



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:24 AM GMT

PDB ID : 3EIO
Title : Crystal Structure Analysis of DPPIV Inhibitor
Authors : Ahn, J.H.; Lee, J.-O.
Deposited on : 2008-09-17
Resolution : 2.00 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

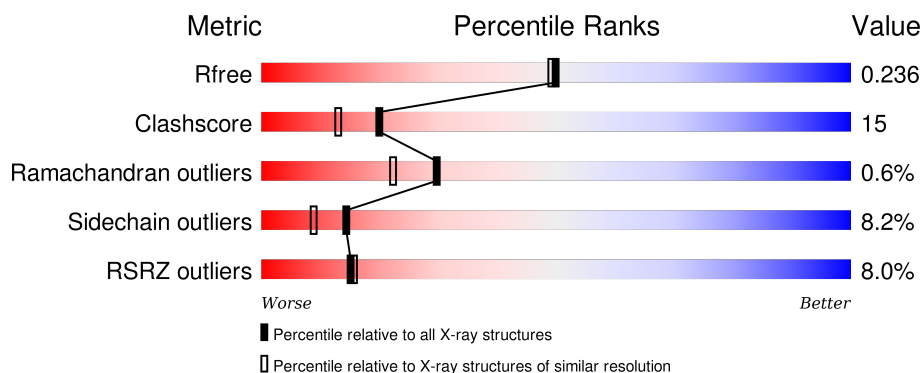
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 ≥ 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	728	<div> <div>10%</div> <div>71%</div> <div>26%</div> <div>.</div> </div>
1	B	728	<div> <div>6%</div> <div>74%</div> <div>23%</div> <div>.</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	941	-	-	-	X
3	NAG	B	971	-	-	-	X
4	NAG	A	841	-	-	-	X
4	NAG	A	842	X	-	-	-
5	NAG	A	861	-	-	-	X
5	NAG	B	901	-	-	-	X
5	NAG	B	932	-	-	-	X
5	NAG	B	951	-	-	-	X
5	NAG	B	952	-	-	-	X
5	NAG	B	961	-	-	-	X

2 Entry composition [i](#)

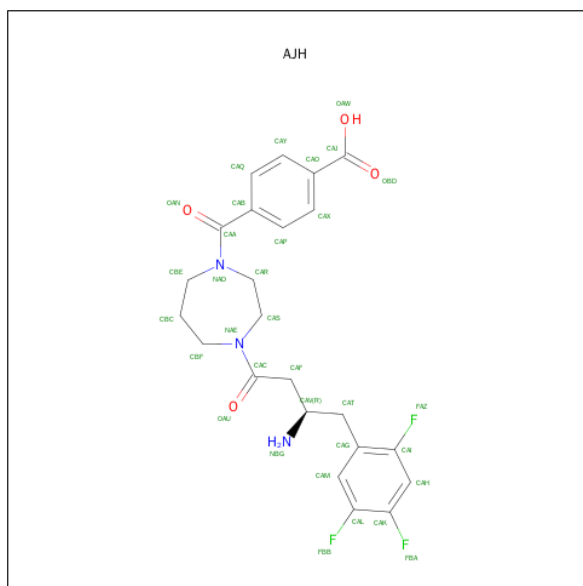
There are 6 unique types of molecules in this entry. The entry contains 12596 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptidyl peptidase 4 soluble form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	0	0
			5948	3816	980	1126	26			
1	B	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			

- Molecule 2 is 4-({4-[(3R)-3-AMINO-4-(2,4,5-TRIFLUOROPHENYL)BUTANOYL]-1,4-DIAZEPAN-1-YL}CARBONYL)BENZOIC ACID (three-letter code: AJH) (formula: C₂₃H₂₄F₃N₃O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			33	23	3	3	4		
2	B	1	Total	C	F	N	O	0	0
			33	23	3	3	4		

- Molecule 3 is SUGAR (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		
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		

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	147	Total	O	0	0
			147	147		
6	B	153	Total	O	0	0
			153	153		

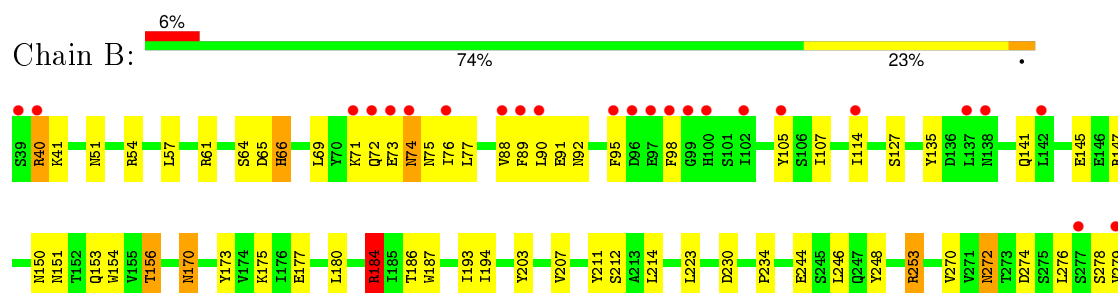
3 Residue-property plots

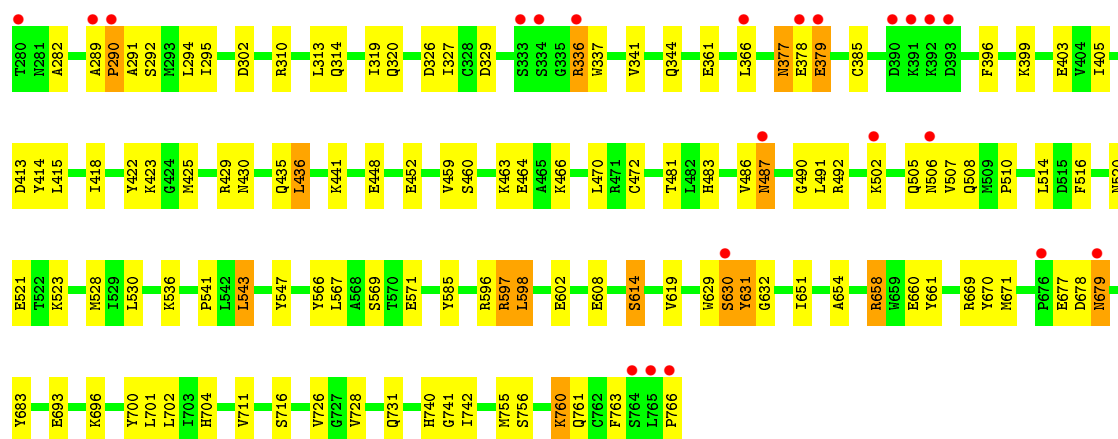
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: Dipeptidyl peptidase 4 soluble form



- Molecule 1: Dipeptidyl peptidase 4 soluble form





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	119.37Å 123.39Å 133.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.26 – 2.00 45.26 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (45.26-2.00) 97.4 (45.26-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.11 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.239 , 0.272 0.237 , 0.236	Depositor DCC
R_{free} test set	6543 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	26.0	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.3	EDS
Estimated twinning fraction	0.011 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 129699 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12596	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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: AJH, NAG, 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	0.69	0/6119	0.84	4/8321 (0.0%)
1	B	0.70	0/6135	0.83	3/8344 (0.0%)
All	All	0.70	0/12254	0.83	7/16665 (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	1
1	B	0	1
4	A	1	0
All	All	1	2

