



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:28 pm GMT

PDB ID : 4KGL
Title : Crystal structure of human alpha-L-iduronidase complex with [2R,3R,4R,5S]-2-carboxy-3,4,5-trihydroxy-piperidine
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Deposited on : 2013-04-29
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28683
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	recalc28949

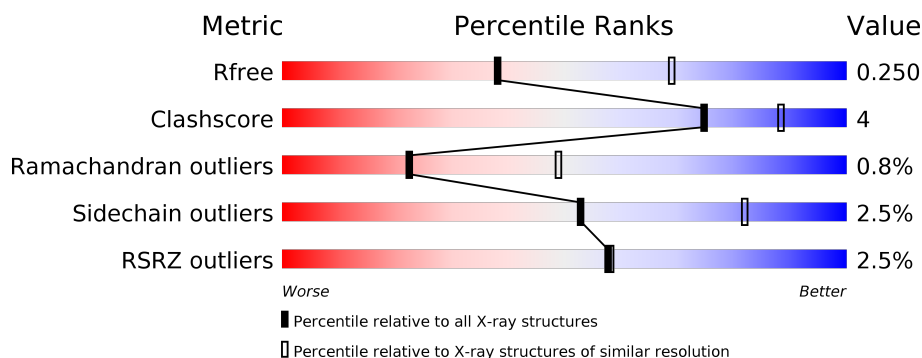
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	627	<div> <div>4%</div> <div>85%</div> <div>10%</div> <div>5%</div> </div>
1	B	627	<div> <div>%</div> <div>84%</div> <div>13%</div> <div>•</div> </div>

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
5	GOL	B	913	-	-	-	X
6	IDJ	A	910	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 9990 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.

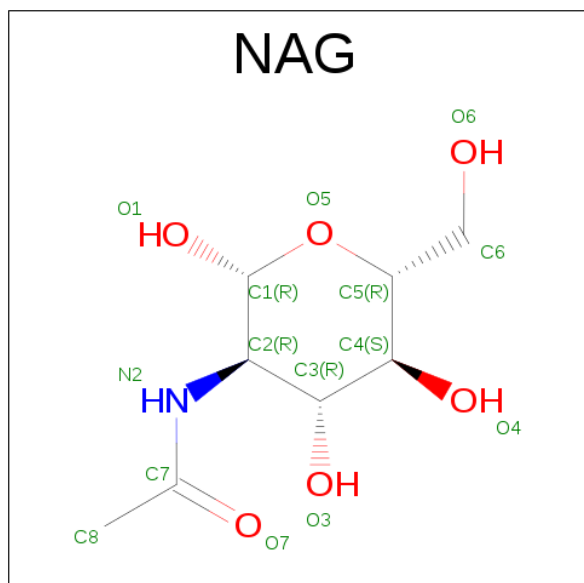
- Molecule 1 is a protein called Alpha-L-iduronidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	0	0
			4734	3030	852	840	12			
1	B	612	Total	C	N	O	S	0	4	0
			4888	3121	886	867	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	GLN	HIS	SEE REMARK 999	UNP P35475
A	63	PRO	GLN	SEE REMARK 999	UNP P35475
A	105	GLN	ARG	SEE REMARK 999	UNP P35475
B	33	GLN	HIS	SEE REMARK 999	UNP P35475
B	63	PRO	GLN	SEE REMARK 999	UNP P35475
B	105	GLN	ARG	SEE REMARK 999	UNP P35475

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

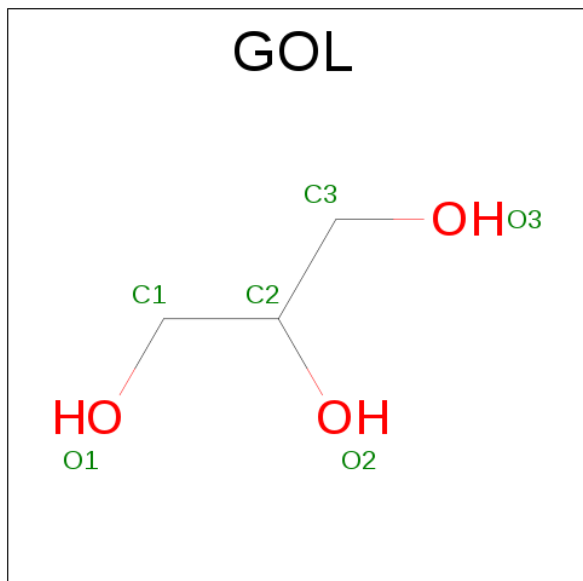
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



