



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 12, 2017 – 06:27 PM EDT

PDB ID : 5LHD
Title : Structure of glycosylated human aminopeptidase N
Authors : Recacha, R.; Mudgal, G.; Santiago, C.; Casasnovas, J.M.
Deposited on : 2016-07-11
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029077
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20029077

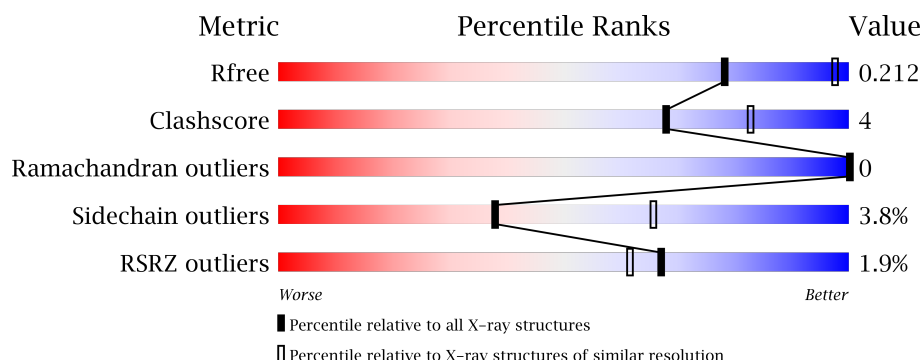
1 Overall quality at a glance

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}	100719	2542 (2.60-2.60)
Clashscore	112137	2895 (2.60-2.60)
Ramachandran outliers	110173	2848 (2.60-2.60)
Sidechain outliers	110143	2848 (2.60-2.60)
RSRZ outliers	101464	2550 (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	950	<div> <div>2%</div> <div>84%</div> <div>10%</div> <div>5%</div> </div>
1	B	950	<div> <div>2%</div> <div>83%</div> <div>12%</div> <div>5%</div> </div>
1	C	950	<div> <div>2%</div> <div>81%</div> <div>13%</div> <div>5%</div> </div>
1	D	950	<div> <div>2%</div> <div>84%</div> <div>11%</div> <div>5%</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1012	-	-	-	X
2	NAG	A	1015	X	-	-	-
2	NAG	A	1018	X	-	-	-
2	NAG	B	1012	-	-	-	X
2	NAG	B	1017	-	-	-	X
2	NAG	B	1019	X	-	-	-
2	NAG	C	1101	-	-	-	X
2	NAG	C	1114	-	-	-	X
2	NAG	C	1117	X	-	-	-
2	NAG	C	1118	X	-	-	-
2	NAG	C	1126	X	-	-	X
2	NAG	C	1128	X	-	-	-
2	NAG	D	1001	-	-	-	X
2	NAG	D	1017	X	-	-	-
2	NAG	D	1019	-	-	-	X
2	NAG	D	1021	X	-	-	-
2	NAG	D	1023	X	-	-	-
5	EDO	A	1024	-	-	-	X
5	EDO	A	1026	-	-	-	X
5	EDO	A	1027	-	-	-	X
5	EDO	A	1028	-	-	-	X
5	EDO	A	1029	-	-	-	X
5	EDO	A	1030	-	-	-	X
5	EDO	A	1031	-	-	-	X
5	EDO	A	1032	-	-	-	X
5	EDO	A	1033	-	-	-	X
5	EDO	A	1034	-	-	-	X
5	EDO	A	1035	-	-	-	X
5	EDO	A	1037	-	-	-	X
5	EDO	B	1025	-	-	-	X
5	EDO	B	1026	-	-	-	X
5	EDO	B	1027	-	-	-	X
5	EDO	B	1028	-	-	-	X
5	EDO	B	1030	-	-	-	X
5	EDO	B	1033	-	-	-	X
5	EDO	B	1034	-	-	-	X
5	EDO	C	1136	-	-	-	X
5	EDO	C	1140	-	-	-	X
5	EDO	C	1142	-	-	-	X
5	EDO	C	1145	-	-	-	X
5	EDO	C	1146	-	-	-	X
5	EDO	D	1027	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	EDO	D	1031	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 31338 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	903	Total	C	N	O	S	0	0	0
			7285	4647	1226	1388	24			
1	B	904	Total	C	N	O	S	0	1	0
			7302	4656	1232	1390	24			
1	C	905	Total	C	N	O	S	0	0	0
			7300	4654	1231	1391	24			
1	D	904	Total	C	N	O	S	0	0	0
			7295	4651	1230	1390	24			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	TYR	-	expression tag	UNP P15144
A	19	PRO	-	expression tag	UNP P15144
A	20	TYR	-	expression tag	UNP P15144
A	21	ASP	-	expression tag	UNP P15144
A	22	VAL	-	expression tag	UNP P15144
A	23	PRO	-	expression tag	UNP P15144
A	24	ASP	-	expression tag	UNP P15144
A	25	TYR	-	expression tag	UNP P15144
A	26	ALA	-	expression tag	UNP P15144
A	27	GLY	-	expression tag	UNP P15144
A	28	ALA	-	expression tag	UNP P15144
A	29	GLN	-	expression tag	UNP P15144
A	30	PRO	-	expression tag	UNP P15144
A	31	ALA	-	expression tag	UNP P15144
A	32	ARG	-	expression tag	UNP P15144
A	33	SER	-	expression tag	UNP P15144
A	34	PRO	-	expression tag	UNP P15144
A	35	GLY	-	expression tag	UNP P15144
B	18	TYR	-	expression tag	UNP P15144
B	19	PRO	-	expression tag	UNP P15144
B	20	TYR	-	expression tag	UNP P15144

