Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:15 PM GMT

PDB ID	:	4BWE
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

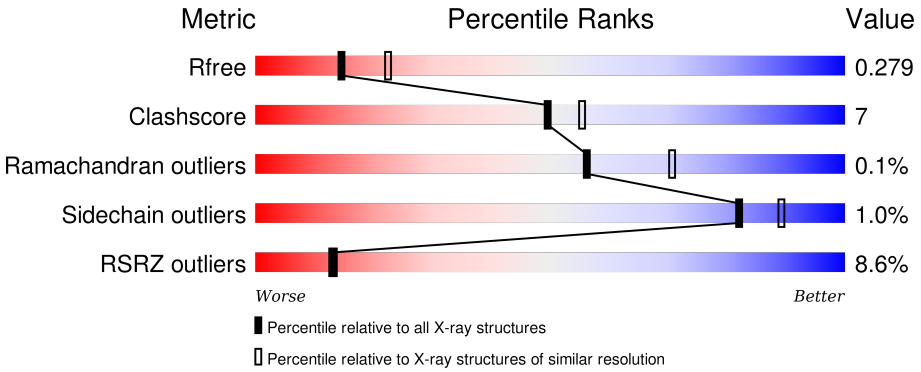
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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}	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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 <=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	7% 72% 12% • 16%
1	B	478	7% 73% 14% • 12%
1	C	478	9% 72% 11% 17%
1	D	478	8% 71% 16% 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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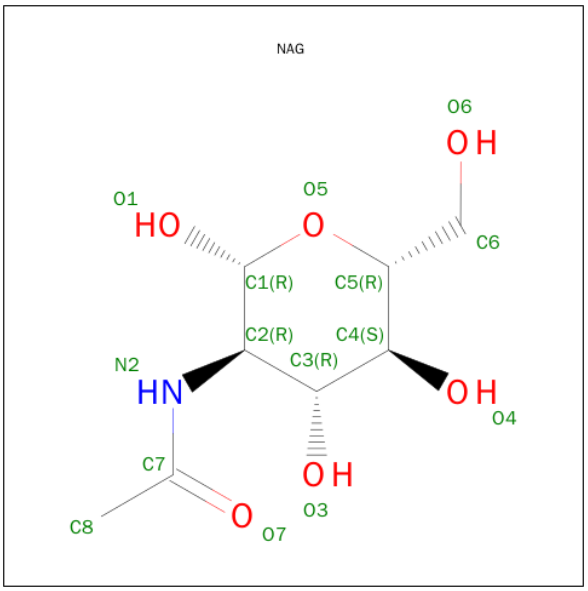
Chain	Residue	Modelled	Actual	Comment	Reference
C	21	GLY	-	EXPRESSION TAG	UNP P35052
C	22	LYS	-	EXPRESSION TAG	UNP P35052
C	23	LEU	-	EXPRESSION TAG	UNP P35052
D	2	ALA	-	EXPRESSION TAG	UNP P35052
D	3	PRO	-	EXPRESSION TAG	UNP P35052
D	4	GLN	-	EXPRESSION TAG	UNP P35052
D	5	LEU	-	EXPRESSION TAG	UNP P35052
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 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 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 4 is water.