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	631	TYR	N-CA-CB	5.67	120.81	110.60
1	A	669	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	669	ARG	NE-CZ-NH2	-5.49	117.55	120.30
1	A	656	VAL	N-CA-C	-5.30	96.69	111.00
1	B	319	ILE	N-CA-C	-5.09	97.24	111.00
1	A	319	ILE	N-CA-C	-5.07	97.32	111.00
1	B	184	ARG	NE-CZ-NH1	5.04	122.82	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	842	NAG	C1

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	700	TYR	Sidechain
1	B	700	TYR	Sidechain

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	5948	0	5657	190	0
1	B	5963	0	5677	160	0
2	A	33	0	23	5	0
2	B	33	0	23	4	0
3	A	84	0	78	6	0
3	B	56	0	52	4	0
4	A	39	0	34	2	0
5	A	28	0	25	0	0
5	B	112	0	100	3	0
6	A	147	0	0	4	0
6	B	153	0	0	1	0
All	All	12596	0	11669	354	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 15.

All (354) 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:760:LYS:HE2	1:B:766:PRO:C	1.60	1.22
2:B:2:AJH:HARA	2:B:2:AJH:HAP	1.17	1.08
1:B:760:LYS:CE	1:B:766:PRO:C	2.24	1.05
1:A:759:ILE:HG23	1:A:763:PHE:CE1	1.90	1.05
1:A:277:SER:CB	1:A:280:THR:HB	1.86	1.04
2:A:1:AJH:HARA	2:A:1:AJH:HAP	1.11	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ALA:CB	1:B:294:LEU:HG	1.92	1.00
1:A:114:ILE:HG22	1:A:135:TYR:HB3	1.43	1.00
1:B:114:ILE:HG22	1:B:135:TYR:HB3	1.44	0.99
2:A:1:AJH:HARA	2:A:1:AJH:CAP	1.91	0.97
2:B:2:AJH:CAP	2:B:2:AJH:HARA	1.95	0.96
1:B:74:ASN:HD22	3:B:911:NAG:H2	1.30	0.96
1:A:147:ARG:NH1	3:A:821:NAG:O6	1.99	0.95
1:A:651:ILE:HG21	1:A:755:MET:HE2	1.45	0.95
1:B:760:LYS:CE	1:B:766:PRO:O	2.16	0.94
1:B:74:ASN:HB2	1:B:92:ASN:HD22	1.31	0.94
1:B:756:SER:O	1:B:760:LYS:HG2	1.70	0.91
1:B:289:ALA:HB3	1:B:294:LEU:CG	2.01	0.91
1:B:74:ASN:O	1:B:92:ASN:HB3	1.70	0.91
2:A:1:AJH:HAP	2:A:1:AJH:CAR	2.01	0.90
1:A:759:ILE:O	1:A:763:PHE:HD1	1.57	0.87
1:A:289:ALA:HB3	1:A:294:LEU:HG	1.57	0.86
2:B:2:AJH:CAR	2:B:2:AJH:HAP	2.06	0.84
1:A:277:SER:OG	1:A:280:THR:HB	1.77	0.84
1:A:697:GLN:HG3	6:A:1043:HOH:O	1.77	0.84
1:A:731:GLN:NE2	1:B:731:GLN:HE22	1.76	0.84
1:B:289:ALA:HB1	1:B:294:LEU:HG	1.59	0.84
1:A:759:ILE:HG23	1:A:763:PHE:HE1	1.41	0.83
1:A:756:SER:O	1:A:760:LYS:HG2	1.78	0.83
1:B:289:ALA:CB	1:B:294:LEU:CG	2.58	0.82
1:A:289:ALA:HB3	1:A:294:LEU:CG	2.09	0.82
1:B:630:SER:HB2	1:B:740:HIS:NE2	1.95	0.81
1:A:731:GLN:HE22	1:B:731:GLN:NE2	1.77	0.81
1:B:630:SER:HB2	1:B:740:HIS:CE1	2.16	0.80
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.63	0.80
1:B:289:ALA:HB3	1:B:294:LEU:HG	1.61	0.80
1:A:193:ILE:HG22	1:A:194:ILE:HG12	1.64	0.79
1:A:230:ASP:OD1	1:A:264:PRO:HB3	1.83	0.78
1:A:184:ARG:HH11	1:A:187:TRP:HA	1.48	0.78
1:B:651:ILE:HG21	1:B:755:MET:HE2	1.65	0.78
1:B:272:ASN:C	1:B:272:ASN:HD22	1.86	0.77
1:A:651:ILE:HG21	1:A:755:MET:CE	2.14	0.77
1:A:272:ASN:HD22	1:A:274:ASP:H	1.33	0.77
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.67	0.76
1:B:760:LYS:NZ	1:B:766:PRO:O	2.19	0.75
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.84	0.75
1:B:184:ARG:HD3	1:B:186:THR:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:272:ASN:ND2	1:A:274:ASP:H	1.84	0.75
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.69	0.75
1:A:196:ASN:OD1	1:A:227:GLN:HG3	1.87	0.74
1:A:183:TYR:CZ	1:A:276:LEU:HD21	2.23	0.74
1:B:72:GLN:O	1:B:74:ASN:OD1	2.05	0.73
1:A:377:ASN:C	1:A:377:ASN:HD22	1.91	0.73
2:A:1:AJH:CAR	2:A:1:AJH:CAP	2.64	0.73
1:B:76:ILE:HG22	1:B:90:LEU:HB3	1.71	0.73
1:B:669:ARG:HD2	1:B:670:TYR:CZ	2.23	0.72
1:B:289:ALA:HB3	1:B:294:LEU:CD1	2.18	0.72
1:B:177:GLU:HB2	1:B:180:LEU:HD13	1.71	0.72
1:A:253:ARG:HH22	1:B:253:ARG:HH22	1.38	0.71
1:A:184:ARG:HD3	1:A:186:THR:O	1.90	0.71
1:B:276:LEU:CD2	1:B:282:ALA:HB2	2.20	0.71
1:B:289:ALA:HB3	1:B:294:LEU:HD11	1.72	0.70
1:A:76:ILE:HG22	1:A:90:LEU:HB3	1.73	0.69
1:B:74:ASN:HB3	3:B:911:NAG:C7	2.23	0.69
1:A:195:TYR:CE1	1:A:230:ASP:OD2	2.46	0.69
1:A:413:ASP:HB3	1:A:414:TYR:CD1	2.26	0.69
1:B:679:ASN:O	1:B:683:TYR:HD2	1.75	0.69
1:A:183:TYR:CD1	1:A:276:LEU:HD11	2.28	0.68
1:A:658:ARG:HG2	1:A:661:TYR:CE2	2.28	0.68
1:A:183:TYR:CE2	1:A:276:LEU:HG	2.29	0.68
1:B:74:ASN:C	1:B:92:ASN:HB3	2.14	0.67
1:A:413:ASP:HB3	1:A:414:TYR:HD1	1.58	0.67
1:A:731:GLN:NE2	1:B:731:GLN:NE2	2.39	0.67
1:A:156:THR:HG21	1:A:214:LEU:HD11	1.74	0.67
