



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 15, 2019 – 07:35 PM EDT

PDB ID : 2JBK  
Title : membrane-bound glutamate carboxypeptidase II (GCPII) in complex with quisqualic acid (quisqualate, alpha-amino-3,5-dioxo-1,2,4-oxadiazolidine-2-propanoic acid)  
Authors : Mesters, J.R.; Henning, K.; Hilgenfeld, R.  
Deposited on : 2006-12-07  
Resolution : 2.99 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.0 (224370), CSD as540be (2019)  
Xtriage (Phenix) : 1.13  
EDS : 2.3.2  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.3.2

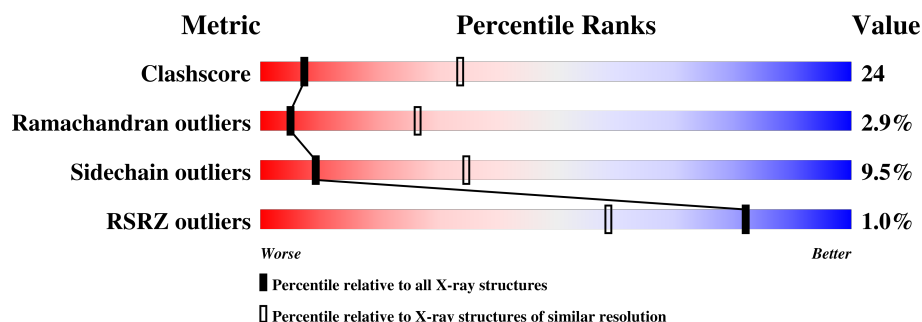
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.99 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	122126	2167 (3.00-3.00)
Ramachandran outliers	120053	2101 (3.00-3.00)
Sidechain outliers	120020	2104 (3.00-3.00)
RSRZ outliers	108989	1751 (3.00-3.00)

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	707	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5532 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 GLUTAMATE CARBOXYPEPTIDASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	687	Total	C	N	O	S	0	0	0
			5318	3430	881	990	17			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

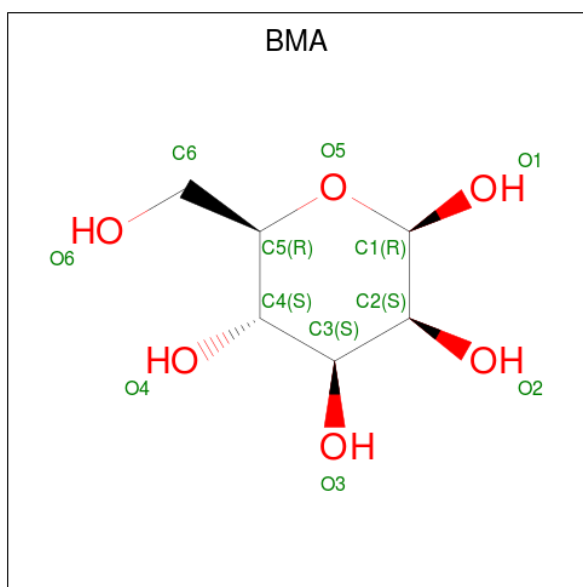
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cl	0	0
			1	1		

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



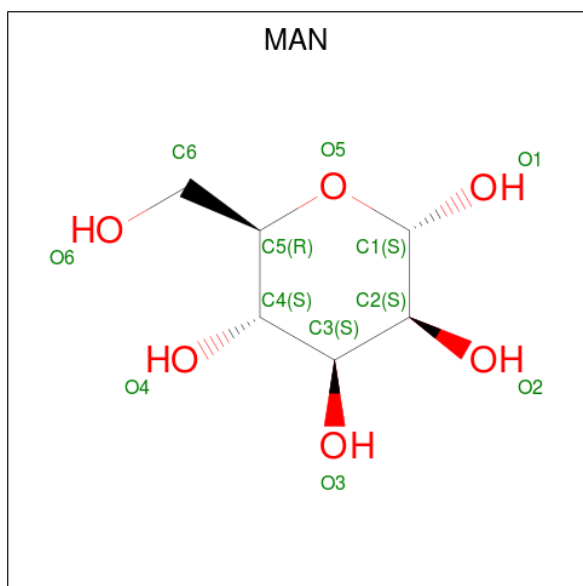
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1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

- Molecule 6 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



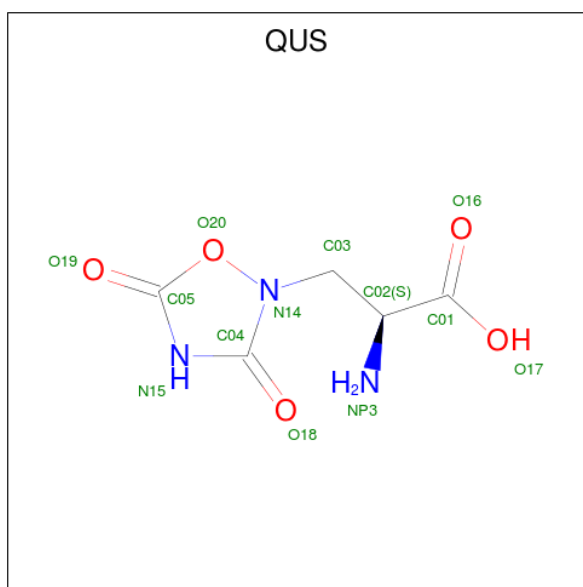
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 7 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is (S)-2-AMINO-3-(3,5-DIOXO-[1,2,4]OXADIAZOLIDIN-2-YL)-PROPIONIC ACID (three-letter code: QUS) (formula:  $C_5H_7N_3O_5$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			13	5	3	5		

