:GLY:HA3	1.95	0.47
1:A:275:THR:HB	1:A:277:GLU:OE1	2.14	0.47
1:A:389:PRO:HD2	1:A:392:LYS:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:PRO:HG2	1:A:53:TRP:CZ3	2.49	0.47
1:A:535:GLU:CD	1:A:535:GLU:N	2.67	0.47
1:A:241:SER:OG	1:A:262:MET:HB3	2.13	0.47
1:A:370:TYR:CE2	1:A:480:HIS:HB3	2.50	0.47
1:A:490:GLN:N	1:A:491:PRO:CD	2.78	0.47
3:A:994:BMA:O2	3:A:996:BMA:O2	2.19	0.47
1:A:242:SER:O	1:A:245:ASN:HB3	2.14	0.47
1:A:77:PHE:CZ	1:A:471:LEU:O	2.66	0.47
1:A:287:ILE:HD13	1:A:308:MET:SD	2.54	0.47
1:A:358:ASP:C	1:A:359:ILE:HD12	2.35	0.47
1:A:380:PHE:HD2	1:A:428:GLN:NE2	2.11	0.47
1:A:431:ILE:O	1:A:435:VAL:HG23	2.15	0.47
1:A:298:LYS:O	1:A:298:LYS:HD2	2.14	0.47
1:A:2:ILE:O	1:A:2:ILE:HG22	2.15	0.47
1:A:71:TYR:HD2	1:A:73:TYR:CE1	2.31	0.47
1:A:347:THR:CG2	1:A:350:LYS:HE2	2.42	0.47
1:A:36:LYS:HB2	1:A:48:VAL:CG2	2.46	0.46
1:A:376:PHE:HB3	1:A:379:TYR:CD2	2.46	0.46
1:A:387:ALA:HA	1:A:424:GLY:C	2.36	0.46
1:A:238:SER:OG	2:A:593:SO4:O1	2.33	0.46
1:A:200:GLU:HG3	5:A:2014:HOH:O	2.16	0.46
1:A:369:THR:HG21	1:A:476:MET:HA	1.97	0.46
1:A:206:VAL:HA	1:A:209:TRP:HD1	1.81	0.46
1:A:491:PRO:O	1:A:503:ARG:HG2	2.16	0.46
1:A:153:MET:CE	1:A:320:GLN:NE2	2.79	0.45
1:A:278:LYS:O	1:A:282:ILE:HG13	2.16	0.45
1:A:285:ALA:O	1:A:289:ASP:HB2	2.16	0.45
1:A:421:GLY:O	1:A:422:ASN:CB	2.63	0.45
1:A:77:PHE:CE2	1:A:382:LYS:HD2	2.51	0.45
1:A:389:PRO:HB2	1:A:391:ASP:OD1	2.17	0.45
1:A:143:ILE:O	1:A:232:MET:HA	2.17	0.45
1:A:233:THR:HG21	1:A:517:ALA:CA	2.38	0.45
1:A:232:MET:HE2	1:A:257:VAL:HG22	1.98	0.45
1:A:408:GLU:OE2	1:A:571:ARG:HG3	2.16	0.45
1:A:72:GLU:OE2	1:A:81:GLU:OE2	2.35	0.45
1:A:528:GLU:HG2	5:A:2121:HOH:O	2.17	0.45
1:A:373:LEU:HD13	1:A:476:MET:CE	2.47	0.45
1:A:440:PHE:C	1:A:443:PRO:HD2	2.37	0.45
1:A:211:GLN:HE21	1:A:247:GLN:HE21	1.66	0.44
1:A:161:ILE:HG23	1:A:162:TYR:CE1	2.53	0.44
1:A:179:GLN:CA	1:A:179:GLN:HE21	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ILE:HG23	1:A:232:MET:HE1	1.99	0.44
1:A:334:PRO:HB2	1:A:341:LEU:CD1	2.48	0.44
1:A:361:MET:O	1:A:460:TYR:HA	2.17	0.44
1:A:146:TRP:HA	1:A:235:PHE:O	2.18	0.44
1:A:307:CYS:O	1:A:310:SER:HB2	2.17	0.44
1:A:36:LYS:HD3	1:A:48:VAL:CG2	2.47	0.44
1:A:291:ASN:O	1:A:292:CYS:SG	2.76	0.43
1:A:144:LEU:N	1:A:144:LEU:HD12	2.33	0.43
1:A:489:GLY:O	1:A:492:LEU:HB2	2.18	0.43
1:A:43:ARG:NH2	1:A:91:GLU:OE2	2.41	0.43
1:A:359:ILE:N	1:A:359:ILE:HD12	2.33	0.43
1:A:65:THR:O	1:A:89:VAL:HA	2.18	0.43
1:A:409:ARG:O	1:A:413:ILE:HG13	2.18	0.43
1:A:8:GLN:HE21	1:A:13:PRO:HB3	1.84	0.43
1:A:572:SER:O	1:A:573:TRP:C	2.56	0.43
1:A:539:TYR:HE2	1:A:541:ILE:HD11	1.84	0.43
1:A:217:TRP:CE2	1:A:221:ASN:ND2	2.87	0.43
