



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:21 PM UTC

PDB ID : 4ACR / pdb_00004acr
Title : Crystal structure of N-glycosylated, C-terminally truncated human glypican-1
Authors : Svensson, G.; Awad, W.; Mani, K.; Logan, D.T.
Deposited on : 2011-12-17
Resolution : 2.55 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

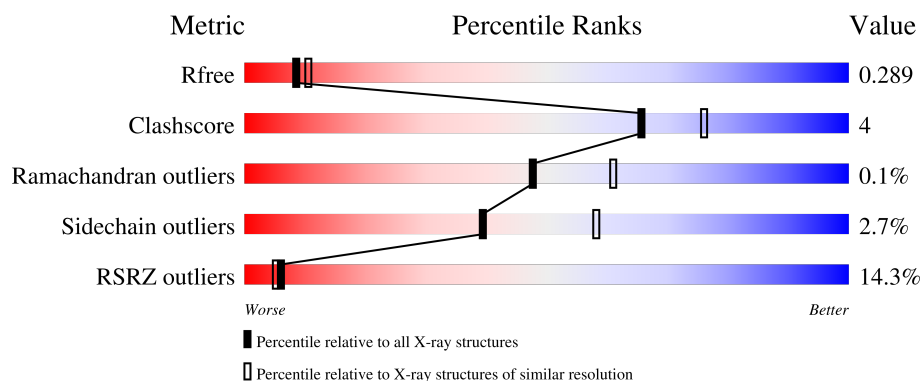
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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 $\leq 5\%$. 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	478	14% 64% 8% • 27%
1	B	478	12% 77% 11% • 11%
1	C	478	11% 72% 10% • 18%
1	D	478	10% 81% 7% • 10%

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
2	NAG	B	500	X	-	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12812 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	347	Total	C	N	O	S	0	0	0
			2723	1696	500	506	21			
1	B	424	Total	C	N	O	S	0	0	0
			3324	2074	605	622	23			
1	C	393	Total	C	N	O	S	0	0	0
			3082	1921	562	577	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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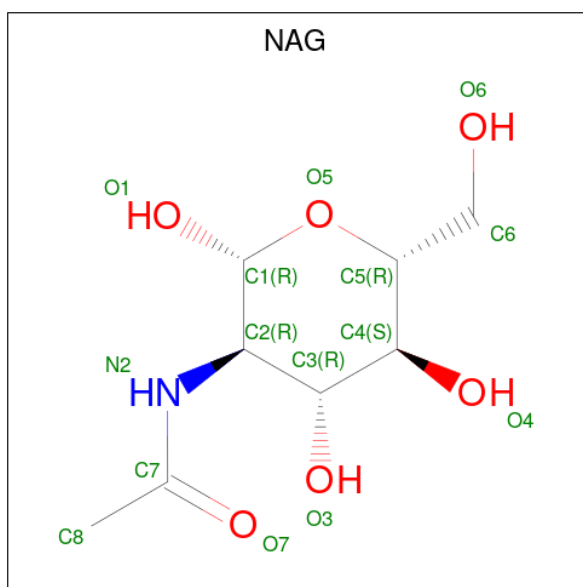
Chain	Residue	Modelled	Actual	Comment	Reference
A	23	LEU	-	expression tag	UNP P35052
B	2	ALA	-	expression tag	UNP P35052
B	3	PRO	-	expression tag	UNP P35052
B	4	GLN	-	expression tag	UNP P35052
B	5	LEU	-	expression tag	UNP P35052
B	6	HIS	-	expression tag	UNP P35052
B	7	HIS	-	expression tag	UNP P35052
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 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: 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		

