Full wwPDB X-ray Structure Validation Report (i)

Oct 8, 2023 – 08:08 AM EDT

PDB ID	:	6E4R
Title	:	Crystal Structure of the Drosophila Melanogaster Polypeptide N-Acetylgalac tosaminyl Transferase PGANT9B
Authors	:	Samara, N.L.; Tabak, L.A.; Ten Hagen, K.G.
Deposited on	:	2018-07-18
Resolution	:	2.06 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

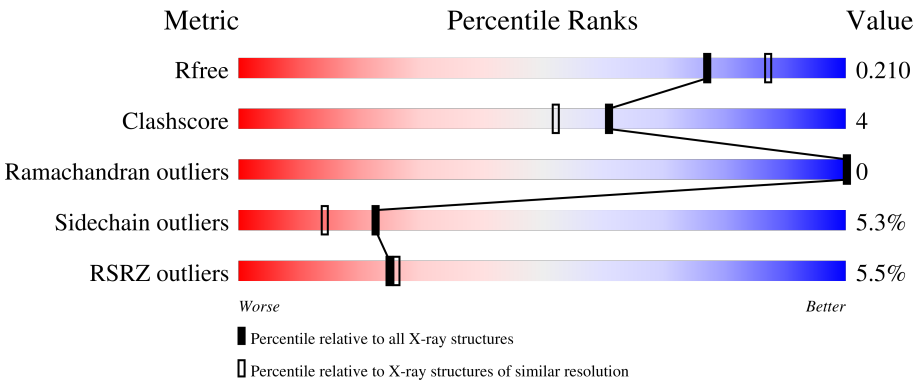
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.06 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	2684 (2.08-2.04)
Clashscore	141614	2801 (2.08-2.04)
Ramachandran outliers	138981	2768 (2.08-2.04)
Sidechain outliers	138945	2768 (2.08-2.04)
RSRZ outliers	127900	2646 (2.08-2.04)

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 of 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% 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	507	5% 86% 11% • •
1	B	507	6% 85% 11% • •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	B	709	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8921 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.

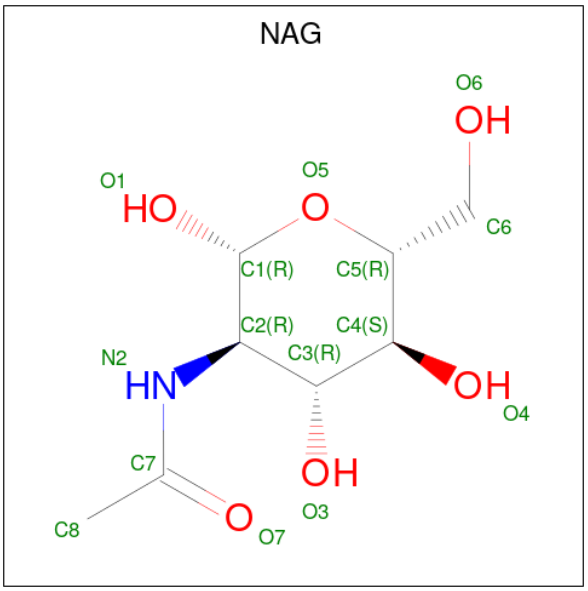
- Molecule 1 is a protein called polypeptide N-acetylgalactosaminyltransferase 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	504	4099	2586	721	769	23	0	7	0
1	B	495	3997	2518	701	755	23	0	3	0

There are 10 discrepancies between the modelled and reference sequences:

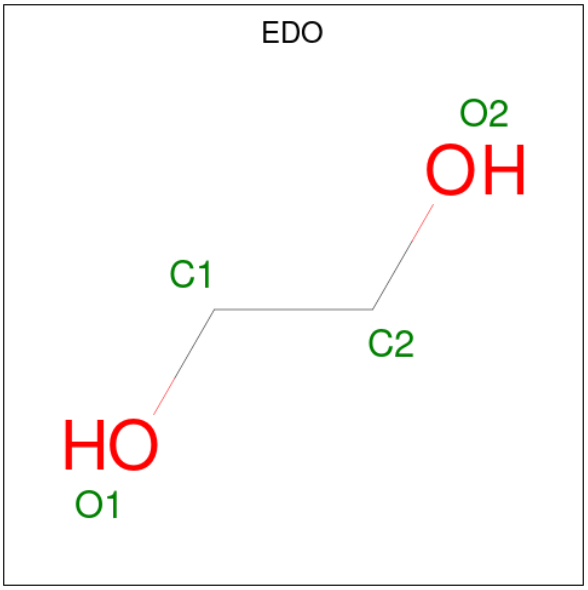
Chain	Residue	Modelled	Actual	Comment	Reference
A	141	GLY	-	expression tag	UNP Q8MRC9
A	142	GLY	-	expression tag	UNP Q8MRC9
A	143	GLY	-	expression tag	UNP Q8MRC9
A	144	GLY	-	expression tag	UNP Q8MRC9
A	145	GLY	-	expression tag	UNP Q8MRC9
B	141	GLY	-	expression tag	UNP Q8MRC9
B	142	GLY	-	expression tag	UNP Q8MRC9
B	143	GLY	-	expression tag	UNP Q8MRC9
B	144	GLY	-	expression tag	UNP Q8MRC9
B	145	GLY	-	expression tag	UNP Q8MRC9

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



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

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
3	A	1	4	2	2		0	0
3	A	1	4	2	2		0	0

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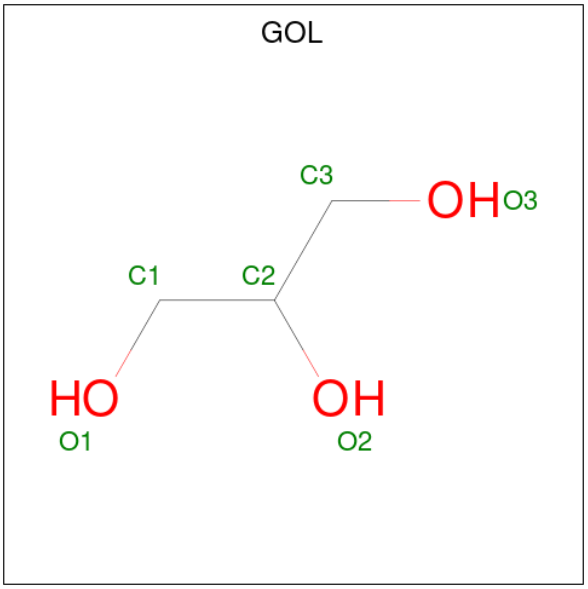
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
3	B	1	4	2	2	0	0
			Total	C	O		
3	B	1	4	2	2	0	0
			Total	C	O		
3	B	1	4	2	2	0	0
			Total	C	O		
3	B	1	4	2	2	0	0
			Total	C	O		
3	B	1	4	2	2	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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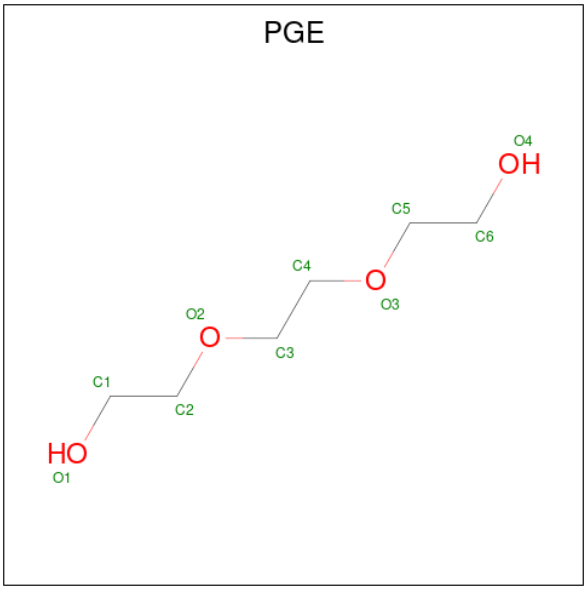
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	B	1	6	3	3	0	0
			Total	C	O		
4	B	1	6	3	3	0	0

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	A	1	10	6	4	0	0

- Molecule 6 is water.

