



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 9, 2018 – 12:42 AM EST

PDB ID : 4AD7
Title : Crystal structure of full-length N-glycosylated human glypican-1
Authors : Svensson, G.; Awad, W.; Mani, K.; Logan, D.T.
Deposited on : 2011-12-22
Resolution : 2.94 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 : rb-20030736
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) : rb-20030736

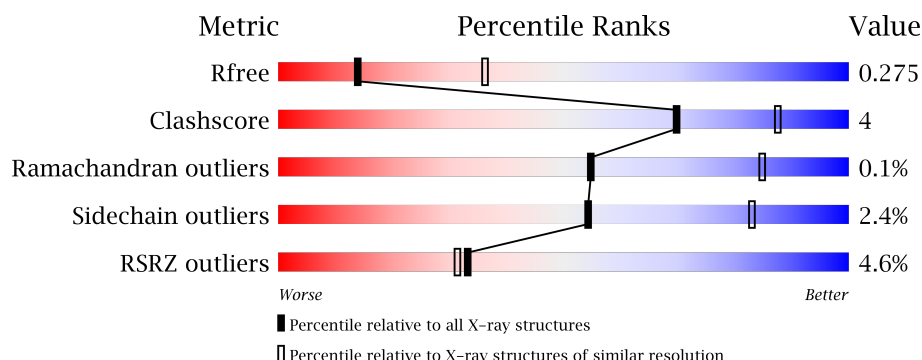
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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	2289 (2.98-2.90)
Clashscore	112137	2543 (2.98-2.90)
Ramachandran outliers	110173	2475 (2.98-2.90)
Sidechain outliers	110143	2477 (2.98-2.90)
RSRZ outliers	101464	2301 (2.98-2.90)

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	528	<div> <div>5%</div> <div>59%</div> <div>9%</div> <div>32%</div> </div>
1	B	528	<div> <div>3%</div> <div>68%</div> <div>13%</div> <div>19%</div> </div>
1	C	528	<div> <div>3%</div> <div>66%</div> <div>7%</div> <div>27%</div> </div>
1	D	528	<div> <div>3%</div> <div>70%</div> <div>11%</div> <div>19%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	1500	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12754 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 GLYPICAN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	358	Total	C	N	O	S	0	0	0
			2811	1751	512	526	22			
1	B	426	Total	C	N	O	S	0	0	0
			3341	2085	608	624	24			
1	C	385	Total	C	N	O	S	0	0	0
			3035	1894	554	565	22			
1	D	428	Total	C	N	O	S	0	0	0
			3357	2093	611	629	24			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	-	expression tag	UNP P35052
A	3	PRO	-	expression tag	UNP P35052
A	4	GLN	-	expression tag	UNP P35052
A	5	LEU	-	expression tag	UNP P35052
A	6	HIS	-	expression tag	UNP P35052
A	7	HIS	-	expression tag	UNP P35052
A	8	HIS	-	expression tag	UNP P35052
A	9	HIS	-	expression tag	UNP P35052
A	10	HIS	-	expression tag	UNP P35052
A	11	HIS	-	expression tag	UNP P35052
A	12	ASP	-	expression tag	UNP P35052
A	13	LEU	-	expression tag	UNP P35052
A	14	TYR	-	expression tag	UNP P35052
A	15	GLU	-	expression tag	UNP P35052
A	16	ASN	-	expression tag	UNP P35052
A	17	LEU	-	expression tag	UNP P35052
A	18	TYR	-	expression tag	UNP P35052
A	19	PHE	-	expression tag	UNP P35052
A	20	GLN	-	expression tag	UNP P35052
A	21	GLY	-	expression tag	UNP P35052
A	22	LYS	-	expression tag	UNP P35052