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

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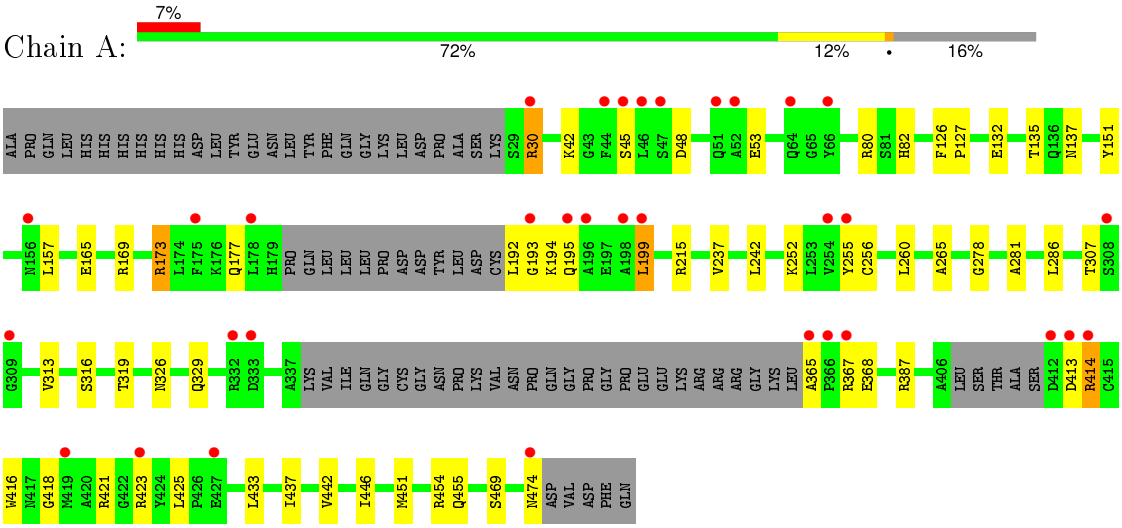
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	82	Total O 82 82	0	0
4	C	84	Total O 84 84	0	0
4	D	88	Total O 88 88	0	0

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 errors 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.

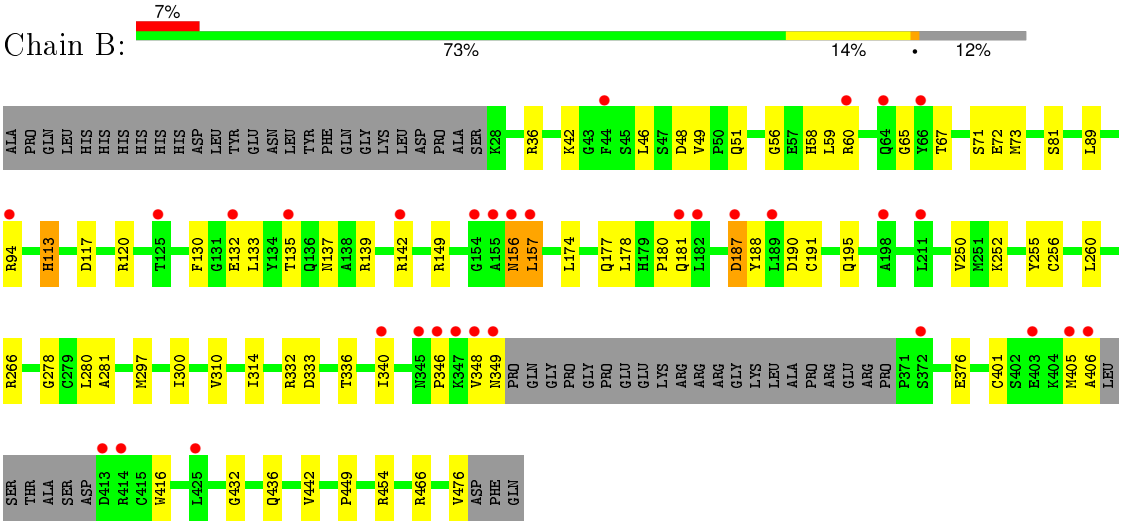
- Molecule 1: GLYPICAN-1

Chain A:



