Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:45 PM GMT

PDB ID	:	1LXK
Title	:	Streptococcus pneumoniae Hyaluronate Lyase in Complex with Tetrasaccharide Hyaluronan Substrate
Authors	:	Jedrzejas, M.J.; Mello, L.V.; De Groot, B.L.; Li, S.
Deposited on	:	2002-06-05
Resolution	:	1.53 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:

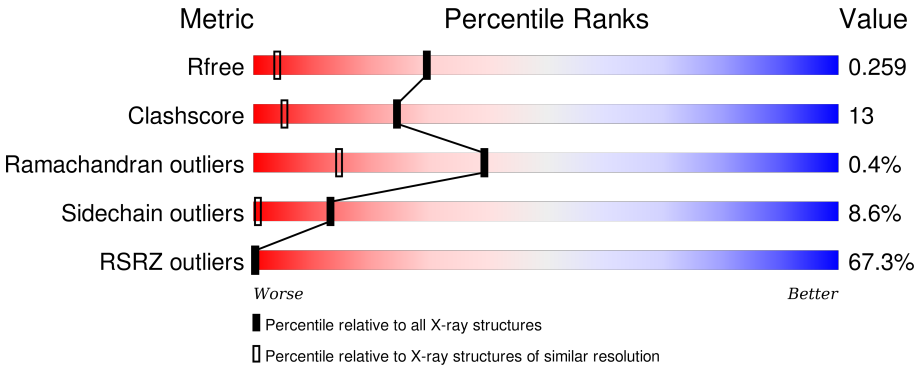
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 1.53 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	1555 (1.56-1.52)
Clashscore	102246	1627 (1.56-1.52)
Ramachandran outliers	100387	1594 (1.56-1.52)
Sidechain outliers	100360	1592 (1.56-1.52)
RSRZ outliers	91569	1555 (1.56-1.52)

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	721	67% 70% 25% ·

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	BDP	A	1001	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BDP	A	1003	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6512 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 Hyaluronate Lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	719	Total	C	N	O	S	0	0	0
			5774	3632	966	1154	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	408	PHE	TYR	ENGINEERED	GB 437705
A	731	VAL	GLY	SEE REMARK 999	GB 437705

- Molecule 2 is a polymer of unknown type called SUGAR (NAG-GCU-NAG-GCU).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	4	Total	C	N	O	0	0
			53	28	2	23		

- Molecule 3 is water.

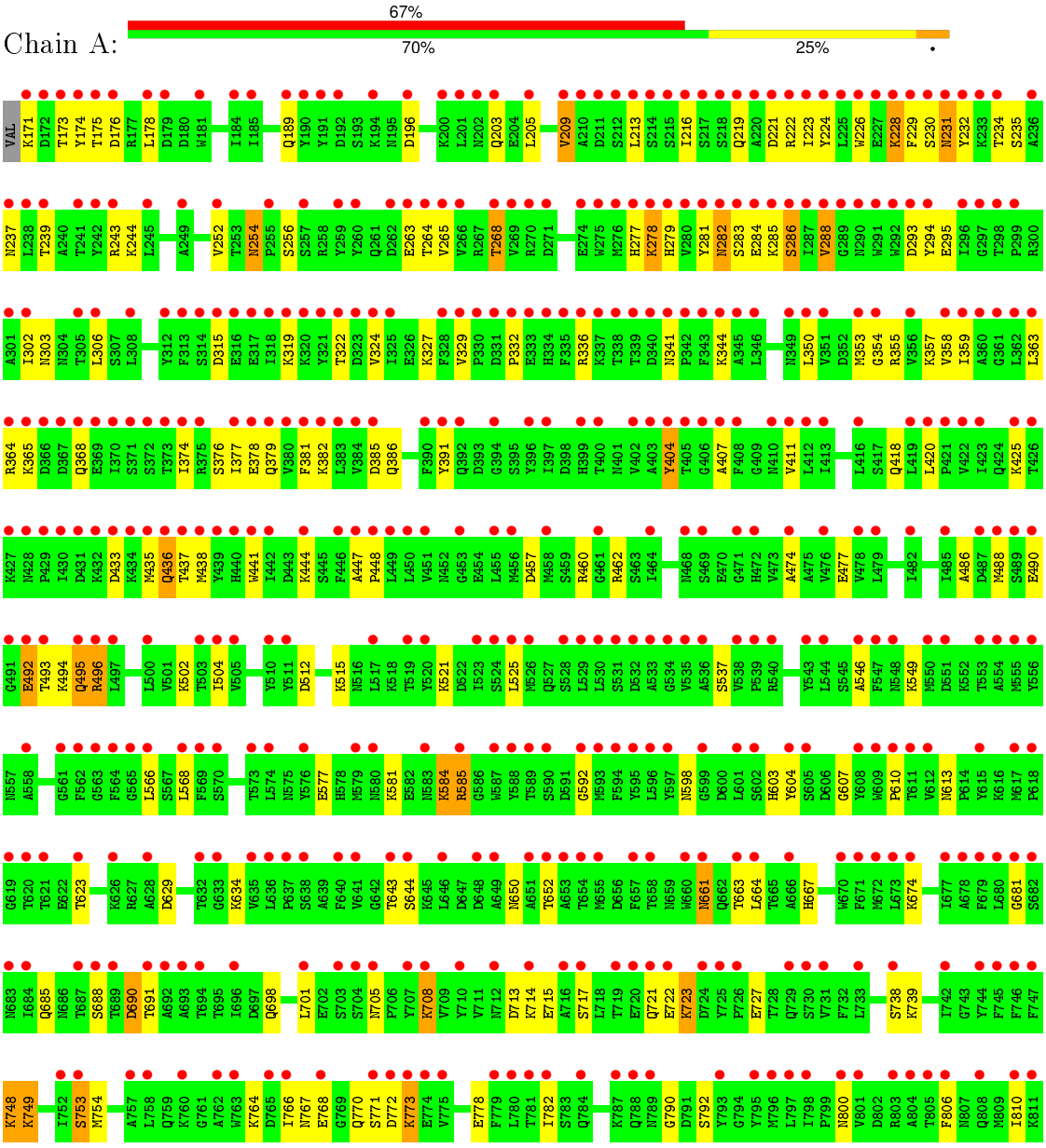
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	685	Total	O	0	0
			685	685		

