Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:36 PM GMT

PDB ID	:	4CPZ
Title	:	Structure of the Neuraminidase from the B-Lyon-CHU-15.216-2011 virus in complex with Zanamivir
Authors	:	Vachieri, S.G.; Collins, P.J.; Escuret, V.; Casalegno, J.S.; Cattle, N.; Ferraris, O.; Sabatier, M.; Frobert, E.; Caro, V.; Skehel, J.J.; Gamblin, S.J.; Valla, F.; Valette, M.; Ottmann, M.; McCauley, J.W.; Daniels, R.S.; Lina, B.
Deposited on	:	2014-02-09
Resolution	:	2.20 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

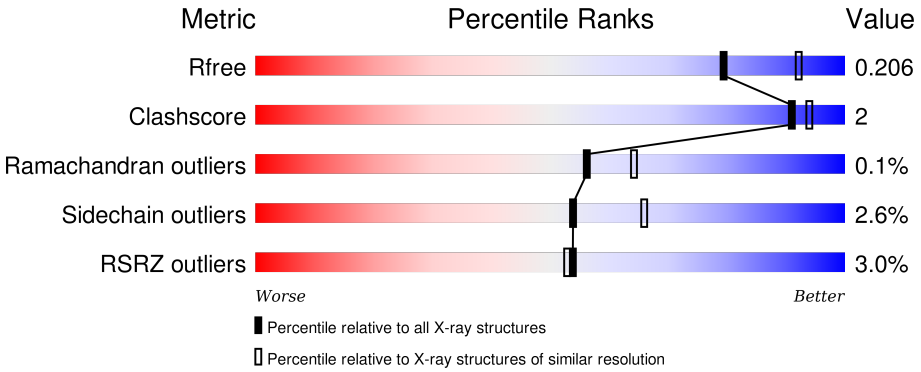
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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.

Mol	Chain	Length	Quality of chain
1	A	466	79% · 16%
1	B	466	80% · 16%
1	C	466	% 80% · 16%
1	D	466	78% 5% 16%
1	E	466	4% 74% 9% · 16%

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Mol	Chain	Length	Quality of chain
1	F	466	6% 77% 6% 16%
1	G	466	3% 74% 10% 16%
1	H	466	4% 76% 7% 16%

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
7	EDO	D	1472	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 25984 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 NEURAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3017	1891	520	577	29			
1	B	390	Total	C	N	O	S	0	0	0
			3017	1891	520	577	29			
1	C	390	Total	C	N	O	S	0	0	0
			3017	1891	520	577	29			
1	D	390	Total	C	N	O	S	0	0	0
			3017	1891	520	577	29			
1	E	390	Total	C	N	O	S	0	0	0
			3013	1890	520	574	29			
1	F	390	Total	C	N	O	S	0	0	0
			3014	1890	520	575	29			
1	G	390	Total	C	N	O	S	0	0	0
			3014	1890	520	575	29			
1	H	390	Total	C	N	O	S	0	0	0
			3017	1891	520	577	29			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	E	1	Total	Ca	0	0
			1	1		
2	H	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

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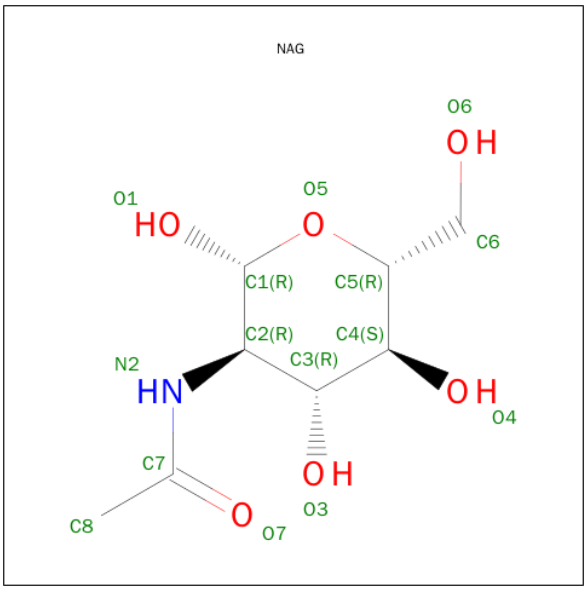
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	F	1	Total Ca 1 1	0	0

- 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 39 22 2 15	0	0
3	B	3	Total C N O 39 22 2 15	0	0
3	D	3	Total C N O 39 22 2 15	0	0
3	E	3	Total C N O 39 22 2 15	0	0
3	F	3	Total C N O 39 22 2 15	0	0
3	G	3	Total C N O 39 22 2 15	0	0

- 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 14 8 1 5	0	0

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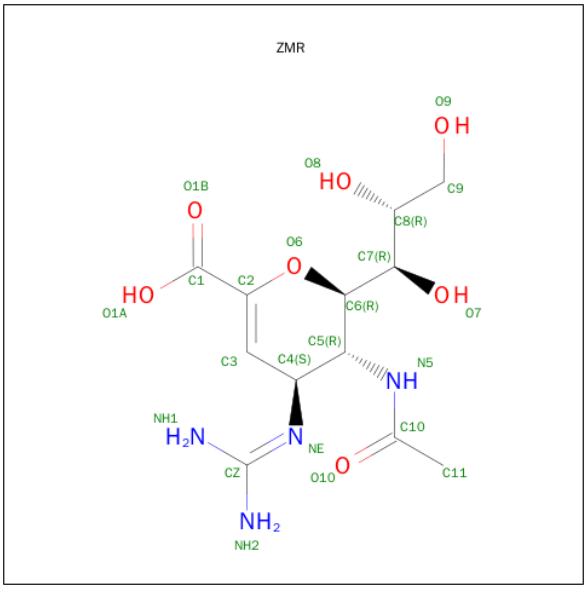
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	E	1	Total C N O 14 8 1 5	0	0
4	G	1	Total C N O 14 8 1 5	0	0
4	H	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is ZANAMIVIR (three-letter code: ZMR) (formula: $C_{12}H_{20}N_4O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C N O 23 12 4 7	0	0
5	B	1	Total C N O 23 12 4 7	0	0
5	C	1	Total C N O 23 12 4 7	0	0
5	D	1	Total C N O 23 12 4 7	0	0
5	E	1	Total C N O 23 12 4 7	0	0

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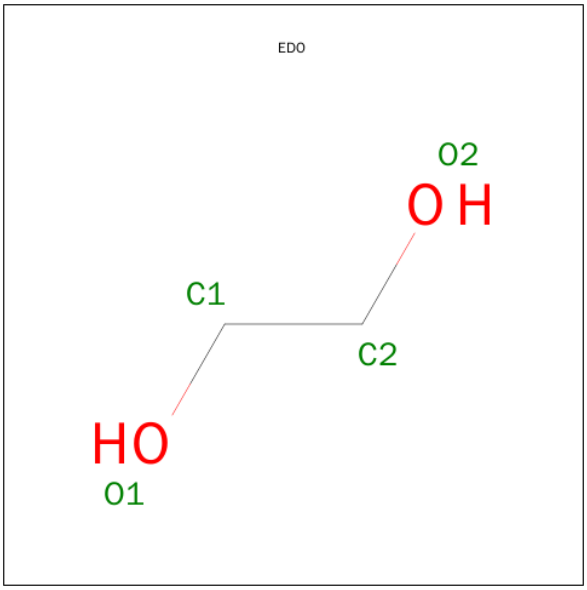
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	F	1	Total C N O 23 12 4 7	0	0
5	G	1	Total C N O 23 12 4 7	0	0
5	H	1	Total C N O 23 12 4 7	0	0

