



Full wwPDB X-ray Structure Validation Report ⓘ

Jul 12, 2014 – 01:40 AM EDT

PDB ID : 4DLO
Title : Crystal structure of the GAIN and HormR domains of brain angiogenesis inhibitor 3 (BAI3)
Authors : Arac, D.; Boucard, A.A.; Bolliger, M.F.; Nguyen, J.; Soltis, M.; Sudhof, T.C.; Brunger, A.T.
Deposited on : 2012-02-06
Resolution : 2.30 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

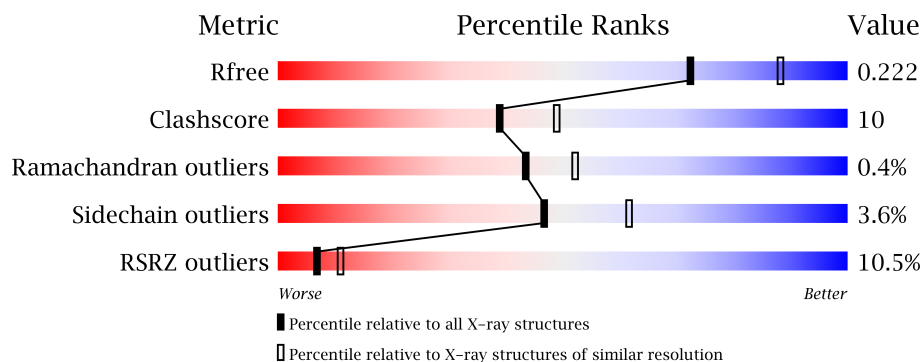
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable23161
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable23161

1 Overall quality at a glance

The reported resolution of this entry is 2.30 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}	66092	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	382	
1	B	382	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	GOL	A	906	-	X
4	GOL	A	908	-	X
4	GOL	A	909	-	X
4	GOL	B	905	-	X
4	GOL	B	906	-	X
4	GOL	B	907	-	X

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Mol	Type	Chain	Res	Geometry	Electron density
4	GOL	B	908	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5755 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Brain-specific angiogenesis inhibitor 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	351	Total	C	N	O	S	0	0	0
			2761	1753	464	524	20			
1	B	337	Total	C	N	O	S	0	0	0
			2656	1688	449	498	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	503	SER	ASN	CONFLICT	UNP O60242

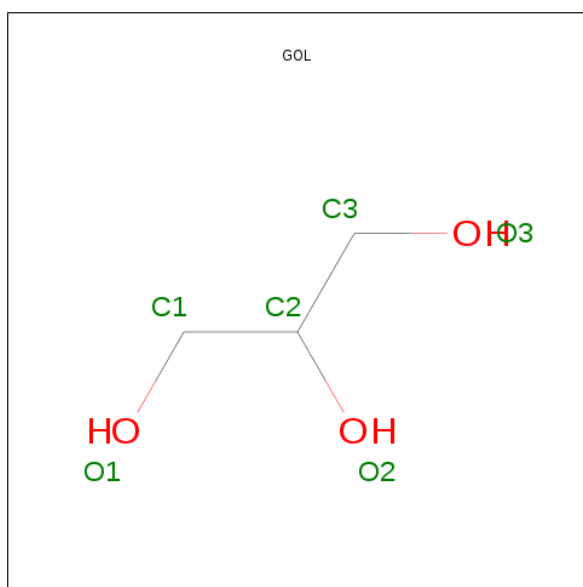
- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			38	22	2	14		
2	B	3	Total	C	N	O	0	0
			38	22	2	14		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

