



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:12 PM GMT

PDB ID : 4KX8
Title : Crystal structure of human aminopeptidase A complexed with amastatin
Authors : Yang, Y.; Liu, C.; Lin, Y.Y.; Li, F.
Deposited on : 2013-05-24
Resolution : 2.40 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 ⓘ 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 (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

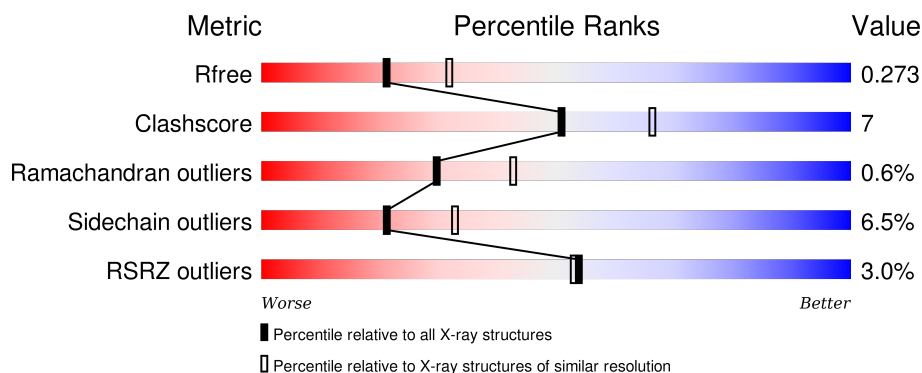
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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	888	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>15%</div> <div>..</div> </div> </div>
2	C	4	<div> <div>25%</div> <div> <div>25%</div> <div>50%</div> <div>25%</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7942 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 Glutamyl aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	875	Total	C	N	O	S	0	1	0
			7151	4580	1190	1356	25			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	213	ARG	GLN	NATURAL VARIANT	UNP Q07075
A	218	ALA	VAL	NATURAL VARIANT	UNP Q07075
A	958	HIS	-	EXPRESSION TAG	UNP Q07075
A	959	HIS	-	EXPRESSION TAG	UNP Q07075
A	960	HIS	-	EXPRESSION TAG	UNP Q07075
A	961	HIS	-	EXPRESSION TAG	UNP Q07075
A	962	HIS	-	EXPRESSION TAG	UNP Q07075
A	963	HIS	-	EXPRESSION TAG	UNP Q07075

- Molecule 2 is a protein called amastatin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	4	Total	C	N	O	0	0	0
			33	21	4	8			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

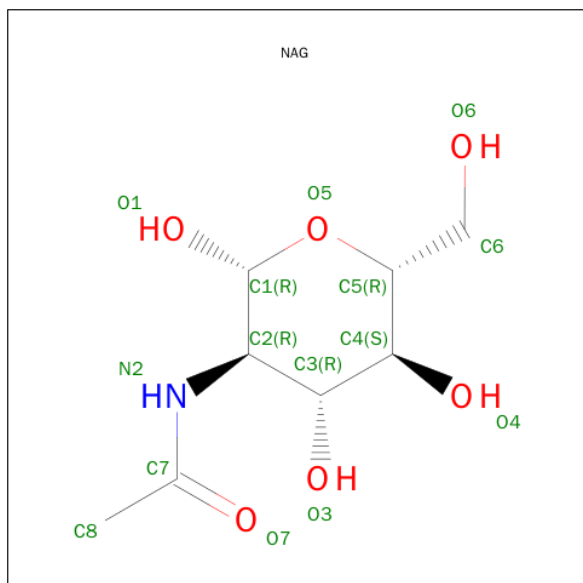
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 6 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	3	Total	C	N	O	0	0
			42	24	3	15		
6	A	3	Total	C	N	O	0	0
			42	24	3	15		