1:B:760:LYS:NZ	1:B:766:PRO:C	2.47	0.67
1:B:74:ASN:OD1	1:B:74:ASN:N	2.25	0.67
1:A:195:TYR:HE1	1:A:230:ASP:OD2	1.77	0.67
1:B:651:ILE:HG21	1:B:755:MET:CE	2.24	0.67
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.76	0.66
1:A:759:ILE:HG23	1:A:763:PHE:CD1	2.31	0.66
1:B:435:GLN:NE2	1:B:441:LYS:HG3	2.10	0.66
1:A:377:ASN:ND2	1:A:379:GLU:H	1.93	0.66
1:B:658:ARG:HG2	1:B:661:TYR:CE2	2.30	0.66
1:A:175:LYS:HE3	1:A:180:LEU:O	1.96	0.66
1:A:277:SER:HB2	1:A:280:THR:HB	1.77	0.66
1:A:759:ILE:O	1:A:763:PHE:CD1	2.46	0.65
1:A:74:ASN:HB3	3:A:811:NAG:C1	2.26	0.65
1:B:173:TYR:CE2	1:B:184:ARG:HG3	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:679:ASN:O	1:B:683:TYR:CD2	2.49	0.65
1:B:74:ASN:HB3	3:B:911:NAG:O7	1.96	0.65
1:B:378:GLU:OE2	1:B:378:GLU:HA	1.94	0.65
1:B:153:GLN:HE22	1:B:170:ASN:ND2	1.95	0.65
1:A:177:GLU:HB2	1:A:180:LEU:HD13	1.79	0.65
1:A:231:THR:HG22	1:A:231:THR:O	1.95	0.64
1:A:320:GLN:OE1	1:A:669:ARG:HD3	1.96	0.64
1:B:57:LEU:HD23	6:B:1114:HOH:O	1.96	0.64
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.33	0.64
1:A:173:TYR:CE2	1:A:184:ARG:HG3	2.33	0.64
1:A:272:ASN:HD21	1:A:274:ASP:HB2	1.61	0.64
2:B:2:AJH:CAP	2:B:2:AJH:CAR	2.67	0.63
1:A:184:ARG:HD2	1:A:187:TRP:CE2	2.35	0.62
1:B:175:LYS:HE3	1:B:180:LEU:O	2.00	0.62
1:A:231:THR:CG2	1:A:231:THR:O	2.47	0.62
1:A:75:ASN:HD21	3:A:811:NAG:C8	2.13	0.62
1:A:625:ALA:CB	1:A:763:PHE:HZ	2.13	0.61
1:B:377:ASN:HD22	1:B:377:ASN:C	2.02	0.61
1:A:625:ALA:HB3	1:A:763:PHE:HZ	1.66	0.61
1:A:596:ARG:O	1:A:597:ARG:HD2	2.01	0.61
1:A:289:ALA:HB3	1:A:294:LEU:CD2	2.29	0.61
1:A:289:ALA:CB	1:A:294:LEU:HG	2.29	0.60
1:B:289:ALA:CB	1:B:294:LEU:CD2	2.80	0.60
1:B:377:ASN:ND2	1:B:379:GLU:H	1.99	0.59
1:A:88:VAL:HG11	1:A:91:GLU:OE2	2.02	0.59
1:A:272:ASN:C	1:A:272:ASN:HD22	2.05	0.59
1:B:74:ASN:O	1:B:92:ASN:CB	2.47	0.59
1:A:74:ASN:C	1:A:92:ASN:HB3	2.23	0.59
1:A:759:ILE:CG2	1:A:763:PHE:CD1	2.85	0.59
1:B:630:SER:C	1:B:632:GLY:H	2.06	0.59
1:B:385:CYS:HB3	1:B:396:PHE:CD1	2.38	0.59
1:A:598:LEU:HD22	1:A:671:MET:HG2	1.85	0.58
1:B:74:ASN:ND2	3:B:911:NAG:H2	2.11	0.58
1:A:203:TYR:CG	1:A:228:PHE:CE2	2.92	0.58
1:A:191:GLU:C	1:A:193:ILE:H	2.07	0.57
1:A:676:PRO:HG2	1:A:677:GLU:OE2	2.05	0.57
1:A:184:ARG:NH1	1:A:187:TRP:HA	2.18	0.57
1:B:184:ARG:HH11	1:B:187:TRP:HA	1.69	0.57
1:B:528:MET:CE	1:B:530:LEU:HD21	2.34	0.57
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.28	0.57
1:B:69:LEU:CD1	1:B:107:ILE:HD12	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:VAL:HG12	1:A:487:ASN:N	2.19	0.56
1:B:71:LYS:HE3	1:B:105:TYR:HE1	1.70	0.56
1:A:341:VAL:O	1:A:344:GLN:HG2	2.06	0.56
1:A:357:PHE:CE1	2:A:1:AJH:HAS	2.41	0.56
1:A:759:ILE:CG2	1:A:763:PHE:CE1	2.78	0.56
1:B:276:LEU:HD21	1:B:282:ALA:HB2	1.87	0.56
1:A:277:SER:CB	1:A:280:THR:CB	2.72	0.56
1:A:272:ASN:HD22	1:A:274:ASP:N	2.04	0.56
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.42	0.55
1:A:289:ALA:HB3	1:A:294:LEU:HD21	1.89	0.55
1:B:276:LEU:HD23	1:B:282:ALA:HB2	1.87	0.55
1:A:156:THR:CG2	1:A:214:LEU:HD11	2.36	0.55
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.42	0.55
1:B:760:LYS:HE3	1:B:766:PRO:O	2.02	0.55
1:B:72:GLN:O	1:B:74:ASN:N	2.36	0.55
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.88	0.55
1:A:90:LEU:HD21	1:A:95:PHE:HE2	1.72	0.55
1:A:541:PRO:HB2	1:A:763:PHE:CD2	2.42	0.54
5:B:951:NAG:H61	5:B:952:NAG:O7	2.08	0.54
1:A:377:ASN:ND2	1:A:377:ASN:C	2.60	0.54
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.90	0.54
1:B:289:ALA:CB	1:B:294:LEU:HD21	2.38	0.54
1:B:90:LEU:HD21	1:B:95:PHE:HE2	1.72	0.54
1:A:415:LEU:HB2	1:A:436:LEU:HD11	1.89	0.53
1:A:290:PRO:O	1:A:291:ALA:CB	2.55	0.53
1:B:658:ARG:HG2	1:B:661:TYR:CD2	2.44	0.53
1:A:689:MET:HE3	1:B:244:GLU:HG3	1.88	0.53
1:B:704:HIS:HD2	1:B:716:SER:OG	1.92	0.53
1:B:422:TYR:CE2	1:B:423:LYS:HD3	2.44	0.53
1:B:272:ASN:C	1:B:272:ASN:ND2	2.60	0.53
1:A:194:ILE:HD12	4:A:841:NAG:H82	1.91	0.53
1:B:203:TYR:HA	1:B:207:VAL:HG13	1.91	0.53
1:B:76:ILE:HD12	1:B:105:TYR:CE2	2.44	0.52
1:A:218:PRO:HB2	1:A:308:GLN:NE2	2.25	0.52
1:A:483:HIS:HD2	6:A:991:HOH:O	1.92	0.52
5:B:951:NAG:O4	5:B:952:NAG:C7	2.57	0.52
1:B:516:PHE:CE2	1:B:523:LYS:HE2	2.45	0.52
1:B:289:ALA:HB3	1:B:294:LEU:CD2	2.39	0.52