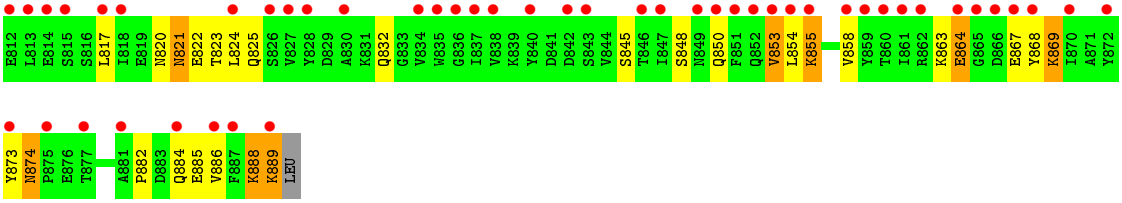
3 Residue-property plots (i)

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: Hyaluronate Lyase

Chain A:




E812
L813
E814
S815
S816
L817
I818
E819
N820
N821
E822
T823
L824
Q825
S826
V827
Y828
D829
A830
K831
Q832
G833
V834
W835
G836
I837
V838
K839
Y840
D841
D842
S843
V844
S845
T846
I847
S848
N849
Q850
F851
Q852
V853
L854
K855
V858
Y859
T860
I861
R862
K863
E864
G865
D866
E867
Y868
K869
I870
A871
Y872
Y873
N874
P875
E876
T877
A881
P882
D883
Q884
E885
V886
F887
K888
K889
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.74Å 103.82Å 101.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.53 64.55 – 1.53	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-1.53) 93.2 (64.55-1.53)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.08 (at 1.52Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.190 , 0.239 0.225 , 0.259	Depositor DCC
R_{free} test set	1227 reflections (0.99%)	DCC
Wilson B-factor (Å^2)	15.9	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 78.6	EDS
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 124794 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	6512	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: NAG, BDP

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	0.35	0/5893	0.58	0/7958

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5774	0	5591	148	0
2	A	53	0	38	1	0
3	A	685	0	0	27	0
All	All	6512	0	5629	148	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 13.