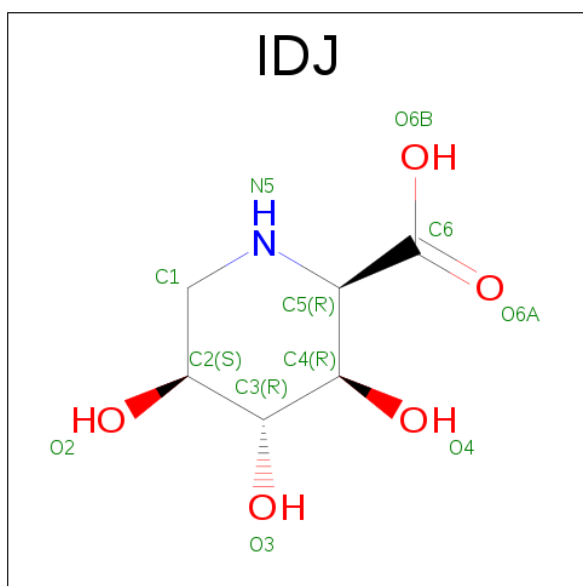
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 6 is (2R,3R,4R,5S)-3,4,5-TRIHIDROXYPIPERIDINE-2-CARBOXYLIC ACID (three-letter code: IDJ) (formula: C₆H₁₁NO₅).

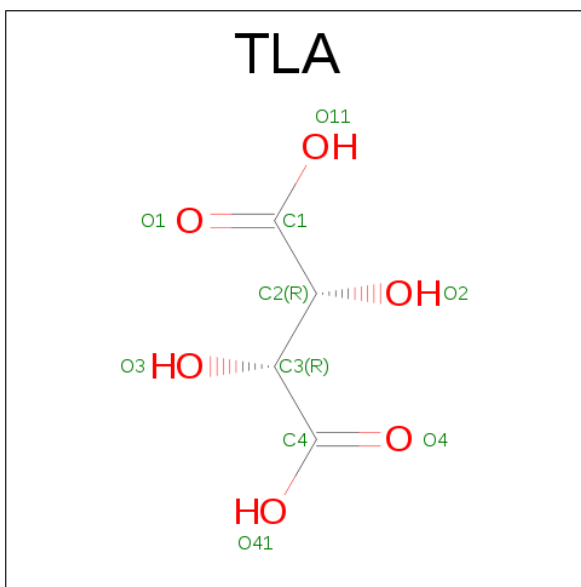


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			12	6	1	5		
6	B	1	Total	C	N	O	0	0
			12	6	1	5		

- Molecule 7 is a polymer of unknown type called SUGAR (9-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	9	Total	C	N	O	0	0
			105	58	2	45		

- Molecule 8 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			10	4	6		

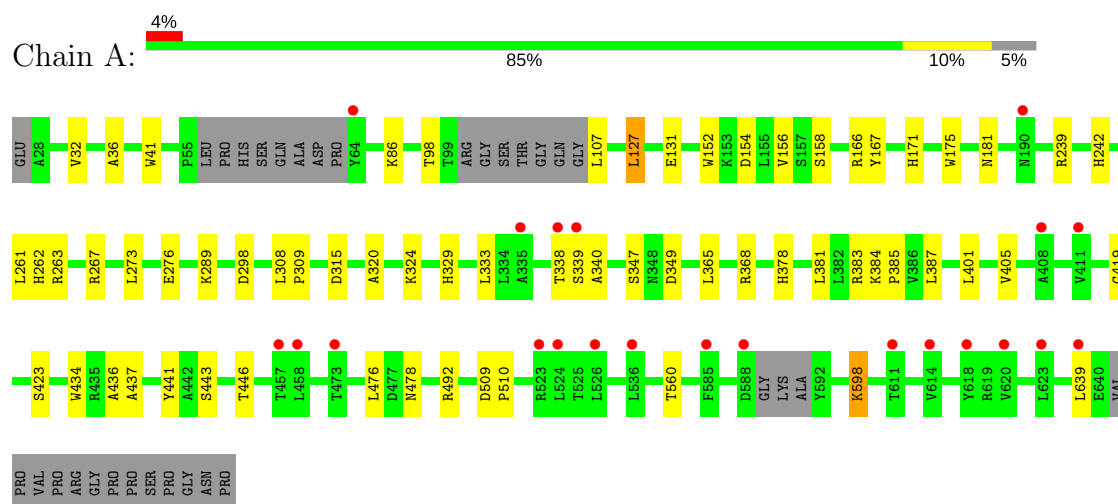
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	20	Total	O	0	0
			20	20		
9	B	34	Total	O	0	0
			34	34		