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

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

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total C O 4 2 2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	314	Total O 314 314	0	0

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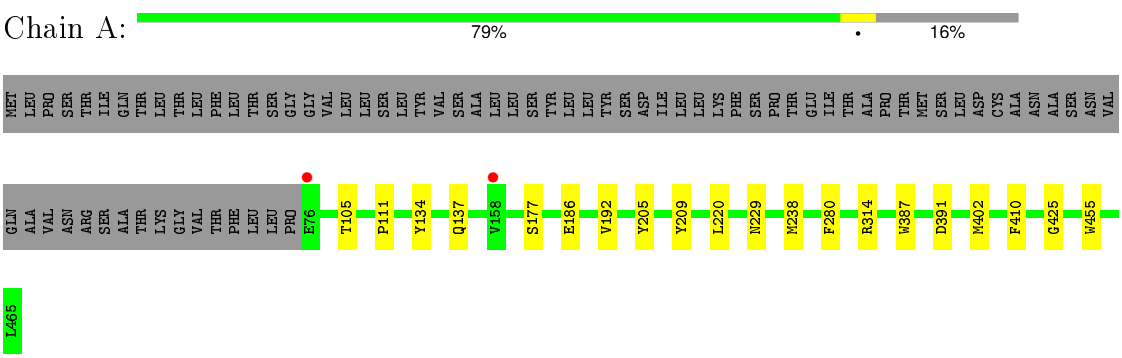
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	251	Total O 251 251	0	0
8	C	255	Total O 255 255	0	0
8	D	188	Total O 188 188	0	0
8	E	102	Total O 102 102	0	0
8	F	50	Total O 50 50	0	0
8	G	58	Total O 58 58	0	0
8	H	56	Total O 56 56	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

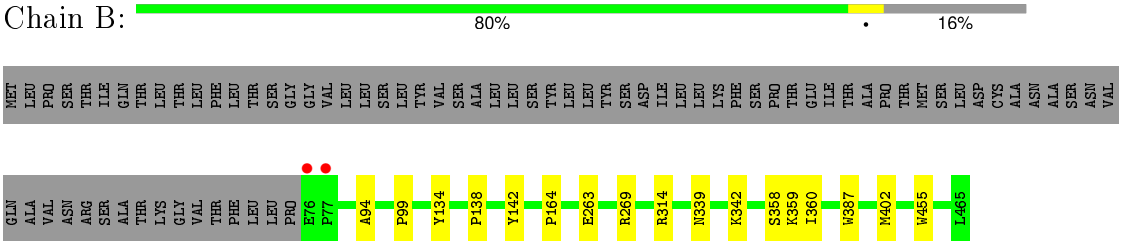
- Molecule 1: NEURAMINIDASE

Chain A:



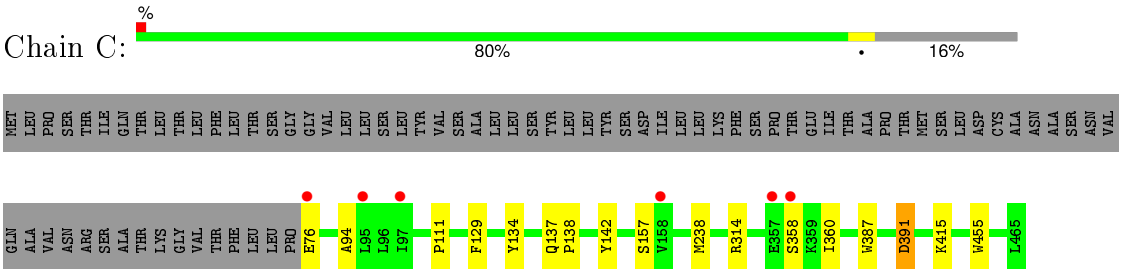
- Molecule 1: NEURAMINIDASE

Chain B:



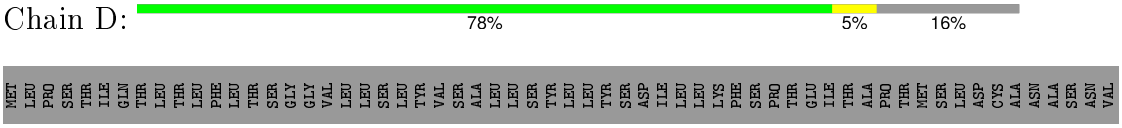
- Molecule 1: NEURAMINIDASE

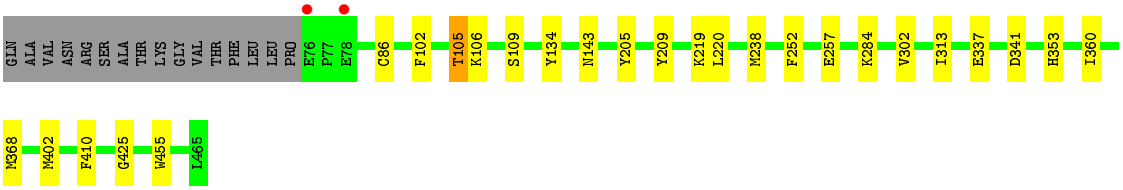
Chain C:



- Molecule 1: NEURAMINIDASE

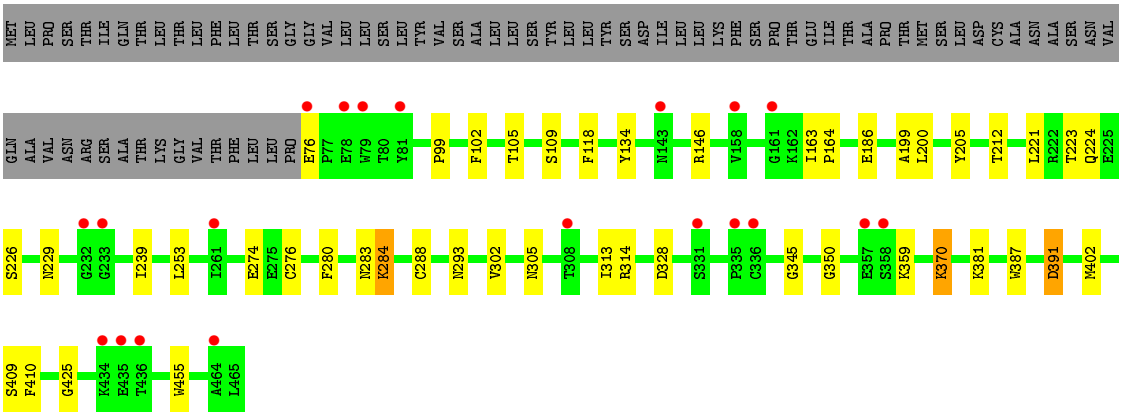
Chain D:





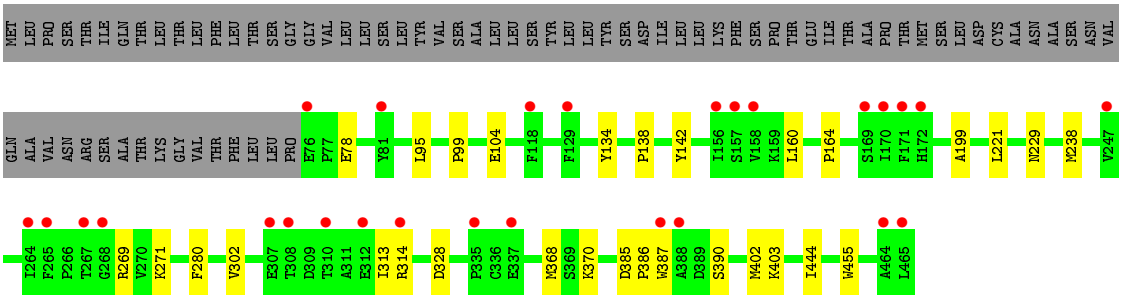
• Molecule 1: NEURAMINIDASE

Chain E:



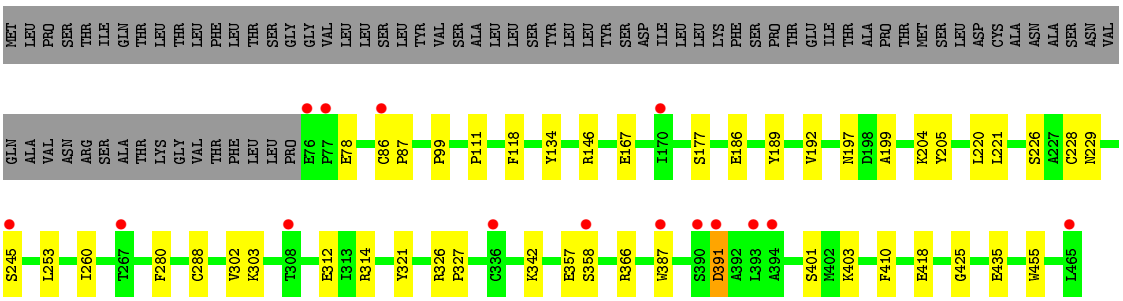
• Molecule 1: NEURAMINIDASE

Chain F:



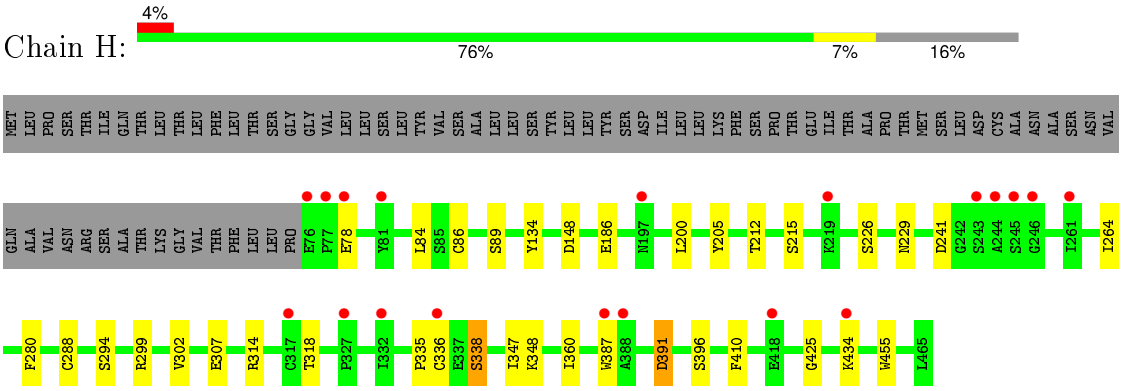
• Molecule 1: NEURAMINIDASE

Chain G:



• Molecule 1: NEURAMINIDASE

Chain H:


4%
76%
7%
16%
MET LEU PRO SER THR ILE GLN THR LEU THR LEU PHE LEU THR SER GLY GLY VAL LEU LEU SER LEU TYR VAL SER ALA LEU LEU SER TYR LEU LEU TYR SER ASP ILE LEU LEU LYS PHE SER PRO THR GLU ILE THR ALA PRO THR MET SER LEU ASP CYS ALA ASN ALA SER ASN VAL
GLN ALA VAL ASN ARG SER ALA THR LYS GLY VAL THR PHE LEU LEU PRO
E76 F77 E78 Y81 L84 S85 C86 S89 Y134 D148 E186 N197 L200 Y205 T212 S215 K219 S226 N229 D241 G242 S243 A244 S245 G246 T261 I264
F280 C288 S294 R299 V302 E307 R314 C317 T318 P327 I332 P335 C336 E337 S338 I347 K348 I360 W387 A388 D391 S396 F410 E418 G425 K434 W455 L465

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	89.34Å 163.25Å 123.45Å 90.00° 108.31° 90.00°	Depositor
Resolution (Å)	48.50 – 2.20 48.50 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.8 (48.50-2.20) 96.4 (48.50-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.31 (at 2.20Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.153 , 0.200 0.165 , 0.206	Depositor DCC
R_{free} test set	8173 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	34.4	Xtriage
Anisotropy	0.711	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.5	EDS
Estimated twinning fraction	0.029 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	1 of 163705 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	25984	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ZMR, CA, BMA, NAG, EDO

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	0.47	0/3091	0.61	0/4176
1	B	0.41	0/3091	0.57	0/4176
1	C	0.45	0/3091	0.60	0/4176
1	D	0.42	0/3091	0.57	0/4176
1	E	0.31	0/3087	0.50	0/4172
1	F	0.31	0/3088	0.50	0/4172
1	G	0.32	0/3088	0.52	0/4172
1	H	0.30	0/3091	0.51	0/4176
All	All	0.38	0/24718	0.55	0/33396

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

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	3017	0	2891	8	0
1	B	3017	0	2891	9	0
1	C	3017	0	2891	6	0
1	D	3017	0	2891	15	0
1	E	3013	0	2889	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3014	0	2890	12	0
1	G	3014	0	2889	20	0
1	H	3017	0	2891	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	39	0	34	1	0
3	B	39	0	34	1	0
3	D	39	0	34	0	0
3	E	39	0	34	1	0
3	F	39	0	34	0	0
3	G	39	0	34	0	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
4	E	14	0	13	0	0
4	G	14	0	13	0	0
4	H	14	0	13	0	0
5	A	23	0	19	0	0
5	B	23	0	19	0	0
5	C	23	0	19	0	0
5	D	23	0	18	0	0
5	E	23	0	19	0	0
5	F	23	0	19	0	0
5	G	23	0	19	0	0
5	H	23	0	19	1	0
6	C	28	0	25	0	0
6	H	28	0	25	0	0
7	D	4	0	6	2	0
8	A	314	0	0	2	1
8	B	251	0	0	3	0
8	C	255	0	0	0	1
8	D	188	0	0	4	0
8	E	102	0	0	1	0
8	F	50	0	0	0	0
8	G	58	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	56	0	0	0	0
All	All	25984	0	23625	105	1

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 2.