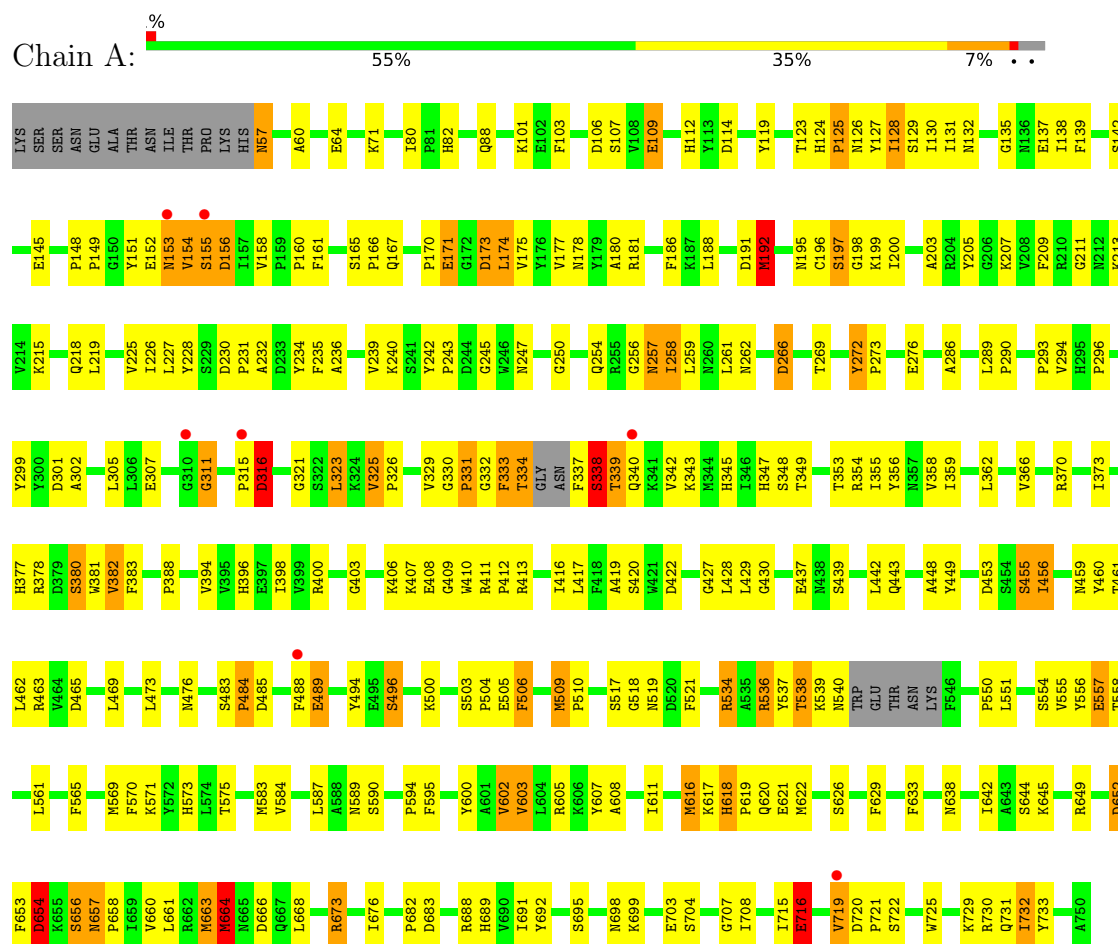
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	21	Total	O	0	0
			21	21		

### 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: GLUTAMATE CARBOXYPEPTIDASE 2



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.14Å 130.76Å 159.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	100.00 – 2.99 49.38 – 2.99	Depositor EDS
% Data completeness (in resolution range)	93.2 (100.00-2.99) 93.2 (49.38-2.99)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.44 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.210 , (Not available) 0.201 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.3	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 32.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5532	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: ZN, BMA, NAG, CL, CA, QUS, MAN

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	1.13	9/5468 (0.2%)	1.05	14/7431 (0.2%)

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	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	654	ASP	CB-CG	5.52	1.63	1.51
1	A	408	GLU	CB-CG	5.44	1.62	1.52
1	A	109	GLU	CD-OE2	5.36	1.31	1.25
1	A	101	LYS	CD-CE	5.19	1.64	1.51
1	A	171	GLU	CD-OE2	5.11	1.31	1.25
1	A	272	TYR	CE2-CZ	-5.10	1.31	1.38
1	A	716	GLU	CG-CD	5.10	1.59	1.51
1	A	333	PHE	CE2-CZ	5.09	1.47	1.37
1	A	64	GLU	CD-OE1	5.03	1.31	1.25

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	664	MET	CG-SD-CE	7.21	111.74	100.20
1	A	654	ASP	CB-CG-OD1	7.18	124.76	118.30
1	A	453	ASP	CB-CG-OD2	7.12	124.70	118.30
1	A	156	ASP	CB-CG-OD2	-6.68	112.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	ASP	CB-CG-OD1	6.45	124.11	118.30
1	A	652	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	A	616	MET	CG-SD-CE	5.85	109.56	100.20
1	A	173	ASP	CB-CG-OD1	-5.76	113.11	118.30
1	A	673	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	A	652	ASP	N-CA-C	5.54	125.97	111.00
1	A	732	ILE	CB-CA-C	-5.49	100.62	111.60
1	A	652	ASP	CB-CA-C	-5.26	99.88	110.40
1	A	719	VAL	CB-CA-C	-5.18	101.56	111.40
1	A	156	ASP	N-CA-C	5.10	124.76	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	152	GLU	Peptide
1	A	338	SER	Peptide
1	A	506	PHE	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	5318	0	5004	251	1
2	A	2	0	0	0	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	154	0	138	11	0
6	A	11	0	9	0	1
7	A	11	0	10	0	0
8	A	13	0	6	2	0
9	A	21	0	0	13	0
All	All	5532	0	5167	253	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 24.

