



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2016 – 08:02 PM EST

PDB ID : 1TK3
Title : Crystal Structure Of Human Apo Dipeptidyl Peptidase IV/CD26
Authors : Bjelke, J.R.; Christensen, J.; Branner, S.; Wagtmann, N.; Olsen, C.; Kanstrup, A.B.; Rasmussen, H.B.
Deposited on : 2004-06-08
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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028320
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-20028320

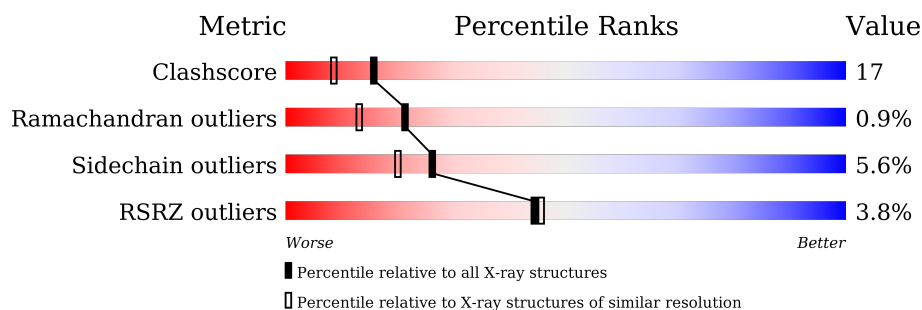
1 Overall quality at a glance

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))
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>2%</div> <div>72%</div> <div>24%</div> <div>.</div> </div>
1	B	728	<div> <div>5%</div> <div>68%</div> <div>28%</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
4	NAG	A	774	-	-	-	X
4	NAG	A	780	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NAG	A	782	-	-	-	X
6	NAG	B	781	-	-	-	X
7	NAG	B	772	-	-	-	X
8	NAG	B	776	-	-	-	X
9	NDG	B	779	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 13536 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 IV.

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
			5964	3827	982	1129	26			

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			38	22	2	14		
2	B	3	Total	C	N	O	0	0
			38	22	2	14		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	3	Total	C	N	O	0	0
			38	22	2	14		

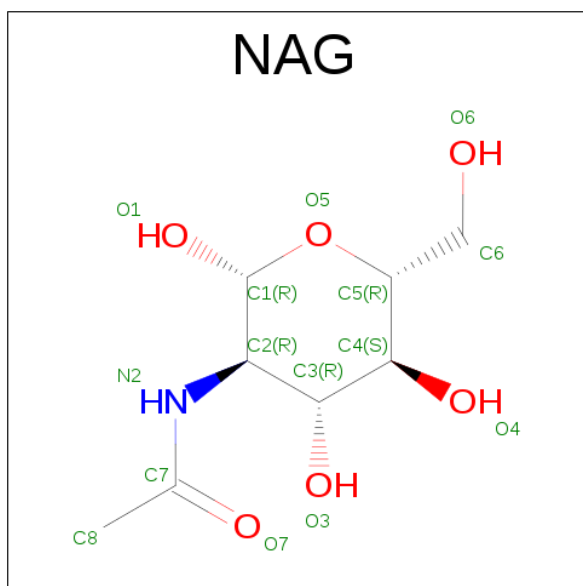
- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

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

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

- Molecule 6 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 8 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 9 is a polymer of unknown type called SUGAR (2-MER).

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

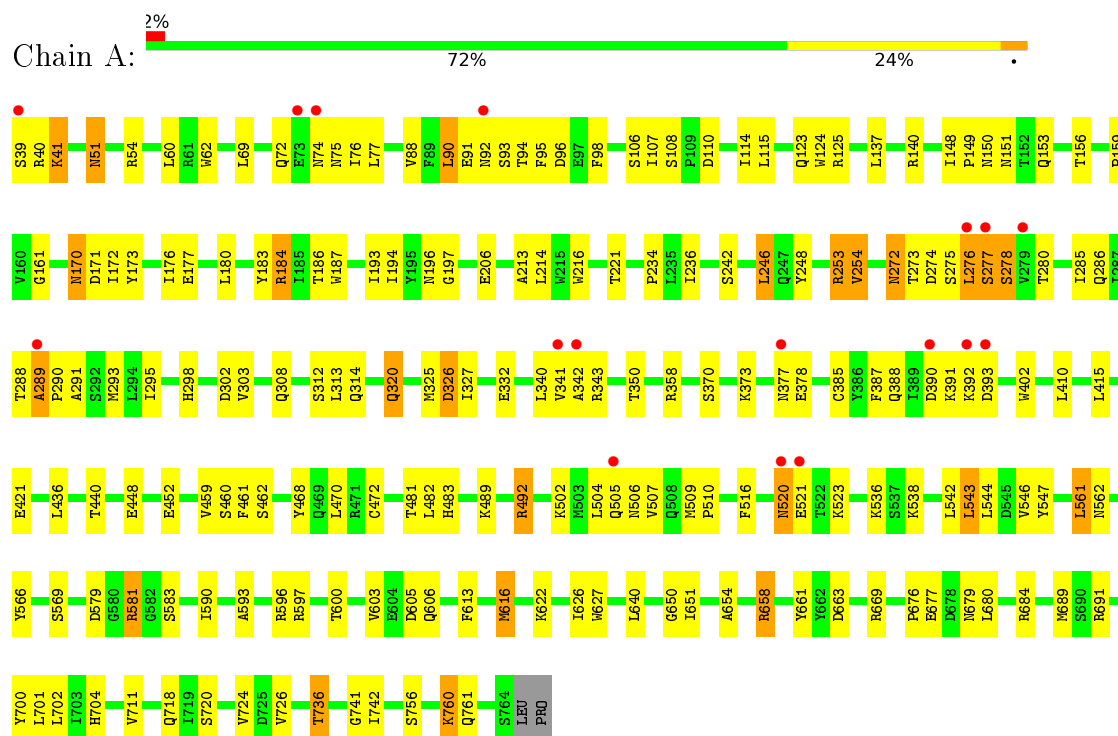
- Molecule 10 is water.

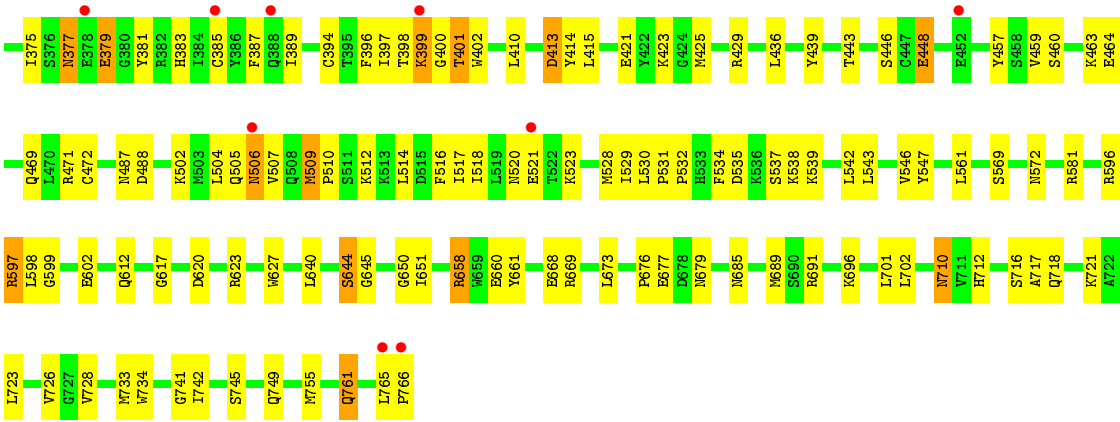
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	627	Total	O	0	0
			627	627		
10	B	584	Total	O	0	0
			584	584		