1:A:183:TYR:CE1	1:A:276:LEU:HD21	2.45	0.52
1:B:631:TYR:O	1:B:631:TYR:CD1	2.63	0.52
1:B:193:ILE:HG22	1:B:194:ILE:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.92	0.51
1:B:630:SER:CB	1:B:740:HIS:NE2	2.71	0.51
1:A:76:ILE:HD12	1:A:105:TYR:OH	2.11	0.51
1:B:74:ASN:CB	1:B:92:ASN:HD22	2.12	0.50
1:A:528:MET:CE	1:A:530:LEU:HD21	2.41	0.50
1:A:625:ALA:HB2	1:A:763:PHE:CZ	2.47	0.50
1:B:658:ARG:HD3	1:B:660:GLU:HB2	1.93	0.50
1:A:625:ALA:CB	1:A:763:PHE:CZ	2.95	0.50
1:B:177:GLU:CB	1:B:180:LEU:HD13	2.40	0.50
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.47	0.50
1:B:486:VAL:C	1:B:487:ASN:HD22	2.16	0.49
1:A:203:TYR:CD1	1:A:228:PHE:CE2	3.01	0.49
1:A:176:ILE:HG13	1:A:276:LEU:HD22	1.93	0.49
1:A:183:TYR:OH	1:A:276:LEU:HD21	2.13	0.49
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.30	0.49
1:A:183:TYR:CZ	1:A:276:LEU:CD2	2.92	0.49
1:B:614:SER:HA	1:B:619:VAL:HB	1.94	0.49
1:A:218:PRO:HB2	1:A:308:GLN:HE22	1.76	0.49
1:B:502:LYS:O	1:B:505:GLN:HG2	2.12	0.49
1:A:183:TYR:CG	1:A:276:LEU:HD11	2.47	0.49
1:B:76:ILE:HD12	1:B:105:TYR:OH	2.12	0.49
1:B:520:ASN:O	1:B:521:GLU:HB2	2.13	0.49
1:B:272:ASN:ND2	1:B:274:ASP:H	2.10	0.49
1:A:203:TYR:HA	1:A:207:VAL:HG13	1.95	0.48
1:A:153:GLN:HE22	1:A:170:ASN:HD21	1.59	0.48
1:A:277:SER:HB2	1:A:280:THR:CB	2.39	0.48
1:B:629:TRP:O	1:B:630:SER:C	2.52	0.48
1:A:378:GLU:HA	1:A:378:GLU:OE2	2.13	0.48
1:B:156:THR:HG21	1:B:214:LEU:HD11	1.96	0.48
1:B:69:LEU:HD13	1:B:107:ILE:HD12	1.95	0.48
1:A:658:ARG:HD3	1:A:660:GLU:HB2	1.94	0.48
1:A:72:GLN:HE22	1:A:77:LEU:HD11	1.78	0.48
1:A:170:ASN:N	1:A:170:ASN:HD22	2.12	0.48
1:A:516:PHE:CE2	1:A:523:LYS:HE2	2.48	0.48
1:A:415:LEU:C	1:A:415:LEU:HD23	2.34	0.48
1:B:598:LEU:HD22	1:B:671:MET:HG2	1.94	0.48
1:B:678:ASP:OD1	1:B:678:ASP:C	2.53	0.47
1:A:718:GLN:HE22	1:A:721:LYS:NZ	2.12	0.47
1:A:630:SER:HB2	1:A:740:HIS:NE2	2.30	0.47
1:A:331:ASP:HB3	1:A:334:SER:HB3	1.96	0.47
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:VAL:O	1:B:344:GLN:HG2	2.15	0.47
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.98	0.47
1:B:630:SER:C	1:B:632:GLY:N	2.68	0.47
1:A:693:GLU:OE2	1:A:696:LYS:HE3	2.15	0.47
1:A:183:TYR:CE1	1:A:276:LEU:HD11	2.49	0.47
1:A:147:ARG:CZ	3:A:821:NAG:O6	2.61	0.47
1:A:65:ASP:OD2	1:A:466:LYS:HB2	2.15	0.47
1:B:413:ASP:HB3	1:B:414:TYR:CD1	2.50	0.47
1:A:71:LYS:HE3	1:A:105:TYR:HE1	1.80	0.46
1:A:741:GLY:O	1:A:742:ILE:C	2.54	0.46
1:B:528:MET:HE2	1:B:528:MET:HB3	1.70	0.46
1:A:626:ILE:O	1:A:650:GLY:HA2	2.15	0.46
1:B:88:VAL:HG11	1:B:91:GLU:OE2	2.16	0.46
1:A:191:GLU:C	1:A:193:ILE:N	2.68	0.46
1:B:704:HIS:HE1	1:B:711:VAL:O	1.99	0.46
1:A:520:ASN:O	1:A:521:GLU:HB2	2.15	0.46
1:A:422:TYR:CE2	1:A:423:LYS:HD3	2.50	0.46
1:B:693:GLU:OE2	1:B:696:LYS:HE3	2.15	0.46
1:B:89:PHE:CE1	1:B:107:ILE:HD13	2.50	0.46
1:A:286:GLN:NE2	1:A:288:THR:HG22	2.31	0.46
1:B:272:ASN:HD21	1:B:274:ASP:HB2	1.81	0.45
1:B:415:LEU:HB2	1:B:436:LEU:HD11	1.98	0.45
1:A:542:LEU:HD23	1:A:542:LEU:C	2.37	0.45
1:B:310:ARG:HG3	1:B:329:ASP:OD1	2.15	0.45
1:A:704:HIS:HD2	1:A:716:SER:OG	2.00	0.45
1:A:69:LEU:HD13	1:A:107:ILE:HD12	1.98	0.45
1:B:65:ASP:CG	1:B:464:GLU:HB2	2.37	0.45
1:B:596:ARG:O	1:B:597:ARG:HD2	2.16	0.45
1:A:177:GLU:CB	1:A:180:LEU:HD13	2.47	0.45
1:B:756:SER:O	1:B:760:LYS:CG	2.55	0.45
1:B:547:TYR:CE2	1:B:630:SER:O	2.70	0.45
1:B:528:MET:HE1	1:B:530:LEU:HD21	1.98	0.45
1:A:528:MET:HE2	1:A:530:LEU:HD21	1.99	0.45
1:B:741:GLY:O	1:B:742:ILE:C	2.54	0.45
1:A:704:HIS:HE1	1:A:711:VAL:O	1.99	0.45
1:B:71:LYS:HE3	1:B:105:TYR:CE1	2.51	0.45
1:A:76:ILE:HD12	1:A:105:TYR:CE2	2.52	0.45
1:A:402:TRP:CD1	1:A:421:GLU:HG3	2.51	0.45
1:A:310:ARG:HG3	1:A:329:ASP:OD1	2.16	0.45
1:B:629:TRP:O	1:B:630:SER:O	2.35	0.45
1:A:191:GLU:O	1:A:193:ILE:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:LEU:O	1:A:140:ARG:NH1	2.50	0.44
1:A:651:ILE:CD1	1:A:755:MET:HE2	2.47	0.44
1:A:291:ALA:O	1:A:295:ILE:HG22	2.16	0.44
1:A:543:LEU:HD12	1:A:567:LEU:HD13	2.00	0.44
1:B:481:THR:OG1	1:B:483:HIS:HE1	2.01	0.44
1:A:290:PRO:O	1:A:291:ALA:HB3	2.17	0.44
1:A:418:ILE:HA	1:A:430:ASN:O	2.16	0.44
1:A:193:ILE:HG22	1:A:194:ILE:N	2.31	0.44
1:A:69:LEU:HB3	1:A:76:ILE:HD11	1.99	0.44
1:B:677:GLU:H	1:B:677:GLU:CD	2.21	0.44
1:B:491:LEU:O	1:B:492:ARG:HB3	2.17	0.44
