



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:27 AM GMT

PDB ID : 2X1W
Title : Crystal Structure of VEGF-C in Complex with Domains 2 and 3 of VEGFR2
Authors : Leppanen, V.M.; Prota, A.E.; Jeltsch, M.; Anisimov, A.; Kalkkinen, N.; Strandin, T.; Lankinen, H.; Goldman, A.; Ballmer-Hofer, K.; Alitalo, K.
Deposited on : 2010-01-08
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) : 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

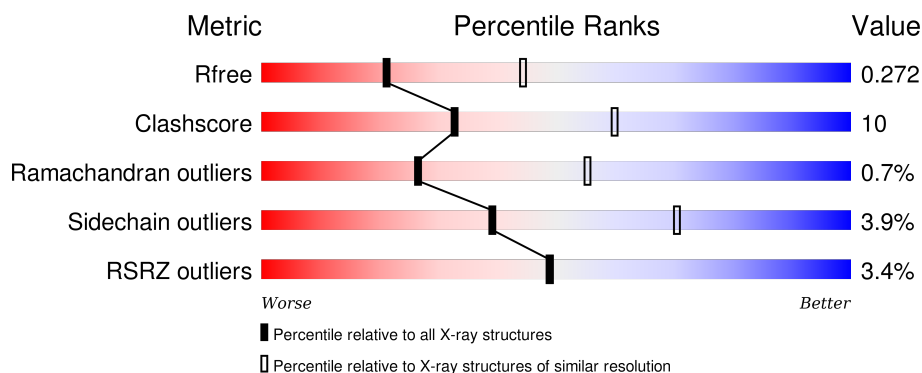
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (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 $\leq 5\%$. 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	110	<div> <div>4%</div> <div>64% 23% • 11%</div> </div>
1	B	110	<div> <div>4%</div> <div>74% 14% • 11%</div> </div>
1	C	110	<div> <div>%</div> <div>69% 18% • 12%</div> </div>
1	D	110	<div> <div>5%</div> <div>68% 17% 5% 10%</div> </div>
2	L	213	<div> <div>3%</div> <div>71% 17% • 8%</div> </div>

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Mol	Chain	Length	Quality of chain
2	M	213	
2	N	213	
2	O	213	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	500	-	-	-	X
3	NAG	M	1301	X	-	-	-
5	NAG	L	2401	X	-	-	-
5	NAG	O	2001	X	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9720 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 VASCULAR ENDOTHELIAL GROWTH FACTOR C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	98	Total	C	N	O	S	0	0	0
			750	468	127	144	11			
1	B	98	Total	C	N	O	S	0	0	0
			752	470	128	143	11			
1	C	97	Total	C	N	O	S	0	0	0
			743	465	127	140	11			
1	D	99	Total	C	N	O	S	0	0	0
			760	476	129	144	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	137	ALA	CYS	ENGINEERED MUTATION	UNP P49767
B	137	ALA	CYS	ENGINEERED MUTATION	UNP P49767
C	137	ALA	CYS	ENGINEERED MUTATION	UNP P49767
D	137	ALA	CYS	ENGINEERED MUTATION	UNP P49767

- Molecule 2 is a protein called VASCULAR ENDOTHELIAL GROWTH FACTOR RECEPTOR 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	196	Total	C	N	O	S	0	0	0
			1535	977	261	287	10			
2	M	179	Total	C	N	O	S	0	0	0
			1402	894	236	262	10			
2	N	194	Total	C	N	O	S	0	0	0
			1522	969	255	288	10			
2	O	193	Total	C	N	O	S	0	0	0
			1516	967	256	283	10			

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

- Molecule 4 is CESIUM ION (three-letter code: CS) (formula: Cs).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cs	0	0
			1	1		
4	C	1	Total	Cs	0	0
			1	1		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 6 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	L	2	Total	C	N	O	0	0
			28	16	2	10		
6	M	2	Total	C	N	O	0	0
			28	16	2	10		
6	N	2	Total	C	N	O	0	0
			28	16	2	10		
6	O	2	Total	C	N	O	0	0
			28	16	2	10		

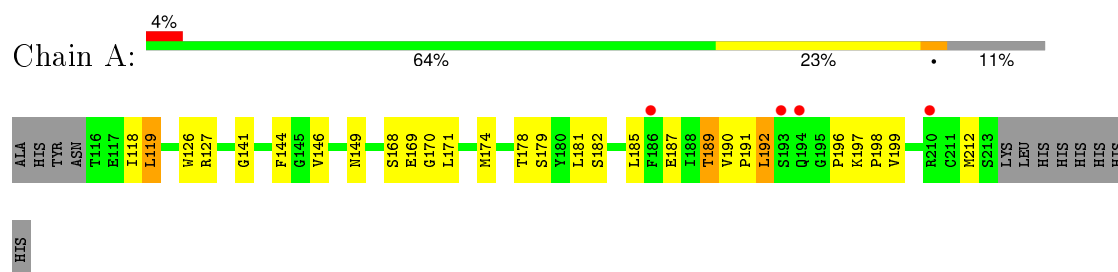
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	14	Total 14	O 14	0	0
7	B	11	Total 11	O 11	0	0
7	C	32	Total 32	O 32	0	0
7	D	19	Total 19	O 19	0	0
7	L	31	Total 31	O 31	0	0
7	M	12	Total 12	O 12	0	0
7	N	34	Total 34	O 34	0	0
7	O	24	Total 24	O 24	0	0

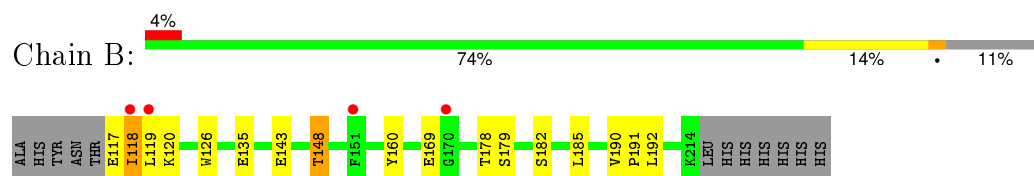
3 Residue-property plots

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.