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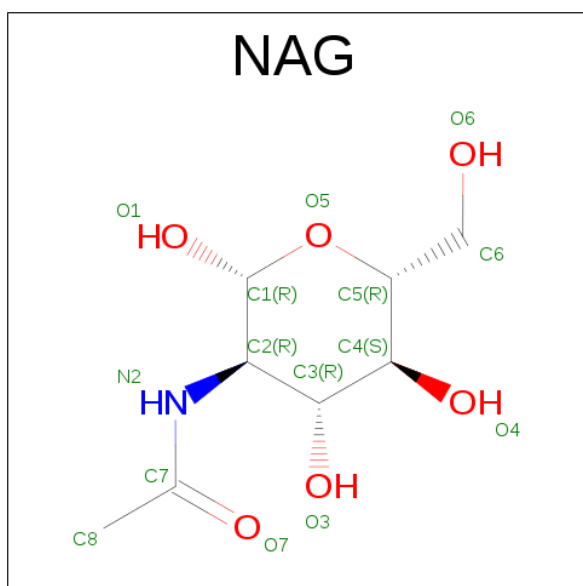
Chain	Residue	Modelled	Actual	Comment	Reference
B	21	ASP	-	expression tag	UNP P15144
B	22	VAL	-	expression tag	UNP P15144
B	23	PRO	-	expression tag	UNP P15144
B	24	ASP	-	expression tag	UNP P15144
B	25	TYR	-	expression tag	UNP P15144
B	26	ALA	-	expression tag	UNP P15144
B	27	GLY	-	expression tag	UNP P15144
B	28	ALA	-	expression tag	UNP P15144
B	29	GLN	-	expression tag	UNP P15144
B	30	PRO	-	expression tag	UNP P15144
B	31	ALA	-	expression tag	UNP P15144
B	32	ARG	-	expression tag	UNP P15144
B	33	SER	-	expression tag	UNP P15144
B	34	PRO	-	expression tag	UNP P15144
B	35	GLY	-	expression tag	UNP P15144
C	18	TYR	-	expression tag	UNP P15144
C	19	PRO	-	expression tag	UNP P15144
C	20	TYR	-	expression tag	UNP P15144
C	21	ASP	-	expression tag	UNP P15144
C	22	VAL	-	expression tag	UNP P15144
C	23	PRO	-	expression tag	UNP P15144
C	24	ASP	-	expression tag	UNP P15144
C	25	TYR	-	expression tag	UNP P15144
C	26	ALA	-	expression tag	UNP P15144
C	27	GLY	-	expression tag	UNP P15144
C	28	ALA	-	expression tag	UNP P15144
C	29	GLN	-	expression tag	UNP P15144
C	30	PRO	-	expression tag	UNP P15144
C	31	ALA	-	expression tag	UNP P15144
C	32	ARG	-	expression tag	UNP P15144
C	33	SER	-	expression tag	UNP P15144
C	34	PRO	-	expression tag	UNP P15144
C	35	GLY	-	expression tag	UNP P15144
D	18	TYR	-	expression tag	UNP P15144
D	19	PRO	-	expression tag	UNP P15144
D	20	TYR	-	expression tag	UNP P15144
D	21	ASP	-	expression tag	UNP P15144
D	22	VAL	-	expression tag	UNP P15144
D	23	PRO	-	expression tag	UNP P15144
D	24	ASP	-	expression tag	UNP P15144
D	25	TYR	-	expression tag	UNP P15144
D	26	ALA	-	expression tag	UNP P15144

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Chain	Residue	Modelled	Actual	Comment	Reference
D	27	GLY	-	expression tag	UNP P15144
D	28	ALA	-	expression tag	UNP P15144
D	29	GLN	-	expression tag	UNP P15144
D	30	PRO	-	expression tag	UNP P15144
D	31	ALA	-	expression tag	UNP P15144
D	32	ARG	-	expression tag	UNP P15144
D	33	SER	-	expression tag	UNP P15144
D	34	PRO	-	expression tag	UNP P15144
D	35	GLY	-	expression tag	UNP P15144

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



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

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

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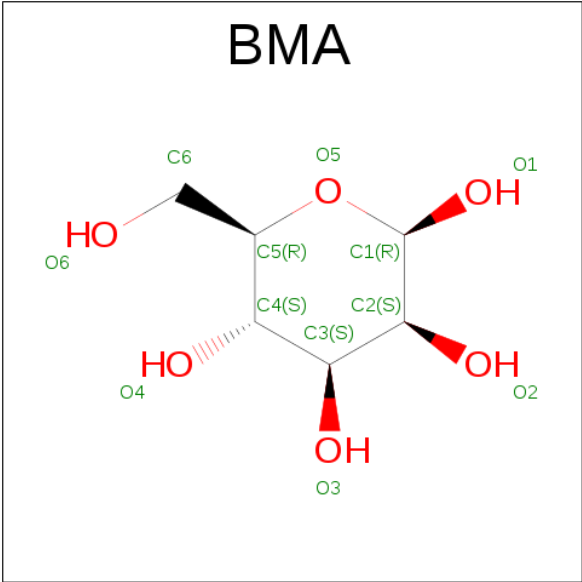
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

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

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	C	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	C	O	0	0
			11	6	5		

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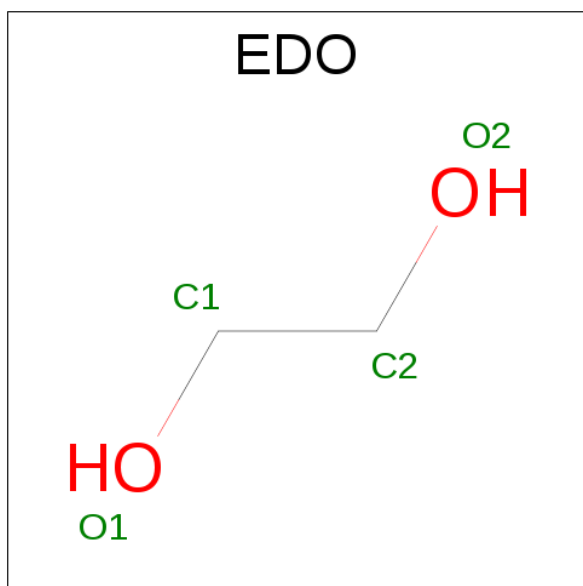
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	C	O	0	0
			11	6	5		
3	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Zn	0	0
			1	1		
4	A	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		
4	C	1	Total	Zn	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	A	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	B	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	C	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0
5	D	1	Total 4	C 2	O 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			4	2	2		

