



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 11:19 AM BST

PDB ID : 3KF5
Title : Structure of invertase from Schwanniomyces occidentalis
Authors : Sanz-Aparicio, J.; Polo, A.
Deposited on : 2009-10-27
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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

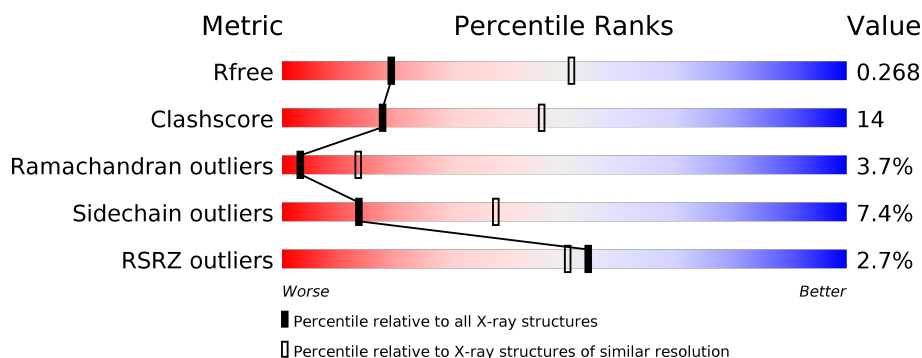
1 Overall quality at a glance

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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	512	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>• •</div> </div> </div>
1	B	512	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>24%</div> <div>• ••</div> </div> </div>

2 Entry composition [i](#)

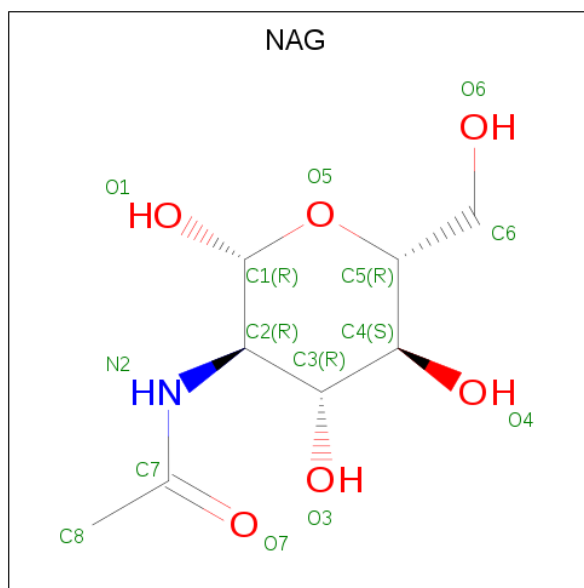
There are 4 unique types of molecules in this entry. The entry contains 8626 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Invertase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	512	Total	C	N	O	S	0	0	0
			4156	2670	680	800	6			
1	B	508	Total	C	N	O	S	0	0	0
			4126	2651	676	793	6			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



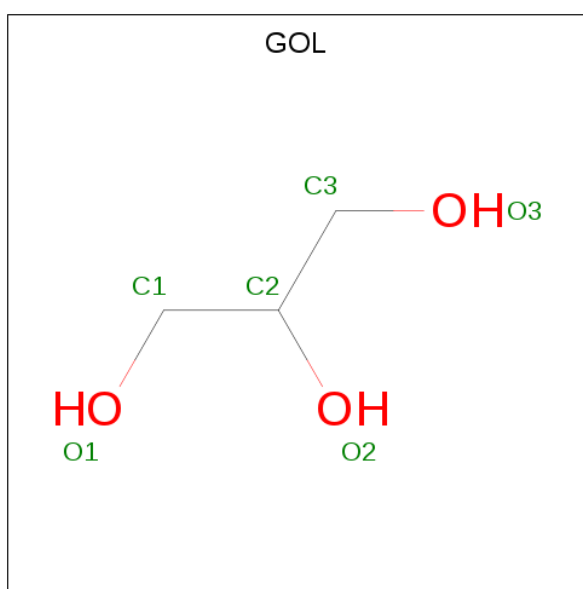
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	119	Total	O	0	0
			119	119		
4	B	95	Total	O	0	0
			95	95		