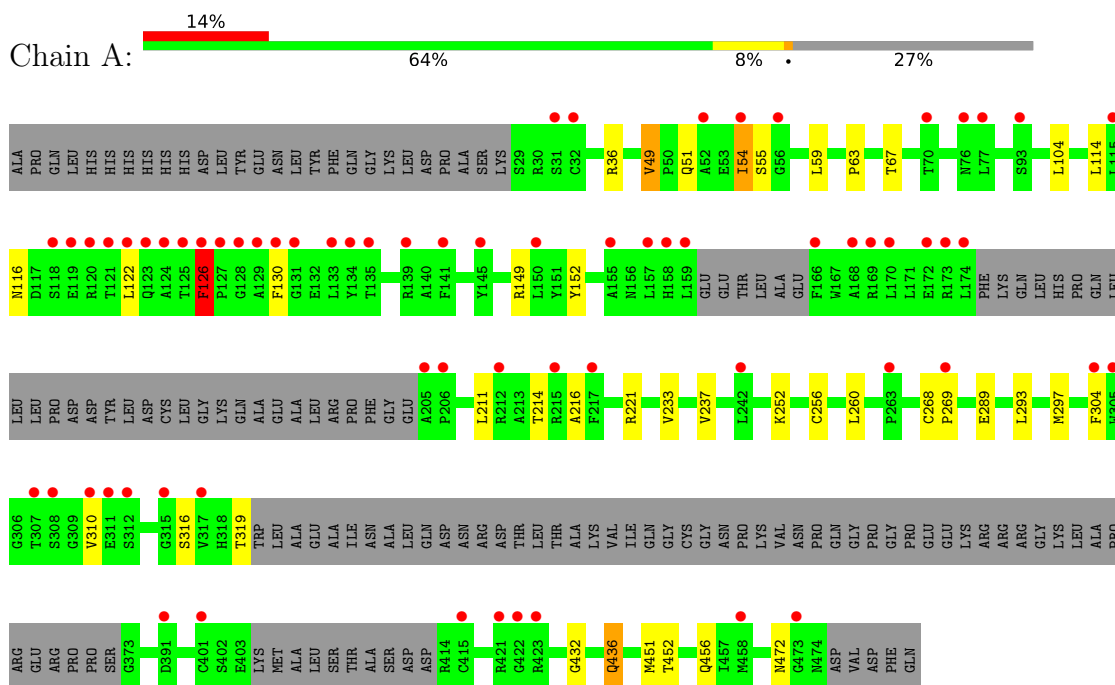
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total	O	0	0
			35	35		
3	B	55	Total	O	0	0
			55	55		
3	C	70	Total	O	0	0
			70	70		
3	D	82	Total	O	0	0
			82	82		

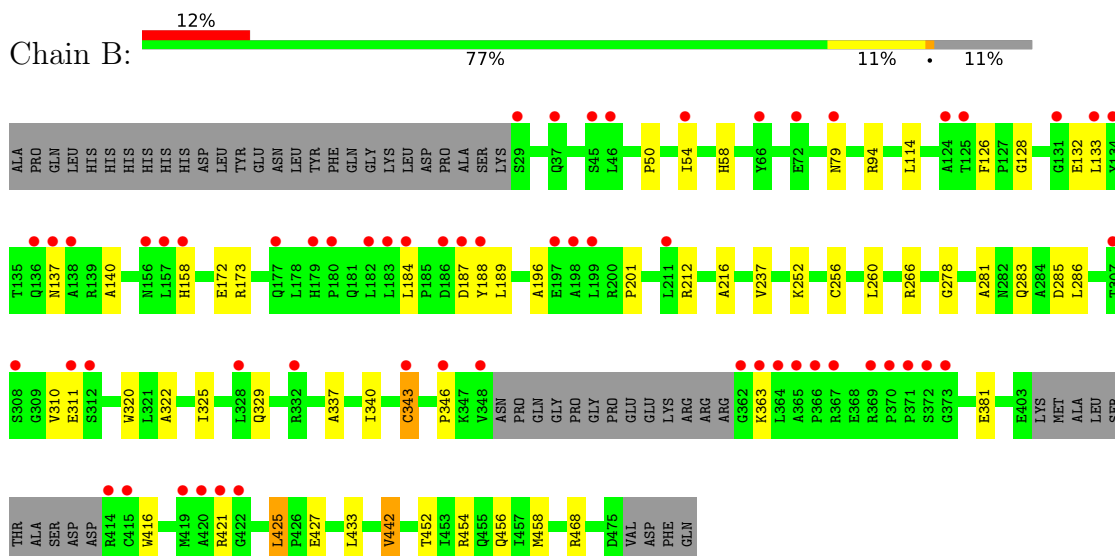
3 Residue-property plots

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.