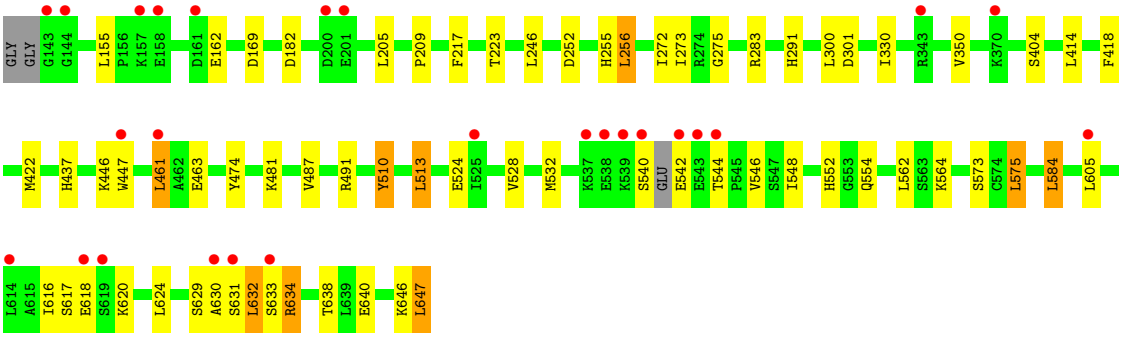
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	388	388	388	0	0
			Total	O		
6	B	322	323	323	0	1

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 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.

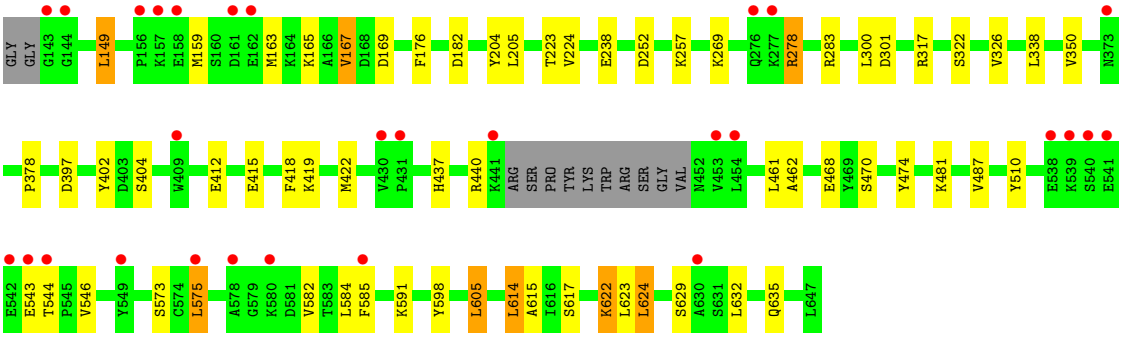
• Molecule 1: polypeptide N-acetylgalactosaminyltransferase 9

Chain A:



• Molecule 1: polypeptide N-acetylgalactosaminyltransferase 9

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	113.91Å 48.44Å 232.04Å 90.00° 91.40° 90.00°	Depositor
Resolution (Å)	20.07 – 2.06 20.07 – 2.06	Depositor EDS
% Data completeness (in resolution range)	97.0 (20.07-2.06) 96.9 (20.07-2.06)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.64 (at 2.06Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.164 , 0.207 0.168 , 0.210	Depositor DCC
R_{free} test set	3758 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	28.0	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 56.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8921	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, GOL, EDO, PGE

