Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:44 AM GMT

PDB ID	:	2ID5
Title	:	Crystal Structure of the Lingo-1 Ectodomain
Authors	:	Mosyak, L.; Wood, A.; Dwyer, B.; Johnson, M.; Stahl, M.L.; Somers, W.S.
Deposited on	:	2006-09-14
Resolution	:	2.70 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:

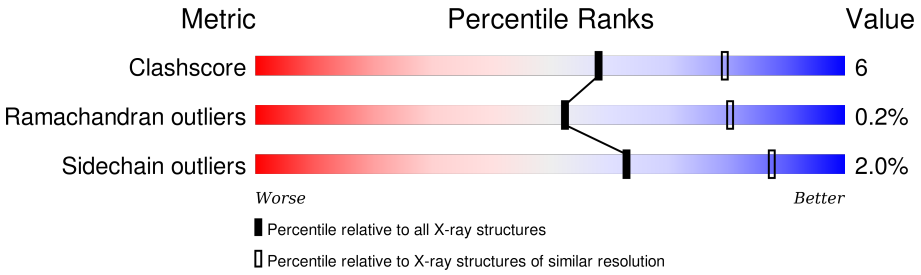
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.70 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	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)

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 <=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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	477	82% 17%
1	B	477	81% 19%
1	C	477	86% 12%
1	D	477	83% 15%

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
2	MAN	A	480	X	-	-	-
2	MAN	A	483	X	-	-	-
2	MAN	A	490	X	-	-	-
2	MAN	B	484	X	-	-	-
2	MAN	B	491	X	-	-	-
2	MAN	C	480	X	-	-	-
2	MAN	C	483	X	-	-	-
2	MAN	C	490	X	-	-	-
3	NAG	B	485	X	-	-	-
3	NAG	C	485	X	-	-	-
4	NAG	A	486	X	-	-	-
4	NAG	A	487	X	-	-	-
5	MAN	B	480	X	-	-	-
5	MAN	D	480	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16119 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.

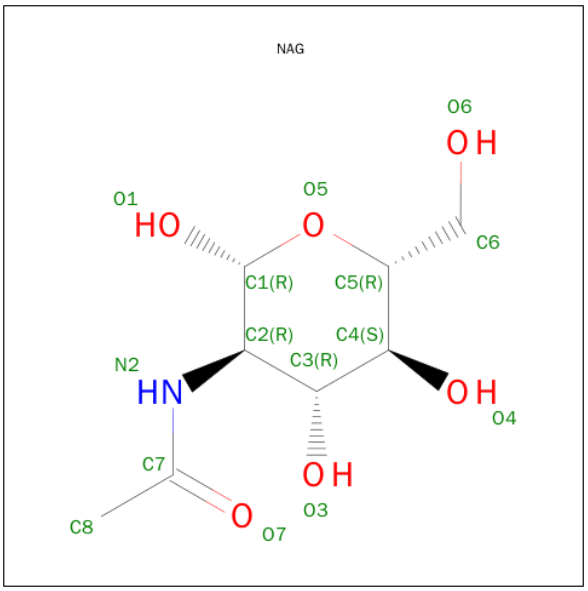
- Molecule 1 is a protein called Leucine rich repeat neuronal 6A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	470	Total	C	N	O	S	0	0	0
			3769	2402	671	679	17			
1	B	473	Total	C	N	O	S	0	0	0
			3790	2414	676	683	17			
1	C	472	Total	C	N	O	S	0	0	0
			3785	2410	677	681	17			
1	D	471	Total	C	N	O	S	0	0	0
			3778	2407	677	677	17			

- 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
			39	22	2	15		
2	A	3	Total	C	N	O	0	0
			39	22	2	15		
2	A	3	Total	C	N	O	0	0
			39	22	2	15		
2	B	3	Total	C	N	O	0	0
			39	22	2	15		
2	B	3	Total	C	N	O	0	0
			39	22	2	15		
2	C	3	Total	C	N	O	0	0
			39	22	2	15		
2	C	3	Total	C	N	O	0	0
			39	22	2	15		
2	C	3	Total	C	N	O	0	0
			39	22	2	15		
2	D	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 5 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	4	Total	C	N	O	0	0
			50	28	2	20		
5	D	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	81	Total	O	0	0
			81	81		
6	B	102	Total	O	0	0
			102	102		
6	C	66	Total	O	0	0
			66	66		
6	D	59	Total	O	0	0
			59	59		

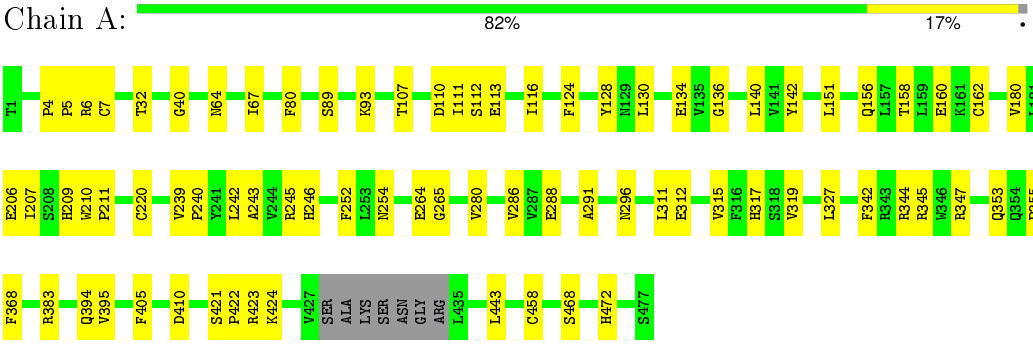
3 Residue-property plots (i)

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.

