



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:47 AM GMT

PDB ID : 2BGR
Title : CRYSTAL STRUCTURE OF HIV-1 TAT DERIVED NONAPEPTIDES
TAT(1-9) BOUND TO THE ACTIVE SITE OF DIPEPTIDYL PEPTIDASE
IV (CD26)
Authors : Weihofen, W.A.; Liu, J.; Reutter, W.; Saenger, W.; Fan, H.
Deposited on : 2005-01-04
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

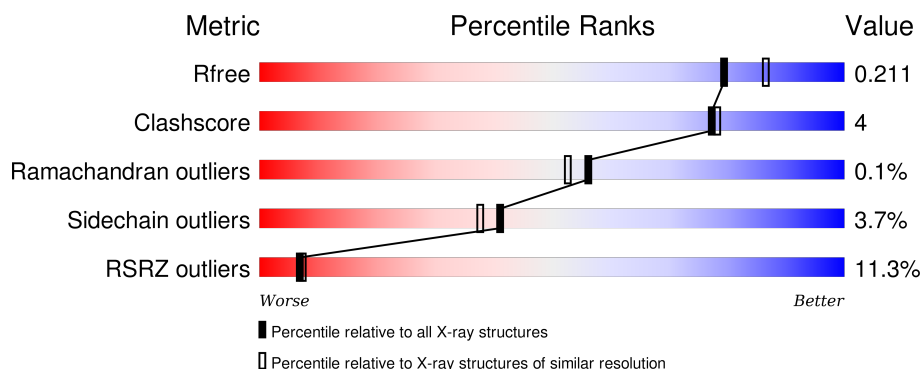
1 Overall quality at a glance

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	738	<div> <div>9%</div> <div>89%</div> <div>8%</div> <div>..</div> </div>
1	B	738	<div> <div>13%</div> <div>89%</div> <div>8%</div> <div>..</div> </div>
2	Y	9	<div> <div>33%</div> <div>11%</div> <div>11%</div> <div>11%</div> <div>67%</div> </div>
2	Z	9	<div> <div>33%</div> <div>22%</div> <div>11%</div> <div>67%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	1767	-	-	-	X
3	FUC	A	1768	X	-	-	-
5	NAG	A	1772	-	-	-	X
5	NAG	A	1778	-	-	-	X
5	NAG	B	1770	-	-	-	X
5	NAG	B	1771	-	-	-	X
5	NAG	B	1777	-	-	-	X
6	NAG	A	1773	-	-	-	X
6	NAG	B	1772	-	-	-	X
7	NAG	B	1767	-	-	-	X
7	FUC	B	1768	X	-	-	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14100 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	729	Total	C	N	O	S	0	0	0
			5972	3831	983	1132	26			
1	B	729	Total	C	N	O	S	0	0	0
			5972	3831	983	1132	26			

- Molecule 2 is a protein called HIV-1 TAT PROTEIN DERIVED N-TERMINAL NONAPEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	Y	3	Total	C	N	O	S	0	0	0
			23	14	3	5	1			
2	Z	3	Total	C	N	O	S	0	0	0
			23	14	3	5	1			

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



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

- 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	A	2	Total	C	N	O	0	0
			28	16	2	10		
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		

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

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

- 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
			24	14	1	9		

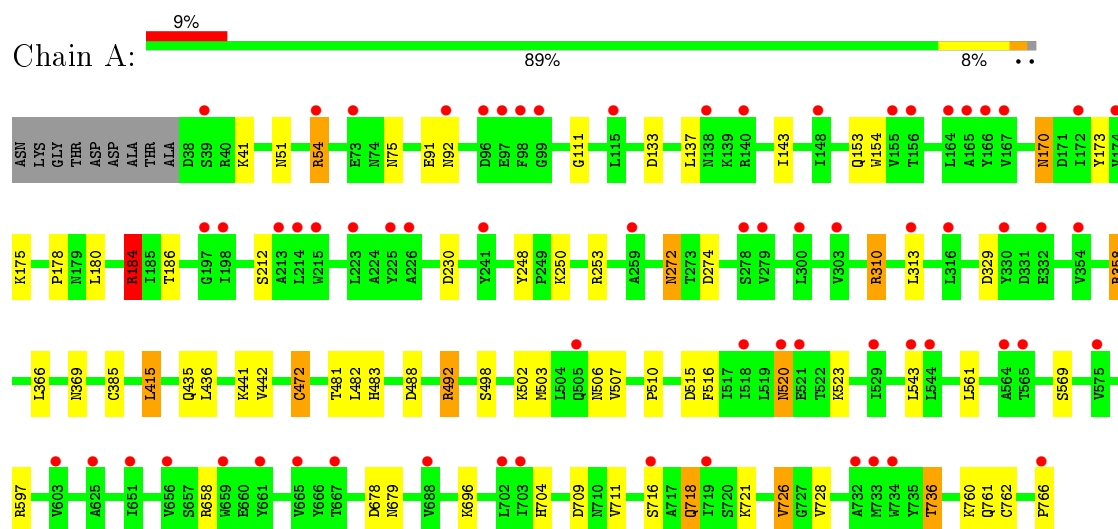
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	892	Total	O	0	0
			892	892		
8	B	845	Total	O	0	0
			845	845		
8	Y	6	Total	O	0	0
			6	6		
8	Z	3	Total	O	0	0
			3	3		