1:A:234:LEU:O	1:A:260:GLY:HA2	2.18	0.43
1:A:354:LEU:O	1:A:456:ALA:HA	2.19	0.43
1:A:327:ILE:HG21	1:A:376:PHE:HE1	1.83	0.43
1:A:387:ALA:HA	1:A:424:GLY:CA	2.48	0.43
1:A:6:VAL:CG2	1:A:15:ARG:HB3	2.49	0.42
1:A:386:THR:HG23	1:A:428:GLN:HE22	1.84	0.42
1:A:54:HIS:CG	1:A:55:GLY:H	2.37	0.42
1:A:308:MET:O	1:A:311:VAL:HG22	2.19	0.42
1:A:251:PRO:HD2	1:A:340:PHE:O	2.18	0.42
1:A:465:HIS:CD2	1:A:544:THR:HG23	2.54	0.42
1:A:89:VAL:O	1:A:89:VAL:HG23	2.17	0.42
1:A:234:LEU:HB2	1:A:244:VAL:HG13	2.00	0.42
1:A:43:ARG:NH1	1:A:308:MET:O	2.52	0.42
1:A:328:LEU:HD21	1:A:371:PHE:CE1	2.54	0.42
1:A:393:TYR:HE2	1:A:413:ILE:HG23	1.83	0.42
1:A:327:ILE:HB	1:A:375:ASP:OD2	2.19	0.42
1:A:524:GLN:OE1	1:A:527:GLU:OE1	2.37	0.42
1:A:315:THR:O	1:A:319:GLN:HG2	2.19	0.42
1:A:142:PRO:HG3	1:A:231:TRP:CZ3	2.55	0.42
1:A:7:VAL:CG1	1:A:14:VAL:HB	2.49	0.42
1:A:340:PHE:O	1:A:342:PRO:HD3	2.20	0.42
1:A:71:TYR:CD2	1:A:73:TYR:HE1	2.35	0.42
3:A:994:BMA:C3	3:A:996:BMA:O2	2.68	0.42
1:A:186:GLY:HA2	1:A:206:VAL:HG23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:LEU:HD11	1:A:334:PRO:HA	2.02	0.42
1:A:238:SER:O	1:A:241:SER:HB3	2.19	0.42
1:A:99:TRP:CD2	1:A:164:ALA:HB3	2.55	0.42
1:A:245:ASN:ND2	1:A:267:MET:HG2	2.35	0.42
1:A:429:GLN:NE2	5:A:2100:HOH:O	2.52	0.42
1:A:449:GLN:HE21	1:A:534:LYS:HG3	1.83	0.42
1:A:401:PHE:HA	1:A:403:LYS:CE	2.49	0.42
1:A:36:LYS:CG	1:A:48:VAL:HG23	2.50	0.42
1:A:466:ARG:NH2	1:A:472:TRP:O	2.53	0.42
1:A:152:PHE:HB3	1:A:187:PHE:CE2	2.55	0.41
1:A:438:HIS:HB2	1:A:563:TRP:CH2	2.55	0.41
1:A:471:LEU:HD12	1:A:471:LEU:HA	1.89	0.41
1:A:380:PHE:CE2	1:A:428:GLN:HG3	2.56	0.41
1:A:99:TRP:HE3	1:A:175:VAL:O	2.04	0.41
1:A:396:ILE:O	1:A:399:ASN:N	2.51	0.41
1:A:166:ILE:HD11	1:A:493:ASN:HB2	2.02	0.41
1:A:24:ARG:NH2	1:A:172:ASN:ND2	2.69	0.41
1:A:271:TRP:HB3	1:A:328:LEU:O	2.20	0.41
1:A:273:HIS:HA	1:A:334:PRO:HG2	2.03	0.41
1:A:344:ASP:O	1:A:348:LEU:HG	2.21	0.41
1:A:22:GLN:HG3	1:A:170:VAL:HG23	2.01	0.41
1:A:207:GLY:O	1:A:210:ASP:HB2	2.20	0.41
1:A:209:TRP:CZ3	1:A:252:VAL:HG11	2.55	0.41
1:A:142:PRO:HG3	1:A:231:TRP:CH2	2.56	0.41
1:A:262:MET:CE	1:A:266:THR:HG22	2.46	0.41
1:A:567:LEU:HD12	1:A:567:LEU:HA	1.83	0.41
1:A:451:LEU:HD12	1:A:451:LEU:HA	1.87	0.41
1:A:154:THR:CG2	1:A:155:GLY:N	2.84	0.41
1:A:3:ASP:HB3	1:A:6:VAL:CG2	2.50	0.41
1:A:386:THR:HG23	1:A:428:GLN:NE2	2.36	0.41
1:A:188:LEU:HD11	1:A:190:LEU:HD11	2.03	0.40
1:A:17:ARG:HD3	1:A:60:THR:HB	2.02	0.40
1:A:274:MET:O	1:A:335:THR:HA	2.21	0.40
1:A:304:VAL:CG2	1:A:305:MET:N	2.84	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	538/585 (92%)	478 (89%)	50 (9%)	10 (2%)	9	22