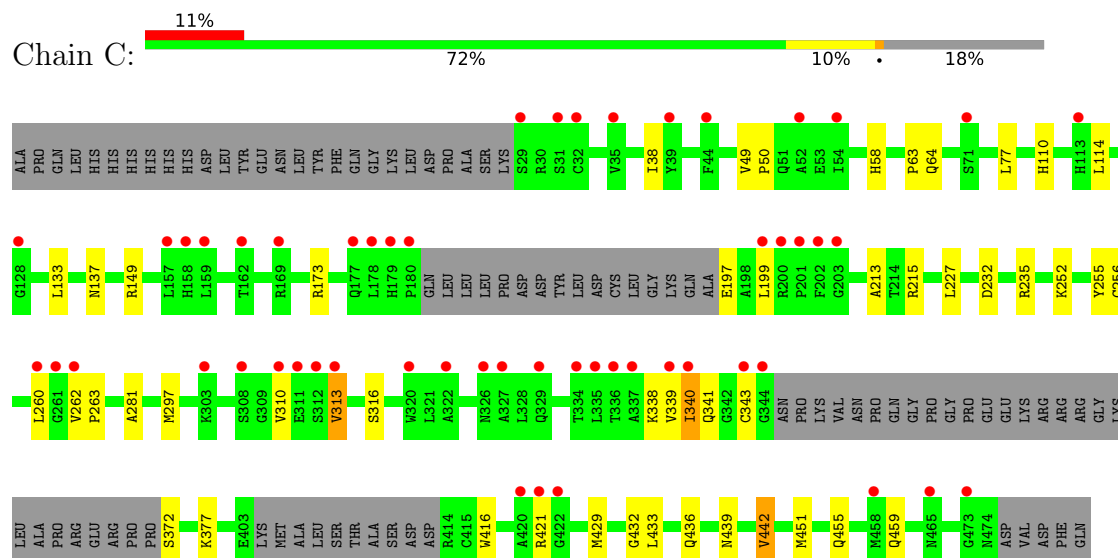
- Molecule 1: GLYPICAN-1



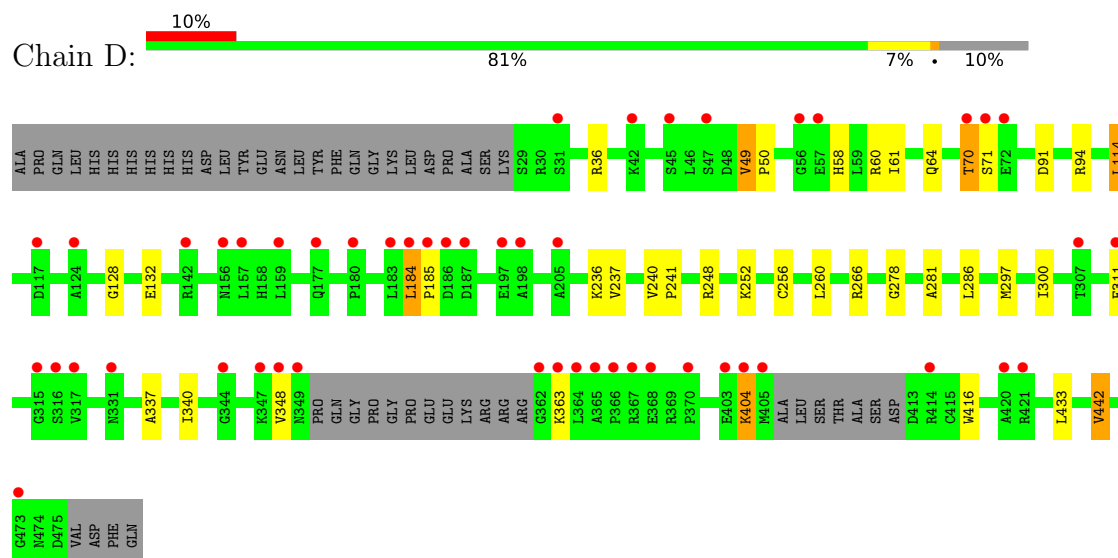
- Molecule 1: GLYPICAN-1



• 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	47.17Å 168.63Å 147.76Å 90.00° 94.59° 90.00°	Depositor
Resolution (Å)	29.71 – 2.55 29.71 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.7 (29.71-2.55) 99.7 (29.71-2.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.18 (at 2.54Å)	Xtrriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.251 , 0.292 0.250 , 0.289	Depositor DCC
R_{free} test set	3757 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtrriage
Anisotropy	0.825	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 57.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12812	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.39 % 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 5.8764e-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	0.28	0/2769	0.74	1/3739 (0.0%)
1	B	0.29	0/3385	0.79	5/4580 (0.1%)
1	C	0.30	0/3136	0.76	1/4239 (0.0%)
1	D	0.30	0/3418	0.78	2/4623 (0.0%)
All	All	0.29	0/12708	0.77	9/17181 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	LEU	CA-C-N	9.03	128.67	119.82
1	B	184	LEU	C-N-CA	9.03	128.67	119.82
1	D	184	LEU	CA-C-N	8.45	128.10	119.82
1	D	184	LEU	C-N-CA	8.45	128.10	119.82
1	B	187	ASP	N-CA-C	-5.82	104.33	112.12
1	A	126	PHE	N-CA-C	5.77	121.35	113.16
1	C	313	VAL	N-CA-C	5.36	118.57	111.17
1	B	266	ARG	CA-C-N	5.14	125.15	119.90
1	B	266	ARG	C-N-CA	5.14	125.15	119.90