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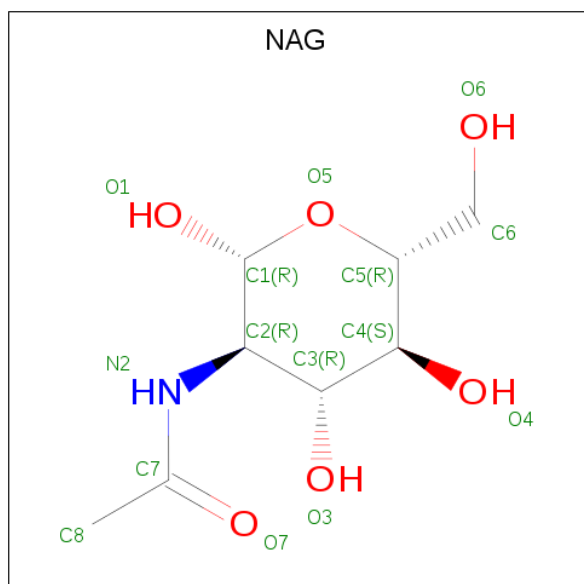
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	LEU	-	expression tag	UNP P35052
B	2	ALA	-	expression tag	UNP P35052
B	3	PRO	-	expression tag	UNP P35052
B	4	GLN	-	expression tag	UNP P35052
B	5	LEU	-	expression tag	UNP P35052
B	6	HIS	-	expression tag	UNP P35052
B	7	HIS	-	expression tag	UNP P35052
B	8	HIS	-	expression tag	UNP P35052
B	9	HIS	-	expression tag	UNP P35052
B	10	HIS	-	expression tag	UNP P35052
B	11	HIS	-	expression tag	UNP P35052
B	12	ASP	-	expression tag	UNP P35052
B	13	LEU	-	expression tag	UNP P35052
B	14	TYR	-	expression tag	UNP P35052
B	15	GLU	-	expression tag	UNP P35052
B	16	ASN	-	expression tag	UNP P35052
B	17	LEU	-	expression tag	UNP P35052
B	18	TYR	-	expression tag	UNP P35052
B	19	PHE	-	expression tag	UNP P35052
B	20	GLN	-	expression tag	UNP P35052
B	21	GLY	-	expression tag	UNP P35052
B	22	LYS	-	expression tag	UNP P35052
B	23	LEU	-	expression tag	UNP P35052
C	2	ALA	-	expression tag	UNP P35052
C	3	PRO	-	expression tag	UNP P35052
C	4	GLN	-	expression tag	UNP P35052
C	5	LEU	-	expression tag	UNP P35052
C	6	HIS	-	expression tag	UNP P35052
C	7	HIS	-	expression tag	UNP P35052
C	8	HIS	-	expression tag	UNP P35052
C	9	HIS	-	expression tag	UNP P35052
C	10	HIS	-	expression tag	UNP P35052
C	11	HIS	-	expression tag	UNP P35052
C	12	ASP	-	expression tag	UNP P35052
C	13	LEU	-	expression tag	UNP P35052
C	14	TYR	-	expression tag	UNP P35052
C	15	GLU	-	expression tag	UNP P35052
C	16	ASN	-	expression tag	UNP P35052
C	17	LEU	-	expression tag	UNP P35052
C	18	TYR	-	expression tag	UNP P35052
C	19	PHE	-	expression tag	UNP P35052
C	20	GLN	-	expression tag	UNP P35052

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Chain	Residue	Modelled	Actual	Comment	Reference
C	21	GLY	-	expression tag	UNP P35052
C	22	LYS	-	expression tag	UNP P35052
C	23	LEU	-	expression tag	UNP P35052
D	2	ALA	-	expression tag	UNP P35052
D	3	PRO	-	expression tag	UNP P35052
D	4	GLN	-	expression tag	UNP P35052
D	5	LEU	-	expression tag	UNP P35052
D	6	HIS	-	expression tag	UNP P35052
D	7	HIS	-	expression tag	UNP P35052
D	8	HIS	-	expression tag	UNP P35052
D	9	HIS	-	expression tag	UNP P35052
D	10	HIS	-	expression tag	UNP P35052
D	11	HIS	-	expression tag	UNP P35052
D	12	ASP	-	expression tag	UNP P35052
D	13	LEU	-	expression tag	UNP P35052
D	14	TYR	-	expression tag	UNP P35052
D	15	GLU	-	expression tag	UNP P35052
D	16	ASN	-	expression tag	UNP P35052
D	17	LEU	-	expression tag	UNP P35052
D	18	TYR	-	expression tag	UNP P35052
D	19	PHE	-	expression tag	UNP P35052
D	20	GLN	-	expression tag	UNP P35052
D	21	GLY	-	expression tag	UNP P35052
D	22	LYS	-	expression tag	UNP P35052
D	23	LEU	-	expression tag	UNP P35052