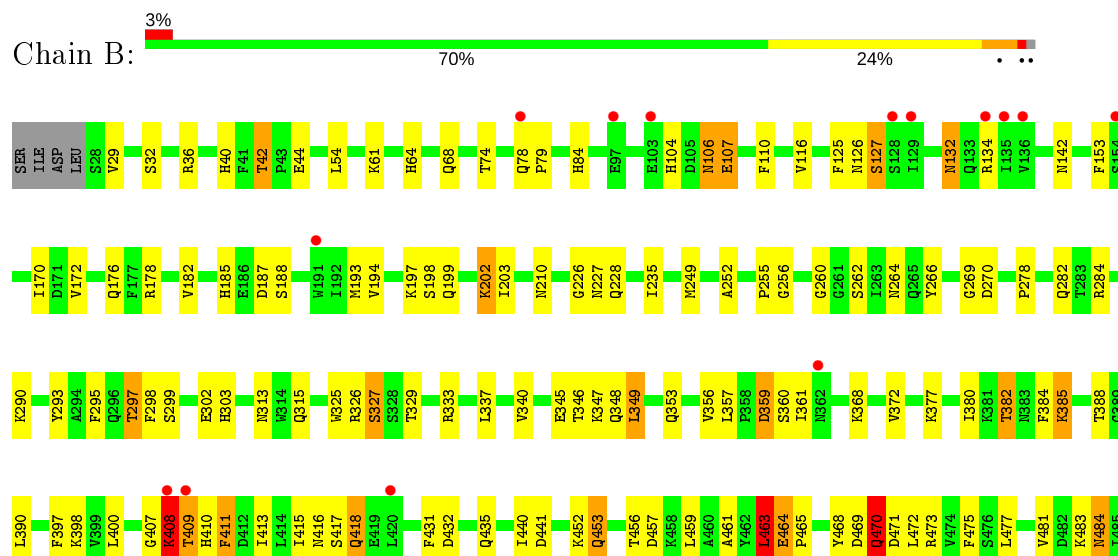
3 Residue-property plots [i](#)

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

• Molecule 1: Invertase



• Molecule 1: Invertase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.78 Å 119.49 Å 137.68 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.65 – 2.90 59.65 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (59.65-2.90) 99.8 (59.65-2.90)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.29 (at 2.91 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.222 , 0.257 0.228 , 0.268	Depositor DCC
R_{free} test set	1979 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	42.0	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.9	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	0.89	EDS
Total number of atoms	8626	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, NAG

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	0.43	0/4277	0.66	2/5825 (0.0%)
1	B	0.42	0/4247	0.65	2/5784 (0.0%)
All	All	0.43	0/8524	0.66	4/11609 (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	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	463	LEU	N-CA-C	5.76	126.55	111.00
1	A	463	LEU	N-CA-C	5.53	125.92	111.00
1	A	502	PHE	N-CA-C	5.31	125.33	111.00
1	B	502	PHE	N-CA-C	5.04	124.59	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	ASP	Peptide
1	A	459	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	B	359	ASP	Peptide
1	B	459	LEU	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	4156	0	3937	117	0
1	B	4126	0	3908	110	0
2	A	70	0	65	1	0
2	B	42	0	39	1	0
3	A	18	0	24	1	0
4	A	119	0	0	2	0
4	B	95	0	0	6	0
All	All	8626	0	7973	222	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 14.