All (105) 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:D:86:CYS:HB2	8:D:2009:HOH:O	1.90	0.71
1:G:312:GLU:OE2	1:G:314:ARG:NH2	2.28	0.66
1:B:358:SER:O	8:B:2209:HOH:O	2.14	0.66
1:E:359:LYS:NZ	8:E:2084:HOH:O	2.21	0.63
1:H:200:LEU:HD11	1:H:212:THR:HB	1.82	0.61
1:B:314:ARG:HB2	1:B:387:TRP:CD1	2.37	0.60
1:F:302:VAL:HG22	1:F:313:ILE:HG12	1.85	0.58
1:H:314:ARG:HB2	1:H:387:TRP:CD1	2.38	0.57
1:E:391:ASP:OD1	1:E:391:ASP:N	2.38	0.57
1:E:350:GLY:N	1:E:409:SER:OG	2.37	0.57
1:G:401:SER:HB2	1:G:403:LYS:HE3	1.88	0.56
1:E:314:ARG:HB2	1:E:387:TRP:CD1	2.41	0.55
1:F:95:LEU:HD23	1:F:444:ILE:HD12	1.87	0.55
1:H:391:ASP:N	1:H:391:ASP:OD1	2.40	0.55
1:E:284:LYS:HD2	1:E:305:ASN:HD21	1.73	0.54
1:D:368:MET:HB2	1:D:402:MET:HG3	1.89	0.53
1:F:368:MET:HB2	1:F:402:MET:HG3	1.91	0.53
1:D:205:TYR:CE1	7:D:1472:EDO:H11	2.44	0.52
1:G:99:PRO:HB2	1:G:111:PRO:HB3	1.92	0.52
1:D:302:VAL:HG22	1:D:313:ILE:HG12	1.92	0.52
1:C:391:ASP:N	1:C:391:ASP:OD1	2.34	0.51
1:E:200:LEU:HD11	1:E:212:THR:HB	1.93	0.51
1:C:314:ARG:HB2	1:C:387:TRP:CD1	2.46	0.51
1:H:229:ASN:HB3	1:H:280:PHE:CE2	2.46	0.51
1:F:199:ALA:HB3	1:F:221:LEU:HB3	1.93	0.51
1:F:328:ASP:OD1	1:F:370:LYS:HE2	2.11	0.50
1:E:223:THR:OG1	1:E:224:GLN:N	2.43	0.49
1:G:391:ASP:OD1	1:G:391:ASP:N	2.44	0.49
1:E:276:CYS:HB3	1:E:288:CYS:HB3	1.95	0.48
1:H:299:ARG:HH22	1:H:347:ILE:HG23	1.77	0.48
1:F:99:PRO:HG3	1:F:164:PRO:HD2	1.94	0.48
1:A:314:ARG:HB2	1:A:387:TRP:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:335:PRO:O	1:H:338:SER:OG	2.32	0.48
1:F:269:ARG:NH2	1:F:271:LYS:HE2	2.30	0.47
1:H:288:CYS:HB2	1:H:302:VAL:HB	1.96	0.47
1:E:99:PRO:HG3	1:E:164:PRO:HD2	1.97	0.46
1:A:391:ASP:OD1	8:A:2275:HOH:O	2.20	0.46
1:D:341:ASP:N	8:D:2137:HOH:O	2.48	0.46
1:F:314:ARG:HB2	1:F:387:TRP:CD1	2.50	0.46
1:A:111:PRO:HD2	1:A:137:GLN:O	2.15	0.46
1:G:118:PHE:CG	1:G:226:SER:HA	2.51	0.46
1:C:111:PRO:HD2	1:C:137:GLN:O	2.16	0.46
1:E:328:ASP:OD1	1:E:370:LYS:HE2	2.16	0.46
1:F:138:PRO:HA	1:F:142:TYR:OH	2.15	0.46
1:D:105:THR:HG22	8:D:2020:HOH:O	2.14	0.45
1:E:229:ASN:HB3	1:E:280:PHE:CE1	2.51	0.45
1:G:253:LEU:HD13	1:G:260:ILE:HD13	1.97	0.45
1:B:138:PRO:HA	1:B:142:TYR:OH	2.16	0.45
1:D:106:LYS:HB2	8:D:2021:HOH:O	2.15	0.45
1:G:229:ASN:HB3	1:G:280:PHE:CE2	2.52	0.45
1:E:199:ALA:HB3	1:E:221:LEU:HB3	1.98	0.45
1:H:148:ASP:OD1	5:H:1470:ZMR:NE	2.49	0.45
1:G:189:TYR:HB2	1:G:204:LYS:HB3	1.99	0.45
1:B:94:ALA:HB1	1:D:209:TYR:CZ	2.52	0.45
1:C:138:PRO:HA	1:C:142:TYR:OH	2.17	0.44
1:A:410:PHE:CZ	1:A:425:GLY:HA3	2.53	0.44
1:G:177:SER:HB3	1:G:192:VAL:HB	2.00	0.44
1:A:177:SER:HB3	1:A:192:VAL:HB	1.98	0.44
1:E:163:ILE:HA	1:E:164:PRO:HD3	1.81	0.44
1:B:402:MET:SD	1:G:435:GLU:HG2	2.57	0.44
1:B:269:ARG:HH21	1:B:339:ASN:HD21	1.65	0.44
1:D:353:HIS:HD2	1:D:360:ILE:HD11	1.82	0.44
1:H:186:GLU:HB3	1:H:205:TYR:CZ	2.52	0.44
1:G:199:ALA:HB3	1:G:221:LEU:HB3	1.99	0.44
1:G:86:CYS:HB3	1:G:87:PRO:HD2	2.00	0.44
1:D:257:GLU:N	7:D:1472:EDO:H22	2.31	0.43
1:G:327:PRO:HD3	1:G:342:LYS:HB2	2.00	0.43
1:H:226:SER:HB3	1:H:348:LYS:HE3	1.99	0.43
1:B:359:LYS:HB3	8:B:2209:HOH:O	2.17	0.43
1:E:302:VAL:HG22	1:E:313:ILE:HG12	2.01	0.43
1:G:167:GLU:OE2	8:G:2029:HOH:O	2.21	0.43
1:E:381:LYS:HE2	1:E:391:ASP:HB2	2.01	0.43
1:D:102:PHE:O	1:D:109:SER:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:TYR:CZ	1:C:94:ALA:HB1	2.54	0.42
1:B:269:ARG:HH21	1:B:339:ASN:ND2	2.17	0.42
1:F:385:ASP:HA	1:F:386:PRO:HD2	1.93	0.42
3:A:1467:NAG:H83	8:A:2207:HOH:O	2.18	0.42
1:F:160:LEU:HD11	1:F:444:ILE:HD11	2.02	0.42
1:E:186:GLU:HB3	1:E:205:TYR:CZ	2.54	0.42
1:G:288:CYS:HB2	1:G:302:VAL:HB	2.01	0.42
1:D:341:ASP:OD1	1:H:434:LYS:HG2	2.19	0.42
1:H:215:SER:OG	1:H:241:ASP:OD2	2.23	0.42
1:G:321:TYR:O	1:G:366:ARG:NH1	2.49	0.42
1:E:239:ILE:HD13	1:E:253:LEU:HD11	2.02	0.42
1:E:274:GLU:OE2	1:E:293:ASN:HB2	2.20	0.41
1:E:283:ASN:HD22	3:E:1467:NAG:H83	1.85	0.41
1:C:129:PHE:CD1	1:C:157:SER:HB3	2.56	0.41
1:E:118:PHE:CG	1:E:226:SER:HA	2.55	0.41
3:B:1467:NAG:H83	8:B:2162:HOH:O	2.20	0.41
1:E:102:PHE:O	1:E:109:SER:HB2	2.21	0.41
1:G:326:ARG:CZ	1:G:366:ARG:HD2	2.50	0.41
1:E:293:ASN:HA	1:E:345:GLY:O	2.21	0.41
1:D:410:PHE:CZ	1:D:425:GLY:HA3	2.56	0.41
1:H:84:LEU:HA	1:H:84:LEU:HD23	1.85	0.41
1:A:229:ASN:HB3	1:A:280:PHE:CE2	2.56	0.41
1:G:410:PHE:CZ	1:G:425:GLY:HA3	2.56	0.41
1:H:410:PHE:CZ	1:H:425:GLY:HA3	2.56	0.41
1:D:353:HIS:CD2	1:D:360:ILE:HD11	2.56	0.40
1:A:186:GLU:HB3	1:A:205:TYR:CZ	2.57	0.40
1:G:303:LYS:HG3	1:G:387:TRP:CZ2	2.57	0.40
1:F:229:ASN:HB3	1:F:280:PHE:CE2	2.57	0.40
1:G:186:GLU:HB3	1:G:205:TYR:CZ	2.56	0.40
1:E:410:PHE:CZ	1:E:425:GLY:HA3	2.57	0.40
1:D:238:MET:HB2	1:D:252:PHE:CE2	2.56	0.40
1:B:99:PRO:HG3	1:B:164:PRO:HD2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:2305:HOH:O	8:C:2147:HOH:O[1_455]	2.19	0.01