3 Residue-property plots [i](#)

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 IV





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	119.26Å 122.36Å 129.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.68 – 2.00 40.68 – 2.00	Depositor EDS
% Data completeness (in resolution range)	90.6 (40.68-2.00) 90.7 (40.68-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 2.00Å)	Xtriage
Refinement program	CNX 2000.1	Depositor
R, R_{free}	0.229 , 0.272 0.220 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 53.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13536	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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: MAN, BMA, NAG, NDG, FUC

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	0/6119	0.64	0/8321
1	B	0.36	0/6136	0.64	0/8344
All	All	0.36	0/12255	0.64	0/16665

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	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	5660	182	0
1	B	5964	0	5677	219	0
2	A	38	0	34	0	0
2	B	38	0	34	1	0
3	A	38	0	34	6	0
4	A	84	0	75	1	0
5	A	39	0	34	5	0
6	A	14	0	13	4	0
6	B	28	0	26	7	0
7	B	28	0	25	3	0
8	B	78	0	68	1	0
9	B	28	0	25	3	0
10	A	627	0	0	20	0
10	B	584	0	0	12	0
All	All	13536	0	11705	410	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 17.

All (410) 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:289:ALA:HB1	1:B:290:PRO:HA	1.44	0.98
1:A:492:ARG:HH11	1:A:492:ARG:HB3	1.25	0.97
1:A:172:ILE:H	1:A:186:THR:HG22	1.29	0.96
1:A:176:ILE:HD11	1:A:276:LEU:HD21	1.49	0.94
1:B:72:GLN:HE21	1:B:77:LEU:HD21	1.35	0.90
1:A:253:ARG:NH2	1:B:253:ARG:HH22	1.71	0.87
1:B:77:LEU:H	1:B:77:LEU:HD23	1.40	0.86
1:A:581:ARG:CZ	6:A:782:NAG:H62	2.07	0.84
1:A:184:ARG:NH1	1:A:187:TRP:HA	1.93	0.83
1:A:289:ALA:HB1	1:A:290:PRO:HA	1.59	0.83
1:B:91:GLU:HG2	1:B:94:THR:OG1	1.79	0.82
1:B:733:MET:HE2	1:B:734:TRP:O	1.79	0.82
1:B:502:LYS:O	1:B:505:GLN:HG2	1.81	0.81
6:B:781:NAG:O7	6:B:781:NAG:H3	1.78	0.80
1:B:289:ALA:HB1	1:B:290:PRO:CA	2.12	0.79
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.18	0.78
1:A:253:ARG:HH22	1:B:253:ARG:HH22	1.30	0.78
1:B:509:MET:HG3	1:B:510:PRO:HD2	1.65	0.76
1:B:702:LEU:HD11	1:B:716:SER:HB3	1.67	0.76
1:B:90:LEU:HD11	1:B:94:THR:HG21	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:GLN:HB3	1:A:391:LYS:HD3	1.69	0.75
1:B:399:LYS:HG3	10:B:817:HOH:O	1.88	0.74
1:B:76:ILE:CG2	1:B:90:LEU:HB3	2.17	0.74
1:B:184:ARG:HD3	1:B:186:THR:O	1.88	0.73
1:A:289:ALA:HB1	1:A:290:PRO:CA	2.18	0.73
1:B:69:LEU:HB3	1:B:76:ILE:HD11	1.71	0.73
1:B:279:VAL:O	1:B:280:THR:HG22	1.90	0.72
1:B:399:LYS:HB2	1:B:402:TRP:CZ2	2.25	0.72
1:B:272:ASN:C	1:B:272:ASN:HD22	1.93	0.72
1:A:173:TYR:CE2	1:A:184:ARG:HG2	2.25	0.71
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.89	0.71
1:B:401:THR:O	1:B:401:THR:HG22	1.89	0.71
5:A:776:NDG:H6C2	5:A:777:MAN:H2	1.71	0.71
1:A:596:ARG:O	1:A:597:ARG:HD2	1.90	0.71
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.71	0.71
1:B:95:PHE:O	1:B:98:PHE:HB2	1.91	0.71
3:A:770:NDG:H4	3:A:771:NAG:N2	2.05	0.70
1:B:41:LYS:HD3	1:B:41:LYS:H	1.56	0.70
1:A:736:THR:HG21	1:B:717:ALA:O	1.90	0.70
1:A:76:ILE:HD12	1:A:90:LEU:HD11	1.72	0.70
1:B:76:ILE:HG23	1:B:90:LEU:HB3	1.73	0.70
1:A:676:PRO:HG2	1:A:677:GLU:OE2	1.91	0.69
1:B:72:GLN:HE21	1:B:77:LEU:CD2	2.05	0.69
1:A:272:ASN:ND2	1:A:274:ASP:H	1.91	0.69
1:B:156:THR:HG21	10:B:1035:HOH:O	1.93	0.68
1:B:154:TRP:NE1	1:B:156:THR:HG23	2.08	0.68
1:A:658:ARG:HG2	1:A:661:TYR:CE2	2.29	0.67
1:A:172:ILE:H	1:A:186:THR:CG2	2.07	0.67
1:B:596:ARG:O	1:B:597:ARG:HD2	1.95	0.67
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.30	0.66
1:A:194:ILE:HD13	5:A:775:NAG:H82	1.78	0.66
1:B:377:ASN:HD22	1:B:377:ASN:C	1.99	0.66
1:B:272:ASN:ND2	1:B:274:ASP:H	1.94	0.65
1:A:156:THR:HG21	1:A:214:LEU:HD11	1.78	0.65
1:B:153:GLN:HE22	1:B:170:ASN:ND2	1.93	0.65
1:B:581:ARG:CZ	6:B:781:NAG:H5	2.26	0.65