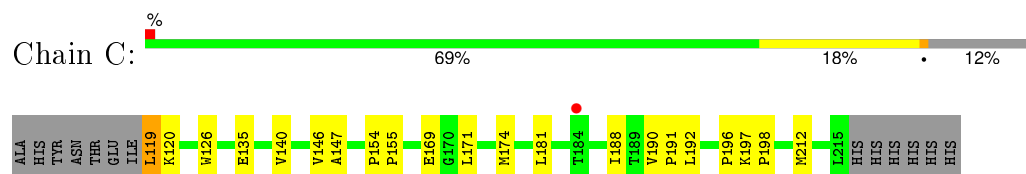
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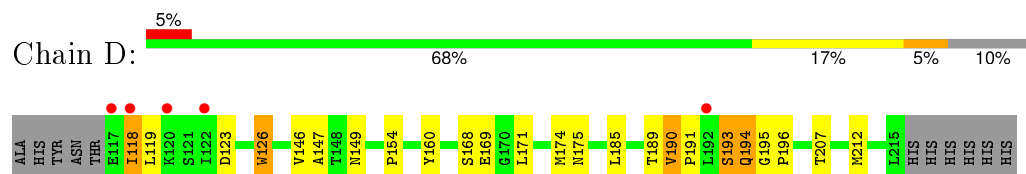
• Molecule 1: VASCULAR ENDOTHELIAL GROWTH FACTOR C



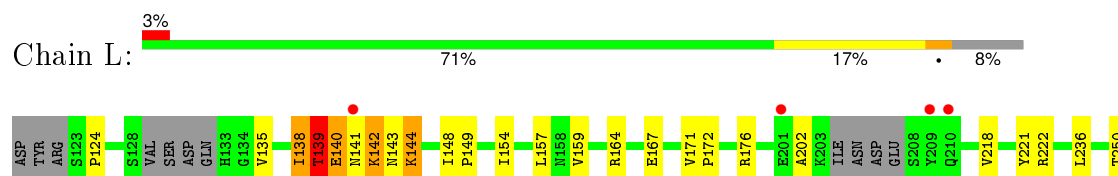
• Molecule 1: VASCULAR ENDOTHELIAL GROWTH FACTOR C

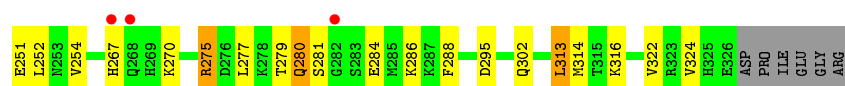


• Molecule 1: VASCULAR ENDOTHELIAL GROWTH FACTOR C

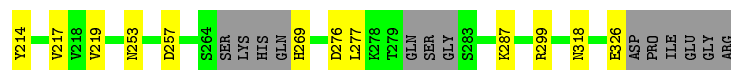
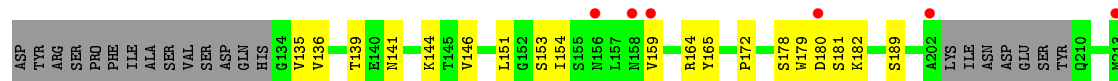


• Molecule 2: VASCULAR ENDOTHELIAL GROWTH FACTOR RECEPTOR 2

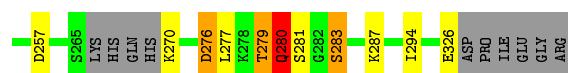
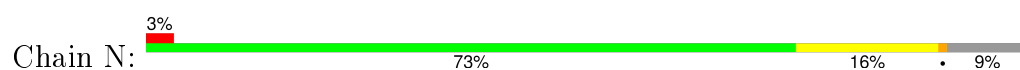




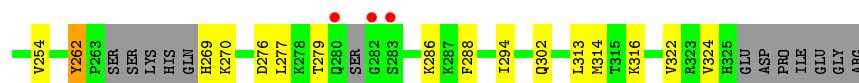
• Molecule 2: VASCULAR ENDOTHELIAL GROWTH FACTOR RECEPTOR 2



• Molecule 2: VASCULAR ENDOTHELIAL GROWTH FACTOR RECEPTOR 2



• Molecule 2: VASCULAR ENDOTHELIAL GROWTH FACTOR RECEPTOR 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.75Å 123.83Å 211.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	52.96 – 2.70 69.65 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (52.96-2.70) 99.6 (69.65-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.69Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.227 , 0.280 0.220 , 0.272	Depositor DCC
R_{free} test set	2746 reflections (5.09%)	DCC
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 57.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 53965 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9720	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/765	0.52	0/1035
1	B	0.34	0/767	0.54	0/1036
1	C	0.35	0/758	0.53	0/1024
1	D	0.34	0/775	0.53	0/1047
2	L	0.31	0/1565	0.48	0/2113
2	M	0.28	0/1426	0.47	0/1925
2	N	0.30	0/1550	0.47	0/2093
2	O	0.32	0/1544	0.50	0/2085
All	All	0.32	0/9150	0.50	0/12358

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
3	M	1	0

There are no bond length outliers.

There are no bond angle outliers.

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	M	1301	NAG	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	750	0	732	20	0
1	B	752	0	738	10	0
1	C	743	0	732	13	0
1	D	760	0	749	22	0
2	L	1535	0	1540	49	0
2	M	1402	0	1415	24	0
2	N	1522	0	1526	37	0
2	O	1516	0	1518	33	0
3	A	78	0	68	3	0
3	B	78	0	68	4	0
3	C	78	0	68	1	0
3	D	78	0	68	5	0
3	M	39	0	34	2	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	L	28	0	26	0	0
5	N	28	0	26	0	0
5	O	42	0	39	3	0
6	L	28	0	25	0	0
6	M	28	0	25	0	0
6	N	28	0	25	0	0
6	O	28	0	25	0	0
7	A	14	0	0	0	0
7	B	11	0	0	1	0
7	C	32	0	0	1	0
7	D	19	0	0	1	0
7	L	31	0	0	0	0
7	M	12	0	0	0	0
7	N	34	0	0	0	0
7	O	24	0	0	0	0
All	All	9720	0	9447	198	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 10.