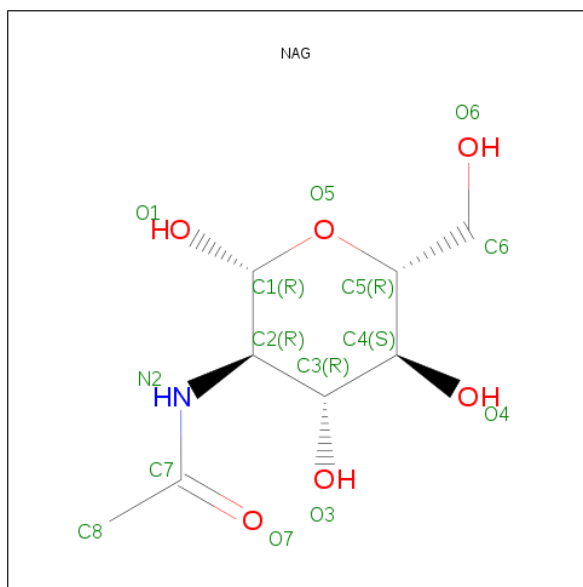
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is water.

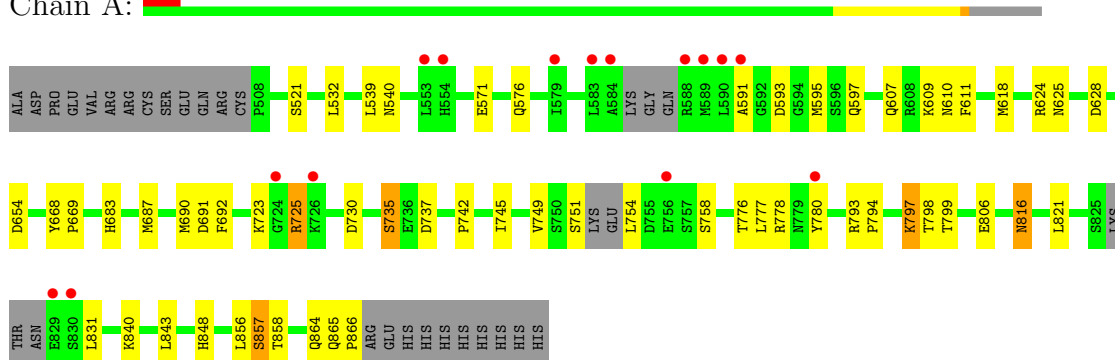
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	106	Total	O	0	0
			106	106		
6	B	60	Total	O	0	0
			60	60		

3 Residue-property plots

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

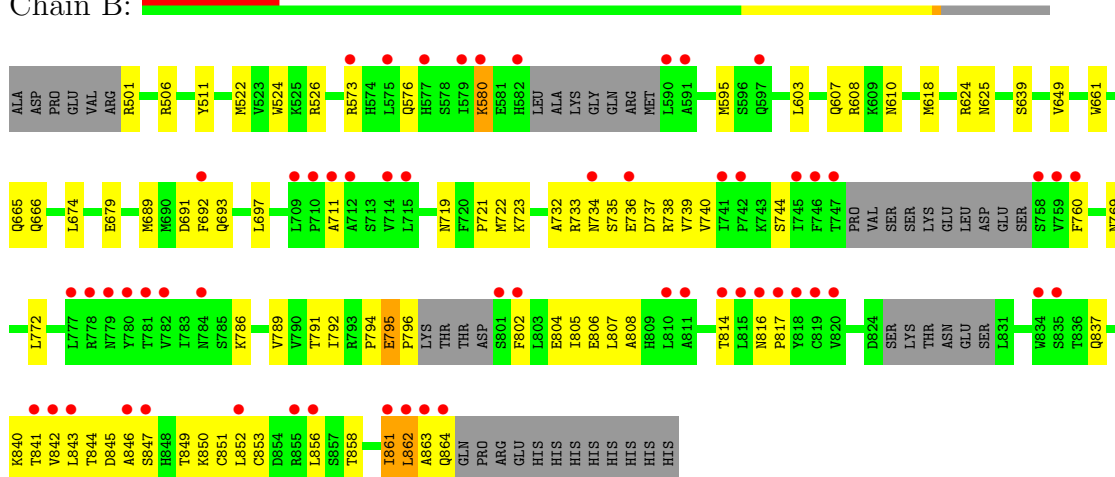
- Molecule 1: Brain-specific angiogenesis inhibitor 3