9:B:779:NDG:H4	9:B:780:NDG:H5	1.78	0.65
1:A:388:GLN:CB	1:A:391:LYS:HD3	2.26	0.65
3:A:771:NAG:H3	3:A:771:NAG:O7	1.95	0.65
1:B:112:GLN:HB3	1:B:138:ASN:HD21	1.61	0.65
1:B:258:LYS:NZ	1:B:712:HIS:HD2	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ASP:OD1	1:A:186:THR:HG23	1.98	0.64
1:A:492:ARG:NH1	1:A:492:ARG:HB3	2.06	0.64
1:A:502:LYS:HB2	10:A:1161:HOH:O	1.98	0.64
1:B:414:TYR:HA	1:B:436:LEU:HD13	1.78	0.64
1:B:125:ARG:HG2	1:B:126:HIS:CE1	2.32	0.64
1:B:658:ARG:HG2	1:B:661:TYR:CE2	2.33	0.64
1:B:139:LYS:HG3	1:B:141:GLN:HB2	1.80	0.63
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.80	0.63
1:A:756:SER:O	1:A:760:LYS:HG2	1.99	0.62
1:B:258:LYS:HZ3	1:B:712:HIS:HD2	1.45	0.62
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.29	0.62
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.80	0.61
1:A:410:LEU:HD13	1:A:415:LEU:HD23	1.81	0.61
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.82	0.61
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.80	0.61
3:A:770:NDG:H4	3:A:771:NAG:HN2	1.66	0.61
1:B:318:ARG:HD3	1:B:668:GLU:OE1	2.00	0.61
1:B:139:LYS:NZ	1:B:139:LYS:HB3	2.16	0.60
5:A:776:NDG:C6	5:A:777:MAN:H2	2.31	0.60
1:B:232:GLU:HB3	1:B:262:VAL:HG11	1.84	0.60
1:B:55:LEU:HD11	1:B:561:LEU:HD12	1.82	0.60
1:A:91:GLU:O	1:A:93:SER:N	2.32	0.60
1:A:320:GLN:OE1	1:A:669:ARG:HD3	2.02	0.59
1:A:272:ASN:C	1:A:272:ASN:HD22	2.05	0.59
1:A:504:LEU:HA	1:A:507:VAL:HG12	1.85	0.59
1:A:377:ASN:ND2	10:A:946:HOH:O	2.34	0.59
1:A:492:ARG:HH11	1:A:492:ARG:CB	2.08	0.59
1:B:651:ILE:HG21	1:B:755:MET:CE	2.33	0.59
1:B:138:ASN:HA	10:B:1178:HOH:O	2.03	0.59
1:B:529:ILE:HD11	10:B:800:HOH:O	2.02	0.59
1:A:579:ASP:HB3	1:A:583:SER:OG	2.02	0.58
1:B:723:LEU:HD22	1:B:728:VAL:HG11	1.85	0.58
1:A:75:ASN:HB3	1:A:91:GLU:HA	1.85	0.58
1:B:658:ARG:HD3	1:B:660:GLU:HB2	1.86	0.58
1:A:74:ASN:O	1:A:92:ASN:HB2	2.04	0.58
8:B:777:NAG:O3	8:B:778:BMA:H2	2.04	0.58
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.39	0.57
1:B:658:ARG:HG3	1:B:658:ARG:O	2.03	0.57
1:B:272:ASN:HD22	1:B:274:ASP:H	1.51	0.57
1:B:676:PRO:HG2	1:B:677:GLU:OE2	2.04	0.57
1:B:290:PRO:HG3	1:B:326:ASP:OD2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:399:LYS:HB2	1:B:402:TRP:HZ2	1.70	0.57
1:A:253:ARG:HH22	1:B:253:ARG:NH2	2.02	0.57
1:B:170:ASN:N	1:B:170:ASN:HD22	2.03	0.57
1:A:272:ASN:HD22	1:A:274:ASP:H	1.51	0.57
1:B:723:LEU:HB3	1:B:728:VAL:HG13	1.86	0.56
1:A:341:VAL:C	1:A:343:ARG:H	2.08	0.56
1:B:40:ARG:HG3	1:B:506:ASN:O	2.05	0.56
1:A:546:VAL:HG22	1:A:547:TYR:N	2.21	0.56
1:B:258:LYS:HZ3	1:B:712:HIS:CD2	2.24	0.56
1:B:49:LEU:HD22	1:B:749:GLN:HA	1.88	0.56
1:B:289:ALA:CB	1:B:290:PRO:HA	2.28	0.56
1:B:512:LYS:HD3	10:B:1099:HOH:O	2.04	0.56
1:A:392:LYS:HG2	10:A:1291:HOH:O	2.05	0.56
1:B:320:GLN:OE1	1:B:669:ARG:HD3	2.06	0.56
1:B:377:ASN:ND2	1:B:379:GLU:H	2.04	0.56
1:A:377:ASN:HB3	10:A:946:HOH:O	2.06	0.56
1:B:691:ARG:HD2	10:B:1130:HOH:O	2.04	0.56
1:B:520:ASN:HD22	6:B:781:NAG:H4	1.70	0.56
1:A:76:ILE:HB	1:A:90:LEU:CD1	2.36	0.56
1:B:385:CYS:HB3	1:B:396:PHE:CD1	2.42	0.55
1:A:72:GLN:HB3	10:A:1057:HOH:O	2.07	0.55
1:B:446:SER:HB2	1:B:457:TYR:CE2	2.41	0.55
1:B:504:LEU:HD22	1:B:509:MET:CE	2.37	0.55
1:B:154:TRP:HE1	1:B:156:THR:CG2	2.21	0.54
1:B:286:GLN:NE2	1:B:288:THR:HG22	2.22	0.54
1:B:90:LEU:HD21	1:B:95:PHE:HE2	1.72	0.54
1:A:341:VAL:O	1:A:342:ALA:HB3	2.06	0.54
1:B:651:ILE:HG21	1:B:755:MET:HE3	1.87	0.54
1:A:194:ILE:CD1	5:A:775:NAG:H82	2.38	0.54
1:B:620:ASP:OD2	1:B:623:ARG:HD3	2.07	0.54
1:A:613:PHE:HA	1:A:616:MET:HG3	1.90	0.54
1:B:504:LEU:HA	1:B:507:VAL:HG12	1.90	0.54
1:A:350:THR:HG22	4:A:780:NAG:H81	1.89	0.54
1:A:704:HIS:HE1	1:A:711:VAL:O	1.91	0.54
1:B:64:SER:O	1:B:463:LYS:HG2	2.08	0.54
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.89	0.54
1:A:507:VAL:HG13	1:A:509:MET:HG2	1.90	0.54
1:B:139:LYS:O	1:B:141:GLN:HG2	2.08	0.54
1:A:171:ASP:OD2	1:A:184:ARG:NH1	2.41	0.54
1:A:197:GLY:C	1:A:213:ALA:HB3	2.29	0.53