All (148) 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:A:613:ASN:H	1:A:698:GLN:HE22	1.08	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:THR:O	1:A:268:THR:HG22	1.70	0.91
1:A:354:GLY:HA3	1:A:377:ILE:HD11	1.58	0.86
1:A:821:ASN:ND2	1:A:824:LEU:H	1.76	0.82
1:A:821:ASN:HD21	1:A:824:LEU:H	1.32	0.74
1:A:171:LYS:HB2	1:A:175:THR:HG21	1.73	0.70
1:A:644:SER:HB3	3:A:1281:HOH:O	1.93	0.67
1:A:650:ASN:HD21	1:A:832:GLN:HE22	1.41	0.67
1:A:754:MET:HG2	1:A:782:ILE:HG12	1.75	0.67
1:A:295:GLU:HB3	1:A:329:VAL:HG22	1.77	0.66
1:A:171:LYS:HE3	1:A:315:ASP:OD2	1.95	0.66
1:A:889:LYS:HG2	3:A:1688:HOH:O	1.95	0.66
1:A:708:LYS:HD3	1:A:715:GLU:HG3	1.78	0.66
1:A:546:ALA:HB1	3:A:1058:HOH:O	1.98	0.64
1:A:821:ASN:ND2	1:A:823:THR:H	1.95	0.63
1:A:288:VAL:HG13	1:A:294:TYR:OH	1.99	0.63
1:A:178:LEU:HD11	1:A:363:LEU:HD23	1.81	0.62
1:A:705:ASN:HB3	3:A:1240:HOH:O	2.00	0.61
1:A:336:ARG:HH12	2:A:1000:NAG:H2	1.64	0.61
1:A:874:ASN:HD22	1:A:874:ASN:C	2.04	0.61
1:A:820:ASN:HD22	1:A:825:GLN:HG2	1.65	0.61
1:A:603:HIS:ND1	3:A:1444:HOH:O	2.31	0.60
1:A:189:GLN:HG2	3:A:1546:HOH:O	2.03	0.59
1:A:821:ASN:C	1:A:821:ASN:HD22	2.06	0.59
1:A:286:SER:O	1:A:288:VAL:HG12	2.03	0.59
1:A:663:THR:HB	1:A:688:SER:HB3	1.85	0.58
1:A:821:ASN:HD22	1:A:823:THR:H	1.50	0.58
1:A:492:GLU:HG3	1:A:493:THR:N	2.18	0.58
1:A:855:LYS:HB2	1:A:886:VAL:HG12	1.84	0.58
1:A:652:THR:HB	3:A:1281:HOH:O	2.03	0.57
1:A:764:LYS:HD2	1:A:772:ASP:HB3	1.86	0.57
1:A:607:GLY:C	1:A:610:PRO:HD2	2.25	0.57
1:A:205:LEU:O	1:A:209:VAL:HG13	2.05	0.57
1:A:411:VAL:HG13	3:A:1623:HOH:O	2.03	0.57
1:A:254:ASN:ND2	1:A:256:SER:H	2.03	0.57
1:A:717:SER:O	1:A:723:LYS:HE3	2.06	0.56
1:A:585:ARG:HG3	1:A:766:ILE:HG22	1.88	0.56
1:A:488:MET:HE2	3:A:1602:HOH:O	2.05	0.55
1:A:845:SER:HB2	1:A:853:VAL:HG23	1.88	0.55
1:A:888:LYS:O	1:A:889:LYS:HB2	2.06	0.55
1:A:355:ARG:HH11	1:A:418:GLN:NE2	2.06	0.54
1:A:376:SER:O	1:A:379:GLN:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:LYS:HD3	3:A:1688:HOH:O	2.07	0.53
1:A:174:TYR:CD2	1:A:365:LYS:HG2	2.43	0.53
1:A:235:SER:HB2	1:A:293:ASP:HB2	1.90	0.53
1:A:288:VAL:HG22	1:A:288:VAL:O	2.09	0.53
1:A:713:ASP:C	1:A:714:LYS:HD2	2.30	0.52
1:A:386:GLN:NE2	3:A:1635:HOH:O	2.41	0.52
1:A:354:GLY:CA	1:A:377:ILE:HD11	2.37	0.52
1:A:495:GLN:CA	1:A:495:GLN:HE21	2.23	0.52
1:A:420:LEU:HD13	1:A:435:MET:CE	2.41	0.51
1:A:462:ARG:HD3	1:A:577:GLU:OE2	2.10	0.50
1:A:355:ARG:NH2	3:A:1623:HOH:O	2.44	0.50
1:A:173:THR:O	1:A:176:ASP:HB2	2.11	0.50
1:A:623:THR:HB	1:A:690:ASP:HB2	1.93	0.50
1:A:566:LEU:HD23	3:A:1062:HOH:O	2.10	0.50
1:A:213:LEU:HD11	1:A:265:VAL:HG22	1.93	0.50
1:A:230:SER:O	1:A:232:TYR:N	2.45	0.50
1:A:254:ASN:HD22	1:A:254:ASN:C	2.15	0.49
1:A:806:PHE:O	1:A:810:ILE:HG23	2.11	0.49
1:A:239:THR:HG22	1:A:243:ARG:HD2	1.94	0.49
1:A:322:THR:OG1	1:A:364:ARG:NH1	2.44	0.49
1:A:723:LYS:HD3	3:A:1203:HOH:O	2.12	0.49
1:A:216:ILE:HD12	1:A:226:TRP:CZ2	2.47	0.49
1:A:224:TYR:CD2	1:A:230:SER:HB3	2.47	0.49
1:A:882:PRO:HB2	1:A:884:GLN:NE2	2.27	0.49
1:A:604:TYR:HA	3:A:1444:HOH:O	2.13	0.48
1:A:882:PRO:HB2	1:A:884:GLN:HE22	1.78	0.48
1:A:228:LYS:HD2	1:A:229:PHE:CE1	2.48	0.48
1:A:598:ASN:HB2	1:A:739:LYS:O	2.14	0.48
1:A:303:ASN:HB3	1:A:359:ILE:HG21	1.96	0.47
1:A:303:ASN:HB3	1:A:359:ILE:CG2	2.44	0.47
1:A:701:LEU:HD12	1:A:778:GLU:HG2	1.96	0.47
1:A:374:ILE:O	1:A:378:GLU:HG3	2.15	0.47
