Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 11:22 PM BST

PDB ID	:	5Y31
Title	:	Crystal structure of human LGI1-ADAM22 complex
Authors	:	Yamagata, A.; Fukai, S.
Deposited on	:	2017-07-27
Resolution	:	7.12 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
https://www.wwpdb.org/validation/2017/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:

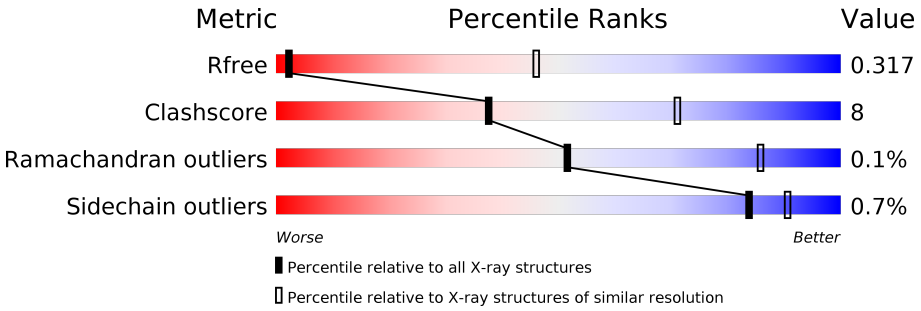
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 7.12 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}	130704	1004 (10.00-3.90)
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)

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 respectively. 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%

Mol	Chain	Length	Quality of chain
1	A	497	84% 13% •
1	C	497	82% 15% •
2	B	544	71% 22% • 6%
2	D	544	73% 20% • 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15832 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 Disintegrin and metalloproteinase domain-containing protein 22.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3696	2283	637	725	51			
1	C	482	Total	C	N	O	S	0	0	0
			3696	2283	637	725	51			

- Molecule 2 is a protein called Leucine-rich glioma-inactivated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	511	Total	C	N	O	S	0	0	0
			4146	2670	689	772	15			
2	D	511	Total	C	N	O	S	0	0	0
			4146	2670	689	772	15			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	21	ASP	-	expression tag	UNP O95970
B	22	ALA	-	expression tag	UNP O95970
B	23	ALA	-	expression tag	UNP O95970
B	24	GLN	-	expression tag	UNP O95970
B	25	PRO	-	expression tag	UNP O95970
B	26	ALA	-	expression tag	UNP O95970
B	27	ARG	-	expression tag	UNP O95970
B	28	ARG	-	expression tag	UNP O95970
B	29	ALA	-	expression tag	UNP O95970
B	30	ARG	-	expression tag	UNP O95970
B	31	ARG	-	expression tag	UNP O95970
B	32	THR	-	expression tag	UNP O95970
B	33	TYR	-	expression tag	UNP O95970
B	34	GLU	-	expression tag	UNP O95970
B	35	ALA	-	expression tag	UNP O95970
B	36	TYR	-	expression tag	UNP O95970

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Chain	Residue	Modelled	Actual	Comment	Reference
B	470	ALA	ARG	engineered mutation	UNP O95970
B	558	LYS	-	expression tag	UNP O95970
B	559	HIS	-	expression tag	UNP O95970
B	560	HIS	-	expression tag	UNP O95970
B	561	HIS	-	expression tag	UNP O95970
B	562	HIS	-	expression tag	UNP O95970
B	563	HIS	-	expression tag	UNP O95970
B	564	HIS	-	expression tag	UNP O95970
D	21	ASP	-	expression tag	UNP O95970
D	22	ALA	-	expression tag	UNP O95970
D	23	ALA	-	expression tag	UNP O95970
D	24	GLN	-	expression tag	UNP O95970
D	25	PRO	-	expression tag	UNP O95970
D	26	ALA	-	expression tag	UNP O95970
D	27	ARG	-	expression tag	UNP O95970
D	28	ARG	-	expression tag	UNP O95970
D	29	ALA	-	expression tag	UNP O95970
D	30	ARG	-	expression tag	UNP O95970
D	31	ARG	-	expression tag	UNP O95970
D	32	THR	-	expression tag	UNP O95970
D	33	TYR	-	expression tag	UNP O95970
D	34	GLU	-	expression tag	UNP O95970
D	35	ALA	-	expression tag	UNP O95970
D	36	TYR	-	expression tag	UNP O95970
D	470	ALA	ARG	engineered mutation	UNP O95970
D	558	LYS	-	expression tag	UNP O95970
D	559	HIS	-	expression tag	UNP O95970
D	560	HIS	-	expression tag	UNP O95970
D	561	HIS	-	expression tag	UNP O95970
D	562	HIS	-	expression tag	UNP O95970
D	563	HIS	-	expression tag	UNP O95970
D	564	HIS	-	expression tag	UNP O95970

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Ca 1 1	0	0
3	A	3	Total Ca 3 3	0	0
3	D	1	Total Ca 1 1	0	0

