



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 05:12 pm GMT

PDB ID : 1LXK
Title : Streptococcus pneumoniae Hyaluronate Lyase in Complex with Tetrasaccharide Hyaluronan Substrate
Authors : Jedrzejewski, 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

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

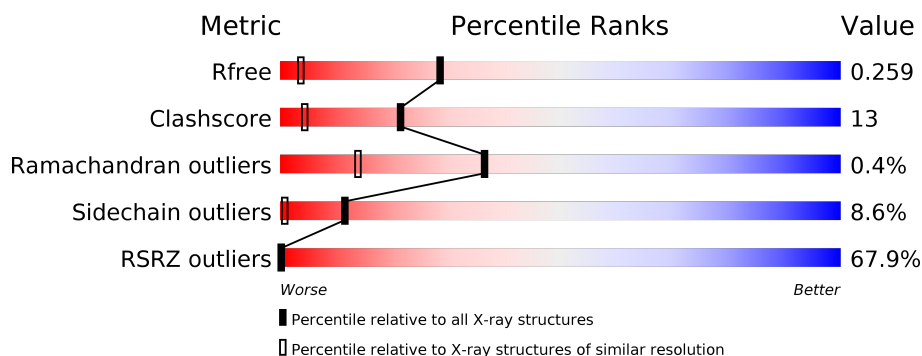
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	111664	2055 (1.56-1.52)
Clashscore	122126	2124 (1.56-1.52)
Ramachandran outliers	120053	2083 (1.56-1.52)
Sidechain outliers	120020	2081 (1.56-1.52)
RSRZ outliers	108989	2027 (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 $\leq 5\%$. 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	721	<div> <div>68%</div> <div>70%25%.</div> </div>

2 Entry composition [i](#)

There are 4 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
			Total	C	N	O	S			
1	A	719	5774	3632	966	1154	22	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

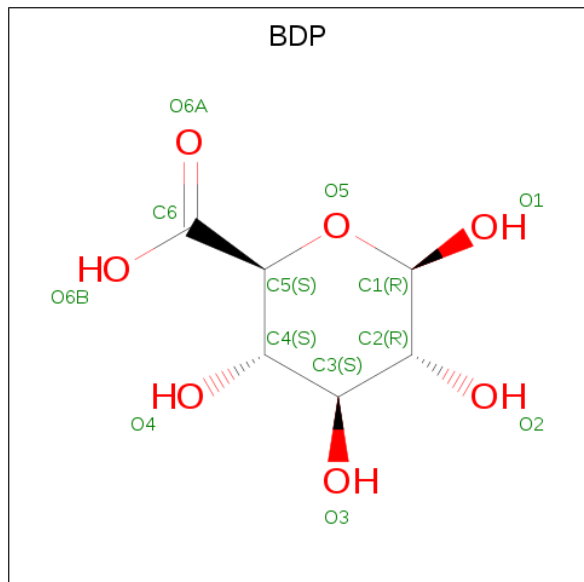
Chain	Residue	Modelled	Actual	Comment	Reference
A	408	PHE	TYR	ENGINEERED	GB 437705
A	731	VAL	GLY	SEE REMARK 999	GB 437705

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	15	8	1	6	0	0
2	A	1	14	8	1	5	0	0

- Molecule 3 is BETA-D-GLUCOPYRANURONIC ACID (three-letter code: BDP) (formula: $C_6H_{10}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	A	1	Total	C	O	0	0
			12	6	6		