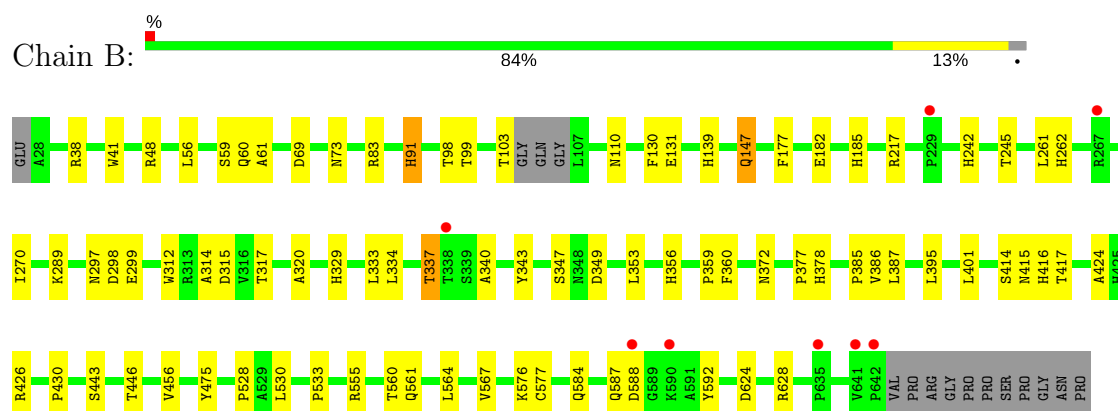
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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: Alpha-L-iduronidase



• Molecule 1: Alpha-L-iduronidase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	259.36Å 259.36Å 71.57Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.06 – 2.70 49.01 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (49.06-2.70) 99.4 (49.01-2.70)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.204 , 0.254 0.202 , 0.250	Depositor DCC
R_{free} test set	2479 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.797	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.007 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9990	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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: GOL, BMA, NAG, TLA, IDJ, MAN

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	0.34	0/4879	0.55	0/6666
1	B	0.36	0/5039	0.57	0/6886
All	All	0.35	0/9918	0.56	0/13552