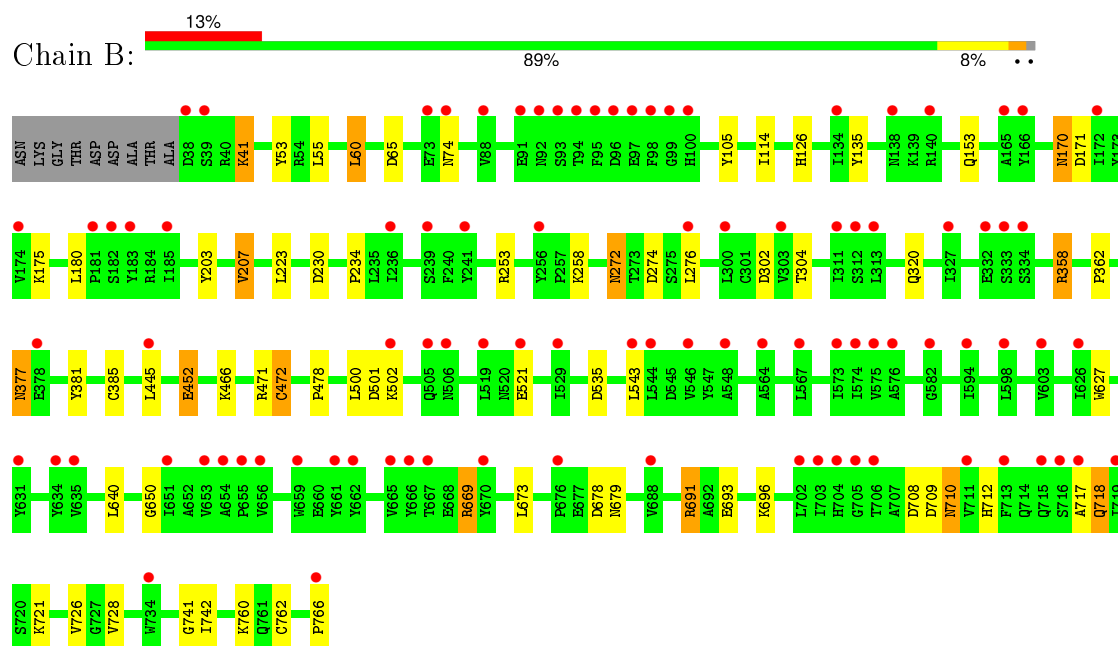
3 Residue-property plots

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.

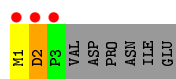
• Molecule 1: DIPEPTIDYL PEPTIDASE IV



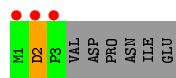
• Molecule 1: DIPEPTIDYL PEPTIDASE IV



• Molecule 2: HIV-1 TAT PROTEIN DERIVED N-TERMINAL NONAPEPTIDE



● Molecule 2: HIV-1 TAT PROTEIN DERIVED N-TERMINAL NONAPEPTIDE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	118.30Å 127.04Å 137.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 29.88 – 2.00	Depositor EDS
% Data completeness (in resolution range)	92.1 (30.00-2.00) 92.1 (29.88-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.1.1999	Depositor
R, R_{free}	0.160 , 0.203 0.170 , 0.211	Depositor DCC
R_{free} test set	1297 reflections (1.02%)	DCC
Wilson B-factor (Å ²)	30.8	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 128767 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14100	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG, 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	0.50	0/6144	0.86	15/8355 (0.2%)
1	B	0.49	0/6144	0.85	13/8355 (0.2%)
2	Y	0.52	0/23	1.51	1/30 (3.3%)
2	Z	0.45	0/23	1.30	0/30
All	All	0.50	0/12334	0.86	29/16770 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0
3	A	1	0
7	B	1	0
All	All	3	0