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	0.40	0/4227	0.62	1/5719 (0.0%)
1	B	0.39	0/4107	0.60	2/5556 (0.0%)
All	All	0.39	0/8334	0.61	3/11275 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	614	LEU	CA-CB-CG	5.71	128.44	115.30
1	B	624	LEU	CA-CB-CG	5.31	127.51	115.30
1	A	461	LEU	CA-CB-CG	5.11	127.05	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4099	0	3949	39	0
1	B	3997	0	3843	31	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
3	A	8	0	12	1	0
3	B	20	0	30	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	30	0	40	4	0
4	B	18	0	24	4	0
5	A	10	0	14	0	0
6	A	388	0	0	3	0
6	B	323	0	0	5	0
All	All	8921	0	7938	72	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (72) 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:B:204:TYR:HE1	3:B:709:EDO:H21	1.44	0.82
1:A:418:PHE:O	1:A:422:MET:HG2	1.87	0.74
1:B:204:TYR:CE1	3:B:709:EDO:H21	2.23	0.73
1:B:418:PHE:O	1:B:422:MET:HG2	1.88	0.73
1:A:528:VAL:HG22	1:A:638:THR:HG23	1.76	0.67
1:B:278:ARG:NH1	6:B:801:HOH:O	2.29	0.66
1:B:629:SER:HB3	1:B:632:LEU:HD12	1.79	0.64
1:A:630:ALA:O	1:A:631:SER:OG	2.12	0.64
1:A:463:GLU:HG3	1:A:491:ARG:HH22	1.62	0.63
1:A:463:GLU:HG3	1:A:491:ARG:NH2	2.16	0.61
1:A:633:SER:H	1:A:634:ARG:HH11	1.48	0.61
1:A:629:SER:HB3	1:A:632:LEU:HD22	1.85	0.59
1:B:591:LYS:NZ	3:B:706:EDO:H21	2.18	0.58
1:A:548:ILE:HD13	1:A:616:ILE:HD11	1.86	0.57
1:A:246:LEU:HB2	1:A:272:ILE:HD13	1.86	0.56
1:A:540:SER:O	1:A:542:GLU:N	2.39	0.56
1:B:598:TYR:HD1	1:B:605:LEU:HD13	1.72	0.55
3:B:709:EDO:H22	6:B:1085:HOH:O	2.07	0.54
1:B:378:PRO:HG3	3:B:709:EDO:H11	1.88	0.54
1:B:617:SER:HB3	1:B:622:LYS:HG2	1.91	0.53
1:B:415:GLU:O	1:B:419:LYS:HG3	2.09	0.52
1:A:510:TYR:CE2	1:A:513:LEU:HG	2.45	0.51
1:A:217:PHE:CE2	1:A:256:LEU:HG	2.47	0.50
1:A:437:HIS:NE2	4:A:705:GOL:O3	2.29	0.49
1:A:255:HIS:CD2	1:A:256:LEU:HD13	2.48	0.49
1:A:275:GLY:HA3	6:A:913:HOH:O	2.12	0.49
1:B:615:ALA:HB2	1:B:635:GLN:HG2	1.94	0.49
1:A:634:ARG:NE	1:A:634:ARG:H	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ARG:HB2	1:B:326:VAL:HG11	1.96	0.48
1:B:163:MET:O	1:B:167:VAL:HG13	2.14	0.48
1:B:440[B]:ARG:NH2	4:B:703:GOL:O3	2.42	0.48