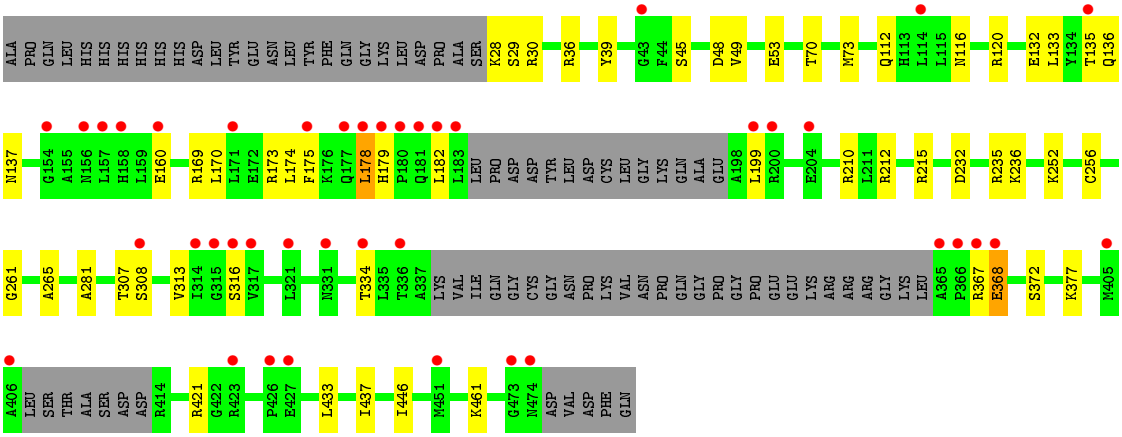
- Molecule 1: GLYPICAN-1

Chain B:



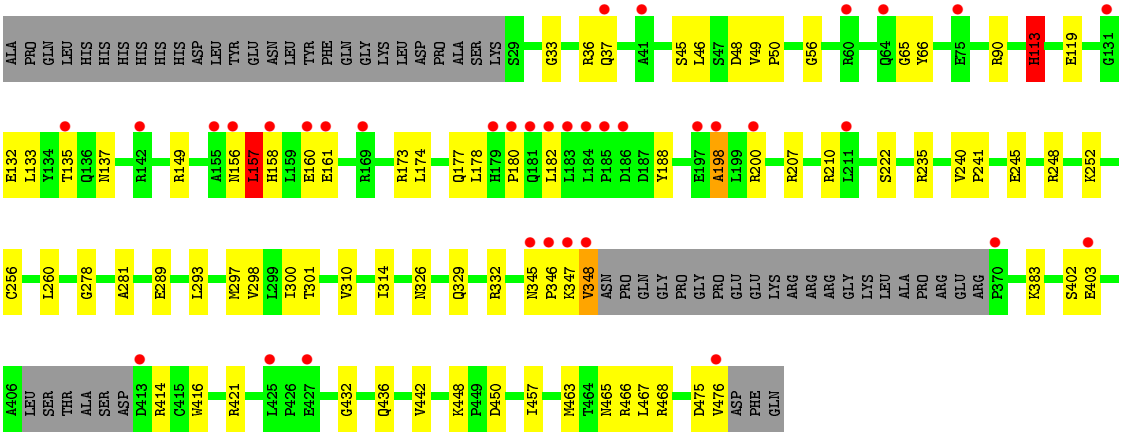
- Molecule 1: GLYPICAN-1

Chain C:



- Molecule 1: GLYPICAN-1

Chain D:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.82 (at 2.45Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.8.4_1496)	Depositor
R, R_{free}	0.229 , 0.280 0.230 , 0.279	Depositor DCC
R_{free} test set	3807 reflections (5.03%)	DCC
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 , 62.0	EDS
Estimated twinning fraction	0.043 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.35$	Xtriage
Outliers	1 of 75752 reflections (0.001%)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 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	0.32	0/3230	0.51	1/4368 (0.0%)
1	B	0.31	0/3377	0.48	3/4570 (0.1%)
1	C	0.28	0/3165	0.44	1/4283 (0.0%)
1	D	0.31	0/3383	0.50	3/4580 (0.1%)
All	All	0.30	0/13155	0.48	8/17801 (0.0%)

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

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	178	LEU	CA-CB-CG	5.77	128.56	115.30
1	B	113[A]	HIS	N-CA-C	5.68	126.34	111.00
1	B	113[B]	HIS	N-CA-C	5.68	126.34	111.00
1	D	157	LEU	CA-CB-CG	5.68	128.36	115.30
1	D	113[A]	HIS	N-CA-C	5.38	125.52	111.00
1	D	113[B]	HIS	N-CA-C	5.38	125.52	111.00
1	A	425	LEU	CA-CB-CG	5.23	127.33	115.30
1	B	157	LEU	CA-CB-CG	5.10	127.04	115.30