All (253) 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)
5:A:1754:NAG:H3	9:A:2019:HOH:O	1.46	1.12
1:A:337:PHE:HB3	1:A:340:GLN:NE2	1.70	1.07
1:A:657:ASN:HD21	1:A:660:VAL:HG23	1.18	1.06
1:A:657:ASN:ND2	1:A:660:VAL:CG2	2.19	1.04
1:A:620:GLN:NE2	1:A:620:GLN:HA	1.71	1.02
1:A:337:PHE:C	1:A:339:THR:HB	1.80	1.01
1:A:337:PHE:HB3	1:A:340:GLN:HE21	0.85	1.01
1:A:315:PRO:O	1:A:316:ASP:HB3	1.56	1.00
1:A:337:PHE:CB	1:A:340:GLN:HE21	1.74	0.99
1:A:509:MET:HA	1:A:509:MET:CE	1.92	0.99
1:A:620:GLN:HE21	1:A:620:GLN:HA	1.27	0.97
1:A:657:ASN:ND2	1:A:660:VAL:HG23	1.79	0.97
1:A:509:MET:HE2	1:A:510:PRO:HD2	1.46	0.96
1:A:257:ASN:ND2	8:A:1764:QUS:O18	2.01	0.92
1:A:197:SER:O	1:A:199:LYS:HD2	1.71	0.91
1:A:494:TYR:OH	1:A:509:MET:CE	2.19	0.91
1:A:509:MET:HA	1:A:509:MET:HE3	1.49	0.91
1:A:638:ASN:O	1:A:642:ILE:HG13	1.71	0.90
1:A:456:ILE:HD13	1:A:573:HIS:CE1	2.07	0.90
1:A:494:TYR:OH	1:A:509:MET:HE1	1.71	0.89
1:A:138:ILE:O	5:A:1754:NAG:C8	2.21	0.89
1:A:175:VAL:CG2	1:A:331:PRO:HB3	2.05	0.86
1:A:138:ILE:O	5:A:1754:NAG:H83	1.74	0.86
1:A:645:LYS:O	1:A:649:ARG:HG3	1.78	0.83
1:A:349:THR:HG21	5:A:1753:NAG:H81	1.61	0.82
1:A:180:ALA:HB3	1:A:213:LYS:HB3	1.62	0.82
1:A:657:ASN:HD21	1:A:660:VAL:CG2	1.81	0.81
1:A:109:GLU:HA	1:A:109:GLU:OE2	1.81	0.80
1:A:618:HIS:HB3	1:A:621:GLU:OE1	1.81	0.80
1:A:654:ASP:OD1	1:A:656:SER:CB	2.30	0.79
1:A:370:ARG:NH2	1:A:666:ASP:OD1	2.17	0.78
1:A:654:ASP:OD1	1:A:656:SER:HB2	1.85	0.77
1:A:339:THR:HA	9:A:2006:HOH:O	1.85	0.76
1:A:337:PHE:HA	9:A:2005:HOH:O	1.86	0.75
1:A:337:PHE:N	9:A:2005:HOH:O	2.19	0.75
1:A:325:VAL:HB	1:A:326:PRO:CD	2.18	0.73
1:A:509:MET:HA	1:A:509:MET:HE2	1.71	0.73
1:A:456:ILE:CD1	1:A:573:HIS:CE1	2.71	0.72
1:A:175:VAL:HG22	1:A:331:PRO:HB3	1.70	0.72
1:A:334:THR:HG23	1:A:334:THR:O	1.90	0.72
1:A:439:SER:O	1:A:443:GLN:HG2	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:460:TYR:CE1	1:A:500:LYS:HE2	2.24	0.72
1:A:337:PHE:O	1:A:339:THR:HB	1.89	0.71
1:A:422:ASP:O	1:A:430:GLY:HA3	1.90	0.70
1:A:235:PHE:HA	1:A:247:ASN:OD1	1.91	0.70
1:A:205:TYR:CE1	1:A:254:GLN:HB3	2.26	0.70
1:A:602:VAL:HG12	1:A:603:VAL:N	2.06	0.69
1:A:616:MET:O	1:A:619:PRO:HD3	1.93	0.68
1:A:166:PRO:HD3	1:A:290:PRO:HG2	1.74	0.68
1:A:657:ASN:ND2	1:A:660:VAL:HG21	2.05	0.68
1:A:138:ILE:O	5:A:1754:NAG:H82	1.93	0.68
1:A:228:TYR:CE1	1:A:230:ASP:HB2	2.29	0.68
1:A:456:ILE:CD1	1:A:573:HIS:HE1	2.05	0.67
1:A:171:GLU:HA	1:A:342:VAL:O	1.95	0.67
1:A:334:THR:O	1:A:334:THR:CG2	2.43	0.66
1:A:719:VAL:O	1:A:721:PRO:HD3	1.96	0.66
1:A:716:GLU:H	1:A:716:GLU:CD	1.97	0.66
1:A:366:VAL:HB	1:A:413:ARG:HG2	1.77	0.65
1:A:180:ALA:CB	1:A:213:LYS:HB3	2.26	0.65
1:A:461:THR:HG23	1:A:462:LEU:O	1.96	0.65
1:A:509:MET:CA	1:A:509:MET:CE	2.72	0.65
1:A:337:PHE:CA	9:A:2005:HOH:O	2.40	0.64
1:A:551:LEU:HD12	1:A:561:LEU:HD22	1.79	0.64
1:A:259:LEU:HD13	1:A:261:LEU:HD21	1.80	0.64
1:A:315:PRO:O	1:A:316:ASP:CB	2.34	0.63
1:A:556:TYR:O	1:A:558:THR:HG23	1.97	0.63
1:A:377:HIS:CE1	1:A:388:PRO:HB3	2.32	0.63
1:A:337:PHE:CD2	1:A:340:GLN:NE2	2.67	0.63
1:A:509:MET:CE	1:A:510:PRO:HD2	2.27	0.63
1:A:538:THR:HG23	1:A:539:LYS:O	1.99	0.62
1:A:448:ALA:HB3	1:A:587:LEU:HD13	1.80	0.62
1:A:137:GLU:OE2	5:A:1754:NAG:H5	1.99	0.62
1:A:232:ALA:HB2	1:A:321:GLY:HA2	1.82	0.62
1:A:460:TYR:CD1	1:A:500:LYS:HE2	2.34	0.62
1:A:337:PHE:O	1:A:340:GLN:N	2.23	0.62
1:A:225:VAL:HB	1:A:294:VAL:HG22	1.82	0.61
1:A:459:ASN:OD1	5:A:1757:NAG:H2	1.99	0.61
1:A:707:GLY:O	1:A:731:GLN:HG3	1.99	0.61
1:A:177:VAL:CG2	1:A:203:ALA:HB2	2.29	0.61
1:A:339:THR:HG23	9:A:2006:HOH:O	2.00	0.61
1:A:394:VAL:O	1:A:398:ILE:HG13	2.00	0.61
1:A:195:ASN:OD1	1:A:197:SER:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:GLN:HE21	1:A:620:GLN:CA	2.06	0.60
1:A:173:ASP:O	1:A:174:LEU:C	2.39	0.60