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 [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	4734	0	4632	34	0
1	B	4888	0	4786	37	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
3	A	28	0	25	0	0
3	B	28	0	25	1	0
4	A	61	0	52	2	0
5	A	6	0	8	3	0
5	B	24	0	32	2	0
6	A	12	0	10	0	0
6	B	12	0	10	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	105	0	88	2	0
8	B	10	0	4	0	0
9	A	20	0	0	0	0
9	B	34	0	0	1	0
All	All	9990	0	9698	73	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 (73) 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:577[A]:CYS:SG	1:B:577[A]:CYS:O	2.33	0.86
1:A:315:ASP:HB2	1:A:478:ASN:OD1	1.77	0.83
4:A:906:BMA:H61	4:A:907:MAN:H5	1.74	0.69
1:B:270:ILE:HD11	3:B:902:NAG:H82	1.80	0.63
1:B:334:LEU:HD21	1:B:343:TYR:HB3	1.80	0.63
1:B:320:ALA:HB1	1:B:443:SER:HB2	1.81	0.61
1:A:152:TRP:O	1:A:156:VAL:HG23	2.01	0.61
1:A:131:GLU:OE2	1:A:181:ASN:HB2	2.01	0.60
1:B:356:HIS:HB2	5:B:914:GOL:H31	1.82	0.60
1:A:273:LEU:HD11	1:A:333:LEU:HD13	1.84	0.59
1:A:298:ASP:HA	1:A:347:SER:HB3	1.84	0.59
1:B:359:PRO:HG3	5:B:914:GOL:H12	1.85	0.58
1:A:324:LYS:NZ	5:A:909:GOL:H11	2.18	0.58
1:A:378:HIS:CD2	1:A:560:THR:HB	2.38	0.58
1:A:36:ALA:HA	1:A:401:LEU:HD13	1.86	0.57
4:A:906:BMA:H61	4:A:907:MAN:C5	2.35	0.57
1:B:414:SER:C	1:B:416:HIS:H	2.11	0.54
1:A:166:ARG:HG3	1:A:166:ARG:HH11	1.75	0.52
1:A:476:LEU:HG	1:A:510:PRO:HB3	1.91	0.52
1:B:242:HIS:CD2	1:B:289:LYS:HB2	2.45	0.51
1:B:56:LEU:HD13	7:B:909:MAN:H3	1.91	0.51
1:A:242:HIS:CD2	1:A:289:LYS:HB2	2.46	0.51
1:A:261:LEU:HD13	1:A:263:ARG:HG2	1.92	0.50
1:B:315:ASP:HA	1:B:385:PRO:HG2	1.93	0.50
1:A:492:ARG:NH2	7:B:906:BMA:O2	2.46	0.49
1:A:368:ARG:HA	1:A:381:LEU:HD23	1.95	0.48
1:A:434:TRP:CH2	1:A:436:ALA:HB2	2.48	0.48
1:A:383:ARG:HG2	1:A:387:LEU:HD23	1.95	0.48
1:B:584:GLN:HB3	1:B:592:TYR:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ARG:HG2	1:A:446:THR:HG21	1.95	0.48
1:B:98:THR:OG1	1:B:110:ASN:HB3	2.13	0.48
1:A:276:GLU:OE1	1:A:329:HIS:NE2	2.44	0.47
1:A:32:VAL:HG22	1:A:405:VAL:HG22	1.96	0.46
1:A:315:ASP:HA	1:A:385:PRO:HG2	1.97	0.46
1:B:242:HIS:NE2	1:B:289:LYS:HB2	2.31	0.46
1:B:401:LEU:HD21	1:B:424:ALA:HB2	1.97	0.46
1:A:365:LEU:O	1:A:384:LYS:HB2	2.16	0.45
1:B:386:VAL:HG13	1:B:387:LEU:N	2.31	0.45
1:B:314:ALA:HB1	1:B:360:PHE:HB3	1.98	0.45
1:B:73:ASN:HB2	1:B:353:LEU:HD21	1.97	0.45
1:A:419:GLY:HA3	1:A:441:TYR:CE1	2.52	0.45
1:A:171:HIS:CD2	1:A:175:TRP:HE1	2.35	0.45
1:A:509:ASP:HB2	1:A:598:LYS:HE3	2.00	0.44
1:A:86:LYS:HE2	1:A:127:LEU:HD11	2.00	0.44
1:A:154:ASP:O	1:A:158:SER:HB2	2.18	0.44
1:A:242:HIS:NE2	1:A:289:LYS:HB2	2.33	0.44
1:B:298:ASP:HA	1:B:347:SER:HB3	1.99	0.43
1:A:166:ARG:HD3	1:A:167:TYR:CZ	2.54	0.43
1:B:99:THR:HG21	1:B:139:HIS:HB2	2.01	0.43
1:B:475:TYR:HE1	1:B:530:LEU:HD22	1.84	0.43
1:A:324:LYS:HZ3	5:A:909:GOL:H11	1.81	0.43
1:B:91:HIS:ND1	1:B:131:GLU:OE1	2.52	0.43
1:B:378:HIS:CD2	1:B:560:THR:HB	2.54	0.43
1:B:456:VAL:O	1:B:528:PRO:HD2	2.18	0.43
1:B:182:GLU:HB3	1:B:185:HIS:HB2	2.01	0.42
1:B:395:LEU:HD22	1:B:576:LYS:HB3	2.01	0.42
1:B:48:ARG:HD2	1:B:83:ARG:O	2.18	0.42
1:A:320:ALA:HB1	1:A:443:SER:HB2	2.01	0.42
1:A:324:LYS:HZ1	5:A:909:GOL:H11	1.83	0.42
1:B:317:THR:HA	1:B:533:PRO:HG3	2.02	0.42
1:B:624:ASP:OD2	1:B:628:ARG:HB2	2.20	0.42
1:A:263:ARG:HD3	1:A:263:ARG:HA	1.87	0.42
1:B:372:ASN:HA	1:B:377:PRO:HB3	2.02	0.41
1:B:337:THR:HG21	9:B:1022:HOH:O	2.19	0.41
1:B:564:LEU:C	1:B:564:LEU:HD12	2.39	0.41
1:B:329:HIS:O	1:B:333:LEU:HB3	2.21	0.41
1:B:298:ASP:O	1:B:299:GLU:HG3	2.19	0.41
1:B:312:TRP:CD2	1:B:446:THR:HG22	2.56	0.41
1:A:423:SER:OG	1:A:437:ALA:HB3	2.21	0.41
1:B:103:THR:HG21	1:B:147:GLN:HE21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:LEU:HA	1:A:309:PRO:HD3	1.91	0.40
1:B:177:PHE:HB2	1:B:217:ARG:O	2.21	0.40
1:B:261:LEU:O	1:B:297:ASN:HA	2.21	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	587/627 (94%)	543 (92%)	41 (7%)	3 (0%)	32 60
1	B	612/627 (98%)	569 (93%)	36 (6%)	7 (1%)	17 40
All	All	1199/1254 (96%)	1112 (93%)	77 (6%)	10 (1%)	22 49

