



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:20 PM UTC

PDB ID : 4BWE / pdb_00004bwe
Title : Crystal structure of C-terminally truncated glypican-1 after controlled dehydration to 86 percent relative humidity
Authors : Awad, W.; Svensson Birkedal, G.; Thunnissen, M.M.G.M.; Mani, K.; Logan, D.T.
Deposited on : 2013-07-01
Resolution : 2.46 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

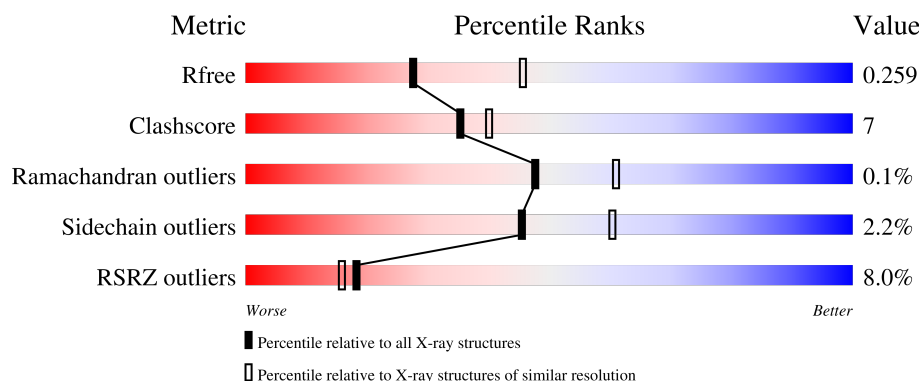
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	6% 70% 13% • 16%
1	B	478	6% 71% 16% • 12%
1	C	478	8% 71% 13% 17%
1	D	478	6% 70% 15% • 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13323 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	402	Total	C	N	O	S	0	6	0
			3157	1970	576	589	22			
1	B	422	Total	C	N	O	S	0	3	0
			3308	2068	596	620	24			
1	C	399	Total	C	N	O	S	0	0	0
			3109	1942	564	581	22			
1	D	421	Total	C	N	O	S	0	5	0
			3307	2069	596	618	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	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		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	B	2	Total	Ca	0	0
			2	2		
3	C	3	Total	Ca	0	0
			3	3		
3	D	2	Total	Ca	0	0
			2	2		

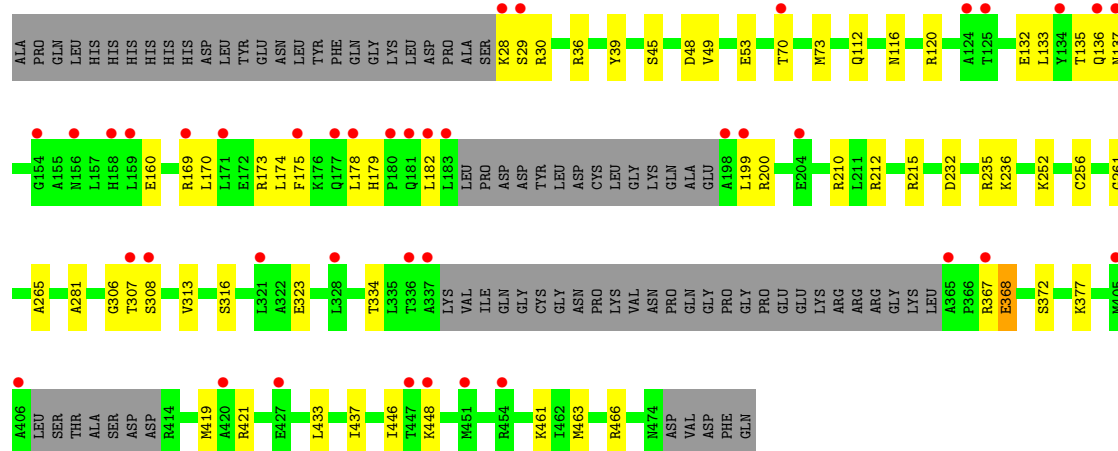
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	123	Total	O	0	0
			123	123		