All (222) 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:B:116:VAL:HG11	1:B:132:ASN:HA	1.42	0.99
1:A:116:VAL:HG11	1:A:132:ASN:HA	1.43	0.97
1:B:36:ARG:HD2	1:B:42:THR:HG21	1.47	0.94
1:B:170:ILE:HD12	1:B:193:MET:HE1	1.49	0.93
1:A:371:ASN:HD22	1:A:371:ASN:N	1.62	0.93
1:A:36:ARG:HD2	1:A:42:THR:HG21	1.51	0.89
1:B:176:GLN:HG2	1:B:199:GLN:HG3	1.56	0.87
1:B:170:ILE:HD12	1:B:193:MET:CE	2.08	0.84
1:A:172:VAL:HG11	1:A:197:LYS:HE3	1.61	0.83
1:B:36:ARG:CD	1:B:42:THR:HG21	2.10	0.82
1:A:176:GLN:HG2	1:A:199:GLN:HG3	1.62	0.80
1:B:203:ILE:HD13	1:B:249:MET:HE2	1.63	0.80
1:A:371:ASN:H	1:A:371:ASN:HD22	1.25	0.79
1:B:172:VAL:HG11	1:B:197:LYS:HE3	1.62	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ILE:HD12	1:A:193:MET:HE1	1.64	0.77
1:A:170:ILE:HD12	1:A:193:MET:CE	2.14	0.77
1:A:463:LEU:O	1:A:464:GLU:HB2	1.83	0.76
1:A:36:ARG:CD	1:A:42:THR:HG21	2.15	0.76
1:B:264:ASN:HD21	1:B:295:PHE:H	1.32	0.76
1:A:371:ASN:ND2	1:A:371:ASN:N	2.29	0.75
1:B:463:LEU:O	1:B:464:GLU:HB2	1.87	0.75
1:A:203:ILE:HD13	1:A:249:MET:CE	2.17	0.74
1:B:36:ARG:HH11	1:B:42:THR:CG2	1.99	0.74
1:A:36:ARG:HH11	1:A:42:THR:CG2	2.00	0.74
1:A:264:ASN:HD21	1:A:295:PHE:H	1.35	0.73
1:A:76:TRP:HE1	3:A:6001:GOL:HO3	1.35	0.72
1:A:107:GLU:HG3	1:A:142:ASN:ND2	2.05	0.71
1:A:203:ILE:HD13	1:A:249:MET:HE2	1.73	0.71
1:B:329:THR:HG23	4:B:594:HOH:O	1.90	0.70
1:B:329:THR:CG2	4:B:594:HOH:O	2.38	0.70
1:A:42:THR:HB	4:A:606:HOH:O	1.91	0.70
1:B:203:ILE:HD13	1:B:249:MET:CE	2.20	0.70
1:A:346:THR:O	1:A:347:LYS:HB2	1.93	0.69
1:A:417:SER:HB3	1:A:503:MET:CE	2.24	0.68
1:B:107:GLU:HG3	1:B:142:ASN:ND2	2.07	0.68
1:A:416:ASN:HD21	1:A:513:GLN:HE21	1.42	0.68
1:B:417:SER:HB3	1:B:503:MET:CE	2.24	0.66
1:B:333:ARG:HH11	1:B:353:GLN:NE2	1.94	0.66
1:A:484:ASN:C	1:A:484:ASN:HD22	1.99	0.65
1:B:68:GLN:HE22	1:B:110:PHE:HA	1.61	0.65
1:A:407:GLY:O	1:A:408:LYS:HB2	1.97	0.64
1:A:333:ARG:HH11	1:A:353:GLN:NE2	1.96	0.64
1:B:407:GLY:O	1:B:408:LYS:HB2	1.97	0.63
1:A:107:GLU:HB3	1:A:142:ASN:O	1.98	0.63
1:A:262:SER:HB2	1:A:293:TYR:CD1	2.34	0.62
1:A:417:SER:HB3	1:A:503:MET:HE1	1.81	0.62
1:A:282:GLN:HE22	1:A:348:GLN:NE2	1.96	0.62
1:A:116:VAL:CG1	1:A:132:ASN:HA	2.26	0.62
1:A:488:LEU:HD12	1:A:497:MET:HE1	1.80	0.62
1:B:262:SER:HB2	1:B:293:TYR:CD1	2.35	0.62
1:B:346:THR:O	1:B:347:LYS:HB2	1.99	0.62
1:B:132:ASN:C	1:B:132:ASN:HD22	2.04	0.61
1:B:416:ASN:HD21	1:B:513:GLN:HE21	1.49	0.61
1:A:68:GLN:HE22	1:A:110:PHE:HA	1.66	0.60
1:B:116:VAL:CG1	1:B:132:ASN:HA	2.26	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:417:SER:HB3	1:B:503:MET:HE1	1.82	0.60
