



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:36 PM GMT

PDB ID : 4FKK
Title : Crystal structure of porcine aminopeptidase-N complexed with bestatin
Authors : Chen, L.; Lin, Y.L.; Peng, G.; Li, F.
Deposited on : 2012-06-13
Resolution : 2.60 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

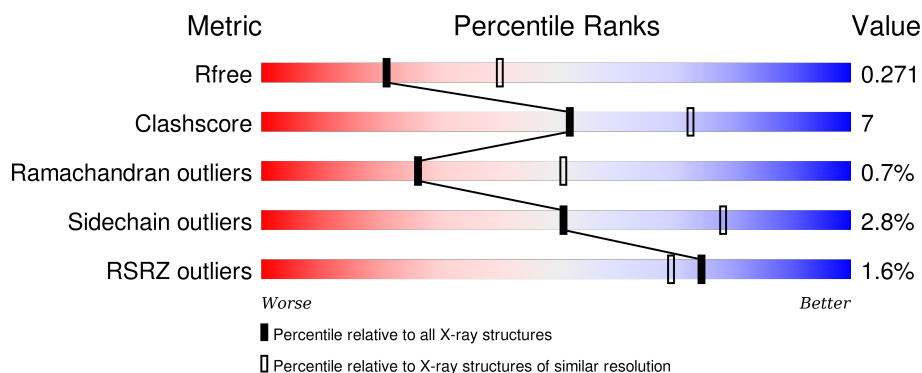
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	909	

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
5	BES	A	1024	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8434 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 Aminopeptidase N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	902	Total	C	N	O	S	0	0	0
			7241	4622	1210	1379	30			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	82	ASN	PHE	CONFLICT	UNP P15145
A	107	PHE	LEU	CONFLICT	UNP P15145
A	964	SER	-	EXPRESSION TAG	UNP P15145
A	965	HIS	-	EXPRESSION TAG	UNP P15145
A	966	HIS	-	EXPRESSION TAG	UNP P15145
A	967	HIS	-	EXPRESSION TAG	UNP P15145
A	968	HIS	-	EXPRESSION TAG	UNP P15145
A	969	HIS	-	EXPRESSION TAG	UNP P15145
A	970	HIS	-	EXPRESSION TAG	UNP P15145

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

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

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

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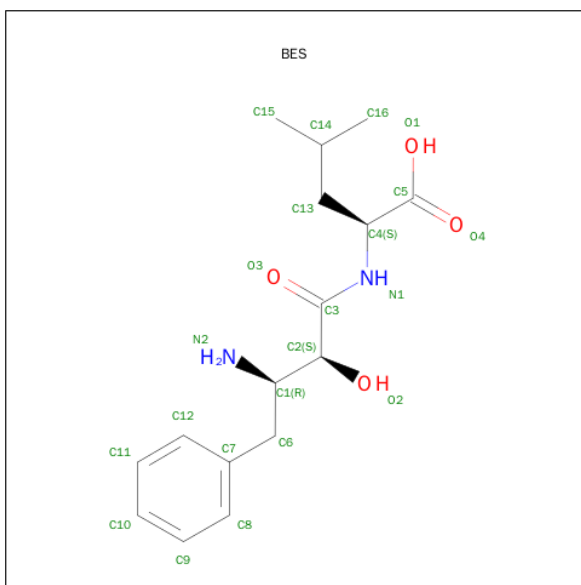
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is 2-(3-AMINO-2-HYDROXY-4-PHENYL-BUTYRYLAMINO)-4-METHYL-PENTANOIC ACID (three-letter code: BES) (formula: $C_{16}H_{24}N_2O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			22	16	2	4		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