Note EDS was not executed.

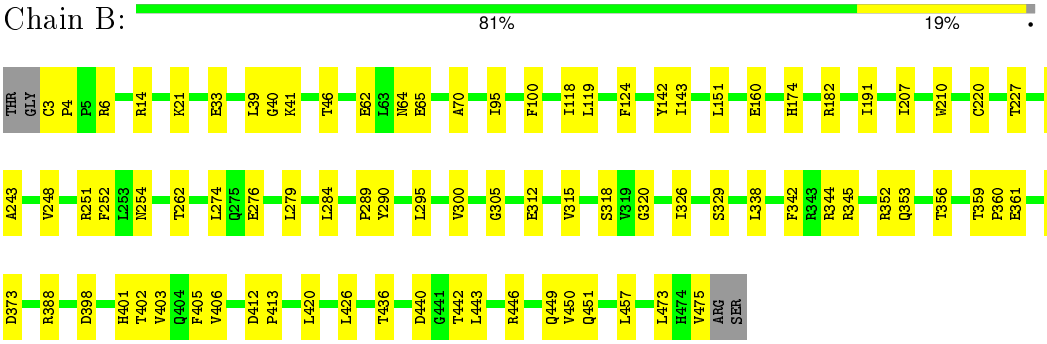
- Molecule 1: Leucine rich repeat neuronal 6A

Chain A:



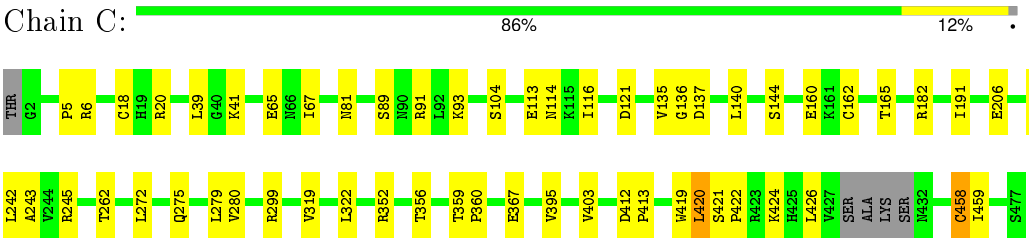
- Molecule 1: Leucine rich repeat neuronal 6A

Chain B:



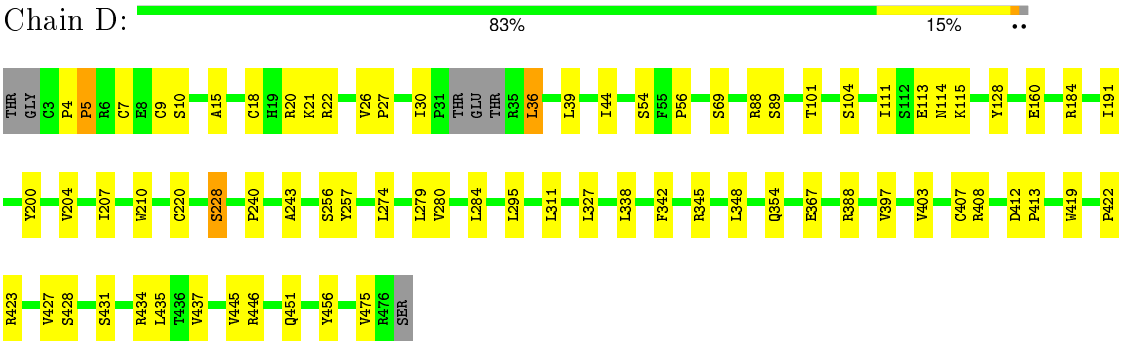
- Molecule 1: Leucine rich repeat neuronal 6A

Chain C:



- Molecule 1: Leucine rich repeat neuronal 6A

Chain D:


83%
15%
THR GLY C3 P4 P5 R6 C7 E8 C9 S10 A15 C18 H19 R20 K21 R22 V26 P27 I30 P31 THR GLU THR R35 L36 L39 I44 S54 F55 P56 S69 R88 S89 T101 S104 I111 S112 E113 N114 K115 Y128 E160 R184 I191
Y200 V204 I207 W210 C220 S228 P240 A243 S256 Y257 L274 L279 V280 L284 L295 L311 L327 L338 F342 R345 L348 Q354 E367 R388 V397 V403 C407 R408 D412 P413 W419 P422
R423 V427 S428 S431 R434 L435 T436 V437 V445 R446 Q451 Y456 V475 R476 SER

4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	201.52Å 149.72Å 157.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	158.11 – 2.70	Depositor
% Data completeness (in resolution range)	98.7 (158.11-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
Refinement program	REFMAC 5.2	Depositor
R, R_{free}	0.214 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16119	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.48	0/3850	0.62	0/5233
1	B	0.48	0/3872	0.59	0/5263
1	C	0.43	0/3866	0.58	0/5253
1	D	0.42	0/3859	0.57	0/5242
All	All	0.45	0/15447	0.59	0/20991

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	0	1
2	A	3	0
2	B	2	0
2	C	3	0
4	A	2	0
5	B	1	0
5	D	1	0
All	All	12	1

There are no bond length outliers.

There are no bond angle outliers.