All (198) 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)
2:N:280:GLN:HB2	2:N:281:SER:HA	1.22	1.14
2:N:280:GLN:CB	2:N:281:SER:HA	1.78	1.11
2:O:138:ILE:HG22	2:O:146:VAL:HG11	1.41	1.00
2:L:142:LYS:HG3	2:L:143:ASN:H	1.37	0.89
2:L:124:PRO:HB2	2:L:157:LEU:HD11	1.60	0.82
1:A:141:GLY:HA2	1:A:146:VAL:HG21	1.59	0.82
2:O:276:ASP:O	2:O:277:LEU:HD23	1.80	0.82
1:D:146:VAL:HG22	1:D:147:ALA:H	1.45	0.81
1:C:140:VAL:HG12	1:C:155:PRO:O	1.82	0.79
1:A:181:LEU:HD21	3:A:500:NAG:H82	1.64	0.78
2:N:280:GLN:CB	2:N:281:SER:CA	2.59	0.78
2:O:190:TYR:CZ	5:O:2001:NAG:H5	2.21	0.76
2:L:141:ASN:CG	2:L:142:LYS:H	1.88	0.76
2:L:142:LYS:HG3	2:L:143:ASN:N	2.04	0.72
1:A:192:LEU:HD22	1:A:192:LEU:H	1.55	0.72
2:L:142:LYS:HA	2:L:142:LYS:HE3	1.72	0.71
1:D:196:PRO:HD2	2:L:135:VAL:HG21	1.71	0.71
2:N:280:GLN:HB3	2:N:281:SER:HA	1.73	0.71
2:O:164:ARG:HG2	2:O:167:GLU:HG2	1.74	0.70
1:D:190:VAL:HA	1:D:191:PRO:C	2.11	0.70
2:O:139:THR:HA	2:O:219:VAL:O	1.93	0.68
2:L:142:LYS:CG	2:L:143:ASN:H	2.07	0.67
2:O:204:ILE:HG23	2:O:204:ILE:O	1.93	0.67
2:L:252:LEU:HG	2:L:284:GLU:HG2	1.76	0.67
2:N:280:GLN:HB2	2:N:281:SER:CA	2.09	0.66
2:L:164:ARG:HG2	2:L:167:GLU:HG2	1.76	0.65
1:D:207:THR:HA	3:D:500:NAG:O6	1.96	0.65
1:D:168:SER:HB2	1:D:171:LEU:HD12	1.78	0.65
2:O:190:TYR:OH	5:O:2001:NAG:H5	1.97	0.64
1:B:148:THR:HG23	2:N:276:ASP:CG	2.18	0.64
2:N:126:ILE:HD13	2:N:151:LEU:HB3	1.78	0.64
2:O:270:LYS:HB3	2:O:294:ILE:HG12	1.80	0.63
2:L:221:TYR:HB2	2:L:313:LEU:HB2	1.81	0.61
2:L:267:HIS:HB2	2:L:270:LYS:HD2	1.83	0.61
2:L:140:GLU:HG3	2:L:140:GLU:O	1.99	0.61
2:O:204:ILE:C	2:O:206:ASP:H	2.02	0.61
2:O:270:LYS:CB	2:O:294:ILE:HG12	2.30	0.60
1:B:117:GLU:HA	1:B:120:LYS:HD2	1.82	0.60
2:L:279:THR:HG23	2:L:280:GLN:N	2.16	0.60
2:N:138:ILE:HG22	2:N:140:GLU:H	1.67	0.60
1:B:169:GLU:OE2	2:M:253:ASN:N	2.35	0.59
1:C:169:GLU:OE1	2:L:286:LYS:HD3	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:217:VAL:HG12	2:M:219:VAL:HG13	1.84	0.59
1:A:178:THR:HG22	1:A:179:SER:O	2.03	0.59
2:M:153:SER:HB2	2:M:154:ILE:HD12	1.85	0.58
1:A:196:PRO:HD3	2:M:135:VAL:HG21	1.85	0.58
2:O:221:TYR:HB2	2:O:313:LEU:HB2	1.85	0.58
2:L:141:ASN:CG	2:L:142:LYS:N	2.57	0.58
2:N:153:SER:HB2	2:N:154:ILE:HD12	1.86	0.58
1:D:118:ILE:HB	1:D:119:LEU:HD12	1.85	0.58
1:D:146:VAL:HG22	1:D:147:ALA:N	2.19	0.58
2:N:159:VAL:HG21	2:N:179:TRP:CE2	2.38	0.58
2:N:280:GLN:CD	2:N:280:GLN:H	2.07	0.57
2:L:143:ASN:O	2:L:176:ARG:NH2	2.37	0.57
1:A:196:PRO:CD	2:M:135:VAL:HG21	2.34	0.57
2:M:159:VAL:HG21	2:M:179:TRP:CE2	2.40	0.57
1:A:170:GLY:HA3	2:N:252:LEU:CD1	2.35	0.57
1:A:149:ASN:ND2	1:A:189:THR:HG22	2.19	0.56
1:A:170:GLY:HA3	2:N:252:LEU:HD13	1.85	0.56
1:A:119:LEU:HD23	2:N:132:GLN:HE21	1.70	0.56
2:L:252:LEU:CD1	2:L:284:GLU:HG2	2.36	0.56
1:A:127:ARG:HG3	2:N:165:TYR:CE2	2.41	0.56
2:O:204:ILE:HG22	2:O:207:GLU:H	1.69	0.56
2:N:146:VAL:HG23	2:N:189:SER:HB3	1.89	0.55
2:L:139:THR:O	2:L:140:GLU:CB	2.54	0.55
2:L:140:GLU:O	2:L:140:GLU:CG	2.54	0.54
2:N:136:VAL:HG23	2:N:214:TYR:HB3	1.90	0.54
1:B:178:THR:HG22	1:B:179:SER:O	2.08	0.54
1:B:169:GLU:HG3	2:M:253:ASN:OD1	2.08	0.53