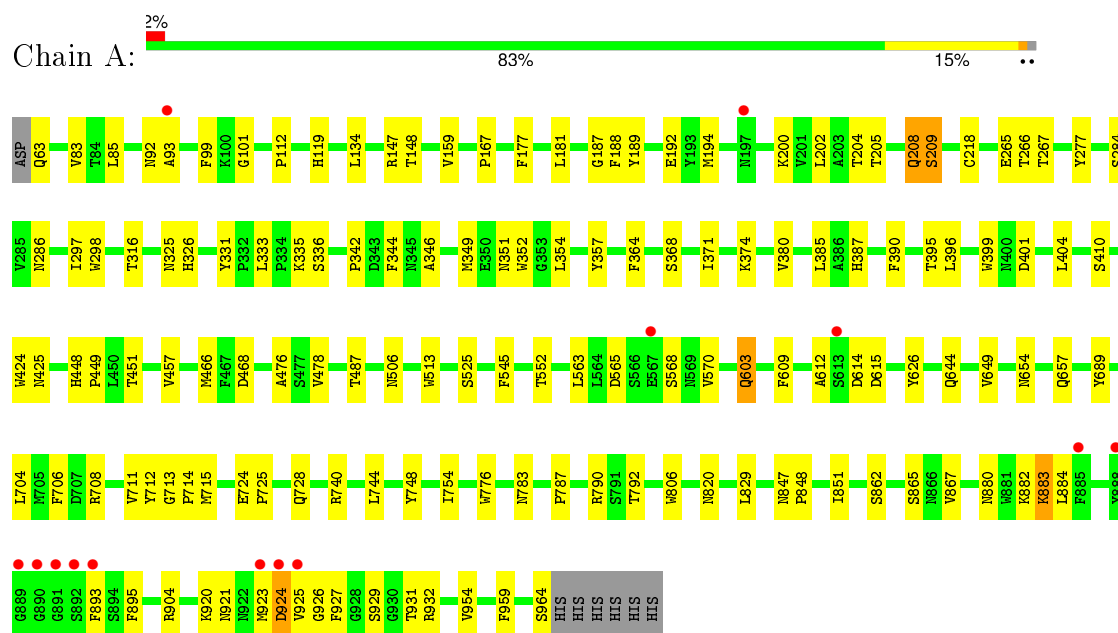
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	848	Total	O	0	0
			848	848		

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: Aminopeptidase N



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	260.61Å 63.01Å 81.70Å 90.00° 100.83° 90.00°	Depositor
Resolution (Å)	28.28 – 2.60 28.27 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.9 (28.28-2.60) 97.0 (28.27-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.24 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.164 , 0.276 0.166 , 0.271	Depositor DCC
R_{free} test set	2022 reflections (5.43%)	DCC
Wilson B-factor (Å ²)	42.5	Xtriage
Anisotropy	0.248	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 54.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	1 of 39197 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8434	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BES, ZN, 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	0.52	0/7429	0.67	0/10124