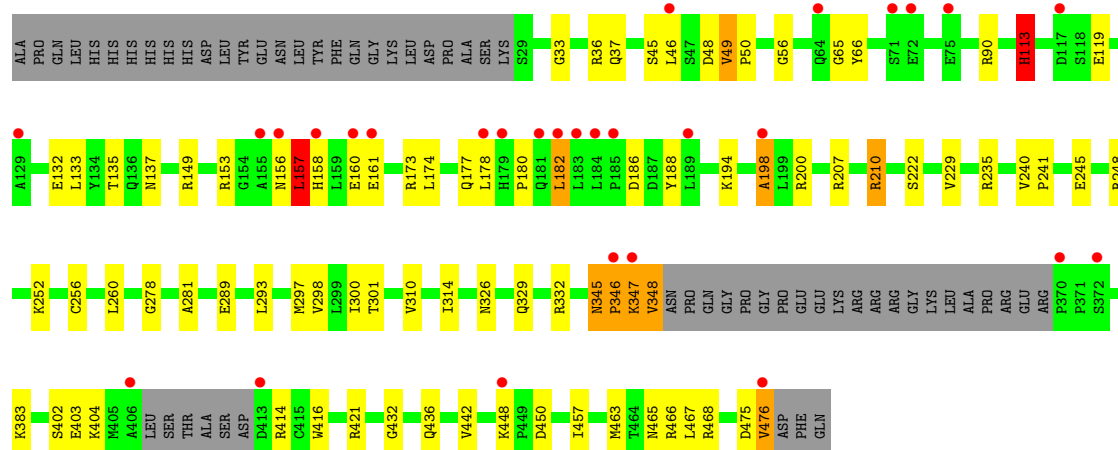
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	82	Total 82	O 82	0	0
4	C	84	Total 84	O 84	0	0
4	D	88	Total 88	O 88	0	0



• 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	47.23Å 166.72Å 139.09Å 90.00° 90.80° 90.00°	Depositor
Resolution (Å)	29.48 – 2.46 29.48 – 2.46	Depositor EDS
% Data completeness (in resolution range)	97.3 (29.48-2.46) 97.3 (29.48-2.46)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.45Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.4_1496)	Depositor
R, R_{free}	0.229 , 0.280 (Not available) , 0.259	Depositor DCC
R_{free} test set	3807 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 66.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	13323	wwPDB-VP
Average B, all atoms (Å ²)	58.0	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 45.73 % 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 1.2663e-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, CA

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	0.43	1/3230 (0.0%)	0.83	4/4368 (0.1%)
1	B	0.42	1/3377 (0.0%)	0.83	5/4570 (0.1%)
1	C	0.39	0/3165	0.77	3/4283 (0.1%)
1	D	0.42	2/3383 (0.1%)	0.84	12/4580 (0.3%)
All	All	0.41	4/13155 (0.0%)	0.82	24/17801 (0.1%)

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	A	0	1
1	B	0	1
1	D	0	3
All	All	0	5

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	109	ASP	C-O	-5.62	1.17	1.24
1	D	113[A]	HIS	C-O	-5.37	1.17	1.24
1	D	113[B]	HIS	C-O	-5.37	1.17	1.24
1	A	116	ASN	C-O	-5.15	1.18	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	345	ASN	CA-C-N	7.43	127.34	120.21
1	B	345	ASN	C-N-CA	7.43	127.34	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	113[A]	HIS	N-CA-C	7.30	126.34	110.80
1	B	113[B]	HIS	N-CA-C	7.30	126.34	110.80
1	D	113[A]	HIS	N-CA-C	6.91	125.51	110.80
1	D	113[B]	HIS	N-CA-C	6.91	125.51	110.80
1	D	345	ASN	CA-C-N	6.30	126.80	119.99
1	D	345	ASN	C-N-CA	6.30	126.80	119.99
1	D	182	LEU	N-CA-C	6.21	119.82	109.95
1	A	404	LYS	N-CA-C	6.02	120.69	113.23
1	C	448	LYS	CA-C-N	5.77	125.75	120.03
1	C	448	LYS	C-N-CA	5.77	125.75	120.03
1	D	346	PRO	CA-C-N	-5.69	111.78	121.85
1	D	346	PRO	C-N-CA	-5.69	111.78	121.85
1	D	113[A]	HIS	CA-C-O	-5.60	112.51	120.51
1	D	113[B]	HIS	CA-C-O	-5.60	112.51	120.51
1	B	157	LEU	N-CA-C	-5.55	98.98	110.80
1	A	370	PRO	O-C-N	5.38	123.68	121.15
1	A	317	VAL	N-CA-C	5.29	115.91	110.36
1	A	308	SER	N-CA-C	5.23	117.43	110.53
1	D	157	LEU	CA-C-N	-5.21	115.49	122.42
1	D	157	LEU	C-N-CA	-5.21	115.49	122.42
1	C	306	GLY	N-CA-C	-5.18	105.91	112.54
1	D	347	LYS	N-CA-C	5.13	117.05	108.99

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	307	THR	Peptide
1	B	156	ASN	Peptide
1	D	113[A]	HIS	Mainchain
1	D	113[B]	HIS	Mainchain
1	D	198	ALA	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of 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	3157	0	3104	39	0
1	B	3308	0	3258	52	0
1	C	3109	0	3049	42	1
1	D	3307	0	3259	54	1
2	A	14	0	13	0	0
2	B	14	0	13	6	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	3	0	0	0	0
3	D	2	0	0	0	0
4	A	123	0	0	4	0
4	B	82	0	0	2	0
4	C	84	0	0	5	0
4	D	88	0	0	3	0
All	All	13323	0	12722	189	1

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 7.