1:A:358:VAL:O	1:A:419:ALA:HA	2.01	0.60
1:A:325:VAL:HB	1:A:326:PRO:HD2	1.84	0.60
1:A:192:MET:HE1	1:A:329:VAL:HG21	1.82	0.60
1:A:476:ASN:HD22	5:A:1758:NAG:H83	1.66	0.60
1:A:195:ASN:ND2	5:A:1756:NAG:C7	2.65	0.60
1:A:338:SER:N	1:A:339:THR:HB	2.16	0.60
1:A:484:PRO:HD2	1:A:485:ASP:OD1	2.02	0.59
1:A:460:TYR:CD2	1:A:540:ASN:HA	2.38	0.59
1:A:174:LEU:HD13	1:A:342:VAL:HG21	1.85	0.58
1:A:232:ALA:HB2	1:A:321:GLY:CA	2.33	0.58
1:A:657:ASN:HD22	1:A:660:VAL:CG2	2.14	0.57
1:A:155:SER:O	1:A:156:ASP:CG	2.42	0.57
1:A:88:GLN:N	1:A:88:GLN:OE1	2.37	0.57
1:A:165:SER:OG	1:A:293:PRO:HA	2.05	0.57
1:A:127:TYR:HE1	1:A:129:SER:OG	1.88	0.57
1:A:703:GLU:HG3	1:A:704:SER:N	2.19	0.57
1:A:175:VAL:HG23	1:A:331:PRO:HB3	1.86	0.57
1:A:349:THR:HG21	5:A:1753:NAG:C8	2.32	0.57
1:A:689:HIS:CE1	1:A:691:ILE:HB	2.40	0.57
1:A:381:TRP:CH2	9:A:2003:HOH:O	2.52	0.56
1:A:382:VAL:HB	9:A:2008:HOH:O	2.06	0.56
1:A:412:PRO:HA	1:A:589:ASN:OD1	2.05	0.56
1:A:494:TYR:OH	1:A:509:MET:HE3	2.04	0.56
1:A:657:ASN:ND2	1:A:660:VAL:CB	2.68	0.56
1:A:656:SER:O	1:A:658:PRO:HD3	2.05	0.56
1:A:258:ILE:HD12	1:A:290:PRO:HG3	1.86	0.55
1:A:483:SER:HB2	1:A:496:SER:OG	2.07	0.55
1:A:82:HIS:HB2	1:A:380:SER:OG	2.06	0.55
1:A:699:LYS:HE2	8:A:1764:QUS:O19	2.07	0.55
1:A:509:MET:HE3	1:A:509:MET:CA	2.30	0.55
1:A:619:PRO:HA	1:A:622:MET:HB2	1.89	0.55
1:A:103:PHE:O	1:A:403:GLY:HA3	2.07	0.54
1:A:129:SER:HA	1:A:139:PHE:O	2.07	0.54
1:A:618:HIS:N	1:A:618:HIS:CD2	2.75	0.54
1:A:484:PRO:HG3	1:A:575:THR:OG1	2.07	0.54
1:A:109:GLU:OE2	1:A:109:GLU:CA	2.53	0.53
1:A:181:ARG:HH11	1:A:207:LYS:HG2	1.74	0.53
1:A:460:TYR:HD2	1:A:540:ASN:HA	1.72	0.53
5:A:1758:NAG:H61	5:A:1759:NAG:C1	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ALA:N	1:A:247:ASN:OD1	2.41	0.53
1:A:311:GLY:HA3	1:A:330:GLY:O	2.08	0.52
1:A:334:THR:HG22	1:A:337:PHE:HD1	1.73	0.52
1:A:338:SER:HB3	1:A:339:THR:OG1	2.09	0.52
1:A:191:ASP:OD1	1:A:191:ASP:N	2.41	0.51
1:A:373:ILE:HG12	1:A:417:LEU:HB2	1.92	0.51
1:A:688:ARG:HD3	9:A:2016:HOH:O	2.10	0.51
1:A:382:VAL:HG12	1:A:383:PHE:N	2.25	0.51
1:A:103:PHE:HB3	1:A:400:ARG:HA	1.93	0.51
1:A:239:VAL:HB	1:A:247:ASN:ND2	2.26	0.51
1:A:225:VAL:O	1:A:294:VAL:HA	2.11	0.51
1:A:608:ALA:O	1:A:611:ILE:HG22	2.11	0.51
1:A:71:LYS:HE2	1:A:570:PHE:CE2	2.46	0.51
1:A:153:ASN:O	1:A:154:VAL:C	2.49	0.51
1:A:242:TYR:CG	1:A:243:PRO:HA	2.46	0.51
1:A:71:LYS:HG3	1:A:570:PHE:CZ	2.46	0.50
1:A:137:GLU:HB2	9:A:2019:HOH:O	2.11	0.50
1:A:231:PRO:HD2	1:A:323:LEU:HD13	1.93	0.50
1:A:695:SER:HB3	1:A:698:ASN:O	2.11	0.50
1:A:330:GLY:HA2	1:A:331:PRO:O	2.11	0.50
1:A:534:ARG:HB2	9:A:2011:HOH:O	2.12	0.50
1:A:455:SER:O	1:A:536:ARG:HB2	2.12	0.50
1:A:148:PRO:HG2	1:A:151:TYR:CD2	2.47	0.49
1:A:302:ALA:O	1:A:305:LEU:N	2.41	0.49
1:A:629:PHE:O	1:A:633:PHE:HD2	1.96	0.49
1:A:130:ILE:HG22	1:A:131:ILE:N	2.28	0.49
1:A:653:PHE:O	1:A:653:PHE:CD1	2.65	0.49
1:A:128:ILE:CD1	1:A:226:ILE:HG12	2.43	0.49
1:A:325:VAL:CB	1:A:326:PRO:CD	2.87	0.49
1:A:551:LEU:HD12	1:A:561:LEU:CD2	2.42	0.49
1:A:494:TYR:HH	1:A:509:MET:HE1	1.72	0.48
1:A:621:GLU:O	1:A:622:MET:C	2.52	0.48
1:A:657:ASN:HD22	1:A:660:VAL:HG21	1.74	0.48
1:A:413:ARG:HG3	1:A:413:ARG:HH11	1.79	0.48
1:A:301:ASP:O	1:A:302:ALA:C	2.52	0.48
1:A:114:ASP:OD1	1:A:354:ARG:HB2	2.13	0.48
1:A:273:PRO:HG3	1:A:437:GLU:HA	1.96	0.48
1:A:356:TYR:O	1:A:378:ARG:NH2	2.30	0.48
1:A:682:PRO:O	1:A:683:ASP:HB2	2.12	0.48
1:A:175:VAL:HG22	1:A:331:PRO:CB	2.41	0.48
1:A:333:PHE:HD1	1:A:340:GLN:O	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:SER:N	1:A:301:ASP:OD2	2.40	0.47
1:A:657:ASN:ND2	1:A:660:VAL:HB	2.29	0.47
1:A:240:LYS:O	1:A:245:GLY:HA3	2.14	0.47
1:A:602:VAL:CG1	1:A:603:VAL:N	2.77	0.47
1:A:620:GLN:NE2	1:A:620:GLN:CA	2.53	0.47
1:A:209:PHE:CE2	1:A:211:GLY:HA3	2.49	0.47