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	7241	0	6994	92	0
2	A	126	0	111	3	0
3	A	168	0	150	3	0
4	A	28	0	26	0	0
5	A	22	0	22	2	0
6	A	1	0	0	0	0
7	A	848	0	0	21	0
All	All	8434	0	7303	99	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 (99) 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:194:MET:SD	7:A:1886:HOH:O	2.07	1.12
1:A:208:GLN:HG3	1:A:349:MET:CE	1.86	1.03
1:A:451:THR:HG22	7:A:1823:HOH:O	1.66	0.94
2:A:1012:NAG:H3	7:A:1787:HOH:O	1.71	0.91
3:A:1009:NAG:O6	7:A:1699:HOH:O	1.81	0.84
1:A:457:VAL:HG21	1:A:466:MET:CE	2.10	0.82
1:A:924:ASP:C	1:A:926:GLY:H	1.85	0.81
1:A:396:LEU:HD11	1:A:404:LEU:HD23	1.61	0.80
3:A:1016:NAG:H61	7:A:1820:HOH:O	1.83	0.77
1:A:208:GLN:HG3	1:A:349:MET:HE1	1.69	0.75
1:A:704:LEU:HD21	1:A:904:ARG:HG2	1.69	0.73
1:A:457:VAL:HG21	1:A:466:MET:HE2	1.71	0.72
1:A:208:GLN:HG3	1:A:349:MET:HE2	1.74	0.69
1:A:364:PHE:CZ	1:A:374:LYS:HG3	2.28	0.69
1:A:208:GLN:HG3	1:A:349:MET:SD	2.35	0.67
1:A:728:GLN:HG3	7:A:1639:HOH:O	1.95	0.65
1:A:924:ASP:O	1:A:926:GLY:N	2.28	0.64
1:A:457:VAL:CG2	1:A:466:MET:CE	2.77	0.63
1:A:371:ILE:CG1	1:A:744:LEU:HD12	2.29	0.63
1:A:371:ILE:HG12	1:A:744:LEU:HD12	1.81	0.62
1:A:147:ARG:NE	7:A:1838:HOH:O	2.15	0.61
1:A:565:ASP:HB3	1:A:568:SER:OG	2.01	0.61
1:A:148:THR:HG22	1:A:159:VAL:HG13	1.81	0.60
1:A:457:VAL:CG2	1:A:466:MET:HE2	2.30	0.60
1:A:924:ASP:C	1:A:926:GLY:N	2.54	0.60
1:A:92:ASN:HB3	7:A:1728:HOH:O	2.01	0.60
1:A:331:TYR:CE2	1:A:333:LEU:HB2	2.38	0.59
3:A:1016:NAG:C6	7:A:1820:HOH:O	2.45	0.59
1:A:689:TYR:CD1	1:A:748:TYR:HB3	2.37	0.59
1:A:457:VAL:HG21	1:A:466:MET:HE3	1.83	0.59
2:A:1003:NAG:H83	7:A:1818:HOH:O	2.03	0.58
1:A:395:THR:O	1:A:506:ASN:HA	2.04	0.57
1:A:724:GLU:HB3	1:A:725:PRO:HD3	1.85	0.56
1:A:424:TRP:O	1:A:425:ASN:HB2	2.06	0.56
1:A:931:THR:HG22	1:A:932:ARG:HG2	1.87	0.55
1:A:904:ARG:HD2	7:A:1656:HOH:O	2.07	0.54
1:A:754:ILE:HG22	1:A:792:THR:HG21	1.90	0.53
1:A:927:PHE:HB2	1:A:931:THR:HA	1.91	0.53
1:A:820:ASN:HB2	7:A:1830:HOH:O	2.08	0.53
1:A:884:LEU:HD11	1:A:927:PHE:C	2.29	0.53
1:A:880:ASN:O	1:A:883:LYS:HD2	2.10	0.52
1:A:806:TRP:CE2	1:A:829:LEU:HD22	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:920:LYS:HE2	7:A:1739:HOH:O	2.11	0.51
1:A:148:THR:CG2	1:A:159:VAL:HG13	2.40	0.50
1:A:351:ASN:HB2	1:A:354:LEU:O	2.11	0.50
1:A:449:PRO:HB2	1:A:451:THR:O	2.12	0.50
2:A:1005:NAG:H4	7:A:1897:HOH:O	2.11	0.50