2:M:146:VAL:HG23	2:M:189:SER:HB3	1.90	0.53
2:L:139:THR:CG2	2:L:140:GLU:N	2.71	0.53
2:N:203:LYS:HG2	2:N:208:SER:HB3	1.90	0.53
2:M:136:VAL:HG23	2:M:214:TYR:HB3	1.91	0.53
1:D:123:ASP:HA	2:O:197:MET:HE1	1.91	0.53
1:C:119:LEU:HD22	1:C:120:LYS:N	2.23	0.53
2:N:279:THR:HG22	2:N:280:GLN:N	2.24	0.53
1:C:190:VAL:HA	1:C:191:PRO:C	2.29	0.53
1:D:118:ILE:HD12	1:D:118:ILE:H	1.73	0.52
2:L:139:THR:HG22	2:L:140:GLU:N	2.25	0.52
2:M:318:ASN:OD1	3:M:1301:NAG:H83	2.10	0.51
2:N:180:ASP:O	2:N:181:SER:HB3	2.11	0.51
2:L:286:LYS:HE3	2:L:288:PHE:CZ	2.45	0.51
2:M:141:ASN:ND2	2:M:144:LYS:HB2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:252:LEU:CG	2:L:284:GLU:HG2	2.41	0.51
2:M:299:ARG:HH21	2:M:326:GLU:HB3	1.76	0.51
2:L:279:THR:HG23	2:L:280:GLN:H	1.76	0.50
2:O:222:ARG:HB2	2:O:251:GLU:CD	2.30	0.50
1:A:192:LEU:HD22	1:A:192:LEU:N	2.24	0.50
2:N:154:ILE:N	2:N:154:ILE:HD12	2.26	0.50
3:B:500:NAG:H2	7:B:2009:HOH:O	2.11	0.50
1:D:196:PRO:CD	2:L:135:VAL:HG21	2.41	0.50
2:M:180:ASP:O	2:M:181:SER:HB3	2.11	0.50
2:N:126:ILE:CD1	2:N:151:LEU:HB3	2.42	0.50
2:L:236:LEU:O	2:L:324:VAL:HA	2.11	0.50
1:D:118:ILE:CD1	1:D:118:ILE:H	2.25	0.49
2:O:286:LYS:HE3	2:O:288:PHE:CZ	2.47	0.49
2:O:302:GLN:HG3	2:O:322:VAL:O	2.12	0.49
2:M:154:ILE:HD12	2:M:154:ILE:N	2.27	0.49
2:O:262:TYR:CD2	2:O:270:LYS:HD2	2.47	0.49
2:L:314:MET:HE1	2:L:316:LYS:HE3	1.94	0.49
3:M:1301:NAG:H4	3:M:1302:NAG:HN2	1.78	0.48
2:L:159:VAL:HG22	2:L:202:ALA:HB2	1.94	0.48
2:O:236:LEU:O	2:O:324:VAL:HA	2.13	0.48
1:D:149:ASN:O	1:D:189:THR:HA	2.14	0.48
2:N:138:ILE:HG23	2:N:189:SER:HB2	1.95	0.48
2:M:277:LEU:HD12	2:M:287:LYS:HG2	1.96	0.48
1:C:135:GLU:HG2	7:C:2013:HOH:O	2.14	0.47
2:N:125:PHE:HA	2:N:151:LEU:O	2.14	0.47
1:C:146:VAL:HG13	1:C:147:ALA:O	2.14	0.47
2:L:252:LEU:HG	2:L:284:GLU:CG	2.43	0.47
1:D:160:TYR:CG	3:D:500:NAG:H5	2.50	0.47
2:L:279:THR:O	2:L:281:SER:N	2.48	0.47
2:N:146:VAL:CG2	2:N:189:SER:HB3	2.44	0.47
2:N:277:LEU:HD12	2:N:287:LYS:HG2	1.96	0.47
2:L:222:ARG:HB2	2:L:251:GLU:CD	2.35	0.47
1:D:154:PRO:HD2	1:D:185:LEU:HD12	1.97	0.47
1:C:181:LEU:HD21	3:C:500:NAG:H82	1.97	0.47
2:L:138:ILE:HG13	2:L:139:THR:HB	1.97	0.46
2:M:146:VAL:CG2	2:M:189:SER:HB3	2.44	0.46
1:D:193:SER:C	1:D:195:GLY:H	2.18	0.46
1:B:169:GLU:OE2	2:M:253:ASN:HA	2.16	0.46
2:L:144:LYS:HB2	2:L:144:LYS:NZ	2.31	0.46
1:A:181:LEU:CD2	3:A:500:NAG:H82	2.41	0.46
2:O:176:ARG:HH11	2:O:176:ARG:HG3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:302:GLN:HG3	2:L:322:VAL:O	2.16	0.45
2:L:221:TYR:HB2	2:L:313:LEU:CB	2.47	0.45
1:D:193:SER:O	1:D:194:GLN:HB2	2.17	0.45
2:L:295:ASP:CG	2:N:169:ARG:HE	2.18	0.45
2:L:138:ILE:O	2:L:218:VAL:HA	2.16	0.45
2:N:280:GLN:NE2	2:N:280:GLN:H	2.14	0.45
2:O:204:ILE:C	2:O:206:ASP:N	2.70	0.45
1:C:154:PRO:HG3	1:D:126:TRP:CD2	2.51	0.45
1:C:188:ILE:HD11	1:C:196:PRO:HG3	1.99	0.45
2:M:141:ASN:ND2	2:M:144:LYS:HE3	2.32	0.45
2:L:275:ARG:HD2	2:L:277:LEU:HD23	1.98	0.45
2:L:142:LYS:CA	2:L:142:LYS:HE3	2.44	0.45
2:M:151:LEU:HD13	2:M:181:SER:O	2.17	0.45
1:D:174:MET:HB2	1:D:212:MET:HE2	1.98	0.45
1:A:187:GLU:OE1	1:A:199:VAL:HG11	2.17	0.44