1:A:456:ILE:HD11	1:A:573:HIS:HE1	1.79	0.47
1:A:463:ARG:HD3	1:A:536:ARG:CZ	2.44	0.47
1:A:652:ASP:N	1:A:652:ASP:OD2	2.48	0.47
1:A:337:PHE:HD2	1:A:340:GLN:NE2	2.13	0.47
1:A:330:GLY:CA	1:A:331:PRO:O	2.63	0.47
1:A:353:THR:HG22	1:A:354:ARG:N	2.30	0.46
1:A:231:PRO:HG2	1:A:323:LEU:CD1	2.45	0.46
1:A:449:TYR:CE2	1:A:521:PHE:HA	2.50	0.46
1:A:250:GLY:CA	1:A:299:TYR:CE2	2.98	0.46
1:A:112:HIS:HA	1:A:355:ILE:O	2.15	0.46
1:A:406:LYS:HA	1:A:410:TRP:O	2.16	0.45
1:A:126:ASN:HA	1:A:345:HIS:O	2.16	0.45
1:A:57:ASN:ND2	1:A:60:ALA:H	2.14	0.45
1:A:518:GLY:O	1:A:519:ASN:HB2	2.16	0.45
1:A:616:MET:CE	1:A:619:PRO:HB3	2.47	0.45
1:A:720:ASP:C	1:A:720:ASP:OD1	2.55	0.45
1:A:715:ILE:HD13	1:A:725:TRP:CE2	2.52	0.45
1:A:188:LEU:HD23	1:A:196:CYS:SG	2.57	0.45
1:A:469:LEU:O	1:A:595:PHE:HA	2.17	0.45
1:A:551:LEU:O	1:A:557:GLU:HG3	2.17	0.45
1:A:488:PHE:O	1:A:489:GLU:C	2.54	0.44
1:A:234:TYR:HD2	1:A:550:PRO:HA	1.82	0.44
1:A:106:ASP:OD1	1:A:411:ARG:NH2	2.45	0.44
1:A:658:PRO:O	1:A:661:LEU:HB3	2.17	0.44
1:A:119:TYR:O	1:A:348:SER:HB3	2.17	0.44
1:A:145:GLU:OE1	1:A:555:VAL:HB	2.18	0.44
1:A:382:VAL:HG11	1:A:555:VAL:HG23	1.99	0.44
1:A:561:LEU:HD12	1:A:565:PHE:HD2	1.82	0.44
1:A:170:PRO:O	1:A:343:LYS:HA	2.17	0.43
1:A:231:PRO:HD3	1:A:299:TYR:CD1	2.53	0.43
1:A:167:GLN:HG2	1:A:347:HIS:HA	2.00	0.43
1:A:654:ASP:C	1:A:656:SER:N	2.71	0.43
1:A:239:VAL:HB	1:A:247:ASN:HD21	1.82	0.43
1:A:663:MET:O	1:A:663:MET:HG3	2.16	0.43
1:A:611:ILE:HD11	1:A:708:ILE:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ASN:HB3	1:A:138:ILE:HD11	2.01	0.43
1:A:266:ASP:HA	1:A:429:LEU:HD22	2.00	0.43
1:A:186:PHE:HD1	1:A:186:PHE:HA	1.70	0.43
1:A:427:GLY:O	1:A:428:LEU:HB2	2.19	0.43
1:A:333:PHE:CD1	1:A:340:GLN:O	2.72	0.43
1:A:80:ILE:HD12	1:A:88:GLN:HG2	2.01	0.42
1:A:131:ILE:HB	1:A:135:GLY:HA2	2.00	0.42
1:A:621:GLU:CD	1:A:621:GLU:H	2.21	0.42
1:A:362:LEU:HD23	1:A:416:ILE:HD12	2.00	0.42
1:A:307:GLU:HA	1:A:325:VAL:HG12	2.02	0.42
1:A:517:SER:OG	1:A:518:GLY:N	2.53	0.42
1:A:603:VAL:HG23	1:A:607:TYR:CE2	2.53	0.42
1:A:127:TYR:C	1:A:127:TYR:CD1	2.93	0.42
1:A:160:PRO:O	1:A:161:PHE:HB3	2.20	0.42
1:A:339:THR:CA	9:A:2006:HOH:O	2.56	0.42
1:A:181:ARG:HB2	1:A:181:ARG:HE	1.39	0.41
1:A:256:GLY:HA2	9:A:2021:HOH:O	2.19	0.41
1:A:732:ILE:O	1:A:732:ILE:HG22	2.18	0.41
1:A:407:LYS:C	1:A:409:GLY:H	2.24	0.41
1:A:504:PRO:O	1:A:506:PHE:N	2.53	0.41
1:A:689:HIS:HB3	1:A:692:TYR:O	2.21	0.41
1:A:442:LEU:HA	1:A:442:LEU:HD23	1.76	0.41
1:A:654:ASP:C	1:A:656:SER:H	2.24	0.41
1:A:272:TYR:CD2	1:A:272:TYR:N	2.89	0.41
1:A:538:THR:HG23	1:A:539:LYS:N	2.36	0.41
1:A:664:MET:HE3	1:A:664:MET:HB3	1.90	0.41
1:A:691:ILE:O	1:A:704:SER:HA	2.21	0.41
1:A:215:LYS:HE2	1:A:219:LEU:HD11	2.01	0.41
1:A:583:MET:O	1:A:584:VAL:C	2.57	0.41
1:A:149:PRO:HG2	1:A:243:PRO:HG3	2.02	0.41
1:A:227:LEU:O	1:A:296:PRO:HA	2.20	0.41
1:A:334:THR:CG2	1:A:337:PHE:HD1	2.34	0.41
1:A:382:VAL:HG12	1:A:383:PHE:CD2	2.56	0.41
1:A:485:ASP:OD1	1:A:485:ASP:N	2.54	0.41
1:A:124:HIS:N	1:A:125:PRO:CD	2.82	0.40
1:A:266:ASP:OD2	1:A:269:THR:OG1	2.39	0.40
1:A:676:ILE:HG23	1:A:688:ARG:HB2	2.02	0.40
1:A:155:SER:O	1:A:156:ASP:CB	2.69	0.40
1:A:261:LEU:O	1:A:262:ASN:HB2	2.21	0.40
1:A:286:ALA:HB3	1:A:289:LEU:HG	2.03	0.40
1:A:378:ARG:HB2	1:A:420:SER:OG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:PHE:CD2	1:A:400:ARG:HB2	2.57	0.40
1:A:616:MET:C	1:A:618:HIS:N	2.75	0.40
1:A:653:PHE:C	1:A:653:PHE:CD1	2.94	0.40
1:A:145:GLU:OE2	1:A:554:SER:HB2	2.20	0.40
1:A:191:ASP:O	1:A:192:MET:C	2.60	0.40
1:A:250:GLY:HA2	1:A:299:TYR:CE2	2.56	0.40
1:A:729:LYS:O	1:A:730:ARG:C	2.58	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:276:GLU:OE2	6:A:1762:BMA:O2[2_565]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	681/707 (96%)	587 (86%)	74 (11%)	20 (3%)	5	26

