



Full wwPDB X-ray Structure Validation Report ⓘ

May 8, 2016 – 07:29 AM EDT

PDB ID : 4ZEL
Title : Human dopamine beta-hydroxylase
Authors : Vendelboe, T.V.; Harris, P.; Christensen, H.E.M.; Harlos, K.; Walter, T.; Zhao, Y.; Omari, K.
Deposited on : 2015-04-20
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027457
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) : rb-20027457

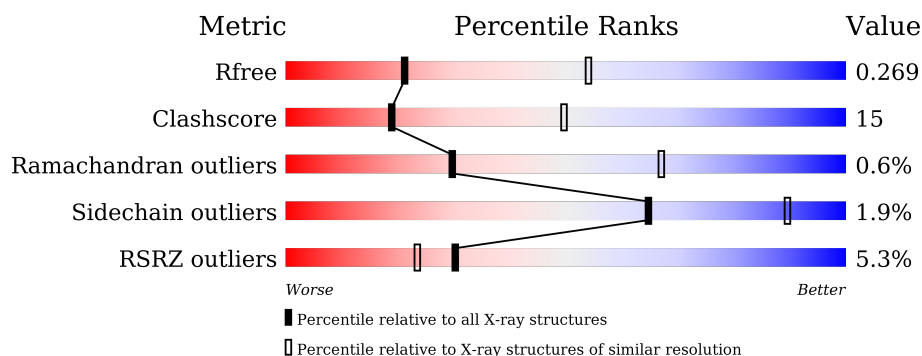
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 ≥ 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	578	
1	B	578	

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
5	MAN	B	704	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8939 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.

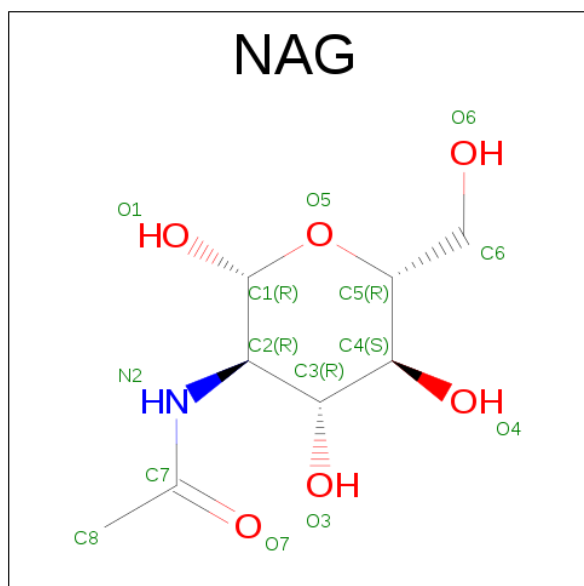
- Molecule 1 is a protein called Dopamine beta-hydroxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	1	0
			4396	2813	747	810	26			
1	B	544	Total	C	N	O	S	0	2	0
			4346	2784	742	795	25			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cu	0	0
			1	1		

- Molecule 3 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



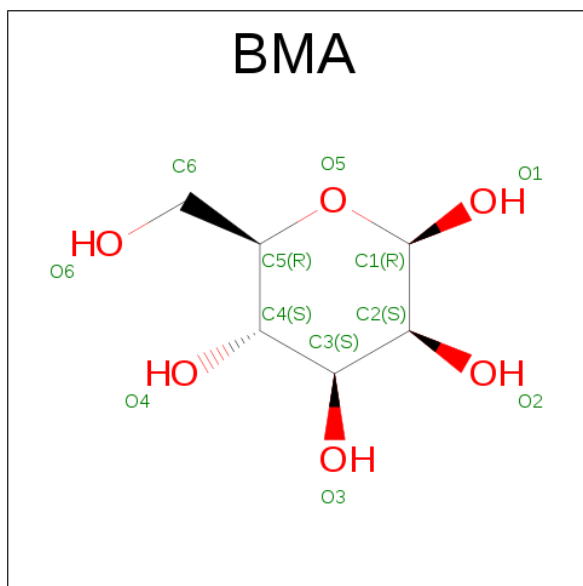
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

Continued on next page...

Continued from previous page...

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

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



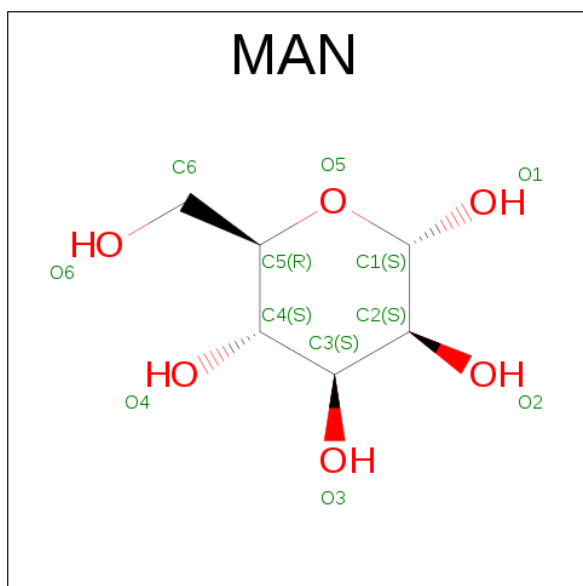
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	B	1	Total	C	O	0	0
			11	6	5		

Continued on next page...