2:O:148:ILE:HA	2:O:149:PRO:HD3	1.74	0.44
3:B:500:NAG:H61	3:B:501:NAG:C7	2.47	0.44
1:A:197:LYS:HA	1:A:198:PRO:HD3	1.87	0.44
1:D:146:VAL:CG2	1:D:147:ALA:H	2.23	0.43
2:L:138:ILE:CG1	2:L:139:THR:HB	2.48	0.43
2:N:240:GLU:OE2	2:N:240:GLU:HA	2.17	0.43
2:L:142:LYS:CE	2:L:143:ASN:H	2.31	0.43
2:O:314:MET:HE1	2:O:316:LYS:HE3	2.00	0.43
1:B:190:VAL:HG13	1:B:191:PRO:HA	2.01	0.43
3:B:401:NAG:H2	3:B:401:NAG:H83	1.88	0.43
1:D:169:GLU:CD	7:D:2011:HOH:O	2.56	0.43
2:N:151:LEU:HD13	2:N:181:SER:O	2.19	0.43
2:O:204:ILE:O	2:O:205:ASN:HB3	2.19	0.43
1:C:197:LYS:HA	1:C:198:PRO:HD3	1.80	0.43
2:N:180:ASP:C	2:N:182:LYS:H	2.23	0.42
3:B:500:NAG:H61	3:B:501:NAG:N2	2.34	0.42
1:B:118:ILE:HD12	1:B:118:ILE:H	1.84	0.42
2:N:138:ILE:HG22	2:N:140:GLU:N	2.33	0.42
1:D:207:THR:HA	3:D:500:NAG:HO6	1.82	0.42
2:O:154:ILE:HB	2:O:157:LEU:HG	2.02	0.42
2:M:164:ARG:HD3	2:M:165:TYR:CE1	2.55	0.42
2:L:250:THR:HG21	2:L:254:VAL:HG11	2.01	0.42
1:A:174:MET:HE2	1:A:212:MET:HB2	2.02	0.42
2:L:142:LYS:HE2	2:L:143:ASN:H	1.84	0.41
2:N:164:ARG:HD3	2:N:165:TYR:CE1	2.55	0.41
1:C:171:LEU:HA	1:C:212:MET:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:286:LYS:HE3	2:L:288:PHE:HZ	1.85	0.41
2:M:180:ASP:C	2:M:182:LYS:H	2.23	0.41
1:C:174:MET:HB2	1:C:212:MET:HE2	2.02	0.41
1:A:168:SER:HB2	1:A:171:LEU:HD22	2.01	0.41
2:L:138:ILE:CB	2:L:139:THR:HB	2.50	0.41
2:M:172:PRO:HB3	2:M:178:SER:HA	2.02	0.41
1:B:135:GLU:HG3	1:B:160:TYR:CE1	2.54	0.41
2:M:299:ARG:HE	2:M:326:GLU:HB3	1.86	0.41
2:O:229:SER:HA	2:O:230:PRO:C	2.40	0.41
2:O:164:ARG:HB3	2:O:165:TYR:CG	2.56	0.41
1:C:188:ILE:HG23	1:C:192:LEU:CD2	2.50	0.41
2:L:154:ILE:HB	2:L:157:LEU:HG	2.03	0.41
2:O:142:LYS:HD3	5:O:2001:NAG:O7	2.21	0.41
2:O:286:LYS:HE3	2:O:288:PHE:HZ	1.84	0.41
2:L:171:VAL:HG13	2:L:172:PRO:HD2	2.02	0.41
2:O:250:THR:HG21	2:O:254:VAL:HG11	2.03	0.41
2:N:280:GLN:HA	2:N:283:SER:HB3	2.03	0.41
1:B:148:THR:HG23	2:N:276:ASP:OD2	2.21	0.41
2:O:221:TYR:HB2	2:O:313:LEU:CB	2.50	0.41
3:A:401:NAG:H4	3:A:402:BMA:H2	1.87	0.41
2:L:148:ILE:HA	2:L:149:PRO:HD3	1.75	0.41
1:A:190:VAL:HA	1:A:191:PRO:C	2.40	0.41
1:A:192:LEU:CD2	1:A:192:LEU:H	2.28	0.41
1:A:169:GLU:C	1:A:171:LEU:H	2.23	0.41
2:L:176:ARG:HH11	2:L:176:ARG:HG3	1.84	0.40
2:O:219:VAL:HB	2:O:220:GLY:HA3	2.04	0.40
3:D:500:NAG:H61	3:D:501:NAG:H82	2.01	0.40
2:O:142:LYS:C	2:O:143:ASN:HD22	2.24	0.40
1:D:175:ASN:ND2	3:D:400:NAG:O7	2.53	0.40
2:M:164:ARG:HA	2:M:165:TYR:HA	1.82	0.40
2:N:139:THR:C	2:N:141:ASN:H	2.25	0.40
2:O:159:VAL:HG21	2:O:179:TRP:CE2	2.56	0.40
2:N:270:LYS:HG2	2:N:294:ILE:HG12	2.03	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	96/110 (87%)	92 (96%)	3 (3%)	1 (1%)	19	45
1	B	96/110 (87%)	95 (99%)	0	1 (1%)	19	45
1	C	95/110 (86%)	93 (98%)	2 (2%)	0	100	100
1	D	97/110 (88%)	89 (92%)	7 (7%)	1 (1%)	19	45
2	L	190/213 (89%)	175 (92%)	12 (6%)	3 (2%)	12	30
2	M	171/213 (80%)	156 (91%)	15 (9%)	0	100	100
2	N	188/213 (88%)	169 (90%)	18 (10%)	1 (0%)	34	63
2	O	185/213 (87%)	174 (94%)	10 (5%)	1 (0%)	34	63
All	All	1118/1292 (86%)	1043 (93%)	67 (6%)	8 (1%)	26	55