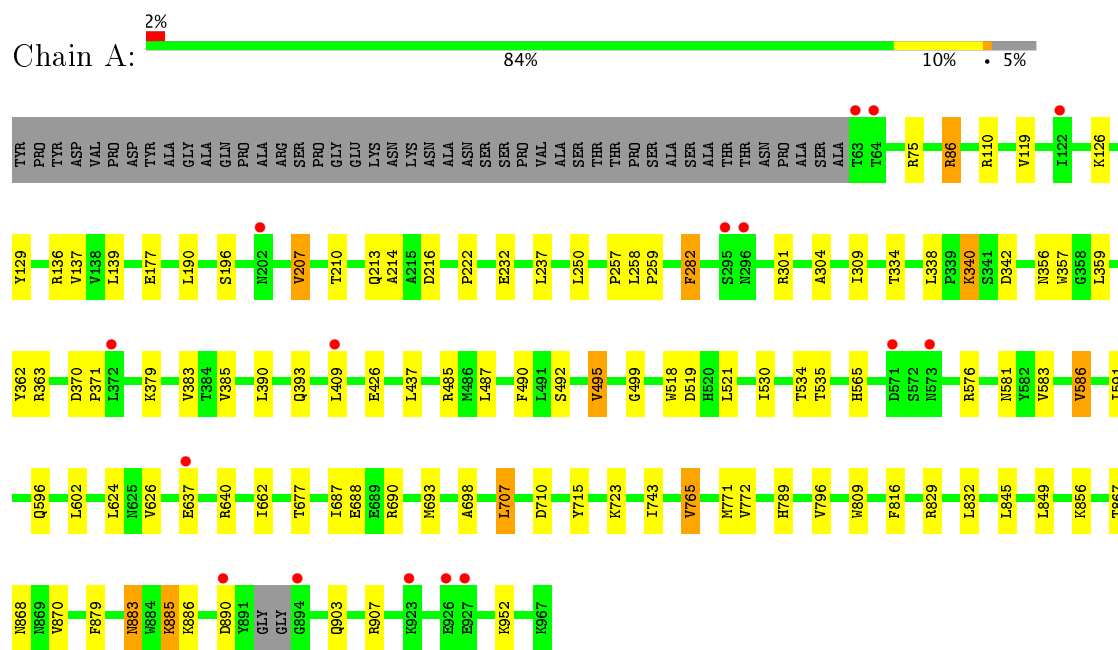
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	157	Total	O	0	0
			157	157		
6	B	186	Total	O	0	0
			186	186		
6	C	154	Total	O	0	0
			154	154		
6	D	168	Total	O	0	0
			168	168		

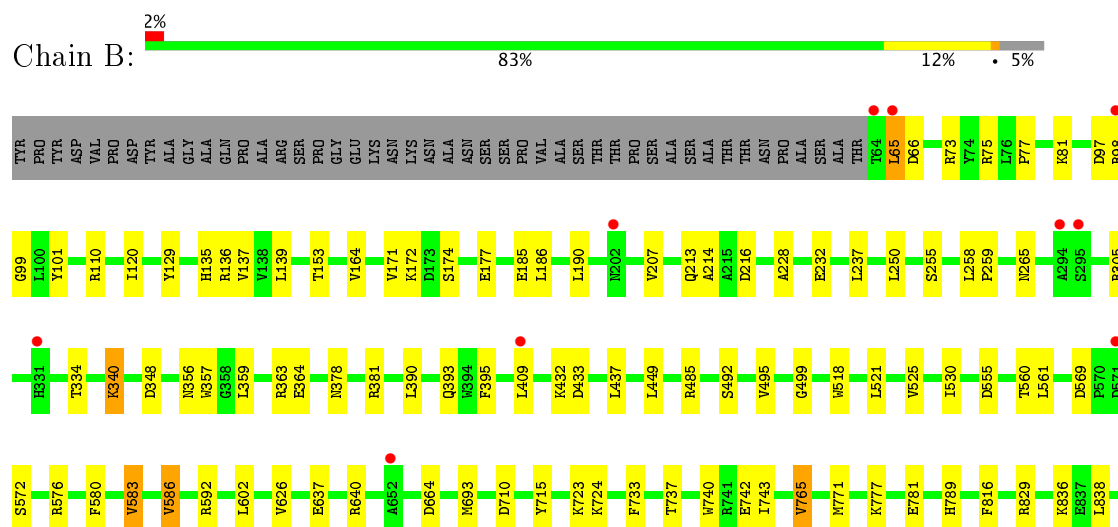
3 Residue-property plots [i](#)

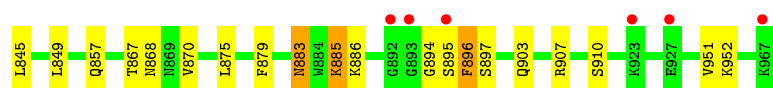
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Aminopeptidase N

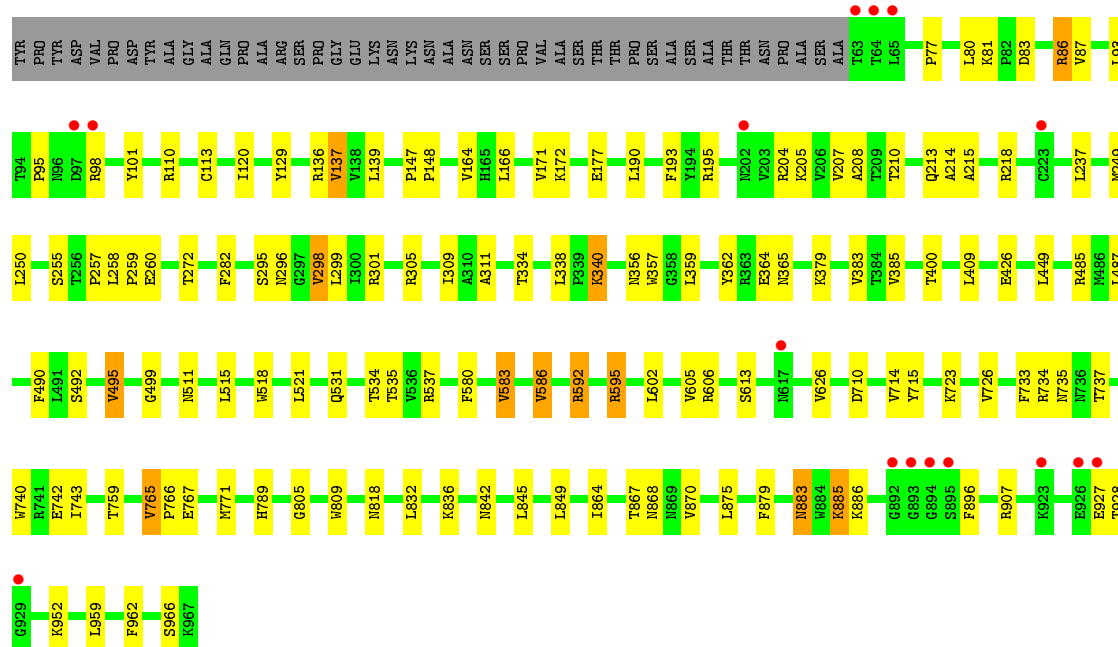
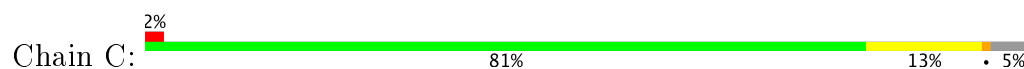