All (189) 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:133:LEU:O	1:D:137:ASN:ND2	1.87	1.08
1:C:232:ASP:OD1	1:C:235:ARG:NH1	1.89	1.05
1:B:133:LEU:HA	1:B:177:GLN:HE22	1.39	0.85
1:D:149:ARG:NH1	4:D:2022:HOH:O	2.06	0.80
1:D:137:ASN:OD1	1:D:173:ARG:NH1	2.14	0.79
1:C:133:LEU:O	1:C:137:ASN:ND2	2.16	0.77
1:B:149:ARG:NH1	4:B:2020:HOH:O	2.11	0.76
1:D:278:GLY:HA3	1:D:442[A]:VAL:HG11	1.66	0.75
1:B:132:GLU:OE1	1:B:135:THR:HB	1.87	0.75
1:B:401:CYS:HA	1:B:405:MET:HB2	1.69	0.73
1:C:132:GLU:OE2	4:C:2027:HOH:O	2.06	0.72
1:B:278:GLY:HA3	1:B:442[A]:VAL:HG11	1.72	0.72
1:B:117:ASP:OD1	1:B:120:ARG:NH2	2.22	0.71
1:A:278:GLY:HA3	1:A:442[A]:VAL:HG11	1.73	0.70
1:C:367:ARG:HD2	1:C:368:GLU:H	1.57	0.68
1:A:265:ALA:HB2	1:A:421:ARG:HD2	1.77	0.66
1:B:260:LEU:HD12	1:B:416:TRP:HH2	1.61	0.66
1:A:469:SER:O	1:A:474:ASN:HB2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:ARG:NH2	4:A:2093:HOH:O	2.28	0.65
1:B:113[A]:HIS:CE1	2:B:501:NAG:H81	2.32	0.65
1:C:175:PHE:HA	1:C:178:LEU:HD13	1.78	0.64
1:C:28:LYS:HD3	1:C:261:GLY:HA3	1.80	0.63
1:B:48:ASP:OD2	1:B:72:GLU:OE2	2.17	0.63
1:C:212:ARG:NH2	4:C:2034:HOH:O	2.31	0.63
1:B:133:LEU:O	1:B:137:ASN:ND2	2.32	0.62
1:D:465:ASN:OD1	1:D:468[B]:ARG:NH2	2.33	0.62
1:B:113[A]:HIS:CD2	2:B:501:NAG:H81	2.36	0.60
1:B:46:LEU:O	1:B:49:VAL:HG12	2.01	0.60
1:D:310:VAL:HG13	1:D:314:ILE:HD12	1.82	0.60
1:D:260:LEU:HD12	1:D:416:TRP:HH2	1.66	0.60
1:D:347:LYS:HG2	1:D:348:VAL:N	2.16	0.60
1:D:475:ASP:OD1	1:D:476:VAL:N	2.35	0.60
1:D:463:MET:HE2	1:D:466:ARG:HH11	1.67	0.60
1:C:169:ARG:HG3	1:C:169:ARG:HH11	1.66	0.59
1:C:367:ARG:HD2	1:C:368:GLU:N	2.16	0.59
1:A:329:GLN:NE2	4:A:2089:HOH:O	2.35	0.59
1:A:413:ASP:HB2	1:A:423:ARG:NH2	2.18	0.59
1:A:30:ARG:HH11	1:A:30:ARG:HG3	1.67	0.59
1:C:367:ARG:HH11	1:C:367:ARG:HG3	1.66	0.58
1:A:260:LEU:HD12	1:A:416:TRP:HH2	1.68	0.57
1:C:28:LYS:HD2	1:C:53:GLU:OE2	2.04	0.57
1:A:451:MET:O	1:A:455:GLN:HG2	2.04	0.57
1:D:448:LYS:C	1:D:448:LYS:HD2	2.29	0.57
1:D:133:LEU:HG	1:D:177:GLN:NE2	2.20	0.57
1:B:178:LEU:HB3	1:B:332:ARG:HD3	1.86	0.57
1:C:169:ARG:HH11	1:C:169:ARG:CG	2.17	0.56
1:C:281:ALA:HB1	1:C:433:LEU:HA	1.87	0.56
1:D:133:LEU:HD23	1:D:174:LEU:HD22	1.87	0.56
1:B:181:GLN:CD	1:B:181:GLN:H	2.12	0.56
1:A:316:SER:O	1:A:319:THR:HB	2.05	0.56
1:A:326:ASN:OD1	1:A:329:GLN:NE2	2.39	0.56
1:B:266:ARG:HH21	1:B:406:ALA:HB3	1.71	0.55
1:A:132:GLU:HA	1:A:135:THR:HB	1.88	0.55
1:C:463:MET:HE2	1:C:466:ARG:HH11	1.71	0.55
1:D:298:VAL:O	1:D:301:THR:OG1	2.24	0.55
1:D:177:GLN:O	1:D:180:PRO:HD3	2.06	0.55
1:B:348:VAL:HG12	1:B:349:ASN:H	1.72	0.55
1:A:45:SER:OG	1:A:48:ASP:OD2	2.21	0.54
1:A:42:LYS:HD3	1:A:80:ARG:NH1	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:ARG:NH1	4:C:2001:HOH:O	2.23	0.54
1:D:297:MET:O	1:D:300:ILE:HG22	2.08	0.54
1:A:173:ARG:O	1:A:177:GLN:HG2	2.08	0.54