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	669	ARG	NE-CZ-NH2	-14.38	113.11	120.30
1	B	669	ARG	NE-CZ-NH1	11.74	126.17	120.30
1	A	492	ARG	NE-CZ-NH2	-10.91	114.85	120.30
1	A	658	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	A	658	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	A	515	ASP	CB-CG-OD2	7.92	125.43	118.30
1	A	492	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	A	310	ARG	NE-CZ-NH2	-7.75	116.42	120.30
1	A	184	ARG	NE-CZ-NH1	7.44	124.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	678	ASP	CB-CG-OD2	7.29	124.86	118.30
1	A	415	LEU	CA-CB-CG	7.24	131.95	115.30
1	B	691	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	B	709	ASP	CB-CG-OD2	6.47	124.12	118.30
1	A	133	ASP	CB-CG-OD2	6.42	124.08	118.30
1	A	184	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	678	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	310	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	415	LEU	CB-CG-CD1	5.92	121.07	111.00
1	B	358	ARG	NE-CZ-NH1	5.72	123.16	120.30
2	Y	2	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	709	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	535	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	691	ARG	NE-CZ-NH2	-5.45	117.57	120.30
1	B	501	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	358	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	B	60	LEU	CA-CB-CG	5.22	127.31	115.30
1	B	708	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	488	ASP	CB-CG-OD2	5.16	122.95	118.30
1	B	171	ASP	CB-CG-OD2	5.09	122.88	118.30

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1768	FUC	C1
1	B	304	THR	CB
7	B	1768	FUC	C1

There are no planarity outliers.

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	5972	0	5682	46	0
1	B	5972	0	5682	43	0
2	Y	23	0	22	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	Z	23	0	22	0	0
3	A	38	0	34	0	0
4	A	28	0	26	1	0
4	B	28	0	26	2	0
5	A	84	0	75	0	0
5	B	84	0	75	1	0
6	A	39	0	34	0	0
6	B	39	0	34	0	0
7	B	24	0	22	0	0
8	A	892	0	0	8	0
8	B	845	0	0	11	0
8	Y	6	0	0	1	0
8	Z	3	0	0	0	0
All	All	14100	0	11734	88	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 4.