• Molecule 1: Aminopeptidase N

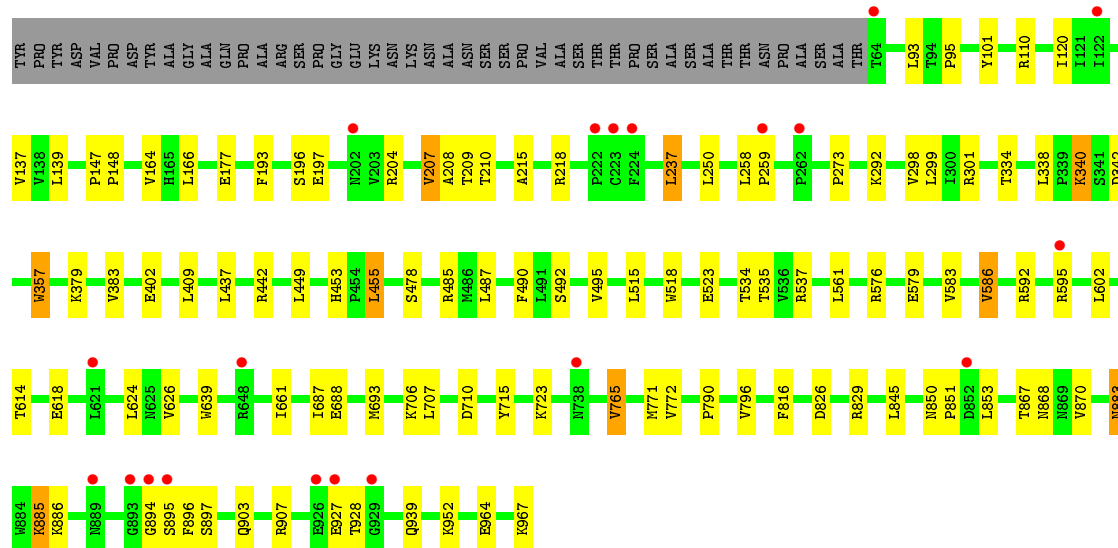
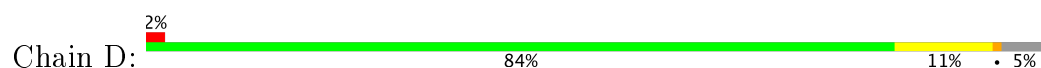




• Molecule 1: Aminopeptidase N



• Molecule 1: Aminopeptidase N



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	127.09Å 168.86Å 244.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 2.60 24.96 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.4 (19.97-2.60) 99.8 (24.96-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.10 (at 2.60Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.181 , 0.214 0.178 , 0.212	Depositor DCC
R_{free} test set	8076 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	52.9	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	31338	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.68 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0639e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: ZN, BMA, NAG, EDO

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	0.23	0/7472	0.40	0/10179
1	B	0.24	0/7494	0.42	0/10208
1	C	0.23	0/7488	0.41	0/10200
1	D	0.23	0/7483	0.41	0/10193
All	All	0.23	0/29937	0.41	0/40780

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	7285	0	7037	56	0
1	B	7302	0	7062	75	0
1	C	7300	0	7056	77	0
1	D	7295	0	7054	53	0
2	A	196	0	172	1	0
2	B	210	0	185	1	0
2	C	238	0	207	2	0
2	D	252	0	222	0	0
3	A	88	0	76	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	66	0	57	2	0
3	C	176	0	150	4	0
3	D	77	0	67	2	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	68	0	102	6	0
5	B	48	0	72	8	0
5	C	48	0	72	2	0
5	D	20	0	30	0	0
6	A	157	0	0	8	1
6	B	186	0	0	15	0
6	C	154	0	0	11	1
6	D	168	0	0	6	0
All	All	31338	0	29621	263	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

The worst 5 of 263 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:232:GLU:OE1	6:A:1101:HOH:O	1.81	0.96
1:C:77:PRO:O	6:C:1201:HOH:O	1.87	0.93
1:A:710:ASP:OD1	6:A:1102:HOH:O	1.95	0.84
1:A:530:ILE:O	6:A:1103:HOH:O	1.97	0.81
1:B:213:GLN:NE2	6:B:1105:HOH:O	2.13	0.81

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1171:HOH:O	6:C:1310:HOH:O[3_555]	2.15	0.05

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	899/950 (95%)	868 (97%)	31 (3%)	0	100	100
1	B	903/950 (95%)	870 (96%)	33 (4%)	0	100	100
1	C	903/950 (95%)	874 (97%)	29 (3%)	0	100	100
1	D	902/950 (95%)	873 (97%)	29 (3%)	0	100	100
All	All	3607/3800 (95%)	3485 (97%)	122 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	800/837 (96%)	768 (96%)	32 (4%)	36	64
1	B	803/837 (96%)	778 (97%)	25 (3%)	45	73
1	C	802/837 (96%)	769 (96%)	33 (4%)	35	63
1	D	802/837 (96%)	770 (96%)	32 (4%)	36	64
All	All	3207/3348 (96%)	3085 (96%)	122 (4%)	38	66

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	885	LYS
1	C	309	ILE
1	D	765	VAL