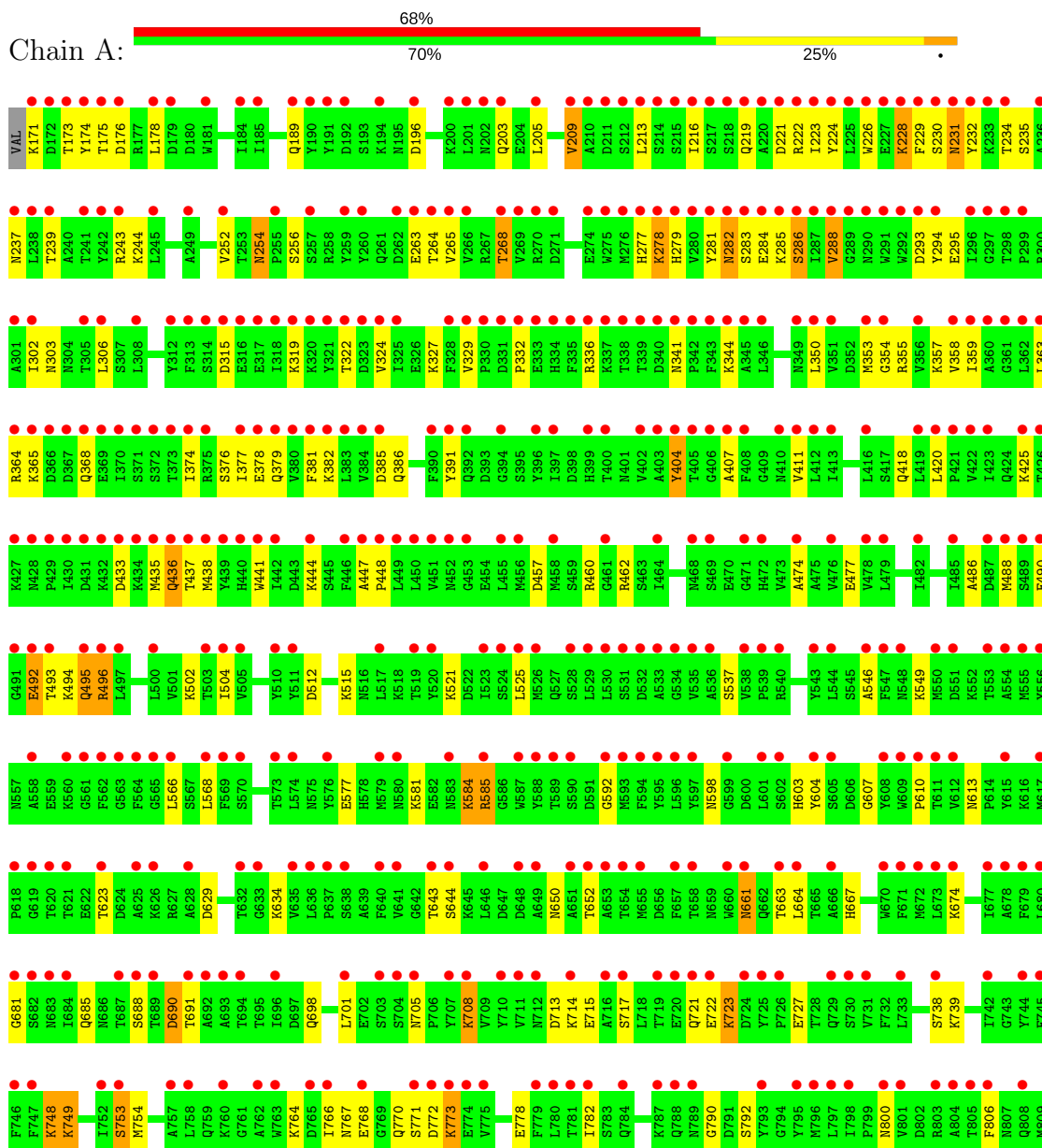
- Molecule 4 is water.

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

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Hyaluronate Lyase





4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 1.52Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.190 , 0.239 0.226 , 0.259	Depositor DCC
R_{free} test set	1227 reflections (0.98%)	wwPDB-VP
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
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	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.*