1:A:387:HIS:HA	1:A:390:PHE:O	2.11	0.50
1:A:364:PHE:CE1	1:A:374:LYS:HG3	2.47	0.49
1:A:565:ASP:HB3	1:A:568:SER:HG	1.78	0.49
1:A:357:TYR:HE2	1:A:380:VAL:HG12	1.77	0.49
1:A:209:SER:HB3	1:A:399:TRP:CH2	2.47	0.49
1:A:776:TRP:CD1	1:A:783:ASN:HA	2.47	0.49
1:A:112:PRO:HD3	1:A:167:PRO:HG3	1.96	0.48
1:A:708:ARG:HG2	1:A:867:VAL:CG2	2.44	0.48
5:A:1024:BES:H152	7:A:1482:HOH:O	2.15	0.47
1:A:349:MET:SD	5:A:1024:BES:H61	2.54	0.47
1:A:954:VAL:HG23	7:A:1471:HOH:O	2.13	0.47
1:A:715:MET:HG3	1:A:959:PHE:CZ	2.50	0.47
1:A:862:SER:O	1:A:865:SER:HB2	2.15	0.47
1:A:448:HIS:HD2	1:A:449:PRO:O	1.99	0.46
1:A:187:GLY:O	1:A:205:THR:HA	2.16	0.46
1:A:202:LEU:C	1:A:202:LEU:HD12	2.35	0.46
1:A:545:PHE:HB3	1:A:626:TYR:CE2	2.51	0.46
1:A:410:SER:HB2	1:A:476:ALA:HB2	1.98	0.46
1:A:368:SER:O	1:A:787:PRO:HB3	2.16	0.45
1:A:847:ASN:HA	1:A:848:PRO:HD3	1.78	0.45
1:A:189:TYR:CZ	1:A:204:THR:HG23	2.52	0.45
1:A:883:LYS:HD3	1:A:883:LYS:C	2.37	0.44
1:A:851:ILE:O	7:A:1781:HOH:O	2.20	0.44
1:A:371:ILE:HG13	1:A:744:LEU:HD12	1.99	0.44
1:A:654:ASN:HA	1:A:657:GLN:HB3	2.00	0.44
1:A:266:THR:HG22	1:A:267:THR:O	2.17	0.44
1:A:448:HIS:HE1	1:A:468:ASP:OD2	2.00	0.43
1:A:101:GLY:HA3	1:A:177:PHE:CE1	2.53	0.43
1:A:396:LEU:HD12	1:A:401:ASP:HB3	1.99	0.43
1:A:932:ARG:N	1:A:932:ARG:HE	2.16	0.43
1:A:344:PHE:CZ	1:A:346:ALA:HB3	2.53	0.43
1:A:612:ALA:H	1:A:615:ASP:HB2	1.84	0.43
1:A:265:GLU:HG3	7:A:1324:HOH:O	2.19	0.43
1:A:884:LEU:HG	1:A:895:PHE:CE2	2.53	0.43
1:A:147:ARG:NH2	7:A:1838:HOH:O	2.52	0.42
1:A:740:ARG:HG2	1:A:740:ARG:HH21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:SER:HB3	1:A:298:TRP:CD2	2.54	0.42
1:A:192:GLU:HA	1:A:200:LYS:O	2.19	0.42
1:A:316:THR:HG23	1:A:385:LEU:HD11	2.02	0.42
1:A:552:THR:HA	1:A:609:PHE:O	2.20	0.42
1:A:603:GLN:HG3	7:A:1884:HOH:O	2.19	0.42
1:A:787:PRO:HA	1:A:790:ARG:HD2	2.01	0.41
1:A:99:PHE:HB3	1:A:181:LEU:HD13	2.02	0.41
1:A:563:LEU:HD11	1:A:570:VAL:CG2	2.51	0.41
1:A:284:SER:HA	1:A:297:ILE:O	2.20	0.41
1:A:706:PHE:HB3	1:A:711:VAL:HB	2.02	0.41
1:A:83:VAL:HG12	1:A:85:LEU:CD2	2.50	0.41
1:A:92:ASN:O	1:A:93:ALA:HB3	2.21	0.41
1:A:119:HIS:HB2	1:A:218:CYS:O	2.21	0.41
1:A:713:GLY:N	1:A:714:PRO:HD2	2.36	0.40
1:A:921:ASN:ND2	7:A:1842:HOH:O	2.54	0.40
1:A:325:ASN:O	1:A:326:HIS:C	2.59	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	900/909 (99%)	853 (95%)	41 (5%)	6 (1%)	26 51