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	338	THR
1	A	339	SER
1	A	340	ALA
1	B	340	ALA
1	B	60	GLN
1	B	415	ASN
1	B	61	ALA
1	B	587	GLN
1	B	588	ASP
1	B	430	PRO

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	503/527 (95%)	494 (98%)	9 (2%)	64	87
1	B	520/527 (99%)	504 (97%)	16 (3%)	45	75
All	All	1023/1054 (97%)	998 (98%)	25 (2%)	53	83

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	TRP
1	A	98	THR
1	A	107	LEU
1	A	127	LEU
1	A	239	ARG
1	A	262	HIS
1	A	349	ASP
1	A	598	LYS
1	A	639	LEU
1	B	38	ARG
1	B	41	TRP
1	B	59	SER
1	B	69	ASP
1	B	91	HIS
1	B	130	PHE
1	B	147	GLN
1	B	245	THR
1	B	262	HIS
1	B	337	THR
1	B	349	ASP
1	B	417	THR
1	B	426	ARG
1	B	555	ARG
1	B	561	GLN
1	B	567	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	GLN
1	A	125	GLN
1	A	281	GLN
1	A	587	GLN
1	B	147	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

18 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	902	1,3	14,14,15	0.52	0	15,19,21	1.48	2 (13%)
3	NAG	A	903	3	14,14,15	0.58	0	15,19,21	0.94	1 (6%)
4	NAG	A	904	1,4	14,14,15	0.57	0	15,19,21	1.20	1 (6%)
4	NAG	A	905	4	14,14,15	0.53	0	15,19,21	1.47	1 (6%)
4	BMA	A	906	4	11,11,12	0.41	0	13,15,17	0.80	0
4	MAN	A	907	4	11,11,12	0.56	0	13,15,17	2.04	3 (23%)
4	MAN	A	908	4	11,11,12	0.58	0	13,15,17	0.65	0
3	NAG	B	902	1,3	14,14,15	0.54	0	15,19,21	0.79	0
3	NAG	B	903	3	14,14,15	0.51	0	15,19,21	1.38	2 (13%)
7	NAG	B	904	1,7	14,14,15	0.49	0	15,19,21	1.23	1 (6%)
7	NAG	B	905	7	14,14,15	0.56	0	15,19,21	1.20	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	BMA	B	906	7	11,11,12	0.64	0	13,15,17	1.47	1 (7%)
7	MAN	B	907	7	11,11,12	0.67	0	13,15,17	0.98	0
7	MAN	B	908	7	11,11,12	0.59	0	13,15,17	1.04	1 (7%)
7	MAN	B	909	7	11,11,12	0.49	0	13,15,17	1.42	1 (7%)
7	MAN	B	910	7	11,11,12	0.57	0	13,15,17	0.70	1 (7%)
7	MAN	B	911	7	11,11,12	0.56	0	13,15,17	0.72	0
7	MAN	B	912	7	11,11,12	0.75	0	13,15,17	1.57	3 (23%)