Continued from previous page...

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

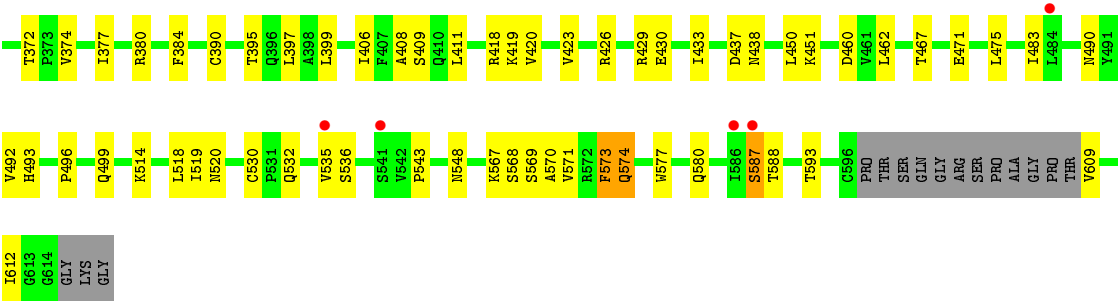
- Molecule 5 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	8	Total	O	0	0
			8	8		
6	B	4	Total	O	0	0
			4	4		



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	102.81Å 119.06Å 224.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.53 – 2.90 63.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.8 (59.53-2.90) 99.9 (63.98-2.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.91Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.230 , 0.270 0.232 , 0.269	Depositor DCC
R_{free} test set	2954 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	68.0	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8939	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, CU, 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	0.37	0/4516	0.71	5/6144 (0.1%)
1	B	0.36	1/4466 (0.0%)	0.64	0/6073
All	All	0.37	1/8982 (0.0%)	0.68	5/12217 (0.0%)

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	7
1	B	0	5
All	All	0	12

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	227	GLU	CG-CD	-5.50	1.43	1.51

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	326	ARG	N-CA-C	7.17	130.35	111.00
1	A	357	LEU	CA-CB-CG	7.07	131.56	115.30
1	A	285	SER	N-CA-C	-6.88	92.43	111.00
1	A	288	LYS	CD-CE-NZ	6.73	127.17	111.70
1	A	269	CYS	CA-CB-SG	5.40	123.72	114.00

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	ARG	Peptide
1	A	189	GLN	Peptide
1	A	206	GLU	Peptide
1	A	288	LYS	Peptide
1	A	289	PRO	Peptide
1	A	291	ARG	Peptide
1	A	324	SER	Peptide
1	B	293	ASN	Peptide
1	B	296	ARG	Peptide
1	B	530	CYS	Peptide
1	B	573	PHE	Peptide
1	B	587	SER	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	4396	0	4284	166	0
1	B	4346	0	4245	108	1
2	A	1	0	0	0	0
3	A	70	0	62	2	0
3	B	70	0	61	0	0
4	A	11	0	10	0	0
4	B	22	0	19	0	0
5	B	11	0	10	0	0
6	A	8	0	0	1	1
6	B	4	0	0	1	1
All	All	8939	0	8691	269	2

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 15.