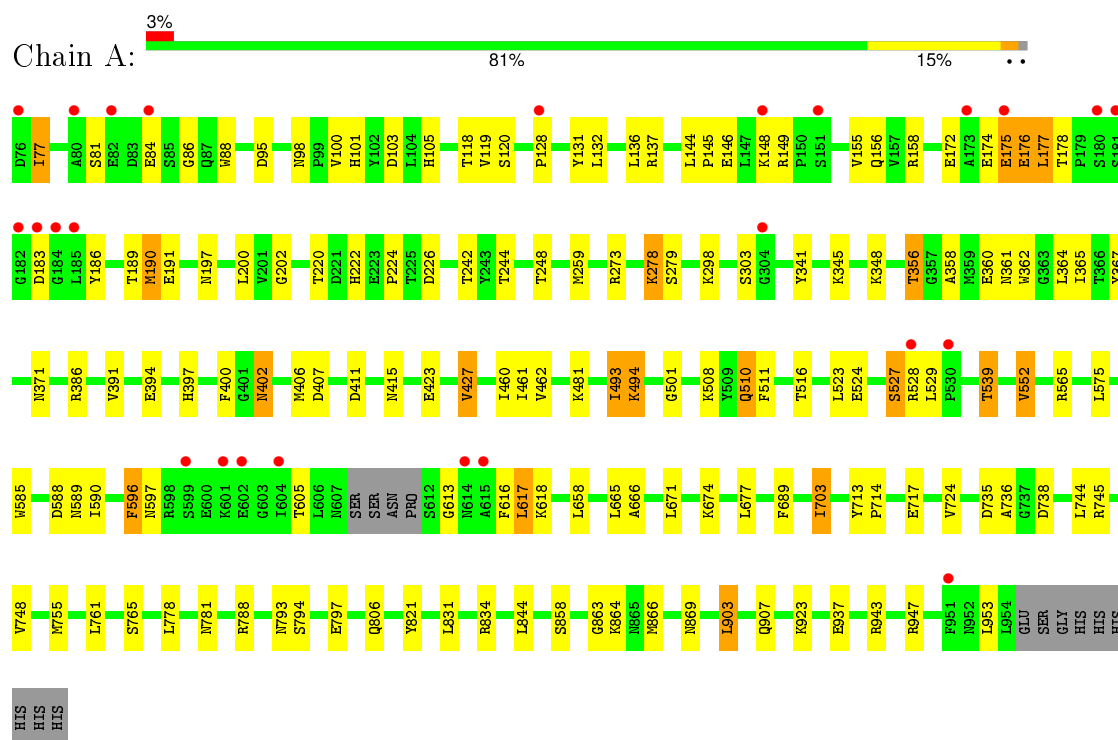
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	531	Total 531	O 531	0	0
7	C	2	Total 2	O 2	0	0

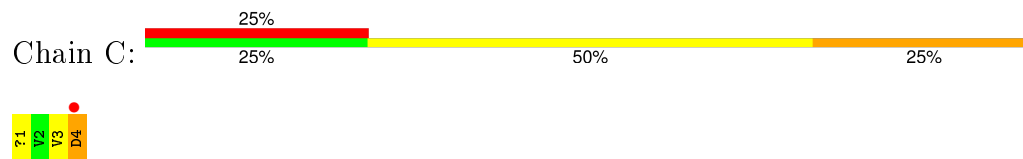
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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: Glutamyl aminopeptidase



• Molecule 2: amastatin



4 Data and refinement statistics

Property	Value	Source
Space group	P 64 2 2	Depositor
Cell constants a, b, c, α , β , γ	142.74Å 142.74Å 237.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.21 – 2.40 41.21 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.0 (41.21-2.40) 95.0 (41.21-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.20 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.210 , 0.276 0.214 , 0.273	Depositor DCC
R_{free} test set	2866 reflections (5.62%)	DCC
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.613	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 56.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	0 of 53672 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7942	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, NAG, L2O