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Mol	Chain	Res	Type
1	B	896	PHE
1	C	190	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 151 ligands modelled in this entry, 4 are monoatomic - leaving 147 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	A	1001	1,2	14,14,15	0.53	0	15,19,21	0.69	0
2	NAG	A	1002	3,2	14,14,15	0.53	0	15,19,21	0.77	0
3	BMA	A	1003	3,2	11,11,12	0.57	0	13,15,17	1.25	2 (15%)
3	BMA	A	1004	3	11,11,12	0.68	0	13,15,17	0.48	0
2	NAG	A	1005	1,2	14,14,15	0.53	0	15,19,21	0.67	0
2	NAG	A	1006	3,2	14,14,15	0.55	0	15,19,21	0.65	0
3	BMA	A	1007	3,2	11,11,12	0.52	0	13,15,17	1.02	1 (7%)
3	BMA	A	1008	3	11,11,12	0.57	0	13,15,17	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	A	1009	3	11,11,12	0.59	0	13,15,17	0.50	0
2	NAG	A	1010	1,2	14,14,15	0.49	0	15,19,21	0.76	0
2	NAG	A	1011	2	14,14,15	0.56	0	15,19,21	0.67	0
2	NAG	A	1012	1,2	14,14,15	0.58	0	15,19,21	0.78	0
2	NAG	A	1013	3,2	14,14,15	0.58	0	15,19,21	0.90	0
3	BMA	A	1014	2	11,11,12	0.62	0	13,15,17	0.56	0
2	NAG	A	1015	1	14,14,15	0.52	0	15,19,21	0.68	0
2	NAG	A	1016	1,2	14,14,15	0.57	0	15,19,21	0.69	0
2	NAG	A	1017	2	14,14,15	0.50	0	15,19,21	0.59	0
2	NAG	A	1018	1,2	14,14,15	0.53	0	15,19,21	0.76	1 (6%)
2	NAG	A	1019	3,2	14,14,15	0.51	0	15,19,21	0.82	1 (6%)
3	BMA	A	1020	3,2	11,11,12	0.53	0	13,15,17	0.50	0
3	BMA	A	1021	3	11,11,12	0.66	0	13,15,17	0.45	0
2	NAG	A	1022	1	14,14,15	0.47	0	15,19,21	0.76	0
5	EDO	A	1024	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	A	1025	-	3,3,3	0.46	0	2,2,2	0.33	0
5	EDO	A	1026	-	3,3,3	0.45	0	2,2,2	0.37	0
5	EDO	A	1027	-	3,3,3	0.45	0	2,2,2	0.43	0
5	EDO	A	1028	-	3,3,3	0.48	0	2,2,2	0.28	0
5	EDO	A	1029	-	3,3,3	0.46	0	2,2,2	0.20	0
5	EDO	A	1030	-	3,3,3	0.45	0	2,2,2	0.38	0
5	EDO	A	1031	-	3,3,3	0.48	0	2,2,2	0.27	0
5	EDO	A	1032	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	A	1033	-	3,3,3	0.45	0	2,2,2	0.34	0
5	EDO	A	1034	-	3,3,3	0.48	0	2,2,2	0.28	0
5	EDO	A	1035	-	3,3,3	0.46	0	2,2,2	0.42	0
5	EDO	A	1036	-	3,3,3	0.46	0	2,2,2	0.35	0
5	EDO	A	1037	-	3,3,3	0.44	0	2,2,2	0.39	0
5	EDO	A	1038	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	A	1039	-	3,3,3	0.44	0	2,2,2	0.38	0
5	EDO	A	1040	-	3,3,3	0.42	0	2,2,2	0.30	0
2	NAG	B	1001	1,2	14,14,15	0.61	0	15,19,21	0.89	0
2	NAG	B	1002	3,2	14,14,15	0.55	0	15,19,21	0.60	0
3	BMA	B	1003	3,2	11,11,12	0.68	0	13,15,17	0.90	0
3	BMA	B	1004	3	11,11,12	0.86	1 (9%)	13,15,17	1.58	3 (23%)
2	NAG	B	1005	1,2	14,14,15	0.55	0	15,19,21	0.67	0
2	NAG	B	1006	3,2	14,14,15	0.43	0	15,19,21	1.47	2 (13%)
3	BMA	B	1007	3,2	11,11,12	0.59	0	13,15,17	1.54	2 (15%)
3	BMA	B	1008	3	11,11,12	0.55	0	13,15,17	1.09	1 (7%)
3	BMA	B	1009	3	11,11,12	0.54	0	13,15,17	1.43	2 (15%)
2	NAG	B	1010	1,2	14,14,15	0.59	0	15,19,21	0.70	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1011	2	14,14,15	0.55	0	15,19,21	0.54	0
2	NAG	B	1012	1,2	14,14,15	0.58	0	15,19,21	0.64	0
2	NAG	B	1013	2	14,14,15	0.49	0	15,19,21	0.74	0
2	NAG	B	1014	1,2	14,14,15	0.45	0	15,19,21	1.11	1 (6%)
2	NAG	B	1015	3,2	14,14,15	0.57	0	15,19,21	0.62	0
3	BMA	B	1016	2	11,11,12	0.55	0	13,15,17	0.94	0
2	NAG	B	1017	1,2	14,14,15	0.55	0	15,19,21	0.72	0
2	NAG	B	1018	2	14,14,15	0.55	0	15,19,21	1.35	2 (13%)
2	NAG	B	1019	1,2	14,14,15	0.53	0	15,19,21	1.00	1 (6%)
2	NAG	B	1020	2	14,14,15	0.49	0	15,19,21	0.75	0
2	NAG	B	1021	1	14,14,15	0.55	0	15,19,21	0.89	0
5	EDO	B	1023	-	3,3,3	0.44	0	2,2,2	0.40	0
5	EDO	B	1024	-	3,3,3	0.45	0	2,2,2	0.37	0
5	EDO	B	1025	-	3,3,3	0.41	0	2,2,2	0.51	0
5	EDO	B	1026	-	3,3,3	0.45	0	2,2,2	0.43	0
5	EDO	B	1027	-	3,3,3	0.41	0	2,2,2	0.42	0
5	EDO	B	1028	-	3,3,3	0.47	0	2,2,2	0.32	0
5	EDO	B	1029	-	3,3,3	0.47	0	2,2,2	0.31	0
5	EDO	B	1030	-	3,3,3	0.49	0	2,2,2	0.30	0
5	EDO	B	1031	-	3,3,3	0.47	0	2,2,2	0.26	0
5	EDO	B	1032	-	3,3,3	0.46	0	2,2,2	0.37	0
5	EDO	B	1033	-	3,3,3	0.45	0	2,2,2	0.36	0
5	EDO	B	1034	-	3,3,3	0.49	0	2,2,2	0.23	0
2	NAG	C	1101	1,2	14,14,15	0.67	0	15,19,21	1.69	3 (20%)
2	NAG	C	1102	3,2	14,14,15	0.58	0	15,19,21	0.96	1 (6%)
3	BMA	C	1103	3,2	11,11,12	0.62	0	13,15,17	0.61	0
3	BMA	C	1104	3	11,11,12	0.62	0	13,15,17	0.40	0
2	NAG	C	1105	1,2	14,14,15	0.54	0	15,19,21	0.59	0
2	NAG	C	1106	3,2	14,14,15	0.54	0	15,19,21	0.72	0
3	BMA	C	1107	3,2	11,11,12	0.75	0	13,15,17	0.78	0
3	BMA	C	1108	3	11,11,12	0.64	0	13,15,17	0.84	0
3	BMA	C	1109	3	11,11,12	0.64	0	13,15,17	0.53	0
2	NAG	C	1110	1,2	14,14,15	0.58	0	15,19,21	0.87	1 (6%)
2	NAG	C	1111	3,2	14,14,15	0.53	0	15,19,21	0.79	1 (6%)
3	BMA	C	1112	3,2	11,11,12	0.59	0	13,15,17	0.66	0
3	BMA	C	1113	3	11,11,12	0.60	0	13,15,17	1.04	1 (7%)
2	NAG	C	1114	1,2	14,14,15	0.55	0	15,19,21	0.63	0
2	NAG	C	1115	3,2	14,14,15	0.58	0	15,19,21	1.00	1 (6%)
3	BMA	C	1116	2	11,11,12	0.64	0	13,15,17	0.61	0
2	NAG	C	1117	1	14,14,15	0.51	0	15,19,21	0.79	0
2	NAG	C	1118	1,2	14,14,15	0.57	0	15,19,21	1.10	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1119	2	14,14,15	0.49	0	15,19,21	0.61	0
2	NAG	C	1120	1,2	14,14,15	0.58	0	15,19,21	0.77	0
2	NAG	C	1121	3,2	14,14,15	0.53	0	15,19,21	0.52	0
3	BMA	C	1122	3,2	11,11,12	0.49	0	13,15,17	0.73	0
3	BMA	C	1123	3	11,11,12	0.60	0	13,15,17	1.97	4 (30%)
3	BMA	C	1124	3	11,11,12	0.59	0	13,15,17	0.99	1 (7%)