All (269) 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:288:LYS:HE2	1:A:289:PRO:HD3	1.45	0.95
1:B:243:ARG:HA	1:B:320:GLY:HA3	1.60	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LYS:HD2	1:A:236:GLU:H	1.43	0.83
1:A:429:ARG:NH1	1:A:587:SER:OG	2.12	0.83
1:A:248:LYS:HB3	1:A:352:TYR:HB2	1.61	0.83
1:B:408:ALA:HB3	1:B:493:HIS:HB2	1.62	0.82
1:A:408:ALA:HB3	1:A:493:HIS:HB2	1.60	0.81
1:A:292:LEU:C	1:A:294:TYR:H	1.85	0.80
1:B:573:PHE:O	1:B:577:TRP:NE1	2.15	0.80
1:A:313:GLU:HA	1:A:358:ARG:HH11	1.45	0.80
1:B:296:ARG:O	1:B:297:HIS:ND1	2.16	0.79
1:A:279:PHE:CE1	1:A:288:LYS:HD2	2.18	0.78
1:B:67:TYR:OH	1:B:199:LYS:O	2.02	0.77
1:B:243:ARG:NH1	1:B:324:SER:OG	2.19	0.76
1:A:235:LYS:HD2	1:A:236:GLU:N	2.00	0.76
1:B:248:LYS:HB3	1:B:352:TYR:HB2	1.66	0.75
1:A:253:VAL:HG11	1:A:258:GLU:HA	1.68	0.74
1:B:103:LEU:HD12	1:B:145:LEU:HD21	1.70	0.73
1:A:292:LEU:O	1:A:294:TYR:N	2.22	0.72
1:A:326:ARG:NH1	1:A:327:TYR:O	2.23	0.72
1:A:184:ASN:HD21	3:A:705:NAG:C7	1.99	0.72
1:A:221:ILE:HG21	1:A:280:SER:OG	1.89	0.72
1:A:534:SER:HB3	1:A:537:GLN:HB3	1.72	0.72
1:B:236:GLU:OE1	1:B:327:TYR:HA	1.91	0.71
1:A:149:ARG:HH22	1:A:158:ASP:HB3	1.56	0.70
1:B:243:ARG:HD3	1:B:318:ALA:HB1	1.73	0.70
1:A:252:ILE:HD11	1:A:350:ARG:HB2	1.74	0.70
1:A:269:CYS:N	1:A:326:ARG:HD3	2.07	0.70
1:A:426:ARG:NH2	1:A:458:PRO:O	2.24	0.70
1:A:83:ALA:O	1:A:105:THR:OG1	2.07	0.70
1:A:126:ASP:OD1	1:A:157:LYS:NZ	2.26	0.69
1:A:289:PRO:HB2	1:A:290:ASP:OD1	1.93	0.69
1:A:518:LEU:HG	1:B:518:LEU:HD22	1.74	0.69
1:B:475:LEU:O	6:B:801:HOH:O	2.11	0.69
1:B:215:GLU:O	1:B:235:LYS:NZ	2.17	0.68
1:B:252:ILE:HD11	1:B:350:ARG:HB2	1.75	0.67
1:A:130:ASP:OD2	1:A:149:ARG:NH1	2.28	0.66
1:B:84:GLY:HA3	1:B:173:LEU:HD12	1.77	0.66
1:A:247:ILE:HG12	1:A:354:THR:HG23	1.78	0.65
1:A:355:ALA:C	1:A:356:LYS:HD2	2.16	0.65
1:A:259:ALA:O	1:A:262:HIS:NE2	2.28	0.65
1:A:521:ARG:HH22	1:B:532:GLN:NE2	1.95	0.64
1:A:590:GLU:N	1:A:590:GLU:OE1	2.29	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:CYS:HA	1:B:295:CYS:HA	1.81	0.62
1:A:426:ARG:NE	1:A:460:ASP:OD1	2.31	0.62
1:A:139:THR:HG23	1:A:141:GLU:H	1.65	0.62
1:B:307:LYS:HG3	1:B:308:ALA:N	2.15	0.61
1:A:269:CYS:H	1:A:326:ARG:HD3	1.62	0.61
1:B:335:HIS:ND1	1:B:337:PRO:HD3	2.15	0.61
1:B:429:ARG:HH12	1:B:588:THR:C	2.04	0.61
1:A:529:THR:HG22	1:A:531:PRO:HD3	1.82	0.61
1:B:419:LYS:HB2	1:B:467:THR:HB	1.83	0.61
1:A:326:ARG:HG3	1:A:327:TYR:N	2.15	0.61
1:A:325:SER:OG	1:A:326:ARG:N	2.33	0.61
1:A:524:ASN:OD1	1:A:525:GLU:N	2.33	0.61
1:A:104:TRP:HE3	1:A:111:TYR:HB2	1.65	0.61
1:A:524:ASN:HB2	1:B:514:LYS:HE2	1.82	0.60
1:A:104:TRP:CE3	1:A:111:TYR:HB2	2.36	0.60
1:A:290:ASP:OD1	1:A:291:ARG:N	2.34	0.60
1:B:294:TYR:HB2	1:B:296:ARG:HG3	1.82	0.60
1:A:357:LEU:HG	1:A:358:ARG:O	2.01	0.60
1:A:219:PRO:HD3	1:A:233:TYR:CD1	2.37	0.59
1:A:295:CYS:O	1:A:329:ARG:NH1	2.35	0.59
1:A:236:GLU:HG2	1:A:327:TYR:CD2	2.37	0.59
1:A:243:ARG:HB2	1:A:321:GLY:HA3	1.84	0.59
1:A:231:TRP:CH2	1:A:281:GLY:HA2	2.38	0.59