1:C:367:ARG:NH1	1:C:368:GLU:O	2.40	0.54
1:C:160:GLU:HG3	1:C:210:ARG:HD3	1.90	0.53
1:D:198:ALA:HA	1:D:200:ARG:HE	1.73	0.53
1:A:313:VAL:HA	1:A:316:SER:OG	2.09	0.53
2:B:501:NAG:O6	2:B:501:NAG:O4	2.16	0.53
1:C:36:ARG:HA	1:C:49:VAL:HG21	1.91	0.53
1:A:151:TYR:HD1	1:A:157:LEU:HB2	1.74	0.53
1:D:403:GLU:HA	1:D:403:GLU:OE1	2.09	0.52
1:B:113[A]:HIS:NE2	2:B:501:NAG:H81	2.23	0.52
1:B:310:VAL:HG13	1:B:314:ILE:HD12	1.91	0.52
1:D:178:LEU:HD22	1:D:332:ARG:HH11	1.74	0.51
1:B:187:ASP:HA	1:B:190:ASP:HB2	1.93	0.51
1:C:116:ASN:O	1:C:120:ARG:HG3	2.10	0.51
1:C:367:ARG:HD2	1:C:368:GLU:HG2	1.92	0.51
1:D:188:TYR:CZ	1:D:346:PRO:HG3	2.46	0.50
1:D:45:SER:OG	1:D:48:ASP:OD1	2.29	0.50
1:C:437:ILE:HB	1:C:446:ILE:HD13	1.93	0.50
1:D:235:ARG:NH1	4:D:2032:HOH:O	2.44	0.50
1:C:179:HIS:CG	1:C:182:LEU:HD12	2.46	0.50
1:B:376:GLU:OE1	1:B:376:GLU:N	2.41	0.50
1:B:266:ARG:NH2	1:B:405:MET:O	2.45	0.49
1:C:132:GLU:HA	1:C:135:THR:HB	1.94	0.49
1:D:421:ARG:NH2	4:D:2036:HOH:O	2.46	0.49
1:A:215:ARG:NH2	4:A:2050:HOH:O	2.45	0.49
1:A:416:TRP:CE2	1:A:418:GLY:HA2	2.47	0.49
1:B:156:ASN:OD1	1:B:157:LEU:N	2.45	0.49
1:D:252:LYS:HA	1:D:256:CYS:SG	2.52	0.49
1:A:30:ARG:HA	1:A:53:GLU:HG3	1.95	0.48
1:D:245:GLU:CD	1:D:248:ARG:HH12	2.20	0.48
1:C:252:LYS:HA	1:C:256:CYS:SG	2.53	0.48
1:A:413:ASP:OD1	1:A:414:ARG:N	2.47	0.48
1:D:132:GLU:HA	1:D:135:THR:HB	1.94	0.48
1:A:281:ALA:HB1	1:A:433:LEU:HA	1.95	0.47
1:B:49:VAL:HG23	1:B:73:MET:HE1	1.96	0.47
1:A:252:LYS:HA	1:A:256:CYS:SG	2.54	0.47
1:A:367:ARG:NE	1:A:368:GLU:O	2.47	0.47
1:B:139:ARG:HA	1:B:142:ARG:NH1	2.29	0.47
1:C:463:MET:HE2	1:C:466:ARG:NH1	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:GLN:HB3	1:C:173:ARG:HH21	1.80	0.47
1:C:313:VAL:HA	1:C:316:SER:OG	2.14	0.47
1:D:240:VAL:HA	1:D:241:PRO:HD3	1.78	0.47
1:A:42:LYS:HD3	1:A:80:ARG:HH11	1.79	0.46
1:C:112:GLN:HG2	4:C:2022:HOH:O	2.15	0.46
1:C:169:ARG:CG	1:C:169:ARG:NH1	2.76	0.46
1:B:449:PRO:HB3	1:B:454:ARG:HH21	1.81	0.46
1:A:437:ILE:HB	1:A:446:ILE:HD13	1.97	0.46
1:C:45:SER:HB3	1:C:48:ASP:OD2	2.15	0.46
1:C:265:ALA:HB2	1:C:421:ARG:HD3	1.98	0.46
1:D:158:HIS:CE1	1:D:160:GLU:HG3	2.50	0.46
1:A:193:GLY:C	1:A:194:LYS:HD2	2.41	0.46
1:B:466:ARG:HG2	1:B:476:VAL:HG21	1.96	0.46
1:A:169:ARG:NH2	4:A:2040:HOH:O	2.35	0.45
1:D:161:GLU:HA	1:D:161:GLU:OE1	2.16	0.45
1:D:156:ASN:OD1	1:D:157:LEU:N	2.49	0.45
1:B:130:PHE:O	1:B:133:LEU:HB2	2.16	0.45
1:B:174:LEU:O	1:B:178:LEU:HG	2.16	0.45
1:D:300:ILE:HD12	1:D:300:ILE:HA	1.87	0.45
1:B:58:HIS:H	1:B:58:HIS:HD1	1.65	0.45
1:B:297:MET:O	1:B:300:ILE:HG22	2.17	0.45
1:C:170:LEU:O	1:C:174:LEU:HB2	2.17	0.45
1:B:113[A]:HIS:CG	2:B:501:NAG:H81	2.52	0.44
1:C:215:ARG:NH1	4:C:2035:HOH:O	2.50	0.44
1:A:137:ASN:HD21	1:A:177:GLN:NE2	2.16	0.44
1:B:252:LYS:HA	1:B:256:CYS:SG	2.57	0.44
1:C:39:TYR:CZ	1:C:73:MET:HG2	2.52	0.44