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	902	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	903	3	-	0/6/23/26	0/1/1/1
4	NAG	A	904	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	905	4	-	0/6/23/26	0/1/1/1
4	BMA	A	906	4	-	0/2/19/22	0/1/1/1
4	MAN	A	907	4	-	0/2/19/22	0/1/1/1
4	MAN	A	908	4	-	0/2/19/22	0/1/1/1
3	NAG	B	902	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	903	3	-	0/6/23/26	0/1/1/1
7	NAG	B	904	1,7	-	0/6/23/26	0/1/1/1
7	NAG	B	905	7	-	0/6/23/26	0/1/1/1
7	BMA	B	906	7	-	0/2/19/22	0/1/1/1
7	MAN	B	907	7	-	0/2/19/22	0/1/1/1
7	MAN	B	908	7	-	0/2/19/22	0/1/1/1
7	MAN	B	909	7	-	0/2/19/22	0/1/1/1
7	MAN	B	910	7	-	0/2/19/22	0/1/1/1
7	MAN	B	911	7	-	0/2/19/22	0/1/1/1
7	MAN	B	912	7	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	904	NAG	O5-C1-C2	-3.49	106.62	111.47
4	A	904	NAG	O5-C1-C2	-3.02	107.27	111.47
3	A	902	NAG	O5-C1-C2	-2.44	108.08	111.47
7	B	910	MAN	C1-O5-C5	2.03	114.97	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	907	MAN	O5-C1-C2	2.45	114.62	110.79
3	A	903	NAG	C1-O5-C5	2.48	115.58	112.17
7	B	912	MAN	C3-C4-C5	2.60	114.81	110.22
3	B	903	NAG	C2-N2-C7	2.70	126.89	122.94
7	B	908	MAN	C1-O5-C5	2.81	116.04	112.17
7	B	905	NAG	C1-O5-C5	2.91	116.18	112.17
7	B	912	MAN	C1-C2-C3	3.07	113.55	109.65
3	B	903	NAG	C1-O5-C5	3.11	116.45	112.17
7	B	912	MAN	C2-C3-C4	3.40	116.80	110.88
4	A	907	MAN	C1-C2-C3	3.81	114.49	109.65
7	B	906	BMA	C1-C2-C3	4.08	114.82	109.65
4	A	905	NAG	C1-O5-C5	4.11	117.83	112.17
3	A	902	NAG	C1-O5-C5	4.35	118.17	112.17
7	B	909	MAN	C1-O5-C5	4.37	118.19	112.17
4	A	907	MAN	C1-O5-C5	5.49	119.74	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	906	BMA	2	0
4	A	907	MAN	2	0
3	B	902	NAG	1	0
7	B	906	BMA	1	0
7	B	909	MAN	1	0

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
2	NAG	A	901	1	14,14,15	0.54	0	15,19,21	1.13	1 (6%)
5	GOL	A	909	-	5,5,5	0.19	0	5,5,5	0.15	0
6	IDJ	A	910	-	8,12,12	1.05	0	7,17,17	2.84	2 (28%)
2	NAG	B	901	1	14,14,15	0.46	0	15,19,21	0.84	1 (6%)
5	GOL	B	913	-	5,5,5	0.32	0	5,5,5	0.25	0
5	GOL	B	914	-	5,5,5	0.30	0	5,5,5	0.22	0
5	GOL	B	915	-	5,5,5	0.29	0	5,5,5	0.34	0
5	GOL	B	916	-	5,5,5	0.32	0	5,5,5	0.63	0
8	TLA	B	917	-	3,9,9	0.58	0	6,12,12	0.95	0
6	IDJ	B	918	-	8,12,12	1.01	0	7,17,17	2.43	2 (28%)

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	-	0/6/23/26	0/1/1/1
5	GOL	A	909	-	-	0/4/4/4	0/0/0/0
6	IDJ	A	910	-	-	0/0/21/21	0/1/1/1
2	NAG	B	901	1	-	0/6/23/26	0/1/1/1
5	GOL	B	913	-	-	0/4/4/4	0/0/0/0
5	GOL	B	914	-	-	0/4/4/4	0/0/0/0
5	GOL	B	915	-	-	0/4/4/4	0/0/0/0
5	GOL	B	916	-	-	0/4/4/4	0/0/0/0
8	TLA	B	917	-	-	0/4/12/12	0/0/0/0
6	IDJ	B	918	-	-	0/0/21/21	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	NAG	C1-O5-C5	2.35	115.41	112.17
2	A	901	NAG	C1-O5-C5	3.16	116.53	112.17
6	B	918	IDJ	C2-C3-C4	3.58	117.11	110.88
6	A	910	IDJ	C2-C3-C4	4.77	119.19	110.88
6	B	918	IDJ	C1-C2-C3	5.05	116.28	110.30
6	A	910	IDJ	C1-C2-C3	5.42	116.72	110.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	909	GOL	3	0
5	B	914	GOL	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