1:B:184:ASN:OD1	1:B:185:GLY:N	2.35	0.58
1:A:275:SER:OG	1:A:276:VAL:N	2.35	0.58
1:A:279:PHE:CZ	1:A:288:LYS:HD2	2.38	0.58
1:A:219:PRO:HD3	1:A:233:TYR:CE1	2.39	0.58
1:A:292:LEU:C	1:A:294:TYR:N	2.57	0.58
1:B:426:ARG:NH1	1:B:460:ASP:OD1	2.32	0.58
1:A:233:TYR:CE2	1:A:235:LYS:HB2	2.39	0.57
1:A:440:TYR:OH	1:A:445:GLN:NE2	2.35	0.57
1:B:397:LEU:HD21	1:B:574:GLN:HB2	1.84	0.57
1:B:227:GLU:O	1:B:336:ASN:N	2.27	0.57
1:A:200:PRO:HA	1:A:451:LYS:HG2	1.86	0.57
1:A:210:ASP:OD2	1:A:355:ALA:N	2.21	0.57
1:A:269:CYS:HB2	1:A:326:ARG:NE	2.19	0.57
1:B:66:SER:OG	1:B:69:GLN:HB3	2.03	0.57
1:B:149:ARG:NH1	1:B:150:PRO:O	2.37	0.57
1:A:290:ASP:CG	1:A:291:ARG:H	2.06	0.57
1:B:208:PRO:HD2	1:B:211:ALA:HB2	1.87	0.56
1:A:356:LYS:N	1:A:356:LYS:HD2	2.20	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:247:ILE:HB	1:B:358:ARG:HH21	1.71	0.56
1:A:104:TRP:HZ3	1:A:609:VAL:HG11	1.71	0.56
1:B:217:GLN:HB3	1:B:346:SER:O	2.05	0.56
1:A:113:ALA:HB2	1:A:609:VAL:HG13	1.88	0.56
1:A:67:TYR:OH	1:A:199:LYS:O	2.12	0.55
1:B:322:PRO:HA	1:B:324:SER:N	2.21	0.55
1:A:326:ARG:CG	1:A:327:TYR:H	2.17	0.55
1:B:128:GLN:CD	1:B:128:GLN:H	2.09	0.55
1:A:414:HIS:ND1	1:A:485:GLU:O	2.30	0.55
1:A:527:VAL:O	1:A:527:VAL:HG12	2.08	0.54
1:B:235:LYS:HG3	1:B:236:GLU:N	2.22	0.54
1:A:243:ARG:O	1:A:356:LYS:HE3	2.07	0.54
1:A:573:PHE:O	1:A:577:TRP:NE1	2.20	0.54
1:A:269:CYS:H	1:A:326:ARG:NH1	2.05	0.54
1:A:196:GLN:NE2	6:A:802:HOH:O	2.30	0.54
1:A:181:GLU:OE1	1:A:181:GLU:N	2.38	0.54
1:A:83:ALA:HB3	1:A:173:LEU:O	2.08	0.53
1:A:585:VAL:C	1:A:587:SER:H	2.11	0.53
1:B:568:SER:C	1:B:570:ALA:H	2.12	0.53
1:B:263[B]:HIS:CE1	1:B:333:HIS:HD1	2.27	0.53
1:B:188:LEU:HG	1:B:190:MET:HG2	1.91	0.53
1:A:271:PRO:HA	1:A:325:SER:HB3	1.91	0.53
1:A:429:ARG:HH22	1:A:589:LEU:HD12	1.73	0.53
1:A:429:ARG:HH11	1:A:430:GLU:H	1.54	0.53
1:A:576:GLU:O	1:A:580:GLN:NE2	2.41	0.53
1:B:181:GLU:N	1:B:181:GLU:OE2	2.42	0.52
1:A:235:LYS:CD	1:A:236:GLU:H	2.18	0.52
1:A:177:PHE:CE1	3:A:705:NAG:H62	2.43	0.52
1:A:299:LEU:HA	1:A:317:LEU:HD21	1.92	0.52
1:B:372:THR:HB	1:B:374:VAL:HG22	1.90	0.52
1:B:139:THR:HG23	1:B:141:GLU:H	1.74	0.52
1:A:221:ILE:HD13	1:A:231:TRP:CZ2	2.45	0.52
1:A:286:LYS:C	1:A:288:LYS:H	2.13	0.52
1:A:313:GLU:HA	1:A:358:ARG:NH1	2.22	0.52
1:A:409:SER:OG	1:A:490:ASN:OD1	2.27	0.52
1:B:125:LEU:HD11	1:B:609:VAL:HG22	1.91	0.52
1:B:216:VAL:HG12	1:B:330:LEU:HD22	1.91	0.51
1:A:261:VAL:HG22	1:A:334:TYR:CE1	2.46	0.51
1:A:326:ARG:CG	1:A:327:TYR:N	2.71	0.51
1:B:171:GLY:HA2	1:B:189:GLN:O	2.10	0.51
1:A:236:GLU:OE1	1:A:237:LEU:N	2.36	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:LYS:HB3	1:A:289:PRO:HD3	1.92	0.51
1:A:587:SER:OG	1:A:588:THR:N	2.43	0.51
1:A:336:ASN:OD1	1:A:338:LEU:HB3	2.10	0.51
1:B:242:SER:HA	1:B:321:GLY:H	1.76	0.51
1:A:64:ASN:OD1	1:A:73:HIS:HB2	2.11	0.50
1:B:88:GLY:HA3	1:B:100:LEU:HD23	1.92	0.50
1:A:286:LYS:C	1:A:288:LYS:N	2.61	0.50
1:A:585:VAL:HG12	1:A:587:SER:HB3	1.94	0.50
1:B:208:PRO:C	1:B:210:ASP:H	2.14	0.50