1:A:502:LYS:O	1:A:505:GLN:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:581:ARG:HG2	1:A:593:ALA:HB1	1.90	0.53
1:A:236:ILE:CG2	1:A:254:VAL:HG13	2.38	0.53
1:A:293:MET:HG3	1:A:298:HIS:CB	2.39	0.53
1:A:325:MET:HE2	1:A:327:ILE:HG12	1.90	0.53
1:B:77:LEU:N	1:B:77:LEU:HD23	2.18	0.53
1:A:183:TYR:CE1	1:A:277:SER:O	2.61	0.52
1:B:504:LEU:HD22	1:B:509:MET:HE2	1.91	0.52
1:A:459:VAL:HG22	1:A:460:SER:N	2.24	0.52
1:A:622:LYS:NZ	1:A:622:LYS:HB2	2.25	0.52
1:B:377:ASN:ND2	1:B:381:TYR:H	2.06	0.52
1:B:74:ASN:O	1:B:92:ASN:HA	2.10	0.52
1:A:183:TYR:HE1	1:A:277:SER:O	1.93	0.52
1:A:140:ARG:HG2	1:A:140:ARG:HH11	1.75	0.52
1:B:154:TRP:NE1	1:B:156:THR:CG2	2.73	0.52
1:B:346:ILE:N	1:B:346:ILE:HD12	2.25	0.52
1:B:98:PHE:CD1	1:B:100:HIS:HB2	2.45	0.52
1:A:489:LYS:HD2	10:A:932:HOH:O	2.10	0.52
1:A:273:THR:O	1:A:276:LEU:HD22	2.10	0.51
1:A:726:VAL:HG12	1:A:726:VAL:O	2.10	0.51
1:A:93:SER:HB2	1:A:96:ASP:OD2	2.10	0.51
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.91	0.51
1:B:710:ASN:C	1:B:710:ASN:HD22	2.14	0.51
1:A:106:SER:HB3	1:A:115:LEU:HB3	1.92	0.51
1:A:377:ASN:OD1	1:A:378:GLU:N	2.44	0.51
1:B:319:ILE:HD11	1:B:673:LEU:HD13	1.93	0.51
1:A:358:ARG:HD2	10:A:961:HOH:O	2.09	0.51
1:A:377:ASN:CB	10:A:946:HOH:O	2.57	0.51
1:B:41:LYS:CD	1:B:41:LYS:H	2.22	0.51
1:B:598:LEU:HA	1:B:602:GLU:OE2	2.11	0.51
2:B:767:NAG:H61	2:B:769:FUC:O2	2.11	0.51
1:A:177:GLU:CG	1:A:180:LEU:HD22	2.41	0.51
1:A:39:SER:O	1:A:40:ARG:HB2	2.10	0.51
1:A:75:ASN:CB	1:A:91:GLU:HA	2.41	0.50
1:B:69:LEU:CD1	1:B:107:ILE:HD12	2.41	0.50
1:A:289:ALA:CB	1:A:290:PRO:CA	2.89	0.50
1:A:718:GLN:HA	1:A:718:GLN:HE21	1.75	0.50
1:B:165:ALA:HB2	1:B:216:TRP:CZ2	2.47	0.50
1:B:448:GLU:HG3	10:B:1180:HOH:O	2.11	0.50
1:A:581:ARG:NH1	6:A:782:NAG:H62	2.25	0.50
1:B:443:THR:HG21	10:B:974:HOH:O	2.11	0.50
1:B:538:LYS:HD3	1:B:539:LYS:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:279:VAL:O	1:B:280:THR:CG2	2.60	0.50
1:A:392:LYS:HG3	1:A:393:ASP:N	2.27	0.50
1:B:250:LYS:NZ	1:B:250:LYS:HB2	2.27	0.50
1:A:75:ASN:HB2	1:A:90:LEU:O	2.12	0.49
1:A:95:PHE:HB3	1:A:98:PHE:HB2	1.93	0.49
1:B:60:LEU:O	1:B:60:LEU:HD23	2.11	0.49
1:A:542:LEU:HD23	1:A:542:LEU:C	2.32	0.49
1:B:765:LEU:HB3	1:B:766:PRO:HA	1.93	0.49
1:A:312:SER:C	1:A:313:LEU:HD12	2.31	0.49
1:B:546:VAL:HG22	1:B:547:TYR:N	2.27	0.49
1:A:276:LEU:HD23	1:A:276:LEU:O	2.12	0.49
1:B:139:LYS:HZ2	1:B:139:LYS:HB3	1.78	0.49
1:A:704:HIS:CE1	1:A:711:VAL:O	2.66	0.49
1:A:193:ILE:HG22	1:A:194:ILE:HG13	1.94	0.49
1:B:236:ILE:HG12	1:B:712:HIS:CE1	2.48	0.49
1:A:581:ARG:HG2	1:A:593:ALA:CB	2.43	0.49
6:A:782:NAG:O7	6:A:782:NAG:H3	2.11	0.49
1:B:272:ASN:C	1:B:272:ASN:ND2	2.65	0.49
1:A:40:ARG:HB3	1:A:506:ASN:O	2.13	0.48
1:A:492:ARG:NE	10:A:1381:HOH:O	2.45	0.48
1:B:72:GLN:C	1:B:74:ASN:H	2.16	0.48
1:A:150:ASN:O	1:A:151:ASN:HB2	2.13	0.48
1:A:214:LEU:O	1:A:214:LEU:HD12	2.13	0.48
1:A:275:SER:HB2	10:A:1253:HOH:O	2.13	0.48
1:A:581:ARG:HB2	1:A:605:ASP:OD2	2.12	0.48
1:B:761:GLN:HG3	10:B:1341:HOH:O	2.12	0.48
1:A:542:LEU:HD23	1:A:543:LEU:N	2.28	0.48
1:B:293:MET:HE3	1:B:315:TRP:HB2	1.94	0.48
1:A:108:SER:C	1:A:110:ASP:H	2.17	0.48
1:B:529:ILE:HD13	10:B:864:HOH:O	2.13	0.48
1:B:387:PHE:CE1	1:B:394:CYS:HB3	2.49	0.48
1:A:69:LEU:HD13	1:A:107:ILE:HD12	1.95	0.48
1:A:170:ASN:N	1:A:170:ASN:HD22	2.11	0.48
1:B:415:LEU:HD23	1:B:415:LEU:C	2.34	0.48
1:B:520:ASN:HD22	6:B:781:NAG:H61	1.78	0.48
1:A:92:ASN:C	1:A:94:THR:N	2.67	0.48
1:B:55:LEU:CD1	1:B:561:LEU:HD12	2.44	0.48
1:A:613:PHE:O	1:A:616:MET:HG3	2.12	0.47
1:B:532:PRO:HD3	1:B:569:SER:HA	1.96	0.47
1:B:268:PHE:CD2	1:B:313:LEU:HD21	2.49	0.47
3:A:771:NAG:C3	3:A:771:NAG:O7	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.96	0.47
1:B:74:ASN:HB3	1:B:92:ASN:CG	2.35	0.47
1:A:110:ASP:HB2	1:A:161:GLY:O	2.14	0.47
1:B:308:GLN:HB3	7:B:771:NDG:H6C1	1.96	0.47
1:A:108:SER:C	1:A:110:ASP:N	2.67	0.47
1:B:69:LEU:HD11	1:B:107:ILE:HD12	1.95	0.47