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	925	VAL
1	A	923	MET
1	A	893	PHE
1	A	882	LYS
1	A	924	ASP

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Mol	Chain	Res	Type
1	A	487	THR

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	797/804 (99%)	775 (97%)	22 (3%)	51 78

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	134	LEU
1	A	188	PHE
1	A	208	GLN
1	A	209	SER
1	A	277	TYR
1	A	286	ASN
1	A	335	LYS
1	A	336	SER
1	A	342	PRO
1	A	352	TRP
1	A	478	VAL
1	A	513	TRP
1	A	525	SER
1	A	603	GLN
1	A	614	ASP
1	A	644	GLN
1	A	649	VAL
1	A	712	TYR
1	A	883	LYS
1	A	929	SER
1	A	964	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	448	HIS
1	A	500	HIS
1	A	886	GLN
1	A	897	ASN
1	A	913	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 ⓘ

21 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	1001	1,2	14,14,15	0.54	0	15,19,21	1.80	2 (13%)
2	NAG	A	1002	2	14,14,15	0.53	0	15,19,21	1.31	1 (6%)
2	NAG	A	1003	2	14,14,15	0.69	0	15,19,21	1.31	2 (13%)
2	NAG	A	1004	1,2	14,14,15	0.56	0	15,19,21	1.17	1 (6%)
2	NAG	A	1005	2	14,14,15	0.63	0	15,19,21	1.18	1 (6%)
2	NAG	A	1006	2	14,14,15	0.78	1 (7%)	15,19,21	1.39	2 (13%)
3	NAG	A	1007	1,3	14,14,15	0.99	1 (7%)	15,19,21	1.26	2 (13%)
3	NAG	A	1008	3	14,14,15	0.62	0	15,19,21	1.02	1 (6%)
3	NAG	A	1009	1,3	14,14,15	0.67	0	15,19,21	1.14	1 (6%)
3	NAG	A	1010	3	14,14,15	0.62	0	15,19,21	1.30	2 (13%)
2	NAG	A	1011	1,2	14,14,15	0.59	0	15,19,21	1.70	3 (20%)
2	NAG	A	1012	2	14,14,15	0.50	0	15,19,21	0.90	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	1013	2	14,14,15	0.73	1 (7%)	15,19,21	2.41	3 (20%)
3	NAG	A	1014	1,3	14,14,15	0.59	0	15,19,21	1.74	1 (6%)
3	NAG	A	1015	3	14,14,15	0.62	0	15,19,21	1.52	4 (26%)
3	NAG	A	1016	1,3	14,14,15	0.60	0	15,19,21	1.40	3 (20%)
3	NAG	A	1017	3	14,14,15	0.54	0	15,19,21	1.30	2 (13%)
3	NAG	A	1018	1,3	14,14,15	0.58	0	15,19,21	1.20	1 (6%)
3	NAG	A	1019	3	14,14,15	0.50	0	15,19,21	1.69	2 (13%)
3	NAG	A	1021	1,3	14,14,15	0.52	0	15,19,21	1.45	2 (13%)
3	NAG	A	1022	3	14,14,15	0.48	0	15,19,21	1.80	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
2	NAG	A	1001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1002	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1003	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1004	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1005	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1006	2	-	0/6/23/26	0/1/1/1
3	NAG	A	1007	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1008	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1009	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1010	3	-	0/6/23/26	0/1/1/1
2	NAG	A	1011	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1012	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1013	2	-	0/6/23/26	0/1/1/1
3	NAG	A	1014	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1015	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1016	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1017	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1018	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1019	3	-	0/6/23/26	0/1/1/1
3	NAG	A	1021	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1022	3	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1007	NAG	O5-C1	-2.52	1.39	1.43
2	A	1013	NAG	C1-C2	2.07	1.55	1.52
2	A	1006	NAG	C1-C2	2.22	1.55	1.52

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1022	NAG	C4-C3-C2	-3.66	105.55	111.23
2	A	1011	NAG	C3-C2-N2	-3.36	102.50	110.56
3	A	1015	NAG	O7-C7-C8	-2.78	116.96	122.06
3	A	1016	NAG	O7-C7-C8	-2.65	117.19	122.06
2	A	1013	NAG	O7-C7-C8	-2.57	117.34	122.06
3	A	1019	NAG	C4-C3-C2	-2.56	107.24	111.23
3	A	1007	NAG	C2-N2-C7	-2.53	119.79	123.04
3	A	1007	NAG	C4-C3-C2	-2.41	107.49	111.23
3	A	1021	NAG	C3-C4-C5	-2.35	106.10	110.20
2	A	1011	NAG	C2-N2-C7	-2.33	120.05	123.04
2	A	1001	NAG	O4-C4-C3	-2.11	105.58	110.34
3	A	1008	NAG	C1-O5-C5	-2.08	109.61	112.25
2	A	1004	NAG	C1-O5-C5	2.11	114.92	112.25
3	A	1015	NAG	C3-C4-C5	2.13	113.91	110.20
3	A	1017	NAG	C2-N2-C7	2.13	125.78	123.04
3	A	1010	NAG	C1-O5-C5	2.22	115.07	112.25
2	A	1012	NAG	C4-C3-C2	2.27	114.75	111.23
2	A	1006	NAG	C4-C3-C2	2.29	114.79	111.23
2	A	1003	NAG	C2-N2-C7	2.39	126.11	123.04
3	A	1015	NAG	C4-C3-C2	2.47	115.07	111.23
3	A	1015	NAG	C8-C7-N2	2.50	120.89	116.11
3	A	1016	NAG	C8-C7-N2	2.51	120.91	116.11
3	A	1010	NAG	C2-N2-C7	2.53	126.29	123.04
2	A	1005	NAG	C1-O5-C5	2.61	115.56	112.25
2	A	1006	NAG	C2-N2-C7	2.75	126.57	123.04
3	A	1018	NAG	C1-O5-C5	2.91	115.94	112.25
3	A	1016	NAG	C2-N2-C7	3.09	127.00	123.04
2	A	1003	NAG	C4-C3-C2	3.12	116.08	111.23
3	A	1017	NAG	C1-O5-C5	3.27	116.40	112.25
3	A	1009	NAG	C1-O5-C5	3.32	116.46	112.25
2	A	1013	NAG	C8-C7-N2	3.53	122.86	116.11
2	A	1002	NAG	C4-C3-C2	3.79	117.12	111.23
2	A	1011	NAG	C1-O5-C5	3.94	117.25	112.25
3	A	1021	NAG	C1-O5-C5	4.06	117.41	112.25
3	A	1022	NAG	C1-O5-C5	4.95	118.53	112.25
3	A	1019	NAG	C1-O5-C5	4.97	118.55	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1001	NAG	C1-O5-C5	5.50	119.22	112.25
3	A	1014	NAG	C1-O5-C5	6.08	119.97	112.25
2	A	1013	NAG	C2-N2-C7	7.70	132.94	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1003	NAG	1	0
2	A	1005	NAG	1	0
3	A	1009	NAG	1	0
2	A	1012	NAG	1	0
3	A	1016	NAG	2	0