1:B:251:PRO:HG3	1:B:302:TRP:NE1	2.27	0.50
1:B:170:TYR:CZ	1:B:191:GLY:HA3	2.46	0.50
1:A:326:ARG:HG3	1:A:327:TYR:H	1.76	0.49
1:A:276:VAL:HG21	1:A:289:PRO:HG2	1.94	0.49
1:A:48:PRO:HD2	1:A:64:ASN:HB3	1.94	0.49
1:B:411:LEU:HD13	1:B:420:VAL:HB	1.95	0.49
1:A:379:PRO:O	1:A:549:ARG:NH1	2.31	0.49
1:A:395:THR:O	1:A:399:LEU:HB2	2.13	0.49
1:A:222:GLN:HG3	1:A:342:GLY:HA3	1.94	0.49
1:A:521:ARG:NH2	1:B:532:GLN:NE2	2.61	0.49
1:A:104:TRP:CZ3	1:A:609:VAL:HG11	2.48	0.49
1:B:236:GLU:CD	1:B:237:LEU:H	2.16	0.49
1:A:406:ILE:HG23	1:A:492:VAL:HG13	1.94	0.49
1:A:231:TRP:O	1:A:331:GLU:HA	2.13	0.48
1:B:69:GLN:HE21	1:B:148:LYS:HD3	1.77	0.48
1:A:263:HIS:HB3	1:A:333:HIS:HB3	1.94	0.48
1:B:177:PHE:CE2	1:B:183:ILE:HA	2.48	0.48
1:A:92:ARG:NH2	1:A:439:HIS:O	2.45	0.48
1:A:326:ARG:NH2	1:A:327:TYR:HB2	2.29	0.48
1:A:521:ARG:HH12	1:B:532:GLN:HE21	1.62	0.48
1:B:72:ILE:HD11	1:B:198:LEU:HD23	1.94	0.48
1:B:543:PRO:O	1:B:548:ASN:ND2	2.47	0.48
1:B:225:SER:O	1:B:226:GLN:HG3	2.14	0.48
1:A:270:ALA:HB1	1:A:272:GLU:OE1	2.14	0.48
1:B:257:ASN:HA	1:B:260:LEU:HD23	1.96	0.48
1:A:380:ARG:NH2	1:A:474:GLU:HG2	2.29	0.48
1:A:231:TRP:CZ2	1:A:281:GLY:HA2	2.49	0.47
1:B:245:HIS:CD2	1:B:357:LEU:HD22	2.49	0.47
1:A:139:THR:HG23	1:A:141:GLU:N	2.27	0.47
1:A:268:GLN:O	1:A:297:HIS:HB3	2.15	0.47
1:A:269:CYS:HA	1:A:295:CYS:HA	1.96	0.47
1:A:534:SER:O	1:A:538:GLN:N	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:395:THR:O	1:B:399:LEU:HB2	2.14	0.47
1:A:139:THR:OG1	1:A:140:PRO:HD2	2.14	0.47
1:A:419:LYS:HB2	1:A:467:THR:HB	1.95	0.47
1:A:149:ARG:NH2	1:A:159:TYR:O	2.48	0.47
1:A:288:LYS:HB3	1:A:288:LYS:HE2	1.57	0.47
1:A:266:VAL:HG23	1:A:349:ILE:HD12	1.97	0.47
1:A:167:HIS:HE1	1:A:439:HIS:O	1.97	0.47
1:A:265:GLU:HB3	1:A:267:PHE:CE1	2.50	0.47
1:A:292:LEU:O	1:A:294:TYR:HD2	1.98	0.47
1:A:326:ARG:HG3	1:A:327:TYR:O	2.14	0.47
1:A:446:GLU:OE2	1:A:448:ARG:NH1	2.48	0.46
1:A:243:ARG:NH2	1:A:361:ASN:HD21	2.14	0.46
1:A:104:TRP:HB3	1:A:106:ASP:CG	2.36	0.46
1:A:295:CYS:C	1:A:296:ARG:HD3	2.35	0.46
1:A:88:GLY:HA3	1:A:100:LEU:HD23	1.98	0.46
1:A:295:CYS:O	1:A:296:ARG:HD3	2.16	0.46
1:B:49:TYR:CE1	1:B:199:LYS:HD2	2.52	0.45
1:A:242:SER:O	1:A:244:HIS:ND1	2.48	0.45
1:B:165:THR:H	1:B:437:ASP:CG	2.19	0.45
1:B:429:ARG:NH1	1:B:587:SER:HB3	2.32	0.45
1:B:390:CYS:HB3	1:B:462:LEU:HB2	1.97	0.45
1:B:535:VAL:HG23	1:B:536:SER:H	1.81	0.45
1:B:406:ILE:HG23	1:B:492:VAL:HG13	1.98	0.45
1:A:221:ILE:HD13	1:A:231:TRP:CE2	2.52	0.45
1:A:279:PHE:CZ	1:A:288:LYS:CD	2.99	0.45
1:A:289:PRO:O	1:A:291:ARG:O	2.34	0.45
1:B:430:GLU:OE1	1:B:588:THR:OG1	2.35	0.45
1:A:225:SER:O	1:A:339:VAL:HG23	2.17	0.45
1:A:610:VAL:HG12	1:A:611:SER:H	1.82	0.45
1:B:269:CYS:HA	1:B:295:CYS:CB	2.47	0.45
1:B:139:THR:HG23	1:B:141:GLU:N	2.32	0.45
1:B:267:PHE:CE1	1:B:298:VAL:HG22	2.52	0.45
1:A:315:ALA:HB1	1:A:362:ALA:HB2	1.99	0.45
1:B:226:GLN:O	1:B:336:ASN:HB3	2.17	0.45
1:B:177:PHE:HD2	1:B:183:ILE:HG12	1.82	0.45
1:B:499:GLN:O	1:B:567:LYS:HB3	2.16	0.44