1:B:107:GLU:HB3	1:B:142:ASN:O	2.02	0.60
1:B:484:ASN:HD22	1:B:484:ASN:C	2.06	0.59
1:A:313:ASN:OD1	1:A:315:GLN:HG2	2.03	0.59
1:B:282:GLN:HE22	1:B:348:GLN:NE2	2.00	0.59
1:A:398:LYS:HD3	1:A:472:LEU:HD23	1.85	0.58
1:A:340:VAL:O	1:A:347:LYS:HA	2.03	0.58
1:A:132:ASN:HD22	1:A:132:ASN:C	2.07	0.58
1:A:107:GLU:HG3	1:A:142:ASN:HD22	1.68	0.57
1:B:388:THR:HG22	1:B:390:LEU:H	1.71	0.56
1:B:313:ASN:OD1	1:B:315:GLN:HG2	2.06	0.56
1:A:36:ARG:HH11	1:A:42:THR:HG21	1.68	0.56
1:A:203:ILE:HD13	1:A:249:MET:HE1	1.88	0.56
1:B:410:HIS:HB2	1:B:432:ASP:HA	1.87	0.56
1:B:452:LYS:O	1:B:453:GLN:CB	2.53	0.56
1:B:226:GLY:HA3	1:B:256:GLY:HA3	1.88	0.55
1:B:398:LYS:HD3	1:B:472:LEU:HD23	1.89	0.55
1:B:452:LYS:O	1:B:453:GLN:HB2	2.05	0.55
1:A:172:VAL:CG1	1:A:197:LYS:HE3	2.36	0.55
1:A:416:ASN:ND2	1:A:513:GLN:HE21	2.04	0.54
1:A:172:VAL:O	1:A:172:VAL:CG1	2.55	0.54
1:B:377:LYS:HD2	4:B:617:HOH:O	2.08	0.54
1:A:185:HIS:HD2	1:A:188:SER:OG	1.91	0.54
1:A:410:HIS:HB2	1:A:432:ASP:HA	1.89	0.54
1:B:185:HIS:HD2	1:B:188:SER:OG	1.90	0.54
1:B:107:GLU:HG3	1:B:142:ASN:HD22	1.72	0.53
1:A:388:THR:HG22	1:A:390:LEU:H	1.73	0.53
1:A:226:GLY:HA3	1:A:256:GLY:HA3	1.89	0.53
1:B:264:ASN:ND2	1:B:295:PHE:H	2.05	0.53
1:A:463:LEU:O	1:A:464:GLU:CB	2.53	0.53
1:A:452:LYS:O	1:A:453:GLN:CB	2.57	0.52
1:B:463:LEU:O	1:B:464:GLU:CB	2.57	0.52
1:A:226:GLY:CA	1:A:256:GLY:HA3	2.40	0.52
1:B:337:LEU:HB3	1:B:349:LEU:HD22	1.91	0.52
1:A:170:ILE:HD12	1:A:193:MET:HE2	1.92	0.52
1:B:340:VAL:O	1:B:347:LYS:HA	2.08	0.52
1:B:397:PHE:CZ	1:B:475:PHE:HB2	2.45	0.52
1:A:64:HIS:CD2	1:A:84:HIS:NE2	2.78	0.51
1:B:36:ARG:NH2	4:B:588:HOH:O	2.43	0.51
1:B:172:VAL:O	1:B:172:VAL:CG1	2.58	0.51
1:B:36:ARG:HH11	1:B:42:THR:HG21	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:HIS:HD2	1:A:84:HIS:NE2	2.09	0.51
1:B:456:THR:O	1:B:457:ASP:HB2	2.10	0.51
1:B:416:ASN:ND2	1:B:513:GLN:HE21	2.08	0.51
1:A:486:ILE:HD11	1:A:488:LEU:HD21	1.93	0.51
1:A:78:GLN:HB2	1:A:79:PRO:HD3	1.93	0.51
1:A:227:ASN:HB3	1:A:255:PRO:HD2	1.92	0.50
1:A:337:LEU:HB3	1:A:349:LEU:HD22	1.93	0.50
1:A:456:THR:O	1:A:457:ASP:HB2	2.11	0.50
1:B:226:GLY:CA	1:B:256:GLY:HA3	2.42	0.50
1:B:488:LEU:HD12	1:B:497:MET:HE1	1.92	0.50
1:A:452:LYS:O	1:A:453:GLN:HB2	2.11	0.50
1:A:440:ILE:HG21	1:A:497:MET:HE3	1.94	0.50
1:B:172:VAL:CG1	1:B:197:LYS:HE3	2.37	0.50
1:A:397:PHE:CZ	1:A:475:PHE:HB2	2.47	0.49
1:B:326:ARG:O	1:B:327:SER:HB2	2.13	0.49
1:A:372:VAL:HG21	1:A:380:ILE:HD11	1.94	0.49