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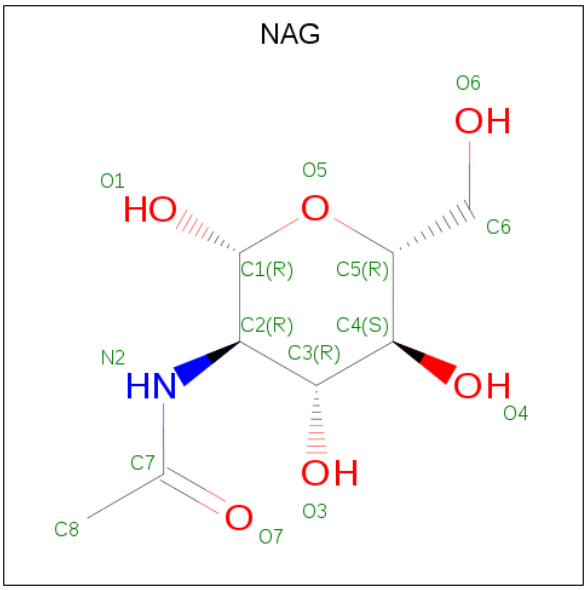
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	3	Total Ca 3 3	0	0

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



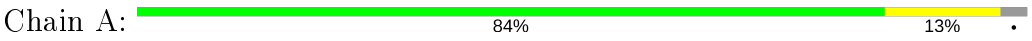
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 14 8 1 5	0	0
4	A	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	B	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	D	1	Total C N O 14 8 1 5	0	0
4	D	1	Total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

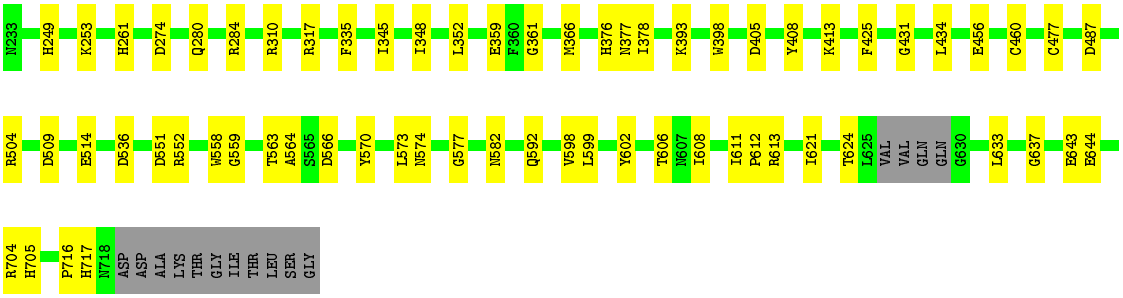
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: Disintegrin and metalloproteinase domain-containing protein 22

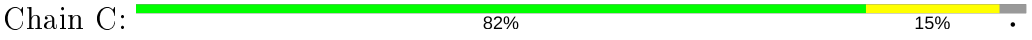
Chain A:

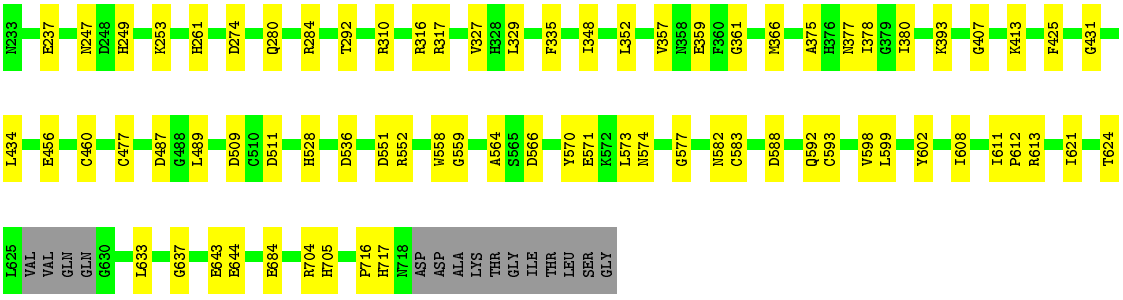




- Molecule 1: Disintegrin and metalloproteinase domain-containing protein 22

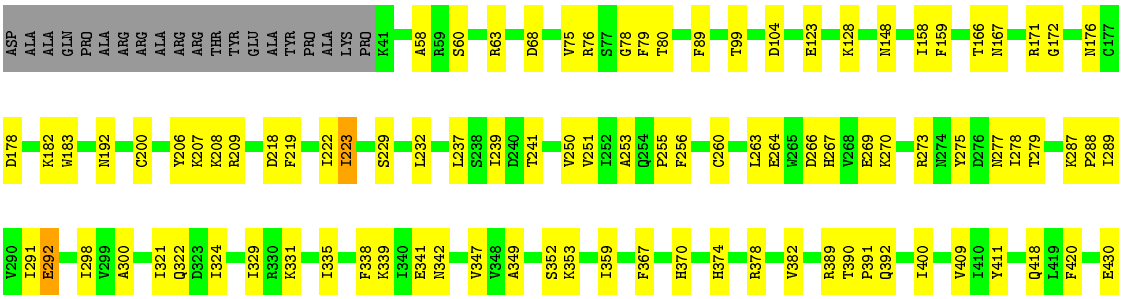
Chain C:

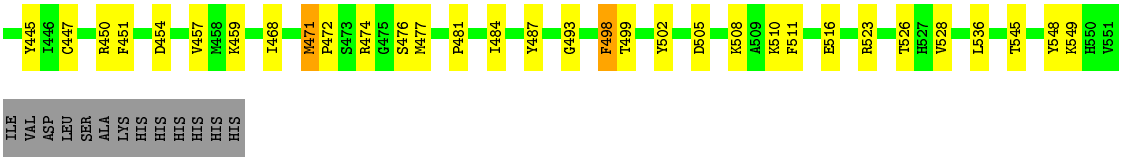




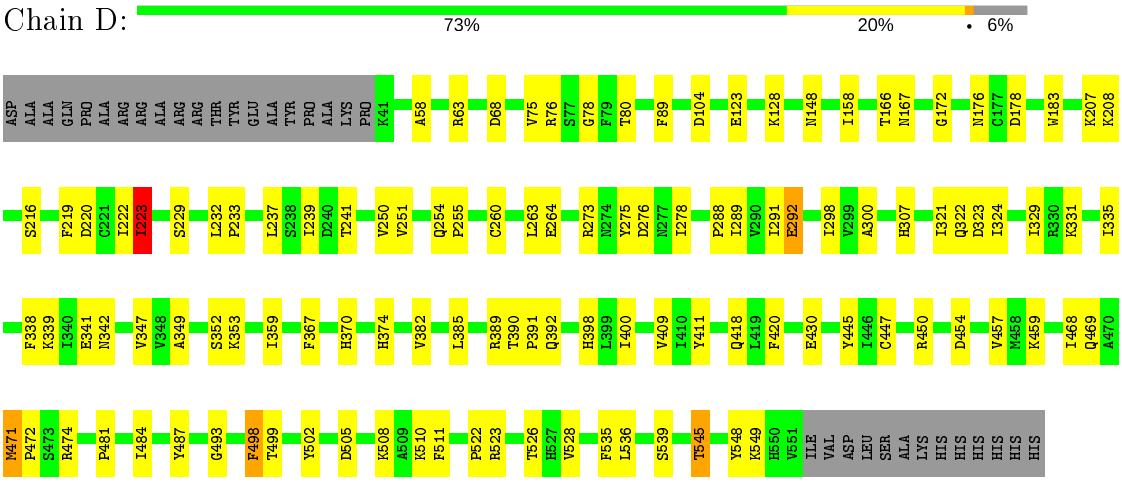
- Molecule 2: Leucine-rich glioma-inactivated protein 1

Chain B:





• Molecule 2: Leucine-rich glioma-inactivated protein 1



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	105.14Å 124.32Å 164.66Å 90.00° 104.80° 90.00°	Depositor
Resolution (Å)	48.99 – 7.12 48.99 – 7.13	Depositor EDS
% Data completeness (in resolution range)	97.2 (48.99-7.12) 97.2 (48.99-7.13)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 7.37Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.265 , 0.316 0.267 , 0.317	Depositor DCC
R_{free} test set	297 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å^2)	275.9	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 380.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.32$, $< L^2 > = 0.15$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.78	EDS
Total number of atoms	15832	wwPDB-VP
Average B, all atoms (Å^2)	447.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.24	0/3759	0.40	0/5058
1	C	0.25	0/3759	0.41	0/5058
2	B	0.27	0/4253	0.45	0/5771
2	D	0.25	0/4253	0.44	0/5771
All	All	0.26	0/16024	0.42	0/21658

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
2	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	222	ILE	Peptide

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	3696	0	3546	50	1
1	C	3696	0	3545	47	2
2	B	4146	0	4058	88	2
2	D	4146	0	4056	78	1
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	3	0	0	0	0
3	D	1	0	0	0	0
4	A	28	0	26	0	0
4	B	42	0	39	4	0
4	C	28	0	26	0	0
4	D	42	0	38	1	0
All	All	15832	0	15334	241	3

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 8.