1:A:297:HIS:HA	1:A:501:GLU:OE1	2.18	0.44
1:A:390:CYS:HB3	1:A:462:LEU:HB2	2.00	0.44
1:A:525:GLU:HG3	1:A:527:VAL:HG23	2.00	0.44
1:B:200:PRO:HB3	1:B:451:LYS:HA	1.99	0.44
1:B:577:TRP:HA	1:B:580:GLN:HE21	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:PHE:CD1	1:B:496:PRO:HB3	2.52	0.44
1:A:262:HIS:CD2	1:A:262:HIS:N	2.84	0.44
1:B:568:SER:OG	1:B:571:VAL:HG22	2.18	0.44
1:A:429:ARG:HD2	1:A:587:SER:CB	2.48	0.44
1:B:573:PHE:HB3	1:B:574:GLN:HG2	1.99	0.44
1:A:419:LYS:HG2	1:A:438:ASN:O	2.18	0.43
1:B:419:LYS:HG2	1:B:438:ASN:O	2.17	0.43
1:A:396:GLN:HA	1:A:458:PRO:HB3	1.99	0.43
1:B:269:CYS:HA	1:B:295:CYS:CA	2.47	0.43
1:B:302:TRP:CD1	1:B:306:ALA:HB3	2.54	0.43
1:B:423:VAL:HG12	1:B:433:ILE:HD13	1.99	0.43
1:B:110:ALA:HB3	1:B:612:ILE:O	2.19	0.43
1:A:233:TYR:HE2	1:A:235:LYS:HB2	1.80	0.43
1:A:128:GLN:HE22	1:A:157:LYS:NZ	2.16	0.43
1:A:437:ASP:HB3	1:A:440:TYR:HB2	2.01	0.43
1:A:429:ARG:HD2	1:A:429:ARG:HA	1.73	0.43
1:A:149:ARG:HG2	1:A:150:PRO:O	2.18	0.43
1:A:235:LYS:CD	1:A:236:GLU:N	2.77	0.43
1:A:538:GLN:O	1:A:542:VAL:HG23	2.19	0.43
1:B:243:ARG:NH1	1:B:319:PHE:HA	2.34	0.43
1:B:244:HIS:CD2	1:B:355:ALA:HA	2.54	0.43
1:A:134:LEU:HD11	1:A:148:LYS:HB2	2.01	0.42
1:B:130:ASP:OD1	1:B:130:ASP:N	2.42	0.42
1:B:139:THR:OG1	1:B:140:PRO:HD2	2.18	0.42
1:A:104:TRP:O	1:A:110:ALA:HA	2.20	0.42
1:B:202:ILE:H	1:B:202:ILE:HG13	1.73	0.42
1:B:206:GLU:HG2	1:B:207:LEU:N	2.34	0.42
1:B:519:ILE:HG13	1:B:520:ASN:N	2.34	0.42
1:A:233:TYR:CD1	1:A:279:PHE:O	2.73	0.42
1:B:337:PRO:C	1:B:339:VAL:H	2.23	0.42
1:B:612:ILE:HD13	1:B:612:ILE:HA	1.89	0.42
1:A:289:PRO:HB2	1:A:290:ASP:CG	2.39	0.42
1:A:312:PRO:HG2	1:A:407:PHE:CD1	2.55	0.42
1:B:177:PHE:CD2	1:B:183:ILE:HG12	2.55	0.42
1:B:247:ILE:HG21	1:B:358:ARG:HE	1.84	0.42
1:B:377:ILE:HG23	1:B:384:PHE:CD2	2.54	0.42
1:B:409:SER:OG	1:B:490:ASN:OD1	2.36	0.42
1:A:311:TYR:HA	1:A:312:PRO:HD3	1.63	0.42
1:A:355:ALA:HB1	1:A:356:LYS:HD2	2.03	0.41
1:A:269:CYS:H	1:A:326:ARG:CD	2.31	0.41
1:B:92:ARG:CZ	1:B:418[B]:ARG:HG2	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:568:SER:OG	1:B:571:VAL:N	2.53	0.41
1:A:417:GLY:O	1:A:418:ARG:NH1	2.51	0.41
1:A:238:PRO:O	1:A:241:PHE:HB2	2.21	0.41
1:A:232:CYS:N	1:A:283:CYS:SG	2.94	0.41
1:A:279:PHE:CZ	1:A:281:GLY:N	2.88	0.41
1:B:408:ALA:HA	1:B:450:LEU:HD13	2.01	0.41
1:A:559:ALA:HA	1:A:560:PRO:HD3	1.91	0.41
1:B:286:LYS:HA	1:B:286:LYS:HD2	1.91	0.41
1:A:577:TRP:HA	1:A:580:GLN:HE21	1.86	0.41
1:B:202:ILE:O	1:B:202:ILE:HD12	2.21	0.41
1:B:380:ARG:HA	1:B:471:GLU:HA	2.03	0.41
1:B:223:ILE:HA	1:B:224:PRO:HD3	1.83	0.41
1:B:243:ARG:CA	1:B:320:GLY:HA3	2.41	0.41
1:A:177:PHE:CD2	1:A:183:ILE:HA	2.57	0.40
1:A:423:VAL:HG12	1:A:433:ILE:HD13	2.03	0.40
1:A:286:LYS:HA	1:A:286:LYS:HD2	1.52	0.40
1:B:210:ASP:OD2	1:B:355:ALA:N	2.55	0.40
1:B:227:GLU:HA	1:B:336:ASN:O	2.20	0.40
1:A:165:THR:H	1:A:437:ASP:CG	2.25	0.40
1:A:297:HIS:HA	1:A:501:GLU:OE2	2.22	0.40
1:B:69:GLN:NE2	1:B:148:LYS:HD3	2.37	0.40