1:A:658:ARG:HG2	1:A:661:TYR:CD2	2.53	0.44
1:B:153:GLN:HE22	1:B:170:ASN:HD22	1.64	0.44
1:B:289:ALA:HB3	1:B:294:LEU:HD21	2.00	0.44
1:A:272:ASN:ND2	1:A:274:ASP:N	2.60	0.44
1:A:677:GLU:CD	1:A:677:GLU:H	2.21	0.44
1:B:276:LEU:HD21	1:B:282:ALA:CB	2.48	0.44
1:A:69:LEU:CD1	1:A:107:ILE:HD12	2.48	0.44
1:B:377:ASN:C	1:B:377:ASN:ND2	2.71	0.44
1:B:40:ARG:NH2	1:B:508:GLN:HG2	2.32	0.44
1:A:535:ASP:C	1:A:537:SER:H	2.21	0.44
1:B:629:TRP:O	1:B:632:GLY:N	2.51	0.44
1:A:334:SER:OG	1:A:336:ARG:HD3	2.18	0.44
1:B:65:ASP:HB3	1:B:66:HIS:CE1	2.53	0.44
1:A:65:ASP:CG	1:A:464:GLU:HB2	2.38	0.43
1:B:470:LEU:HD12	1:B:483:HIS:CE1	2.54	0.43
1:A:110:ASP:OD1	1:A:112:GLN:HG3	2.18	0.43
1:B:528:MET:HE2	1:B:530:LEU:HD21	1.99	0.43
1:B:704:HIS:CE1	1:B:711:VAL:O	2.71	0.43
1:A:279:VAL:O	1:A:280:THR:OG1	2.28	0.43
1:A:76:ILE:HD12	1:A:105:TYR:CZ	2.54	0.43
1:B:64:SER:HA	1:B:463:LYS:HG3	2.00	0.43
1:A:405:ILE:HG13	1:A:429:ARG:HD3	2.01	0.43
1:A:502:LYS:O	1:A:505:GLN:HG2	2.18	0.43
1:B:658:ARG:HG3	1:B:658:ARG:O	2.18	0.43
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.18	0.43
1:A:191:GLU:O	1:A:193:ILE:HG12	2.18	0.43
1:A:369:ASN:C	1:A:389:ILE:HG23	2.39	0.43
1:B:415:LEU:HD23	1:B:415:LEU:C	2.39	0.43
1:A:203:TYR:CD2	1:A:228:PHE:HE2	2.37	0.43
1:B:76:ILE:O	1:B:76:ILE:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:VAL:HG22	1:B:460:SER:N	2.34	0.42
1:A:310:ARG:HD3	1:A:327:ILE:CG2	2.49	0.42
1:B:541:PRO:HB2	1:B:763:PHE:CE1	2.54	0.42
1:A:513:LYS:HE3	1:A:513:LYS:HB2	1.83	0.42
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.55	0.42
1:B:150:ASN:O	1:B:151:ASN:HB2	2.19	0.42
1:B:631:TYR:O	1:B:631:TYR:HD1	2.03	0.42
1:A:571:GLU:CD	1:A:760:LYS:HE3	2.40	0.42
1:B:336:ARG:HG3	1:B:336:ARG:HH11	1.84	0.42
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.55	0.42
1:A:190:LYS:CE	1:A:193:ILE:HG21	2.50	0.42
1:B:654:ALA:HA	1:B:704:HIS:CD2	2.55	0.42
1:A:528:MET:CE	1:A:574:ILE:HG21	2.50	0.42
1:B:65:ASP:OD2	1:B:466:LYS:HB2	2.19	0.42
1:A:81:ALA:O	1:A:492:ARG:NH2	2.44	0.42
1:A:74:ASN:HD22	3:A:811:NAG:HN2	1.68	0.42
1:A:654:ALA:HA	1:A:704:HIS:CD2	2.55	0.42
1:B:483:HIS:CD2	1:B:490:GLY:HA2	2.55	0.42
1:B:290:PRO:O	1:B:291:ALA:HB3	2.20	0.42
1:A:280:THR:HG22	1:A:281:ASN:O	2.20	0.41
1:A:195:TYR:HD1	1:A:228:PHE:O	2.03	0.41
1:B:76:ILE:HD12	1:B:105:TYR:CZ	2.54	0.41
1:B:571:GLU:OE2	1:B:760:LYS:HE3	2.20	0.41
1:B:651:ILE:HD13	1:B:755:MET:HE2	2.01	0.41
5:B:951:NAG:C6	5:B:952:NAG:O7	2.68	0.41
1:A:759:ILE:HG22	1:A:763:PHE:CD1	2.55	0.41
1:A:199:THR:HA	1:A:228:PHE:CE1	2.55	0.41
1:A:149:PRO:HB2	1:A:168:TRP:CD1	2.55	0.41
1:A:760:LYS:H	1:A:760:LYS:HG2	1.69	0.41
1:A:597:ARG:HH12	1:A:679:ASN:HD21	1.67	0.41
1:A:336:ARG:HG3	1:A:336:ARG:HH11	1.85	0.41
1:B:310:ARG:HD3	1:B:327:ILE:CG2	2.50	0.41
1:A:535:ASP:OD1	1:A:537:SER:HB3	2.20	0.41
1:B:289:ALA:HB2	1:B:294:LEU:HD21	2.01	0.41
1:A:190:LYS:HE3	1:A:193:ILE:HG21	2.01	0.41
1:B:76:ILE:HG23	1:B:89:PHE:HB3	2.02	0.41
1:A:41:LYS:HB2	6:A:1007:HOH:O	2.20	0.41
1:B:156:THR:CG2	1:B:214:LEU:HD11	2.51	0.41
1:A:602:GLU:N	1:A:602:GLU:OE2	2.51	0.41
1:B:602:GLU:OE2	1:B:602:GLU:N	2.53	0.41
1:B:127:SER:HB3	1:B:211:TYR:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:ILE:CD1	4:A:841:NAG:H82	2.50	0.41
1:A:74:ASN:HB3	1:A:92:ASN:ND2	2.36	0.41
1:A:109:PRO:HG2	1:A:158:SER:O	2.21	0.41
1:A:704:HIS:CE1	1:A:711:VAL:O	2.74	0.41
1:B:405:ILE:HG13	1:B:429:ARG:HD3	2.03	0.41
1:A:510:PRO:HD3	1:A:569:SER:HB2	2.03	0.41
1:B:74:ASN:O	1:B:92:ASN:HA	2.21	0.41
1:B:76:ILE:HG22	1:B:90:LEU:CB	2.48	0.41
1:B:502:LYS:HD2	1:B:502:LYS:HA	1.89	0.40
1:A:64:SER:HA	1:A:463:LYS:HG3	2.03	0.40
1:A:237:GLU:CD	1:A:253:ARG:HH21	2.22	0.40
1:A:75:ASN:HD21	3:A:811:NAG:H82	1.85	0.40
1:A:195:TYR:O	1:A:227:GLN:HA	2.21	0.40
1:B:290:PRO:O	1:B:292:SER:N	2.49	0.40
1:A:162:HIS:HD2	1:A:178:PRO:HD3	1.87	0.40
1:B:270:VAL:HG11	1:B:337:TRP:CZ2	2.56	0.40
1:A:72:GLN:O	1:A:72:GLN:HG2	2.22	0.40
1:A:523:LYS:HD2	6:A:997:HOH:O	2.21	0.40
1:B:418:ILE:HA	1:B:430:ASN:O	2.21	0.40
1:B:543:LEU:HD12	1:B:567:LEU:HD13	2.03	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	724/728 (100%)	687 (95%)	33 (5%)	4 (1%)	30	22
1	B	726/728 (100%)	692 (95%)	30 (4%)	4 (1%)	30	22
All	All	1450/1456 (100%)	1379 (95%)	63 (4%)	8 (1%)	30	22