Chain A:



- Molecule 1: Brain-specific angiogenesis inhibitor 3

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	123.36Å 128.01Å 160.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.40 – 2.30 44.41 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.40-2.30) 99.7 (44.41-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.1.357)	Depositor
R, R_{free}	0.186 , 0.228 0.177 , 0.222	Depositor DCC
R_{free} test set	2901 reflections (5.14%)	DCC
Wilson B-factor (Å ²)	45.0	Xtriage
Anisotropy	0.289	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 56.8	EDS
Estimated twinning fraction	0.024 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 56491 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5755	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, FUL, 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	0.46	0/2817	0.58	0/3822
1	B	0.40	0/2709	0.53	0/3673
All	All	0.44	0/5526	0.56	0/7495

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2761	0	2735	45	0
1	B	2656	0	2623	63	0
2	A	38	0	34	1	0
2	B	38	0	34	3	0
3	A	28	0	25	1	0
4	A	30	0	40	1	0
4	B	24	0	32	3	0
5	B	14	0	13	1	0
6	A	106	0	0	1	0
6	B	60	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5755	0	5536	108	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 10.

All (108) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:814:THR:HB	1:B:863:ALA:HB1	1.52	0.90
1:B:736:GLU:HB2	1:B:808:ALA:HB2	1.60	0.83
1:A:797:LYS:HE3	1:A:799:THR:HB	1.60	0.82
1:B:732:ALA:O	1:B:735:SER:HB3	1.87	0.74
1:A:865:GLN:N	1:A:866:PRO:HD2	2.07	0.69
1:A:865:GLN:N	1:A:866:PRO:CD	2.58	0.66
1:B:721:PRO:O	1:B:723:LYS:HD2	1.95	0.66
1:B:807:LEU:HD12	1:B:861:ILE:HD13	1.80	0.64
1:A:754:LEU:HA	1:A:758:SER:OG	1.99	0.61
1:A:725:ARG:N	1:A:725:ARG:HD2	2.15	0.61
1:A:864:GLN:HB3	1:A:866:PRO:HD2	1.82	0.60
1:B:526:ARG:NE	6:B:1034:HOH:O	1.98	0.60
1:A:749:VAL:HG12	1:A:751:SER:H	1.67	0.59
1:A:776:THR:O	1:A:778:ARG:HD2	2.02	0.59
1:B:852:LEU:HG	6:B:1059:HOH:O	2.03	0.59
1:A:840:LYS:HD3	1:B:722:MET:HE2	1.85	0.58
1:A:840:LYS:HD3	1:B:722:MET:CE	2.32	0.58