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	0.45	1/7336 (0.0%)	0.61	1/9974 (0.0%)
2	C	1.51	0/22	1.72	0/28
All	All	0.45	1/7358 (0.0%)	0.61	1/10002 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	158	ARG	CG-CD	5.11	1.64	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	903	LEU	CA-CB-CG	5.30	127.49	115.30

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	7151	0	6943	98	0
2	C	33	0	35	6	0
3	A	1	0	0	0	0
4	A	84	0	75	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	56	0	52	2	0
6	A	84	0	74	1	0
7	A	531	0	0	18	0
7	C	2	0	0	0	0
All	All	7942	0	7179	100	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 7.

All (100) 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:907:GLN:HB3	7:A:1482:HOH:O	1.43	1.16
1:A:244:THR:HB	7:A:1595:HOH:O	1.62	0.98
1:A:175:GLU:O	1:A:176:GLU:HB3	1.68	0.94
1:A:761:LEU:HD22	1:A:793:ASN:HD21	1.41	0.83
1:A:423:GLU:O	1:A:427:VAL:HG12	1.81	0.81
1:A:356:THR:HG21	2:C:1:L2O:H8	1.68	0.75
1:A:793:ASN:HB3	7:A:1501:HOH:O	1.90	0.72
1:A:501:GLY:HA3	1:A:523:LEU:HD23	1.72	0.72
1:A:736:ALA:O	1:A:745:ARG:NH1	2.20	0.70
1:A:120:SER:OG	1:A:189:THR:HG22	1.92	0.70
1:A:146:GLU:HA	7:A:1563:HOH:O	1.91	0.70
1:A:834:ARG:HD2	7:A:1612:HOH:O	1.91	0.70
1:A:100:VAL:O	1:A:242:THR:HG22	1.92	0.69
1:A:386:ARG:NH2	2:C:4:ASP:OD1	2.26	0.68
1:A:118:THR:HG22	1:A:191:GLU:HG2	1.74	0.68
1:A:943:ARG:HH12	1:A:947:ARG:HH11	1.42	0.68
1:A:674:LYS:HD3	6:A:1007:NAG:H62	1.77	0.67
1:A:703:ILE:HD12	1:A:713:TYR:CE2	2.29	0.67
1:A:511:PHE:CZ	7:A:1411:HOH:O	2.47	0.66
5:A:1004:NAG:H83	7:A:1591:HOH:O	1.98	0.64
1:A:244:THR:HG22	1:A:278:LYS:HA	1.79	0.64
1:A:735:ASP:OD1	1:A:781:ASN:HB2	1.98	0.63
1:A:101:HIS:CD2	1:A:242:THR:HG23	2.33	0.62
1:A:224:PRO:HD2	7:A:1241:HOH:O	2.01	0.60
1:A:137:ARG:NH2	1:A:226:ASP:OD1	2.34	0.60
1:A:103:ASP:HB2	1:A:120:SER:HB2	1.84	0.59
1:A:923:LYS:HG3	7:A:1409:HOH:O	2.02	0.58
1:A:869:ASN:HB2	7:A:1515:HOH:O	2.03	0.58
1:A:597:ASN:HD22	5:A:1017:NAG:H83	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:552:VAL:HG12	1:A:617:LEU:HD12	1.86	0.56
1:A:703:ILE:CD1	1:A:713:TYR:CE2	2.89	0.56
1:A:717:GLU:HG2	1:A:755:MET:O	2.06	0.56
1:A:119:VAL:O	1:A:189:THR:HA	2.06	0.55
1:A:175:GLU:CG	1:A:176:GLU:N	2.71	0.54
1:A:689:PHE:HA	1:A:744:LEU:HD13	1.90	0.54
1:A:713:TYR:HB3	1:A:714:PRO:HD3	1.90	0.53
1:A:365:ILE:HG22	1:A:367:TYR:CE1	2.44	0.53
1:A:177:LEU:CD1	1:A:178:THR:H	2.23	0.52
1:A:565:ARG:CZ	1:A:937:GLU:HG3	2.40	0.52
1:A:128:PRO:HB3	1:A:176:GLU:OE2	2.11	0.51
1:A:273:ARG:HD2	7:A:1508:HOH:O	2.09	0.51
1:A:402:ASN:HD22	1:A:402:ASN:N	2.07	0.51
1:A:278:LYS:HB2	7:A:1596:HOH:O	2.10	0.51