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	291	ALA
1	B	40	ARG
1	B	630	SER
1	A	192	ASP
1	B	73	GLU
1	B	320	GLN
1	A	536	LYS

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	651/653 (100%)	598 (92%)	53 (8%)	15	9
1	B	653/653 (100%)	599 (92%)	54 (8%)	14	8
All	All	1304/1306 (100%)	1197 (92%)	107 (8%)	14	9

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	51	ASN
1	A	54	ARG
1	A	61	ARG
1	A	74	ASN
1	A	75	ASN
1	A	77	LEU
1	A	98	PHE
1	A	141	GLN
1	A	145	GLU
1	A	147	ARG
1	A	156	THR
1	A	184	ARG
1	A	223	LEU
1	A	246	LEU
1	A	253	ARG

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Mol	Chain	Res	Type
1	A	272	ASN
1	A	290	PRO
1	A	295	ILE
1	A	303	VAL
1	A	326	ASP
1	A	329	ASP
1	A	336	ARG
1	A	343	ARG
1	A	361	GLU
1	A	366	LEU
1	A	377	ASN
1	A	379	GLU
1	A	385	CYS
1	A	399	LYS
1	A	425	MET
1	A	436	LEU
1	A	448	GLU
1	A	452	GLU
1	A	472	CYS
1	A	487	ASN
1	A	506	ASN
1	A	507	VAL
1	A	514	LEU
1	A	536	LYS
1	A	543	LEU
1	A	566	TYR
1	A	597	ARG
1	A	598	LEU
1	A	608	GLU
1	A	612	GLN
1	A	614	SER
1	A	658	ARG
1	A	679	ASN
1	A	701	LEU
1	A	702	LEU
1	A	760	LYS
1	A	761	GLN
1	B	41	LYS
1	B	51	ASN
1	B	54	ARG
1	B	61	ARG
1	B	66	HIS

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Mol	Chain	Res	Type
1	B	74	ASN
1	B	75	ASN
1	B	77	LEU
1	B	98	PHE
1	B	141	GLN
1	B	145	GLU
1	B	147	ARG
1	B	156	THR
1	B	170	ASN
1	B	184	ARG
1	B	223	LEU
1	B	230	ASP
1	B	246	LEU
1	B	253	ARG
1	B	272	ASN
1	B	278	SER
1	B	279	VAL
1	B	290	PRO
1	B	295	ILE
1	B	313	LEU
1	B	326	ASP
1	B	336	ARG
1	B	361	GLU
1	B	366	LEU
1	B	377	ASN
1	B	379	GLU
1	B	399	LYS
1	B	425	MET
1	B	436	LEU
1	B	448	GLU
1	B	452	GLU
1	B	472	CYS
1	B	487	ASN
1	B	506	ASN
1	B	507	VAL
1	B	514	LEU
1	B	536	LYS
1	B	543	LEU
1	B	566	TYR
1	B	597	ARG
1	B	598	LEU
1	B	608	GLU

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Mol	Chain	Res	Type
1	B	614	SER
1	B	658	ARG
1	B	679	ASN
1	B	701	LEU
1	B	702	LEU
1	B	760	LYS
1	B	761	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	112	GLN
1	A	123	GLN
1	A	169	ASN
1	A	170	ASN
1	A	227	GLN
1	A	247	GLN
1	A	272	ASN
1	A	314	GLN
1	A	377	ASN
1	A	435	GLN
1	A	483	HIS
1	A	487	ASN
1	A	586	GLN
1	A	606	GLN
1	A	612	GLN
1	A	679	ASN
1	A	694	ASN
1	A	704	HIS
1	A	718	GLN
1	A	731	GLN
1	A	761	GLN
1	B	72	GLN
1	B	112	GLN
1	B	123	GLN
1	B	169	ASN
1	B	170	ASN
1	B	227	GLN
1	B	247	GLN
1	B	272	ASN
1	B	314	GLN

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Mol	Chain	Res	Type
1	B	377	ASN
1	B	435	GLN
1	B	483	HIS
1	B	487	ASN
1	B	533	HIS
1	B	572	ASN
1	B	586	GLN
1	B	612	GLN
1	B	679	ASN
1	B	694	ASN
1	B	704	HIS
1	B	718	GLN
1	B	748	HIS
1	B	761	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 ⓘ