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	153	ASN
1	A	154	VAL
1	A	338	SER
1	A	505	GLU
1	A	192	MET
1	A	332	GLY
1	A	339	THR
1	A	602	VAL
1	A	178	ASN

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Mol	Chain	Res	Type
1	A	617	LYS
1	A	125	PRO
1	A	382	VAL
1	A	557	GLU
1	A	594	PRO
1	A	316	ASP
1	A	484	PRO
1	A	657	ASN
1	A	311	GLY
1	A	198	GLY
1	A	331	PRO

### 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	536/603 (89%)	485 (90%)	51 (10%)	9	35

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	ASN
1	A	107	SER
1	A	123	THR
1	A	128	ILE
1	A	155	SER
1	A	158	VAL
1	A	174	LEU
1	A	192	MET
1	A	197	SER
1	A	200	ILE
1	A	218	GLN
1	A	257	ASN
1	A	258	ILE
1	A	266	ASP
1	A	316	ASP

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Mol	Chain	Res	Type
1	A	323	LEU
1	A	325	VAL
1	A	334	THR
1	A	359	ILE
1	A	380	SER
1	A	396	HIS
1	A	455	SER
1	A	456	ILE
1	A	465	ASP
1	A	473	LEU
1	A	489	GLU
1	A	496	SER
1	A	503	SER
1	A	509	MET
1	A	534	ARG
1	A	536	ARG
1	A	537	TYR
1	A	538	THR
1	A	569	MET
1	A	571	LYS
1	A	590	SER
1	A	600	TYR
1	A	603	VAL
1	A	605	ARG
1	A	618	HIS
1	A	626	SER
1	A	644	SER
1	A	654	ASP
1	A	656	SER
1	A	663	MET
1	A	664	MET
1	A	668	LEU
1	A	673	ARG
1	A	716	GLU
1	A	722	SER
1	A	733	TYR

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	57	ASN
1	A	340	GLN

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Mol	Chain	Res	Type
1	A	345	HIS
1	A	443	GLN
1	A	618	HIS
1	A	620	GLN
1	A	657	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 4 are monoatomic - leaving 14 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	$\# Z  > 2$
5	NAG	A	1751	1,5	14,14,15	1.01	1 (7%)	17,19,21	2.00	5 (29%)
5	NAG	A	1752	5	14,14,15	0.95	1 (7%)	17,19,21	2.79	6 (35%)
5	NAG	A	1753	1	14,14,15	1.35	3 (21%)	17,19,21	3.19	7 (41%)
5	NAG	A	1754	1,5	14,14,15	1.46	3 (21%)	17,19,21	2.95	9 (52%)
5	NAG	A	1755	5	14,14,15	1.09	1 (7%)	17,19,21	2.92	7 (41%)
5	NAG	A	1756	1	14,14,15	1.85	5 (35%)	17,19,21	2.74	8 (47%)
5	NAG	A	1757	1	14,14,15	1.09	1 (7%)	17,19,21	2.71	7 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	1758	1,5	14,14,15	0.88	0	17,19,21	2.78	7 (41%)
5	NAG	A	1759	5	14,14,15	0.77	0	17,19,21	3.19	6 (35%)
5	NAG	A	1760	1,5	14,14,15	0.58	0	17,19,21	2.37	6 (35%)
5	NAG	A	1761	5,6	14,14,15	1.29	3 (21%)	17,19,21	3.55	7 (41%)
6	BMA	A	1762	5,7	11,11,12	1.06	1 (9%)	15,15,17	1.51	2 (13%)
7	MAN	A	1763	6	11,11,12	0.87	0	15,15,17	2.64	8 (53%)
8	QUS	A	1764	-	4,13,13	1.68	2 (50%)	0,18,18	0.00	-

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
5	NAG	A	1751	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1752	5	-	4/6/23/26	0/1/1/1
5	NAG	A	1753	1	-	4/6/23/26	0/1/1/1
5	NAG	A	1754	1,5	-	2/6/23/26	0/1/1/1
5	NAG	A	1755	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1756	1	-	6/6/23/26	0/1/1/1
5	NAG	A	1757	1	-	6/6/23/26	0/1/1/1
5	NAG	A	1758	1,5	-	4/6/23/26	0/1/1/1
5	NAG	A	1759	5	-	1/6/23/26	0/1/1/1
5	NAG	A	1760	1,5	-	2/6/23/26	0/1/1/1
5	NAG	A	1761	5,6	-	4/6/23/26	0/1/1/1
6	BMA	A	1762	5,7	-	0/2/19/22	0/1/1/1
7	MAN	A	1763	6	-	0/2/19/22	0/1/1/1
8	QUS	A	1764	-	-	1/2/8/8	0/1/1/1