1:B:802:PHE:HA	1:B:853:CYS:O	2.04	0.58
1:B:723:LYS:HZ2	1:B:735:SER:CB	2.17	0.57
1:A:571:GLU:H	1:A:571:GLU:CD	2.07	0.57
1:A:856:LEU:O	1:A:857:SER:HB2	2.05	0.56
1:B:737:ASP:OD1	1:B:786:LYS:HD2	2.06	0.56
1:B:679:GLU:CD	1:B:791:THR:HG21	2.25	0.56
1:A:609:LYS:HA	1:A:611:PHE:CE2	2.41	0.56
1:A:624:ARG:O	1:A:624:ARG:HD3	2.06	0.55
1:A:816:ASN:O	1:A:816:ASN:CG	2.45	0.55
1:B:816:ASN:N	1:B:817:PRO:HD3	2.22	0.55
1:A:777:LEU:O	1:A:778:ARG:HG3	2.07	0.55
1:B:814:THR:CB	1:B:863:ALA:HB1	2.31	0.53
1:A:793:ARG:HA	1:A:794:PRO:C	2.29	0.52
1:B:666:GLN:OE1	4:B:908:GOL:H11	2.09	0.52
1:A:848:HIS:HB3	6:A:1104:HOH:O	2.09	0.51
1:A:624:ARG:HD3	1:A:624:ARG:C	2.31	0.51
1:B:624:ARG:HD3	1:B:624:ARG:O	2.10	0.51
1:B:526:ARG:NH2	6:B:1034:HOH:O	2.38	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:749:VAL:H	1:A:754:LEU:HB2	1.76	0.50
1:B:625:ASN:OD1	5:B:904:NAG:C7	2.59	0.50
1:B:817:PRO:HD2	1:B:843:LEU:HD21	1.94	0.50
1:B:719:ASN:OD1	1:B:740:VAL:HG22	2.12	0.50
1:A:532:LEU:HD21	4:A:906:GOL:H32	1.94	0.50
1:A:798:THR:HG21	1:A:856:LEU:HG	1.94	0.49
1:B:814:THR:HA	1:B:864:GLN:O	2.13	0.49
1:A:683:HIS:O	1:A:687:MET:HG2	2.12	0.49
1:A:625:ASN:OD1	3:A:904:NAG:O5	2.25	0.49
2:B:901:NAG:H3	2:B:903:FUL:O2	2.13	0.49
1:B:845:ASP:OD1	1:B:846:ALA:N	2.46	0.48
1:B:576:GLN:HG3	1:B:618:MET:SD	2.54	0.48
1:B:789:VAL:HG22	1:B:858:THR:HG23	1.94	0.48
1:B:522:MET:HE3	1:B:524:TRP:CZ2	2.49	0.48
1:B:691:ASP:O	1:B:692:PHE:HB2	2.14	0.47
1:A:725:ARG:N	1:A:725:ARG:CD	2.77	0.47
1:A:864:GLN:C	1:A:866:PRO:HD2	2.33	0.47
1:B:723:LYS:NZ	1:B:735:SER:HB2	2.29	0.47
1:A:624:ARG:HD2	1:A:628:ASP:OD2	2.15	0.47
1:B:845:ASP:CG	1:B:847:SER:H	2.18	0.47
1:A:865:GLN:O	1:A:866:PRO:C	2.52	0.47
4:B:908:GOL:HO3	4:B:908:GOL:HO1	1.62	0.47
1:B:733:ARG:O	1:B:735:SER:N	2.48	0.46
1:B:769:ASN:HB2	1:B:772:LEU:HD12	1.97	0.46
1:A:725:ARG:H	1:A:725:ARG:HD2	1.80	0.46
1:A:843:LEU:HD12	1:B:697:LEU:HD22	1.98	0.46
1:B:607:GLN:HA	1:B:607:GLN:OE1	2.15	0.46
1:B:738:ARG:HD2	1:B:806:GLU:OE2	2.15	0.46
1:B:711:ALA:HB2	1:B:760:PHE:HE1	1.80	0.46
1:B:845:ASP:OD2	1:B:847:SER:HB2	2.15	0.46