1:A:634:LYS:HD2	3:A:1459:HOH:O	2.15	0.47
1:A:585:ARG:NH1	1:A:629:ASP:OD2	2.48	0.47
1:A:229:PHE:HE2	1:A:244:LYS:HE2	1.80	0.47
1:A:504:ILE:HG23	3:A:1016:HOH:O	2.15	0.47
1:A:354:GLY:O	1:A:358:VAL:HB	2.15	0.47
1:A:722:GLU:HG2	1:A:753:SER:OG	2.15	0.47
1:A:850:GLN:O	1:A:889:LYS:HD2	2.14	0.46
1:A:708:LYS:HD3	1:A:715:GLU:CG	2.45	0.46
1:A:254:ASN:ND2	1:A:254:ASN:C	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:888:LYS:O	1:A:889:LYS:CB	2.64	0.46
1:A:447:ALA:HB3	1:A:448:PRO:HD3	1.98	0.46
1:A:295:GLU:HB3	1:A:329:VAL:CG2	2.46	0.46
1:A:420:LEU:HD13	1:A:435:MET:HE3	1.96	0.46
1:A:764:LYS:HA	1:A:767:ASN:O	2.16	0.45
1:A:667:HIS:HD2	3:A:1142:HOH:O	1.99	0.45
1:A:329:VAL:HG12	1:A:357:LYS:HD2	1.98	0.45
1:A:381:PHE:O	1:A:437:THR:HG21	2.17	0.45
1:A:643:THR:HB	3:A:1058:HOH:O	2.16	0.45
1:A:277:HIS:CD2	3:A:1528:HOH:O	2.69	0.45
1:A:581:LYS:O	1:A:584:LYS:HD2	2.15	0.45
1:A:661:ASN:C	1:A:661:ASN:HD22	2.20	0.45
1:A:708:LYS:CD	1:A:715:GLU:HG3	2.46	0.45
1:A:607:GLY:O	1:A:610:PRO:HD2	2.16	0.45
1:A:502:LYS:HD3	1:A:537:SER:HB2	1.98	0.45
1:A:203:GLN:HG3	3:A:1374:HOH:O	2.17	0.45
1:A:768:GLU:HG3	3:A:1536:HOH:O	2.17	0.45
1:A:224:TYR:CG	1:A:230:SER:HB3	2.52	0.44
1:A:738:SER:O	1:A:800:ASN:HA	2.17	0.44
1:A:864:GLU:OE2	1:A:869:LYS:HD3	2.18	0.44
1:A:644:SER:HB2	1:A:873:TYR:HB3	1.98	0.44
1:A:568:LEU:HD23	1:A:592:GLY:HA2	2.00	0.44
1:A:420:LEU:HD12	1:A:488:MET:HE1	1.99	0.44
1:A:244:LYS:HE2	3:A:1366:HOH:O	2.16	0.44
1:A:585:ARG:HD3	1:A:629:ASP:OD1	2.17	0.44
1:A:231:ASN:O	1:A:237:ASN:ND2	2.49	0.44
1:A:771:SER:OG	1:A:773:LYS:HB2	2.17	0.44
1:A:661:ASN:H	1:A:661:ASN:HD22	1.66	0.44
1:A:436:GLN:O	1:A:436:GLN:HG2	2.17	0.44
1:A:858:VAL:HG12	3:A:1281:HOH:O	2.17	0.44
1:A:790:GLY:HA2	3:A:1132:HOH:O	2.17	0.43
1:A:863:LYS:HD2	1:A:868:TYR:OH	2.18	0.43
1:A:512:ASP:HB3	1:A:515:LYS:HG3	2.00	0.43
1:A:278:LYS:HG2	1:A:279:HIS:CD2	2.53	0.43
1:A:664:LEU:HA	1:A:685:GLN:O	2.18	0.43
1:A:623:THR:HA	1:A:691:THR:O	2.18	0.43
1:A:332:PRO:O	1:A:353:MET:HG2	2.18	0.43
1:A:749:LYS:HZ3	1:A:749:LYS:HG2	1.57	0.43
1:A:521:LYS:HD2	1:A:521:LYS:HA	1.80	0.43
1:A:681:GLY:O	1:A:792:SER:HB2	2.18	0.43
1:A:282:ASN:HD22	1:A:284:GLU:N	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:ALA:O	1:A:477:GLU:HB2	2.19	0.42
1:A:495:GLN:NE2	3:A:1005:HOH:O	2.51	0.42
1:A:486:ALA:O	1:A:494:LYS:HG3	2.20	0.42
1:A:882:PRO:O	1:A:885:GLU:HB2	2.19	0.42
1:A:223:ILE:HD13	1:A:223:ILE:N	2.34	0.42
1:A:496:ARG:HG3	1:A:496:ARG:HH11	1.85	0.42
1:A:457:ASP:HA	1:A:460:ARG:HG3	2.01	0.42
1:A:178:LEU:HA	1:A:178:LEU:HD23	1.90	0.41
1:A:302:ILE:O	1:A:306:LEU:HG	2.19	0.41
1:A:175:THR:HA	1:A:178:LEU:HB2	2.02	0.41
1:A:585:ARG:HH11	1:A:629:ASP:CG	2.23	0.41
1:A:350:LEU:O	1:A:353:MET:HB3	2.20	0.41
1:A:438:MET:HG2	1:A:441:TRP:CZ3	2.55	0.41
1:A:822:GLU:HG2	1:A:823:THR:HG23	2.03	0.41
1:A:767:ASN:HB3	1:A:770:GLN:CG	2.51	0.41
1:A:521:LYS:HE3	1:A:525:LEU:HG	2.02	0.41
1:A:282:ASN:HD22	1:A:284:GLU:H	1.67	0.41
1:A:821:ASN:HD21	1:A:824:LEU:N	2.07	0.41
1:A:748:LYS:O	1:A:749:LYS:C	2.59	0.40
1:A:869:LYS:HD2	1:A:869:LYS:N	2.36	0.40
1:A:404:TYR:CD1	1:A:407:ALA:HB3	2.57	0.40
1:A:281:TYR:CD2	1:A:324:VAL:HG11	2.57	0.40
1:A:234:THR:HG22	3:A:1533:HOH:O	2.20	0.40
1:A:391:TYR:CD2	1:A:549:LYS:HG3	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	717/721 (99%)	676 (94%)	38 (5%)	3 (0%)	39 14