1:B:134:ARG:HH22	1:B:153:PHE:HB2	1.77	0.49
1:B:227:ASN:HB3	1:B:255:PRO:HD2	1.95	0.49
1:A:264:ASN:ND2	1:A:295:PHE:H	2.05	0.48
1:B:78:GLN:HB2	1:B:79:PRO:HD3	1.95	0.48
1:A:526:GLU:HB3	4:A:625:HOH:O	2.13	0.48
1:B:486:ILE:HD11	1:B:488:LEU:HD21	1.94	0.48
1:B:417:SER:HB3	1:B:503:MET:HE3	1.95	0.48
1:B:126:ASN:O	1:B:127:SER:HB3	2.12	0.48
1:A:326:ARG:O	1:A:327:SER:HB2	2.14	0.47
1:A:282:GLN:CD	1:A:284:ARG:HE	2.17	0.47
1:B:32:SER:O	1:B:483:LYS:NZ	2.48	0.47
1:B:418:GLN:HG2	1:B:510:HIS:CD2	2.50	0.47
1:B:202:LYS:NZ	2:B:3001:NAG:H61	2.29	0.47
1:A:134:ARG:HH22	1:A:153:PHE:HB2	1.79	0.47
1:B:408:LYS:O	1:B:409:THR:HB	2.14	0.47
1:A:170:ILE:CD1	1:A:193:MET:HE2	2.45	0.47
1:B:260:GLY:HA3	1:B:290:LYS:NZ	2.30	0.47
1:B:260:GLY:HA3	1:B:290:LYS:HZ3	1.80	0.47
1:B:64:HIS:CD2	1:B:84:HIS:NE2	2.82	0.47
1:B:372:VAL:HG11	1:B:380:ILE:HD11	1.97	0.46
1:B:440:ILE:HG21	1:B:497:MET:HE3	1.97	0.46
1:A:176:GLN:HG3	1:A:178:ARG:HH12	1.79	0.46
1:A:126:ASN:O	1:A:127:SER:HB3	2.14	0.46
1:A:417:SER:HB3	1:A:503:MET:HE3	1.94	0.46
1:A:384:PHE:O	1:A:385:LYS:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:GLN:HA	1:A:470:GLN:HE21	1.81	0.46
1:B:64:HIS:HD2	1:B:84:HIS:NE2	2.14	0.46
1:B:410:HIS:HB3	1:B:523:PHE:CZ	2.51	0.46
1:A:260:GLY:HA3	1:A:290:LYS:NZ	2.31	0.46
1:A:415:ILE:HD13	1:A:481:VAL:HG21	1.97	0.46
1:B:471:ASP:HB2	4:B:561:HOH:O	2.14	0.45
1:B:125:PHE:CE2	1:B:127:SER:HA	2.51	0.45
1:B:269:GLY:HA3	1:B:278:PRO:HA	1.98	0.45
1:A:32:SER:O	1:A:483:LYS:NZ	2.50	0.45
1:A:408:LYS:O	1:A:409:THR:HB	2.17	0.45
1:B:170:ILE:CD1	1:B:193:MET:CE	2.87	0.45
1:A:227:ASN:ND2	1:A:255:PRO:HD2	2.32	0.45
1:A:484:ASN:ND2	1:A:484:ASN:C	2.70	0.45
1:B:252:ALA:HB1	1:B:293:TYR:CE1	2.52	0.45
1:B:516:THR:HG22	1:B:518:THR:H	1.82	0.45
1:A:194:VAL:HG13	1:A:232:PRO:HB2	1.98	0.44
1:A:176:GLN:HE21	1:A:178:ARG:HH12	1.65	0.44
1:A:389:GLY:HA3	1:A:483:LYS:CG	2.47	0.44
1:A:227:ASN:HD22	1:A:255:PRO:HD2	1.82	0.44
1:A:418:GLN:HG2	1:A:510:HIS:CD2	2.51	0.44
1:A:125:PHE:CE2	1:A:127:SER:HA	2.52	0.44
1:A:438:PHE:O	1:A:460:ALA:O	2.36	0.44
1:A:36:ARG:O	1:A:483:LYS:HD3	2.18	0.44
1:A:380:ILE:O	1:A:513:GLN:HA	2.18	0.44
1:A:516:THR:HG22	1:A:518:THR:H	1.81	0.44
1:A:199:GLN:HE21	1:B:345:GLU:HB2	1.82	0.44
1:A:269:GLY:HA3	1:A:278:PRO:HA	1.98	0.44
1:A:370:LYS:HB3	1:A:371:ASN:ND2	2.33	0.44
1:B:227:ASN:ND2	1:B:228:GLN:HG3	2.33	0.44
1:A:450:PRO:HB3	1:B:407:GLY:CA	2.48	0.44
1:A:368:LYS:HG2	1:A:529:ILE:HG12	2.00	0.43
1:A:441:ASP:HA	1:A:457:ASP:O	2.18	0.43
1:B:104:HIS:C	1:B:106:ASN:H	2.20	0.43