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, 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 [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	5774	0	5591	148	0
2	A	29	0	26	1	0
3	A	24	0	12	0	0
4	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
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	4: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	4: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	4:A:1058:HOH:O	1.98	0.64
1:A:288:VAL:HG13	1:A:294:TYR:OH	1.99	0.63
1:A:821:ASN:ND2	1:A:823:THR:H	1.95	0.63
1:A:178:LEU:HD11	1:A:363:LEU:HD23	1.81	0.62
1:A:336:ARG:HH12	2:A:1000:NAG:H2	1.64	0.61
1:A:705:ASN:HB3	4:A:1240:HOH:O	2.00	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	4:A:1444:HOH:O	2.31	0.60
1:A:189:GLN:HG2	4: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	4: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	4: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	4: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:SER:HB2	1:A:293:ASP:HB2	1.90	0.53
1:A:174:TYR:CD2	1:A:365:LYS:HG2	2.43	0.53
1:A:889:LYS:HD3	4:A:1688:HOH:O	2.07	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	4: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	4:A:1623:HOH:O	2.44	0.50
1:A:173:THR:O	1:A:176:ASP:HB2	2.11	0.50
1:A:566:LEU:HD23	4:A:1062:HOH:O	2.10	0.50
1:A:623:THR:HB	1:A:690:ASP:HB2	1.93	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:216:ILE:HD12	1:A:226:TRP:CZ2	2.47	0.49
1:A:723:LYS:HD3	4:A:1203:HOH:O	2.12	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	4: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	4: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	4: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

Continued on next page...

Continued from previous page...

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:667:HIS:HD2	4:A:1142:HOH:O	1.99	0.45
1:A:764:LYS:HA	1:A:767:ASN:O	2.16	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:277:HIS:CD2	4:A:1528:HOH:O	2.69	0.45
1:A:581:LYS:O	1:A:584:LYS:HD2	2.15	0.45
1:A:643:THR:HB	4:A:1058:HOH:O	2.16	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	4:A:1374:HOH:O	2.17	0.45
1:A:768:GLU:HG3	4: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:568:LEU:HD23	1:A:592:GLY:HA2	2.00	0.44
1:A:644:SER:HB2	1:A:873:TYR:HB3	1.98	0.44
1:A:244:LYS:HE2	4:A:1366:HOH:O	2.16	0.44
1:A:420:LEU:HD12	1:A:488:MET:HE1	1.99	0.44
1:A:231:ASN:O	1:A:237:ASN:ND2	2.49	0.44
1:A:585:ARG:HD3	1:A:629:ASP:OD1	2.17	0.44
1:A:771:SER:OG	1:A:773:LYS:HB2	2.17	0.44
1:A:436:GLN:O	1:A:436:GLN:HG2	2.17	0.44
1:A:661:ASN:H	1:A:661:ASN:HD22	1.66	0.44
1:A:858:VAL:HG12	4:A:1281:HOH:O	2.17	0.44
1:A:790:GLY:HA2	4: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:HG2	1:A:749:LYS:HZ3	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

Continued on next page...

Continued from previous page...

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:486:ALA:O	1:A:494:LYS:HG3	2.20	0.42
1:A:495:GLN:NE2	4:A:1005:HOH:O	2.51	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:350:LEU:O	1:A:353:MET:HB3	2.20	0.41
1:A:585:ARG:HH11	1:A:629:ASP:CG	2.23	0.41
1:A:438:MET:HG2	1:A:441:TRP:CZ3	2.55	0.41
1:A:521:LYS:HE3	1:A:525:LEU:HG	2.02	0.41
1:A:767:ASN:HB3	1:A:770:GLN:CG	2.51	0.41
1:A:822:GLU:HG2	1:A:823:THR:HG23	2.03	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:404:TYR:CD1	1:A:407:ALA:HB3	2.57	0.40
1:A:869:LYS:HD2	1:A:869:LYS:N	2.36	0.40
1:A:234:THR:HG22	4:A:1533:HOH:O	2.20	0.40
1:A:281:TYR:CD2	1:A:324:VAL:HG11	2.57	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%)	36 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 [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	638/640 (100%)	583 (91%)	55 (9%)	11 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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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 ⓘ

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 ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	1000	3	15,15,15	2.17	7 (46%)	21,21,21	1.19	3 (14%)
3	BDP	A	1001	2	9,12,13	6.58	2 (22%)	12,17,19	3.37	5 (41%)
2	NAG	A	1002	3	14,14,15	2.56	6 (42%)	17,19,21	0.92	2 (11%)
3	BDP	A	1003	2	9,12,13	3.14	4 (44%)	12,17,19	1.67	4 (33%)