All (88) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:472:CYS:SG	8:A:2625:HOH:O	2.01	1.15
1:A:762:CYS:HB2	8:A:2874:HOH:O	1.48	1.12
1:B:472:CYS:SG	8:B:2571:HOH:O	2.14	1.06
1:A:503:MET:HG3	8:A:2028:HOH:O	1.76	0.85
1:B:762:CYS:HB2	8:B:2766:HOH:O	1.75	0.85
1:A:310:ARG:HD3	1:A:329:ASP:OD1	1.77	0.84
1:A:736:THR:HG21	1:B:717:ALA:O	1.85	0.75
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.88	0.73
1:B:74:ASN:HD22	4:B:1779:NAG:H81	1.53	0.71
1:B:304:THR:HG22	8:B:2454:HOH:O	1.92	0.70
1:B:762:CYS:CB	8:B:2766:HOH:O	2.36	0.69
1:A:272:ASN:HD22	1:A:274:ASP:H	1.40	0.68
1:A:310:ARG:CD	1:A:329:ASP:OD1	2.43	0.66
1:A:272:ASN:ND2	1:A:274:ASP:H	1.93	0.66
1:A:704:HIS:HD2	1:A:716:SER:OG	1.78	0.66
1:A:173:TYR:CE2	1:A:184:ARG:HG3	2.32	0.65
1:B:760:LYS:HE2	1:B:766:PRO:OXT	1.99	0.62
1:B:272:ASN:HD21	1:B:274:ASP:HB2	1.64	0.62
1:A:153:GLN:HE22	1:A:170:ASN:ND2	1.98	0.62
1:B:258:LYS:NZ	1:B:712:HIS:HD2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:377:ASN:HD22	1:B:377:ASN:C	2.03	0.61
1:A:435:GLN:NE2	1:A:441:LYS:HD2	2.16	0.60
1:B:272:ASN:C	1:B:272:ASN:HD22	2.05	0.60
1:A:184:ARG:HD3	1:A:186:THR:O	2.01	0.60
1:A:760:LYS:CE	1:A:766:PRO:OXT	2.51	0.59
1:A:760:LYS:NZ	1:A:766:PRO:OXT	2.35	0.58
1:A:435:GLN:HE22	1:A:441:LYS:HD2	1.69	0.58
1:A:696:LYS:HG2	1:A:728:VAL:HG22	1.85	0.58
1:B:203:TYR:HA	1:B:207:VAL:HG13	1.86	0.57
2:Y:1:MET:HA	8:Y:2004:HOH:O	2.04	0.57
1:B:65:ASP:OD2	1:B:466:LYS:HB2	2.06	0.56
1:A:272:ASN:HD21	1:A:274:ASP:HB2	1.70	0.56
1:A:111:GLY:O	1:A:137:LEU:HD12	2.05	0.56
1:B:472:CYS:CB	8:B:2571:HOH:O	2.49	0.56
1:A:726:VAL:HG13	1:A:728:VAL:HG23	1.87	0.55
1:A:272:ASN:HD22	1:A:272:ASN:C	2.12	0.54
1:B:276:LEU:O	8:B:2348:HOH:O	2.19	0.53
1:B:302:ASP:OD1	1:B:304:THR:HG23	2.08	0.53
1:B:760:LYS:CE	1:B:766:PRO:OXT	2.58	0.52
1:B:304:THR:HG21	1:B:362:PRO:HD2	1.91	0.51
1:B:452:GLU:H	1:B:452:GLU:CD	2.14	0.51
1:B:691:ARG:HD2	8:B:2752:HOH:O	2.10	0.51
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.91	0.50
1:A:310:ARG:HH22	1:A:369:ASN:ND2	2.09	0.50
1:A:516:PHE:CE2	1:A:523:LYS:HD2	2.47	0.49
1:A:696:LYS:CG	1:A:728:VAL:HG22	2.42	0.48
1:A:762:CYS:CB	8:A:2874:HOH:O	2.30	0.48
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.97	0.48
1:A:92:ASN:ND2	4:A:1780:NAG:C7	2.77	0.48
1:B:693:GLU:OE2	1:B:696:LYS:NZ	2.38	0.47
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.49	0.47
1:A:250:LYS:HD3	8:A:2351:HOH:O	2.14	0.47
1:A:503:MET:HE3	8:A:2650:HOH:O	2.15	0.47
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.97	0.47
1:A:597:ARG:HH12	1:A:679:ASN:HD21	1.62	0.47
1:A:704:HIS:HE1	1:A:711:VAL:O	1.97	0.47
1:B:710:ASN:C	1:B:710:ASN:HD22	2.19	0.46
1:B:170:ASN:ND2	8:B:2190:HOH:O	2.48	0.46
1:A:154:TRP:CE2	1:A:212:SER:HB3	2.50	0.46
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.63	0.46
1:B:258:LYS:HZ1	1:B:712:HIS:HD2	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LYS:NZ	1:A:180:LEU:O	2.47	0.46
1:B:377:ASN:ND2	1:B:381:TYR:H	2.14	0.45
1:B:175:LYS:NZ	1:B:180:LEU:O	2.49	0.45
1:B:74:ASN:ND2	4:B:1779:NAG:H81	2.28	0.45
1:B:126:HIS:HD2	8:B:2057:HOH:O	1.98	0.45
1:B:153:GLN:HE22	1:B:170:ASN:ND2	2.15	0.44
1:A:520:ASN:OD1	1:A:520:ASN:O	2.36	0.44
1:B:41:LYS:HE3	1:B:53:TYR:OH	2.17	0.44
1:B:55:LEU:HD23	1:B:500:LEU:CD2	2.48	0.44
1:A:704:HIS:CD2	1:A:716:SER:OG	2.66	0.43
5:B:1778:NAG:O7	8:B:2844:HOH:O	2.21	0.43
1:B:105:TYR:HB2	1:B:114:ILE:HD11	2.00	0.43
1:B:114:ILE:HG23	1:B:135:TYR:HB3	2.00	0.43
1:B:718:GLN:HE22	1:B:721:LYS:NZ	2.17	0.42
1:B:272:ASN:HD22	1:B:274:ASP:H	1.67	0.42
1:A:51:ASN:HB3	8:A:2017:HOH:O	2.20	0.42
1:A:718:GLN:HE22	1:A:721:LYS:NZ	2.17	0.42
1:B:472:CYS:CA	8:B:2571:HOH:O	2.67	0.42
1:A:510:PRO:HD3	1:A:569:SER:HB2	2.01	0.42
1:B:741:GLY:O	1:B:742:ILE:C	2.57	0.42
1:A:75:ASN:ND2	1:A:92:ASN:H	2.17	0.41
1:A:143:ILE:HD13	1:A:178:PRO:HB2	2.03	0.41
1:A:54:ARG:HE	1:A:54:ARG:HB2	1.69	0.41
1:A:170:ASN:N	1:A:170:ASN:HD22	2.19	0.41
1:A:498:SER:O	1:A:502:LYS:HG2	2.21	0.41
1:B:472:CYS:O	1:B:478:PRO:HA	2.21	0.40
1:A:358:ARG:HD3	8:A:2100:HOH:O	2.21	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	727/738 (98%)	702 (97%)	24 (3%)	1 (0%)	56	53
1	B	727/738 (98%)	703 (97%)	24 (3%)	0	100	100
2	Y	1/9 (11%)	1 (100%)	0	0	100	100
2	Z	1/9 (11%)	0	0	1 (100%)	0	0
All	All	1456/1494 (98%)	1406 (97%)	48 (3%)	2 (0%)	56	53