1:A:176:GLN:CG	1:A:199:GLN:HG3	2.43	0.43
1:B:368:LYS:HG2	1:B:529:ILE:HG12	2.01	0.43
1:A:54:LEU:HB3	1:A:298:PHE:CD2	2.53	0.43
1:A:409:THR:O	1:A:410:HIS:C	2.57	0.43
1:B:54:LEU:HB3	1:B:298:PHE:CD2	2.53	0.43
1:B:415:ILE:HD13	1:B:481:VAL:HG21	2.00	0.43
1:B:266:TYR:CE1	1:B:284:ARG:NH1	2.86	0.43
1:B:384:PHE:O	1:B:385:LYS:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:ARG:CD	1:B:353:GLN:HE21	2.31	0.43
1:B:36:ARG:HD3	1:B:42:THR:HG21	1.98	0.43
1:A:172:VAL:O	1:A:172:VAL:HG12	2.19	0.42
1:A:306:LEU:HD21	2:A:4001:NAG:H82	2.01	0.42
1:A:410:HIS:HB3	1:A:523:PHE:CZ	2.54	0.42
1:B:125:PHE:CZ	1:B:127:SER:HA	2.54	0.42
1:B:176:GLN:HG3	1:B:178:ARG:HH12	1.84	0.42
1:A:125:PHE:CZ	1:A:127:SER:HA	2.54	0.42
1:B:470:GLN:HA	1:B:470:GLN:HE21	1.85	0.42
1:B:410:HIS:HB3	1:B:523:PHE:HZ	1.84	0.42
1:A:450:PRO:HB3	1:B:407:GLY:HA2	2.01	0.42
1:A:349:LEU:HA	1:A:349:LEU:HD23	1.92	0.42
1:B:40:HIS:CE1	4:B:4:HOH:O	2.73	0.42
1:B:441:ASP:HA	1:B:457:ASP:O	2.20	0.42
1:B:170:ILE:CD1	1:B:193:MET:HE2	2.50	0.42
1:A:252:ALA:HB1	1:A:293:TYR:CE1	2.55	0.42
1:A:410:HIS:O	1:A:431:PHE:O	2.38	0.42
1:B:382:THR:HB	1:B:512:ILE:H	1.84	0.42
1:A:333:ARG:HD3	1:A:353:GLN:HE21	1.84	0.42
1:B:410:HIS:O	1:B:431:PHE:O	2.37	0.42
1:B:176:GLN:HE21	1:B:178:ARG:HH22	1.67	0.41
1:B:409:THR:O	1:B:410:HIS:C	2.57	0.41
1:B:333:ARG:HD3	1:B:353:GLN:HE21	1.85	0.41
1:B:465:PRO:HG2	1:B:468:TYR:CZ	2.54	0.41
1:A:329:THR:HG23	1:A:330:SER:O	2.20	0.41
1:A:369:LYS:HB3	1:A:372:VAL:CG1	2.51	0.41
1:B:176:GLN:CG	1:B:199:GLN:HG3	2.38	0.41
1:A:315:GLN:HA	1:B:435:GLN:NE2	2.35	0.41
1:B:36:ARG:HH11	1:B:42:THR:HG23	1.82	0.41
1:B:282:GLN:CD	1:B:284:ARG:HE	2.24	0.41
1:A:345:GLU:HB2	1:B:199:GLN:HE21	1.86	0.41
1:A:186:GLU:C	1:A:188:SER:H	2.24	0.41
1:A:382:THR:HB	1:A:512:ILE:H	1.86	0.41
1:A:484:ASN:HD22	1:A:485:ILE:N	2.19	0.41
1:B:74:THR:O	1:B:326:ARG:HD2	2.21	0.41
1:A:227:ASN:CB	1:A:255:PRO:HD2	2.51	0.40
1:A:227:ASN:ND2	1:A:228:GLN:HG3	2.36	0.40
1:A:379:PRO:HB3	1:A:515:VAL:HG12	2.03	0.40
1:A:70:ASN:ND2	1:A:77:GLY:HA3	2.36	0.40
1:B:235:ILE:HD12	1:B:297:THR:HG21	2.03	0.40
1:A:232:PRO:HA	1:A:250:PHE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:MET:HE2	1:B:497:MET:HB3	1.93	0.40
1:B:176:GLN:HE21	1:B:178:ARG:HH12	1.69	0.40
1:B:198:SER:HB3	1:B:228:GLN:HB3	2.04	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	510/512 (100%)	446 (88%)	44 (9%)	20 (4%)	3	12
1	B	506/512 (99%)	447 (88%)	41 (8%)	18 (4%)	3	14
All	All	1016/1024 (99%)	893 (88%)	85 (8%)	38 (4%)	3	13