1:A:573:SER:HB3	1:A:584:LEU:HD22	1.96	0.47
1:B:257:LYS:NZ	6:B:811:HOH:O	2.48	0.47
1:A:273:ILE:HD11	1:A:291[A]:HIS:CE1	2.50	0.46
1:B:573:SER:HB3	1:B:584:LEU:HG	1.97	0.46
1:B:462:ALA:HB1	1:B:470:SER:HB2	1.98	0.45
1:B:182:ASP:HA	1:B:223:THR:HG21	1.98	0.45
1:A:182:ASP:HA	1:A:223:THR:HG21	1.99	0.45
1:A:330:ILE:O	4:A:704:GOL:H12	2.17	0.45
1:B:437:HIS:HE2	4:B:703:GOL:C1	2.28	0.45
1:A:283:ARG:NH2	1:A:404:SER:O	2.46	0.44
1:A:634:ARG:H	1:A:634:ARG:HE	1.65	0.44
1:B:149:LEU:HD12	1:B:149:LEU:HA	1.88	0.44
1:A:169:ASP:OD1	6:A:801:HOH:O	2.21	0.44
1:A:474:TYR:CZ	1:A:481:LYS:HE3	2.53	0.44
1:B:591:LYS:HZ1	3:B:706:EDO:H21	1.83	0.43
1:B:322:SER:HB3	4:B:705:GOL:H32	1.99	0.43
1:B:474:TYR:CZ	1:B:481:LYS:HE3	2.53	0.43
1:A:510:TYR:HH	3:A:702:EDO:HO1	1.60	0.43
1:A:301:ASP:HB2	6:A:1070:HOH:O	2.18	0.42
1:A:532:MET:HB3	1:A:548:ILE:HG13	2.01	0.42
1:B:283:ARG:NH1	1:B:404:SER:O	2.52	0.42
1:A:162:GLU:OE2	1:A:162:GLU:N	2.51	0.42
1:A:246:LEU:HD12	1:A:272:ILE:CD1	2.50	0.42
1:B:575:LEU:HD22	1:B:582:VAL:HG12	2.02	0.41
1:A:446:LYS:HE3	1:A:447:TRP:CZ2	2.55	0.41
1:A:620:LYS:HE2	1:A:620:LYS:HB3	1.74	0.41
1:B:402:TYR:CD1	1:B:412:GLU:HB2	2.55	0.41
1:B:238:GLU:O	1:B:269:LYS:NZ	2.53	0.41
1:B:440[B]:ARG:HH21	4:B:703:GOL:H11	1.85	0.41
4:A:709:GOL:H12	6:B:823:HOH:O	2.21	0.41
1:A:209:PRO:HG3	4:A:706:GOL:H2	2.03	0.41
1:A:524:GLU:HG2	1:A:640[B]:GLU:OE1	2.21	0.41
1:A:546:VAL:HG11	1:A:575:LEU:HD21	2.02	0.41
1:A:646:LYS:O	1:A:647:LEU:HB2	2.20	0.41
1:B:176:PHE:CZ	1:B:224:VAL:HG21	2.56	0.41
1:A:552:HIS:O	1:A:554:GLN:HG2	2.21	0.40
1:B:301:ASP:HB2	6:B:992:HOH:O	2.20	0.40
1:A:616:ILE:HD13	1:A:616:ILE:HA	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:LYS:HG3	1:A:647:LEU:HG	2.02	0.40
1:A:616:ILE:HG22	1:A:617:SER:O	2.21	0.40
1:B:546:VAL:HG21	1:B:575:LEU:CD2	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	507/507 (100%)	494 (97%)	13 (3%)	0	100	100
1	B	494/507 (97%)	480 (97%)	14 (3%)	0	100	100
All	All	1001/1014 (99%)	974 (97%)	27 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	448/442 (101%)	427 (95%)	21 (5%)	26	18
1	B	436/442 (99%)	411 (94%)	25 (6%)	20	12
All	All	884/884 (100%)	838 (95%)	46 (5%)	22	14