1:B:139:LYS:HG3	1:B:141:GLN:CB	2.44	0.47
1:B:397:ILE:HG22	1:B:439:TYR:CE2	2.49	0.47
1:B:93:SER:HA	1:B:96:ASP:OD2	2.15	0.47
1:A:370:SER:HB2	1:A:387:PHE:O	2.14	0.47
1:A:91:GLU:C	1:A:93:SER:H	2.17	0.47
1:B:272:ASN:HD21	1:B:274:ASP:HB2	1.79	0.47
1:B:184:ARG:HD2	1:B:187:TRP:NE1	2.30	0.47
1:A:718:GLN:NE2	10:A:818:HOH:O	2.48	0.47
1:B:399:LYS:HB3	1:B:400:GLY:H	1.44	0.47
1:A:285:ILE:N	1:A:285:ILE:HD12	2.30	0.46
1:A:291:ALA:O	1:A:295:ILE:HG23	2.14	0.46
1:B:308:GLN:HB3	7:B:771:NDG:C6	2.45	0.46
1:B:51:ASN:ND2	1:B:54:ARG:NE	2.62	0.46
1:B:75:ASN:ND2	1:B:92:ASN:H	2.12	0.46
1:A:39:SER:O	1:A:40:ARG:CB	2.62	0.46
1:A:60:LEU:C	1:A:60:LEU:HD12	2.35	0.46
3:A:770:NDG:C4	3:A:771:NAG:N2	2.75	0.46
1:B:106:SER:HB3	1:B:115:LEU:HB3	1.97	0.46
1:B:344:GLN:HE21	1:B:346:ILE:HD11	1.80	0.46
1:A:184:ARG:HH12	1:A:187:TRP:HA	1.74	0.46
1:A:290:PRO:HG3	1:A:326:ASP:OD2	2.15	0.46
1:A:340:LEU:O	1:A:343:ARG:HB3	2.16	0.46
1:B:199:THR:HG21	1:B:208:PHE:HD2	1.80	0.46
1:B:401:THR:O	1:B:401:THR:CG2	2.61	0.46
1:A:140:ARG:HG2	1:A:140:ARG:NH1	2.31	0.46
1:A:177:GLU:HG3	1:A:180:LEU:HD22	1.96	0.46
1:A:742:ILE:O	1:A:742:ILE:HG22	2.16	0.46
1:B:135:TYR:CE2	1:B:137:LEU:HD23	2.50	0.46
1:B:377:ASN:HD21	1:B:381:TYR:H	1.63	0.46
1:B:446:SER:HB2	1:B:457:TYR:CD2	2.50	0.46
1:B:77:LEU:H	1:B:77:LEU:CD2	2.20	0.46
1:A:123:GLN:HG2	1:A:124:TRP:CD2	2.51	0.46
1:A:272:ASN:HD22	1:A:273:THR:N	2.14	0.46
1:A:590:ILE:HG12	10:A:1015:HOH:O	2.15	0.46
1:B:114:ILE:HG22	1:B:135:TYR:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:ASN:C	1:B:377:ASN:ND2	2.69	0.46
1:A:314:GLN:HE22	1:A:373:LYS:NZ	2.14	0.45
1:B:147:ARG:NH2	6:B:770:NAG:HN2	2.14	0.45
1:B:520:ASN:HB2	6:B:781:NAG:H61	1.98	0.45
1:B:718:GLN:HE22	1:B:721:LYS:NZ	2.14	0.45
1:B:90:LEU:HD21	1:B:95:PHE:CE2	2.50	0.45
1:B:733:MET:HE3	1:B:733:MET:HA	1.98	0.45
1:B:72:GLN:O	1:B:74:ASN:N	2.44	0.45
1:B:69:LEU:HD23	1:B:78:VAL:HB	1.97	0.45
1:A:402:TRP:CD2	1:A:421:GLU:HB2	2.52	0.45
1:A:600:THR:O	1:A:603:VAL:CG1	2.64	0.45
1:A:600:THR:O	1:A:603:VAL:HG13	2.16	0.45
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.47	0.45
1:A:718:GLN:HA	1:A:718:GLN:NE2	2.31	0.45
1:B:741:GLY:O	1:B:742:ILE:C	2.54	0.45
1:A:622:LYS:HB2	1:A:622:LYS:HZ1	1.82	0.45
1:B:46:THR:HG23	10:B:993:HOH:O	2.16	0.45
1:B:535:ASP:OD1	1:B:537:SER:HB2	2.17	0.45
1:A:184:ARG:HH11	1:A:187:TRP:HA	1.77	0.44
1:A:341:VAL:HG22	1:A:342:ALA:H	1.82	0.44
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.98	0.44
1:A:658:ARG:HD2	1:A:661:TYR:CE1	2.52	0.44
1:B:517:ILE:HG12	1:B:518:ILE:N	2.33	0.44
1:B:487:ASN:O	1:B:488:ASP:HB2	2.17	0.44
1:B:516:PHE:CD2	1:B:523:LYS:HE3	2.52	0.44
1:B:96:ASP:O	1:B:97:GLU:HB2	2.18	0.44
1:A:114:ILE:HG13	1:A:137:LEU:HD11	2.00	0.44
1:B:139:LYS:HG3	1:B:141:GLN:CG	2.48	0.44
1:B:207:VAL:O	1:B:358:ARG:HD3	2.18	0.44
1:A:691:ARG:HG3	1:A:691:ARG:HH11	1.82	0.44
1:A:654:ALA:HA	1:A:704:HIS:CD2	2.52	0.44
1:A:92:ASN:C	1:A:94:THR:H	2.19	0.44
1:B:279:VAL:O	1:B:280:THR:CB	2.66	0.44
1:A:544:LEU:HD21	1:A:606:GLN:HE21	1.83	0.44
1:B:293:MET:HG2	1:B:315:TRP:HB3	2.00	0.44
1:A:680:LEU:HD11	1:A:684:ARG:CZ	2.48	0.43
1:A:720:SER:O	1:A:724:VAL:HG23	2.18	0.43
1:B:469:GLN:OE1	1:B:471:ARG:NE	2.51	0.43
1:B:546:VAL:CG2	1:B:547:TYR:N	2.81	0.43
1:A:177:GLU:HB2	1:A:180:LEU:HD22	2.00	0.43
1:B:517:ILE:CD1	1:B:612:GLN:HG3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:TRP:CD2	1:B:421:GLU:HB2	2.53	0.43
1:B:184:ARG:HH11	1:B:187:TRP:HA	1.83	0.43
1:B:193:ILE:HG22	1:B:194:ILE:HG12	2.01	0.43
1:B:644:SER:OG	1:B:645:GLY:N	2.50	0.43
1:A:41:LYS:HD3	1:A:41:LYS:H	1.83	0.43
1:A:332:GLU:HG3	10:A:1271:HOH:O	2.19	0.43
3:A:770:NDG:HB	3:A:771:NAG:H83	1.84	0.43
1:B:343:ARG:HA	1:B:389:ILE:O	2.19	0.43
1:B:208:PHE:O	1:B:209:SER:HB2	2.19	0.43
1:B:56:LYS:NZ	1:B:56:LYS:HB3	2.34	0.43
1:A:277:SER:OG	1:A:280:THR:HB	2.19	0.43
1:A:289:ALA:CB	1:A:290:PRO:HA	2.39	0.43
1:A:546:VAL:CG2	1:A:547:TYR:N	2.82	0.43