All (241) 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:B:206:TYR:OH	2:B:218:ASP:O	1.86	0.91
2:D:220:ASP:HB3	2:D:222:ILE:HG12	1.56	0.86
1:A:359:GLU:OE2	2:B:378:ARG:NH1	2.07	0.86
2:D:289:ILE:HD11	2:D:298:ILE:HD11	1.62	0.81
2:D:75:VAL:HG12	2:D:76:ARG:HG3	1.64	0.79
2:B:289:ILE:HD11	2:B:298:ILE:HD11	1.64	0.78
2:D:222:ILE:HB	2:D:223:ILE:HA	1.66	0.77
2:B:75:VAL:HG12	2:B:76:ARG:HG3	1.66	0.76
2:B:260:CYS:HB2	2:B:278:ILE:HB	1.68	0.75
2:D:260:CYS:HB2	2:D:278:ILE:HB	1.68	0.74
1:C:407:GLY:HA3	2:D:331:LYS:HG2	1.71	0.71
2:D:291:ILE:HG22	2:D:292:GLU:HG2	1.72	0.71
2:B:291:ILE:HG22	2:B:292:GLU:HG2	1.73	0.71
1:C:378:ILE:HD11	1:C:434:LEU:HD21	1.73	0.71
2:B:237:LEU:HB2	2:B:255:PRO:HG3	1.72	0.70
1:C:280:GLN:HE22	1:C:413:LYS:HA	1.55	0.70
2:D:166:THR:HG22	2:D:167:ASN:ND2	2.07	0.69
2:D:232:LEU:HB2	2:D:545:THR:HG23	1.75	0.69
2:D:229:SER:HB2	2:D:549:LYS:HG3	1.75	0.68
1:C:598:VAL:HG13	1:C:599:LEU:HD22	1.76	0.67
2:B:229:SER:HB2	2:B:549:LYS:HG3	1.74	0.67
2:D:430:GLU:H	2:D:450:ARG:HH21	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:331:LYS:HB2	2:B:352:SER:HB3	1.78	0.66
1:A:378:ILE:HD11	1:A:434:LEU:HD21	1.77	0.66
2:B:430:GLU:H	2:B:450:ARG:HH21	1.43	0.65
1:A:280:GLN:HE22	1:A:413:LYS:HA	1.61	0.65
2:B:536:LEU:HB3	2:B:548:TYR:HB2	1.80	0.64
2:B:516:GLU:OE1	2:D:76:ARG:NH2	2.29	0.64
2:B:459:LYS:HB2	2:B:468:ILE:HD11	1.80	0.64
1:A:598:VAL:HG13	1:A:599:LEU:HD22	1.80	0.63
2:B:232:LEU:HB2	2:B:545:THR:HG23	1.80	0.63
1:A:398:TRP:CD2	2:B:256:PHE:HE1	2.17	0.62
1:A:359:GLU:OE1	2:B:353:LYS:NZ	2.27	0.62
2:B:264:GLU:HB2	2:B:275:TYR:HB2	1.81	0.62
1:C:536:ASP:OD2	1:C:552:ARG:NH1	2.33	0.61
2:B:166:THR:HG22	2:B:167:ASN:ND2	2.16	0.61
2:B:321:ILE:HD12	2:B:322:GLN:HB2	1.82	0.61
2:D:237:LEU:HB2	2:D:255:PRO:HG3	1.83	0.60
2:D:459:LYS:HB2	2:D:468:ILE:HD11	1.84	0.60
2:D:454:ASP:OD1	2:D:454:ASP:N	2.36	0.59
1:C:704:ARG:HG2	1:C:705:HIS:ND1	2.17	0.59
1:A:261:HIS:CE1	2:D:166:THR:HG23	2.37	0.59
1:A:704:ARG:HG2	1:A:705:HIS:ND1	2.17	0.59
2:B:341:GLU:O	2:B:342:ASN:ND2	2.36	0.58
1:A:509:ASP:OD1	1:A:509:ASP:N	2.36	0.58
2:B:516:GLU:CD	2:D:76:ARG:HH21	2.06	0.58
2:D:347:VAL:HG22	2:D:359:ILE:HG12	1.86	0.57
1:A:335:PHE:O	2:B:353:LYS:NZ	2.37	0.57
2:B:474:ARG:NH2	2:D:123:GLU:OE1	2.37	0.57
1:A:536:ASP:OD2	1:A:552:ARG:NH1	2.37	0.57
2:B:347:VAL:HG22	2:B:359:ILE:HG12	1.86	0.57
1:A:348:ILE:HG12	1:A:378:ILE:HD12	1.86	0.57
2:B:339:LYS:HE2	2:B:342:ASN:HA	1.86	0.57
2:B:454:ASP:N	2:B:454:ASP:OD1	2.36	0.57
2:D:536:LEU:HB3	2:D:548:TYR:HB2	1.86	0.57
2:D:321:ILE:HD12	2:D:322:GLN:HB2	1.86	0.56
1:C:551:ASP:HA	1:C:564:ALA:HB2	1.88	0.56
1:A:398:TRP:CG	2:B:256:PHE:HE1	2.24	0.56
2:B:158:ILE:HG22	2:B:183:TRP:CH2	2.41	0.56