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	ILE
1	A	139	ASN
1	A	152	PHE
1	A	335	THR
1	A	293	ASN
1	A	423	PRO
1	A	54	HIS
1	A	256	LEU
1	A	150	GLY
1	A	422	ASN

### 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	447/480 (93%)	418 (94%)	29 (6%)	20	43

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ASP

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Mol	Chain	Res	Type
1	A	65	THR
1	A	72	GLU
1	A	85	PRO
1	A	86	ASN
1	A	87	THR
1	A	136	ASN
1	A	179	GLN
1	A	233	THR
1	A	238	SER
1	A	289	ASP
1	A	293	ASN
1	A	327	ILE
1	A	341	LEU
1	A	370	TYR
1	A	384	ASP
1	A	386	THR
1	A	390	ARG
1	A	399	ASN
1	A	403	LYS
1	A	420	GLU
1	A	433	ARG
1	A	444	THR
1	A	451	LEU
1	A	479	LEU
1	A	524	GLN
1	A	538	VAL
1	A	551	LEU
1	A	553	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	68	GLN
1	A	86	ASN
1	A	97	ASN
1	A	172	ASN
1	A	179	GLN
1	A	211	GLN
1	A	245	ASN
1	A	263	GLN
1	A	320	GLN

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Mol	Chain	Res	Type
1	A	363	ASN
1	A	399	ASN
1	A	415	GLN
1	A	429	GLN
1	A	438	HIS
1	A	445	ASN
1	A	449	GLN
1	A	465	HIS
1	A	564	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 ⓘ

5 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	$\# Z  > 2$
3	NAG	A	991	1,3	14,14,15	0.49	0	15,19,21	0.97	2 (13%)
3	NAG	A	993	3	14,14,15	0.54	0	15,19,21	0.78	0
3	BMA	A	994	3	11,11,12	0.82	0	13,15,17	1.37	1 (7%)
3	BMA	A	995	3	11,11,12	0.58	0	13,15,17	0.87	1 (7%)
3	BMA	A	996	3	11,11,12	0.67	0	13,15,17	0.79	0

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
3	NAG	A	991	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	993	3	-	0/6/23/26	0/1/1/1
3	BMA	A	994	3	1/1/4/5	0/2/19/22	0/1/1/1
3	BMA	A	995	3	1/1/4/5	0/2/19/22	1/1/1/1
3	BMA	A	996	3	1/1/4/5	0/2/19/22	1/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	991	NAG	C4-C3-C2	-2.38	107.54	111.02
3	A	991	NAG	O5-C1-C2	-2.11	108.54	111.47
3	A	995	BMA	C1-O5-C5	2.83	116.06	112.17
3	A	994	BMA	C3-C4-C5	3.72	116.76	110.22