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

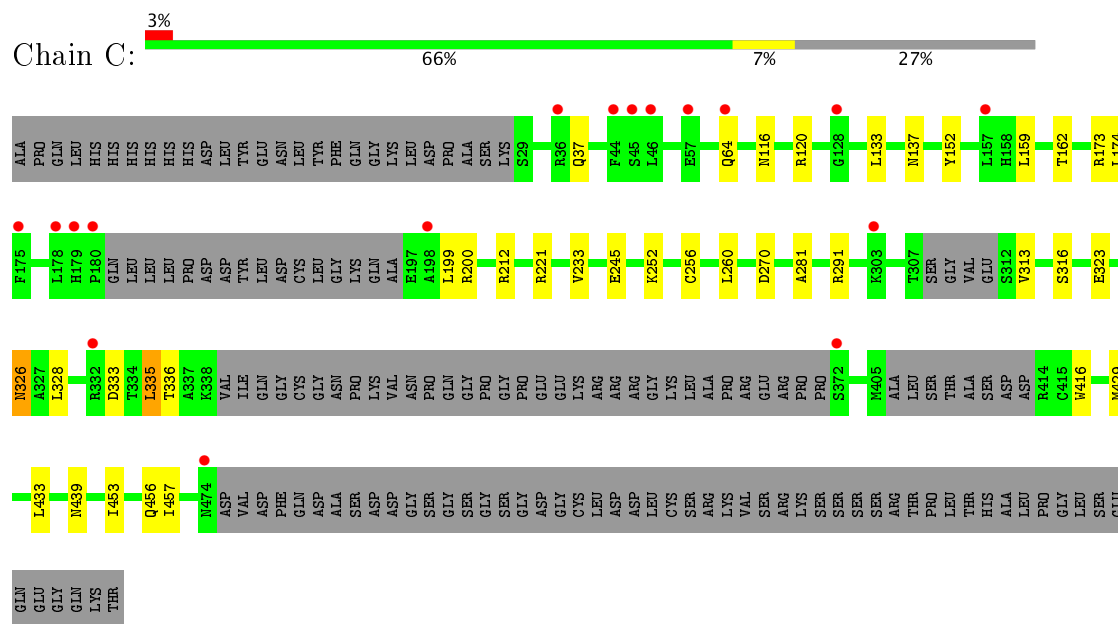


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

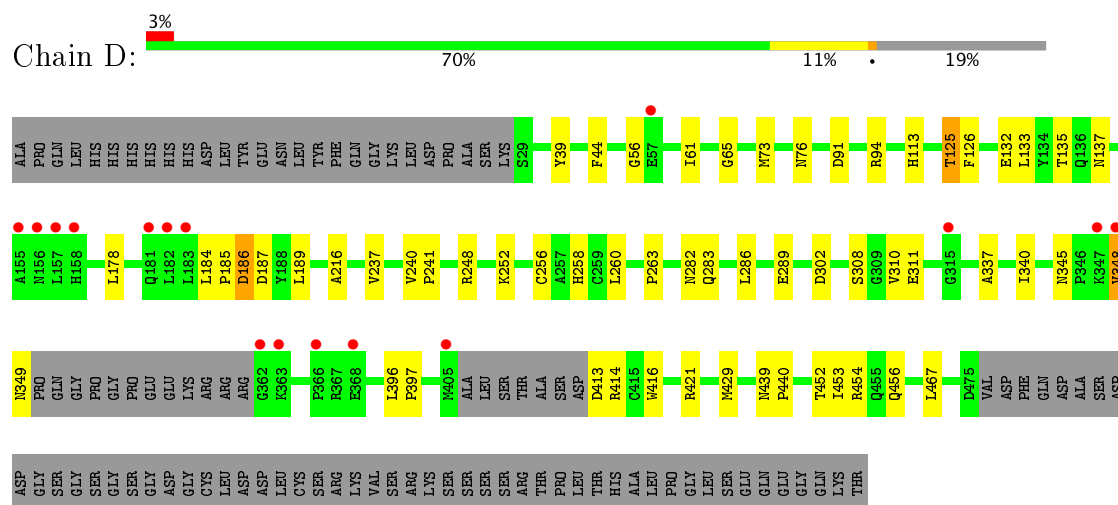
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		
3	B	39	Total	O	0	0
			39	39		
3	C	30	Total	O	0	0
			30	30		
3	D	39	Total	O	0	0
			39	39		