2:D:341:GLU:O	2:D:342:ASN:ND2	2.38	0.56
1:C:249:HIS:CD2	1:C:253:LYS:HE2	2.41	0.56
2:B:277:ASN:HB3	4:B:603:NAG:C7	2.36	0.56
2:B:182:LYS:HA	2:B:219:PHE:CZ	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:509:ASP:N	1:C:509:ASP:OD1	2.38	0.55
1:A:566:ASP:HB3	1:A:633:LEU:HD13	1.87	0.55
2:D:158:ILE:HG22	2:D:183:TRP:CH2	2.41	0.55
1:A:361:GLY:H	1:A:366:MET:HE2	1.72	0.55
2:B:166:THR:HA	1:C:261:HIS:CE1	2.41	0.55
2:B:192:ASN:HD22	4:B:602:NAG:C7	2.21	0.54
1:A:398:TRP:CD2	2:B:256:PHE:CE1	2.96	0.54
2:B:58:ALA:O	2:B:78:GLY:N	2.38	0.54
1:C:359:GLU:OE1	2:D:353:LYS:NZ	2.35	0.54
1:C:611:ILE:HD12	1:C:612:PRO:HD2	1.90	0.54
2:D:324:ILE:HG21	2:D:329:ILE:HD12	1.89	0.54
1:A:249:HIS:CD2	1:A:253:LYS:HE2	2.43	0.53
2:D:339:LYS:HE2	2:D:342:ASN:HA	1.89	0.53
2:B:176:ASN:ND2	2:B:178:ASP:OD2	2.35	0.53
1:C:361:GLY:H	1:C:366:MET:HE2	1.72	0.53
2:B:324:ILE:HG21	2:B:329:ILE:HD12	1.89	0.53
1:A:558:TRP:CE2	1:A:608:ILE:HD11	2.44	0.53
1:C:460:CYS:HA	1:C:487:ASP:OD2	2.09	0.53
2:B:171:ARG:HH21	2:D:472:PRO:HG3	1.74	0.53
1:A:574:ASN:HB2	1:A:598:VAL:HG23	1.91	0.52
1:A:705:HIS:HD2	1:A:716:PRO:HA	1.73	0.52
1:A:408:TYR:OH	2:B:477:MET:SD	2.57	0.52
2:B:80:THR:O	2:B:104:ASP:N	2.33	0.52
2:D:176:ASN:ND2	2:D:178:ASP:OD2	2.35	0.52
1:C:577:GLY:HA3	1:C:592:GLN:HA	1.91	0.52
2:D:505:ASP:HB3	2:D:508:LYS:HB2	1.90	0.52
1:A:582:ASN:H	1:A:602:TYR:HB2	1.75	0.52
1:A:611:ILE:HD12	1:A:612:PRO:HD2	1.91	0.52
1:A:559:GLY:HA2	1:A:613:ARG:HD2	1.91	0.52
2:D:276:ASP:HA	4:D:603:NAG:H82	1.92	0.52
2:B:445:TYR:HE2	2:B:459:LYS:HZ1	1.58	0.52
2:D:222:ILE:CB	2:D:223:ILE:HA	2.37	0.52
2:D:445:TYR:HE2	2:D:459:LYS:HZ1	1.58	0.52
1:A:551:ASP:HA	1:A:564:ALA:HB2	1.93	0.51
1:C:348:ILE:HG12	1:C:378:ILE:HD12	1.91	0.51
1:C:566:ASP:HB3	1:C:633:LEU:HD13	1.93	0.51
2:D:370:HIS:NE2	2:D:418:GLN:O	2.40	0.51
1:C:558:TRP:CE2	1:C:608:ILE:HD11	2.45	0.51
2:D:338:PHE:HE1	2:D:347:VAL:HG23	1.75	0.51
2:B:471:MET:N	2:B:471:MET:HE2	2.25	0.51
1:A:570:TYR:HD2	1:A:574:ASN:HD21	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:317:ARG:HD3	1:C:352:LEU:HD21	1.92	0.51
2:B:241:THR:HG21	2:B:528:VAL:HG22	1.93	0.51
1:C:559:GLY:HA2	1:C:613:ARG:HD2	1.92	0.51
1:C:335:PHE:O	2:D:353:LYS:NZ	2.40	0.51
2:B:266:ASP:OD2	2:B:273:ARG:NH2	2.44	0.50
1:A:460:CYS:HA	1:A:487:ASP:OD2	2.11	0.50
2:D:430:GLU:H	2:D:450:ARG:NH2	2.09	0.50
1:A:274:ASP:OD2	1:A:284:ARG:NH1	2.44	0.50
2:D:471:MET:N	2:D:471:MET:HE2	2.27	0.50
2:D:241:THR:HG21	2:D:528:VAL:HG22	1.92	0.50
2:B:502:TYR:HB3	2:B:511:PHE:HB3	1.93	0.50
1:A:348:ILE:HG13	1:A:377:ASN:O	2.12	0.50
1:A:563:THR:OG1	1:A:606:THR:OG1	2.30	0.49
2:D:80:THR:O	2:D:104:ASP:N	2.33	0.49
1:A:398:TRP:CZ3	2:B:255:PRO:HB3	2.48	0.49