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	3	-	0/6/26/26	0/1/1/1
3	BDP	A	1001	2	-	0/0/21/24	0/1/1/1
2	NAG	A	1002	3	-	0/6/23/26	0/1/1/1
3	BDP	A	1003	2	-	0/0/21/24	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003	BDP	C4-C5	-7.31	1.37	1.53
2	A	1002	NAG	C7-N2	2.07	1.41	1.34
2	A	1000	NAG	C7-N2	2.08	1.41	1.34
2	A	1000	NAG	O5-C5	2.26	1.49	1.44
2	A	1002	NAG	C4-C5	2.33	1.58	1.53
2	A	1000	NAG	C4-C3	2.41	1.58	1.52
2	A	1000	NAG	C4-C5	2.74	1.58	1.53
3	A	1003	BDP	C2-C3	2.79	1.56	1.52
3	A	1003	BDP	O4-C4	2.82	1.49	1.43
2	A	1000	NAG	C1-C2	3.00	1.56	1.52
2	A	1002	NAG	O5-C5	3.38	1.50	1.43
2	A	1002	NAG	C2-N2	3.39	1.52	1.46
2	A	1002	NAG	C1-C2	3.57	1.57	1.52
2	A	1000	NAG	C2-N2	3.85	1.52	1.45
2	A	1000	NAG	O5-C1	4.12	1.53	1.42
3	A	1003	BDP	O5-C5	4.13	1.47	1.43
2	A	1002	NAG	O5-C1	6.36	1.54	1.43
3	A	1001	BDP	C4-C5	6.77	1.68	1.53
3	A	1001	BDP	O5-C5	18.22	1.61	1.43

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1001	BDP	O4-C4-C5	-4.17	101.98	110.04
3	A	1003	BDP	C1-C2-C3	-3.24	105.55	109.66
2	A	1000	NAG	C8-C7-N2	-2.57	111.61	116.10
2	A	1002	NAG	C8-C7-N2	-2.21	112.23	116.10
3	A	1001	BDP	C1-C2-C3	-2.11	106.98	109.66
3	A	1003	BDP	O4-C4-C5	-2.06	106.07	110.04
3	A	1003	BDP	O2-C2-C3	2.01	114.10	110.19
2	A	1002	NAG	O7-C7-N2	2.08	125.87	121.94
2	A	1000	NAG	O7-C7-N2	2.22	126.14	121.94
2	A	1000	NAG	O5-C1-C2	2.45	111.97	109.52
3	A	1003	BDP	C1-O5-C5	2.58	116.72	112.17
3	A	1001	BDP	C3-C4-C5	5.35	120.14	109.01
3	A	1001	BDP	C6-C5-C4	5.44	127.14	113.04
3	A	1001	BDP	C1-O5-C5	7.30	125.05	112.17

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

5.7 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	719/721 (99%)	2.76	488 (67%) 0 0	31, 41, 68, 98	0