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	ASP
1	A	127	SER
1	A	187	ASP
1	A	303	HIS
1	A	360	SER
1	A	409	THR
1	A	411	PHE
1	B	127	SER
1	B	303	HIS
1	B	360	SER
1	B	409	THR
1	B	411	PHE
1	A	359	ASP
1	A	371	ASN
1	A	453	GLN

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Mol	Chain	Res	Type
1	A	470	GLN
1	B	187	ASP
1	B	359	ASP
1	B	453	GLN
1	B	470	GLN
1	A	408	LYS
1	B	357	LEU
1	B	408	LYS
1	A	356	VAL
1	A	357	LEU
1	A	461	ALA
1	A	327	SER
1	A	460	ALA
1	B	327	SER
1	B	385	LYS
1	B	461	ALA
1	A	385	LYS
1	A	464	GLU
1	A	503	MET
1	B	356	VAL
1	B	473	ARG
1	B	503	MET
1	B	464	GLU

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	464/464 (100%)	428 (92%)	36 (8%)	12	34
1	B	460/464 (99%)	428 (93%)	32 (7%)	15	41
All	All	924/928 (100%)	856 (93%)	68 (7%)	13	38

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASP
1	A	29	VAL
1	A	42	THR
1	A	44	GLU
1	A	61	LYS
1	A	106	ASN
1	A	107	GLU
1	A	132	ASN
1	A	176	GLN
1	A	182	VAL
1	A	194	VAL
1	A	202	LYS
1	A	210	ASN
1	A	270	ASP
1	A	297	THR
1	A	302	GLU
1	A	325	TRP
1	A	349	LEU
1	A	361	ILE
1	A	371	ASN
1	A	372	VAL
1	A	378	LYS
1	A	382	THR
1	A	400	LEU
1	A	408	LYS
1	A	411	PHE
1	A	413	ILE
1	A	418	GLN
1	A	463	LEU
1	A	469	ASP
1	A	470	GLN
1	A	483	LYS
1	A	484	ASN
1	A	486	ILE
1	A	495	VAL
1	A	533	LEU
1	B	29	VAL
1	B	42	THR
1	B	44	GLU
1	B	61	LYS
1	B	106	ASN
1	B	107	GLU
1	B	132	ASN

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Mol	Chain	Res	Type
1	B	182	VAL
1	B	194	VAL
1	B	202	LYS
1	B	210	ASN
1	B	270	ASP
1	B	297	THR
1	B	299	SER
1	B	302	GLU
1	B	325	TRP
1	B	349	LEU
1	B	361	ILE
1	B	382	THR
1	B	400	LEU
1	B	408	LYS
1	B	411	PHE
1	B	413	ILE
1	B	418	GLN
1	B	463	LEU
1	B	469	ASP
1	B	470	GLN
1	B	477	LEU
1	B	484	ASN
1	B	486	ILE
1	B	495	VAL
1	B	533	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	64	HIS
1	A	68	GLN
1	A	106	ASN
1	A	132	ASN
1	A	176	GLN
1	A	185	HIS
1	A	199	GLN
1	A	227	ASN
1	A	228	GLN
1	A	241	ASN
1	A	264	ASN
1	A	296	GLN

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Mol	Chain	Res	Type
1	A	348	GLN
1	A	353	GLN
1	A	362	ASN
1	A	371	ASN
1	A	403	ASN
1	A	470	GLN
1	A	484	ASN
1	A	510	HIS
1	A	513	GLN
1	B	52	ASN
1	B	64	HIS
1	B	68	GLN
1	B	106	ASN
1	B	132	ASN
1	B	176	GLN
1	B	185	HIS
1	B	227	ASN
1	B	228	GLN
1	B	264	ASN
1	B	296	GLN
1	B	348	GLN
1	B	353	GLN
1	B	362	ASN
1	B	403	ASN
1	B	453	GLN
1	B	470	GLN
1	B	484	ASN
1	B	513	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

11 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	NAG	A	5001	1	14,14,15	0.65	0	17,19,21	1.64	3 (17%)
2	NAG	A	4001	1	14,14,15	0.45	0	17,19,21	1.71	4 (23%)
2	NAG	A	3001	1	14,14,15	0.65	0	17,19,21	1.73	2 (11%)
2	NAG	A	2001	1	14,14,15	0.44	0	17,19,21	1.17	1 (5%)
2	NAG	B	5001	1	14,14,15	0.59	0	17,19,21	1.99	3 (17%)
3	GOL	A	6001	-	5,5,5	0.40	0	5,5,5	0.15	0
3	GOL	A	6002	-	5,5,5	0.33	0	5,5,5	0.38	0
2	NAG	B	4001	1	14,14,15	0.60	0	17,19,21	1.39	3 (17%)
3	GOL	A	6003	-	5,5,5	0.38	0	5,5,5	0.42	0
2	NAG	A	1001	1	14,14,15	0.54	0	17,19,21	1.65	2 (11%)
2	NAG	B	3001	1	14,14,15	0.59	0	17,19,21	2.20	2 (11%)