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	520	ASN
2	Z	2	ASP

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	654/660 (99%)	629 (96%)	25 (4%)	40	36
1	B	654/660 (99%)	632 (97%)	22 (3%)	44	41
2	Y	3/9 (33%)	2 (67%)	1 (33%)	0	0
2	Z	3/9 (33%)	2 (67%)	1 (33%)	0	0
All	All	1314/1338 (98%)	1265 (96%)	49 (4%)	41	38

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	LYS
1	A	54	ARG
1	A	91	GLU
1	A	170	ASN
1	A	184	ARG
1	A	230	ASP
1	A	272	ASN
1	A	313	LEU
1	A	358	ARG

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Mol	Chain	Res	Type
1	A	366	LEU
1	A	385	CYS
1	A	415	LEU
1	A	436	LEU
1	A	442	VAL
1	A	472	CYS
1	A	482	LEU
1	A	492	ARG
1	A	506	ASN
1	A	507	VAL
1	A	543	LEU
1	A	561	LEU
1	A	718	GLN
1	A	726	VAL
1	A	736	THR
1	A	761	GLN
1	B	41	LYS
1	B	60	LEU
1	B	170	ASN
1	B	207	VAL
1	B	223	LEU
1	B	230	ASP
1	B	272	ASN
1	B	358	ARG
1	B	377	ASN
1	B	385	CYS
1	B	445	LEU
1	B	452	GLU
1	B	471	ARG
1	B	472	CYS
1	B	502	LYS
1	B	521	GLU
1	B	543	LEU
1	B	627	TRP
1	B	673	LEU
1	B	679	ASN
1	B	710	ASN
1	B	718	GLN
2	Y	2	ASP
2	Z	2	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	169	ASN
1	A	170	ASN
1	A	247	GLN
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	572	ASN
1	A	586	GLN
1	A	679	ASN
1	A	685	ASN
1	A	694	ASN
1	A	704	HIS
1	A	718	GLN
1	A	761	GLN
1	B	112	GLN
1	B	126	HIS
1	B	169	ASN
1	B	170	ASN
1	B	247	GLN
1	B	272	ASN
1	B	314	GLN
1	B	345	HIS
1	B	377	ASN
1	B	435	GLN
1	B	572	ASN
1	B	606	GLN
1	B	679	ASN
1	B	694	ASN
1	B	710	ASN
1	B	712	HIS
1	B	718	GLN
1	B	731	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 ⓘ