All (488) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	224	TYR	12.2
1	A	221	ASP	12.1
1	A	689	THR	9.3
1	A	287	ILE	8.3
1	A	220	ALA	7.8
1	A	174	TYR	7.7
1	A	335	PHE	7.3
1	A	286	SER	7.2
1	A	430	ILE	7.1
1	A	339	THR	7.1
1	A	375	ARG	7.0
1	A	233	LYS	6.9
1	A	275	TRP	6.9
1	A	223	ILE	6.7
1	A	281	TYR	6.7
1	A	217	SER	6.7
1	A	279	HIS	6.6
1	A	427	LYS	6.5
1	A	367	ASP	6.3
1	A	227	GLU	6.3
1	A	232	TYR	6.2
1	A	219	GLN	6.2
1	A	865	GLY	6.2
1	A	325	ILE	6.2
1	A	278	LYS	6.1
1	A	189	GLN	5.6
1	A	342	PRO	5.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	371	SER	5.5
1	A	171	LYS	5.4
1	A	225	LEU	5.4
1	A	226	TRP	5.3
1	A	431	ASP	5.3
1	A	341	ASN	5.3
1	A	283	SER	5.3
1	A	324	VAL	5.3
1	A	368	GLN	5.2
1	A	236	ALA	5.2
1	A	284	GLU	5.2
1	A	216	ILE	5.2
1	A	289	GLY	5.1
1	A	721	GLN	5.1
1	A	432	LYS	5.0
1	A	381	PHE	5.0
1	A	810	ILE	5.0
1	A	849	ASN	4.9
1	A	343	PHE	4.9
1	A	209	VAL	4.9
1	A	178	LEU	4.9
1	A	314	SER	4.9
1	A	228	LYS	4.9
1	A	328	PHE	4.8
1	A	322	THR	4.8
1	A	173	THR	4.8
1	A	436	GLN	4.8
1	A	345	ALA	4.7
1	A	338	THR	4.7
1	A	231	ASN	4.7
1	A	363	LEU	4.7
1	A	291	TRP	4.7
1	A	433	ASP	4.7
1	A	290	ASN	4.6
1	A	333	GLU	4.6
1	A	268	THR	4.6
1	A	788	GLN	4.6
1	A	359	ILE	4.5
1	A	464	ILE	4.5
1	A	677	ILE	4.5
1	A	218	SER	4.5
1	A	308	LEU	4.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	264	THR	4.5
1	A	425	LYS	4.5
1	A	265	VAL	4.4
1	A	196	ASP	4.4
1	A	280	VAL	4.4
1	A	691	THR	4.4
1	A	351	VAL	4.4
1	A	215	SER	4.4
1	A	259	TYR	4.4
1	A	377	ILE	4.3
1	A	703	SER	4.3
1	A	370	ILE	4.3
1	A	234	THR	4.2
1	A	569	PHE	4.2
1	A	353	MET	4.2
1	A	758	LEU	4.2
1	A	564	PHE	4.2
1	A	635	VAL	4.2
1	A	374	ILE	4.2
1	A	632	THR	4.2
1	A	858	VAL	4.2
1	A	827	VAL	4.1
1	A	292	TRP	4.1
1	A	316	GLU	4.1
1	A	260	TYR	4.1
1	A	636	LEU	4.1
1	A	319	LYS	4.1
1	A	867	GLU	4.1
1	A	299	PRO	4.0
1	A	782	ILE	4.0
1	A	679	PHE	4.0
1	A	271	ASP	4.0
1	A	331	ASP	4.0
1	A	492	GLU	4.0
1	A	658	THR	4.0
1	A	646	LEU	3.9
1	A	429	PRO	3.9
1	A	230	SER	3.9
1	A	315	ASP	3.9
1	A	421	PRO	3.9
1	A	176	ASP	3.9
1	A	238	LEU	3.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	420	LEU	3.9
1	A	423	ILE	3.9
1	A	861	ILE	3.9
1	A	358	VAL	3.9
1	A	757	ALA	3.9
1	A	229	PHE	3.9
1	A	556	TYR	3.9
1	A	568	LEU	3.9
1	A	222	ARG	3.8
1	A	294	TYR	3.8
1	A	595	TYR	3.8
1	A	657	PHE	3.8
1	A	337	LYS	3.8