1:A:691:ASP:O	1:A:692:PHE:HB2	2.17	0.45
1:A:668:TYR:CG	1:A:669:PRO:HD2	2.52	0.45
1:B:817:PRO:HA	1:B:862:LEU:O	2.17	0.45
1:A:843:LEU:HD12	1:B:697:LEU:CD2	2.47	0.44
1:A:780:TYR:HB3	1:A:866:PRO:HD3	1.98	0.44
1:A:737:ASP:HA	1:A:806:GLU:O	2.18	0.44
1:B:792:ILE:N	1:B:792:ILE:HD12	2.32	0.44
2:B:901:NAG:N2	2:B:903:FUL:C1	2.80	0.44
1:A:742:PRO:HG2	1:A:745:ILE:HG23	2.00	0.44
1:A:591:ALA:O	1:A:595:MET:HG2	2.18	0.43
1:B:841:THR:HG22	1:B:842:VAL:N	2.33	0.43
1:A:539:LEU:O	1:A:540:ASN:HB2	2.17	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:901:NAG:H62	2:A:902:NAG:C7	2.49	0.43
1:B:804:GLU:CG	1:B:850:LYS:HD2	2.49	0.43
1:B:580:LYS:H	1:B:580:LYS:HG2	1.40	0.43
1:B:723:LYS:CG	1:B:735:SER:OG	2.67	0.43
1:B:760:PHE:CD2	1:B:794:PRO:HD2	2.54	0.43
1:B:805:ILE:HD12	1:B:805:ILE:N	2.34	0.42
1:B:610:ASN:OD1	2:B:903:FUL:H4	2.20	0.42
1:B:649:VAL:HG22	1:B:674:LEU:HD11	2.02	0.42
1:A:821:LEU:HD12	1:A:821:LEU:C	2.40	0.42
1:B:851:CYS:SG	1:B:861:ILE:HD11	2.58	0.42
1:B:739:VAL:HG13	1:B:739:VAL:O	2.20	0.42
1:A:576:GLN:HG3	1:A:618:MET:SD	2.60	0.42
1:B:769:ASN:HB2	1:B:772:LEU:CD1	2.50	0.42
1:B:506:ARG:NH2	6:B:1043:HOH:O	2.42	0.41
1:B:501:ARG:N	6:B:1044:HOH:O	2.52	0.41
1:B:689:MET:HE2	1:B:693:GLN:HB3	2.03	0.41
1:B:850:LYS:HG2	6:B:1059:HOH:O	2.20	0.41
1:B:603:LEU:O	1:B:607:GLN:HG2	2.21	0.41
1:B:689:MET:CE	1:B:693:GLN:HB3	2.51	0.41
1:B:849:THR:CG2	1:B:850:LYS:N	2.83	0.41
1:A:821:LEU:HA	1:A:858:THR:O	2.20	0.41
1:B:795:GLU:HA	1:B:796:PRO:HD3	1.69	0.41
1:A:821:LEU:HD12	1:A:821:LEU:O	2.21	0.41
1:B:856:LEU:N	1:B:856:LEU:HD22	2.36	0.41
1:A:797:LYS:HE3	1:A:799:THR:CB	2.42	0.41
1:A:669:PRO:HG2	1:A:831:LEU:HG	2.03	0.40
1:A:593:ASP:O	1:A:597:GLN:HG3	2.21	0.40
1:B:661:TRP:O	1:B:665:GLN:HG3	2.22	0.40
1:B:723:LYS:HG3	1:B:735:SER:OG	2.21	0.40
1:B:595:MET:HA	1:B:595:MET:HE2	2.04	0.40
1:B:511:TYR:HA	4:B:907:GOL:H12	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	343/382 (90%)	334 (97%)	7 (2%)	2 (1%)	33	39
1	B	327/382 (86%)	316 (97%)	10 (3%)	1 (0%)	50	60
All	All	670/764 (88%)	650 (97%)	17 (2%)	3 (0%)	43	52