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	ASN
1	A	848	SER
1	A	674	LYS

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	638/640 (100%)	583 (91%)	55 (9%)	13 1

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	196	ASP
1	A	209	VAL
1	A	219	GLN
1	A	221	ASP
1	A	222	ARG
1	A	228	LYS
1	A	252	VAL
1	A	254	ASN
1	A	263	GLU
1	A	268	THR
1	A	278	LYS
1	A	282	ASN
1	A	283	SER
1	A	285	LYS
1	A	286	SER
1	A	288	VAL
1	A	319	LYS
1	A	327	LYS
1	A	341	ASN
1	A	344	LYS
1	A	368	GLN
1	A	382	LYS

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Mol	Chain	Res	Type
1	A	385	ASP
1	A	404	TYR
1	A	425	LYS
1	A	433	ASP
1	A	436	GLN
1	A	444	LYS
1	A	490	GLU
1	A	492	GLU
1	A	495	GLN
1	A	496	ARG
1	A	584	LYS
1	A	585	ARG
1	A	661	ASN
1	A	690	ASP
1	A	708	LYS
1	A	721	GLN
1	A	723	LYS
1	A	727	GLU
1	A	748	LYS
1	A	749	LYS
1	A	753	SER
1	A	773	LYS
1	A	817	LEU
1	A	821	ASN
1	A	853	VAL
1	A	854	LEU
1	A	855	LYS
1	A	864	GLU
1	A	867	GLU
1	A	869	LYS
1	A	874	ASN
1	A	888	LYS
1	A	889	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	197	GLN
1	A	202	ASN
1	A	254	ASN
1	A	277	HIS
1	A	282	ASN

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Mol	Chain	Res	Type
1	A	349	ASN
1	A	368	GLN
1	A	379	GLN
1	A	418	GLN
1	A	436	GLN
1	A	495	GLN
1	A	580	ASN
1	A	661	ASN
1	A	667	HIS
1	A	683	ASN
1	A	698	GLN
1	A	705	ASN
1	A	729	GLN
1	A	759	GLN
1	A	820	ASN
1	A	821	ASN
1	A	825	GLN
1	A	832	GLN
1	A	874	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)

4 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	NAG	A	1000	2	15,15,15	2.34	6 (40%)	17,21,21	1.00	2 (11%)
2	BDP	A	1001	2	9,12,13	6.68	2 (22%)	13,17,19	3.93	6 (46%)
2	NAG	A	1002	2	14,14,15	2.48	5 (35%)	15,19,21	0.94	1 (6%)
2	BDP	A	1003	2	9,12,13	3.23	4 (44%)	13,17,19	1.79	3 (23%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1000	2	-	0/6/26/26	0/1/1/1
2	BDP	A	1001	2	-	0/0/21/24	0/1/1/1
2	NAG	A	1002	2	-	0/6/23/26	0/1/1/1
2	BDP	A	1003	2	-	0/0/21/24	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1003	BDP	C4-C5	-7.54	1.37	1.53
2	A	1000	NAG	O5-C5	2.22	1.49	1.44
2	A	1002	NAG	C4-C5	2.32	1.58	1.53
2	A	1000	NAG	C4-C3	2.34	1.58	1.52
2	A	1000	NAG	C4-C5	2.73	1.58	1.53
2	A	1003	BDP	O4-C4	2.91	1.49	1.43
2	A	1000	NAG	C1-C2	2.94	1.56	1.53
2	A	1003	BDP	C2-C3	2.98	1.56	1.52
2	A	1002	NAG	O5-C5	3.18	1.50	1.43
2	A	1002	NAG	C2-N2	3.27	1.52	1.46
2	A	1002	NAG	C1-C2	3.55	1.57	1.52
2	A	1000	NAG	C2-N2	3.81	1.52	1.45
2	A	1003	BDP	O5-C5	4.13	1.47	1.43
2	A	1000	NAG	O5-C1	5.45	1.53	1.43
2	A	1002	NAG	O5-C1	6.16	1.54	1.43
2	A	1001	BDP	C4-C5	7.11	1.68	1.53
2	A	1001	BDP	O5-C5	18.42	1.61	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	BDP	O5-C5-C4	-6.24	98.20	108.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	BDP	O4-C4-C5	-4.48	101.98	110.42
2	A	1003	BDP	C1-C2-C3	-3.37	105.55	109.54
2	A	1000	NAG	C8-C7-N2	-2.35	111.61	116.11
2	A	1003	BDP	O4-C4-C5	-2.31	106.07	110.42
2	A	1001	BDP	C1-C2-C3	-2.16	106.98	109.54
2	A	1002	NAG	C8-C7-N2	-2.03	112.23	116.11
2	A	1000	NAG	O7-C7-N2	2.10	126.14	121.86
2	A	1003	BDP	C1-O5-C5	3.17	116.72	111.84
2	A	1001	BDP	C6-C5-C4	5.00	127.14	113.00
2	A	1001	BDP	C3-C4-C5	5.93	120.14	108.66
2	A	1001	BDP	C1-O5-C5	8.57	125.05	111.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	NAG	1	0

5.6 Ligand geometry (i)

There are no ligands in this entry.