1:D:207:ARG:HG3	1:D:210:ARG:HH21	1.81	0.44
1:B:89:LEU:HD11	1:B:280:LEU:HD21	1.99	0.44
1:B:278:GLY:HA3	1:B:442[A]:VAL:CG1	2.46	0.44
1:D:49:VAL:HA	1:D:50:PRO:HD3	1.83	0.44
1:D:281:ALA:HB2	1:D:436:GLN:HG3	1.99	0.44
2:B:501:NAG:HO4	2:B:501:NAG:HO6	1.60	0.44
1:C:307:THR:OG1	1:C:308:SER:N	2.51	0.43
1:C:372:SER:HB3	1:C:377:LYS:NZ	2.33	0.43
1:C:307:THR:O	1:C:308:SER:HB3	2.16	0.43
1:B:188:TYR:OH	1:B:346:PRO:HD3	2.18	0.43
1:A:319:THR:HG23	1:A:365:ALA:HB1	2.00	0.43
1:D:345:ASN:HA	1:D:346:PRO:HD2	1.90	0.43
1:B:30:ARG:HA	1:B:53:GLU:CD	2.44	0.43
1:B:332:ARG:NH1	4:B:2027:HOH:O	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:ARG:HE	1:D:90:ARG:HB2	1.62	0.43
1:A:237:VAL:HG21	1:A:286:LEU:HD11	2.01	0.43
1:C:461:LYS:HE3	1:C:461:LYS:HB2	1.88	0.43
1:D:448:LYS:NZ	1:D:450:ASP:HA	2.33	0.43
1:B:49:VAL:HA	1:B:73:MET:SD	2.59	0.43
1:B:336:THR:O	1:B:340:ILE:HG23	2.19	0.42
1:D:36:ARG:HG2	1:D:46:LEU:HD22	2.01	0.42
1:B:58:HIS:HD2	1:B:71:SER:H	1.66	0.42
1:D:245:GLU:OE2	1:D:248:ARG:NH1	2.30	0.42
1:A:126:PHE:N	1:A:127:PRO:HD2	2.35	0.42
1:A:165:GLU:OE1	1:A:169:ARG:NH2	2.53	0.42
1:D:182:LEU:HD13	1:D:346:PRO:HG2	2.02	0.42
1:D:432:GLY:O	1:D:436:GLN:HG2	2.19	0.42
1:B:281:ALA:HB2	1:B:436:GLN:HG3	2.02	0.42
1:D:402:SER:OG	1:D:403:GLU:N	2.52	0.42
1:C:235:ARG:NH2	1:C:236:LYS:NZ	2.67	0.42
1:D:33:GLY:O	1:D:37[A]:GLN:HG3	2.20	0.42
1:D:229:VAL:HG21	1:D:463:MET:HE3	2.02	0.42
1:D:36:ARG:HG3	1:D:49:VAL:HG11	2.02	0.42
1:A:451:MET:HA	1:A:454[B]:ARG:HB2	2.02	0.41
1:C:70:THR:HG22	1:C:73:MET:HG3	2.02	0.41
1:D:289:GLU:HG3	1:D:457:ILE:HG23	2.02	0.41
1:D:414:ARG:HD3	1:D:421:ARG:HD2	2.02	0.41
1:B:191:CYS:O	1:B:195:GLN:HG2	2.19	0.41
1:D:222:SER:HB3	1:D:467:LEU:HD23	2.02	0.41
1:B:133:LEU:HD23	1:B:177:GLN:CD	2.45	0.41
1:A:82:HIS:CE1	1:A:242:LEU:HB2	2.56	0.41
1:A:195:GLN:HB3	1:A:199:LEU:HD21	2.01	0.41
1:D:133:LEU:HD22	1:D:329:GLN:HE21	1.85	0.41
1:D:119:GLU:OE1	1:D:149:ARG:NH2	2.54	0.41
1:B:261:GLY:C	1:B:263:PRO:HD3	2.45	0.41
1:D:293:LEU:O	1:D:297:MET:HG3	2.20	0.41
1:A:42:LYS:HE2	1:A:255:TYR:OH	2.20	0.41
1:A:82:HIS:HE1	1:A:242:LEU:HB2	1.86	0.41
1:B:60:ARG:HA	1:B:60:ARG:HD3	1.86	0.41
1:C:199:LEU:HD12	1:C:199:LEU:HA	1.78	0.41
1:B:177:GLN:O	1:B:180:PRO:HD3	2.21	0.41
1:D:178:LEU:HB3	1:D:332:ARG:HD2	2.02	0.41
1:B:59:LEU:HD21	1:B:67:THR:HG21	2.03	0.40
1:B:432:GLY:O	1:B:436:GLN:HG2	2.21	0.40
1:A:192:LEU:HB3	1:A:194:LYS:NZ	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:LYS:NZ	1:B:255:TYR:CE1	2.89	0.40
1:C:170:LEU:HG	1:C:174:LEU:HD12	2.03	0.40
1:D:56:GLY:HA3	1:D:65:GLY:O	2.21	0.40
1:B:36:ARG:HH21	1:B:51:GLN:HG3	1.86	0.40
1:B:56:GLY:HA3	1:B:65:GLY:O	2.22	0.40
1:B:81:SER:HB2	1:B:250:VAL:HG12	2.03	0.40
1:D:298:VAL:HG13	1:D:383:LYS:HG2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:29:SER:O	1:D:66:TYR:OH[2_445]	2.00	0.20