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1754	NAG	C1-C2	3.48	1.57	1.52
5	A	1756	NAG	O5-C1	3.05	1.48	1.43
5	A	1756	NAG	O5-C5	2.96	1.49	1.43
5	A	1757	NAG	O5-C1	2.70	1.48	1.43
5	A	1761	NAG	C8-C7	2.63	1.56	1.50
8	A	1764	QUS	O19-C05	2.62	1.22	1.19
5	A	1756	NAG	C8-C7	2.59	1.56	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1761	NAG	O5-C1	-2.49	1.39	1.43
5	A	1754	NAG	O7-C7	2.48	1.29	1.23
5	A	1751	NAG	O7-C7	2.43	1.28	1.23
5	A	1756	NAG	O7-C7	2.41	1.28	1.23
5	A	1753	NAG	O5-C1	2.35	1.47	1.43
5	A	1753	NAG	O5-C5	2.34	1.48	1.43
5	A	1754	NAG	C2-N2	2.24	1.50	1.46
5	A	1761	NAG	O5-C5	-2.17	1.39	1.43
5	A	1753	NAG	C6-C5	2.15	1.59	1.51
5	A	1755	NAG	C1-C2	2.06	1.55	1.52
6	A	1762	BMA	C2-C3	2.06	1.55	1.52
5	A	1756	NAG	C4-C3	2.06	1.57	1.52
5	A	1752	NAG	O5-C5	2.04	1.47	1.43
8	A	1764	QUS	C04-N15	-2.01	1.32	1.34

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1759	NAG	C2-N2-C7	-10.78	107.48	122.92
5	A	1761	NAG	C2-N2-C7	-9.77	108.92	122.92
5	A	1753	NAG	O5-C5-C6	7.45	118.94	107.15
5	A	1758	NAG	C2-N2-C7	-7.42	112.29	122.92
5	A	1761	NAG	C1-O5-C5	-6.74	103.04	112.20
5	A	1754	NAG	C2-N2-C7	-6.66	113.38	122.92
5	A	1752	NAG	C1-O5-C5	6.64	121.23	112.20
5	A	1755	NAG	C2-N2-C7	-6.49	113.62	122.92
5	A	1757	NAG	C4-C3-C2	-6.26	101.85	111.02
5	A	1756	NAG	C1-O5-C5	6.15	120.56	112.20
5	A	1752	NAG	O3-C3-C2	-6.09	96.53	109.38
5	A	1761	NAG	C3-C4-C5	-5.86	99.69	110.23
5	A	1757	NAG	C1-O5-C5	5.51	119.69	112.20
5	A	1753	NAG	C3-C4-C5	-5.48	100.38	110.23
5	A	1756	NAG	O5-C5-C6	5.33	115.58	107.15
5	A	1760	NAG	C2-N2-C7	5.20	130.38	122.92
5	A	1755	NAG	O3-C3-C2	-5.20	98.41	109.38
7	A	1763	MAN	C1-O5-C5	-5.07	105.32	112.20
5	A	1753	NAG	C1-O5-C5	5.01	119.01	112.20
5	A	1754	NAG	O5-C5-C6	4.96	115.00	107.15
5	A	1753	NAG	C4-C3-C2	-4.94	103.78	111.02
5	A	1754	NAG	C1-O5-C5	-4.72	105.79	112.20
5	A	1755	NAG	O5-C5-C4	-4.61	99.60	110.83
5	A	1758	NAG	O5-C5-C6	-4.43	100.14	107.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1752	NAG	O5-C5-C4	4.43	121.59	110.83
5	A	1759	NAG	O4-C4-C5	4.26	119.94	109.29
7	A	1763	MAN	O5-C5-C6	4.21	113.81	107.15
5	A	1751	NAG	O5-C5-C6	4.12	113.67	107.15
5	A	1754	NAG	C1-C2-N2	4.06	117.43	110.49
5	A	1751	NAG	O4-C4-C3	-3.90	101.30	110.34
5	A	1757	NAG	O5-C5-C6	3.85	113.24	107.15
5	A	1760	NAG	C6-C5-C4	-3.83	104.02	113.00
7	A	1763	MAN	O5-C5-C4	-3.72	101.78	110.83
5	A	1758	NAG	O3-C3-C2	-3.72	101.53	109.38
5	A	1756	NAG	O4-C4-C3	3.63	118.77	110.34
5	A	1753	NAG	C2-N2-C7	-3.62	117.74	122.92
5	A	1755	NAG	C1-C2-N2	3.57	116.59	110.49
6	A	1762	BMA	O4-C4-C5	3.57	118.20	109.29
5	A	1751	NAG	C1-O5-C5	3.48	116.93	112.20
5	A	1757	NAG	C2-N2-C7	-3.42	118.02	122.92
5	A	1761	NAG	O5-C1-C2	-3.41	106.01	111.36
5	A	1754	NAG	C3-C4-C5	3.37	116.29	110.23
5	A	1760	NAG	O7-C7-C8	-3.37	116.09	122.07
5	A	1756	NAG	C6-C5-C4	-3.29	105.28	113.00
5	A	1760	NAG	O4-C4-C3	3.20	117.78	110.34
5	A	1758	NAG	O3-C3-C4	-3.19	102.94	110.34
7	A	1763	MAN	C3-C4-C5	-3.18	104.52	110.23
5	A	1754	NAG	O7-C7-C8	-3.17	116.44	122.07
5	A	1755	NAG	O7-C7-C8	-3.05	116.66	122.07
5	A	1755	NAG	C8-C7-N2	3.04	121.34	116.10
5	A	1756	NAG	C1-C2-N2	3.00	115.61	110.49
5	A	1753	NAG	O4-C4-C5	2.99	116.76	109.29
7	A	1763	MAN	O4-C4-C3	-2.96	103.47	110.34
5	A	1759	NAG	O5-C1-C2	2.94	115.98	111.36
5	A	1760	NAG	O7-C7-N2	2.92	127.40	121.95
7	A	1763	MAN	C6-C5-C4	2.92	119.85	113.00
7	A	1763	MAN	O2-C2-C1	2.91	115.08	109.17
5	A	1756	NAG	O5-C1-C2	-2.90	106.80	111.36
6	A	1762	BMA	C1-C2-C3	2.88	113.20	109.66
5	A	1757	NAG	O7-C7-N2	2.82	127.21	121.95
5	A	1758	NAG	O4-C4-C5	2.79	116.26	109.29
5	A	1760	NAG	O5-C5-C6	2.78	111.55	107.15
5	A	1758	NAG	O6-C6-C5	-2.72	101.87	111.29
5	A	1754	NAG	C8-C7-N2	2.71	120.77	116.10
5	A	1751	NAG	C4-C3-C2	-2.68	107.09	111.02
5	A	1752	NAG	C6-C5-C4	-2.67	106.73	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1761	NAG	O4-C4-C3	2.65	116.49	110.34
5	A	1751	NAG	C3-C4-C5	-2.62	105.52	110.23
5	A	1759	NAG	O6-C6-C5	-2.56	102.43	111.29
5	A	1755	NAG	O4-C4-C5	2.37	115.21	109.29
5	A	1754	NAG	C4-C3-C2	2.35	114.46	111.02
5	A	1761	NAG	O5-C5-C6	-2.33	103.47	107.15
5	A	1752	NAG	C8-C7-N2	2.32	120.11	116.10
5	A	1759	NAG	C1-C2-N2	-2.28	106.59	110.49
5	A	1757	NAG	C8-C7-N2	-2.28	112.17	116.10
7	A	1763	MAN	C2-C3-C4	2.21	114.72	110.89
5	A	1757	NAG	O5-C1-C2	2.21	114.83	111.36
5	A	1756	NAG	C2-N2-C7	2.17	126.03	122.92
5	A	1756	NAG	C3-C4-C5	2.16	114.12	110.23
5	A	1752	NAG	O4-C4-C5	2.16	114.68	109.29
5	A	1754	NAG	O4-C4-C3	-2.11	105.46	110.34
5	A	1761	NAG	C6-C5-C4	2.10	117.93	113.00
5	A	1759	NAG	C3-C4-C5	-2.08	106.48	110.23
5	A	1758	NAG	O5-C1-C2	-2.03	108.17	111.36
5	A	1753	NAG	O6-C6-C5	2.02	118.29	111.29