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, 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	719/721 (99%)	2.75	484 (67%)	0	0	31, 41, 68, 98	0

All (484) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	224	TYR	12.1
1	A	221	ASP	11.9
1	A	689	THR	9.2
1	A	287	ILE	8.2
1	A	220	ALA	7.8
1	A	174	TYR	7.7
1	A	335	PHE	7.4
1	A	286	SER	7.2
1	A	430	ILE	7.1
1	A	375	ARG	7.0
1	A	339	THR	6.9
1	A	233	LYS	6.8
1	A	275	TRP	6.8
1	A	217	SER	6.7
1	A	223	ILE	6.7
1	A	281	TYR	6.6
1	A	279	HIS	6.5
1	A	427	LYS	6.5
1	A	227	GLU	6.3
1	A	367	ASP	6.3
1	A	865	GLY	6.2
1	A	232	TYR	6.2
1	A	325	ILE	6.2
1	A	219	GLN	6.1
1	A	278	LYS	6.0
1	A	342	PRO	5.6
1	A	189	GLN	5.5

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Mol	Chain	Res	Type	RSRZ
1	A	371	SER	5.4
1	A	225	LEU	5.4
1	A	171	LYS	5.4
1	A	341	ASN	5.3
1	A	236	ALA	5.3
1	A	283	SER	5.3
1	A	431	ASP	5.3
1	A	226	TRP	5.2
1	A	284	GLU	5.2
1	A	289	GLY	5.2
1	A	324	VAL	5.2
1	A	368	GLN	5.2
1	A	216	ILE	5.2
1	A	721	GLN	5.1
1	A	381	PHE	5.1
1	A	432	LYS	5.0
1	A	178	LEU	4.9
1	A	810	ILE	4.9
1	A	849	ASN	4.9
1	A	328	PHE	4.9
1	A	343	PHE	4.9
1	A	209	VAL	4.9
1	A	436	GLN	4.9
1	A	314	SER	4.8
1	A	322	THR	4.8
1	A	363	LEU	4.8
1	A	228	LYS	4.8
1	A	173	THR	4.8
1	A	345	ALA	4.7
1	A	433	ASP	4.7
1	A	333	GLU	4.7
1	A	338	THR	4.7
1	A	231	ASN	4.7
1	A	291	TRP	4.6
1	A	788	GLN	4.6
1	A	290	ASN	4.6
1	A	218	SER	4.6
1	A	268	THR	4.5
1	A	359	ILE	4.5
1	A	677	ILE	4.5
1	A	464	ILE	4.5
1	A	308	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	265	VAL	4.4
1	A	264	THR	4.4
1	A	196	ASP	4.4
1	A	425	LYS	4.4
1	A	280	VAL	4.4
1	A	351	VAL	4.4
1	A	215	SER	4.3
1	A	259	TYR	4.3
1	A	691	THR	4.3
1	A	377	ILE	4.3
1	A	703	SER	4.3
1	A	370	ILE	4.3
1	A	569	PHE	4.3
1	A	353	MET	4.2
1	A	564	PHE	4.2
1	A	374	ILE	4.2
1	A	635	VAL	4.2
1	A	234	THR	4.2
1	A	632	THR	4.2
1	A	758	LEU	4.2
1	A	827	VAL	4.1
1	A	858	VAL	4.1
1	A	316	GLU	4.1
1	A	636	LEU	4.1
1	A	299	PRO	4.1
1	A	292	TRP	4.1
1	A	260	TYR	4.1
1	A	319	LYS	4.0
1	A	867	GLU	4.0
1	A	679	PHE	4.0
1	A	782	ILE	4.0
1	A	492	GLU	4.0
1	A	429	PRO	4.0
1	A	646	LEU	4.0
1	A	331	ASP	3.9
1	A	315	ASP	3.9
1	A	421	PRO	3.9
1	A	229	PHE	3.9
1	A	658	THR	3.9
1	A	271	ASP	3.9
1	A	230	SER	3.9
1	A	420	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	176	ASP	3.9
1	A	861	ILE	3.9
1	A	238	LEU	3.9
1	A	568	LEU	3.9
1	A	757	ALA	3.9
1	A	294	TYR	3.8
1	A	556	TYR	3.8
1	A	423	ILE	3.8
1	A	562	PHE	3.8
1	A	657	PHE	3.8
1	A	222	ARG	3.8
1	A	358	VAL	3.8
1	A	538	VAL	3.8
1	A	866	ASP	3.8
1	A	595	TYR	3.8
1	A	172	ASP	3.8
1	A	488	MET	3.8
1	A	814	GLU	3.7
1	A	237	ASN	3.7
1	A	239	THR	3.7
1	A	337	LYS	3.7
1	A	609	TRP	3.7
1	A	350	LEU	3.7
1	A	716	ALA	3.7
1	A	594	PHE	3.7
1	A	704	SER	3.7
1	A	441	TRP	3.7
1	A	566	LEU	3.7
1	A	671	PHE	3.7
1	A	479	LEU	3.7
1	A	870	ILE	3.6
1	A	334	HIS	3.6
1	A	604	TYR	3.6
1	A	719	THR	3.6
1	A	744	TYR	3.6
1	A	828	TYR	3.6
1	A	779	PHE	3.6
1	A	504	ILE	3.6
1	A	285	LYS	3.6
1	A	451	VAL	3.6
1	A	597	TYR	3.6
1	A	282	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	404	TYR	3.6
1	A	213	LEU	3.6
1	A	766	ILE	3.6
1	A	428	ASN	3.5