- Molecule 1: GLYPICAN-1



- Molecule 1: GLYPICAN-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.25Å 169.20Å 151.71Å 90.00° 94.96° 90.00°	Depositor
Resolution (Å)	29.76 – 2.94 29.76 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.76-2.94) 99.2 (29.76-2.95)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.95Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: DEV_938)	Depositor
R, R_{free}	0.218 , 0.278 0.213 , 0.275	Depositor DCC
R_{free} test set	2528 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.945	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 67.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	12754	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.33 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 3.2232e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 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	0.23	0/2859	0.41	0/3860
1	B	0.25	0/3402	0.43	0/4601
1	C	0.24	0/3088	0.41	0/4171
1	D	0.24	0/3418	0.41	0/4623
All	All	0.24	0/12767	0.42	0/17255

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
1	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
1	B	39	TYR	Peptide

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	2811	0	2763	23	0
1	B	3341	0	3299	36	0
1	C	3035	0	2989	19	0
1	D	3357	0	3308	28	0
2	A	14	0	13	0	0
2	B	28	0	26	0	0
2	C	14	0	13	0	0
2	D	28	0	26	0	0
3	A	18	0	0	0	0
3	B	39	0	0	2	0
3	C	30	0	0	0	0
3	D	39	0	0	1	0
All	All	12754	0	12437	105	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 (105) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:VAL:HA	1:C:316:SER:HB3	1.72	0.71
1:D:61:ILE:HG23	1:D:248:ARG:HG2	1.71	0.71
1:D:414:ARG:HH21	1:D:421:ARG:HD3	1.58	0.67
1:D:454:ARG:NH2	3:D:2018:HOH:O	2.29	0.65
1:B:133:LEU:O	1:B:137:ASN:ND2	2.30	0.64
1:C:133:LEU:O	1:C:137:ASN:ND2	2.26	0.64
1:A:212:ARG:NH2	1:A:307:THR:O	2.30	0.63
1:B:114:LEU:HD21	1:B:311:GLU:HG3	1.80	0.63
1:B:260:LEU:HD12	1:B:416:TRP:HH2	1.63	0.62
1:D:125:THR:HG22	1:D:126:PHE:HD1	1.64	0.62
1:D:133:LEU:O	1:D:137:ASN:ND2	2.34	0.61
1:A:36:ARG:HG3	1:A:49:VAL:HG11	1.82	0.60
1:A:260:LEU:HD12	1:A:416:TRP:HH2	1.65	0.60
1:B:176:LYS:HE3	1:B:189:LEU:HD11	1.84	0.59