1:B:219:ASN:ND2	7:B:771:NDG:C7	2.82	0.43
1:A:278:SER:HB3	10:A:1301:HOH:O	2.18	0.42
1:B:459:VAL:HG22	1:B:460:SER:N	2.34	0.42
1:B:658:ARG:HG2	1:B:661:TYR:CD2	2.53	0.42
1:A:340:LEU:C	1:A:341:VAL:O	2.57	0.42
1:A:77:LEU:HD23	1:A:88:VAL:HA	2.02	0.42
1:B:289:ALA:HA	1:B:294:LEU:HD11	2.01	0.42
1:B:651:ILE:HG21	1:B:755:MET:HE2	2.00	0.42
1:B:70:TYR:O	1:B:77:LEU:HD23	2.19	0.42
1:A:186:THR:HG21	1:A:196:ASN:CB	2.50	0.42
1:B:530:LEU:HA	1:B:531:PRO:HD3	1.92	0.42
1:A:562:ASN:HB2	10:A:1343:HOH:O	2.20	0.42
1:B:41:LYS:N	1:B:41:LYS:HD3	2.30	0.42
1:B:520:ASN:HD22	6:B:781:NAG:C4	2.28	0.42
1:A:581:ARG:CZ	6:A:782:NAG:C6	2.89	0.42
1:A:75:ASN:HD21	1:A:77:LEU:HD21	1.84	0.42
1:B:115:LEU:HD11	1:B:132:TYR:HB3	2.02	0.42
1:B:93:SER:O	1:B:94:THR:C	2.57	0.42
1:A:626:ILE:O	1:A:650:GLY:HA2	2.19	0.42
1:B:531:PRO:HB3	1:B:572:ASN:HD22	1.84	0.42
1:B:65:ASP:HB3	1:B:66:HIS:CE1	2.55	0.42
1:B:726:VAL:HG23	1:B:728:VAL:HG12	2.01	0.42
1:B:75:ASN:OD1	1:B:92:ASN:HB2	2.19	0.42
1:A:312:SER:O	1:A:313:LEU:HD12	2.20	0.42
1:A:62:TRP:CG	1:A:462:SER:HA	2.55	0.42
1:B:423:LYS:HB3	1:B:425:MET:HG3	2.01	0.42
1:B:528:MET:HE2	1:B:528:MET:HB3	1.87	0.42
1:A:148:ILE:HA	1:A:149:PRO:HD3	1.94	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:538:LYS:HG3	10:A:1162:HOH:O	2.19	0.42
1:B:375:ILE:HD11	1:B:385:CYS:SG	2.59	0.42
1:A:470:LEU:HD23	1:A:470:LEU:HA	1.92	0.42
1:A:90:LEU:HD22	1:A:92:ASN:H	1.85	0.42
1:B:112:GLN:HB3	1:B:138:ASN:ND2	2.33	0.42
1:B:317:ARG:HD2	1:B:322:TYR:HB3	2.02	0.42
1:B:80:ASN:OD1	1:B:82:GLU:HB3	2.20	0.42
1:A:452:GLU:OE1	1:A:452:GLU:HA	2.20	0.41
1:B:154:TRP:HE1	1:B:156:THR:HG21	1.85	0.41
1:B:65:ASP:OD1	1:B:464:GLU:HB2	2.20	0.41
1:A:377:ASN:CG	1:A:378:GLU:N	2.74	0.41
1:A:658:ARG:O	1:A:658:ARG:HG3	2.19	0.41
1:A:461:PHE:CD2	1:A:468:TYR:HB3	2.54	0.41
1:B:289:ALA:CB	1:B:290:PRO:CA	2.86	0.41
1:B:627:TRP:CE3	1:B:755:MET:HE1	2.55	0.41
1:B:348:MET:HE3	9:B:779:NDG:H8C1	2.02	0.41
1:A:125:ARG:HD3	10:A:934:HOH:O	2.19	0.41
1:B:237:GLU:HA	1:B:252:VAL:O	2.21	0.41
1:B:55:LEU:N	1:B:55:LEU:HD12	2.36	0.41
1:B:599:GLY:H	1:B:602:GLU:CD	2.24	0.41
1:B:93:SER:O	1:B:95:PHE:N	2.53	0.41
1:A:341:VAL:C	1:A:343:ARG:N	2.73	0.41
1:A:51:ASN:OD1	1:A:54:ARG:NH1	2.54	0.41
1:A:627:TRP:HB2	1:A:651:ILE:HB	2.02	0.41
1:A:677:GLU:CD	1:A:677:GLU:H	2.23	0.41
1:B:136:ASP:CG	1:B:139:LYS:HG2	2.41	0.41
1:B:383:HIS:HB3	1:B:398:THR:OG1	2.20	0.41
1:B:530:LEU:HD13	1:B:534:PHE:CD2	2.56	0.41
1:A:520:ASN:O	1:A:521:GLU:CB	2.69	0.41
5:A:776:NDG:H6C2	5:A:777:MAN:C2	2.46	0.41
1:B:521:GLU:HA	1:B:521:GLU:OE2	2.20	0.41
1:B:745:SER:O	1:B:749:GLN:HG3	2.21	0.41
1:A:289:ALA:HB3	10:A:1251:HOH:O	2.21	0.41
1:B:696:LYS:HB3	1:B:696:LYS:HE2	1.90	0.41
1:A:206:GLU:OE2	1:A:663:ASP:OD2	2.39	0.41
1:B:250:LYS:NZ	1:B:250:LYS:CB	2.83	0.41
1:B:542:LEU:HD23	1:B:542:LEU:C	2.41	0.41
1:B:77:LEU:N	1:B:77:LEU:CD2	2.82	0.41
1:B:41:LYS:O	1:B:507:VAL:HG23	2.21	0.41
1:A:741:GLY:O	1:A:742:ILE:C	2.58	0.41
1:B:289:ALA:HA	1:B:294:LEU:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:LEU:C	1:A:415:LEU:HD13	2.41	0.41
1:A:481:THR:OG1	1:A:483:HIS:CE1	2.73	0.41
1:A:221:THR:HB	10:A:901:HOH:O	2.21	0.40
1:B:250:LYS:HZ2	1:B:250:LYS:HB2	1.85	0.40
1:B:316:LEU:HD12	1:B:322:TYR:O	2.20	0.40
1:B:90:LEU:CD1	1:B:94:THR:HG21	2.43	0.40
1:A:286:GLN:NE2	1:A:288:THR:HG22	2.36	0.40
1:A:314:GLN:HE22	1:A:373:LYS:HZ3	1.68	0.40
1:A:516:PHE:CE2	1:A:523:LYS:HE2	2.56	0.40
1:A:561:LEU:HA	1:A:561:LEU:HD12	1.91	0.40
1:A:308:GLN:HG2	10:A:1386:HOH:O	2.21	0.40
1:A:51:ASN:OD1	1:A:54:ARG:CZ	2.69	0.40
1:B:51:ASN:HD21	1:B:54:ARG:NE	2.19	0.40
1:A:718:GLN:CA	1:A:718:GLN:HE21	2.34	0.40
1:B:280:THR:HA	10:B:963:HOH:O	2.22	0.40
1:B:370:SER:HB2	1:B:387:PHE:O	2.21	0.40
1:B:517:ILE:HD11	1:B:612:GLN:OE1	2.21	0.40
1:B:539:LYS:HE3	1:B:617:GLY:O	2.21	0.40
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.51	0.40
1:B:413:ASP:HB3	1:B:414:TYR:CD1	2.56	0.40
9:B:779:NDG:H4	9:B:780:NDG:C5	2.48	0.40