2:B:505:ASP:HB3	2:B:508:LYS:HB2	1.95	0.49
2:B:68:ASP:N	2:B:68:ASP:OD1	2.40	0.49
1:C:310:ARG:CZ	1:C:310:ARG:HB2	2.42	0.49
2:B:338:PHE:HE1	2:B:347:VAL:HG23	1.78	0.49
1:C:621:ILE:HG23	1:C:637:GLY:O	2.12	0.49
2:B:411:TYR:HB3	2:B:420:PHE:HB3	1.95	0.49
1:C:582:ASN:H	1:C:602:TYR:HB2	1.78	0.48
1:A:317:ARG:HD3	1:A:352:LEU:HD21	1.96	0.48
1:A:573:LEU:HD21	1:A:624:THR:HG21	1.94	0.48
1:A:348:ILE:HD11	1:A:425:PHE:CE2	2.48	0.48
2:D:502:TYR:HB3	2:D:511:PHE:HB3	1.94	0.48
1:C:643:GLU:HG2	1:C:644:GLU:N	2.29	0.48
1:A:335:PHE:N	2:B:353:LYS:HZ3	2.12	0.48
2:B:430:GLU:N	2:B:450:ARG:HH21	2.11	0.48
2:D:331:LYS:HB2	2:D:352:SER:HB3	1.96	0.47
1:A:456:GLU:HB2	1:A:477:CYS:HB3	1.96	0.47
1:C:570:TYR:HD2	1:C:574:ASN:HD21	1.62	0.47
2:D:307:HIS:ND1	2:D:323:ASP:OD1	2.36	0.47
1:A:577:GLY:HA3	1:A:592:GLN:HA	1.95	0.47
2:B:60:SER:HA	2:B:79:PHE:HB3	1.97	0.47
2:D:264:GLU:HB2	2:D:275:TYR:HB2	1.96	0.47
1:C:274:ASP:OD2	1:C:284:ARG:NH1	2.47	0.47
2:D:216:SER:HA	2:D:219:PHE:HE2	1.80	0.47
2:D:300:ALA:HB2	2:D:335:ILE:HD11	1.97	0.47
2:D:430:GLU:N	2:D:450:ARG:HH21	2.12	0.47
2:D:68:ASP:OD1	2:D:68:ASP:N	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:621:ILE:HG23	1:A:637:GLY:O	2.15	0.46
2:B:104:ASP:O	2:B:128:LYS:HB2	2.16	0.46
1:C:280:GLN:NE2	1:C:413:LYS:HA	2.25	0.46
2:D:411:TYR:HB3	2:D:420:PHE:HB3	1.97	0.46
1:C:705:HIS:HD2	1:C:716:PRO:HA	1.81	0.46
2:B:322:GLN:NE2	2:B:367:PHE:O	2.49	0.46
1:A:310:ARG:CZ	1:A:310:ARG:HB2	2.45	0.46
1:A:643:GLU:HG2	1:A:644:GLU:N	2.31	0.46
2:B:267:HIS:O	2:B:270:LYS:NZ	2.31	0.46
1:C:348:ILE:HD11	1:C:425:PHE:CE2	2.50	0.46
1:C:329:LEU:HD23	1:C:357:VAL:HG23	1.98	0.46
1:A:280:GLN:NE2	1:A:413:LYS:HA	2.29	0.46
2:B:498:PHE:CE2	2:D:75:VAL:HG11	2.52	0.46
2:B:370:HIS:NE2	2:B:418:GLN:O	2.44	0.45
2:B:287:LYS:HA	2:B:288:PRO:HD3	1.80	0.45
1:A:348:ILE:HD13	1:A:431:GLY:HA2	1.97	0.45
2:D:58:ALA:O	2:D:78:GLY:N	2.38	0.45
2:B:279:THR:HG22	4:B:603:NAG:H83	1.98	0.45
2:B:389:ARG:O	2:B:392:GLN:HB2	2.17	0.45
2:D:493:GLY:HA2	2:D:499:THR:HG23	1.98	0.45
2:D:510:LYS:NZ	2:D:511:PHE:O	2.37	0.45
2:B:200:CYS:HB2	2:B:206:TYR:O	2.17	0.45
2:B:239:ILE:O	2:B:526:THR:HG21	2.16	0.45
1:C:571:GLU:HA	1:C:598:VAL:HG21	1.98	0.45
2:D:220:ASP:O	2:D:222:ILE:HG23	2.17	0.44
2:B:400:ILE:HA	2:B:409:VAL:O	2.18	0.44
2:B:493:GLY:HA2	2:B:499:THR:HG23	1.99	0.44
1:C:316:ARG:HD3	1:C:327:VAL:HG21	1.99	0.44
1:C:348:ILE:HG13	1:C:348:ILE:H	1.63	0.44
1:A:574:ASN:ND2	1:A:598:VAL:O	2.50	0.44
2:B:430:GLU:H	2:B:450:ARG:NH2	2.11	0.44
2:B:474:ARG:CZ	2:D:123:GLU:OE1	2.65	0.44
1:C:375:ALA:HB1	1:C:380:ILE:HB	1.99	0.44
2:B:207:LYS:HG2	2:B:208:LYS:HG2	2.00	0.44
1:C:705:HIS:CD2	1:C:717:HIS:H	2.35	0.44