1:A:616:PHE:HE2	1:A:618:LYS:HG3	1.76	0.51
1:A:197:ASN:O	4:A:1002:NAG:H82	2.10	0.51
1:A:202:GLY:O	1:A:220:THR:HA	2.11	0.50
1:A:131:TYR:CD2	1:A:172:GLU:HB3	2.46	0.50
1:A:397:HIS:HA	1:A:400:PHE:O	2.12	0.50
1:A:341:TYR:HA	7:A:1483:HOH:O	2.12	0.50
1:A:131:TYR:CE2	1:A:172:GLU:HB3	2.47	0.49
1:A:511:PHE:HZ	7:A:1411:HOH:O	1.92	0.49
1:A:361:ASN:HB2	1:A:364:LEU:O	2.13	0.49
1:A:175:GLU:O	1:A:176:GLU:CB	2.49	0.49
1:A:174:GLU:O	1:A:175:GLU:CB	2.61	0.48
1:A:493:ILE:O	1:A:494:LYS:HB2	2.14	0.48
1:A:585:TRP:CD1	1:A:617:LEU:HD23	2.47	0.48
1:A:175:GLU:CG	1:A:176:GLU:H	2.26	0.48
1:A:356:THR:HG21	2:C:1:L2O:H12	1.96	0.48
1:A:493:ILE:HG13	1:A:529:LEU:HD12	1.95	0.47
1:A:461:ILE:HD12	1:A:539:THR:HG23	1.95	0.47
1:A:460:ILE:HD11	1:A:481:LYS:HG2	1.96	0.47
1:A:145:PRO:HB3	1:A:190:MET:HB3	1.97	0.47
1:A:101:HIS:HD2	1:A:242:THR:HG23	1.78	0.47
1:A:358:ALA:O	2:C:1:L2O:H15	2.14	0.47
1:A:943:ARG:HH22	1:A:947:ARG:NH1	2.13	0.47
1:A:411:ASP:OD1	1:A:516:THR:OG1	2.31	0.46
1:A:348:LYS:HZ3	1:A:365:ILE:HD13	1.79	0.46
1:A:348:LYS:HE3	1:A:391:VAL:HG13	1.97	0.46
1:A:177:LEU:HD12	1:A:178:THR:H	1.81	0.46
1:A:360:GLU:O	1:A:361:ASN:C	2.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:863:GLY:HA2	1:A:866:MET:HB2	1.97	0.46
1:A:259:MET:SD	1:A:279:SER:HA	2.56	0.46
1:A:348:LYS:NZ	1:A:365:ILE:HD13	2.32	0.45
1:A:527:SER:C	1:A:529:LEU:H	2.19	0.45
1:A:175:GLU:HG2	1:A:176:GLU:H	1.82	0.45
1:A:588:ASP:O	1:A:589:ASN:HB2	2.15	0.45
7:A:1264:HOH:O	2:C:3:VAL:HG13	2.17	0.45
1:A:77:ILE:HD11	1:A:144:LEU:N	2.32	0.45
1:A:177:LEU:HB3	1:A:186:TYR:OH	2.18	0.44
1:A:371:ASN:HD21	2:C:4:ASP:CG	2.21	0.44
1:A:86:GLY:HA3	1:A:88:TRP:CZ3	2.53	0.44
1:A:360:GLU:HG3	1:A:397:HIS:HB3	1.99	0.44
1:A:105:HIS:HE1	1:A:248:THR:OG1	2.00	0.44
1:A:510:GLN:HE21	1:A:510:GLN:HB2	1.65	0.43
1:A:407:ASP:HB3	7:A:1603:HOH:O	2.18	0.43
1:A:596:PHE:CD1	1:A:596:PHE:C	2.92	0.43
1:A:175:GLU:HG3	1:A:176:GLU:N	2.34	0.43
1:A:174:GLU:O	1:A:175:GLU:CG	2.67	0.42
1:A:788:ARG:HD2	7:A:1141:HOH:O	2.20	0.42
1:A:222:HIS:HA	1:A:226:ASP:HB2	2.01	0.42
1:A:666:ALA:HA	1:A:671:LEU:O	2.20	0.42
1:A:415:ASN:N	1:A:415:ASN:HD22	2.18	0.41
1:A:858:SER:O	1:A:864:LYS:HA	2.20	0.41
1:A:806:GLN:NE2	7:A:1328:HOH:O	2.53	0.41
1:A:175:GLU:HG3	1:A:176:GLU:O	2.20	0.41
1:A:923:LYS:HA	1:A:923:LYS:HD2	1.85	0.41
1:A:797:GLU:HG3	1:A:831:LEU:HD21	2.03	0.40
1:A:174:GLU:O	1:A:175:GLU:HG2	2.21	0.40
1:A:149:ARG:CZ	1:A:155:VAL:HG22	2.51	0.40
1:A:120:SER:CB	1:A:189:THR:HG22	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	872/888 (98%)	838 (96%)	29 (3%)	5 (1%)	30	43
2	C	2/4 (50%)	2 (100%)	0	0	100	100
All	All	874/892 (98%)	840 (96%)	29 (3%)	5 (1%)	30	43