All (2) 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)
6:A:807:HOH:O	6:B:804:HOH:O[5_555]	2.08	0.12
1:B:359:ARG:NH1	1:B:593:THR:OG1[4_555]	2.17	0.03

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	545/578 (94%)	513 (94%)	27 (5%)	5 (1%)	21	57
1	B	536/578 (93%)	507 (95%)	27 (5%)	2 (0%)	39	74
All	All	1081/1156 (94%)	1020 (94%)	54 (5%)	7 (1%)	30	67

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	293	ASN
1	A	190[A]	MET
1	A	190[B]	MET
1	B	569	SER
1	A	527	VAL
1	A	339	VAL
1	B	339	VAL

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	485/504 (96%)	478 (99%)	7 (1%)	74	93
1	B	479/504 (95%)	466 (97%)	13 (3%)	52	84
All	All	964/1008 (96%)	944 (98%)	20 (2%)	65	88

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	101	VAL
1	A	190[A]	MET
1	A	190[B]	MET
1	A	236	GLU
1	A	288	LYS
1	A	346	SER
1	A	426	ARG
1	B	64	ASN
1	B	128	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	129	GLN
1	B	225	SER
1	B	227	GLU
1	B	263[A]	HIS
1	B	263[B]	HIS
1	B	268	GLN
1	B	276	VAL
1	B	286	LYS
1	B	294	TYR
1	B	483	ILE
1	B	574	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	333	HIS
1	A	335	HIS
1	B	532	GLN
1	B	580	GLN

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 15 ligands modelled in this entry, 1 is 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
3	NAG	A	702	1	14,14,15	0.30	0	15,19,21	0.43	0
3	NAG	A	703	1,3	14,14,15	0.73	1 (7%)	15,19,21	1.07	1 (6%)
3	NAG	A	704	3	14,14,15	0.24	0	15,19,21	0.38	0
3	NAG	A	705	1,3	14,14,15	0.91	1 (7%)	15,19,21	0.98	2 (13%)
3	NAG	A	706	3,4	14,14,15	0.50	0	15,19,21	0.39	0
4	BMA	A	707	3	11,11,12	0.52	0	15,15,17	0.95	1 (6%)
3	NAG	B	701	1,3	14,14,15	0.32	0	15,19,21	0.64	0
3	NAG	B	702	3,4	14,14,15	0.40	0	15,19,21	0.68	0
4	BMA	B	703	3,5	11,11,12	0.79	0	15,15,17	1.37	2 (13%)
5	MAN	B	704	4	11,11,12	0.73	0	15,15,17	1.57	3 (20%)
3	NAG	B	705	1	14,14,15	1.43	2 (14%)	15,19,21	1.46	1 (6%)
3	NAG	B	706	1,3	14,14,15	0.50	0	15,19,21	0.33	0
3	NAG	B	707	3,4	14,14,15	0.25	0	15,19,21	0.37	0
4	BMA	B	708	3	11,11,12	0.71	0	15,15,17	0.78	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	702	1	-	0/6/23/26	0/1/1/1
3	NAG	A	703	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	704	3	-	0/6/23/26	0/1/1/1
3	NAG	A	705	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	706	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	707	3	-	0/2/19/22	0/1/1/1
3	NAG	B	701	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	702	3,4	-	0/6/23/26	0/1/1/1
4	BMA	B	703	3,5	-	0/2/19/22	1/1/1/1
5	MAN	B	704	4	-	0/2/19/22	0/1/1/1
3	NAG	B	705	1	-	0/6/23/26	0/1/1/1
3	NAG	B	706	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	707	3,4	-	0/6/23/26	0/1/1/1
4	BMA	B	708	3	-	0/2/19/22	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	705	NAG	O5-C1	-2.57	1.39	1.43
3	B	705	NAG	C1-C2	2.29	1.55	1.52
3	A	703	NAG	O5-C1	2.58	1.47	1.43
3	B	705	NAG	O5-C1	4.33	1.50	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	703	BMA	O2-C2-C3	-2.36	105.44	110.19
4	A	707	BMA	O2-C2-C3	-2.34	105.46	110.19
5	B	704	MAN	O2-C2-C3	-2.10	105.95	110.19
3	A	705	NAG	C3-C4-C5	2.14	114.03	110.23
3	A	705	NAG	O5-C5-C4	2.15	113.69	110.13
5	B	704	MAN	O5-C1-C2	2.76	115.31	110.89
4	B	703	BMA	C1-O5-C5	3.74	117.64	112.14
3	A	703	NAG	C1-O5-C5	3.96	117.97	112.14
5	B	704	MAN	C1-O5-C5	4.17	118.27	112.14
3	B	705	NAG	C1-O5-C5	5.25	119.86	112.14