There are no symmetry-related clashes.

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	724/728 (100%)	676 (93%)	43 (6%)	5 (1%)	26	19
1	B	726/728 (100%)	684 (94%)	34 (5%)	8 (1%)	17	9
All	All	1450/1456 (100%)	1360 (94%)	77 (5%)	13 (1%)	21	13

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	SER
1	B	399	LYS
1	A	289	ALA
1	A	520	ASN
1	B	280	THR
1	B	289	ALA
1	B	320	GLN
1	B	401	THR
1	A	320	GLN
1	B	94	THR
1	A	277	SER
1	B	40	ARG
1	B	73	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	651/653 (100%)	617 (95%)	34 (5%)	29	23
1	B	653/653 (100%)	614 (94%)	39 (6%)	24	17
All	All	1304/1306 (100%)	1231 (94%)	73 (6%)	26	20

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	51	ASN
1	A	90	LEU
1	A	170	ASN
1	A	184	ARG
1	A	246	LEU
1	A	253	ARG
1	A	254	VAL
1	A	272	ASN
1	A	276	LEU

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Mol	Chain	Res	Type
1	A	303	VAL
1	A	326	ASP
1	A	385	CYS
1	A	390	ASP
1	A	436	LEU
1	A	440	THR
1	A	448	GLU
1	A	472	CYS
1	A	482	LEU
1	A	492	ARG
1	A	536	LYS
1	A	543	LEU
1	A	561	LEU
1	A	566	TYR
1	A	581	ARG
1	A	616	MET
1	A	658	ARG
1	A	679	ASN
1	A	689	MET
1	A	701	LEU
1	A	702	LEU
1	A	736	THR
1	A	760	LYS
1	A	761	GLN
1	B	41	LYS
1	B	60	LEU
1	B	61	ARG
1	B	66	HIS
1	B	73	GLU
1	B	77	LEU
1	B	92	ASN
1	B	125	ARG
1	B	139	LYS
1	B	170	ASN
1	B	223	LEU
1	B	230	ASP
1	B	232	GLU
1	B	246	LEU
1	B	253	ARG
1	B	272	ASN
1	B	303	VAL
1	B	304	THR

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Mol	Chain	Res	Type
1	B	366	LEU
1	B	377	ASN
1	B	379	GLU
1	B	410	LEU
1	B	413	ASP
1	B	429	ARG
1	B	448	GLU
1	B	472	CYS
1	B	506	ASN
1	B	509	MET
1	B	514	LEU
1	B	543	LEU
1	B	597	ARG
1	B	644	SER
1	B	658	ARG
1	B	679	ASN
1	B	685	ASN
1	B	689	MET
1	B	701	LEU
1	B	710	ASN
1	B	761	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	75	ASN
1	A	92	ASN
1	A	169	ASN
1	A	170	ASN
1	A	272	ASN
1	A	314	GLN
1	A	345	HIS
1	A	369	ASN
1	A	435	GLN
1	A	483	HIS
1	A	505	GLN
1	A	572	ASN
1	A	595	ASN
1	A	606	GLN
1	A	612	GLN
1	A	679	ASN

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Mol	Chain	Res	Type
1	A	694	ASN
1	A	704	HIS
1	A	718	GLN
1	B	51	ASN
1	B	72	GLN
1	B	112	GLN
1	B	119	ASN
1	B	123	GLN
1	B	126	HIS
1	B	138	ASN
1	B	169	ASN
1	B	170	ASN
1	B	272	ASN
1	B	286	GLN
1	B	314	GLN
1	B	344	GLN
1	B	345	HIS
1	B	377	ASN
1	B	388	GLN
1	B	435	GLN
1	B	572	ASN
1	B	621	ASN
1	B	679	ASN
1	B	685	ASN
1	B	694	ASN
1	B	710	ASN
1	B	712	HIS
1	B	718	GLN
1	B	731	GLN
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 ⓘ

28 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
2	NAG	A	767	1,2	14,14,15	0.55	0	15,19,21	0.73	1 (6%)
2	NAG	A	768	2	14,14,15	0.49	0	15,19,21	0.76	1 (6%)
2	FUC	A	769	2	10,10,11	0.46	0	13,14,16	0.30	0
3	NDG	A	770	1,3	14,14,15	0.73	0	15,19,21	0.78	1 (6%)
3	NAG	A	771	3	14,14,15	0.71	1 (7%)	15,19,21	0.58	0
3	FUC	A	772	3	10,10,11	0.50	0	13,14,16	0.36	0
4	NAG	A	773	1,4	14,14,15	0.47	0	15,19,21	0.81	1 (6%)
4	NAG	A	774	4	14,14,15	0.49	0	15,19,21	0.71	1 (6%)
5	NAG	A	775	1,5	14,14,15	0.49	0	15,19,21	0.91	1 (6%)
5	NDG	A	776	5	14,14,15	0.70	0	15,19,21	0.96	1 (6%)
5	MAN	A	777	5	11,11,12	0.63	0	15,15,17	0.37	0
4	NAG	A	778	1,4	14,14,15	0.47	0	15,19,21	0.78	1 (6%)
4	NAG	A	779	4	14,14,15	0.51	0	15,19,21	0.61	0
4	NAG	A	780	1,4	14,14,15	0.54	0	15,19,21	0.76	1 (6%)
4	NAG	A	781	4	14,14,15	0.51	0	15,19,21	0.72	0
2	NAG	B	767	1,2	14,14,15	0.52	0	15,19,21	0.75	1 (6%)
2	NAG	B	768	2	14,14,15	0.55	0	15,19,21	0.78	1 (6%)
2	FUC	B	769	2	10,10,11	0.51	0	13,14,16	0.47	0
7	NDG	B	771	1,7	14,14,15	0.74	0	15,19,21	1.11	2 (13%)
7	NAG	B	772	7	14,14,15	0.54	0	15,19,21	0.85	1 (6%)
8	NAG	B	773	1,8	14,14,15	0.43	0	15,19,21	0.84	1 (6%)
8	NAG	B	774	8	14,14,15	0.46	0	15,19,21	0.75	1 (6%)
8	BMA	B	775	8	11,11,12	0.49	0	15,15,17	0.23	0
8	NAG	B	776	1,8	14,14,15	0.61	0	15,19,21	0.94	1 (6%)
8	NAG	B	777	8	14,14,15	0.72	0	15,19,21	1.19	2 (13%)
8	BMA	B	778	8	11,11,12	0.49	0	15,15,17	0.38	0
9	NDG	B	779	1,9	14,14,15	0.62	0	15,19,21	0.84	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	NDG	B	780	9	14,14,15	0.69	0	15,19,21	0.89	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	NAG	A	767	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	768	2	-	0/6/23/26	0/1/1/1
2	FUC	A	769	2	-	0/0/17/20	0/1/1/1
3	NDG	A	770	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	771	3	-	0/6/23/26	0/1/1/1
3	FUC	A	772	3	-	0/0/17/20	0/1/1/1
4	NAG	A	773	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	774	4	-	0/6/23/26	0/1/1/1
5	NAG	A	775	1,5	-	0/6/23/26	0/1/1/1
5	NDG	A	776	5	-	0/6/23/26	0/1/1/1
5	MAN	A	777	5	-	0/2/19/22	0/1/1/1
4	NAG	A	778	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	779	4	-	0/6/23/26	0/1/1/1
4	NAG	A	780	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	781	4	-	0/6/23/26	0/1/1/1
2	NAG	B	767	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	768	2	-	0/6/23/26	0/1/1/1
2	FUC	B	769	2	-	0/0/17/20	0/1/1/1
7	NDG	B	771	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	772	7	-	0/6/23/26	0/1/1/1
8	NAG	B	773	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	774	8	-	0/6/23/26	0/1/1/1
8	BMA	B	775	8	-	0/2/19/22	0/1/1/1
8	NAG	B	776	1,8	-	0/6/23/26	0/1/1/1
8	NAG	B	777	8	-	0/6/23/26	0/1/1/1
8	BMA	B	778	8	-	0/2/19/22	0/1/1/1
9	NDG	B	779	1,9	-	0/6/23/26	0/1/1/1
9	NDG	B	780	9	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	771	NAG	C1-C2	2.04	1.55	1.52