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	400/478 (84%)	390 (98%)	10 (2%)	0	100	100
1	B	419/478 (88%)	408 (97%)	11 (3%)	0	100	100
1	C	391/478 (82%)	382 (98%)	9 (2%)	0	100	100
1	D	420/478 (88%)	411 (98%)	7 (2%)	2 (0%)	24	32
All	All	1630/1912 (85%)	1591 (98%)	37 (2%)	2 (0%)	48	61

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	113[A]	HIS
1	D	113[B]	HIS

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	334/403 (83%)	324 (97%)	10 (3%)	36	51
1	B	355/403 (88%)	349 (98%)	6 (2%)	53	67
1	C	329/403 (82%)	324 (98%)	5 (2%)	57	70
1	D	355/403 (88%)	344 (97%)	11 (3%)	35	50
All	All	1373/1612 (85%)	1341 (98%)	32 (2%)	45	59

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

Mol	Chain	Res	Type
1	A	30	ARG
1	A	49	VAL
1	A	51	GLN
1	A	173	ARG
1	A	199	LEU
1	A	245	GLU
1	A	387[A]	ARG
1	A	387[B]	ARG
1	A	414	ARG
1	A	425	LEU
1	B	35	VAL
1	B	90	ARG
1	B	181	GLN
1	B	311	GLU
1	B	347	LYS
1	B	348	VAL
1	C	200	ARG
1	C	323	GLU
1	C	334	THR
1	C	368	GLU
1	C	419	MET
1	D	49	VAL
1	D	153	ARG
1	D	157	LEU

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Mol	Chain	Res	Type
1	D	186	ASP
1	D	194	LYS
1	D	210	ARG
1	D	326[A]	ASN
1	D	326[B]	ASN
1	D	348	VAL
1	D	404	LYS
1	D	476	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	177	GLN
1	A	179	HIS
1	B	97	GLN
1	B	177	GLN
1	C	329	GLN
1	D	97	GLN
1	D	158	HIS
1	D	177	GLN
1	D	329	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 9 are monoatomic - leaving 4 for Mogul analysis.