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	857	SER
1	A	735	SER
1	B	734	ASN

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	312/341 (92%)	301 (96%)	11 (4%)	48	63
1	B	298/341 (87%)	287 (96%)	11 (4%)	45	60
All	All	610/682 (89%)	588 (96%)	22 (4%)	47	61

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	521	SER
1	A	607	GLN
1	A	610	ASN
1	A	654	ASP
1	A	690	MET
1	A	723	LYS
1	A	725	ARG
1	A	730	ASP
1	A	735	SER
1	A	797	LYS
1	A	816	ASN
1	B	573	ARG
1	B	580	LYS
1	B	608	ARG

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Mol	Chain	Res	Type
1	B	639	SER
1	B	744	SER
1	B	795	GLU
1	B	837	GLN
1	B	840	LYS
1	B	844	THR
1	B	861	ILE
1	B	862	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

8 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	901	1,2	12,14,15	0.90	1 (8%)	15,19,21	1.07	1 (6%)
2	NAG	A	902	2	12,14,15	0.85	1 (8%)	15,19,21	1.02	1 (6%)
2	FUL	A	903	2	9,10,11	0.97	1 (11%)	10,14,16	0.78	0
3	NAG	A	904	1,3	12,14,15	0.75	1 (8%)	15,19,21	0.86	0
3	NAG	A	905	3	12,14,15	0.62	0	15,19,21	1.13	1 (6%)
2	NAG	B	901	1,2	12,14,15	0.69	1 (8%)	15,19,21	1.92	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	902	2	12,14,15	0.75	1 (8%)	15,19,21	0.83	0
2	FUL	B	903	2	9,10,11	1.03	1 (11%)	10,14,16	0.80	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
2	NAG	A	901	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	902	2	-	0/6/23/26	0/1/1/1
2	FUL	A	903	2	-	0/0/17/20	0/1/1/1
3	NAG	A	904	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	905	3	-	0/6/23/26	0/1/1/1
2	NAG	B	901	1,2	-	2/6/23/26	0/1/1/1
2	NAG	B	902	2	-	0/6/23/26	0/1/1/1
2	FUL	B	903	2	-	0/0/17/20	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	NAG	O5-C5	-2.70	1.41	1.45
2	A	902	NAG	O5-C5	-2.68	1.41	1.45
2	B	903	FUL	O5-C5	-2.68	1.41	1.45
2	A	903	FUL	O5-C5	-2.37	1.41	1.45
2	B	902	NAG	O5-C5	-2.33	1.41	1.45
3	A	904	NAG	O5-C5	-2.16	1.42	1.45
2	B	901	NAG	O5-C5	-2.06	1.42	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	NAG	O5-C5-C6	4.84	112.06	106.98
3	A	905	NAG	O5-C5-C6	3.48	110.64	106.98
2	B	901	NAG	O4-C4-C3	3.45	118.07	110.36
2	A	901	NAG	O5-C5-C6	2.71	109.83	106.98
2	B	901	NAG	C2-N2-C7	-2.61	120.24	123.39
2	B	901	NAG	C4-C3-C2	-2.52	105.43	110.74
2	A	902	NAG	O5-C5-C6	2.13	109.22	106.98

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	901	NAG	O7-C7-N2-C2
2	B	901	NAG	C8-C7-N2-C2

There are no ring outliers.

5.6 Ligand geometry

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	GOL	A	906	-	5,5,5	0.42	0	5,5,5	0.23	0
4	GOL	A	907	-	5,5,5	0.27	0	5,5,5	0.41	0
4	GOL	A	908	-	5,5,5	0.30	0	5,5,5	0.28	0
4	GOL	A	909	-	5,5,5	0.35	0	5,5,5	0.68	0
4	GOL	A	910	-	5,5,5	0.33	0	5,5,5	0.71	0
5	NAG	B	904	1	12,14,15	0.69	1 (8%)	15,19,21	0.90	1 (6%)
4	GOL	B	905	-	5,5,5	0.45	0	5,5,5	0.80	0
4	GOL	B	906	-	5,5,5	0.31	0	5,5,5	1.04	0
4	GOL	B	907	-	5,5,5	0.28	0	5,5,5	0.67	0
4	GOL	B	908	-	5,5,5	0.31	0	5,5,5	0.55	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	GOL	A	906	-	-	0/4/4/4	0/0/0/0
4	GOL	A	907	-	-	0/4/4/4	0/0/0/0
4	GOL	A	908	-	-	0/4/4/4	0/0/0/0
4	GOL	A	909	-	-	0/4/4/4	0/0/0/0
4	GOL	A	910	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	904	1	-	0/6/23/26	0/1/1/1
4	GOL	B	905	-	-	0/4/4/4	0/0/0/0
4	GOL	B	906	-	-	0/4/4/4	0/0/0/0
4	GOL	B	907	-	-	0/4/4/4	0/0/0/0
4	GOL	B	908	-	-	0/4/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	904	NAG	O5-C5	-2.09	1.42	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	904	NAG	O5-C5-C6	2.80	109.91	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