1:C:137:ASN:OD1	1:C:173:ARG:NH1	2.36	0.59
1:A:216:ALA:HA	1:A:310:VAL:HG22	1.85	0.58
1:B:285:ASP:OD2	1:B:454:ARG:NH2	2.39	0.56
1:D:91:ASP:OD1	1:D:94:ARG:NH2	2.39	0.56
1:B:172:GLU:HG3	1:B:189:LEU:HD13	1.87	0.55
1:D:216:ALA:HB1	1:D:310:VAL:HA	1.88	0.55
1:B:37:GLN:O	1:B:40:GLY:HA3	2.07	0.55
1:B:163:LEU:HD12	1:B:210:ARG:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:335:LEU:O	1:C:336:THR:OG1	2.25	0.54
1:A:373:GLY:HA2	1:A:377:LYS:HE2	1.91	0.53
1:B:429:MET:HG3	1:B:439:ASN:HD22	1.74	0.52
1:A:316:SER:OG	1:A:319:THR:OG1	2.27	0.52
1:B:282:ASN:HB3	1:B:453:ILE:HD12	1.92	0.52
1:A:110:HIS:CE1	1:A:375:LEU:HB2	2.45	0.52
1:D:337:ALA:O	1:D:340:ILE:HG13	2.11	0.51
1:B:319:THR:HG21	1:B:367:ARG:HB3	1.91	0.51
1:D:282:ASN:HB3	1:D:453:ILE:HD12	1.92	0.50
1:B:474:ASN:ND2	3:B:2039:HOH:O	2.37	0.49
1:C:233:VAL:HG13	1:C:456:GLN:HB3	1.94	0.49
1:A:252:LYS:HA	1:A:256:CYS:SG	2.53	0.48
1:B:186:ASP:HA	1:B:189:LEU:HB2	1.95	0.48
1:C:281:ALA:HB1	1:C:433:LEU:HA	1.95	0.48
1:D:260:LEU:HD12	1:D:416:TRP:HH2	1.79	0.48
1:D:132:GLU:HA	1:D:135:THR:OG1	2.13	0.47
1:B:132:GLU:HA	1:B:135:THR:OG1	2.14	0.47
1:B:421:ARG:NH2	3:B:2018:HOH:O	2.46	0.47
1:A:54:ILE:HG22	1:A:55:SER:H	1.79	0.47
1:A:304:PHE:HA	1:A:310:VAL:HB	1.97	0.47
1:C:323:GLU:O	1:C:326:ASN:ND2	2.47	0.47
1:D:348:VAL:HG12	1:D:349:ASN:H	1.80	0.46
1:D:429:MET:HG3	1:D:439:ASN:HD22	1.79	0.46
1:C:159:LEU:O	1:C:162:THR:OG1	2.25	0.46
1:C:252:LYS:HA	1:C:256:CYS:SG	2.55	0.46
1:C:429:MET:HG3	1:C:439:ASN:HD22	1.81	0.46
1:D:186:ASP:HA	1:D:189:LEU:HB2	1.96	0.46
1:A:77:LEU:HD13	1:A:255:TYR:HB3	1.98	0.46
1:B:237:VAL:HG21	1:B:286:LEU:HD11	1.97	0.46
1:A:236:LYS:HD2	1:A:456:GLN:NE2	2.31	0.46
1:C:116:ASN:HB3	1:C:120:ARG:HH12	1.80	0.45
1:A:58:HIS:HD1	1:A:58:HIS:H	1.63	0.45
1:C:453:ILE:O	1:C:457:ILE:HG13	2.17	0.45
1:D:240:VAL:HA	1:D:241:PRO:HD3	1.78	0.45
1:B:216:ALA:HB1	1:B:310:VAL:HA	1.99	0.45
1:D:439:ASN:HA	1:D:440:PRO:HD3	1.76	0.45
1:B:61:ILE:HG23	1:B:248:ARG:HB2	1.99	0.44
1:D:452:THR:O	1:D:456:GLN:HG2	2.17	0.44
1:D:258:HIS:CD2	1:D:263:PRO:HB3	2.53	0.44
1:D:56:GLY:HA3	1:D:65:GLY:O	2.17	0.44
1:A:237:VAL:HG21	1:A:286:LEU:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:ARG:HB3	1:C:313:VAL:HG11	2.00	0.44