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	175	GLU
1	A	176	GLU
1	A	613	GLY
1	A	494	LYS
1	A	552	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	786/797 (99%)	736 (94%)	50 (6%)	22	34
2	C	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	789/800 (99%)	738 (94%)	51 (6%)	21	33

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	ILE
1	A	81	SER
1	A	84	GLU
1	A	95	ASP
1	A	98	ASN
1	A	132	LEU
1	A	136	LEU
1	A	148	LYS

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Mol	Chain	Res	Type
1	A	156	GLN
1	A	177	LEU
1	A	183	ASP
1	A	190	MET
1	A	200	LEU
1	A	278	LYS
1	A	298	LYS
1	A	303	SER
1	A	345	LYS
1	A	356	THR
1	A	362	TRP
1	A	394	GLU
1	A	402	ASN
1	A	406	MET
1	A	427	VAL
1	A	462	VAL
1	A	493	ILE
1	A	508	LYS
1	A	510	GLN
1	A	524	GLU
1	A	527	SER
1	A	528	ARG
1	A	539	THR
1	A	575	LEU
1	A	590	ILE
1	A	596	PHE
1	A	605	THR
1	A	617	LEU
1	A	658	LEU
1	A	665	LEU
1	A	677	LEU
1	A	703	ILE
1	A	724	VAL
1	A	738	ASP
1	A	748	VAL
1	A	765	SER
1	A	778	LEU
1	A	794	SER
1	A	821	TYR
1	A	844	LEU
1	A	903	LEU
1	A	953	LEU

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Mol	Chain	Res	Type
2	C	4	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	HIS
1	A	402	ASN
1	A	415	ASN
1	A	510	GLN
1	A	570	GLN
1	A	792	GLN
1	A	793	ASN
1	A	843	ASN
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 ⓘ

1 non-standard protein/DNA/RNA residue is 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	L2O	C	1	3,2	8,9,10	0.87	0	8,11,13	2.29	5 (62%)

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	L2O	C	1	3,2	-	0/8/10/12	0/0/0/0