3	BMA	C	1125	3	11,11,12	0.60	0	13,15,17	1.12	1 (7%)
2	NAG	C	1126	1,2	14,14,15	0.56	0	15,19,21	0.68	0
2	NAG	C	1127	2	14,14,15	0.53	0	15,19,21	0.65	0
2	NAG	C	1128	1,2	14,14,15	0.50	0	15,19,21	0.65	0
2	NAG	C	1129	3,2	14,14,15	0.59	0	15,19,21	0.75	1 (6%)
3	BMA	C	1130	3,2	11,11,12	0.62	0	13,15,17	0.69	0
3	BMA	C	1131	3	11,11,12	0.66	0	13,15,17	0.68	0
3	BMA	C	1132	3	11,11,12	0.65	0	13,15,17	0.41	0
3	BMA	C	1133	3	11,11,12	0.63	0	13,15,17	0.57	0
5	EDO	C	1135	-	3,3,3	0.45	0	2,2,2	0.38	0
5	EDO	C	1136	-	3,3,3	0.44	0	2,2,2	0.37	0
5	EDO	C	1137	-	3,3,3	0.45	0	2,2,2	0.37	0
5	EDO	C	1138	-	3,3,3	0.46	0	2,2,2	0.37	0
5	EDO	C	1139	-	3,3,3	0.45	0	2,2,2	0.39	0
5	EDO	C	1140	-	3,3,3	0.51	0	2,2,2	0.22	0
5	EDO	C	1141	-	3,3,3	0.46	0	2,2,2	0.38	0
5	EDO	C	1142	-	3,3,3	0.46	0	2,2,2	0.32	0
5	EDO	C	1143	-	3,3,3	0.46	0	2,2,2	0.34	0
5	EDO	C	1144	-	3,3,3	0.46	0	2,2,2	0.38	0
5	EDO	C	1145	-	3,3,3	0.47	0	2,2,2	0.38	0
5	EDO	C	1146	-	3,3,3	0.49	0	2,2,2	0.24	0
2	NAG	D	1001	1,2	14,14,15	0.53	0	15,19,21	0.64	0
2	NAG	D	1002	3,2	14,14,15	0.50	0	15,19,21	0.70	0
3	BMA	D	1003	2	11,11,12	0.62	0	13,15,17	1.05	0
2	NAG	D	1004	1,2	14,14,15	0.57	0	15,19,21	0.58	0
2	NAG	D	1005	3,2	14,14,15	0.53	0	15,19,21	0.69	0
3	BMA	D	1006	3,2	11,11,12	0.62	0	13,15,17	1.26	1 (7%)
3	BMA	D	1007	3	11,11,12	0.81	0	13,15,17	0.74	0
3	BMA	D	1008	3	11,11,12	0.58	0	13,15,17	1.24	2 (15%)
3	BMA	D	1009	3	11,11,12	0.58	0	13,15,17	1.09	0
2	NAG	D	1010	1,2	14,14,15	0.49	0	15,19,21	0.99	1 (6%)
2	NAG	D	1011	3,2	14,14,15	0.57	0	15,19,21	0.70	0
3	BMA	D	1012	2	11,11,12	0.56	0	13,15,17	1.11	1 (7%)
2	NAG	D	1013	1,2	14,14,15	0.55	0	15,19,21	0.52	0
2	NAG	D	1014	3,2	14,14,15	0.49	0	15,19,21	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	BMA	D	1015	2	11,11,12	0.63	0	13,15,17	0.51	0
2	NAG	D	1016	1	14,14,15	0.47	0	15,19,21	0.74	0
2	NAG	D	1017	1,2	14,14,15	0.52	0	15,19,21	0.71	0
2	NAG	D	1018	2	14,14,15	0.51	0	15,19,21	1.23	1 (6%)
2	NAG	D	1019	1,2	14,14,15	0.58	0	15,19,21	1.07	2 (13%)
2	NAG	D	1020	2	14,14,15	0.45	0	15,19,21	0.75	0
2	NAG	D	1021	1,2	14,14,15	0.61	0	15,19,21	1.24	2 (13%)
2	NAG	D	1022	2	14,14,15	0.50	0	15,19,21	1.13	2 (13%)
2	NAG	D	1023	1,2	14,14,15	0.48	0	15,19,21	0.67	0
2	NAG	D	1024	2	14,14,15	0.52	0	15,19,21	0.98	1 (6%)
2	NAG	D	1025	1	14,14,15	0.53	0	15,19,21	0.51	0
5	EDO	D	1027	-	3,3,3	0.44	0	2,2,2	0.40	0
5	EDO	D	1028	-	3,3,3	0.45	0	2,2,2	0.39	0
5	EDO	D	1029	-	3,3,3	0.44	0	2,2,2	0.35	0
5	EDO	D	1030	-	3,3,3	0.47	0	2,2,2	0.24	0
5	EDO	D	1031	-	3,3,3	0.48	0	2,2,2	0.29	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
2	NAG	A	1001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1002	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1003	3,2	-	0/2/19/22	0/1/1/1
3	BMA	A	1004	3	-	0/2/19/22	0/1/1/1
2	NAG	A	1005	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1006	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1007	3,2	-	0/2/19/22	0/1/1/1
3	BMA	A	1008	3	-	0/2/19/22	0/1/1/1
3	BMA	A	1009	3	-	0/2/19/22	0/1/1/1
2	NAG	A	1010	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1011	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1012	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1013	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1014	2	-	0/2/19/22	0/1/1/1
2	NAG	A	1015	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	1016	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	1017	2	-	0/6/23/26	0/1/1/1
2	NAG	A	1018	1,2	1/1/5/7	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1019	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	1020	3,2	-	0/2/19/22	1/1/1/1
3	BMA	A	1021	3	-	0/2/19/22	0/1/1/1
2	NAG	A	1022	1	-	0/6/23/26	0/1/1/1
5	EDO	A	1024	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1025	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1026	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1027	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1028	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1029	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1030	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1031	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1032	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1033	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1034	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1035	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1036	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1037	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1038	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1039	-	-	0/1/1/1	0/0/0/0
5	EDO	A	1040	-	-	0/1/1/1	0/0/0/0
2	NAG	B	1001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1002	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1003	3,2	-	0/2/19/22	0/1/1/1
3	BMA	B	1004	3	-	0/2/19/22	0/1/1/1
2	NAG	B	1005	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1006	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1007	3,2	-	0/2/19/22	0/1/1/1
3	BMA	B	1008	3	-	0/2/19/22	1/1/1/1
3	BMA	B	1009	3	-	0/2/19/22	1/1/1/1