23 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	$\# Z > 2$
3	NAG	A	1767	1,3	14,14,15	0.75	0	15,19,21	1.39	3 (20%)
3	FUC	A	1768	3	10,10,11	0.59	0	14,14,16	1.61	2 (14%)
3	NAG	A	1769	3	14,14,15	0.56	0	15,19,21	1.46	3 (20%)
5	NAG	A	1771	1,5	14,14,15	0.63	0	15,19,21	1.25	1 (6%)
5	NAG	A	1772	5	14,14,15	0.43	0	15,19,21	1.56	2 (13%)
6	NAG	A	1773	1,6	14,14,15	0.72	0	15,19,21	0.91	0
6	NAG	A	1774	6	14,14,15	0.56	0	15,19,21	1.26	3 (20%)
6	BMA	A	1775	6	11,11,12	0.66	0	14,15,17	1.46	3 (21%)
5	NAG	A	1776	1,5	14,14,15	0.59	0	15,19,21	1.79	2 (13%)
5	NAG	A	1777	5	14,14,15	0.48	0	15,19,21	1.18	2 (13%)
5	NAG	A	1778	1,5	14,14,15	0.59	0	15,19,21	1.13	2 (13%)
5	NAG	A	1779	5	14,14,15	0.47	0	15,19,21	1.70	3 (20%)
7	NAG	B	1767	1,7	14,14,15	0.61	0	15,19,21	1.09	1 (6%)
7	FUC	B	1768	7	10,10,11	0.60	0	14,14,16	1.02	1 (7%)
5	NAG	B	1770	1,5	14,14,15	0.42	0	15,19,21	1.09	0
5	NAG	B	1771	5	14,14,15	0.61	0	15,19,21	1.67	3 (20%)
6	NAG	B	1772	1,6	14,14,15	0.50	0	15,19,21	1.18	0
6	NAG	B	1773	6	14,14,15	0.54	0	15,19,21	0.99	0
6	BMA	B	1774	6	11,11,12	0.59	0	14,15,17	1.02	0
5	NAG	B	1775	1,5	14,14,15	0.59	0	15,19,21	1.00	0
5	NAG	B	1776	5	14,14,15	0.54	0	15,19,21	1.11	1 (6%)
5	NAG	B	1777	1,5	14,14,15	0.56	0	15,19,21	1.22	2 (13%)
5	NAG	B	1778	5	14,14,15	0.62	0	15,19,21	1.31	2 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1767	1,3	-	0/6/23/26	0/1/1/1
3	FUC	A	1768	3	1/1/4/5	0/0/17/20	0/1/1/1
3	NAG	A	1769	3	-	0/6/23/26	0/1/1/1
5	NAG	A	1771	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1772	5	-	0/6/23/26	0/1/1/1
6	NAG	A	1773	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1774	6	-	0/6/23/26	0/1/1/1
6	BMA	A	1775	6	-	0/2/19/22	0/1/1/1
5	NAG	A	1776	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1777	5	-	0/6/23/26	0/1/1/1
5	NAG	A	1778	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1779	5	-	0/6/23/26	0/1/1/1
7	NAG	B	1767	1,7	-	0/6/23/26	0/1/1/1
7	FUC	B	1768	7	1/1/4/5	0/0/17/20	0/1/1/1
5	NAG	B	1770	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1771	5	-	0/6/23/26	0/1/1/1
6	NAG	B	1772	1,6	-	0/6/23/26	0/1/1/1
6	NAG	B	1773	6	-	0/6/23/26	0/1/1/1
6	BMA	B	1774	6	-	0/2/19/22	0/1/1/1
5	NAG	B	1775	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1776	5	-	0/6/23/26	0/1/1/1
5	NAG	B	1777	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	1778	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1779	NAG	C4-C3-C2	-3.64	105.58	111.23
3	A	1769	NAG	C2-N2-C7	-2.84	119.39	123.04
5	A	1776	NAG	O4-C4-C3	-2.39	104.95	110.34
6	A	1774	NAG	O7-C7-C8	-2.35	117.75	122.06
5	A	1772	NAG	C2-N2-C7	-2.22	120.19	123.04
5	B	1777	NAG	O7-C7-C8	-2.20	118.02	122.06
3	A	1767	NAG	O4-C4-C5	-2.20	103.40	109.24
7	B	1767	NAG	O7-C7-C8	-2.04	118.32	122.06
6	A	1774	NAG	C4-C3-C2	-2.01	108.11	111.23
3	A	1767	NAG	O6-C6-C5	-2.01	104.70	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1771	NAG	C4-C3-C2	2.01	114.35	111.23
5	A	1778	NAG	O7-C7-N2	2.11	126.16	121.86
5	B	1771	NAG	C1-O5-C5	2.12	114.94	112.25
5	A	1779	NAG	C3-C2-N2	2.25	115.96	110.56
7	B	1768	FUC	O5-C5-C6	2.37	110.04	106.13
5	A	1778	NAG	C1-O5-C5	2.46	115.38	112.25
5	A	1777	NAG	C2-N2-C7	2.47	126.21	123.04
6	A	1775	BMA	C3-C4-C5	2.50	114.56	110.20
3	A	1768	FUC	C1-O5-C5	2.51	116.25	112.38
5	B	1778	NAG	C4-C3-C2	2.53	115.17	111.23
3	A	1769	NAG	C1-O5-C5	2.55	115.49	112.25
6	A	1774	NAG	C8-C7-N2	2.94	121.73	116.11
5	B	1777	NAG	C1-O5-C5	2.96	116.01	112.25
6	A	1775	BMA	C2-C3-C4	2.97	116.09	111.04
5	A	1777	NAG	C3-C2-N2	2.97	117.68	110.56
5	B	1776	NAG	C1-O5-C5	3.31	116.45	112.25
6	A	1775	BMA	C1-C2-C3	3.32	113.47	109.54
3	A	1767	NAG	C1-O5-C5	3.34	116.48	112.25
3	A	1769	NAG	C3-C4-C5	3.46	116.22	110.20
5	B	1771	NAG	C3-C4-C5	3.55	116.38	110.20
5	B	1778	NAG	C2-N2-C7	3.78	127.89	123.04
5	A	1779	NAG	C1-O5-C5	4.07	117.41	112.25
3	A	1768	FUC	O5-C5-C6	4.17	113.03	106.13
5	B	1771	NAG	C4-C3-C2	4.21	117.77	111.23
5	A	1772	NAG	C1-O5-C5	4.77	118.30	112.25
5	A	1776	NAG	C1-O5-C5	5.38	119.08	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1768	FUC	C1
7	B	1768	FUC	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1778	NAG	1	0

5.6 Ligand geometry

4 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$
4	NAG	A	1770	1	14,14,15	0.43	0	15,19,21	1.13	1 (6%)
4	NAG	A	1780	1	14,14,15	0.51	0	15,19,21	1.72	4 (26%)
4	NAG	B	1769	1	14,14,15	0.47	0	15,19,21	0.89	0
4	NAG	B	1779	1	14,14,15	0.46	0	15,19,21	1.30	2 (13%)