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	501	1	14,14,15	1.16	1 (7%)	17,19,21	2.74	4 (23%)
2	NAG	B	501	1	14,14,15	1.39	2 (14%)	17,19,21	2.54	6 (35%)
2	NAG	C	501	1	14,14,15	1.23	1 (7%)	17,19,21	2.92	6 (35%)
2	NAG	D	501	1	14,14,15	1.06	1 (7%)	17,19,21	3.07	4 (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
2	NAG	A	501	1	-	6/6/23/26	0/1/1/1
2	NAG	B	501	1	-	1/6/23/26	0/1/1/1
2	NAG	C	501	1	-	4/6/23/26	0/1/1/1
2	NAG	D	501	1	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAG	C1-C2	3.56	1.57	1.52
2	C	501	NAG	C1-C2	3.55	1.57	1.52
2	B	501	NAG	C3-C2	-2.57	1.47	1.52
2	D	501	NAG	C3-C2	-2.46	1.47	1.52
2	A	501	NAG	O7-C7	-2.01	1.18	1.23

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	NAG	C1-O5-C5	10.34	126.04	112.19
2	A	501	NAG	C1-O5-C5	8.93	124.16	112.19
2	C	501	NAG	C1-O5-C5	7.40	122.10	112.19
2	C	501	NAG	C4-C3-C2	-5.87	102.41	111.02
2	B	501	NAG	C1-O5-C5	5.82	119.98	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAG	C4-C3-C2	-4.93	103.80	111.02
2	D	501	NAG	O3-C3-C2	-4.70	99.64	109.40
2	A	501	NAG	C4-C3-C2	-4.69	104.14	111.02
2	B	501	NAG	O3-C3-C2	-4.45	100.15	109.40
2	C	501	NAG	C2-N2-C7	-4.42	116.97	122.90
2	D	501	NAG	C1-C2-N2	3.83	116.47	110.43
2	C	501	NAG	C1-C2-N2	3.41	115.81	110.43
2	C	501	NAG	C6-C5-C4	-3.34	104.82	113.02
2	B	501	NAG	C1-C2-N2	3.04	115.23	110.43
2	C	501	NAG	O5-C5-C6	2.56	112.64	107.66
2	D	501	NAG	O5-C5-C4	2.34	116.51	110.83
2	B	501	NAG	C6-C5-C4	-2.32	107.33	113.02
2	B	501	NAG	O5-C5-C6	2.21	111.96	107.66
2	A	501	NAG	O3-C3-C4	-2.17	105.27	110.38
2	A	501	NAG	C1-C2-N2	2.15	113.82	110.43