13 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	NAG	A	841	1,4	14,14,15	0.79	1 (7%)	15,19,21	0.61	0
4	NAG	A	842	4	14,14,15	2.74	6 (42%)	15,19,21	2.37	5 (33%)
4	MAN	A	843	4	11,11,12	1.51	4 (36%)	14,15,17	1.55	2 (14%)
5	NAG	A	861	1,5	14,14,15	0.92	0	15,19,21	1.06	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	A	862	5	14,14,15	0.60	0	15,19,21	0.77	0
5	NAG	B	901	1,5	14,14,15	1.02	1 (7%)	15,19,21	0.75	0
5	NAG	B	902	5	14,14,15	0.82	0	15,19,21	0.74	0
5	NAG	B	931	1,5	14,14,15	0.69	0	15,19,21	0.81	0
5	NAG	B	932	5	14,14,15	0.65	0	15,19,21	1.09	1 (6%)
5	NAG	B	951	1,5	14,14,15	0.87	0	15,19,21	1.73	3 (20%)
5	NAG	B	952	5	14,14,15	0.61	0	15,19,21	1.31	2 (13%)
5	NAG	B	961	1,5	14,14,15	0.91	0	15,19,21	1.28	2 (13%)
5	NAG	B	962	5	14,14,15	0.72	0	15,19,21	0.87	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
4	NAG	A	841	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	842	4	1/1/5/7	0/6/23/26	0/1/1/1
4	MAN	A	843	4	-	0/2/19/22	0/1/1/1
5	NAG	A	861	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	862	5	-	0/6/23/26	0/1/1/1
5	NAG	B	901	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	902	5	-	0/6/23/26	0/1/1/1
5	NAG	B	931	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	932	5	-	0/6/23/26	0/1/1/1
5	NAG	B	951	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	952	5	-	0/6/23/26	0/1/1/1
5	NAG	B	961	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	962	5	-	0/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	841	NAG	C1-C2	2.09	1.55	1.52
4	A	843	MAN	O5-C1	2.23	1.47	1.43
5	B	901	NAG	C1-C2	2.38	1.55	1.52
4	A	843	MAN	C1-C2	2.52	1.58	1.52
4	A	843	MAN	C2-C3	2.55	1.56	1.52
4	A	843	MAN	O5-C5	2.58	1.49	1.43
4	A	842	NAG	C4-C5	2.72	1.58	1.53
4	A	842	NAG	C3-C2	2.90	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	842	NAG	C1-C2	3.69	1.57	1.52
4	A	842	NAG	O4-C4	4.29	1.53	1.43
4	A	842	NAG	O5-C1	5.08	1.52	1.43
4	A	842	NAG	O5-C5	5.18	1.54	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	842	NAG	C2-N2-C7	-3.85	118.09	123.04
5	B	951	NAG	C1-O5-C5	-3.34	108.00	112.25
4	A	842	NAG	C3-C4-C5	-3.23	104.57	110.20
5	B	952	NAG	C4-C3-C2	-3.14	106.35	111.23
5	A	861	NAG	C2-N2-C7	-2.85	119.37	123.04
5	B	952	NAG	C2-N2-C7	-2.66	119.63	123.04
4	A	842	NAG	C6-C5-C4	-2.64	106.50	113.02
5	B	961	NAG	C2-N2-C7	-2.52	119.80	123.04
5	B	951	NAG	O4-C4-C3	-2.08	105.66	110.34
5	B	932	NAG	C3-C4-C5	2.21	114.04	110.20
4	A	842	NAG	C4-C3-C2	2.23	114.69	111.23
5	B	961	NAG	C1-O5-C5	3.21	116.33	112.25
4	A	843	MAN	C1-C2-C3	3.56	113.75	109.54
4	A	843	MAN	C1-O5-C5	3.85	117.13	112.25
5	B	951	NAG	C6-C5-C4	4.25	123.49	113.02
4	A	842	NAG	C1-O5-C5	6.11	120.00	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	842	NAG	C1

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	841	NAG	2	0
5	B	951	NAG	3	0
5	B	952	NAG	3	0

5.6 Ligand geometry

12 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	AJH	A	1	-	32,35,35	1.86	1 (3%)	34,49,49	1.55	7 (20%)
3	NAG	A	801	1	14,14,15	1.46	1 (7%)	15,19,21	1.10	2 (13%)
3	NAG	A	811	1	14,14,15	0.93	1 (7%)	15,19,21	0.82	1 (6%)
3	NAG	A	821	1	14,14,15	1.19	1 (7%)	15,19,21	1.03	1 (6%)
3	NAG	A	831	1	14,14,15	0.79	1 (7%)	15,19,21	0.62	0
3	NAG	A	851	1	14,14,15	1.05	1 (7%)	15,19,21	0.77	0
3	NAG	A	871	1	14,14,15	0.60	0	15,19,21	1.42	3 (20%)
2	AJH	B	2	-	32,35,35	1.87	1 (3%)	34,49,49	1.50	7 (20%)
3	NAG	B	911	1	14,14,15	0.66	0	15,19,21	0.65	0
3	NAG	B	921	1	14,14,15	0.71	0	15,19,21	0.58	0
3	NAG	B	941	1	14,14,15	0.88	0	15,19,21	1.73	3 (20%)
3	NAG	B	971	1	14,14,15	0.61	0	15,19,21	0.91	1 (6%)

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	AJH	A	1	-	-	0/18/35/35	0/2/3/3
3	NAG	A	801	1	-	0/6/23/26	0/1/1/1
3	NAG	A	811	1	-	0/6/23/26	0/1/1/1
3	NAG	A	821	1	-	0/6/23/26	0/1/1/1
3	NAG	A	831	1	-	0/6/23/26	0/1/1/1
3	NAG	A	851	1	-	0/6/23/26	0/1/1/1
3	NAG	A	871	1	-	0/6/23/26	0/1/1/1
2	AJH	B	2	-	-	0/18/35/35	0/2/3/3
3	NAG	B	911	1	-	0/6/23/26	0/1/1/1
3	NAG	B	921	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	941	1	-	0/6/23/26	0/1/1/1
3	NAG	B	971	1	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	AJH	CAB-CAA	-9.92	1.34	1.50
2	B	2	AJH	CAB-CAA	-9.92	1.34	1.50
3	A	831	NAG	C1-C2	2.07	1.55	1.52
3	A	821	NAG	C8-C7	2.17	1.54	1.50
3	A	811	NAG	O5-C5	2.39	1.48	1.43
3	A	851	NAG	C1-C2	2.92	1.56	1.52
3	A	801	NAG	C1-C2	4.86	1.59	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	941	NAG	C1-O5-C5	-3.35	108.00	112.25
2	A	1	AJH	CAH-CAI-CAG	-3.15	120.12	124.13
3	A	871	NAG	C4-C3-C2	-2.95	106.65	111.23
3	A	871	NAG	C2-N2-C7	-2.91	119.29	123.04
2	B	2	AJH	CAH-CAI-CAG	-2.91	120.42	124.13
2	A	1	AJH	CAM-CAL-CAK	-2.61	118.76	121.13
2	B	2	AJH	CAM-CAL-CAK	-2.53	118.83	121.13
2	B	2	AJH	OAN-CAA-CAB	-2.50	115.44	120.17
2	A	1	AJH	OAN-CAA-CAB	-2.39	115.65	120.17
3	B	971	NAG	C2-N2-C7	-2.29	120.10	123.04
3	A	801	NAG	C2-N2-C7	-2.26	120.14	123.04
3	A	811	NAG	C2-N2-C7	-2.19	120.22	123.04
3	A	801	NAG	O7-C7-C8	-2.13	118.16	122.06
3	B	941	NAG	O4-C4-C3	-2.11	105.60	110.34
2	B	2	AJH	CBF-NAE-CAS	2.08	119.86	116.29
2	B	2	AJH	CAM-CAG-CAI	2.11	118.16	116.52
2	B	2	AJH	FAZ-CAI-CAG	2.30	121.22	117.91
3	A	871	NAG	C1-O5-C5	2.35	115.23	112.25
3	A	821	NAG	C6-C5-C4	2.51	119.21	113.02
2	A	1	AJH	CBF-NAE-CAS	2.56	120.68	116.29
2	A	1	AJH	FAZ-CAI-CAG	2.61	121.67	117.91
2	A	1	AJH	CAM-CAG-CAI	2.85	118.74	116.52
2	A	1	AJH	CAB-CAA-NAD	3.85	123.89	118.76
3	B	941	NAG	C6-C5-C4	4.24	123.46	113.02
2	B	2	AJH	CAB-CAA-NAD	4.32	124.52	118.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	AJH	5	0
3	A	811	NAG	4	0
3	A	821	NAG	2	0
2	B	2	AJH	4	0
3	B	911	NAG	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	726/728 (99%)	0.53	71 (9%) 10 10	13, 28, 67, 96	0
1	B	728/728 (100%)	0.37	46 (6%) 23 24	13, 27, 57, 94	0
All	All	1454/1456 (99%)	0.45	117 (8%) 15 16	13, 28, 64, 96	0