1	A	596	LEU	3.5
1	A	408	PHE	3.5
1	A	815	SER	3.5
1	A	402	VAL	3.5
1	A	813	LEU	3.5
1	A	745	PHE	3.5
1	A	413	ILE	3.5
1	A	210	ALA	3.5
1	A	372	SER	3.5
1	A	670	TRP	3.5
1	A	834	VAL	3.5
1	A	192	ASP	3.5
1	A	194	LYS	3.5
1	A	859	TYR	3.4
1	A	574	LEU	3.4
1	A	653	ALA	3.4
1	A	266	VAL	3.4
1	A	390	PHE	3.4
1	A	422	VAL	3.4
1	A	843	SER	3.4
1	A	889	LYS	3.4
1	A	608	TYR	3.4
1	A	530	LEU	3.4
1	A	356	VAL	3.4
1	A	837	ILE	3.4
1	A	373	THR	3.4
1	A	705	ASN	3.4
1	A	637	PRO	3.4
1	A	383	LEU	3.4
1	A	673	LEU	3.4
1	A	797	LEU	3.4
1	A	838	VAL	3.4
1	A	312	TYR	3.3
1	A	615	TYR	3.3
1	A	862	ARG	3.3
1	A	505	VAL	3.3
1	A	277	HIS	3.3
1	A	873	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	633	GLY	3.3
1	A	293	ASP	3.3
1	A	419	LEU	3.3
1	A	439	TYR	3.3
1	A	517	LEU	3.3
1	A	269	VAL	3.3
1	A	298	THR	3.3
1	A	455	LEU	3.3
1	A	854	LEU	3.3
1	A	731	VAL	3.3
1	A	437	THR	3.2
1	A	360	ALA	3.2
1	A	563	GLY	3.2
1	A	733	LEU	3.2
1	A	321	TYR	3.2
1	A	329	VAL	3.2
1	A	678	ALA	3.2
1	A	692	ALA	3.2
1	A	804	ALA	3.2
1	A	382	LYS	3.2
1	A	720	GLU	3.2
1	A	203	GLN	3.2
1	A	684	ILE	3.2
1	A	742	ILE	3.2
1	A	392	GLN	3.2
1	A	435	MET	3.2
1	A	544	LEU	3.2
1	A	354	GLY	3.2
1	A	565	GLY	3.2
1	A	588	TYR	3.2
1	A	641	VAL	3.2
1	A	798	ILE	3.1
1	A	450	LEU	3.1
1	A	396	TYR	3.1
1	A	805	THR	3.1
1	A	547	PHE	3.1
1	A	346	LEU	3.1
1	A	362	LEU	3.1
1	A	553	THR	3.1
1	A	787	LYS	3.1
1	A	847	ILE	3.1
1	A	332	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	775	VAL	3.1
1	A	576	TYR	3.1
1	A	812	GLU	3.1
1	A	652	THR	3.1
1	A	860	THR	3.1
1	A	406	GLY	3.1
1	A	525	LEU	3.0
1	A	789	ASN	3.0
1	A	753	SER	3.0
1	A	601	LEU	3.0
1	A	478	VAL	3.0
1	A	621	THR	3.0
1	A	801	VAL	3.0
1	A	205	LEU	3.0
1	A	397	ILE	3.0
1	A	836	GLY	3.0
1	A	726	PRO	3.0
1	A	772	ASP	3.0
1	A	587	TRP	3.0
1	A	680	LEU	3.0
1	A	855	LYS	3.0
1	A	448	PRO	2.9
1	A	405	THR	2.9
1	A	532	ASP	2.9
1	A	643	THR	2.9
1	A	490	GLU	2.9
1	A	349	ASN	2.9
1	A	617	MET	2.9
1	A	449	LEU	2.9
1	A	853	VAL	2.9
1	A	385	ASP	2.9
1	A	306	LEU	2.9
1	A	589	THR	2.9
1	A	555	MET	2.9
1	A	379	GLN	2.9
1	A	558	ALA	2.9
1	A	666	ALA	2.9
1	A	811	LYS	2.9
1	A	458	MET	2.9
1	A	655	MET	2.9
1	A	252	VAL	2.9
1	A	288	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	302	ILE	2.9
1	A	344	LYS	2.9
1	A	447	ALA	2.9
1	A	241	THR	2.8
1	A	687	THR	2.8
1	A	593	MET	2.8
1	A	590	SER	2.8
1	A	497	LEU	2.8
1	A	708	LYS	2.8
1	A	442	ILE	2.8
1	A	495	GLN	2.8
1	A	640	PHE	2.8
1	A	717	SER	2.8
1	A	365	LYS	2.8
1	A	403	ALA	2.8
1	A	526	MET	2.8
1	A	426	THR	2.8
1	A	573	THR	2.8
1	A	340	ASP	2.8
1	A	366	ASP	2.8
1	A	520	TYR	2.8
1	A	818	ILE	2.8
1	A	620	THR	2.8
1	A	320	LYS	2.7
1	A	313	PHE	2.7
1	A	301	ALA	2.7
1	A	533	ALA	2.7
1	A	654	THR	2.7
1	A	846	THR	2.7
1	A	297	GLY	2.7
1	A	610	PRO	2.7
1	A	661	ASN	2.7
1	A	579	MET	2.7
1	A	434	LYS	2.7
1	A	664	LEU	2.7
1	A	781	THR	2.7
1	A	768	GLU	2.7
1	A	543	TYR	2.7
1	A	175	THR	2.7
1	A	190	TYR	2.6
1	A	795	TYR	2.6
1	A	482	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	808	GLN	2.6
1	A	546	ALA	2.6
1	A	384	VAL	2.6
1	A	580	ASN	2.6
1	A	493	THR	2.6
1	A	763	TRP	2.6
1	A	835	TRP	2.6
1	A	323	ASP	2.6
1	A	765	ASP	2.6