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	775	NAG	C2-N2-C7	-3.00	119.21	123.11
8	B	776	NAG	C2-N2-C7	-2.80	119.46	123.11
8	B	777	NAG	C2-N2-C7	-2.72	119.56	123.11
9	B	779	NDG	C2-N2-C7	-2.65	119.65	123.11
7	B	771	NDG	C2-N2-C7	-2.55	119.79	123.11
4	A	773	NAG	C2-N2-C7	-2.54	119.81	123.11
8	B	773	NAG	C2-N2-C7	-2.49	119.86	123.11
2	A	768	NAG	C2-N2-C7	-2.46	119.91	123.11
8	B	777	NAG	C4-C3-C2	-2.42	107.59	111.34
4	A	780	NAG	C2-N2-C7	-2.31	120.10	123.11
8	B	774	NAG	C2-N2-C7	-2.29	120.13	123.11
5	A	776	NDG	C2-N2-C7	-2.27	120.15	123.11
3	A	770	NDG	C2-N2-C7	-2.27	120.16	123.11
7	B	772	NAG	C2-N2-C7	-2.23	120.20	123.11
9	B	780	NDG	C2-N2-C7	-2.18	120.27	123.11
2	B	767	NAG	C2-N2-C7	-2.16	120.29	123.11
2	A	767	NAG	C2-N2-C7	-2.15	120.31	123.11
2	B	768	NAG	C2-N2-C7	-2.14	120.33	123.11
7	B	771	NDG	C4-C3-C2	-2.13	108.04	111.34
4	A	774	NAG	C2-N2-C7	-2.06	120.43	123.11
4	A	778	NAG	C2-N2-C7	-2.05	120.43	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	770	NDG	4	0
3	A	771	NAG	6	0
5	A	775	NAG	2	0
5	A	776	NDG	3	0
5	A	777	MAN	3	0
4	A	780	NAG	1	0
2	B	767	NAG	1	0
2	B	769	FUC	1	0
7	B	771	NDG	3	0
8	B	777	NAG	1	0
8	B	778	BMA	1	0
9	B	779	NDG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	780	NDG	2	0

5.6 Ligand geometry

3 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
6	NAG	A	782	1	14,14,15	0.52	0	15,19,21	0.66	0
6	NAG	B	770	1	14,14,15	0.50	0	15,19,21	0.77	1 (6%)
6	NAG	B	781	1	14,14,15	0.71	0	15,19,21	0.65	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
6	NAG	A	782	1	-	0/6/23/26	0/1/1/1
6	NAG	B	770	1	-	0/6/23/26	0/1/1/1
6	NAG	B	781	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	770	NAG	C2-N2-C7	-2.38	120.01	123.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	782	NAG	4	0
6	B	770	NAG	1	0
6	B	781	NAG	6	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%)	0.05	17 (2%) 64 64	10, 22, 44, 59	0
1	B	728/728 (100%)	0.20	38 (5%) 31 33	10, 24, 50, 70	0
All	All	1454/1456 (99%)	0.12	55 (3%) 44 45	10, 23, 47, 70	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	SER	7.1
1	B	39	SER	6.2
1	B	73	GLU	5.9
1	B	98	PHE	5.9
1	B	105	TYR	5.4
1	B	97	GLU	5.1
1	A	289	ALA	4.9
1	B	766	PRO	4.5
1	A	92	ASN	4.5
1	A	73	GLU	4.4
1	A	279	VAL	4.4
1	B	94	THR	4.1
1	B	92	ASN	4.0
1	A	392	LYS	3.9
1	A	276	LEU	3.8
1	B	333	SER	3.7
1	B	72	GLN	3.6
1	B	40	ARG	3.6
1	B	289	ALA	3.4
1	A	521	GLU	3.4
1	B	75	ASN	3.3
1	B	99	GLY	3.3
1	B	96	ASP	3.3
1	A	277	SER	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	140	ARG	3.1
1	B	138	ASN	3.1
1	B	91	GLU	3.1
1	A	393	ASP	3.1
1	B	334	SER	3.0
1	A	342	ALA	2.8
1	B	399	LYS	2.8
1	B	95	PHE	2.8
1	B	385	CYS	2.8
1	A	74	ASN	2.8
1	B	378	GLU	2.8
1	B	141	GLN	2.7
1	B	93	SER	2.7
1	A	341	VAL	2.6
1	B	88	VAL	2.6
1	B	765	LEU	2.5
1	B	77	LEU	2.4
1	A	520	ASN	2.4
1	A	390	ASP	2.4
1	B	506	ASN	2.4
1	B	76	ILE	2.4
1	B	139	LYS	2.3
1	B	452	GLU	2.2
1	B	521	GLU	2.2
1	A	377	ASN	2.2
1	B	154	TRP	2.1
1	A	505	GLN	2.1
1	B	388	GLN	2.1
1	B	74	ASN	2.1
1	B	100	HIS	2.1
1	B	102	ILE	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 ⓘ

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
9	NDG	B	779	14/15	0.66	0.28	6.91	50,53,56,60	0
8	NAG	B	776	14/15	0.93	0.13	4.83	29,32,36,40	0
4	NAG	A	780	14/15	0.89	0.15	3.98	38,41,44,48	0
7	NAG	B	772	14/15	0.64	0.30	3.20	63,65,65,66	0
4	NAG	A	774	14/15	0.85	0.24	3.04	49,52,53,53	0
2	NAG	A	767	14/15	0.81	0.17	0.88	50,51,54,57	0
5	NAG	A	775	14/15	0.91	0.13	0.78	37,39,44,50	0
2	NAG	B	767	14/15	0.84	0.18	0.64	58,60,63,65	0
8	NAG	B	773	14/15	0.95	0.09	-0.82	28,31,35,41	0
3	NDG	A	770	14/15	0.64	0.36	-	62,66,70,70	0
5	NDG	A	776	14/15	0.63	0.29	-	56,60,62,66	0
5	MAN	A	777	11/12	0.33	0.44	-	69,70,71,71	0
3	FUC	A	772	10/11	0.72	0.46	-	71,72,73,73	0
8	BMA	B	778	11/12	0.61	0.37	-	57,60,61,61	0
4	NAG	A	781	14/15	0.74	0.32	-	49,52,53,54	0
2	FUC	A	769	10/11	0.84	0.17	-	53,54,54,54	0
2	NAG	A	768	14/15	0.64	0.37	-	61,63,64,64	0
2	NAG	B	768	14/15	0.72	0.43	-	67,69,70,70	0
7	NDG	B	771	14/15	0.72	0.33	-	52,57,58,61	0
4	NAG	A	779	14/15	0.73	0.37	-	63,64,65,65	0
9	NDG	B	780	14/15	0.65	0.41	-	63,65,67,67	0
4	NAG	A	773	14/15	0.88	0.15	-	36,39,41,45	0
8	NAG	B	777	14/15	0.87	0.18	-	44,46,49,53	0
4	NAG	A	778	14/15	0.83	0.20	-	55,56,58,60	0
8	BMA	B	775	11/12	0.67	0.31	-	60,62,63,63	0
2	FUC	B	769	10/11	0.78	0.29	-	64,65,65,65	0
8	NAG	B	774	14/15	0.84	0.22	-	46,50,53,57	0
3	NAG	A	771	14/15	0.44	0.49	-	73,74,75,76	0

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(\AA^2)	Q<0.9
6	NAG	B	781	14/15	0.66	0.39	4.99	59,61,62,62	0
6	NAG	A	782	14/15	0.55	0.48	4.75	65,67,67,67	0
6	NAG	B	770	14/15	0.70	0.30	-	50,53,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.