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	480	MAN	C1
2	A	483	MAN	C1
4	A	486	NAG	C1
4	A	487	NAG	C1

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Mol	Chain	Res	Type	Atom
2	A	490	MAN	C1
5	B	480	MAN	C5
2	B	484	MAN	C1
2	B	491	MAN	C1
2	C	480	MAN	C1
2	C	483	MAN	C1
2	C	490	MAN	C1
5	D	480	MAN	C1

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	344	ARG	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3769	0	3787	47	0
1	B	3790	0	3807	58	0
1	C	3785	0	3797	42	0
1	D	3778	0	3801	41	0
2	A	117	0	102	1	0
2	B	78	0	68	2	0
2	C	117	0	102	2	0
2	D	39	0	34	0	0
3	A	42	0	39	1	0
3	B	56	0	52	0	0
3	C	56	0	52	2	0
3	D	28	0	26	0	0
4	A	28	0	25	0	0
4	D	28	0	25	0	0
5	B	50	0	43	1	0
5	D	50	0	43	1	0
6	A	81	0	0	0	0
6	B	102	0	0	5	0
6	C	66	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	59	0	0	0	0
All	All	16119	0	15803	186	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 6.

All (186) 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:C:352:ARG:HH12	2:C:483:MAN:H3	1.24	0.97
1:C:41:LYS:HE3	1:C:65:GLU:OE1	1.74	0.86
1:B:276:GLU:HG2	1:B:300:VAL:HB	1.58	0.85
1:B:356:THR:HG22	1:B:367:GLU:HG2	1.60	0.82
1:B:46:THR:HG22	1:B:70:ALA:HB3	1.60	0.81
1:C:395:VAL:HG11	1:C:403:VAL:CG2	2.11	0.81
1:B:62:GLU:HG3	1:B:64:ASN:ND2	1.96	0.81
1:A:245:ARG:HH21	1:A:246:HIS:CD2	1.99	0.81
1:A:245:ARG:NH2	1:A:246:HIS:NE2	2.29	0.80
1:B:3:CYS:HB2	1:B:4:PRO:HD2	1.65	0.78
1:C:420:LEU:HD13	1:C:459:ILE:HD11	1.67	0.76
1:C:395:VAL:HG11	1:C:403:VAL:HG21	1.66	0.76
1:A:245:ARG:NH2	1:A:246:HIS:CD2	2.53	0.76
1:B:352:ARG:NH1	2:B:484:MAN:H5	2.03	0.74
1:C:412:ASP:OD1	1:C:413:PRO:HA	1.88	0.73
1:A:242:LEU:O	1:A:245:ARG:HG2	1.90	0.72
1:B:352:ARG:HH12	2:B:484:MAN:H5	1.54	0.71
1:B:174:HIS:HE1	6:B:508:HOH:O	1.73	0.71
1:B:227:THR:HG21	1:B:251:ARG:HH21	1.54	0.70
1:B:342:PHE:O	1:B:345:ARG:HB3	1.92	0.70
1:A:383:ARG:HH12	1:A:410:ASP:HB3	1.55	0.69
1:B:191:ILE:HG22	1:B:220:CYS:HB2	1.75	0.69
1:C:395:VAL:CG1	1:C:403:VAL:HG21	2.24	0.68
1:B:356:THR:CG2	1:B:367:GLU:HG2	2.25	0.67
1:A:191:ILE:HG22	1:A:220:CYS:HB2	1.78	0.65
1:B:356:THR:HG22	1:B:367:GLU:CG	2.25	0.65
1:C:20:ARG:HE	1:C:41:LYS:HD3	1.61	0.65
1:C:191:ILE:HG22	1:C:220:CYS:HB2	1.80	0.65
5:B:479:NAG:H3	6:B:515:HOH:O	1.96	0.64
1:B:62:GLU:HG3	1:B:64:ASN:HD21	1.64	0.62
1:A:296:ASN:OD1	1:A:317:HIS:CD2	2.53	0.62
1:B:239:VAL:HG13	1:B:240:PRO:HD2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:423:ARG:NH1	1:D:451:GLN:OE1	2.35	0.59
1:B:3:CYS:CB	1:B:4:PRO:HD2	2.33	0.59
1:A:182:ARG:HG2	1:A:206:GLU:HB3	1.83	0.59
1:A:142:TYR:HE2	1:B:426:LEU:HD22	1.67	0.59
1:A:142:TYR:CE2	1:B:426:LEU:HD22	2.38	0.58
1:C:239:VAL:HG13	1:C:240:PRO:HD2	1.85	0.58
1:C:352:ARG:NH1	2:C:483:MAN:H3	2.08	0.58
1:D:240:PRO:HB2	1:D:243:ALA:HB3	1.85	0.58
1:C:121:ASP:OD1	1:C:144:SER:HB3	2.02	0.58
1:B:14:ARG:HE	1:B:33:GLU:HB2	1.68	0.58
1:B:207:ILE:HG23	1:B:210:TRP:CE2	2.39	0.58
1:B:46:THR:CG2	1:B:70:ALA:HB3	2.31	0.57
1:C:41:LYS:CE	1:C:65:GLU:OE1	2.48	0.57
1:D:397:VAL:HB	1:D:403:VAL:HG21	1.86	0.57
1:D:397:VAL:CG2	1:D:403:VAL:HG21	2.36	0.56
1:B:124:PHE:HB3	1:B:151:LEU:HD21	1.88	0.56
1:C:421:SER:HB2	1:C:422:PRO:HD2	1.87	0.55