1	A	609	TRP	3.8
1	A	488	MET	3.8
1	A	538	VAL	3.8
1	A	562	PHE	3.8
1	A	172	ASP	3.8
1	A	866	ASP	3.8
1	A	237	ASN	3.7
1	A	814	GLU	3.7
1	A	239	THR	3.7
1	A	441	TRP	3.7
1	A	716	ALA	3.7
1	A	350	LEU	3.7
1	A	704	SER	3.7
1	A	566	LEU	3.7
1	A	594	PHE	3.7
1	A	334	HIS	3.7
1	A	285	LYS	3.7
1	A	870	ILE	3.7
1	A	604	TYR	3.6
1	A	671	PHE	3.6
1	A	451	VAL	3.6
1	A	504	ILE	3.6
1	A	719	THR	3.6
1	A	479	LEU	3.6
1	A	744	TYR	3.6
1	A	828	TYR	3.6
1	A	766	ILE	3.6
1	A	282	ASN	3.6
1	A	404	TYR	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	597	TYR	3.6
1	A	213	LEU	3.6
1	A	428	ASN	3.6
1	A	815	SER	3.6
1	A	779	PHE	3.5
1	A	402	VAL	3.5
1	A	596	LEU	3.5
1	A	670	TRP	3.5
1	A	408	PHE	3.5
1	A	745	PHE	3.5
1	A	413	ILE	3.5
1	A	889	LYS	3.5
1	A	372	SER	3.5
1	A	834	VAL	3.5
1	A	210	ALA	3.5
1	A	653	ALA	3.5
1	A	194	LYS	3.5
1	A	608	TYR	3.5
1	A	422	VAL	3.5
1	A	843	SER	3.5
1	A	192	ASP	3.4
1	A	813	LEU	3.4
1	A	373	THR	3.4
1	A	837	ILE	3.4
1	A	859	TYR	3.4
1	A	266	VAL	3.4
1	A	356	VAL	3.4
1	A	705	ASN	3.4
1	A	390	PHE	3.4
1	A	637	PRO	3.4
1	A	574	LEU	3.4
1	A	277	HIS	3.4
1	A	383	LEU	3.4
1	A	530	LEU	3.4
1	A	673	LEU	3.4
1	A	797	LEU	3.4
1	A	862	ARG	3.4
1	A	312	TYR	3.4
1	A	615	TYR	3.4
1	A	505	VAL	3.4
1	A	838	VAL	3.4
1	A	298	THR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	293	ASP	3.3
1	A	437	THR	3.3
1	A	873	TYR	3.3
1	A	419	LEU	3.3
1	A	269	VAL	3.3
1	A	329	VAL	3.3
1	A	439	TYR	3.3
1	A	720	GLU	3.3
1	A	633	GLY	3.3
1	A	517	LEU	3.3
1	A	733	LEU	3.3
1	A	854	LEU	3.3
1	A	692	ALA	3.3
1	A	382	LYS	3.2
1	A	321	TYR	3.2
1	A	731	VAL	3.2
1	A	804	ALA	3.2
1	A	455	LEU	3.2
1	A	203	GLN	3.2
1	A	641	VAL	3.2
1	A	435	MET	3.2
1	A	392	GLN	3.2
1	A	360	ALA	3.2
1	A	563	GLY	3.2
1	A	678	ALA	3.2
1	A	684	ILE	3.2
1	A	742	ILE	3.2
1	A	588	TYR	3.2
1	A	553	THR	3.2
1	A	805	THR	3.2
1	A	544	LEU	3.2
1	A	565	GLY	3.2
1	A	798	ILE	3.2
1	A	787	LYS	3.1
1	A	396	TYR	3.1
1	A	354	GLY	3.1
1	A	362	LEU	3.1
1	A	450	LEU	3.1
1	A	547	PHE	3.1
1	A	652	THR	3.1
1	A	860	THR	3.1
1	A	775	VAL	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	332	PRO	3.1
1	A	812	GLU	3.1
1	A	576	TYR	3.1
1	A	789	ASN	3.1
1	A	406	GLY	3.1
1	A	621	THR	3.1
1	A	346	LEU	3.0
1	A	478	VAL	3.0
1	A	525	LEU	3.0
1	A	753	SER	3.0
1	A	801	VAL	3.0
1	A	847	ILE	3.0
1	A	205	LEU	3.0
1	A	601	LEU	3.0