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 (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	3157	0	3104	39	0
1	B	3308	0	3258	48	0
1	C	3109	0	3049	40	1
1	D	3307	0	3259	52	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	181	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 (181) 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
1:B:113[A]:HIS:CE1	2:B:501:NAG:H81	2.32	0.65
1:A:367:ARG:NH2	4:A:2093:HOH:O	2.28	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: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:260:LEU:HD12	1:D:416:TRP:HH2	1.66	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:C:28:LYS:HD2	1:C:53:GLU:OE2	2.04	0.57
1:A:260:LEU:HD12	1:A:416:TRP:HH2	1.68	0.57
1:A:451:MET:O	1:A:455:GLN:HG2	2.04	0.57
1:D:133:LEU:HG	1:D:177:GLN:NE2	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:LEU:HB3	1:B:332:ARG:HD3	1.86	0.57
1:D:133:LEU:HD23	1:D:174:LEU:HD22	1.87	0.56
1:C:169:ARG:CG	1:C:169:ARG:HH11	2.17	0.56
1:C:281:ALA:HB1	1:C:433:LEU:HA	1.87	0.56
1:A:326:ASN:OD1	1:A:329:GLN:NE2	2.39	0.56
1:A:316:SER:O	1:A:319:THR:HB	2.05	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: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:C:30:ARG:NH1	4:C:2001:HOH:O	2.23	0.54
1:A:42:LYS:HD3	1:A:80:ARG:NH1	2.22	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:O4	2:B:501:NAG:O6	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:448:LYS:HD2	1:D:448:LYS:C	2.29	0.52
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:181:GLN:CD	1:B:181:GLN:H	2.12	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:367:ARG:HD2	1:C:368:GLU:HG2	1.92	0.51
1:C:116:ASN:O	1:C:120:ARG:HG3	2.10	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:D:235:ARG:NH1	4:D:2032:HOH:O	2.44	0.50
1:C:437:ILE:HB	1:C:446:ILE:HD13	1.93	0.50
1:C:179:HIS:CG	1:C:182:LEU:HD12	2.46	0.50
1:B:376:GLU:N	1:B:376:GLU:OE1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:298:VAL:O	1:D:301:THR:OG1	2.24	0.49
1:A:30:ARG:HA	1:A:53:GLU:HG3	1.95	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: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: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:C:136:GLN:HB3	1:C:173:ARG:HH21	1.80	0.47
1:C:169:ARG:CG	1:C:169:ARG:NH1	2.76	0.46
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: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:D:158:HIS:CE1	1:D:160:GLU:HG3	2.50	0.46
1:C:265:ALA:HB2	1:C:421:ARG:HD3	1.98	0.46
1:B:466:ARG:HG2	1:B:476:VAL:HG21	1.96	0.46
1:D:161:GLU:HA	1:D:161:GLU:OE1	2.16	0.45
1:A:169:ARG:NH2	4:A:2040:HOH:O	2.35	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
2:B:501:NAG:HO6	2:B:501:NAG:HO4	1.59	0.45
1:C:307:THR:O	1:C:308:SER:HB3	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:HD1	1:B:58:HIS:H	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: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:252:LYS:HA	1:B:256:CYS:SG	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:89:LEU:HD11	1:B:280:LEU:HD21	1.99	0.44
1:D:281:ALA:HB2	1:D:436:GLN:HG3	1.99	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: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:332:ARG:NH1	4:B:2027:HOH:O	2.43	0.43
1:D:90:ARG:HB2	1:D:90:ARG:HE	1.62	0.43
1:A:237:VAL:HG21	1:A:286:LEU:HD11	2.01	0.43
1:D:448:LYS:NZ	1:D:450:ASP:HA	2.33	0.43
1:C:461:LYS:HB2	1:C:461:LYS:HE3	1.88	0.43
1:B:49:VAL:HA	1:B:73:MET:SD	2.59	0.43
1:D:36:ARG:HG2	1:D:46:LEU:HD22	2.01	0.42
1:B:336:THR:O	1:B:340:ILE:HG23	2.19	0.42
1:B:58:HIS:HD2	1:B:71:SER:H	1.66	0.42
1:D:463:MET:HE2	1:D:466:ARG:HH11	1.85	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:D:182:LEU:HD13	1:D:346:PRO:HG2	2.02	0.42
1:A:165:GLU:OE1	1:A:169:ARG:NH2	2.53	0.42
1:D:432:GLY:O	1:D:436:GLN:HG2	2.19	0.42
1:D:402:SER:OG	1:D:403:GLU:N	2.52	0.42
1:B:281:ALA:HB2	1:B:436:GLN:HG3	2.02	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: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:D:414:ARG:HD3	1:D:421:ARG:HD2	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: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:A:193:GLY:C	1:A:194:LYS:HD2	2.41	0.41
1:D:133:LEU:HD22	1:D:329:GLN:HE21	1.85	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:119:GLU:OE1	1:D:149:ARG:NH2	2.54	0.41
1:D:293:LEU:O	1:D:297:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:199:LEU:HA	1:C:199:LEU:HD12	1.78	0.41
1:B:60:ARG:HD3	1:B:60:ARG:HA	1.86	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:432:GLY:O	1:B:436:GLN:HG2	2.21	0.40
1:B:59:LEU:HD21	1:B:67:THR:HG21	2.03	0.40
1:A:192:LEU:HB3	1:A:194:LYS:NZ	2.36	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:42:LYS:NZ	1:B:255:TYR:CE1	2.89	0.40
1:B:36:ARG:HH21	1:B:51:GLN:HG3	1.86	0.40
1:D:298:VAL:HG13	1:D:383:LYS:HG2	2.04	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