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	2723	0	2681	21	0
1	B	3324	0	3277	28	0
1	C	3082	0	3030	27	0
1	D	3357	0	3309	19	0
2	A	14	0	13	0	0
2	B	28	0	26	1	0
2	C	14	0	13	0	0
2	D	28	0	26	0	0
3	A	35	0	0	0	0
3	B	55	0	0	1	0
3	C	70	0	0	2	0
3	D	82	0	0	1	0
All	All	12812	0	12375	95	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 (95) 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:D:128:GLY:HA3	1:D:363:LYS:HD3	1.69	0.74
1:C:63:PRO:HG2	1:C:260:LEU:HD11	1.71	0.71
1:C:137:ASN:OD1	1:C:173:ARG:NH1	2.27	0.67
1:A:116:ASN:OD1	1:A:149:ARG:NH1	2.28	0.66
1:D:114:LEU:HD21	1:D:311:GLU:HG3	1.77	0.65
1:B:260:LEU:HD12	1:B:416:TRP:HH2	1.62	0.64
1:B:133:LEU:O	1:B:137:ASN:ND2	2.33	0.62
1:A:216:ALA:HA	1:A:310:VAL:HG22	1.84	0.59
1:A:122:LEU:O	1:A:126:PHE:HB2	2.05	0.56
1:B:340:ILE:HG22	1:B:346:PRO:HD2	1.87	0.56
1:D:91:ASP:OD1	1:D:94:ARG:NH2	2.39	0.55
1:C:260:LEU:HD12	1:C:416:TRP:HH2	1.70	0.55
1:C:313:VAL:HA	1:C:316:SER:HB2	1.88	0.55
1:C:372:SER:OG	1:C:377:LYS:NZ	2.40	0.55
1:C:262:VAL:HG11	1:C:421:ARG:HE	1.73	0.54
1:D:260:LEU:HD12	1:D:416:TRP:HH2	1.72	0.54
1:B:421:ARG:NH2	3:B:2021:HOH:O	2.42	0.52
1:A:293:LEU:HG	1:A:297:MET:HE2	1.91	0.52
1:C:232:ASP:OD1	1:C:235:ARG:NH1	2.43	0.51
1:D:61:ILE:HG23	1:D:248:ARG:HG2	1.90	0.51
1:C:262:VAL:HG13	1:C:421:ARG:HH21	1.75	0.51
1:A:211:LEU:O	1:A:214:THR:OG1	2.28	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:ARG:NH1	3:C:2020:HOH:O	2.44	0.50
1:D:281:ALA:HB1	1:D:433:LEU:HA	1.94	0.50
1:A:316:SER:OG	1:A:319:THR:OG1	2.23	0.50
1:D:236:LYS:NZ	3:D:2028:HOH:O	2.45	0.50
1:B:128:GLY:HA3	1:B:363:LYS:HD2	1.94	0.49
1:B:140:ALA:HB2	1:B:173:ARG:HH12	1.77	0.49
1:C:133:LEU:O	1:C:137:ASN:ND2	2.44	0.49
1:B:188:TYR:CE2	1:B:343:CYS:HB3	2.47	0.49
1:D:248:ARG:HH12	1:D:442:VAL:HA	1.78	0.49
1:D:266:ARG:HD2	1:D:404:LYS:HD2	1.94	0.49
1:B:188:TYR:CZ	1:B:343:CYS:HB3	2.48	0.48
1:C:149:ARG:NH1	3:C:2012:HOH:O	2.42	0.48
1:C:227:LEU:HG	1:C:297:MET:HE1	1.95	0.48
1:D:237:VAL:HG21	1:D:286:LEU:HD11	1.96	0.48
1:B:278:GLY:HA3	1:B:442:VAL:HG11	1.96	0.48
1:C:38:ILE:HD12	1:C:263:PRO:HB3	1.94	0.48
1:C:439:ASN:HD22	1:C:442:VAL:H	1.62	0.48
1:C:455:GLN:O	1:C:459:GLN:HG2	2.14	0.48
1:A:59:LEU:HD11	1:A:67:THR:HG21	1.97	0.47
1:B:281:ALA:HB1	1:B:433:LEU:HA	1.96	0.47
1:A:51:GLN:N	1:A:51:GLN:OE1	2.47	0.47
1:C:213:ALA:HA	1:C:313:VAL:HG21	1.96	0.47
1:C:439:ASN:ND2	1:C:442:VAL:H	2.14	0.46
1:C:281:ALA:HB1	1:C:433:LEU:HA	1.97	0.46
1:A:63:PRO:HG2	1:A:260:LEU:HD21	1.97	0.46