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	PHE
2	L	140	GLU
2	N	280	GLN
2	L	280	GLN
1	B	192	LEU
1	D	193	SER
2	L	139	THR
2	O	220	GLY

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	89/100 (89%)	82 (92%)	7 (8%)	15	34
1	B	89/100 (89%)	82 (92%)	7 (8%)	15	34
1	C	88/100 (88%)	86 (98%)	2 (2%)	58	85
1	D	90/100 (90%)	86 (96%)	4 (4%)	35	65
2	L	176/192 (92%)	170 (97%)	6 (3%)	44	75
2	M	161/192 (84%)	157 (98%)	4 (2%)	55	84
2	N	175/192 (91%)	167 (95%)	8 (5%)	33	64
2	O	173/192 (90%)	170 (98%)	3 (2%)	68	90
All	All	1041/1168 (89%)	1000 (96%)	41 (4%)	39	70

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	ILE
1	A	119	LEU
1	A	126	TRP
1	A	182	SER
1	A	185	LEU
1	A	189	THR
1	A	192	LEU
1	B	118	ILE
1	B	119	LEU
1	B	126	TRP
1	B	143	GLU
1	B	148	THR
1	B	182	SER
1	B	185	LEU
1	C	119	LEU
1	C	126	TRP
1	D	118	ILE
1	D	126	TRP
1	D	190	VAL
1	D	194	GLN
2	L	138	ILE
2	L	139	THR
2	L	142	LYS
2	L	144	LYS
2	L	275	ARG
2	L	313	LEU
2	M	139	THR

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Mol	Chain	Res	Type
2	M	257	ASP
2	M	269	HIS
2	M	276	ASP
2	N	210	GLN
2	N	219	VAL
2	N	257	ASP
2	N	276	ASP
2	N	279	THR
2	N	280	GLN
2	N	283	SER
2	N	326	GLU
2	O	262	TYR
2	O	269	HIS
2	O	279	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	M	141	ASN
2	N	132	GLN
2	N	280	GLN
2	O	280	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 ⓘ

35 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	400	1,3	14,14,15	0.64	0	15,19,21	1.06	1 (6%)
3	NAG	A	401	3	14,14,15	0.48	0	15,19,21	0.76	0
3	BMA	A	402	3	11,11,12	0.61	0	14,15,17	0.90	0
3	NAG	A	500	1,3	14,14,15	0.59	0	15,19,21	0.96	1 (6%)
3	NAG	A	501	3	14,14,15	0.51	0	15,19,21	0.95	1 (6%)
3	BMA	A	502	3	11,11,12	0.67	0	14,15,17	0.60	0
3	NAG	B	400	1,3	14,14,15	0.51	0	15,19,21	1.06	1 (6%)
3	NAG	B	401	3	14,14,15	0.46	0	15,19,21	0.89	1 (6%)
3	BMA	B	402	3	11,11,12	0.58	0	14,15,17	1.08	1 (7%)
3	NAG	B	500	1,3	14,14,15	0.69	0	15,19,21	1.39	3 (20%)
3	NAG	B	501	3	14,14,15	0.56	0	15,19,21	0.97	1 (6%)
3	BMA	B	502	3	11,11,12	0.62	0	14,15,17	0.79	0
3	NAG	C	400	1,3	14,14,15	0.52	0	15,19,21	1.05	1 (6%)
3	NAG	C	401	3	14,14,15	0.53	0	15,19,21	0.69	0
3	BMA	C	402	3	11,11,12	0.61	0	14,15,17	0.94	1 (7%)
3	NAG	C	500	1,3	14,14,15	0.61	0	15,19,21	0.99	1 (6%)
3	NAG	C	501	3	14,14,15	0.63	0	15,19,21	0.57	0
3	BMA	C	502	3	11,11,12	0.66	0	14,15,17	0.91	0
3	NAG	D	400	1,3	14,14,15	0.49	0	15,19,21	1.42	1 (6%)
3	NAG	D	401	3	14,14,15	0.36	0	15,19,21	1.14	1 (6%)
3	BMA	D	402	3	11,11,12	0.58	0	14,15,17	0.82	1 (7%)
3	NAG	D	500	1,3	14,14,15	0.45	0	15,19,21	1.08	2 (13%)
3	NAG	D	501	3	14,14,15	0.61	0	15,19,21	0.95	0
3	BMA	D	502	3	11,11,12	0.67	0	14,15,17	0.92	1 (7%)
6	NAG	L	2601	2,6	14,14,15	0.53	0	15,19,21	0.84	1 (6%)
6	NAG	L	2602	6	14,14,15	0.52	0	15,19,21	0.65	0
6	NAG	M	1201	2,6	14,14,15	0.51	0	15,19,21	0.88	0
6	NAG	M	1202	6	14,14,15	0.51	0	15,19,21	0.74	1 (6%)
3	NAG	M	1301	3,2	14,14,15	0.57	0	15,19,21	1.76	3 (20%)
3	NAG	M	1302	3	14,14,15	0.61	0	15,19,21	1.25	2 (13%)
3	BMA	M	1303	3	11,11,12	0.58	0	14,15,17	1.16	2 (14%)
6	NAG	N	1701	2,6	14,14,15	0.45	0	15,19,21	1.48	3 (20%)
6	NAG	N	1702	6	14,14,15	0.46	0	15,19,21	1.26	3 (20%)
6	NAG	O	2201	2,6	14,14,15	0.60	0	15,19,21	0.81	0
6	NAG	O	2202	6	14,14,15	0.57	0	15,19,21	1.16	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	400	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	401	3	-	0/6/23/26	0/1/1/1
3	BMA	A	402	3	-	0/2/19/22	0/1/1/1
3	NAG	A	500	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	501	3	-	0/6/23/26	0/1/1/1
3	BMA	A	502	3	-	0/2/19/22	0/1/1/1
3	NAG	B	400	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	401	3	-	0/6/23/26	0/1/1/1
3	BMA	B	402	3	-	0/2/19/22	0/1/1/1
3	NAG	B	500	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	501	3	-	0/6/23/26	0/1/1/1
3	BMA	B	502	3	-	0/2/19/22	0/1/1/1
3	NAG	C	400	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	401	3	-	0/6/23/26	0/1/1/1
3	BMA	C	402	3	-	0/2/19/22	0/1/1/1
3	NAG	C	500	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	501	3	-	0/6/23/26	0/1/1/1
3	BMA	C	502	3	-	0/2/19/22	0/1/1/1
3	NAG	D	400	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	401	3	-	0/6/23/26	0/1/1/1
3	BMA	D	402	3	-	0/2/19/22	0/1/1/1
3	NAG	D	500	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	501	3	-	0/6/23/26	0/1/1/1
3	BMA	D	502	3	-	0/2/19/22	0/1/1/1
6	NAG	L	2601	2,6	-	0/6/23/26	0/1/1/1
6	NAG	L	2602	6	-	0/6/23/26	0/1/1/1
6	NAG	M	1201	2,6	-	0/6/23/26	0/1/1/1
6	NAG	M	1202	6	-	0/6/23/26	0/1/1/1
3	NAG	M	1301	3,2	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	M	1302	3	-	0/6/23/26	0/1/1/1
3	BMA	M	1303	3	-	0/2/19/22	0/1/1/1
6	NAG	N	1701	2,6	-	0/6/23/26	0/1/1/1
6	NAG	N	1702	6	-	0/6/23/26	0/1/1/1
6	NAG	O	2201	2,6	-	0/6/23/26	0/1/1/1
6	NAG	O	2202	6	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	1301	NAG	C3-C4-C5	-4.14	102.97	110.20
3	D	400	NAG	C2-N2-C7	-3.80	118.15	123.04
3	A	400	NAG	C2-N2-C7	-3.08	119.08	123.04
3	C	400	NAG	C2-N2-C7	-3.04	119.14	123.04
3	D	502	BMA	C1-O5-C5	-2.79	108.70	112.25
3	B	500	NAG	C2-N2-C7	-2.76	119.49	123.04
6	N	1701	NAG	C6-C5-C4	-2.50	106.86	113.02
6	N	1702	NAG	C2-N2-C7	-2.43	119.91	123.04
3	C	500	NAG	C2-N2-C7	-2.40	119.95	123.04
3	D	500	NAG	C2-N2-C7	-2.38	119.98	123.04
3	M	1303	BMA	O5-C1-C2	-2.32	107.09	110.86
3	A	501	NAG	C2-N2-C7	-2.30	120.09	123.04
3	B	402	BMA	O5-C1-C2	-2.26	107.20	110.86
3	M	1301	NAG	C4-C3-C2	-2.22	107.78	111.23
6	N	1702	NAG	C4-C3-C2	-2.19	107.82	111.23
3	C	402	BMA	C1-O5-C5	-2.15	109.52	112.25
6	L	2601	NAG	C2-N2-C7	-2.15	120.28	123.04
3	A	500	NAG	C2-N2-C7	-2.14	120.28	123.04
3	D	401	NAG	C6-C5-C4	-2.08	107.89	113.02
6	M	1202	NAG	C2-N2-C7	-2.07	120.38	123.04
3	D	402	BMA	C1-O5-C5	-2.07	109.62	112.25
6	N	1701	NAG	C3-C4-C5	2.00	113.69	110.20
3	B	500	NAG	C1-O5-C5	2.13	114.95	112.25
3	B	400	NAG	C3-C4-C5	2.14	113.92	110.20
3	D	500	NAG	C1-O5-C5	2.15	114.98	112.25
6	O	2202	NAG	C4-C3-C2	2.19	114.64	111.23
3	B	501	NAG	C4-C3-C2	2.23	114.69	111.23
3	B	401	NAG	C1-O5-C5	2.36	115.24	112.25
3	M	1302	NAG	C1-O5-C5	2.59	115.53	112.25
3	M	1302	NAG	C2-N2-C7	2.76	126.58	123.04
3	M	1303	BMA	C3-C4-C5	2.85	115.16	110.20
3	B	500	NAG	C4-C3-C2	2.91	115.75	111.23
6	N	1702	NAG	C1-O5-C5	2.99	116.05	112.25
3	M	1301	NAG	O4-C4-C3	3.19	117.51	110.34
6	N	1701	NAG	C1-O5-C5	3.61	116.83	112.25