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	LEU
1	A	205	LEU
1	A	252	ASP
1	A	256	LEU
1	A	300	LEU
1	A	350	VAL
1	A	414	LEU
1	A	461	LEU
1	A	487	VAL
1	A	510	TYR
1	A	513	LEU
1	A	544	THR
1	A	562	LEU
1	A	575	LEU
1	A	584	LEU
1	A	605	LEU
1	A	618	GLU
1	A	624	LEU
1	A	632	LEU
1	A	634	ARG
1	A	647	LEU
1	B	149	LEU
1	B	159	MET
1	B	165	LYS
1	B	167	VAL
1	B	169	ASP
1	B	205	LEU
1	B	252	ASP
1	B	278	ARG
1	B	300	LEU
1	B	338	LEU
1	B	350	VAL
1	B	397	ASP
1	B	461	LEU
1	B	468	GLU
1	B	487	VAL
1	B	510	TYR
1	B	543	GLU
1	B	544	THR
1	B	575	LEU
1	B	585	PHE
1	B	605	LEU
1	B	614	LEU

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Mol	Chain	Res	Type
1	B	622	LYS
1	B	623	LEU
1	B	624	LEU

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

18 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	709	-	5,5,5	0.38	0	5,5,5	0.41	0
3	EDO	B	708	-	3,3,3	0.43	0	2,2,2	0.40	0
4	GOL	A	705	-	5,5,5	0.43	0	5,5,5	0.24	0
2	NAG	B	701	1	14,14,15	0.36	0	17,19,21	0.57	0
3	EDO	B	709	-	3,3,3	0.35	0	2,2,2	0.29	0
4	GOL	A	704	-	5,5,5	0.33	0	5,5,5	0.51	0
4	GOL	B	705	-	5,5,5	0.43	0	5,5,5	0.21	0
4	GOL	A	706	-	5,5,5	0.32	0	5,5,5	0.62	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	EDO	A	702	-	3,3,3	0.39	0	2,2,2	0.51	0
4	GOL	B	703	-	5,5,5	0.32	0	5,5,5	1.00	0
4	GOL	A	708	-	5,5,5	0.41	0	5,5,5	0.22	0
4	GOL	B	704	-	5,5,5	0.32	0	5,5,5	0.39	0
5	PGE	A	707	-	9,9,9	0.33	0	8,8,8	0.24	0
3	EDO	B	702	-	3,3,3	0.53	0	2,2,2	0.24	0
3	EDO	B	706	-	3,3,3	0.48	0	2,2,2	0.14	0
3	EDO	B	707	-	3,3,3	0.46	0	2,2,2	0.31	0
3	EDO	A	703	-	3,3,3	0.51	0	2,2,2	0.15	0
2	NAG	A	701	1	14,14,15	0.26	0	17,19,21	0.47	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	709	-	-	2/4/4/4	-
3	EDO	B	708	-	-	1/1/1/1	-
4	GOL	A	705	-	-	4/4/4/4	-
2	NAG	B	701	1	-	2/6/23/26	0/1/1/1
3	EDO	B	709	-	-	1/1/1/1	-
4	GOL	A	704	-	-	0/4/4/4	-
4	GOL	B	705	-	-	4/4/4/4	-
4	GOL	A	706	-	-	0/4/4/4	-
3	EDO	A	702	-	-	0/1/1/1	-
4	GOL	B	703	-	-	1/4/4/4	-
4	GOL	A	708	-	-	4/4/4/4	-
4	GOL	B	704	-	-	2/4/4/4	-
5	PGE	A	707	-	-	4/7/7/7	-
3	EDO	B	702	-	-	0/1/1/1	-
3	EDO	B	706	-	-	0/1/1/1	-
3	EDO	B	707	-	-	0/1/1/1	-
3	EDO	A	703	-	-	1/1/1/1	-
2	NAG	A	701	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	705	GOL	O1-C1-C2-C3
4	A	705	GOL	C1-C2-C3-O3
4	A	708	GOL	O1-C1-C2-O2
4	A	708	GOL	O1-C1-C2-C3
4	A	708	GOL	C1-C2-C3-O3
4	A	708	GOL	O2-C2-C3-O3
4	A	709	GOL	O1-C1-C2-C3
2	B	701	NAG	C8-C7-N2-C2
2	B	701	NAG	O7-C7-N2-C2
4	B	703	GOL	C1-C2-C3-O3
4	B	704	GOL	C1-C2-C3-O3
4	B	705	GOL	O1-C1-C2-C3
4	B	705	GOL	C1-C2-C3-O3
5	A	707	PGE	O2-C3-C4-O3
4	A	709	GOL	O1-C1-C2-O2
4	B	704	GOL	O2-C2-C3-O3
4	B	705	GOL	O2-C2-C3-O3
4	A	705	GOL	O1-C1-C2-O2
4	A	705	GOL	O2-C2-C3-O3
4	B	705	GOL	O1-C1-C2-O2
3	B	708	EDO	O1-C1-C2-O2
5	A	707	PGE	O1-C1-C2-O2
5	A	707	PGE	C3-C4-O3-C5
3	A	703	EDO	O1-C1-C2-O2
3	B	709	EDO	O1-C1-C2-O2
5	A	707	PGE	O3-C5-C6-O4