1	A	855	LYS	3.0
1	A	726	PRO	3.0
1	A	836	GLY	3.0
1	A	397	ILE	3.0
1	A	587	TRP	3.0
1	A	589	THR	3.0
1	A	643	THR	3.0
1	A	772	ASP	3.0
1	A	680	LEU	3.0
1	A	448	PRO	3.0
1	A	617	MET	3.0
1	A	490	GLU	2.9
1	A	532	ASP	2.9
1	A	241	THR	2.9
1	A	405	THR	2.9
1	A	349	ASN	2.9
1	A	385	ASP	2.9
1	A	853	VAL	2.9
1	A	811	LYS	2.9
1	A	555	MET	2.9
1	A	379	GLN	2.9
1	A	302	ILE	2.9
1	A	306	LEU	2.9
1	A	344	LYS	2.9
1	A	449	LEU	2.9
1	A	708	LYS	2.9
1	A	458	MET	2.9
1	A	655	MET	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	687	THR	2.9
1	A	666	ALA	2.9
1	A	252	VAL	2.9
1	A	426	THR	2.9
1	A	495	GLN	2.9
1	A	288	VAL	2.9
1	A	593	MET	2.8
1	A	403	ALA	2.8
1	A	447	ALA	2.8
1	A	558	ALA	2.8
1	A	497	LEU	2.8
1	A	590	SER	2.8
1	A	526	MET	2.8
1	A	573	THR	2.8
1	A	365	LYS	2.8
1	A	717	SER	2.8
1	A	442	ILE	2.8
1	A	366	ASP	2.8
1	A	654	THR	2.8
1	A	640	PHE	2.8
1	A	520	TYR	2.8
1	A	340	ASP	2.8
1	A	320	LYS	2.8
1	A	818	ILE	2.8
1	A	620	THR	2.8
1	A	301	ALA	2.8
1	A	781	THR	2.7
1	A	846	THR	2.7
1	A	533	ALA	2.7
1	A	579	MET	2.7
1	A	434	LYS	2.7
1	A	297	GLY	2.7
1	A	768	GLU	2.7
1	A	661	ASN	2.7
1	A	313	PHE	2.7
1	A	543	TYR	2.7
1	A	610	PRO	2.7
1	A	795	TYR	2.7
1	A	664	LEU	2.7
1	A	493	THR	2.7
1	A	580	ASN	2.7
1	A	175	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	763	TRP	2.6
1	A	482	ILE	2.6
1	A	808	GLN	2.6
1	A	384	VAL	2.6
1	A	270	ARG	2.6
1	A	190	TYR	2.6
1	A	323	ASP	2.6
1	A	765	ASP	2.6
1	A	546	ALA	2.6
1	A	523	ILE	2.6
1	A	476	VAL	2.6
1	A	835	TRP	2.6
1	A	399	HIS	2.6
1	A	585	ARG	2.6
1	A	887	PHE	2.6
1	A	249	ALA	2.6
1	A	489	SER	2.6
1	A	554	ALA	2.6
1	A	864	GLU	2.6
1	A	296	ILE	2.6
1	A	243	ARG	2.6
1	A	648	ASP	2.6
1	A	724	ASP	2.6
1	A	651	ALA	2.6
1	A	693	ALA	2.6
1	A	707	TYR	2.6
1	A	710	TYR	2.6
1	A	529	LEU	2.6
1	A	780	LEU	2.6
1	A	602	SER	2.6
1	A	561	GLY	2.5
1	A	456	MET	2.5
1	A	410	ASN	2.5
1	A	570	SER	2.5
1	A	274	GLU	2.5
1	A	485	ILE	2.5
1	A	752	ILE	2.5
1	A	626	LYS	2.5
1	A	242	TYR	2.5
1	A	200	LYS	2.5
1	A	830	ALA	2.5
1	A	318	ILE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	181	TRP	2.5
1	A	201	LEU	2.5
1	A	511	TYR	2.5
1	A	824	LEU	2.5
1	A	649	ALA	2.5
1	A	380	VAL	2.5
1	A	305	THR	2.5
1	A	255	PRO	2.4
1	A	817	LEU	2.4
1	A	438	MET	2.4
1	A	262	ASP	2.4
1	A	773	LYS	2.4
1	A	474	ALA	2.4
1	A	672	MET	2.4
1	A	179	ASP	2.4
1	A	263	GLU	2.4