1:A:134:GLU:HG2	1:A:158:THR:HB	1.87	0.55
1:B:240:PRO:HB2	1:B:243:ALA:HB3	1.89	0.54
1:B:345:ARG:NH1	1:B:373:ASP:OD1	2.41	0.54
1:D:10:SER:HB3	1:D:15:ALA:HB3	1.89	0.54
1:D:397:VAL:CG2	1:D:403:VAL:CG2	2.86	0.53
1:C:240:PRO:HB2	1:C:243:ALA:HB3	1.90	0.53
1:C:140:LEU:HD23	1:C:162:CYS:SG	2.49	0.53
1:D:354:GLN:HG2	1:D:367:GLU:HB3	1.90	0.53
1:A:355:PRO:HG2	1:A:368:PHE:CG	2.44	0.53
1:D:15:ALA:HA	1:D:36:LEU:HB3	1.92	0.52
1:D:428:SER:H	1:D:431:SER:HB2	1.74	0.52
1:A:458:CYS:O	1:A:468:SER:HA	2.10	0.52
1:B:406:VAL:HA	1:B:442:THR:HG22	1.91	0.52
1:D:54:SER:C	1:D:56:PRO:HD3	2.30	0.51
1:D:427:VAL:HG12	1:D:437:VAL:HG23	1.92	0.51
1:A:136:GLY:HA3	1:A:160:GLU:O	2.11	0.51
1:C:67:ILE:HG12	1:C:91:ARG:HG3	1.93	0.51
1:D:279:LEU:HD13	1:D:284:LEU:HD11	1.93	0.51
1:D:434:ARG:HB2	1:D:446:ARG:HB3	1.92	0.51
1:C:356:THR:HG22	1:C:367:GLU:HG2	1.92	0.51
1:B:262:THR:HG22	6:B:513:HOH:O	2.11	0.51
1:A:5:PRO:O	1:A:6:ARG:HB2	2.10	0.51
1:A:89:SER:HA	1:A:113:GLU:O	2.11	0.50
1:C:420:LEU:HD23	1:C:424:LYS:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:PHE:CE2	1:B:254:ASN:HB2	2.46	0.50
1:C:104:SER:HB2	3:C:484:NAG:H83	1.94	0.50
1:B:359:THR:HB	1:B:360:PRO:HA	1.93	0.50
1:D:20:ARG:HH22	1:D:22:ARG:HH11	1.60	0.50
1:A:359:THR:HB	1:A:360:PRO:HA	1.94	0.50
1:B:40:GLY:HA2	1:B:64:ASN:O	2.12	0.49
1:B:450:VAL:HA	1:B:475:VAL:HG11	1.94	0.49
1:D:388:ARG:NH1	1:D:408:ARG:HD3	2.26	0.49
1:B:402:THR:HG23	1:B:446:ARG:HA	1.95	0.49
1:A:239:VAL:HG13	1:A:240:PRO:HD2	1.95	0.49
1:C:182:ARG:HG2	1:C:206:GLU:HB3	1.95	0.49
1:A:264:GLU:HA	1:A:288:GLU:HG3	1.95	0.49
1:C:114:ASN:N	1:C:137:ASP:OD1	2.44	0.48
1:A:405:PHE:HD2	1:A:443:LEU:HD23	1.78	0.48
1:C:136:GLY:HA3	1:C:160:GLU:O	2.13	0.48
1:B:95:ILE:HG21	1:B:100:PHE:CE2	2.48	0.48
1:B:312:GLU:O	1:B:315:VAL:HG13	2.13	0.48
1:A:124:PHE:HB3	1:A:151:LEU:HD21	1.95	0.48
1:D:7:CYS:HA	1:D:21:LYS:HE3	1.96	0.48
1:C:89:SER:HA	1:C:113:GLU:O	2.13	0.48
1:B:305:GLY:HA2	1:B:329:SER:HB2	1.94	0.48
1:B:449:GLN:HG3	1:B:451:GLN:HB2	1.96	0.48
1:A:107:THR:HA	1:A:130:LEU:HA	1.96	0.47
1:D:89:SER:HA	1:D:113:GLU:O	2.15	0.47
1:B:326:ILE:HG23	1:B:353:GLN:HB3	1.96	0.47
1:A:421:SER:HB2	1:A:422:PRO:HD2	1.97	0.47
1:D:435:LEU:HD23	1:D:445:VAL:HG22	1.96	0.47
1:C:5:PRO:O	1:C:6:ARG:HB2	2.15	0.47
1:C:359:THR:HB	1:C:360:PRO:HA	1.96	0.47
1:A:311:LEU:HD22	1:A:327:LEU:HD21	1.97	0.47
1:A:240:PRO:HB2	1:A:243:ALA:HB3	1.97	0.46
1:D:422:PRO:HD3	1:D:456:TYR:CE1	2.50	0.46
1:A:342:PHE:O	1:A:345:ARG:HG3	2.16	0.46
1:A:156:GLN:HG3	1:A:180:VAL:HB	1.98	0.46
1:A:265:GLY:HA2	1:A:291:ALA:HA	1.97	0.46
1:A:252:PHE:HE2	1:A:254:ASN:HB2	1.81	0.46
1:C:137:ASP:O	1:C:162:CYS:HA	2.16	0.46
1:A:4:PRO:HB2	1:A:7:CYS:SG	2.56	0.46
1:A:209:HIS:O	1:A:211:PRO:HD3	2.17	0.45
1:B:252:PHE:HB2	6:B:548:HOH:O	2.15	0.45
1:D:204:VAL:HG22	1:D:228:SER:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ARG:NE	6:B:537:HOH:O	2.19	0.45
1:C:419:TRP:CZ2	1:C:458:CYS:HB3	2.51	0.45
1:D:207:ILE:HG23	1:D:210:TRP:CE2	2.51	0.45
1:C:81:ASN:OD1	3:C:484:NAG:H61	2.16	0.45
1:A:395:VAL:HG22	1:A:405:PHE:CE1	2.51	0.45
1:A:252:PHE:CE2	1:A:254:ASN:HB2	2.52	0.45
1:B:119:LEU:HD12	1:B:143:ILE:HG12	1.99	0.45