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 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	$\# Z > 2$
4	NAG	A	1020	1	14,14,15	0.61	0	15,19,21	1.91	2 (13%)
4	NAG	A	1023	1	14,14,15	0.62	0	15,19,21	0.92	0
5	BES	A	1024	6	19,22,22	0.88	0	19,29,29	1.22	3 (15%)

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	1020	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1023	1	-	0/6/23/26	0/1/1/1
5	BES	A	1024	6	-	0/20/24/24	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1024	BES	O3-C3-C2	-2.23	115.50	120.05
4	A	1020	NAG	C3-C2-N2	2.31	116.09	110.56
5	A	1024	BES	C2-C3-N1	2.41	119.76	116.33
5	A	1024	BES	O2-C2-C1	3.05	115.84	109.66
4	A	1020	NAG	C2-N2-C7	6.11	130.89	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1024	BES	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	902/909 (99%)	-0.50	14 (1%) 74 69	14, 38, 83, 169	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	888	TYR	7.0
1	A	889	GLY	5.9
1	A	93	ALA	4.4
1	A	924	ASP	3.5
1	A	890	GLY	3.2
1	A	885	PHE	3.1
1	A	891	GLY	3.0
1	A	925	VAL	2.9
1	A	197	ASN	2.7
1	A	892	SER	2.4
1	A	923	MET	2.3
1	A	567	GLU	2.2
1	A	613	SER	2.2
1	A	893	PHE	2.1

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, 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(\AA^2)	Q<0.9
2	NAG	A	1011	14/15	0.94	0.14	1.51	50,63,93,93	0
2	NAG	A	1004	14/15	0.95	0.14	1.02	37,53,76,78	0
3	NAG	A	1021	14/15	0.95	0.10	-0.77	51,65,71,76	0
3	NAG	A	1014	14/15	0.97	0.10	-0.94	24,33,36,42	0
2	NAG	A	1001	14/15	0.98	0.10	-0.97	28,35,41,49	0
3	NAG	A	1007	14/15	0.98	0.08	-1.98	21,25,39,40	0
2	NAG	A	1006	14/15	0.59	0.47	-	93,154,174,178	0
2	NAG	A	1003	14/15	0.77	0.42	-	109,131,149,169	0
3	NAG	A	1009	14/15	0.94	0.13	-	41,56,77,90	0
3	NAG	A	1010	14/15	0.90	0.25	-	54,87,102,106	0
3	NAG	A	1022	14/15	0.88	0.31	-	54,89,114,120	0
2	NAG	A	1013	14/15	0.70	0.41	-	96,140,171,173	0
3	NAG	A	1015	14/15	0.95	0.24	-	50,61,71,82	0
2	NAG	A	1012	14/15	0.89	0.24	-	61,102,133,174	0
3	NAG	A	1019	14/15	0.83	0.44	-	60,113,125,125	0
3	NAG	A	1018	14/15	0.89	0.27	-	53,88,115,116	0
3	NAG	A	1016	14/15	0.88	0.28	-	78,98,108,119	0
2	NAG	A	1005	14/15	0.89	0.36	-	75,115,136,137	0
3	NAG	A	1008	14/15	0.96	0.23	-	43,52,66,79	0
3	NAG	A	1017	14/15	0.82	0.46	-	94,134,150,156	0
2	NAG	A	1002	14/15	0.92	0.25	-	53,77,95,127	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(\AA^2)	Q<0.9
5	BES	A	1024	22/22	0.92	0.24	4.24	51,70,86,88	0
6	ZN	A	1025	1/1	1.00	0.10	-1.02	27,27,27,27	0
4	NAG	A	1020	14/15	0.84	0.60	-	101,135,160,186	0
4	NAG	A	1023	14/15	0.93	0.32	-	98,106,117,124	0

6.5 Other polymers [i](#)

There are no such residues in this entry.