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	595/627 (94%)	0.07	22 (3%) 42 41	34, 52, 81, 105	0
1	B	612/627 (97%)	-0.13	8 (1%) 77 78	33, 47, 76, 112	0
All	All	1207/1254 (96%)	-0.03	30 (2%) 58 58	33, 49, 79, 112	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	339	SER	5.2
1	B	338	THR	3.8
1	B	588	ASP	3.6
1	B	641	VAL	3.4
1	A	338	THR	3.2
1	A	639	LEU	3.2
1	B	635	PRO	3.1
1	A	524	LEU	3.0
1	A	64	TYR	3.0
1	B	642	PRO	2.9
1	A	614	VAL	2.7
1	A	623	LEU	2.7
1	A	618	TYR	2.7
1	A	526	LEU	2.6
1	A	523	ARG	2.6
1	B	229	PRO	2.5
1	B	590	LYS	2.5
1	A	611	THR	2.5
1	A	536	LEU	2.4
1	A	585	PHE	2.4
1	A	411	VAL	2.4
1	A	588	ASP	2.3
1	A	620	VAL	2.3
1	A	458	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	473	THR	2.2
1	A	190	ASN	2.1
1	A	408	ALA	2.1
1	A	457	THR	2.1
1	B	267	ARG	2.1
1	A	335	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	NAG	B	904	14/15	0.96	0.17	0.64	40,41,44,45	0
7	NAG	B	905	14/15	0.96	0.16	-0.18	42,43,49,49	0
7	MAN	B	909	11/12	0.84	0.17	-0.23	92,99,103,105	0
7	BMA	B	906	11/12	0.95	0.12	-	50,53,61,61	0
4	NAG	A	904	14/15	0.96	0.14	-	56,58,61,63	0
7	MAN	B	911	11/12	0.94	0.12	-	70,73,76,83	0
4	MAN	A	907	11/12	0.79	0.21	-	75,82,85,91	0
3	NAG	A	903	14/15	0.84	0.32	-	94,102,109,115	0
7	MAN	B	907	11/12	0.94	0.13	-	69,76,84,90	0
7	MAN	B	910	11/12	0.86	0.17	-	85,93,100,101	0
3	NAG	B	902	14/15	0.94	0.21	-	53,59,64,71	0
7	MAN	B	912	11/12	0.75	0.21	-	78,89,91,92	0
4	MAN	A	908	11/12	0.80	0.29	-	98,102,105,107	0
3	NAG	B	903	14/15	0.84	0.35	-	75,77,80,81	0
4	NAG	A	905	14/15	0.96	0.13	-	53,61,68,74	0
3	NAG	A	902	14/15	0.94	0.19	-	56,64,70,83	0
7	MAN	B	908	11/12	0.81	0.19	-	80,89,92,95	0
4	BMA	A	906	11/12	0.93	0.12	-	74,78,83,93	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	GOL	B	913	6/6	0.88	0.28	7.01	55,62,64,65	0
6	IDJ	A	910	12/12	0.86	0.22	4.74	82,86,88,89	0
5	GOL	B	914	6/6	0.92	0.19	1.38	51,57,57,58	0
5	GOL	A	909	6/6	0.92	0.17	1.23	50,52,54,56	0
5	GOL	B	916	6/6	0.89	0.21	1.03	41,45,47,51	0
8	TLA	B	917	10/10	0.91	0.23	0.62	63,66,70,71	0
5	GOL	B	915	6/6	0.94	0.19	0.39	51,52,53,54	0
6	IDJ	B	918	12/12	0.92	0.16	0.06	69,73,75,77	0
2	NAG	A	901	14/15	0.78	0.25	-	87,95,99,99	0
2	NAG	B	901	14/15	0.93	0.19	-	55,58,61,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.