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	388/466 (83%)	375 (97%)	12 (3%)	1 (0%)	46 50
1	B	388/466 (83%)	376 (97%)	12 (3%)	0	100 100
1	C	388/466 (83%)	376 (97%)	12 (3%)	0	100 100
1	D	388/466 (83%)	373 (96%)	14 (4%)	1 (0%)	46 50
1	E	388/466 (83%)	375 (97%)	13 (3%)	0	100 100
1	F	388/466 (83%)	375 (97%)	13 (3%)	0	100 100
1	G	388/466 (83%)	372 (96%)	15 (4%)	1 (0%)	46 50
1	H	388/466 (83%)	374 (96%)	14 (4%)	0	100 100
All	All	3104/3728 (83%)	2996 (96%)	105 (3%)	3 (0%)	56 64

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	220	LEU
1	A	220	LEU
1	D	220	LEU

5.3.2 Protein sidechains (i)

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	323/390 (83%)	318 (98%)	5 (2%)	72 84
1	B	323/390 (83%)	318 (98%)	5 (2%)	72 84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	323/390 (83%)	315 (98%)	8 (2%)	55 67
1	D	323/390 (83%)	316 (98%)	7 (2%)	60 72
1	E	322/390 (83%)	313 (97%)	9 (3%)	51 63
1	F	322/390 (83%)	315 (98%)	7 (2%)	60 72
1	G	322/390 (83%)	311 (97%)	11 (3%)	44 54
1	H	323/390 (83%)	309 (96%)	14 (4%)	35 43
All	All	2581/3120 (83%)	2515 (97%)	66 (3%)	54 66

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	THR
1	A	134	TYR
1	A	238	MET
1	A	402	MET
1	A	455	TRP
1	B	134	TYR
1	B	263	GLU
1	B	342	LYS
1	B	360	ILE
1	B	455	TRP
1	C	76	GLU
1	C	134	TYR
1	C	238	MET
1	C	358	SER
1	C	360	ILE
1	C	391	ASP
1	C	415	LYS
1	C	455	TRP
1	D	105	THR
1	D	134	TYR
1	D	143	ASN
1	D	219	LYS
1	D	284	LYS
1	D	337	GLU
1	D	455	TRP
1	E	76	GLU
1	E	105	THR
1	E	134	TYR
1	E	146	ARG

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Mol	Chain	Res	Type
1	E	284	LYS
1	E	370	LYS
1	E	391	ASP
1	E	402	MET
1	E	455	TRP
1	F	78	GLU
1	F	104	GLU
1	F	134	TYR
1	F	238	MET
1	F	390	SER
1	F	403	LYS
1	F	455	TRP
1	G	78	GLU
1	G	134	TYR
1	G	146	ARG
1	G	197	ASN
1	G	228	CYS
1	G	245	SER
1	G	357	GLU
1	G	358	SER
1	G	391	ASP
1	G	418	GLU
1	G	455	TRP
1	H	78	GLU
1	H	86	CYS
1	H	89	SER
1	H	134	TYR
1	H	264	ILE
1	H	294	SER
1	H	307	GLU
1	H	318	THR
1	H	336	CYS
1	H	338	SER
1	H	360	ILE
1	H	391	ASP
1	H	396	SER
1	H	455	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	339	ASN