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	NAG	O5-C5-C6-O6
2	A	501	NAG	C8-C7-N2-C2
2	A	501	NAG	O7-C7-N2-C2
2	A	501	NAG	C4-C5-C6-O6
2	D	501	NAG	C4-C5-C6-O6
2	C	501	NAG	C8-C7-N2-C2
2	C	501	NAG	O7-C7-N2-C2
2	A	501	NAG	O5-C5-C6-O6
2	B	501	NAG	O5-C5-C6-O6
2	C	501	NAG	O5-C5-C6-O6
2	C	501	NAG	C4-C5-C6-O6
2	A	501	NAG	C1-C2-N2-C7
2	A	501	NAG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	NAG	6	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	402/478 (84%)	0.44	31 (7%) 19 17	19, 47, 107, 170	8 (1%)
1	B	422/478 (88%)	0.50	31 (7%) 21 18	22, 53, 101, 144	8 (1%)
1	C	399/478 (83%)	0.65	40 (10%) 12 10	31, 54, 112, 167	2 (0%)
1	D	421/478 (88%)	0.56	29 (6%) 23 20	22, 53, 109, 172	10 (2%)
All	All	1644/1912 (85%)	0.54	131 (7%) 18 16	19, 52, 108, 172	28 (1%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	406	ALA	7.5
1	B	406	ALA	6.1
1	A	365	ALA	5.0
1	C	406	ALA	4.7
1	C	365	ALA	4.7
1	D	413	ASP	4.6
1	C	159	LEU	4.2
1	B	413	ASP	4.0
1	A	192	LEU	3.9
1	D	182	LEU	3.9
1	C	307	THR	3.8
1	C	180	PRO	3.8
1	B	154	GLY	3.8
1	A	196	ALA	3.7
1	C	177	GLN	3.7
1	C	183	LEU	3.6
1	C	308	SER	3.6
1	D	346	PRO	3.6
1	D	185	PRO	3.5
1	A	29	SER	3.5
1	C	182	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	370	PRO	3.4
1	A	309	GLY	3.4
1	A	175	PHE	3.4
1	D	347	LYS	3.4
1	C	171	LEU	3.3
1	D	129	ALA	3.3
1	A	308	SER	3.3
1	A	307	THR	3.3
1	C	405	MET	3.3
1	C	158	HIS	3.2
1	C	136	GLN	3.2
1	D	158	HIS	3.1
1	A	51	GLN	3.1
1	D	448	LYS	3.1
1	C	178	LEU	3.1
1	D	372	SER	3.1
1	B	156	ASN	3.1
1	B	349	ASN	3.1
1	C	28	LYS	3.0
1	B	405	MET	3.0
1	D	198	ALA	3.0
1	B	414	ARG	3.0
1	A	198	ALA	3.0
1	D	406	ALA	3.0
1	C	154	GLY	2.9
1	A	49	VAL	2.9
1	B	347	LYS	2.9
1	D	156	ASN	2.9
1	B	346	PRO	2.9
1	A	194	LYS	2.8
1	A	474	ASN	2.8
1	D	155	ALA	2.8
1	B	159	LEU	2.8
1	B	473	GLY	2.8
1	D	183	LEU	2.8
1	B	43	GLY	2.7
1	A	30	ARG	2.7
1	C	204	GLU	2.7
1	C	199	LEU	2.7
1	D	75	GLU	2.7
1	D	161	GLU	2.7
1	D	71	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	137	ASN	2.6
1	A	197	GLU	2.6
1	B	372	SER	2.6
1	D	160	GLU	2.6
1	D	181	GLN	2.6
1	A	334	THR	2.6
1	B	158	HIS	2.6
1	C	448	LYS	2.6
1	A	48	ASP	2.6
1	A	366	PRO	2.6
1	A	419	MET	2.6
1	C	454	ARG	2.5
1	B	333	ASP	2.5
1	D	184	LEU	2.5
1	D	179	HIS	2.5
1	A	193	GLY	2.5
1	A	372	SER	2.5
1	A	195	GLN	2.5
1	A	70	THR	2.4
1	B	75	GLU	2.4
1	B	311	GLU	2.4
1	C	447	THR	2.4
1	B	402	SER	2.4
1	B	157	LEU	2.4
1	D	476	VAL	2.4
1	B	132	GLU	2.4
1	C	29	SER	2.3
1	C	125	THR	2.3
1	C	175	PHE	2.3
1	C	427	GLU	2.3
1	C	337	ALA	2.3
1	C	181	GLN	2.3
1	B	345	ASN	2.3
1	C	156	ASN	2.3
1	C	367	ARG	2.3
1	B	260	LEU	2.3
1	D	178	LEU	2.3
1	A	333	ASP	2.3
1	A	370	PRO	2.3
1	C	134	TYR	2.3
1	C	198	ALA	2.2
1	B	182	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	189	LEU	2.2
1	D	117	ASP	2.2
1	C	124	ALA	2.2
1	C	420	ALA	2.2
1	B	40	GLY	2.2
1	A	337	ALA	2.2
1	C	336	THR	2.2
1	A	45	SER	2.2
1	B	155	ALA	2.2
1	B	183	LEU	2.2
1	C	328	LEU	2.2
1	C	70	THR	2.1
1	B	28	LYS	2.1
1	A	265	ALA	2.1
1	D	64	GLN	2.1
1	C	169	ARG	2.1
1	B	185	PRO	2.1
1	B	387	ARG	2.0
1	A	156	ASN	2.0
1	B	184	LEU	2.0
1	C	321	LEU	2.0
1	B	344	GLY	2.0
1	D	72	GLU	2.0
1	A	414	ARG	2.0
1	D	46	LEU	2.0
1	C	451	MET	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	C	501	14/15	0.73	0.15	88,95,102,111	0
2	NAG	B	501	14/15	0.82	0.14	66,73,95,104	0
2	NAG	A	501	14/15	0.83	0.12	56,67,83,84	0
3	CA	A	502	1/1	0.85	0.09	88,88,88,88	0
2	NAG	D	501	14/15	0.87	0.11	50,71,104,104	0
3	CA	B	502	1/1	0.92	0.08	90,90,90,90	0
3	CA	C	503	1/1	0.93	0.07	86,86,86,86	0
3	CA	C	502	1/1	0.94	0.05	64,64,64,64	0
3	CA	B	503	1/1	0.95	0.05	83,83,83,83	0
3	CA	C	504	1/1	0.96	0.08	54,54,54,54	0
3	CA	D	503	1/1	0.96	0.07	82,82,82,82	0
3	CA	D	502	1/1	0.97	0.06	77,77,77,77	0
3	CA	A	503	1/1	0.98	0.03	49,49,49,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.