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	NAG	A	5001	1	-	2/6/23/26	0/1/1/1
2	NAG	A	4001	1	-	2/6/23/26	0/1/1/1
2	NAG	A	3001	1	-	1/6/23/26	0/1/1/1
2	NAG	A	2001	1	-	1/6/23/26	0/1/1/1
2	NAG	B	5001	1	-	1/6/23/26	0/1/1/1
3	GOL	A	6001	-	-	2/4/4/4	-
3	GOL	A	6002	-	-	4/4/4/4	-
2	NAG	B	4001	1	-	2/6/23/26	0/1/1/1
3	GOL	A	6003	-	-	2/4/4/4	-
2	NAG	A	1001	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	3001	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3001	NAG	C1-O5-C5	7.51	122.37	112.19
2	B	5001	NAG	C1-O5-C5	6.37	120.82	112.19
2	A	3001	NAG	C1-O5-C5	5.48	119.62	112.19
2	A	1001	NAG	C1-O5-C5	4.98	118.94	112.19
2	A	5001	NAG	C4-C3-C2	3.84	116.64	111.02
2	A	4001	NAG	C4-C3-C2	3.81	116.60	111.02
2	A	5001	NAG	C1-O5-C5	3.52	116.97	112.19
2	B	5001	NAG	C4-C3-C2	3.27	115.81	111.02
2	A	4001	NAG	O5-C1-C2	-3.11	106.38	111.29
2	B	4001	NAG	C3-C4-C5	-2.91	105.04	110.24
2	B	4001	NAG	C1-O5-C5	2.84	116.03	112.19
2	B	3001	NAG	C6-C5-C4	-2.75	106.55	113.00
2	A	2001	NAG	C1-O5-C5	2.72	115.88	112.19
2	A	3001	NAG	O5-C5-C6	-2.60	103.13	107.20
2	B	4001	NAG	O4-C4-C5	2.51	115.53	109.30
2	A	4001	NAG	C1-O5-C5	2.48	115.56	112.19
2	A	1001	NAG	C2-N2-C7	2.35	126.25	122.90
2	A	5001	NAG	O5-C1-C2	-2.29	107.67	111.29
2	A	4001	NAG	C6-C5-C4	-2.06	108.17	113.00
2	B	5001	NAG	C6-C5-C4	-2.04	108.22	113.00

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	6001	GOL	C1-C2-C3-O3
3	A	6001	GOL	O2-C2-C3-O3
3	A	6002	GOL	O1-C1-C2-C3
3	A	6003	GOL	C1-C2-C3-O3
2	A	5001	NAG	O5-C5-C6-O6
2	A	5001	NAG	C4-C5-C6-O6
2	A	1001	NAG	O5-C5-C6-O6
2	A	1001	NAG	C4-C5-C6-O6
2	A	3001	NAG	O5-C5-C6-O6
2	A	4001	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	A	6002	GOL	C1-C2-C3-O3
3	A	6002	GOL	O1-C1-C2-O2
3	A	6003	GOL	O2-C2-C3-O3
2	B	3001	NAG	C4-C5-C6-O6
2	B	4001	NAG	C4-C5-C6-O6
2	A	4001	NAG	C4-C5-C6-O6
2	B	3001	NAG	O5-C5-C6-O6
2	A	2001	NAG	O5-C5-C6-O6
3	A	6002	GOL	O2-C2-C3-O3
2	B	5001	NAG	C4-C5-C6-O6
2	B	4001	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	4001	NAG	1	0
3	A	6001	GOL	1	0
2	B	3001	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	512/512 (100%)	0.15	14 (2%) 54 50	10, 19, 33, 46	0
1	B	508/512 (99%)	0.21	14 (2%) 53 49	10, 19, 32, 46	0
All	All	1020/1024 (99%)	0.18	28 (2%) 54 50	10, 19, 32, 46	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	128	SER	4.5
1	B	409	THR	4.0
1	A	127	SER	3.8
1	A	24	SER	3.7
1	A	26	ASP	3.3
1	A	409	THR	3.3
1	B	128	SER	3.1
1	B	408	LYS	3.0
1	A	419	GLU	2.9
1	A	126	ASN	2.7
1	A	125	PHE	2.7
1	A	25	ILE	2.7
1	B	103	GLU	2.6
1	B	362	ASN	2.6
1	B	97	GLU	2.6
1	A	303	HIS	2.6
1	A	469	ASP	2.5
1	B	78	GLN	2.4
1	B	129	ILE	2.3
1	B	134	ARG	2.2
1	B	154	SER	2.2
1	B	191	TRP	2.2
1	A	422	SER	2.2
1	B	420	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	302	GLU	2.1
1	B	135	ILE	2.1
1	A	359	ASP	2.1
1	B	136	VAL	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 monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GOL	A	6003	6/6	0.80	0.29	51,52,52,53	0
2	NAG	B	4001	14/15	0.83	0.26	30,36,37,37	0
2	NAG	A	2001	14/15	0.84	0.47	51,57,59,59	0
2	NAG	B	5001	14/15	0.87	0.21	37,42,44,44	0
2	NAG	B	3001	14/15	0.87	0.21	31,36,38,38	0
2	NAG	A	3001	14/15	0.89	0.21	30,34,38,39	0
2	NAG	A	4001	14/15	0.91	0.18	30,34,36,37	0
2	NAG	A	5001	14/15	0.91	0.29	37,43,46,46	0
2	NAG	A	1001	14/15	0.91	0.21	36,39,42,43	0
3	GOL	A	6002	6/6	0.91	0.19	59,60,61,61	0
3	GOL	A	6001	6/6	0.95	0.19	31,35,37,38	0

6.5 Other polymers [i](#)

There are no such residues in this entry.