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	1770	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1780	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1769	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1779	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1780	NAG	C4-C3-C2	-3.89	105.18	111.23
4	A	1780	NAG	C3-C4-C5	-2.55	105.76	110.20
4	A	1780	NAG	O5-C5-C6	2.10	111.90	107.35
4	B	1779	NAG	C3-C4-C5	2.40	114.39	110.20
4	A	1770	NAG	C1-O5-C5	2.73	115.72	112.25
4	A	1780	NAG	C1-O5-C5	2.74	115.73	112.25
4	B	1779	NAG	C1-O5-C5	3.31	116.45	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1780	NAG	1	0
4	B	1779	NAG	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	729/738 (98%)	0.73	66 (9%) 11 12	35, 44, 55, 66	0
1	B	729/738 (98%)	0.79	93 (12%) 5 5	36, 44, 55, 70	0
2	Y	3/9 (33%)	5.00	3 (100%) 0 0	65, 65, 69, 72	0
2	Z	3/9 (33%)	7.43	3 (100%) 0 0	75, 75, 78, 79	0
All	All	1464/1494 (97%)	0.78	165 (11%) 7 7	35, 44, 55, 79	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Z	3	PRO	11.9
2	Z	2	ASP	7.5
2	Y	3	PRO	6.7
1	B	766	PRO	6.3
2	Y	2	ASP	5.6
1	A	766	PRO	5.4
1	B	97	GLU	5.0
1	A	279	VAL	4.8
1	B	95	PHE	4.7
1	B	96	ASP	4.6
1	B	73	GLU	4.6
1	A	140	ARG	4.5
1	B	575	VAL	4.4
1	A	97	GLU	4.3
1	B	138	ASN	4.3
1	A	155	VAL	4.1
1	B	713	PHE	4.1
1	B	39	SER	4.1
1	B	172	ILE	4.0
1	B	93	SER	4.0
1	A	165	ALA	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	140	ARG	3.8
1	A	734	TRP	3.8
1	B	656	VAL	3.7
1	B	543	LEU	3.7
1	A	543	LEU	3.6
1	A	167	VAL	3.6
1	B	74	ASN	3.6
1	B	529	ILE	3.6
1	B	185	ILE	3.5
1	A	214	LEU	3.5
1	B	706	THR	3.4
1	A	164	LEU	3.4
1	B	38	ASP	3.4
1	B	300	LEU	3.3
1	B	635	VAL	3.3
1	B	332	GLU	3.3
1	A	300	LEU	3.2
1	A	166	TYR	3.2
1	B	716	SER	3.1
1	B	546	VAL	3.1
1	B	719	ILE	3.1
1	B	333	SER	3.1
1	B	702	LEU	3.1
1	A	564	ALA	3.1
1	A	115	LEU	3.1
1	A	148	ILE	3.1
1	A	529	ILE	3.1
1	A	172	ILE	3.0
1	B	564	ALA	3.0
1	A	223	LEU	3.0
1	B	717	ALA	3.0
1	B	311	ILE	3.0
1	B	574	ILE	3.0
1	B	567	LEU	3.0
2	Z	1	MET	3.0
1	B	573	ILE	2.9
1	B	665	VAL	2.9
1	A	92	ASN	2.9
1	B	734	TRP	2.9
1	B	92	ASN	2.9
1	A	702	LEU	2.9
1	B	445	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	659	TRP	2.9
1	B	313	LEU	2.8
1	A	656	VAL	2.8
1	B	659	TRP	2.8
1	A	278	SER	2.8
1	B	91	GLU	2.8
1	B	576	ALA	2.8
1	A	99	GLY	2.8
1	B	99	GLY	2.8
1	B	667	THR	2.8
1	B	715	GLN	2.8
1	B	378	GLU	2.8
1	B	174	VAL	2.8
1	A	226	ALA	2.7
1	B	711	VAL	2.7
2	Y	1	MET	2.7
1	A	332	GLU	2.7
1	A	575	VAL	2.7
1	B	506	ASN	2.7
1	A	521	GLU	2.7
1	A	138	ASN	2.6
1	A	198	ILE	2.6
1	A	651	ILE	2.6
1	B	603	VAL	2.6
1	B	505	GLN	2.6
1	A	316	LEU	2.6
1	B	312	SER	2.5
1	A	716	SER	2.5
1	A	156	THR	2.5
1	B	100	HIS	2.5
1	A	96	ASP	2.5
1	B	594	ILE	2.5
1	B	666	TYR	2.5
1	A	544	LEU	2.5