1:B:425:LEU:H	1:B:425:LEU:HD22	1.81	0.46
1:A:36:ARG:HG3	1:A:49:VAL:HG11	1.98	0.45
1:C:252:LYS:HA	1:C:256:CYS:SG	2.56	0.45
1:B:337:ALA:O	1:B:340:ILE:HG13	2.16	0.45
1:A:126:PHE:CE2	1:A:130:PHE:HD2	2.35	0.45
1:A:216:ALA:HB1	1:A:310:VAL:HG13	1.98	0.45
1:B:79:ASN:OD1	2:B:500:NAG:N2	2.50	0.45
1:D:337:ALA:O	1:D:340:ILE:HG13	2.17	0.45
1:A:252:LYS:HA	1:A:256:CYS:SG	2.57	0.44
1:A:54:ILE:HG22	1:A:55:SER:H	1.82	0.44
1:A:304:PHE:HA	1:A:310:VAL:HB	2.00	0.44
1:B:126:PHE:HE1	1:B:322:ALA:HB2	1.82	0.44
1:B:158:HIS:ND1	1:B:158:HIS:O	2.50	0.44
1:B:283:GLN:OE1	1:B:283:GLN:N	2.49	0.44
1:D:36:ARG:HG3	1:D:49:VAL:HG11	1.99	0.44
1:C:199:LEU:HD23	1:C:199:LEU:HA	1.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:ARG:HH11	1:B:320:TRP:HZ2	1.65	0.44
1:B:216:ALA:HB1	1:B:310:VAL:HA	2.00	0.44
1:B:172:GLU:HG2	1:B:189:LEU:HD13	2.00	0.43
1:B:114:LEU:HD13	1:B:311:GLU:HA	1.99	0.43
1:C:77:LEU:HD13	1:C:255:TYR:HB3	2.00	0.43
1:D:240:VAL:HA	1:D:241:PRO:HD3	1.85	0.43
1:A:233:VAL:HG13	1:A:456:GLN:HB3	2.01	0.43
1:D:297:MET:O	1:D:300:ILE:HG22	2.19	0.43
1:B:252:LYS:HA	1:B:256:CYS:SG	2.58	0.43
1:B:285:ASP:OD2	1:B:454:ARG:NH2	2.52	0.43
1:C:432:GLY:O	1:C:436:GLN:HG2	2.19	0.43
1:B:325:ILE:O	1:B:329:GLN:HG2	2.19	0.42
1:C:49:VAL:HA	1:C:50:PRO:HD3	1.87	0.42
1:D:252:LYS:HA	1:D:256:CYS:SG	2.58	0.42
1:A:432:GLY:O	1:A:436:GLN:NE2	2.49	0.42
1:C:340:ILE:HG23	1:C:341:GLN:H	1.85	0.42
1:B:50:PRO:HB3	1:B:54:ILE:HD11	2.02	0.42
1:A:152:TYR:O	1:A:221:ARG:HG3	2.19	0.42
1:B:196:ALA:O	1:B:201:PRO:HD3	2.20	0.41
1:D:184:LEU:HA	1:D:185:PRO:HD2	1.81	0.41
1:A:237:VAL:HG23	1:A:456:GLN:HG3	2.02	0.41
1:B:237:VAL:HG21	1:B:286:LEU:HD11	2.02	0.41
1:D:278:GLY:HA3	1:D:442:VAL:HG11	2.01	0.41
1:B:188:TYR:CE2	1:B:346:PRO:HD3	2.56	0.41
1:A:452:THR:O	1:A:456:GLN:HG2	2.21	0.41
1:B:452:THR:O	1:B:456:GLN:HG2	2.21	0.41
1:A:268:CYS:HA	1:A:269:PRO:HD3	1.92	0.41
1:D:49:VAL:HA	1:D:50:PRO:HD3	1.78	0.40
1:C:429:MET:HG3	1:C:439:ASN:OD1	2.22	0.40
1:C:451:MET:HA	1:C:451:MET:HE2	2.03	0.40
1:D:70:THR:HG22	1:D:71:SER:H	1.85	0.40
1:C:110:HIS:O	1:C:114:LEU:HB2	2.22	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	337/478 (70%)	332 (98%)	5 (2%)	0	100	100
1	B	418/478 (87%)	409 (98%)	9 (2%)	0	100	100
1	C	385/478 (80%)	377 (98%)	6 (2%)	2 (0%)	24	34
1	D	422/478 (88%)	410 (97%)	12 (3%)	0	100	100
All	All	1562/1912 (82%)	1528 (98%)	32 (2%)	2 (0%)	48	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	340	ILE
1	C	339	VAL