2	NAG	B	1010	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1011	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1012	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1013	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1014	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1015	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	1016	2	-	0/2/19/22	0/1/1/1
2	NAG	B	1017	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	1018	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1019	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	1020	2	-	0/6/23/26	0/1/1/1
2	NAG	B	1021	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	1023	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1024	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1025	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1026	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1027	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1028	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1029	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1030	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1031	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1032	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1033	-	-	0/1/1/1	0/0/0/0
5	EDO	B	1034	-	-	0/1/1/1	0/0/0/0
2	NAG	C	1101	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1102	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	1103	3,2	-	0/2/19/22	0/1/1/1
3	BMA	C	1104	3	-	0/2/19/22	0/1/1/1
2	NAG	C	1105	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1106	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	1107	3,2	-	0/2/19/22	0/1/1/1
3	BMA	C	1108	3	-	0/2/19/22	0/1/1/1
3	BMA	C	1109	3	-	0/2/19/22	0/1/1/1
2	NAG	C	1110	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1111	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	1112	3,2	-	0/2/19/22	0/1/1/1
3	BMA	C	1113	3	-	0/2/19/22	0/1/1/1
2	NAG	C	1114	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1115	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	1116	2	-	0/2/19/22	0/1/1/1
2	NAG	C	1117	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	C	1118	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	C	1119	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1120	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	1121	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	1122	3,2	-	0/2/19/22	0/1/1/1
3	BMA	C	1123	3	-	0/2/19/22	0/1/1/1
3	BMA	C	1124	3	-	0/2/19/22	0/1/1/1
3	BMA	C	1125	3	-	0/2/19/22	0/1/1/1
2	NAG	C	1126	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	C	1127	2	-	0/6/23/26	0/1/1/1
2	NAG	C	1128	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	C	1129	3,2	-	0/6/23/26	0/1/1/1
3	BMA	C	1130	3,2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	C	1131	3	-	0/2/19/22	0/1/1/1
3	BMA	C	1132	3	-	0/2/19/22	0/1/1/1
3	BMA	C	1133	3	-	0/2/19/22	0/1/1/1
5	EDO	C	1135	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1136	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1137	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1138	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1139	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1140	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1141	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1142	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1143	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1144	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1145	-	-	0/1/1/1	0/0/0/0
5	EDO	C	1146	-	-	0/1/1/1	0/0/0/0
2	NAG	D	1001	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	1002	3,2	-	0/6/23/26	0/1/1/1
3	BMA	D	1003	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1004	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	1005	3,2	-	0/6/23/26	0/1/1/1
3	BMA	D	1006	3,2	-	0/2/19/22	0/1/1/1
3	BMA	D	1007	3	-	0/2/19/22	0/1/1/1
3	BMA	D	1008	3	-	0/2/19/22	0/1/1/1
3	BMA	D	1009	3	-	0/2/19/22	0/1/1/1
2	NAG	D	1010	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	1011	3,2	-	0/6/23/26	0/1/1/1
3	BMA	D	1012	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1013	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	1014	3,2	-	0/6/23/26	0/1/1/1
3	BMA	D	1015	2	-	0/2/19/22	0/1/1/1
2	NAG	D	1016	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1017	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	D	1018	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1019	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	1020	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1021	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	D	1022	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1023	1,2	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	D	1024	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1025	1	-	0/6/23/26	0/1/1/1
5	EDO	D	1027	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1028	-	-	0/1/1/1	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	D	1029	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1030	-	-	0/1/1/1	0/0/0/0
5	EDO	D	1031	-	-	0/1/1/1	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1004	BMA	O5-C1	-2.08	1.40	1.43