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

22 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	1467	1,3	14,14,15	0.36	0	15,19,21	0.28	0
3	NAG	A	1468	3	14,14,15	0.42	0	15,19,21	0.31	0
3	BMA	A	1469	3	11,11,12	0.96	0	14,15,17	0.79	0
3	NAG	B	1467	1,3	14,14,15	0.55	0	15,19,21	0.47	0
3	NAG	B	1468	3	14,14,15	0.25	0	15,19,21	0.42	0
3	BMA	B	1469	3	11,11,12	1.56	2 (18%)	14,15,17	1.94	4 (28%)
6	NAG	C	1467	1,6	14,14,15	0.39	0	15,19,21	0.20	0
6	NAG	C	1468	6	14,14,15	0.17	0	15,19,21	0.37	0
3	NAG	D	1467	1,3	14,14,15	0.43	0	15,19,21	0.37	0
3	NAG	D	1468	3	14,14,15	0.31	0	15,19,21	0.51	0
3	BMA	D	1469	3	11,11,12	0.78	0	14,15,17	0.84	0
3	NAG	E	1467	1,3	14,14,15	0.39	0	15,19,21	0.23	0
3	NAG	E	1468	3	14,14,15	0.28	0	15,19,21	0.31	0
3	BMA	E	1469	3	11,11,12	0.53	0	14,15,17	0.95	1 (7%)
3	NAG	F	1467	1,3	14,14,15	0.41	0	15,19,21	0.58	0
3	NAG	F	1468	3	14,14,15	0.76	1 (7%)	15,19,21	1.21	1 (6%)
3	BMA	F	1469	3	11,11,12	1.08	1 (9%)	14,15,17	0.92	0
3	NAG	G	1467	1,3	14,14,15	0.26	0	15,19,21	0.34	0
3	NAG	G	1468	3	14,14,15	0.29	0	15,19,21	0.31	0
3	BMA	G	1469	3	11,11,12	1.07	1 (9%)	14,15,17	0.80	0
6	NAG	H	1467	1,6	14,14,15	0.41	0	15,19,21	1.67	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	NAG	H	1468	6	14,14,15	0.40	0	15,19,21	0.43	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
3	NAG	A	1467	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1468	3	-	0/6/23/26	0/1/1/1
3	BMA	A	1469	3	-	0/2/19/22	0/1/1/1
3	NAG	B	1467	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1468	3	-	0/6/23/26	0/1/1/1
3	BMA	B	1469	3	-	0/2/19/22	0/1/1/1
6	NAG	C	1467	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	1468	6	-	0/6/23/26	0/1/1/1
3	NAG	D	1467	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	1468	3	-	0/6/23/26	0/1/1/1
3	BMA	D	1469	3	-	0/2/19/22	0/1/1/1
3	NAG	E	1467	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	1468	3	-	0/6/23/26	0/1/1/1
3	BMA	E	1469	3	-	0/2/19/22	0/1/1/1
3	NAG	F	1467	1,3	-	0/6/23/26	0/1/1/1
3	NAG	F	1468	3	-	0/6/23/26	0/1/1/1
3	BMA	F	1469	3	-	0/2/19/22	0/1/1/1
3	NAG	G	1467	1,3	-	0/6/23/26	0/1/1/1
3	NAG	G	1468	3	-	0/6/23/26	0/1/1/1
3	BMA	G	1469	3	-	0/2/19/22	0/1/1/1
6	NAG	H	1467	1,6	-	0/6/23/26	0/1/1/1
6	NAG	H	1468	6	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1469	BMA	C1-C2	2.04	1.57	1.52
3	F	1469	BMA	C4-C3	2.21	1.58	1.52
3	F	1468	NAG	O5-C1	2.39	1.47	1.43
3	B	1469	BMA	C1-C2	2.88	1.59	1.52
3	B	1469	BMA	C2-C3	3.94	1.57	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	H	1467	NAG	C4-C3-C2	-2.36	107.56	111.23
3	E	1469	BMA	O2-C2-C3	-2.24	105.61	110.12
3	B	1469	BMA	O2-C2-C3	-2.02	106.06	110.12
6	H	1467	NAG	C1-O5-C5	2.21	115.06	112.25
3	B	1469	BMA	C2-C3-C4	2.63	115.51	111.04
3	B	1469	BMA	O5-C1-C2	2.88	115.53	110.86
3	F	1468	NAG	C1-O5-C5	4.59	118.08	112.25
6	H	1467	NAG	C2-N2-C7	5.21	129.73	123.04
3	B	1469	BMA	C1-C2-C3	5.43	115.96	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1467	NAG	1	0
3	B	1467	NAG	1	0
3	E	1467	NAG	1	0

5.6 Ligand geometry (i)

Of 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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	$\#\|Z\| > 2$
4	NAG	A	1470	1	14,14,15	0.36	0	15,19,21	0.36	0
5	ZMR	A	1471	-	15,23,23	5.79	8 (53%)	18,32,32	3.83	5 (27%)
4	NAG	B	1470	1	14,14,15	0.63	0	15,19,21	0.42	0
5	ZMR	B	1471	-	15,23,23	5.80	8 (53%)	18,32,32	3.28	4 (22%)
4	NAG	C	1469	1	14,14,15	0.26	0	15,19,21	0.37	0
5	ZMR	C	1470	-	15,23,23	5.41	8 (53%)	18,32,32	4.13	5 (27%)
4	NAG	D	1470	1	14,14,15	0.48	0	15,19,21	0.43	0
5	ZMR	D	1471	-	15,23,23	5.51	8 (53%)	18,32,32	3.93	4 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	EDO	D	1472	-	3,3,3	0.47	0	2,2,2	0.20	0
4	NAG	E	1470	1	14,14,15	0.44	0	15,19,21	0.38	0
5	ZMR	E	1471	-	15,23,23	5.53	8 (53%)	18,32,32	4.05	5 (27%)
5	ZMR	F	1470	-	15,23,23	5.50	8 (53%)	18,32,32	3.87	4 (22%)
4	NAG	G	1470	1	14,14,15	0.38	0	15,19,21	0.64	1 (6%)
5	ZMR	G	1471	-	15,23,23	5.60	8 (53%)	18,32,32	3.36	4 (22%)
4	NAG	H	1469	1	14,14,15	0.48	0	15,19,21	0.45	0
5	ZMR	H	1470	-	15,23,23	5.47	8 (53%)	18,32,32	4.12	5 (27%)

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	1470	1	-	0/6/23/26	0/1/1/1
5	ZMR	A	1471	-	-	0/14/38/38	0/1/1/1
4	NAG	B	1470	1	-	0/6/23/26	0/1/1/1
5	ZMR	B	1471	-	-	0/14/38/38	0/1/1/1
4	NAG	C	1469	1	-	0/6/23/26	0/1/1/1
5	ZMR	C	1470	-	-	0/14/38/38	0/1/1/1
4	NAG	D	1470	1	-	0/6/23/26	0/1/1/1
5	ZMR	D	1471	-	-	0/14/38/38	0/1/1/1
7	EDO	D	1472	-	-	0/1/1/1	0/0/0/0
4	NAG	E	1470	1	-	0/6/23/26	0/1/1/1
5	ZMR	E	1471	-	-	0/14/38/38	0/1/1/1
5	ZMR	F	1470	-	-	0/14/38/38	0/1/1/1
4	NAG	G	1470	1	-	0/6/23/26	0/1/1/1
5	ZMR	G	1471	-	-	0/14/38/38	0/1/1/1
4	NAG	H	1469	1	-	0/6/23/26	0/1/1/1
5	ZMR	H	1470	-	-	0/14/38/38	0/1/1/1