1:C:67:ILE:HD11	1:C:91:ARG:NH1	2.33	0.44
1:A:344:ARG:HG2	1:A:347:ARG:HH21	1.83	0.44
1:D:39:LEU:HD23	1:D:44:ILE:HD11	1.98	0.44
1:B:398:ASP:HB2	1:B:401:HIS:ND1	2.32	0.44
1:B:440:ASP:OD1	1:B:442:THR:HG23	2.17	0.44
1:B:41:LYS:HE2	1:B:65:GLU:OE1	2.18	0.44
1:C:239:VAL:HB	1:C:241:TYR:CZ	2.52	0.44
1:A:207:ILE:HG23	1:A:210:TRP:CE2	2.52	0.44
1:D:397:VAL:HG21	1:D:403:VAL:CG2	2.48	0.43
1:D:191:ILE:HG22	1:D:220:CYS:HB2	2.00	0.43
1:C:412:ASP:OD1	1:C:413:PRO:CA	2.63	0.43
1:A:312:GLU:O	1:A:315:VAL:HG13	2.18	0.43
1:D:27:PRO:HG2	1:D:30:ILE:HG13	1.99	0.43
1:C:18:CYS:HB2	1:C:39:LEU:HD23	2.00	0.43
1:C:419:TRP:CH2	1:C:458:CYS:HB3	2.53	0.43
5:D:478:NAG:H61	5:D:479:NAG:HN2	1.83	0.43
1:A:93:LYS:O	1:A:116:ILE:HA	2.19	0.43
1:C:93:LYS:O	1:C:116:ILE:HA	2.19	0.43
1:D:311:LEU:HD22	1:D:327:LEU:HD21	2.01	0.43
1:B:436:THR:O	1:B:443:LEU:HA	2.19	0.43
1:B:239:VAL:HB	1:B:241:TYR:CE1	2.53	0.43
1:D:114:ASN:HB3	1:D:115:LYS:H	1.70	0.43
1:B:420:LEU:HB3	1:B:457:LEU:HB3	2.00	0.43
1:B:289:PRO:O	1:B:290:TYR:HB2	2.18	0.43
1:D:89:SER:HB2	1:D:113:GLU:HG3	2.00	0.43
1:B:353:GLN:N	1:B:353:GLN:OE1	2.52	0.43
1:A:353:GLN:NE2	2:A:482:NAG:H2	2.33	0.43
1:D:4:PRO:HA	1:D:5:PRO:HD3	1.83	0.43
1:D:20:ARG:HD2	1:D:20:ARG:HA	1.90	0.42
1:A:394:GLN:HG2	1:A:472:HIS:HB2	2.00	0.42
1:D:160:GLU:HA	1:D:184:ARG:O	2.19	0.42
1:D:342:PHE:O	1:D:345:ARG:HG3	2.20	0.42
1:D:274:LEU:HD23	1:D:295:LEU:HD21	2.01	0.42
1:C:322:LEU:HA	1:C:322:LEU:HD12	1.91	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:PHE:HZ	1:B:473:LEU:HB2	1.85	0.42
1:B:342:PHE:CE1	1:B:371:PHE:HB2	2.54	0.42
1:B:239:VAL:CG1	1:B:240:PRO:HD2	2.49	0.42
1:D:397:VAL:CB	1:D:403:VAL:HG21	2.48	0.42
1:D:256:SER:HB3	1:D:257:TYR:CD2	2.54	0.42
1:B:342:PHE:HE1	1:B:371:PHE:HB2	1.84	0.42
1:C:275:GLN:OE1	1:C:299:ARG:NH2	2.53	0.42
1:A:110:ASP:OD1	1:A:112:SER:OG	2.35	0.42
1:B:279:LEU:HD13	1:B:284:LEU:HD11	2.00	0.42
1:C:242:LEU:O	1:C:245:ARG:HG2	2.20	0.41
1:D:412:ASP:HA	1:D:413:PRO:C	2.41	0.41
1:D:397:VAL:HG21	1:D:403:VAL:HG23	2.02	0.41
1:C:356:THR:HG22	1:C:367:GLU:CG	2.51	0.41
1:A:423:ARG:O	1:A:424:LYS:HB2	2.20	0.41
1:A:40:GLY:HA2	1:A:64:ASN:O	2.19	0.41
1:A:128:TYR:CE2	1:B:320:GLY:HA3	2.56	0.41
1:D:104:SER:HB2	1:D:128:TYR:CZ	2.56	0.41
1:A:140:LEU:HD23	1:A:162:CYS:SG	2.61	0.41
1:B:412:ASP:HA	1:B:413:PRO:C	2.41	0.41
1:B:142:TYR:HB2	1:C:420:LEU:HD21	2.03	0.41
1:A:111:ILE:HD13	1:A:111:ILE:HA	1.93	0.41
1:C:420:LEU:CD1	1:C:459:ILE:HD11	2.44	0.41
1:C:412:ASP:HA	1:C:413:PRO:C	2.40	0.41
1:B:6:ARG:HB3	1:B:21:LYS:HD2	2.03	0.41
1:B:274:LEU:HD23	1:B:295:LEU:HD21	2.03	0.40
1:B:227:THR:HG21	1:B:251:ARG:NH2	2.29	0.40
1:A:296:ASN:OD1	1:A:317:HIS:NE2	2.54	0.40
1:D:407:CYS:HB2	1:D:419:TRP:CZ2	2.56	0.40
1:D:7:CYS:HB3	1:D:18:CYS:HB2	1.94	0.40
1:A:80:PHE:O	3:A:484:NAG:H2	2.21	0.40
1:D:111:ILE:O	1:D:111:ILE:CG2	2.69	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	466/477 (98%)	439 (94%)	27 (6%)	0	100 100
1	B	471/477 (99%)	445 (94%)	24 (5%)	2 (0%)	39 69
1	C	468/477 (98%)	443 (95%)	25 (5%)	0	100 100
1	D	467/477 (98%)	422 (90%)	44 (9%)	1 (0%)	52 80
All	All	1872/1908 (98%)	1749 (93%)	120 (6%)	3 (0%)	52 80