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1752	NAG	C8-C7-N2-C2
5	A	1756	NAG	C8-C7-N2-C2
5	A	1756	NAG	O7-C7-N2-C2
8	A	1764	QUS	C01-C02-C03-N14
5	A	1758	NAG	C8-C7-N2-C2
5	A	1758	NAG	O7-C7-N2-C2
5	A	1753	NAG	C8-C7-N2-C2
5	A	1753	NAG	O7-C7-N2-C2
5	A	1752	NAG	O7-C7-N2-C2
5	A	1753	NAG	O5-C5-C6-O6
5	A	1756	NAG	O5-C5-C6-O6
5	A	1757	NAG	C4-C5-C6-O6
5	A	1752	NAG	C4-C5-C6-O6
5	A	1756	NAG	C4-C5-C6-O6
5	A	1757	NAG	O5-C5-C6-O6
5	A	1753	NAG	C4-C5-C6-O6
5	A	1757	NAG	C8-C7-N2-C2
5	A	1761	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
5	A	1757	NAG	O7-C7-N2-C2
5	A	1761	NAG	C8-C7-N2-C2
5	A	1761	NAG	O7-C7-N2-C2
5	A	1756	NAG	C1-C2-N2-C7
5	A	1758	NAG	O5-C5-C6-O6
5	A	1758	NAG	C4-C5-C6-O6
5	A	1752	NAG	O5-C5-C6-O6
5	A	1757	NAG	C1-C2-N2-C7
5	A	1760	NAG	C4-C5-C6-O6
5	A	1761	NAG	O5-C5-C6-O6
5	A	1754	NAG	C8-C7-N2-C2
5	A	1759	NAG	C4-C5-C6-O6
5	A	1760	NAG	O5-C5-C6-O6
5	A	1754	NAG	O7-C7-N2-C2
5	A	1756	NAG	C3-C2-N2-C7
5	A	1757	NAG	C3-C2-N2-C7

There are no ring outliers.

8 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1753	NAG	2	0
5	A	1754	NAG	5	0
5	A	1756	NAG	1	0
5	A	1757	NAG	1	0
5	A	1758	NAG	2	0
5	A	1759	NAG	1	0
6	A	1762	BMA	0	1
8	A	1764	QUS	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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	687/707 (97%)	-0.22	7 (1%) 82 59	35, 35, 35, 35	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	340	GLN	2.8
1	A	719	VAL	2.7
1	A	310	GLY	2.3
1	A	155	SER	2.2
1	A	153	ASN	2.0
1	A	315	PRO	2.0
1	A	488	PHE	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	A	1756	14/15	0.85	0.30	35,35,35,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	A	1755	14/15	0.89	0.42	35,35,35,35	0
5	NAG	A	1753	14/15	0.91	0.36	35,35,35,35	0
5	NAG	A	1761	14/15	0.91	0.19	35,35,35,35	0
5	NAG	A	1754	14/15	0.92	0.28	35,35,35,35	0
6	BMA	A	1762	11/12	0.93	0.15	35,35,35,35	0
7	MAN	A	1763	11/12	0.93	0.15	35,35,35,35	0
5	NAG	A	1757	14/15	0.93	0.21	35,35,35,35	0
5	NAG	A	1759	14/15	0.93	0.22	35,35,35,35	0
5	NAG	A	1752	14/15	0.94	0.37	35,35,35,35	0
5	NAG	A	1760	14/15	0.95	0.14	35,35,35,35	0
5	NAG	A	1751	14/15	0.96	0.23	35,35,35,35	0
4	CL	A	804	1/1	0.97	0.16	35,35,35,35	0
8	QUS	A	1764	13/13	0.97	0.19	35,35,35,35	0
5	NAG	A	1758	14/15	0.97	0.18	35,35,35,35	0
2	ZN	A	802	1/1	0.98	0.11	35,35,35,35	0
2	ZN	A	801	1/1	0.98	0.12	35,35,35,35	0
3	CA	A	803	1/1	1.00	0.13	35,35,35,35	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.