1:D:252:LYS:HA	1:D:256:CYS:SG	2.58	0.44
1:C:328:LEU:HA	1:C:328:LEU:HD23	1.84	0.43
1:C:291:ARG:NH2	1:D:302:ASP:OD2	2.30	0.43
1:A:163:LEU:HD12	1:A:210:ARG:HG3	2.01	0.43
1:A:318:HIS:ND1	1:A:319:THR:HG23	2.33	0.43
1:A:152:TYR:O	1:A:221:ARG:HG3	2.18	0.43
1:A:269:PRO:O	1:A:273:ARG:HB2	2.17	0.43
1:B:139:ARG:HG3	1:B:142:ARG:HH21	1.84	0.43
1:B:240:VAL:HA	1:B:241:PRO:HD3	1.83	0.43
1:A:110:HIS:HE1	1:A:375:LEU:HB2	1.82	0.43
1:A:240:VAL:HG21	1:A:453:ILE:HD11	2.01	0.43
1:B:316:SER:HB2	1:B:320:TRP:CZ3	2.53	0.43
1:B:139:ARG:HG3	1:B:142:ARG:NH2	2.34	0.42
1:B:196:ALA:O	1:B:201:PRO:HD3	2.18	0.42
1:C:260:LEU:HD12	1:C:416:TRP:HH2	1.83	0.42
1:D:44:PHE:CZ	1:D:76:ASN:HB3	2.55	0.42
1:B:281:ALA:HB1	1:B:433:LEU:HA	2.01	0.42
1:B:252:LYS:HA	1:B:256:CYS:SG	2.59	0.42
1:B:452:THR:O	1:B:456:GLN:HG2	2.20	0.42
1:B:338:LYS:HB3	1:B:338:LYS:HE2	1.84	0.42
1:B:337:ALA:O	1:B:340:ILE:HG13	2.20	0.42
1:D:283:GLN:N	1:D:283:GLN:OE1	2.47	0.42
1:B:49:VAL:HA	1:B:50:PRO:HD3	1.79	0.42
1:D:39:TYR:CZ	1:D:73:MET:HG2	2.55	0.42
1:D:178:LEU:HD23	1:D:178:LEU:HA	1.92	0.41
1:B:126:PHE:HB3	1:B:134:TYR:CG	2.55	0.41
1:A:447:THR:O	1:A:449:PRO:HD3	2.20	0.41
1:D:237:VAL:HG21	1:D:286:LEU:HD11	2.02	0.41
1:B:218:VAL:HG12	1:B:221:ARG:HH12	1.85	0.41
1:B:390:GLN:HE21	1:B:390:GLN:HB3	1.66	0.41
1:D:396:LEU:HB2	1:D:397:PRO:HD3	2.03	0.41
1:B:300:ILE:HA	1:B:300:ILE:HD12	1.93	0.41
1:C:199:LEU:HD12	1:C:199:LEU:HA	1.86	0.41
1:D:184:LEU:HA	1:D:185:PRO:HD2	1.79	0.41
1:B:170:LEU:HG	1:B:174:LEU:HD13	2.03	0.41
1:C:245:GLU:CD	1:C:245:GLU:H	2.24	0.41
1:A:387:ARG:O	1:A:390:GLN:HG2	2.20	0.41
1:B:183:LEU:HB3	1:B:347:LYS:HG3	2.03	0.40
1:B:450:ASP:O	1:B:454:ARG:HG2	2.22	0.40
1:C:152:TYR:O	1:C:221:ARG:HG3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASN:OD1	1:A:149:ARG:NH1	2.54	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	350/528 (66%)	339 (97%)	10 (3%)	1 (0%)	44	75
1	B	420/528 (80%)	410 (98%)	10 (2%)	0	100	100
1	C	375/528 (71%)	363 (97%)	12 (3%)	0	100	100
1	D	422/528 (80%)	412 (98%)	10 (2%)	0	100	100
All	All	1567/2112 (74%)	1524 (97%)	42 (3%)	1 (0%)	55	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	PRO