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	M	1301	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	O	2202	NAG	C8-C7-N2-C2
6	O	2202	NAG	O7-C7-N2-C2

There are no ring outliers.

12 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	NAG	1	0
3	A	402	BMA	1	0
3	A	500	NAG	2	0
3	B	401	NAG	1	0
3	B	500	NAG	3	0
3	B	501	NAG	2	0
3	C	500	NAG	1	0
3	D	400	NAG	1	0
3	D	500	NAG	4	0
3	D	501	NAG	1	0
3	M	1301	NAG	2	0
3	M	1302	NAG	1	0

5.6 Ligand geometry

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 for Mogul analysis.

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	$\# Z > 2$
5	NAG	L	2401	2	14,14,15	0.44	0	15,19,21	0.81	0
5	NAG	L	2701	2	14,14,15	0.43	0	15,19,21	1.22	2 (13%)
5	NAG	N	1401	2	14,14,15	0.58	0	15,19,21	0.81	0
5	NAG	N	1601	2	14,14,15	0.48	0	15,19,21	0.82	1 (6%)
5	NAG	O	2001	2	14,14,15	0.55	0	15,19,21	1.73	4 (26%)
5	NAG	O	2101	2	14,14,15	0.43	0	15,19,21	1.01	1 (6%)
5	NAG	O	2301	2	14,14,15	0.42	0	15,19,21	1.00	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
5	NAG	L	2401	2	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	L	2701	2	-	0/6/23/26	0/1/1/1
5	NAG	N	1401	2	-	0/6/23/26	0/1/1/1
5	NAG	N	1601	2	-	0/6/23/26	0/1/1/1
5	NAG	O	2001	2	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	O	2101	2	-	0/6/23/26	0/1/1/1
5	NAG	O	2301	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	2001	NAG	C3-C4-C5	-2.52	105.80	110.20
5	O	2001	NAG	C2-N2-C7	-2.27	120.12	123.04
5	L	2701	NAG	C6-C5-C4	-2.26	107.44	113.02
5	O	2001	NAG	C4-C3-C2	-2.13	107.92	111.23
5	N	1601	NAG	C2-N2-C7	-2.03	120.44	123.04
5	O	2101	NAG	C1-O5-C5	2.43	115.34	112.25
5	L	2701	NAG	O5-C5-C6	2.98	113.80	107.35
5	O	2001	NAG	C1-O5-C5	4.58	118.06	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	O	2001	NAG	C1
5	L	2401	NAG	C1