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%)	34	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1630/1912 (85%)	1591 (98%)	37 (2%)	2 (0%)	56 71

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 (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	334/403 (83%)	328 (98%)	6 (2%)	66 81
1	B	355/403 (88%)	352 (99%)	3 (1%)	86 92
1	C	329/403 (82%)	327 (99%)	2 (1%)	90 94
1	D	355/403 (88%)	351 (99%)	4 (1%)	80 88
All	All	1373/1612 (85%)	1358 (99%)	15 (1%)	82 88

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	173	ARG
1	A	199	LEU
1	A	387[A]	ARG
1	A	387[B]	ARG
1	A	414	ARG
1	B	94	ARG
1	B	187	ASP
1	B	333	ASP
1	C	334	THR
1	C	368	GLU
1	D	157	LEU
1	D	326[A]	ASN

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Mol	Chain	Res	Type
1	D	326[B]	ASN
1	D	348	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	137	ASN
1	A	177	GLN
1	B	136	GLN
1	B	177	GLN
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 carbohydrates 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	1.09	0	15,19,21	2.91	3 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	B	501	1	14,14,15	1.32	2 (14%)	15,19,21	2.64	5 (33%)
2	NAG	C	501	1	14,14,15	1.18	1 (7%)	15,19,21	3.02	5 (33%)
2	NAG	D	501	1	14,14,15	0.98	1 (7%)	15,19,21	3.32	3 (20%)