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	361	GLU
1	D	5	PRO
1	B	388	ARG

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	422/427 (99%)	417 (99%)	5 (1%)	78 93
1	B	424/427 (99%)	417 (98%)	7 (2%)	68 90
1	C	423/427 (99%)	413 (98%)	10 (2%)	57 85
1	D	422/427 (99%)	410 (97%)	12 (3%)	51 81
All	All	1691/1708 (99%)	1657 (98%)	34 (2%)	63 87

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	THR
1	A	67	ILE
1	A	280	VAL
1	A	286	VAL
1	A	319	VAL

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Mol	Chain	Res	Type
1	B	39	LEU
1	B	118	ILE
1	B	160	GLU
1	B	248	VAL
1	B	318	SER
1	B	338	LEU
1	B	403	VAL
1	C	135	VAL
1	C	165	THR
1	C	262	THR
1	C	272	LEU
1	C	279	LEU
1	C	280	VAL
1	C	319	VAL
1	C	420	LEU
1	C	426	LEU
1	C	458	CYS
1	D	9	CYS
1	D	26	VAL
1	D	36	LEU
1	D	69	SER
1	D	88	ARG
1	D	101	THR
1	D	200	TYR
1	D	228	SER
1	D	280	VAL
1	D	338	LEU
1	D	348	LEU
1	D	475	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	HIS
1	D	296	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

39 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	478	1,2	14,14,15	0.50	0	15,19,21	1.29	2 (13%)
2	NAG	A	479	2	14,14,15	0.59	0	15,19,21	1.29	2 (13%)
2	MAN	A	480	2	11,11,12	0.64	0	14,15,17	0.89	1 (7%)
2	NAG	A	481	1,2	14,14,15	0.49	0	15,19,21	0.78	0
2	NAG	A	482	2	14,14,15	0.53	0	15,19,21	1.14	1 (6%)
2	MAN	A	483	2	11,11,12	0.59	0	14,15,17	0.96	1 (7%)
4	NAG	A	486	1,4	14,14,15	0.41	0	15,19,21	1.65	2 (13%)
4	NAG	A	487	4	14,14,15	0.47	0	15,19,21	1.18	2 (13%)
2	NAG	A	488	1,2	14,14,15	0.51	0	15,19,21	1.00	0
2	NAG	A	489	2	14,14,15	0.60	0	15,19,21	1.47	2 (13%)
2	MAN	A	490	2	11,11,12	0.76	0	14,15,17	1.24	2 (14%)
5	NAG	B	478	1,5	14,14,15	0.49	0	15,19,21	1.81	3 (20%)
5	NAG	B	479	5	14,14,15	0.57	0	15,19,21	1.42	2 (13%)
5	MAN	B	480	5	11,11,12	0.62	0	14,15,17	1.44	2 (14%)
5	MAN	B	481	5	11,11,12	0.65	0	14,15,17	1.17	2 (14%)
2	NAG	B	482	1,2	14,14,15	0.59	0	15,19,21	0.80	0
2	NAG	B	483	2	14,14,15	0.53	0	15,19,21	0.98	1 (6%)
2	MAN	B	484	2	11,11,12	0.73	0	14,15,17	1.25	1 (7%)
2	NAG	B	489	1,2	14,14,15	0.57	0	15,19,21	1.11	2 (13%)
2	NAG	B	490	2	14,14,15	0.68	0	15,19,21	1.45	3 (20%)
2	MAN	B	491	2	11,11,12	0.73	0	14,15,17	1.38	2 (14%)
2	NAG	C	478	1,2	14,14,15	0.50	0	15,19,21	1.31	1 (6%)
2	NAG	C	479	2	14,14,15	0.52	0	15,19,21	0.83	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	MAN	C	480	2	11,11,12	0.62	0	14,15,17	0.85	1 (7%)
2	NAG	C	481	1,2	14,14,15	0.52	0	15,19,21	0.86	0
2	NAG	C	482	2	14,14,15	0.41	0	15,19,21	1.89	1 (6%)
2	MAN	C	483	2	11,11,12	0.55	0	14,15,17	1.17	1 (7%)
2	NAG	C	488	1,2	14,14,15	0.49	0	15,19,21	1.12	0
2	NAG	C	489	2	14,14,15	0.65	0	15,19,21	1.75	4 (26%)
2	MAN	C	490	2	11,11,12	0.61	0	14,15,17	2.06	2 (14%)
5	NAG	D	478	1,5	14,14,15	0.48	0	15,19,21	1.21	1 (6%)
5	NAG	D	479	5	14,14,15	0.51	0	15,19,21	1.12	1 (6%)
5	MAN	D	480	5	11,11,12	0.73	0	14,15,17	0.91	1 (7%)
5	MAN	D	481	5	11,11,12	0.57	0	14,15,17	1.51	2 (14%)
4	NAG	D	482	1,4	14,14,15	0.50	0	15,19,21	0.81	0
4	NAG	D	483	4	14,14,15	0.44	0	15,19,21	1.13	1 (6%)
2	NAG	D	486	1,2	14,14,15	0.49	0	15,19,21	0.91	0
2	NAG	D	487	2	14,14,15	0.54	0	15,19,21	1.08	1 (6%)
2	MAN	D	488	2	11,11,12	0.59	0	14,15,17	1.65	2 (14%)