1:A:348:ILE:H	1:A:348:ILE:HG13	1.64	0.43
1:C:348:ILE:HD13	1:C:431:GLY:HA2	1.99	0.43
2:B:523:ARG:HD3	2:B:523:ARG:HA	1.80	0.43
2:B:349:ALA:HB2	2:B:382:VAL:HG23	2.00	0.43
1:C:574:ASN:HB2	1:C:598:VAL:HG23	2.00	0.43
2:D:148:ASN:ND2	2:D:172:GLY:HA3	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:456:GLU:HB2	1:C:477:CYS:HB3	1.99	0.43
2:D:216:SER:HA	2:D:219:PHE:CE2	2.53	0.43
1:A:348:ILE:HG23	1:A:377:ASN:HB3	1.99	0.43
1:A:704:ARG:HE	1:A:705:HIS:CE1	2.36	0.43
1:C:573:LEU:HD21	1:C:624:THR:HG21	2.01	0.43
2:D:528:VAL:HB	2:D:535:PHE:HB2	2.00	0.43
2:D:63:ARG:HB3	2:D:89:PHE:CD2	2.54	0.43
2:D:250:VAL:HB	2:D:263:LEU:HB2	2.00	0.43
2:B:300:ALA:HB2	2:B:335:ILE:HD11	2.01	0.42
2:D:523:ARG:HA	2:D:523:ARG:HD3	1.80	0.42
2:B:123:GLU:OE2	2:D:474:ARG:NH1	2.53	0.42
2:D:207:LYS:HG2	2:D:208:LYS:HG2	2.01	0.42
1:A:405:ASP:HB2	2:B:331:LYS:NZ	2.34	0.42
1:C:348:ILE:HG13	1:C:377:ASN:O	2.20	0.42
2:D:349:ALA:HB2	2:D:382:VAL:HG23	2.01	0.42
1:A:504:ARG:HH11	1:A:514:GLU:HG3	1.85	0.42
1:C:237:GLU:HG2	1:C:489:LEU:HD11	2.01	0.42
1:A:705:HIS:CD2	1:A:717:HIS:H	2.37	0.42
2:D:104:ASP:O	2:D:128:LYS:HB2	2.19	0.42
2:D:232:LEU:HA	2:D:233:PRO:HD3	1.74	0.42
2:B:99:THR:HA	2:B:123:GLU:O	2.20	0.42
1:C:574:ASN:ND2	1:C:598:VAL:O	2.53	0.42
2:D:385:LEU:O	2:D:398:HIS:N	2.47	0.42
2:B:148:ASN:ND2	2:B:172:GLY:HA3	2.35	0.42
2:B:266:ASP:OD2	2:B:269:GLU:HB2	2.20	0.42
2:B:484:ILE:O	2:B:487:TYR:HB2	2.19	0.42
2:D:390:THR:HA	2:D:391:PRO:HA	1.82	0.42
2:D:498:PHE:O	2:D:498:PHE:HD1	2.02	0.42
2:D:484:ILE:O	2:D:487:TYR:HB2	2.20	0.41
2:B:253:ALA:O	2:B:255:PRO:HD3	2.20	0.41
2:B:390:THR:HA	2:B:391:PRO:HA	1.81	0.41
1:C:511:ASP:OD1	1:C:528:HIS:HB3	2.20	0.41
1:C:583:CYS:N	1:C:593:CYS:SG	2.93	0.41
2:B:251:VAL:HG21	2:B:288:PRO:HG3	2.02	0.41
2:D:239:ILE:O	2:D:526:THR:HG21	2.19	0.41
2:D:254:GLN:HA	2:D:255:PRO:HD3	1.91	0.41
2:D:322:GLN:NE2	2:D:367:PHE:O	2.54	0.41
2:D:389:ARG:O	2:D:392:GLN:HB2	2.21	0.41
2:D:447:CYS:SG	2:D:481:PRO:HG3	2.60	0.41
2:B:447:CYS:SG	2:B:481:PRO:HG3	2.60	0.41
1:C:247:ASN:HB2	1:C:292:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:400:ILE:HA	2:D:409:VAL:O	2.20	0.41
2:D:457:VAL:HB	2:D:469:GLN:HG2	2.03	0.41
2:B:250:VAL:HB	2:B:263:LEU:HB2	2.02	0.41
2:B:457:VAL:HG23	2:B:471:MET:HE1	2.02	0.41
1:A:345:ILE:HA	1:A:376:HIS:O	2.21	0.41
2:B:510:LYS:NZ	2:B:511:PHE:O	2.39	0.41
2:B:451:PHE:HA	2:B:476:SER:O	2.21	0.40
1:C:378:ILE:HA	1:C:378:ILE:HD12	1.96	0.40
2:B:63:ARG:HB3	2:B:89:PHE:CD2	2.57	0.40
2:D:522:PRO:HA	2:D:539:SER:O	2.21	0.40
2:B:279:THR:HG22	4:B:603:NAG:C8	2.51	0.40
2:B:471:MET:HA	2:B:472:PRO:HD3	1.91	0.40
2:D:251:VAL:HG21	2:D:288:PRO:HG3	2.02	0.40
2:B:158:ILE:HG23	2:B:159:PHE:CD1	2.57	0.40