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 ⓘ

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	351/382 (91%)	0.12	15 (4%) 34 44	29, 44, 95, 137	0
1	B	337/382 (88%)	0.80	58 (17%) 2 4	27, 70, 161, 192	0
All	All	688/764 (90%)	0.45	73 (10%) 7 11	27, 52, 144, 192	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	780	TYR	10.7
1	A	584	ALA	9.2
1	B	863	ALA	9.0
1	B	846	ALA	8.3
1	B	864	GLN	7.6
1	B	811	ALA	7.2
1	A	590	LEU	6.6
1	B	814	THR	6.2
1	B	862	LEU	5.8
1	B	819	CYS	5.6
1	B	758	SER	5.6
1	B	712	ALA	5.4
1	A	588	ARG	5.4
1	B	777	LEU	5.2
1	B	710	PRO	5.1
1	B	856	LEU	5.1
1	B	711	ALA	5.0
1	B	843	LEU	5.0
1	A	553	LEU	4.9
1	B	760	PHE	4.9
1	B	746	PHE	4.8
1	A	589	MET	4.6
1	B	590	LEU	4.6
1	B	816	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	778	ARG	4.5
1	B	781	THR	4.4
1	B	779	ASN	4.4
1	B	815	LEU	4.3
1	A	780	TYR	4.3
1	B	580	LYS	4.2
1	B	818	TYR	4.1
1	A	724	GLY	4.0
1	B	847	SER	3.9
1	B	759	VAL	3.7
1	B	855	ARG	3.6
1	B	820	VAL	3.5
1	B	782	VAL	3.5
1	A	583	LEU	3.4
1	B	715	LEU	3.3
1	B	802	PHE	3.2
1	B	784	ASN	3.2
1	B	579	ILE	3.1
1	B	745	ILE	3.1
1	A	591	ALA	3.0
1	B	861	ILE	3.0
1	A	726	LYS	2.9
1	B	747	THR	2.9
1	B	801	SER	2.8
1	B	709	LEU	2.8
1	B	852	LEU	2.8
1	B	835	SER	2.7
1	B	714	VAL	2.6
1	B	736	GLU	2.5
1	A	756	GLU	2.5
1	B	692	PHE	2.5
1	B	842	VAL	2.5
1	B	742	PRO	2.4
1	B	834	TRP	2.4
1	A	829	GLU	2.4
1	B	810	LEU	2.4
1	B	841	THR	2.4
1	A	830	SER	2.4
1	B	591	ALA	2.3
1	B	741	ILE	2.3
1	B	734	ASN	2.3
1	B	582	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	817	PRO	2.2
1	B	575	LEU	2.1
1	A	554	HIS	2.1
1	B	597	GLN	2.1
1	A	579	ILE	2.1
1	B	573	ARG	2.0
1	B	577	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

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

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	NAG	B	902	14/15	0.30	19.32	141,153,160,161	0
2	FUL	B	903	10/11	0.24	4.58	121,127,128,130	0
2	NAG	B	901	14/15	0.20	3.85	89,98,123,135	0
2	NAG	A	901	14/15	0.15	0.27	93,110,132,146	0
3	NAG	A	904	14/15	0.14	-0.82	76,96,119,139	0
2	NAG	A	902	14/15	0.40	-	159,172,176,176	0
2	FUL	A	903	10/11	0.28	-	137,140,144,148	0
3	NAG	A	905	14/15	0.32	-	156,171,174,177	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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	GOL	A	908	6/6	0.48	33.32	48,69,78,85	0
4	GOL	A	906	6/6	0.39	20.54	65,93,98,99	0
4	GOL	A	909	6/6	0.30	6.86	88,93,95,97	0
4	GOL	B	905	6/6	0.22	5.97	53,67,75,83	0
4	GOL	B	908	6/6	0.25	5.56	95,98,102,105	0
4	GOL	B	906	6/6	0.24	3.59	55,78,87,87	0
4	GOL	B	907	6/6	0.28	2.07	79,83,88,92	0
4	GOL	A	910	6/6	0.23	1.54	44,77,83,87	0
4	GOL	A	907	6/6	0.12	0.51	62,71,74,81	0
5	NAG	B	904	14/15	0.24	0.26	93,110,122,129	0

6.5 Other polymers ⓘ

There are no such residues in this entry.