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	-	0/6/23/26	0/1/1/1
2	NAG	B	501	1	-	0/6/23/26	0/1/1/1
2	NAG	C	501	1	-	0/6/23/26	0/1/1/1
2	NAG	D	501	1	-	0/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	NAG	C3-C2	-2.26	1.47	1.52
2	D	501	NAG	C3-C2	-2.16	1.47	1.52
2	C	501	NAG	C1-C2	3.40	1.57	1.52
2	B	501	NAG	C1-C2	3.42	1.57	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	501	NAG	C4-C3-C2	-5.67	102.41	111.23
2	D	501	NAG	O3-C3-C2	-4.78	99.64	109.11
2	B	501	NAG	C4-C3-C2	-4.78	103.80	111.23
2	C	501	NAG	C2-N2-C7	-4.72	116.97	123.04
2	A	501	NAG	C4-C3-C2	-4.56	104.14	111.23
2	B	501	NAG	O3-C3-C2	-4.52	100.15	109.11
2	D	501	NAG	C3-C2-N2	-3.74	101.60	110.56
2	C	501	NAG	C6-C5-C4	-3.32	104.82	113.02
2	B	501	NAG	C6-C5-C4	-2.31	107.33	113.02
2	A	501	NAG	O3-C3-C4	-2.25	105.27	110.34
2	B	501	NAG	O5-C5-C6	2.13	111.96	107.35
2	C	501	NAG	O5-C5-C6	2.44	112.64	107.35
2	B	501	NAG	C1-O5-C5	6.10	119.98	112.25
2	C	501	NAG	C1-O5-C5	7.76	122.10	112.25
2	A	501	NAG	C1-O5-C5	9.38	124.16	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	501	NAG	C1-O5-C5	10.87	126.04	112.25

There are no chirality outliers.

There are no torsion outliers.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	0.34	33 (8%) 14 15	21, 47, 108, 170	2 (0%)
1	B	422/478 (88%)	0.25	32 (7%) 17 17	24, 54, 102, 144	5 (1%)
1	C	399/478 (83%)	0.51	41 (10%) 9 8	31, 54, 113, 167	2 (0%)
1	D	421/478 (88%)	0.39	36 (8%) 13 13	26, 53, 110, 172	5 (1%)
All	All	1644/1912 (85%)	0.37	142 (8%) 13 13	21, 52, 110, 172	14 (0%)