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	478	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	479	2	-	0/6/23/26	0/1/1/1
2	MAN	A	480	2	1/1/4/5	0/2/19/22	0/1/1/1
2	NAG	A	481	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	482	2	-	0/6/23/26	0/1/1/1
2	MAN	A	483	2	1/1/4/5	0/2/19/22	0/1/1/1
4	NAG	A	486	1,4	1/1/5/7	0/6/23/26	0/1/1/1
4	NAG	A	487	4	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	488	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	489	2	-	0/6/23/26	0/1/1/1
2	MAN	A	490	2	1/1/4/5	0/2/19/22	0/1/1/1
5	NAG	B	478	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	479	5	-	0/6/23/26	0/1/1/1
5	MAN	B	480	5	1/1/4/5	0/2/19/22	0/1/1/1
5	MAN	B	481	5	-	0/2/19/22	0/1/1/1
2	NAG	B	482	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	483	2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MAN	B	484	2	1/1/4/5	0/2/19/22	0/1/1/1
2	NAG	B	489	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	490	2	-	0/6/23/26	0/1/1/1
2	MAN	B	491	2	1/1/4/5	0/2/19/22	0/1/1/1
2	NAG	C	478	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	479	2	-	0/6/23/26	0/1/1/1
2	MAN	C	480	2	1/1/4/5	0/2/19/22	0/1/1/1
2	NAG	C	481	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	482	2	-	0/6/23/26	0/1/1/1
2	MAN	C	483	2	1/1/4/5	0/2/19/22	0/1/1/1
2	NAG	C	488	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	489	2	-	0/6/23/26	0/1/1/1
2	MAN	C	490	2	1/1/4/5	0/2/19/22	1/1/1/1
5	NAG	D	478	1,5	-	0/6/23/26	0/1/1/1
5	NAG	D	479	5	-	0/6/23/26	0/1/1/1
5	MAN	D	480	5	1/1/4/5	0/2/19/22	0/1/1/1
5	MAN	D	481	5	-	0/2/19/22	0/1/1/1
4	NAG	D	482	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	483	4	-	0/6/23/26	0/1/1/1
2	NAG	D	486	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	487	2	-	0/6/23/26	0/1/1/1
2	MAN	D	488	2	-	0/2/19/22	1/1/1/1

There are no bond length outliers.

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	489	NAG	C3-C4-C5	-2.77	105.37	110.20
2	A	489	NAG	O4-C4-C3	-2.44	104.84	110.34
2	C	489	NAG	C4-C3-C2	-2.31	107.64	111.23
2	B	490	NAG	O4-C4-C3	-2.26	105.25	110.34
4	A	487	NAG	C4-C3-C2	-2.22	107.77	111.23
2	A	478	NAG	C3-C4-C5	-2.22	106.32	110.20
5	B	480	MAN	O3-C3-C2	-2.07	106.26	110.00
2	B	489	NAG	C3-C4-C5	-2.05	106.62	110.20
2	A	490	MAN	O2-C2-C1	2.05	113.31	109.21
2	A	483	MAN	C1-O5-C5	2.10	114.91	112.25
2	B	491	MAN	C1-O5-C5	2.12	114.94	112.25
5	D	479	NAG	C2-N2-C7	2.18	125.83	123.04
5	D	480	MAN	C1-C2-C3	2.25	112.20	109.54
4	A	486	NAG	O5-C5-C6	2.26	112.25	107.35
2	A	480	MAN	O5-C5-C6	2.29	112.31	107.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	479	NAG	O5-C5-C6	2.30	112.32	107.35
5	B	478	NAG	C2-N2-C7	2.32	126.02	123.04
2	A	479	NAG	C4-C3-C2	2.34	114.87	111.23
2	B	490	NAG	C1-O5-C5	2.36	115.24	112.25
5	B	481	MAN	C1-C2-C3	2.36	112.33	109.54
2	A	479	NAG	C3-C4-C5	2.42	114.41	110.20
5	D	481	MAN	C1-C2-C3	2.59	112.60	109.54
2	D	487	NAG	C4-C3-C2	2.60	115.26	111.23
2	D	488	MAN	C1-C2-C3	2.67	112.70	109.54
2	C	480	MAN	C1-O5-C5	2.69	115.66	112.25
5	B	478	NAG	C8-C7-N2	2.69	121.26	116.11
2	A	490	MAN	C1-C2-C3	2.71	112.75	109.54
5	B	481	MAN	C1-O5-C5	2.73	115.71	112.25
2	C	489	NAG	O4-C4-C5	2.92	116.97	109.24
2	B	489	NAG	C1-O5-C5	2.96	116.00	112.25
4	A	487	NAG	C1-O5-C5	2.99	116.04	112.25
5	B	479	NAG	C4-C3-C2	3.03	115.94	111.23
2	B	491	MAN	C1-C2-C3	3.13	113.24	109.54
2	B	483	NAG	C1-O5-C5	3.18	116.28	112.25
2	A	478	NAG	C1-O5-C5	3.19	116.30	112.25
5	D	478	NAG	C1-O5-C5	3.19	116.30	112.25
4	D	483	NAG	C1-O5-C5	3.30	116.43	112.25
2	A	482	NAG	C1-O5-C5	3.35	116.50	112.25
2	B	490	NAG	C4-C3-C2	3.53	116.71	111.23
2	C	478	NAG	C1-O5-C5	3.59	116.81	112.25
5	B	480	MAN	C1-C2-C3	3.62	113.82	109.54
2	C	483	MAN	C1-O5-C5	3.67	116.90	112.25
2	B	484	MAN	C1-C2-C3	3.82	114.06	109.54
2	C	490	MAN	C1-C2-C3	4.12	114.41	109.54
2	C	489	NAG	O4-C4-C3	4.15	119.68	110.34
2	A	489	NAG	C4-C3-C2	4.19	117.74	111.23
5	D	481	MAN	C1-O5-C5	4.45	117.89	112.25
4	A	486	NAG	C1-O5-C5	4.81	118.35	112.25
2	D	488	MAN	C1-O5-C5	5.02	118.62	112.25
5	B	478	NAG	C1-O5-C5	5.21	118.86	112.25
2	C	490	MAN	C1-O5-C5	6.05	119.93	112.25
2	C	482	NAG	C1-O5-C5	6.57	120.58	112.25