1	A	39	SER	2.5
1	B	521	GLU	2.5
1	A	225	TYR	2.5
1	B	544	LEU	2.5
1	A	303	VAL	2.5
1	B	236	ILE	2.5
1	B	327	ILE	2.5
1	A	215	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	631	TYR	2.4
1	B	334	SER	2.4
1	B	582	GLY	2.4
1	B	676	PRO	2.4
1	B	634	TYR	2.4
1	B	653	VAL	2.4
1	A	98	PHE	2.4
1	B	662	TYR	2.4
1	A	213	ALA	2.3
1	A	732	ALA	2.3
1	B	181	PRO	2.3
1	A	703	ILE	2.3
1	A	719	ILE	2.3
1	B	654	ALA	2.3
1	B	134	ILE	2.3
1	A	667	THR	2.3
1	B	548	ALA	2.3
1	B	598	LEU	2.3
1	A	733	MET	2.3
1	A	505	GLN	2.3
1	A	174	VAL	2.3
1	B	655	PRO	2.3
1	B	276	LEU	2.3
1	A	54	ARG	2.2
1	A	518	ILE	2.2
1	B	241	TYR	2.2
1	B	502	LYS	2.2
1	B	703	ILE	2.2
1	A	197	GLY	2.2
1	B	519	LEU	2.2
1	B	183	TYR	2.2
1	A	565	THR	2.2
1	B	88	VAL	2.2
1	B	182	SER	2.2
1	A	313	LEU	2.2
1	A	520	ASN	2.2
1	A	241	TYR	2.2
1	B	98	PHE	2.2
1	B	166	TYR	2.2
1	A	603	VAL	2.2
1	A	73	GLU	2.2
1	A	688	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	661	TYR	2.1
1	B	661	TYR	2.1
1	A	354	VAL	2.1
1	A	330	TYR	2.1
1	B	670	TYR	2.1
1	A	665	VAL	2.1
1	B	94	THR	2.1
1	B	704	HIS	2.1
1	B	303	VAL	2.1
1	B	651	ILE	2.1
1	B	256	TYR	2.1
1	B	688	VAL	2.1
1	B	626	ILE	2.1
1	B	239	SER	2.1
1	A	259	ALA	2.0
1	A	625	ALA	2.0
1	B	165	ALA	2.0
1	B	705	GLY	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
5	NAG	B	1770	14/15	0.89	0.35	7.74	46,54,57,59	0
5	NAG	A	1778	14/15	0.89	0.37	7.73	47,52,56,59	0
7	NAG	B	1767	14/15	0.84	0.25	6.24	51,57,64,68	0
3	NAG	A	1767	14/15	0.92	0.29	5.49	43,52,64,65	0
5	NAG	B	1777	14/15	0.85	0.30	4.63	50,54,57,61	0
5	NAG	B	1771	14/15	0.80	0.45	3.02	61,64,66,67	0
5	NAG	A	1772	14/15	0.75	0.42	2.92	61,66,69,70	0
6	NAG	A	1773	14/15	0.91	0.24	2.65	43,47,57,59	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	B	1772	14/15	0.94	0.25	2.61	32,36,44,49	0
5	NAG	B	1775	14/15	0.94	0.12	-1.36	29,32,37,39	0
6	NAG	B	1773	14/15	0.86	0.46	-	54,56,61,66	0
5	NAG	A	1771	14/15	0.82	0.33	-	49,56,64,65	0
5	NAG	A	1779	14/15	0.65	0.51	-	63,67,68,69	0
6	NAG	A	1774	14/15	0.81	0.40	-	62,66,72,77	0
5	NAG	B	1776	14/15	0.86	0.31	-	40,46,50,51	0
6	BMA	A	1775	11/12	0.52	0.54	-	81,83,85,86	0
5	NAG	B	1778	14/15	0.75	0.53	-	65,68,70,70	0
5	NAG	A	1777	14/15	0.62	0.56	-	77,80,81,82	0
3	FUC	A	1768	10/11	0.80	0.26	-	64,65,65,67	0
3	NAG	A	1769	14/15	0.76	0.56	-	72,76,78,78	0
5	NAG	A	1776	14/15	0.81	0.32	-	60,63,67,72	0
6	BMA	B	1774	11/12	0.87	0.41	-	69,72,73,74	0
7	FUC	B	1768	10/11	0.85	0.35	-	70,72,72,74	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(\AA^2)	Q<0.9
4	NAG	B	1769	14/15	0.80	0.47	-	59,63,66,67	0
4	NAG	A	1770	14/15	0.73	0.45	-	58,60,61,63	0
4	NAG	A	1780	14/15	0.78	0.42	-	72,75,76,77	0
4	NAG	B	1779	14/15	0.83	0.47	-	72,73,76,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.