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	292/403 (72%)	283 (97%)	9 (3%)	35	53
1	B	356/403 (88%)	346 (97%)	10 (3%)	38	57
1	C	329/403 (82%)	322 (98%)	7 (2%)	47	66
1	D	360/403 (89%)	350 (97%)	10 (3%)	38	57
All	All	1337/1612 (83%)	1301 (97%)	36 (3%)	39	58

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	VAL
1	A	54	ILE
1	A	104	LEU
1	A	114	LEU

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Mol	Chain	Res	Type
1	A	126	PHE
1	A	289	GLU
1	A	436	GLN
1	A	451	MET
1	A	472	ASN
1	B	58	HIS
1	B	94	ARG
1	B	132	GLU
1	B	343	CYS
1	B	381	GLU
1	B	425	LEU
1	B	427	GLU
1	B	442	VAL
1	B	458	MET
1	B	468	ARG
1	C	58	HIS
1	C	64	GLN
1	C	197	GLU
1	C	310	VAL
1	C	338	LYS
1	C	343	CYS
1	C	442	VAL
1	D	49	VAL
1	D	58	HIS
1	D	60	ARG
1	D	64	GLN
1	D	70	THR
1	D	114	LEU
1	D	132	GLU
1	D	348	VAL
1	D	404	LYS
1	D	442	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	282	ASN
1	B	58	HIS
1	B	103	GLN
1	B	156	ASN
1	B	179	HIS
1	B	282	ASN

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Mol	Chain	Res	Type
1	B	345	ASN
1	C	136	GLN
1	C	239	GLN
1	C	436	GLN
1	D	326	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	501	1	14,14,15	0.48	0	17,19,21	0.84	1 (5%)
2	NAG	A	501	1	14,14,15	0.44	0	17,19,21	1.37	2 (11%)
2	NAG	D	500	1	14,14,15	0.57	0	17,19,21	0.62	0
2	NAG	D	501	1	14,14,15	0.49	0	17,19,21	0.83	1 (5%)
2	NAG	B	500	1	14,14,15	0.57	0	17,19,21	0.82	1 (5%)
2	NAG	B	501	1	14,14,15	0.49	0	17,19,21	0.83	1 (5%)

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	C	501	1	-	1/6/23/26	0/1/1/1
2	NAG	A	501	1	-	4/6/23/26	0/1/1/1
2	NAG	D	500	1	-	2/6/23/26	0/1/1/1
2	NAG	D	501	1	-	2/6/23/26	0/1/1/1
2	NAG	B	500	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	501	1	-	3/6/23/26	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	A	501	NAG	C1-O5-C5	4.10	117.69	112.19
2	C	501	NAG	C1-O5-C5	2.35	115.33	112.19
2	B	500	NAG	O5-C1-C2	-2.27	107.78	111.29
2	B	501	NAG	C1-O5-C5	2.22	115.17	112.19
2	A	501	NAG	C3-C4-C5	2.22	114.26	110.23
2	D	501	NAG	C1-O5-C5	2.08	114.97	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	500	NAG	C1