1	A	330	PRO	2.4
1	A	361	GLY	2.4
1	A	694	THR	2.4
1	A	191	TYR	2.4
1	A	725	TYR	2.4
1	A	550	MET	2.4
1	A	612	VAL	2.4
1	A	528	SER	2.4
1	A	660	TRP	2.4
1	A	185	ILE	2.4
1	A	774	GLU	2.4
1	A	245	LEU	2.4
1	A	500	LEU	2.4
1	A	674	LYS	2.3
1	A	760	LYS	2.3
1	A	663	THR	2.3
1	A	491	GLY	2.3
1	A	599	GLY	2.3
1	A	276	MET	2.3
1	A	683	ASN	2.3
1	A	793	TYR	2.3
1	A	868	TYR	2.3
1	A	394	GLY	2.3
1	A	592	GLY	2.3
1	A	535	VAL	2.3
1	A	524	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	446	PHE	2.3
1	A	747	PHE	2.3
1	A	796	MET	2.3
1	A	806	PHE	2.3
1	A	534	GLY	2.3
1	A	681	GLY	2.3
1	A	400	THR	2.3
1	A	444	LYS	2.3
1	A	872	TYR	2.3
1	A	886	VAL	2.3
1	A	800	ASN	2.3
1	A	738	SER	2.3
1	A	696	ILE	2.3
1	A	378	GLU	2.3
1	A	416	LEU	2.3
1	A	461	GLY	2.3
1	A	212	SER	2.2
1	A	618	PRO	2.2
1	A	628	ALA	2.2
1	A	496	ARG	2.2
1	A	803	ARG	2.2
1	A	369	GLU	2.2
1	A	257	SER	2.2
1	A	638	SER	2.2
1	A	729	GLN	2.2
1	A	211	ASP	2.2
1	A	583	ASN	2.2
1	A	471	GLY	2.2
1	A	336	ARG	2.2
1	A	391	TYR	2.2
1	A	611	THR	2.2
1	A	214	SER	2.2
1	A	317	GLU	2.2
1	A	540	ARG	2.2
1	A	407	ALA	2.2
1	A	536	ALA	2.2
1	A	623	THR	2.2
1	A	762	ALA	2.2
1	A	453	GLY	2.2
1	A	411	VAL	2.2
1	A	202	ASN	2.2
1	A	548	ASN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	746	PHE	2.1
1	A	826	SER	2.1
1	A	619	GLY	2.1
1	A	412	LEU	2.1
1	A	510	TYR	2.1
1	A	364	ARG	2.1
1	A	644	SER	2.1
1	A	503	THR	2.1
1	A	712	ASN	2.1
1	A	784	GLN	2.1
1	A	440	HIS	2.1
1	A	469	SER	2.1
1	A	730	SER	2.1
1	A	850	GLN	2.1
1	A	852	GLN	2.1
1	A	468	ASN	2.1
1	A	701	LEU	2.1
1	A	877	THR	2.1
1	A	840	TYR	2.1
1	A	842	ASP	2.1
1	A	605	SER	2.1
1	A	682	SER	2.1
1	A	688	SER	2.1
1	A	771	SER	2.1
1	A	487	ASP	2.1
1	A	714	LYS	2.1
1	A	519	THR	2.1
1	A	881	ALA	2.1
1	A	539	PRO	2.0
1	A	875	PRO	2.0
1	A	884	GLN	2.0
1	A	711	VAL	2.0
1	A	472	HIS	2.0
1	A	560	LYS	2.0
1	A	851	PHE	2.0
1	A	551	ASP	2.0
1	A	722	GLU	2.0
1	A	184	ILE	2.0
1	A	531	SER	2.0
1	A	452	ASN	2.0
1	A	625	ALA	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. 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(\AA^2)	Q<0.9
2	NAG	A	1000	15/15	0.42	0.29	66,70,76,85	0
3	BDP	A	1001	12/13	0.50	0.35	68,70,81,84	0
3	BDP	A	1003	12/13	0.51	0.37	62,64,71,82	0
2	NAG	A	1002	14/15	0.67	0.24	40,60,63,65	0

6.5 Other polymers [i](#)

There are no such residues in this entry.