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	L2O	O1-C6-C	-3.11	102.79	110.22
2	C	1	L2O	O-C-C6	-3.05	116.72	125.60
2	C	1	L2O	C3-C2-C1	-2.04	111.28	115.77
2	C	1	L2O	C2-C1-N	2.14	115.28	109.13
2	C	1	L2O	O1-C6-C1	3.74	113.73	107.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1	L2O	3	0

5.5 Carbohydrates [i](#)

12 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	$\# Z > 2$
4	NAG	A	1002	1,4	14,14,15	0.48	0	15,19,21	0.85	0
4	NAG	A	1003	4	14,14,15	0.44	0	15,19,21	0.77	0
6	NAG	A	1007	1,6	14,14,15	0.49	0	15,19,21	0.94	0
6	NAG	A	1008	6	14,14,15	0.59	0	15,19,21	0.65	0
6	NAG	A	1009	6	14,14,15	0.50	0	15,19,21	1.18	1 (6%)
6	NAG	A	1010	1,6	14,14,15	0.52	0	15,19,21	1.40	1 (6%)
6	NAG	A	1011	6	14,14,15	0.63	0	15,19,21	1.89	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	1012	6	14,14,15	1.36	1 (7%)	15,19,21	2.09	4 (26%)
4	NAG	A	1013	1,4	14,14,15	0.57	0	15,19,21	1.01	1 (6%)
4	NAG	A	1014	4	14,14,15	0.44	0	15,19,21	1.04	1 (6%)
4	NAG	A	1015	1,4	14,14,15	0.57	0	15,19,21	0.72	0
4	NAG	A	1016	4	14,14,15	0.48	0	15,19,21	0.87	0

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
4	NAG	A	1002	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1003	4	-	0/6/23/26	0/1/1/1
6	NAG	A	1007	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1008	6	-	0/6/23/26	0/1/1/1
6	NAG	A	1009	6	-	0/6/23/26	0/1/1/1
6	NAG	A	1010	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1011	6	-	0/6/23/26	0/1/1/1
6	NAG	A	1012	6	-	0/6/23/26	0/1/1/1
4	NAG	A	1013	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1014	4	-	0/6/23/26	0/1/1/1
4	NAG	A	1015	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1016	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1012	NAG	O6-C6	4.06	1.59	1.42

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1011	NAG	C4-C3-C2	-2.17	107.86	111.23
4	A	1013	NAG	C4-C3-C2	2.26	114.74	111.23
6	A	1011	NAG	C3-C2-N2	2.40	116.31	110.56
6	A	1011	NAG	O4-C4-C3	2.43	115.82	110.34
4	A	1014	NAG	C2-N2-C7	2.54	126.30	123.04
6	A	1009	NAG	C1-O5-C5	2.73	115.71	112.25
6	A	1012	NAG	C1-O5-C5	2.89	115.91	112.25
6	A	1012	NAG	C3-C4-C5	3.49	116.29	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1011	NAG	C2-N2-C7	3.59	127.66	123.04
6	A	1012	NAG	C2-N2-C7	3.77	127.89	123.04
6	A	1011	NAG	C1-O5-C5	3.93	117.23	112.25
6	A	1010	NAG	C1-O5-C5	4.38	117.80	112.25
6	A	1012	NAG	C4-C3-C2	4.47	118.18	111.23

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1002	NAG	1	0
6	A	1007	NAG	1	0

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 1 is 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	$\# Z > 2$
5	NAG	A	1004	1	14,14,15	0.49	0	15,19,21	1.64	4 (26%)
5	NAG	A	1005	1	14,14,15	0.57	0	15,19,21	1.39	1 (6%)
5	NAG	A	1006	1	14,14,15	0.49	0	15,19,21	1.99	4 (26%)
5	NAG	A	1017	1	14,14,15	0.53	0	15,19,21	1.19	2 (13%)