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	365	ALA	8.0
1	D	346	PRO	7.8
1	B	406	ALA	7.3
1	A	198	ALA	7.1
1	A	196	ALA	6.7
1	A	195	GLN	6.5
1	C	180	PRO	6.2
1	C	182	LEU	6.1
1	D	348	VAL	6.1
1	A	413	ASP	6.1
1	C	175	PHE	6.0
1	A	365	ALA	5.9
1	C	156	ASN	5.5
1	C	199	LEU	5.5
1	C	178	LEU	5.3
1	A	175	PHE	5.3
1	C	181	GLN	5.1
1	D	347	LYS	5.0
1	B	346	PRO	4.8
1	D	182	LEU	4.8
1	B	413	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	185	PRO	4.5
1	A	412	ASP	4.5
1	B	347	LYS	4.3
1	C	317	VAL	4.2
1	D	155	ALA	4.2
1	A	474	ASN	4.2
1	C	366	PRO	4.1
1	D	180	PRO	4.0
1	B	156	ASN	4.0
1	D	370	PRO	3.9
1	D	198	ALA	3.9
1	A	64	GLN	3.9
1	D	181	GLN	3.7
1	A	366	PRO	3.7
1	B	155	ALA	3.7
1	D	158	HIS	3.6
1	D	156	ASN	3.6
1	C	406	ALA	3.5
1	D	37[A]	GLN	3.5
1	A	414	ARG	3.5
1	D	476	VAL	3.4
1	C	427	GLU	3.4
1	D	345	ASN	3.3
1	C	368	GLU	3.3
1	A	193	GLY	3.3
1	D	413	ASP	3.3
1	D	60	ARG	3.2
1	A	254	VAL	3.2
1	B	345	ASN	3.2
1	A	178	LEU	3.2
1	C	183	LEU	3.2
1	C	423	ARG	3.2
1	C	367	ARG	3.2
1	D	142	ARG	3.2
1	B	211	LEU	3.1
1	A	309	GLY	3.1
1	C	336	THR	3.1
1	A	45	SER	3.1
1	B	403	GLU	3.0
1	A	308	SER	3.0
1	C	43	GLY	3.0
1	A	367	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	44	PHE	3.0
1	B	132	GLU	3.0
1	B	44	PHE	2.9
1	B	60	ARG	2.9
1	A	47	SER	2.9
1	A	46	LEU	2.8
1	D	64	GLN	2.8
1	C	321	LEU	2.8
1	D	135	THR	2.8
1	A	423	ARG	2.8
1	C	157	LEU	2.7
1	D	200	ARG	2.7
1	C	426	PRO	2.7
1	A	51	GLN	2.7
1	B	181	GLN	2.7
1	B	66	TYR	2.7
1	D	183	LEU	2.7
1	C	405	MET	2.6
1	C	331	ASN	2.6
1	B	154	GLY	2.6
1	B	135	THR	2.6
1	C	179	HIS	2.6
1	A	333	ASP	2.6
1	D	161	GLU	2.6
1	C	315	GLY	2.5
1	B	182	LEU	2.5
1	A	156	ASN	2.5
1	D	211	LEU	2.5
1	D	186	ASP	2.5
1	B	405	MET	2.5
1	C	308	SER	2.5
1	C	154	GLY	2.4
1	C	314	ILE	2.4
1	B	348	VAL	2.4
1	C	474	ASN	2.4
1	D	403	GLU	2.3
1	A	199	LEU	2.3
1	D	184	LEU	2.3
1	A	52	ALA	2.3
1	C	171	LEU	2.3
1	C	334	THR	2.3
1	C	473	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	204	GLU	2.3
1	C	177	GLN	2.3
1	B	349	ASN	2.3
1	D	425	LEU	2.3
1	B	125	THR	2.2
1	B	340	ILE	2.2
1	C	160	GLU	2.2
1	A	427	GLU	2.2
1	D	179	HIS	2.2
1	D	75	GLU	2.2
1	D	160	GLU	2.2
1	B	187	ASP	2.2
1	D	197	GLU	2.2
1	B	189	LEU	2.2
1	B	425	LEU	2.2
1	B	142	ARG	2.2
1	C	200	ARG	2.2
1	B	64	GLN	2.1
1	C	451	MET	2.1
1	D	169	ARG	2.1
1	B	157	LEU	2.1
1	C	158	HIS	2.1
1	B	372	SER	2.1
1	B	414	ARG	2.1
1	A	419	MET	2.1
1	C	135	THR	2.1
1	B	198	ALA	2.1
1	D	41	ALA	2.1
1	A	255	TYR	2.1
1	A	332	ARG	2.1
1	D	131	GLY	2.1
1	D	427	GLU	2.1
1	A	30	ARG	2.1
1	B	94	ARG	2.0
1	A	66	TYR	2.0
1	C	316	SER	2.0
1	C	114	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, 95^{th} 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
2	NAG	D	501	14/15	0.90	0.21	1.76	50,71,104,104	0
2	NAG	C	501	14/15	0.86	0.23	1.18	88,95,102,111	0
2	NAG	A	501	14/15	0.84	0.15	0.32	56,67,83,84	0
2	NAG	B	501	14/15	0.86	0.16	-0.54	66,73,95,104	0
3	CA	A	503	1/1	0.97	0.11	-1.82	49,49,49,49	0
3	CA	A	502	1/1	0.85	0.08	-2.92	88,88,88,88	0
3	CA	B	502	1/1	0.90	0.04	-3.32	90,90,90,90	0
3	CA	D	502	1/1	0.95	0.05	-3.88	77,77,77,77	0
3	CA	C	502	1/1	0.96	0.06	-	64,64,64,64	0
3	CA	C	504	1/1	0.95	0.15	-	54,54,54,54	0
3	CA	D	503	1/1	0.95	0.04	-	82,82,82,82	0
3	CA	C	503	1/1	0.81	0.08	-	86,86,86,86	0
3	CA	B	503	1/1	0.90	0.05	-	83,83,83,83	0

6.5 Other polymers (i)

There are no such residues in this entry.