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	301/444 (68%)	297 (99%)	4 (1%)	73	91

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	358/444 (81%)	349 (98%)	9 (2%)	53	82
1	C	324/444 (73%)	316 (98%)	8 (2%)	53	82
1	D	360/444 (81%)	349 (97%)	11 (3%)	45	78
All	All	1343/1776 (76%)	1311 (98%)	32 (2%)	54	83

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	136	GLN
1	A	208	GLU
1	A	402	SER
1	A	442	VAL
1	B	58	HIS
1	B	114	LEU
1	B	174	LEU
1	B	186	ASP
1	B	187	ASP
1	B	369	ARG
1	B	380	SER
1	B	387	ARG
1	B	465	ASN
1	C	37	GLN
1	C	64	GLN
1	C	174	LEU
1	C	200	ARG
1	C	270	ASP
1	C	326	ASN
1	C	333	ASP
1	C	335	LEU
1	D	113	HIS
1	D	125	THR
1	D	186	ASP
1	D	187	ASP
1	D	289	GLU
1	D	308	SER
1	D	311	GLU
1	D	345	ASN
1	D	348	VAL
1	D	413	ASP
1	D	467	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	390	GLN
1	C	97	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

6 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	1501	1	14,14,15	0.52	0	15,19,21	0.78	0
2	NAG	B	1500	1	14,14,15	0.64	0	15,19,21	0.67	0
2	NAG	B	1501	1	14,14,15	0.49	0	15,19,21	0.86	1 (6%)
2	NAG	C	1501	1	14,14,15	0.60	0	15,19,21	1.24	3 (20%)
2	NAG	D	1500	1	14,14,15	0.64	0	15,19,21	1.02	2 (13%)
2	NAG	D	1501	1	14,14,15	0.50	0	15,19,21	0.84	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	1501	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1500	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	1501	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1501	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1500	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1501	1	-	0/6/23/26	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	C	1501	NAG	O5-C1-C2	-2.50	108.00	111.47
2	C	1501	NAG	C4-C3-C2	-2.29	107.66	111.02
2	D	1500	NAG	O5-C1-C2	-2.23	108.36	111.47
2	B	1501	NAG	C1-O5-C5	2.25	115.27	112.17
2	D	1500	NAG	C4-C3-C2	2.42	114.56	111.02
2	C	1501	NAG	C1-O5-C5	2.62	115.77	112.17

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1500	NAG	C1

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	358/528 (67%)	0.21	26 (7%)	16 13	33, 75, 142, 171	0
1	B	426/528 (80%)	-0.13	14 (3%)	47 44	24, 64, 110, 146	0
1	C	385/528 (72%)	0.09	17 (4%)	35 33	34, 75, 134, 174	0
1	D	428/528 (81%)	-0.06	16 (3%)	42 40	28, 66, 117, 150	0
All	All	1597/2112 (75%)	0.02	73 (4%)	33 31	24, 69, 127, 174	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	372	SER	5.6
1	C	474	ASN	5.4
1	A	127	PRO	4.9
1	A	205	ALA	4.9
1	D	366	PRO	4.4
1	A	207	ARG	4.0
1	C	45	SER	3.9
1	A	48	ASP	3.9
1	B	181	GLN	3.9
1	B	155	ALA	3.5
1	A	211	LEU	3.5
1	A	204	GLU	3.5
1	D	158	HIS	3.5
1	B	182	LEU	3.5
1	B	57	GLU	3.4
1	D	348	VAL	3.4
1	B	403	GLU	3.4
1	D	57	GLU	3.2
1	B	347	LYS	3.2
1	A	130	PHE	3.2
1	C	36	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	368	GLU	3.1
1	D	362	GLY	3.0
1	A	472	ASN	3.0
1	C	46	LEU	3.0
1	C	157	LEU	2.9
1	C	179	HIS	2.9
1	C	57	GLU	2.9
1	C	44	PHE	2.9
1	D	182	LEU	2.8
1	A	206	PRO	2.8
1	B	371	PRO	2.8
1	A	123	GLN	2.7
1	D	181	GLN	2.7
1	C	198	ALA	2.7
1	D	155	ALA	2.7
1	D	157	LEU	2.6
1	D	405	MET	2.6
1	B	362	GLY	2.6
1	A	305	TRP	2.6
1	C	303	LYS	2.5
1	C	178	LEU	2.5
1	D	363	LYS	2.5
1	A	72	GLU	2.5
1	B	419	MET	2.5
1	A	158	HIS	2.5
1	B	183	LEU	2.5
1	D	183	LEU	2.5
1	A	266	ARG	2.4
1	A	36	ARG	2.4
1	B	363	LYS	2.4
1	C	332	ARG	2.4
1	A	172	GLU	2.3
1	A	46	LEU	2.2
1	A	168	ALA	2.2
1	A	132	GLU	2.2
1	A	126	PHE	2.2
1	A	164	ALA	2.2
1	A	128	GLY	2.2
1	A	41	ALA	2.2
1	B	158	HIS	2.1
1	B	402	SER	2.1
1	C	180	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	347	LYS	2.1
1	A	161	GLU	2.1
1	A	316	SER	2.1
1	C	175	PHE	2.1
1	C	64	GLN	2.1
1	B	414	ARG	2.0
1	D	156	ASN	2.0
1	C	128	GLY	2.0
1	D	315	GLY	2.0
1	A	171	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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. 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(\AA^2)	Q<0.9
2	NAG	B	1501	14/15	0.93	0.22	1.03	77,87,102,117	0
2	NAG	B	1500	14/15	0.84	0.20	-	77,104,117,121	0
2	NAG	D	1501	14/15	0.86	0.25	-	65,88,119,140	0
2	NAG	A	1501	14/15	0.89	0.15	-	89,99,102,104	0
2	NAG	C	1501	14/15	0.92	0.21	-	66,75,87,92	0
2	NAG	D	1500	14/15	0.75	0.26	-	103,125,137,142	0

6.5 Other polymers [i](#)

There are no such residues in this entry.