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	995	BMA	C1
3	A	994	BMA	C1
3	A	996	BMA	C1

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	995	BMA	C1-C2-C3-C4-C5-O5
3	A	996	BMA	C1-C2-C3-C4-C5-O5

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	991	NAG	1	0
3	A	993	NAG	2	0
3	A	994	BMA	4	0
3	A	996	BMA	4	0

## 5.6 Ligand geometry

2 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	SO4	A	593	1	4,4,4	0.39	0	6,6,6	0.64	0
4	I40	A	997	-	25,26,26	3.15	16 (64%)	33,36,36	2.86	14 (42%)

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	SO4	A	593	1	-	0/0/0/0	0/0/0/0
4	I40	A	997	-	-	0/5/12/12	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	997	I40	C3-C2	-2.92	1.39	1.51
4	A	997	I40	C10-N1	-2.55	1.29	1.32
4	A	997	I40	C16-C17	-2.52	1.34	1.38
4	A	997	I40	C17-I1	-2.24	2.04	2.10
4	A	997	I40	C19-C18	-2.21	1.34	1.38
4	A	997	I40	C5-C12	2.02	1.46	1.43
4	A	997	I40	C9-C13	2.11	1.45	1.41
4	A	997	I40	C14-C15	2.14	1.56	1.51
4	A	997	I40	C3-C4	2.25	1.59	1.51
4	A	997	I40	C19-C20	2.32	1.43	1.38
4	A	997	I40	C20-C15	2.43	1.43	1.38
4	A	997	I40	C1-C10	3.57	1.56	1.50
4	A	997	I40	C11-C10	3.89	1.45	1.40
4	A	997	I40	C4-C11	5.26	1.59	1.51
4	A	997	I40	C12-C13	7.30	1.53	1.42
4	A	997	I40	C5-C11	8.18	1.51	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	997	I40	C1-C10-C11	-7.43	114.15	121.61
4	A	997	I40	C11-C5-N2	-5.44	108.90	119.55
4	A	997	I40	C15-C14-N2	-4.89	101.84	113.77
4	A	997	I40	C18-C17-I1	-3.08	115.05	119.67
4	A	997	I40	C6-C12-C13	-2.26	115.99	118.34
4	A	997	I40	C19-C20-C15	-2.14	117.37	120.64
4	A	997	I40	C5-C12-C13	-2.14	114.78	117.14
4	A	997	I40	C18-C17-C16	2.05	123.54	121.21
4	A	997	I40	C2-C1-C10	2.19	117.31	113.56
4	A	997	I40	C6-C12-C5	2.55	129.23	124.92
4	A	997	I40	C7-C6-C12	2.64	124.64	120.88
4	A	997	I40	C10-N1-C13	2.83	120.90	117.72
4	A	997	I40	C11-C10-N1	5.99	128.54	123.47
4	A	997	I40	C4-C11-C10	6.58	126.44	121.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	593	SO4	5	0
4	A	997	I40	4	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 [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, 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	540/585 (92%)	0.12	18 (3%)	47 47	23, 51, 88, 100	5 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	VAL	6.7
1	A	136	ASN	6.7
1	A	2	ILE	4.5
1	A	573	TRP	4.3
1	A	421	GLY	3.9
1	A	54	HIS	3.8
1	A	137	THR	3.8
1	A	422	ASN	3.7
1	A	153	MET	3.7
1	A	3	ASP	3.4
1	A	157	ALA	3.3
1	A	351	THR	3.2
1	A	334	PRO	2.6
1	A	352	ALA	2.6
1	A	56	VAL	2.5
1	A	333	ALA	2.1
1	A	16	GLY	2.1
1	A	332	SER	2.1

### 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](#)

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	NAG	A	991	14/15	0.88	0.19	0.54	64,66,74,75	0
3	BMA	A	995	11/12	0.44	0.46	-	91,94,95,95	11
3	BMA	A	994	11/12	0.80	0.29	-	94,96,98,99	0
3	NAG	A	993	14/15	0.90	0.24	-	80,84,87,91	0
3	BMA	A	996	11/12	0.70	0.37	-	93,94,94,94	11

### 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. 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
4	I40	A	997	23/23	0.81	0.32	3.19	80,82,87,87	1
2	SO4	A	593	5/5	0.95	0.24	1.37	55,56,61,62	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.