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	NAG	C3-C2-N2-C7
2	A	501	NAG	C8-C7-N2-C2
2	A	501	NAG	O7-C7-N2-C2
2	B	501	NAG	C8-C7-N2-C2
2	B	501	NAG	O7-C7-N2-C2
2	D	500	NAG	C8-C7-N2-C2
2	D	500	NAG	O7-C7-N2-C2
2	D	501	NAG	C8-C7-N2-C2
2	D	501	NAG	O7-C7-N2-C2
2	C	501	NAG	O5-C5-C6-O6
2	A	501	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
2	B	501	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	500	NAG	1	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	347/478 (72%)	1.08	67 (19%) 3 2	41, 81, 136, 152	0
1	B	424/478 (88%)	0.88	58 (13%) 6 5	27, 67, 125, 159	0
1	C	393/478 (82%)	0.90	53 (13%) 7 5	28, 67, 131, 154	0
1	D	428/478 (89%)	0.66	50 (11%) 9 8	26, 60, 114, 146	0
All	All	1592/1912 (83%)	0.87	228 (14%) 6 5	26, 68, 128, 159	0

All (228) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	364	LEU	7.6
1	B	157	LEU	6.3
1	A	159	LEU	6.0
1	D	365	ALA	5.6
1	A	305	TRP	5.5
1	C	311	GLU	5.1
1	B	364	LEU	4.9
1	C	336	THR	4.8
1	B	199	LEU	4.8
1	C	326	ASN	4.7
1	B	362	GLY	4.6
1	C	337	ALA	4.4
1	D	156	ASN	4.4
1	A	125	THR	4.3
1	C	180	PRO	4.2
1	B	372	SER	4.2
1	B	133	LEU	4.2
1	C	201	PRO	4.2
1	C	308	SER	4.2
1	B	365	ALA	4.1
1	D	404	LYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	366	PRO	4.0
1	C	31	SER	3.9
1	D	362	GLY	3.9
1	C	335	LEU	3.8
1	A	311	GLU	3.8
1	B	348	VAL	3.8
1	A	126	PHE	3.7
1	A	122	LEU	3.7
1	B	182	LEU	3.7
1	C	312	SER	3.7
1	C	179	HIS	3.7
1	D	70	THR	3.7
1	B	422	GLY	3.7
1	A	168	ALA	3.6
1	A	127	PRO	3.5
1	A	157	LEU	3.5
1	C	465	ASN	3.5
1	B	184	LEU	3.5
1	B	197	GLU	3.5
1	D	349	ASN	3.4
1	C	310	VAL	3.4
1	B	183	LEU	3.4
1	C	199	LEU	3.4
1	B	370	PRO	3.4
1	C	157	LEU	3.4
1	B	29	SER	3.4
1	A	169	ARG	3.4
1	A	124	ALA	3.3
1	A	134	TYR	3.3
1	D	370	PRO	3.3
1	A	173	ARG	3.3
1	B	308	SER	3.2
1	A	129	ALA	3.2
1	D	405	MET	3.2
1	A	128	GLY	3.2
1	C	334	THR	3.2
1	C	35	VAL	3.1
1	B	125	THR	3.1
1	C	44	PHE	3.1
1	A	31	SER	3.1
1	D	421	ARG	3.1
1	A	304	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	339	VAL	3.1
1	A	170	LEU	3.0
1	B	198	ALA	3.0
1	D	331	ASN	3.0
1	B	419	MET	3.0
1	A	205	ALA	3.0
1	D	31	SER	3.0
1	C	162	THR	2.9
1	C	158	HIS	2.9
1	B	332	ARG	2.9
1	B	366	PRO	2.9
1	D	187	ASP	2.9
1	B	138	ALA	2.9
1	B	180	PRO	2.9
1	A	123	GLN	2.9
1	D	317	VAL	2.9
1	C	52	ALA	2.9
1	D	316	SER	2.9
1	D	348	VAL	2.9
1	D	177	GLN	2.9
1	A	54	ILE	2.8
1	A	135	THR	2.8
1	B	307	THR	2.8
1	C	169	ARG	2.8
1	D	367	ARG	2.8
1	A	133	LEU	2.8
1	A	120	ARG	2.8
1	D	363	LYS	2.8
1	A	118	SER	2.8
1	B	312	SER	2.8
1	A	415	CYS	2.8
1	C	200	ARG	2.8
1	C	329	GLN	2.8
1	C	113	HIS	2.8
1	B	131	GLY	2.7
1	A	166	PHE	2.7
1	A	150	LEU	2.7
1	B	415	CYS	2.7