1	A	249	ALA	2.6
1	A	523	ILE	2.6
1	A	887	PHE	2.6
1	A	476	VAL	2.6
1	A	780	LEU	2.6
1	A	270	ARG	2.6
1	A	554	ALA	2.6
1	A	651	ALA	2.6
1	A	489	SER	2.6
1	A	296	ILE	2.6
1	A	485	ILE	2.6
1	A	410	ASN	2.6
1	A	864	GLU	2.6
1	A	529	LEU	2.6
1	A	602	SER	2.6
1	A	585	ARG	2.6
1	A	693	ALA	2.6
1	A	399	HIS	2.6
1	A	648	ASP	2.6
1	A	724	ASP	2.6
1	A	242	TYR	2.6
1	A	707	TYR	2.6
1	A	561	GLY	2.6
1	A	456	MET	2.5
1	A	243	ARG	2.5
1	A	570	SER	2.5
1	A	710	TYR	2.5
1	A	752	ILE	2.5
1	A	201	LEU	2.5
1	A	274	GLU	2.5
1	A	830	ALA	2.5
1	A	318	ILE	2.5
1	A	181	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	824	LEU	2.5
1	A	200	LYS	2.5
1	A	361	GLY	2.5
1	A	649	ALA	2.5
1	A	511	TYR	2.5
1	A	626	LYS	2.5
1	A	380	VAL	2.4
1	A	817	LEU	2.4
1	A	305	THR	2.4
1	A	438	MET	2.4
1	A	672	MET	2.4
1	A	245	LEU	2.4
1	A	255	PRO	2.4
1	A	179	ASP	2.4
1	A	262	ASP	2.4
1	A	191	TYR	2.4
1	A	725	TYR	2.4
1	A	263	GLU	2.4
1	A	474	ALA	2.4
1	A	491	GLY	2.4
1	A	330	PRO	2.4
1	A	660	TRP	2.4
1	A	773	LYS	2.4
1	A	528	SER	2.4
1	A	612	VAL	2.4
1	A	185	ILE	2.4
1	A	760	LYS	2.4
1	A	500	LEU	2.4
1	A	550	MET	2.4
1	A	694	THR	2.4
1	A	774	GLU	2.4
1	A	806	PHE	2.4
1	A	394	GLY	2.3
1	A	599	GLY	2.3
1	A	683	ASN	2.3
1	A	868	TYR	2.3
1	A	276	MET	2.3
1	A	663	THR	2.3
1	A	674	LYS	2.3
1	A	446	PHE	2.3
1	A	592	GLY	2.3
1	A	747	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	796	MET	2.3
1	A	793	TYR	2.3
1	A	524	SER	2.3
1	A	535	VAL	2.3
1	A	886	VAL	2.3
1	A	534	GLY	2.3
1	A	681	GLY	2.3
1	A	400	THR	2.3
1	A	800	ASN	2.3
1	A	872	TYR	2.3
1	A	444	LYS	2.3
1	A	696	ILE	2.3
1	A	738	SER	2.3
1	A	378	GLU	2.3
1	A	461	GLY	2.3
1	A	212	SER	2.2
1	A	257	SER	2.2
1	A	369	GLU	2.2
1	A	628	ALA	2.2
1	A	618	PRO	2.2
1	A	416	LEU	2.2
1	A	583	ASN	2.2
1	A	336	ARG	2.2
1	A	496	ARG	2.2
1	A	536	ALA	2.2
1	A	803	ARG	2.2
1	A	471	GLY	2.2
1	A	211	ASP	2.2
1	A	411	VAL	2.2
1	A	729	GLN	2.2
1	A	638	SER	2.2
1	A	317	GLU	2.2
1	A	453	GLY	2.2
1	A	214	SER	2.2
1	A	412	LEU	2.2
1	A	407	ALA	2.2
1	A	619	GLY	2.2
1	A	202	ASN	2.2
1	A	540	ARG	2.2
1	A	548	ASN	2.2
1	A	611	THR	2.2
1	A	746	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	391	TYR	2.2
1	A	712	ASN	2.1
1	A	623	THR	2.1
1	A	762	ALA	2.1
1	A	826	SER	2.1
1	A	644	SER	2.1
1	A	784	GLN	2.1
1	A	701	LEU	2.1
1	A	469	SER	2.1
1	A	364	ARG	2.1
1	A	510	TYR	2.1
1	A	840	TYR	2.1
1	A	539	PRO	2.1
1	A	730	SER	2.1
1	A	771	SER	2.1
1	A	503	THR	2.1
1	A	877	THR	2.1
1	A	468	ASN	2.1
1	A	722	GLU	2.1
1	A	842	ASP	2.1
1	A	850	GLN	2.1
1	A	851	PHE	2.1
1	A	852	GLN	2.1
1	A	605	SER	2.1
1	A	682	SER	2.1
1	A	440	HIS	2.1
1	A	519	THR	2.0
1	A	881	ALA	2.0
1	A	688	SER	2.0
1	A	714	LYS	2.0
1	A	875	PRO	2.0
1	A	884	GLN	2.0
1	A	531	SER	2.0
1	A	487	ASP	2.0
1	A	551	ASP	2.0
1	A	472	HIS	2.0
1	A	184	ILE	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)

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	BDP	A	1003	12/13	0.52	0.37	6.70	62,64,71,82	0
2	BDP	A	1001	12/13	0.50	0.35	3.01	68,70,81,84	0
2	NAG	A	1000	15/15	0.41	0.29	1.12	66,70,76,85	0
2	NAG	A	1002	14/15	0.67	0.24	0.68	40,60,63,65	0

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.