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1471	ZMR	C6-C5	-4.87	1.45	1.53
5	B	1471	ZMR	C6-C5	-4.61	1.45	1.53
5	F	1470	ZMR	C6-C5	-4.61	1.45	1.53
5	H	1470	ZMR	C6-C5	-4.53	1.45	1.53
5	D	1471	ZMR	C6-C5	-4.51	1.45	1.53
5	C	1470	ZMR	C6-C5	-4.42	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1471	ZMR	C6-C5	-4.22	1.46	1.53
5	G	1471	ZMR	C6-C5	-4.22	1.46	1.53
5	D	1471	ZMR	O7-C7	-2.61	1.36	1.43
5	G	1471	ZMR	O7-C7	-2.55	1.36	1.43
5	A	1471	ZMR	O7-C7	-2.46	1.37	1.43
5	B	1471	ZMR	O7-C7	-2.44	1.37	1.43
5	C	1470	ZMR	O7-C7	-2.42	1.37	1.43
5	F	1470	ZMR	O8-C8	-2.41	1.37	1.43
5	H	1470	ZMR	O8-C8	-2.38	1.38	1.43
5	G	1471	ZMR	O8-C8	-2.36	1.38	1.43
5	H	1470	ZMR	O7-C7	-2.34	1.37	1.43
5	E	1471	ZMR	O7-C7	-2.33	1.37	1.43
5	D	1471	ZMR	O8-C8	-2.31	1.38	1.43
5	F	1470	ZMR	O7-C7	-2.31	1.37	1.43
5	C	1470	ZMR	O8-C8	-2.24	1.38	1.43
5	E	1471	ZMR	O8-C8	-2.23	1.38	1.43
5	A	1471	ZMR	O8-C8	-2.13	1.38	1.43
5	B	1471	ZMR	O8-C8	-2.11	1.38	1.43
5	C	1470	ZMR	C10-N5	2.17	1.42	1.34
5	A	1471	ZMR	C10-N5	2.30	1.43	1.34
5	B	1471	ZMR	C10-N5	2.44	1.43	1.34
5	D	1471	ZMR	C10-N5	2.46	1.43	1.34
5	F	1470	ZMR	C10-N5	2.50	1.43	1.34
5	G	1471	ZMR	C10-N5	2.54	1.44	1.34
5	H	1470	ZMR	C10-N5	2.58	1.44	1.34
5	E	1471	ZMR	C10-N5	2.71	1.44	1.34
5	C	1470	ZMR	O6-C2	5.46	1.48	1.37
5	H	1470	ZMR	O6-C2	5.59	1.48	1.37
5	D	1471	ZMR	O6-C2	5.63	1.48	1.37
5	A	1471	ZMR	C5-N5	5.79	1.55	1.45
5	C	1470	ZMR	C5-N5	5.86	1.55	1.45
5	A	1471	ZMR	O6-C2	6.15	1.49	1.37
5	E	1471	ZMR	O6-C2	6.27	1.50	1.37
5	F	1470	ZMR	O6-C2	6.38	1.50	1.37
5	G	1471	ZMR	O6-C2	6.41	1.50	1.37
5	D	1471	ZMR	C5-N5	6.41	1.56	1.45
5	F	1470	ZMR	C5-N5	6.41	1.56	1.45
5	B	1471	ZMR	C5-N5	6.49	1.56	1.45
5	B	1471	ZMR	O6-C2	6.56	1.50	1.37
5	H	1470	ZMR	C5-N5	6.61	1.56	1.45
5	G	1471	ZMR	C5-N5	6.69	1.56	1.45
5	E	1471	ZMR	C5-N5	6.86	1.57	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	1471	ZMR	C4-NE	8.22	1.55	1.46
5	C	1470	ZMR	C4-NE	8.29	1.56	1.46
5	D	1471	ZMR	C4-NE	8.32	1.56	1.46
5	A	1471	ZMR	C4-NE	8.36	1.56	1.46
5	F	1470	ZMR	C4-NE	8.46	1.56	1.46
5	G	1471	ZMR	C4-NE	8.50	1.56	1.46
5	B	1471	ZMR	C4-NE	8.69	1.56	1.46
5	H	1470	ZMR	C4-NE	8.98	1.56	1.46
5	H	1470	ZMR	C3-C2	15.92	1.54	1.32
5	F	1470	ZMR	C3-C2	16.12	1.54	1.32
5	C	1470	ZMR	C3-C2	16.38	1.55	1.32
5	E	1471	ZMR	C3-C2	16.39	1.55	1.32
5	D	1471	ZMR	C3-C2	16.55	1.55	1.32
5	G	1471	ZMR	C3-C2	16.60	1.55	1.32
5	B	1471	ZMR	C3-C2	17.46	1.56	1.32
5	A	1471	ZMR	C3-C2	17.84	1.57	1.32

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	1470	ZMR	O6-C2-C3	-12.61	105.85	124.12
5	A	1471	ZMR	O6-C2-C3	-12.39	106.17	124.12
5	F	1470	ZMR	O6-C2-C3	-12.23	106.39	124.12
5	C	1470	ZMR	O6-C2-C3	-12.13	106.54	124.12
5	D	1471	ZMR	O6-C2-C3	-11.60	107.31	124.12
5	C	1470	ZMR	C4-C3-C2	-11.43	111.78	122.76
5	E	1471	ZMR	O6-C2-C3	-11.42	107.56	124.12
5	E	1471	ZMR	C4-C3-C2	-10.88	112.30	122.76
5	G	1471	ZMR	O6-C2-C3	-10.63	108.71	124.12
5	B	1471	ZMR	O6-C2-C3	-10.32	109.17	124.12
5	D	1471	ZMR	C4-C3-C2	-10.03	113.12	122.76
5	H	1470	ZMR	C4-C3-C2	-9.23	113.89	122.76
5	A	1471	ZMR	C4-C3-C2	-8.75	114.35	122.76
5	F	1470	ZMR	C4-C3-C2	-8.32	114.77	122.76
5	B	1471	ZMR	C4-C3-C2	-6.29	116.72	122.76
5	G	1471	ZMR	C4-C5-N5	-6.22	105.37	110.89
5	B	1471	ZMR	C4-C5-N5	-5.44	106.07	110.89
5	G	1471	ZMR	C4-C3-C2	-5.39	117.59	122.76
5	H	1470	ZMR	C4-C5-N5	-4.60	106.81	110.89
5	F	1470	ZMR	C4-C5-N5	-4.57	106.84	110.89
5	E	1471	ZMR	C6-O6-C2	-4.56	107.74	114.79
5	D	1471	ZMR	C6-O6-C2	-4.06	108.52	114.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	H	1470	ZMR	C6-O6-C2	-3.80	108.92	114.79
5	A	1471	ZMR	C4-C5-N5	-3.59	107.71	110.89
5	C	1470	ZMR	C4-C5-N5	-3.35	107.92	110.89
5	C	1470	ZMR	C6-O6-C2	-2.38	111.12	114.79
5	A	1471	ZMR	C6-C5-N5	-2.36	106.96	111.07
5	E	1471	ZMR	C11-C10-N5	2.07	120.07	116.11
4	G	1470	NAG	C1-O5-C5	2.21	115.06	112.25
5	A	1471	ZMR	C6-O6-C2	2.23	118.24	114.79
5	B	1471	ZMR	C6-O6-C2	2.40	118.50	114.79
5	E	1471	ZMR	O9-C9-C8	2.79	117.16	111.10
5	C	1470	ZMR	O9-C9-C8	2.89	117.38	111.10
5	G	1471	ZMR	O9-C9-C8	2.91	117.42	111.10
5	D	1471	ZMR	O9-C9-C8	2.91	117.43	111.10
5	H	1470	ZMR	O9-C9-C8	3.51	118.74	111.10
5	F	1470	ZMR	O9-C9-C8	3.78	119.31	111.10