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
5	NAG	A	1004	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1005	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1006	1	-	0/6/23/26	0/1/1/1
5	NAG	A	1017	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1004	NAG	O7-C7-C8	-2.92	116.70	122.06
5	A	1017	NAG	C2-N2-C7	2.29	125.98	123.04
5	A	1006	NAG	C3-C4-C5	2.31	114.22	110.20
5	A	1004	NAG	C8-C7-N2	2.36	120.62	116.11
5	A	1006	NAG	C1-O5-C5	2.38	115.27	112.25
5	A	1004	NAG	C2-N2-C7	2.40	126.12	123.04
5	A	1017	NAG	C1-O5-C5	2.44	115.34	112.25
5	A	1006	NAG	C3-C2-N2	2.55	116.66	110.56
5	A	1004	NAG	C1-O5-C5	3.85	117.13	112.25
5	A	1005	NAG	C1-O5-C5	4.70	118.21	112.25
5	A	1006	NAG	C2-N2-C7	5.63	130.28	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1004	NAG	1	0
5	A	1017	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	875/888 (98%)	-0.05	25 (2%) 55 54	20, 51, 97, 139	0
2	C	3/4 (75%)	1.36	1 (33%) 0 1	22, 22, 31, 57	0
All	All	878/892 (98%)	-0.04	26 (2%) 54 53	20, 51, 97, 139	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	183	ASP	5.7
1	A	184	GLY	5.6
1	A	615	ALA	4.5
1	A	182	GLY	3.9
1	A	181	SER	3.7
1	A	175	GLU	3.6
1	A	185	LEU	3.6
1	A	128	PRO	3.6
1	A	173	ALA	3.5
1	A	76	ASP	3.1
1	A	84	GLU	3.0
1	A	528	ARG	3.0
1	A	951	PHE	3.0
1	A	304	GLY	2.9
1	A	151	SER	2.9
1	A	602	GLU	2.9
1	A	530	PRO	2.8
1	A	180	SER	2.7
1	A	599	SER	2.6
2	C	4	ASP	2.4
1	A	80	ALA	2.4
1	A	82	GLU	2.3
1	A	614	ASN	2.2
1	A	604	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	148	LYS	2.0
1	A	601	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	L2O	C	1	10/11	0.85	0.23	-	13,16,17,18	0

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, 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	LLDF	B-factors(Å ²)	Q<0.9
6	NAG	A	1010	14/15	0.87	0.17	0.52	61,82,94,130	0
6	NAG	A	1007	14/15	0.91	0.13	-0.63	67,92,107,110	0
4	NAG	A	1013	14/15	0.93	0.26	-	50,77,90,92	0
4	NAG	A	1003	14/15	0.84	0.35	-	106,135,149,150	0
6	NAG	A	1011	14/15	0.90	0.22	-	96,110,126,129	0
4	NAG	A	1002	14/15	0.88	0.16	-	61,85,105,112	0
4	NAG	A	1014	14/15	0.77	0.36	-	106,120,137,139	0
6	NAG	A	1009	14/15	0.84	0.26	-	113,148,164,177	0
4	NAG	A	1016	14/15	0.88	0.29	-	100,117,131,135	0
6	NAG	A	1012	14/15	0.84	0.22	-	95,137,155,160	0
4	NAG	A	1015	14/15	0.94	0.11	-	43,71,81,97	0
6	NAG	A	1008	14/15	0.91	0.20	-	112,135,161,175	0

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, 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	LLDF	B-factors(Å ²)	Q<0.9
3	ZN	A	1001	1/1	0.83	0.10	-1.81	76,76,76,76	0
5	NAG	A	1006	14/15	0.77	0.30	-	111,131,154,171	0
5	NAG	A	1017	14/15	0.76	0.39	-	90,122,144,150	0
5	NAG	A	1005	14/15	0.74	0.35	-	106,139,160,168	0
5	NAG	A	1004	14/15	0.92	0.14	-	63,88,99,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.