All (117) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	766	PRO	15.0
1	B	765	LEU	10.2
1	A	98	PHE	8.4
1	B	39	SER	8.1
1	A	39	SER	8.1
1	A	73	GLU	7.4
1	B	73	GLU	6.9
1	A	180	LEU	6.1
1	B	97	GLU	6.0
1	A	289	ALA	6.0
1	A	93	SER	5.8
1	A	99	GLY	5.7
1	A	763	PHE	5.6
1	A	97	GLU	5.3
1	B	105	TYR	5.3
1	A	279	VAL	5.3
1	B	98	PHE	5.2
1	B	289	ALA	5.1
1	A	71	LYS	5.1
1	A	228	PHE	4.9
1	A	105	TYR	4.9
1	B	487	ASN	4.6
1	B	391	LYS	4.6
1	B	40	ARG	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	335	GLY	4.5
1	A	276	LEU	4.4
1	B	277	SER	4.4
1	B	392	LYS	4.4
1	B	99	GLY	4.3
1	A	179	ASN	4.2
1	B	71	LYS	4.0
1	A	283	THR	4.0
1	A	278	SER	3.9
1	B	74	ASN	3.8
1	A	114	ILE	3.8
1	B	280	THR	3.8
1	B	89	PHE	3.8
1	A	160	VAL	3.7
1	A	332	GLU	3.7
1	A	139	LYS	3.7
1	A	137	LEU	3.6
1	B	393	ASP	3.5
1	B	76	ILE	3.5
1	A	136	ASP	3.4
1	A	134	ILE	3.4
1	A	135	TYR	3.4
1	A	140	ARG	3.4
1	A	72	GLN	3.4
1	A	183	TYR	3.4
1	A	333	SER	3.3
1	A	764	SER	3.3
1	B	366	LEU	3.3
1	B	72	GLN	3.3
1	A	277	SER	3.2
1	A	181	PRO	3.2
1	A	145	GLU	3.2
1	A	92	ASN	3.2
1	A	76	ILE	3.1
1	A	231	THR	3.1
1	A	273	THR	3.1
1	A	187	TRP	3.1
1	A	336	ARG	3.1
1	A	141	GLN	3.1
1	B	290	PRO	3.0
1	A	75	ASN	3.0
1	A	142	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	280	THR	3.0
1	B	334	SER	3.0
1	A	100	HIS	3.0
1	A	615	LYS	3.0
1	A	392	LYS	2.9
1	B	95	PHE	2.9
1	A	290	PRO	2.9
1	B	333	SER	2.9
1	B	630	SER	2.8
1	B	96	ASP	2.8
1	B	390	ASP	2.7
1	B	88	VAL	2.7
1	A	74	ASN	2.7
1	B	676	PRO	2.7
1	A	138	ASN	2.7
1	A	40	ARG	2.6
1	A	146	GLU	2.6
1	B	138	ASN	2.5
1	B	100	HIS	2.5
1	A	113	PHE	2.5
1	A	103	ASN	2.5
1	A	366	LEU	2.5
1	B	502	LYS	2.5
1	A	90	LEU	2.4
1	A	95	PHE	2.4
1	A	96	ASP	2.4
1	A	537	SER	2.4
1	A	616	MET	2.4
1	B	90	LEU	2.3
1	B	137	LEU	2.3
1	B	764	SER	2.3
1	A	162	HIS	2.3
1	A	275	SER	2.3
1	A	390	ASP	2.3
1	A	222	PHE	2.2
1	A	340	LEU	2.2
1	B	142	LEU	2.2
1	B	102	ILE	2.2
1	A	144	THR	2.2
1	A	295	ILE	2.2
1	B	379	GLU	2.2
1	A	116	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	506	ASN	2.2
1	B	679	ASN	2.1
1	B	279	VAL	2.1
1	B	336	ARG	2.1
1	B	114	ILE	2.0
1	A	521	GLU	2.0
1	A	132	TYR	2.0
1	B	378	GLU	2.0
1	A	143	ILE	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](#)

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	NAG	B	952	14/15	0.62	0.46	22.85	67,72,76,79	0
5	NAG	A	861	14/15	0.69	0.28	12.34	52,56,63,71	0
5	NAG	B	932	14/15	0.74	0.31	4.24	66,70,71,73	0
5	NAG	B	961	14/15	0.71	0.24	3.78	47,51,58,61	0
5	NAG	B	901	14/15	0.75	0.22	2.89	56,61,73,75	0
4	NAG	A	841	14/15	0.77	0.28	2.32	56,63,66,68	0
5	NAG	B	951	14/15	0.75	0.20	2.10	48,50,57,60	0
5	NAG	A	862	14/15	0.73	0.41	-	75,79,81,84	0
4	MAN	A	843	11/12	0.46	0.40	-	78,80,82,85	0
4	NAG	A	842	14/15	0.77	0.27	-	65,72,74,76	0
5	NAG	B	962	14/15	0.77	0.30	-	68,74,76,77	0
5	NAG	B	902	14/15	0.76	0.50	-	80,84,86,88	0
5	NAG	B	931	14/15	0.86	0.16	-	42,51,57,60	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
3	NAG	B	941	14/15	0.78	0.26	3.05	48,50,57,60	0
3	NAG	B	971	14/15	0.61	0.27	3.03	63,70,73,77	0
2	AJH	A	1	33/33	0.92	0.20	1.99	17,26,49,50	0
3	NAG	A	871	14/15	0.64	0.35	1.50	69,71,73,74	0
2	AJH	B	2	33/33	0.92	0.20	1.04	14,23,44,48	0
3	NAG	A	801	14/15	0.69	0.19	-	55,62,64,67	0
3	NAG	A	811	14/15	0.44	0.43	-	81,85,87,87	0
3	NAG	A	831	14/15	0.82	0.22	-	56,63,66,68	0
3	NAG	A	851	14/15	0.70	0.22	-	64,66,69,70	0
3	NAG	B	921	14/15	0.69	0.32	-	61,67,70,73	0
3	NAG	B	911	14/15	0.40	0.36	-	74,78,79,80	0
3	NAG	A	821	14/15	0.55	0.43	-	15,20,30,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.