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	709	GOL	1	0
4	A	705	GOL	1	0
3	B	709	EDO	4	0
4	A	704	GOL	1	0
4	B	705	GOL	1	0
4	A	706	GOL	1	0
3	A	702	EDO	1	0
4	B	703	GOL	3	0
3	B	706	EDO	2	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 (i)

6.1 Protein, DNA and RNA chains (i)

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	504/507 (99%)	-0.05	26 (5%)	27	27	17, 30, 61, 107	0
1	B	495/507 (97%)	0.08	29 (5%)	22	23	21, 35, 64, 133	0
All	All	999/1014 (98%)	0.01	55 (5%)	25	26	17, 33, 62, 133	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	539	LYS	9.2
1	B	542	GLU	8.3
1	A	631	SER	7.8
1	B	541	GLU	6.8
1	B	540	SER	6.5
1	B	453	VAL	5.3
1	B	543	GLU	4.9
1	A	537	LYS	4.5
1	B	630	ALA	4.4
1	A	143	GLY	4.4
1	A	157	LYS	4.4
1	B	161	ASP	4.2
1	B	157	LYS	4.1
1	A	540	SER	4.0
1	B	143	GLY	4.0
1	A	539	LYS	3.9
1	B	409	TRP	3.8
1	A	447	TRP	3.7
1	A	630	ALA	3.7
1	B	162	GLU	3.4
1	B	144	GLY	3.4
1	B	158	GLU	3.2
1	A	158	GLU	3.2
1	B	580	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	200	ASP	3.0
1	A	544	THR	2.9
1	A	542	GLU	2.9
1	B	441	LYS	2.8
1	A	618	GLU	2.8
1	A	614	LEU	2.7
1	A	543	GLU	2.6
1	B	585	PHE	2.6
1	A	144	GLY	2.6
1	A	633	SER	2.6
1	B	430	VAL	2.5
1	A	619	SER	2.5
1	B	575	LEU	2.5
1	B	277	LYS	2.5
1	A	343	ARG	2.4
1	B	431	PRO	2.4
1	B	276	GLN	2.3
1	B	156	PRO	2.3
1	A	461	LEU	2.3
1	B	454	LEU	2.3
1	B	544	THR	2.2
1	B	373	ASN	2.2
1	A	370	LYS	2.2
1	B	549	TYR	2.2
1	A	525	ILE	2.2
1	A	605	LEU	2.1
1	A	201	GLU	2.1
1	A	161	ASP	2.1
1	B	538	GLU	2.1
1	A	538	GLU	2.0
1	B	578	ALA	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)

There are no monosaccharides in this entry.

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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	GOL	A	709	6/6	0.53	0.33	69,73,76,77	0
3	EDO	B	706	4/4	0.74	0.27	63,64,65,69	0
4	GOL	A	706	6/6	0.82	0.28	39,53,58,59	0
5	PGE	A	707	10/10	0.83	0.27	61,69,71,72	0
4	GOL	A	708	6/6	0.85	0.29	60,66,71,74	0
2	NAG	B	701	14/15	0.86	0.32	40,56,66,66	0
3	EDO	B	708	4/4	0.86	0.12	57,58,58,59	0
3	EDO	B	702	4/4	0.86	0.22	46,50,56,64	0
4	GOL	A	705	6/6	0.87	0.21	39,60,70,73	0
3	EDO	A	702	4/4	0.88	0.16	52,52,58,60	0
4	GOL	B	703	6/6	0.88	0.15	32,64,69,69	0
3	EDO	A	703	4/4	0.88	0.17	56,59,59,60	0
4	GOL	B	704	6/6	0.89	0.19	54,63,64,65	0
4	GOL	B	705	6/6	0.90	0.30	49,62,62,63	0
3	EDO	B	707	4/4	0.92	0.22	67,70,72,74	0
2	NAG	A	701	14/15	0.93	0.23	34,40,50,56	0
4	GOL	A	704	6/6	0.93	0.10	41,47,53,57	0
3	EDO	B	709	4/4	0.97	0.11	27,34,37,40	0

6.5 Other polymers (i)

There are no such residues in this entry.