1	B	134	TYR	2.7
1	A	70	THR	2.7
1	A	215	ARG	2.7
1	A	308	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	145	TYR	2.7
1	A	130	PHE	2.6
1	B	363	LYS	2.6
1	C	54	ILE	2.6
1	A	76	ASN	2.6
1	A	141	PHE	2.6
1	B	369	ARG	2.6
1	C	458	MET	2.6
1	D	159	LEU	2.6
1	D	347	LYS	2.6
1	B	421	ARG	2.6
1	A	206	PRO	2.6
1	B	373	GLY	2.5
1	A	317	VAL	2.5
1	B	136	GLN	2.5
1	B	343	CYS	2.5
1	A	131	GLY	2.5
1	A	242	LEU	2.5
1	B	211	LEU	2.5
1	C	178	LEU	2.5
1	C	313	VAL	2.5
1	B	414	ARG	2.5
1	B	346	PRO	2.5
1	C	344	GLY	2.5
1	A	391	ASP	2.5
1	B	420	ALA	2.5
1	C	327	ALA	2.5
1	A	119	GLU	2.5
1	B	72	GLU	2.5
1	B	187	ASP	2.5
1	B	158	HIS	2.5
1	A	315	GLY	2.4
1	D	414	ARG	2.4
1	B	371	PRO	2.4
1	C	340	ILE	2.4
1	C	202	PHE	2.4
1	B	156	ASN	2.4
1	A	269	PRO	2.4
1	C	71	SER	2.4
1	A	310	VAL	2.4
1	A	52	ALA	2.4
1	C	420	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	54	ILE	2.4
1	A	212	ARG	2.4
1	B	179	HIS	2.4
1	C	422	GLY	2.3
1	D	56	GLY	2.3
1	A	421	ARG	2.3
1	A	174	LEU	2.3
1	C	320	TRP	2.3
1	C	303	LYS	2.3
1	B	37	GLN	2.3
1	B	186	ASP	2.3
1	C	262	VAL	2.3
1	C	473	GLY	2.3
1	B	45	SER	2.3
1	B	311	GLU	2.3
1	D	311	GLU	2.3
1	C	421	ARG	2.3
1	A	121	THR	2.2
1	C	203	GLY	2.2
1	D	315	GLY	2.2
1	A	458	MET	2.2
1	D	71	SER	2.2
1	D	180	PRO	2.2
1	B	66	TYR	2.2
1	C	343	CYS	2.2
1	C	177	GLN	2.2
1	C	29	SER	2.2
1	D	186	ASP	2.2
1	B	79	ASN	2.2
1	B	137	ASN	2.2
1	A	158	HIS	2.2
1	C	32	CYS	2.2
1	A	422	GLY	2.2
1	B	46	LEU	2.2
1	C	128	GLY	2.2
1	D	117	ASP	2.2
1	D	57	GLU	2.2
1	D	368	GLU	2.2
1	A	423	ARG	2.2
1	D	197	GLU	2.2
1	D	403	GLU	2.2
1	B	328	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	184	LEU	2.1
1	A	172	GLU	2.1
1	D	42	LYS	2.1
1	B	124	ALA	2.1
1	D	420	ALA	2.1
1	A	77	LEU	2.1
1	A	307	THR	2.1
1	C	261	GLY	2.1
1	D	183	LEU	2.1
1	B	188	TYR	2.1
1	D	72	GLU	2.1
1	A	32	CYS	2.1
1	D	45	SER	2.1
1	D	47	SER	2.1
1	B	177	GLN	2.1
1	A	155	ALA	2.1
1	D	198	ALA	2.1
1	D	205	ALA	2.1
1	D	157	LEU	2.1
1	D	307	THR	2.1
1	C	39	TYR	2.1
1	C	260	LEU	2.1
1	A	56	GLY	2.1
1	D	142	ARG	2.1
1	A	401	CYS	2.1
1	A	217	PHE	2.0
1	A	139	ARG	2.0
1	A	115	LEU	2.0
1	D	344	GLY	2.0
1	A	263	PRO	2.0
1	B	367	ARG	2.0
1	C	159	LEU	2.0
1	C	322	ALA	2.0
1	D	124	ALA	2.0
1	A	473	GLY	2.0
1	D	473	GLY	2.0
1	D	185	PRO	2.0
1	A	93	SER	2.0
1	A	312	SER	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	NAG	D	500	14/15	0.51	0.15	115,118,120,120	0
2	NAG	B	500	14/15	0.65	0.14	80,92,97,99	0
2	NAG	A	501	14/15	0.69	0.20	107,116,118,118	0
2	NAG	B	501	14/15	0.74	0.15	88,98,103,107	0
2	NAG	D	501	14/15	0.81	0.17	75,85,96,102	0
2	NAG	C	501	14/15	0.85	0.15	60,66,77,85	0

6.5 Other polymers [i](#)

There are no such residues in this entry.