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	O	2001	NAG	3	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	98/110 (89%)	0.28	4 (4%)	41	41	43, 69, 129, 148	0
1	B	98/110 (89%)	0.37	4 (4%)	41	41	44, 65, 109, 125	0
1	C	97/110 (88%)	0.28	1 (1%)	84	85	35, 53, 93, 137	0
1	D	99/110 (90%)	0.29	5 (5%)	32	30	35, 57, 118, 142	0
2	L	196/213 (92%)	0.24	7 (3%)	46	46	41, 61, 120, 166	0
2	M	179/213 (84%)	0.37	6 (3%)	49	49	43, 68, 130, 150	0
2	N	194/213 (91%)	0.53	6 (3%)	52	52	37, 67, 125, 143	0
2	O	193/213 (90%)	0.27	6 (3%)	52	52	35, 62, 114, 159	0
All	All	1154/1292 (89%)	0.34	39 (3%)	49	49	35, 62, 121, 166	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	280	GLN	8.0
2	O	282	GLY	4.4
2	N	205	ASN	4.2
2	M	156	ASN	3.4
2	L	201	GLU	3.3
2	L	268	GLN	3.3
2	M	202	ALA	3.1
2	N	206	ASP	3.1
2	O	153	SER	3.0
1	D	117	GLU	2.9
2	O	236	LEU	2.9
1	A	186	PHE	2.8
2	L	209	TYR	2.7
2	N	154	ILE	2.7
1	B	119	LEU	2.5
1	D	192	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	120	LYS	2.4
1	C	184	THR	2.4
2	M	158	ASN	2.4
1	D	118	ILE	2.4
2	M	213	MET	2.4
2	N	209	TYR	2.3
1	A	194	GLN	2.3
1	B	170	GLY	2.2
1	B	118	ILE	2.2
2	L	267	HIS	2.2
2	M	180	ASP	2.2
2	N	157	LEU	2.2
2	O	283	SER	2.2
2	L	141	ASN	2.2
1	A	193	SER	2.1
2	O	157	LEU	2.1
2	M	159	VAL	2.1
2	L	282	GLY	2.1
2	N	138	ILE	2.1
1	D	122	ILE	2.1
1	B	151	PHE	2.0
2	L	210	GLN	2.0
1	A	210	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	A	500	14/15	0.95	0.21	2.60	62,80,96,97	0
3	NAG	A	400	14/15	0.95	0.18	0.49	40,70,88,97	0
3	NAG	M	1301	14/15	0.87	0.17	0.09	64,89,127,133	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	NAG	N	1701	14/15	0.92	0.21	-0.06	39,52,73,81	0
3	NAG	D	500	14/15	0.93	0.17	-0.06	56,71,89,91	0
3	NAG	B	500	14/15	0.94	0.17	-0.18	56,83,105,109	0
3	NAG	C	500	14/15	0.97	0.20	-0.18	32,55,61,75	0
3	NAG	B	400	14/15	0.92	0.13	-0.39	59,77,85,101	0
3	NAG	D	400	14/15	0.92	0.16	-0.41	50,72,92,103	0
3	NAG	C	400	14/15	0.97	0.18	-0.77	36,50,63,66	0
6	NAG	M	1201	14/15	0.94	0.14	-0.82	57,70,96,96	0
6	NAG	O	2201	14/15	0.96	0.14	-1.20	56,77,100,102	0
6	NAG	L	2601	14/15	0.90	0.13	-1.24	59,82,106,112	0
6	NAG	M	1202	14/15	0.91	0.14	-	91,110,119,119	0
3	NAG	B	501	14/15	0.92	0.14	-	57,90,111,128	0
3	NAG	D	401	14/15	0.89	0.14	-	74,105,121,133	0
3	BMA	B	402	11/12	0.65	0.16	-	107,138,147,149	0
6	NAG	L	2602	14/15	0.86	0.18	-	80,124,130,132	0
6	NAG	N	1702	14/15	0.88	0.17	-	29,98,118,119	0
3	NAG	D	501	14/15	0.88	0.19	-	64,89,111,123	0
3	BMA	M	1303	11/12	0.73	0.19	-	119,134,140,141	0
3	BMA	C	502	11/12	0.91	0.14	-	57,81,102,112	0
3	BMA	D	402	11/12	0.63	0.16	-	91,130,139,139	0
3	BMA	C	402	11/12	0.69	0.32	-	92,123,139,140	0
3	BMA	B	502	11/12	0.59	0.18	-	90,122,131,131	0
3	NAG	M	1302	14/15	0.84	0.19	-	89,121,127,140	0
3	NAG	A	501	14/15	0.91	0.22	-	89,106,114,120	0
3	NAG	B	401	14/15	0.88	0.13	-	93,118,130,141	0
3	NAG	A	401	14/15	0.90	0.11	-	114,125,140,150	0
6	NAG	O	2202	14/15	0.88	0.15	-	105,122,131,132	0
3	NAG	C	501	14/15	0.96	0.14	-	53,64,75,81	0
3	NAG	C	401	14/15	0.95	0.16	-	50,60,72,83	0
3	BMA	A	402	11/12	0.73	0.17	-	125,142,155,155	0
3	BMA	A	502	11/12	0.82	0.26	-	85,115,129,137	0
3	BMA	D	502	11/12	0.77	0.15	-	94,126,135,139	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
5	NAG	O	2001	14/15	0.77	0.34	3.76	72,132,193,197	0
5	NAG	O	2301	14/15	0.93	0.17	-0.25	49,71,78,90	0
5	NAG	L	2701	14/15	0.91	0.17	-0.50	55,72,90,100	0
5	NAG	N	1601	14/15	0.91	0.19	-0.55	34,61,71,78	0
4	CS	C	1216	1/1	0.89	0.13	-1.47	135,135,135,135	0
5	NAG	O	2101	14/15	0.71	0.20	-	88,114,133,134	0
5	NAG	N	1401	14/15	0.85	0.23	-	99,119,126,128	0
4	CS	B	1215	1/1	0.97	0.17	-	85,85,85,85	1
5	NAG	L	2401	14/15	0.58	0.33	-	111,164,183,184	0

6.5 Other polymers [i](#)

There are no such residues in this entry.