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	703	BMA	C1-C2-C3-C4-C5-O5

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	705	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	550/578 (95%)	0.52	46 (8%) 14 9	39, 69, 137, 197	0
1	B	544/578 (94%)	0.25	12 (2%) 65 60	41, 64, 116, 170	0
All	All	1094/1156 (94%)	0.38	58 (5%) 30 23	39, 67, 131, 197	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	592	PRO	7.3
1	A	287	MET	4.9
1	A	280	SER	4.5
1	A	105	THR	4.4
1	A	106	ASP	4.3
1	A	228	THR	3.9
1	A	230	TYR	3.9
1	A	323	GLY	3.8
1	A	338	LEU	3.8
1	A	356	LYS	3.6
1	B	67	TYR	3.5
1	A	339	VAL	3.5
1	A	569	SER	3.4
1	A	108	ASP	3.4
1	A	340	ILE	3.4
1	A	231	TRP	3.3
1	A	240	GLY	3.2
1	A	104	TRP	3.1
1	A	290	ASP	3.1
1	A	225	SER	3.1
1	B	186	SER	3.1
1	A	279	PHE	3.0
1	A	269	CYS	3.0
1	A	328	LEU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	341	GLU	2.9
1	A	278	HIS	2.8
1	A	286	LYS	2.7
1	A	292	LEU	2.7
1	A	270	ALA	2.7
1	B	587	SER	2.7
1	A	524	ASN	2.7
1	A	289	PRO	2.7
1	A	217	GLN	2.7
1	A	110	ALA	2.6
1	B	270	ALA	2.6
1	A	214	MET	2.6
1	A	293	ASN	2.6
1	A	355	ALA	2.5
1	A	291	ARG	2.5
1	B	187	GLY	2.5
1	B	287	MET	2.4
1	B	586	ILE	2.4
1	B	541	SER	2.3
1	A	82	LYS	2.3
1	A	235	LYS	2.3
1	A	229	THR	2.3
1	A	46	PRO	2.3
1	A	533	ALA	2.2
1	A	588	THR	2.2
1	A	207	LEU	2.2
1	B	276	VAL	2.2
1	A	209	SER	2.1
1	A	299	LEU	2.1
1	A	221	ILE	2.1
1	B	535	VAL	2.0
1	A	216	VAL	2.0
1	B	46	PRO	2.0
1	B	484	LEU	2.0

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 ⓘ

There are no carbohydrates in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	MAN	B	704	11/12	0.74	0.33	3.78	100,110,119,127	0
3	NAG	B	705	14/15	0.81	0.28	0.72	79,91,103,104	0
3	NAG	B	706	14/15	0.92	0.22	-0.18	61,74,94,98	0
3	NAG	A	702	14/15	0.89	0.19	-0.44	69,78,83,90	0
3	NAG	B	701	14/15	0.94	0.18	-0.50	43,48,57,63	0
3	NAG	A	705	14/15	0.86	0.19	-0.74	70,99,122,134	0
3	NAG	A	703	14/15	0.91	0.19	-1.04	64,77,94,99	0
3	NAG	B	707	14/15	0.80	0.19	-	105,113,121,125	0
3	NAG	B	702	14/15	0.88	0.19	-	71,94,103,105	0
4	BMA	B	708	11/12	0.73	0.18	-	121,129,147,152	0
3	NAG	A	704	14/15	0.87	0.26	-	89,97,101,102	0
4	BMA	B	703	11/12	0.81	0.21	-	105,107,115,117	0
3	NAG	A	706	14/15	0.70	0.27	-	153,155,166,169	0
2	CU	A	701	1/1	0.92	0.09	-	151,151,151,151	0
4	BMA	A	707	11/12	0.67	0.32	-	155,156,159,160	0

6.5 Other polymers ⓘ

There are no such residues in this entry.