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	486	NAG	C1

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Mol	Chain	Res	Type	Atom
4	A	487	NAG	C1
2	C	490	MAN	C1
2	B	491	MAN	C1
2	A	480	MAN	C1
5	B	480	MAN	C5
2	C	480	MAN	C1
2	C	483	MAN	C1
2	A	490	MAN	C1
2	B	484	MAN	C1
5	D	480	MAN	C1
2	A	483	MAN	C1

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	490	MAN	C1-C2-C3-C4-C5-O5
2	D	488	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	482	NAG	1	0
5	B	479	NAG	1	0
2	B	484	MAN	2	0
2	C	483	MAN	2	0
5	D	478	NAG	1	0
5	D	479	NAG	1	0

5.6 Ligand geometry (i)

13 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	$\#\|Z\|>2$
3	NAG	A	484	1	14,14,15	0.85	1 (7%)	15,19,21	1.35	2 (13%)
3	NAG	A	485	1	14,14,15	0.45	0	15,19,21	1.06	2 (13%)
3	NAG	A	491	1	14,14,15	0.56	0	15,19,21	0.82	0
3	NAG	B	485	1	14,14,15	0.67	0	15,19,21	1.50	4 (26%)
3	NAG	B	486	1	14,14,15	0.54	0	15,19,21	0.59	0
3	NAG	B	487	1	14,14,15	0.53	0	15,19,21	1.43	2 (13%)
3	NAG	B	488	1	14,14,15	0.53	0	15,19,21	0.85	0
3	NAG	C	484	1	14,14,15	0.70	0	15,19,21	1.52	3 (20%)
3	NAG	C	485	1	14,14,15	0.63	0	15,19,21	0.92	0
3	NAG	C	486	1	14,14,15	1.15	1 (7%)	15,19,21	1.42	2 (13%)
3	NAG	C	487	1	14,14,15	0.47	0	15,19,21	1.33	2 (13%)
3	NAG	D	484	1	14,14,15	0.59	0	15,19,21	0.86	0
3	NAG	D	485	1	14,14,15	0.48	0	15,19,21	1.11	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
3	NAG	A	484	1	-	0/6/23/26	0/1/1/1
3	NAG	A	485	1	-	0/6/23/26	0/1/1/1
3	NAG	A	491	1	-	0/6/23/26	0/1/1/1
3	NAG	B	485	1	1/1/5/7	0/6/23/26	1/1/1/1
3	NAG	B	486	1	-	0/6/23/26	0/1/1/1
3	NAG	B	487	1	-	0/6/23/26	0/1/1/1
3	NAG	B	488	1	-	1/6/23/26	0/1/1/1
3	NAG	C	484	1	-	0/6/23/26	0/1/1/1
3	NAG	C	485	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	C	486	1	-	0/6/23/26	0/1/1/1
3	NAG	C	487	1	-	2/6/23/26	0/1/1/1
3	NAG	D	484	1	-	0/6/23/26	0/1/1/1
3	NAG	D	485	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	486	NAG	O5-C1	-4.05	1.36	1.43
3	A	484	NAG	C1-C2	2.67	1.56	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	487	NAG	C4-C3-C2	-3.02	106.54	111.23
3	C	486	NAG	C4-C3-C2	-2.69	107.05	111.23
3	B	485	NAG	C4-C3-C2	-2.60	107.19	111.23
3	B	485	NAG	O7-C7-C8	-2.22	117.99	122.06
3	C	484	NAG	C3-C2-N2	-2.07	105.59	110.56
3	B	487	NAG	C2-N2-C7	-2.02	120.44	123.04
3	C	484	NAG	C3-C4-C5	-2.00	106.71	110.20
3	A	485	NAG	C2-N2-C7	2.06	125.69	123.04
3	A	485	NAG	C1-O5-C5	2.10	114.91	112.25
3	B	485	NAG	C8-C7-N2	2.13	120.19	116.11
3	C	487	NAG	C1-O5-C5	2.24	115.09	112.25
3	B	485	NAG	O5-C5-C6	2.48	112.72	107.35
3	A	484	NAG	C2-N2-C7	2.74	126.56	123.04
3	A	484	NAG	C1-O5-C5	3.16	116.26	112.25
3	D	485	NAG	C1-O5-C5	3.18	116.28	112.25
3	C	484	NAG	C2-N2-C7	3.66	127.75	123.04
3	C	486	NAG	C1-O5-C5	3.73	116.98	112.25
3	B	487	NAG	C1-O5-C5	4.32	117.73	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	485	NAG	C1
3	B	485	NAG	C5

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	488	NAG	O7-C7-N2-C2
3	C	487	NAG	O7-C7-N2-C2
3	C	487	NAG	C8-C7-N2-C2

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	485	NAG	C1-C2-C3-C4-C5-O5

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	484	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	484	NAG	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.