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
7	D	1472	EDO	2	0
5	H	1470	ZMR	1	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, 95^{th} 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	390/466 (83%)	-0.24	2 (0%)	91	91	15, 24, 41, 78	0
1	B	390/466 (83%)	-0.35	2 (0%)	91	91	17, 27, 44, 100	0
1	C	390/466 (83%)	-0.13	6 (1%)	76	75	18, 29, 44, 94	0
1	D	390/466 (83%)	-0.21	2 (0%)	91	91	20, 34, 54, 100	0
1	E	390/466 (83%)	0.19	20 (5%)	32	31	32, 49, 73, 106	0
1	F	390/466 (83%)	0.16	27 (6%)	20	19	30, 48, 67, 106	0
1	G	390/466 (83%)	0.13	15 (3%)	44	43	32, 52, 81, 109	0
1	H	390/466 (83%)	0.25	19 (4%)	33	33	35, 55, 80, 102	0
All	All	3120/3728 (83%)	-0.02	93 (2%)	54	53	15, 40, 71, 109	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	76	GLU	5.3
1	E	336	CYS	5.3
1	G	358	SER	4.7
1	H	76	GLU	4.3
1	H	244	ALA	4.2
1	H	317	CYS	4.1
1	D	76	GLU	4.1
1	C	76	GLU	3.9
1	G	86	CYS	3.5
1	F	265	PHE	3.5
1	G	465	LEU	3.4
1	H	81	TYR	3.4
1	E	358	SER	3.4
1	F	268	GLY	3.2
1	F	76	GLU	3.2
1	H	387	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
1	E	434	LYS	3.2
1	G	76	GLU	3.1
1	F	464	ALA	3.1
1	E	78	GLU	3.1
1	F	267	THR	3.0
1	F	465	LEU	3.0
1	H	243	SER	3.0
1	E	435	GLU	3.0
1	A	76	GLU	2.9
1	H	332	ILE	2.9
1	G	390	SER	2.9
1	E	79	TRP	2.9
1	F	335	PRO	2.9
1	E	464	ALA	2.8
1	H	434	LYS	2.8
1	F	156	ILE	2.7
1	F	81	TYR	2.7
1	E	143	ASN	2.7
1	H	78	GLU	2.7
1	E	331	SER	2.7
1	E	436	THR	2.6
1	H	245	SER	2.6
1	E	158	VAL	2.6
1	F	388	ALA	2.6
1	F	170	ILE	2.6
1	F	118	PHE	2.5
1	C	95	LEU	2.5
1	E	357	GLU	2.5
1	G	308	THR	2.5
1	F	387	TRP	2.5
1	H	219	LYS	2.5
1	C	357	GLU	2.5
1	G	170	ILE	2.5
1	G	336	CYS	2.4
1	E	161	GLY	2.4
1	H	246	GLY	2.4
1	H	418	GLU	2.4
1	F	307	GLU	2.4
1	E	308	THR	2.4
1	H	77	PRO	2.4
1	B	76	GLU	2.3
1	C	358	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	314	ARG	2.3
1	F	264	ILE	2.3
1	B	77	PRO	2.3
1	H	336	CYS	2.3
1	D	78	GLU	2.3
1	A	158	VAL	2.3
1	H	388	ALA	2.3
1	G	387	TRP	2.3
1	E	233	GLY	2.3
1	H	327	PRO	2.2
1	F	312	GLU	2.2
1	F	337	GLU	2.2
1	F	169	SER	2.2
1	F	172	HIS	2.2
1	F	171	PHE	2.2
1	F	129	PHE	2.2
1	E	335	PRO	2.2
1	G	77	PRO	2.1
1	F	247	VAL	2.1
1	F	157	SER	2.1
1	E	261	ILE	2.1
1	H	197	ASN	2.1
1	E	232	GLY	2.1
1	G	245	SER	2.1
1	H	261	ILE	2.1
1	C	158	VAL	2.1
1	G	267	THR	2.1
1	G	394	ALA	2.1
1	F	158	VAL	2.1
1	F	310	THR	2.0
1	G	391	ASP	2.0
1	C	97	ILE	2.0
1	F	308	THR	2.0
1	E	81	TYR	2.0
1	G	393	LEU	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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	B	1467	14/15	0.90	0.18	1.43	34,43,54,62	0
3	NAG	G	1467	14/15	0.92	0.18	0.24	64,72,85,87	0
3	BMA	F	1469	11/12	0.73	0.44	-	80,107,110,110	0
6	NAG	C	1467	14/15	0.95	0.21	-	40,53,65,77	0
6	NAG	C	1468	14/15	0.88	0.30	-	70,83,93,99	0
3	BMA	A	1469	11/12	0.73	0.37	-	96,101,113,114	0
3	NAG	G	1468	14/15	0.81	0.31	-	80,88,96,107	0
3	BMA	B	1469	11/12	0.58	0.44	-	92,96,116,117	0
3	BMA	D	1469	11/12	0.83	0.42	-	83,93,103,106	0
3	BMA	E	1469	11/12	0.75	0.31	-	81,84,87,90	0
3	NAG	F	1468	14/15	0.87	0.35	-	64,83,92,101	0
6	NAG	H	1467	14/15	0.83	0.27	-	74,79,85,90	0
3	NAG	A	1467	14/15	0.92	0.17	-	37,50,55,60	0
3	NAG	E	1468	14/15	0.89	0.30	-	63,75,79,86	0
3	NAG	F	1467	14/15	0.94	0.20	-	58,64,69,72	0
3	NAG	A	1468	14/15	0.85	0.29	-	50,68,81,91	0
3	NAG	D	1468	14/15	0.89	0.33	-	65,74,83,92	0
3	NAG	D	1467	14/15	0.96	0.22	-	29,47,56,58	0
3	NAG	B	1468	14/15	0.82	0.35	-	51,67,78,88	0
6	NAG	H	1468	14/15	0.88	0.36	-	92,99,102,103	0
3	NAG	E	1467	14/15	0.91	0.21	-	53,60,69,75	0
3	BMA	G	1469	11/12	0.26	0.36	-	80,92,112,113	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, 95^{th} 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
7	EDO	D	1472	4/4	0.95	0.23	3.71	26,31,32,37	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	ZMR	G	1471	23/23	0.92	0.13	-0.18	36,47,56,65	0
5	ZMR	H	1470	23/23	0.93	0.12	-0.28	45,57,61,65	0
5	ZMR	D	1471	23/23	0.94	0.12	-0.28	26,34,40,44	0
5	ZMR	F	1470	23/23	0.95	0.11	-0.46	38,46,55,56	0
2	CA	C	1466	1/1	0.99	0.10	-0.56	34,34,34,34	0
5	ZMR	A	1471	23/23	0.97	0.11	-0.56	15,22,27,30	0
5	ZMR	E	1471	23/23	0.97	0.11	-0.78	48,51,60,61	0
5	ZMR	B	1471	23/23	0.97	0.09	-0.79	19,27,33,35	0
2	CA	E	1466	1/1	0.99	0.09	-1.11	66,66,66,66	0
2	CA	F	1466	1/1	0.98	0.07	-1.17	59,59,59,59	0
5	ZMR	C	1470	23/23	0.97	0.10	-1.25	21,27,32,33	0
2	CA	H	1466	1/1	0.94	0.04	-1.94	74,74,74,74	0
2	CA	A	1466	1/1	0.99	0.07	-2.26	28,28,28,28	0
2	CA	D	1466	1/1	0.97	0.05	-2.38	42,42,42,42	0
2	CA	G	1466	1/1	0.92	0.04	-2.87	70,70,70,70	0
2	CA	B	1466	1/1	0.99	0.05	-3.21	35,35,35,35	0
4	NAG	C	1469	14/15	0.84	0.25	-	64,70,78,85	0
4	NAG	E	1470	14/15	0.84	0.39	-	78,89,99,99	0
4	NAG	G	1470	14/15	0.87	0.17	-	69,79,91,92	0
4	NAG	H	1469	14/15	0.66	0.47	-	86,98,103,103	0
4	NAG	D	1470	14/15	0.93	0.12	-	73,80,85,86	0
4	NAG	A	1470	14/15	0.91	0.19	-	48,54,72,74	0
4	NAG	B	1470	14/15	0.78	0.34	-	79,86,99,99	0

6.5 Other polymers

There are no such residues in this entry.