All (3) 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)
2:B:266:ASP:OD1	2:D:273:ARG:NH1[1_655]	2.04	0.16
1:A:704:ARG:NH1	1:C:588:ASP:OD2[1_656]	2.14	0.06
2:B:209:ARG:NE	1:C:684:GLU:OE1[2_555]	2.14	0.06

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	478/497 (96%)	460 (96%)	18 (4%)	0	100	100
1	C	478/497 (96%)	460 (96%)	18 (4%)	0	100	100
2	B	509/544 (94%)	489 (96%)	19 (4%)	1 (0%)	47	81
2	D	509/544 (94%)	486 (96%)	22 (4%)	1 (0%)	47	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1974/2082 (95%)	1895 (96%)	77 (4%)	2 (0%)	51 86

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	223	ILE
2	D	223	ILE

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	416/428 (97%)	415 (100%)	1 (0%)	93 96
1	C	416/428 (97%)	415 (100%)	1 (0%)	93 96
2	B	468/494 (95%)	463 (99%)	5 (1%)	73 84
2	D	468/494 (95%)	462 (99%)	6 (1%)	69 81
All	All	1768/1844 (96%)	1755 (99%)	13 (1%)	84 90

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	393	LYS
2	B	223	ILE
2	B	292	GLU
2	B	374	HIS
2	B	471	MET
2	B	498	PHE
1	C	393	LYS
2	D	223	ILE
2	D	292	GLU
2	D	374	HIS
2	D	471	MET
2	D	498	PHE
2	D	545	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	247	ASN
1	A	705	HIS
2	B	148	ASN
2	B	167	ASN
2	B	342	ASN
2	B	406	GLN
2	B	412	GLN
2	B	418	GLN
2	B	437	HIS
1	C	247	ASN
1	C	705	HIS
2	D	148	ASN
2	D	167	ASN
2	D	342	ASN
2	D	406	GLN
2	D	412	GLN
2	D	418	GLN
2	D	437	HIS

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 8 are monoatomic - leaving 10 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	D	602	2	14,14,15	0.43	0	17,19,21	0.32	0
4	NAG	A	804	1	14,14,15	0.28	0	17,19,21	0.72	1 (5%)
4	NAG	C	804	1	14,14,15	0.81	1 (7%)	17,19,21	0.49	0
4	NAG	C	805	1	14,14,15	0.95	1 (7%)	17,19,21	1.42	1 (5%)
4	NAG	B	604	2	14,14,15	0.65	1 (7%)	17,19,21	0.48	0
4	NAG	A	805	1	14,14,15	0.45	0	17,19,21	0.72	1 (5%)
4	NAG	D	603	2	14,14,15	0.21	0	17,19,21	0.43	0
4	NAG	D	604	2	14,14,15	0.39	0	17,19,21	0.61	0
4	NAG	B	603	2	14,14,15	0.57	0	17,19,21	0.81	1 (5%)
4	NAG	B	602	2	14,14,15	0.67	1 (7%)	17,19,21	0.39	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
4	NAG	D	602	2	-	2/6/23/26	0/1/1/1
4	NAG	A	804	1	-	0/6/23/26	0/1/1/1
4	NAG	C	804	1	-	2/6/23/26	0/1/1/1
4	NAG	C	805	1	-	2/6/23/26	0/1/1/1
4	NAG	B	604	2	-	2/6/23/26	0/1/1/1
4	NAG	A	805	1	-	2/6/23/26	0/1/1/1
4	NAG	D	603	2	-	2/6/23/26	0/1/1/1
4	NAG	D	604	2	-	2/6/23/26	0/1/1/1
4	NAG	B	603	2	-	2/6/23/26	0/1/1/1
4	NAG	B	602	2	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	805	NAG	C1-C2	2.99	1.56	1.52
4	C	804	NAG	O5-C1	-2.84	1.39	1.43
4	B	602	NAG	C1-C2	2.35	1.55	1.52
4	B	604	NAG	O5-C1	-2.19	1.40	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	805	NAG	C1-O5-C5	5.11	119.12	112.19
4	B	603	NAG	C1-O5-C5	2.84	116.03	112.19
4	A	805	NAG	C1-O5-C5	2.51	115.60	112.19
4	A	804	NAG	C1-O5-C5	2.50	115.58	112.19

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	603	NAG	O5-C5-C6-O6
4	B	603	NAG	O5-C5-C6-O6
4	D	603	NAG	C4-C5-C6-O6
4	B	603	NAG	C4-C5-C6-O6
4	B	604	NAG	O5-C5-C6-O6
4	B	602	NAG	O5-C5-C6-O6
4	D	602	NAG	C4-C5-C6-O6
4	B	602	NAG	C4-C5-C6-O6
4	D	602	NAG	O5-C5-C6-O6
4	A	805	NAG	O5-C5-C6-O6
4	D	604	NAG	C4-C5-C6-O6
4	D	604	NAG	O5-C5-C6-O6
4	B	604	NAG	C4-C5-C6-O6
4	C	804	NAG	C4-C5-C6-O6
4	A	805	NAG	C4-C5-C6-O6
4	C	805	NAG	O5-C5-C6-O6
4	C	804	NAG	O5-C5-C6-O6
4	C	805	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	603	NAG	1	0
4	B	603	NAG	3	0
4	B	602	NAG	1	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

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.