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1004	BMA	O5-C1-C2	-4.42	103.87	110.79
3	C	1123	BMA	O3-C3-C2	-4.23	102.32	110.02
2	C	1118	NAG	O5-C1-C2	-3.35	106.82	111.47
2	B	1018	NAG	O5-C1-C2	-2.88	107.46	111.47
3	B	1007	BMA	O5-C1-C2	-2.80	106.40	110.79

5 of 10 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1015	NAG	C1
2	B	1019	NAG	C1
2	C	1126	NAG	C1
2	C	1118	NAG	C1
2	C	1128	NAG	C1

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1023	NAG	C8-C7-N2-C2
2	C	1117	NAG	O7-C7-N2-C2
2	C	1117	NAG	C8-C7-N2-C2
2	D	1023	NAG	O7-C7-N2-C2

All (3) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1008	BMA	C1-C2-C3-C4-C5-O5
3	A	1020	BMA	C1-C2-C3-C4-C5-O5
3	B	1009	BMA	C1-C2-C3-C4-C5-O5

25 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1010	NAG	1	0
5	A	1028	EDO	2	0
5	A	1029	EDO	2	0
5	A	1032	EDO	1	0
5	A	1040	EDO	1	0
3	B	1003	BMA	1	0
3	B	1004	BMA	1	0
3	B	1008	BMA	1	0
2	B	1017	NAG	1	0
2	B	1018	NAG	1	0
5	B	1025	EDO	1	0
5	B	1027	EDO	3	0
5	B	1028	EDO	1	0
5	B	1031	EDO	1	0
5	B	1034	EDO	2	0
3	C	1103	BMA	1	0
3	C	1104	BMA	2	0
2	C	1110	NAG	1	0
2	C	1121	NAG	1	0
3	C	1122	BMA	1	0
3	C	1123	BMA	2	0
5	C	1141	EDO	1	0
5	C	1146	EDO	1	0
3	D	1006	BMA	1	0
3	D	1007	BMA	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	903/950 (95%)	-0.18	16 (1%) 69 63	31, 55, 87, 120	0
1	B	904/950 (95%)	-0.21	16 (1%) 69 63	31, 51, 83, 124	0
1	C	905/950 (95%)	-0.22	16 (1%) 69 63	34, 53, 85, 126	0
1	D	904/950 (95%)	-0.20	20 (2%) 62 56	33, 55, 85, 123	0
All	All	3616/3800 (95%)	-0.20	68 (1%) 67 61	31, 53, 85, 126	0

The worst 5 of 68 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	895	SER	6.8
1	A	63	THR	6.8
1	B	64	THR	6.7
1	C	894	GLY	6.7
1	D	894	GLY	6.5

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	EDO	C	1142	4/4	0.82	0.38	17.27	73,75,77,77	0
5	EDO	B	1030	4/4	0.55	0.40	15.18	69,70,71,71	0
5	EDO	A	1031	4/4	0.75	0.49	15.17	57,62,63,67	0
5	EDO	B	1028	4/4	0.91	0.27	13.77	54,55,56,57	0
5	EDO	B	1034	4/4	0.75	0.47	12.09	63,66,66,66	0
5	EDO	C	1136	4/4	0.88	0.31	11.76	67,67,68,71	0
5	EDO	B	1027	4/4	0.87	0.37	10.44	57,59,63,66	0
5	EDO	A	1026	4/4	0.91	0.25	9.65	81,82,82,83	0
5	EDO	A	1037	4/4	0.88	0.40	9.47	77,80,82,84	0
5	EDO	A	1034	4/4	0.82	0.39	9.45	65,69,69,70	0
5	EDO	B	1025	4/4	0.84	0.66	7.29	79,79,80,81	0
5	EDO	A	1024	4/4	0.92	0.20	6.93	71,71,72,73	0
5	EDO	A	1028	4/4	0.80	0.35	6.59	63,66,66,69	0
5	EDO	A	1027	4/4	0.90	0.26	6.14	73,73,75,75	0
5	EDO	A	1033	4/4	0.89	0.35	6.08	71,72,75,76	0
5	EDO	C	1146	4/4	0.77	0.27	5.98	72,73,74,74	0
5	EDO	D	1031	4/4	0.80	0.26	5.88	64,64,65,66	0
5	EDO	A	1030	4/4	0.83	0.36	5.81	73,76,77,78	0
2	NAG	C	1114	14/15	0.83	0.27	4.90	84,96,100,105	0
2	NAG	B	1012	14/15	0.69	0.30	4.46	92,102,108,113	0
2	NAG	A	1012	14/15	0.79	0.30	4.15	76,90,95,99	0
5	EDO	A	1035	4/4	0.73	0.34	4.00	90,90,91,92	0
5	EDO	C	1140	4/4	0.86	0.28	3.80	68,70,71,71	0
5	EDO	D	1027	4/4	0.97	0.20	3.62	69,69,70,71	0
2	NAG	C	1101	14/15	0.84	0.29	3.30	92,112,119,123	0
2	NAG	D	1019	14/15	0.92	0.20	3.02	73,75,79,88	0
2	NAG	C	1126	14/15	0.82	0.25	2.78	106,117,122,125	0
5	EDO	B	1033	4/4	0.91	0.22	2.58	69,69,69,70	0
2	NAG	B	1017	14/15	0.91	0.19	2.57	68,72,79,82	0
5	EDO	B	1026	4/4	0.89	0.24	2.38	67,68,68,68	0
2	NAG	D	1001	14/15	0.89	0.29	2.27	106,114,117,120	0
5	EDO	C	1145	4/4	0.91	0.27	2.14	58,58,60,62	0
5	EDO	A	1029	4/4	0.82	0.29	2.06	59,63,65,68	0
5	EDO	A	1032	4/4	0.79	0.23	2.05	61,62,64,64	0
5	EDO	B	1031	4/4	0.90	0.29	1.90	58,62,63,63	0
5	EDO	C	1143	4/4	0.93	0.26	1.89	65,68,69,71	0
5	EDO	C	1141	4/4	0.71	0.29	1.73	79,80,82,84	0
5	EDO	B	1032	4/4	0.94	0.16	1.69	81,81,82,82	0
5	EDO	D	1029	4/4	0.91	0.23	1.68	58,58,58,58	0
2	NAG	B	1010	14/15	0.87	0.27	1.64	81,100,109,109	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	C	1120	14/15	0.94	0.17	1.55	77,85,87,90	0
2	NAG	A	1018	14/15	0.71	0.25	1.45	86,97,102,106	0
2	NAG	A	1010	14/15	0.87	0.27	1.19	84,92,98,105	0
5	EDO	C	1139	4/4	0.95	0.20	1.09	62,63,64,66	0
2	NAG	B	1001	14/15	0.90	0.20	0.69	80,88,93,98	0
2	NAG	A	1001	14/15	0.96	0.19	0.68	59,65,69,76	0
5	EDO	C	1144	4/4	0.94	0.17	0.60	62,63,63,64	0
5	EDO	A	1039	4/4	0.91	0.20	0.56	81,82,82,83	0
5	EDO	A	1040	4/4	0.94	0.22	0.42	54,56,59,61	0
2	NAG	D	1011	14/15	0.93	0.23	0.34	90,93,100,100	0
2	NAG	A	1016	14/15	0.96	0.17	0.31	67,70,74,81	0
5	EDO	C	1135	4/4	0.92	0.17	0.13	67,69,71,71	0
2	NAG	A	1005	14/15	0.93	0.16	-0.10	49,55,60,61	0
2	NAG	D	1010	14/15	0.95	0.17	-0.14	67,78,79,85	0
2	NAG	C	1105	14/15	0.93	0.14	-0.15	58,61,64,66	0
2	NAG	C	1110	14/15	0.95	0.16	-0.17	67,76,81,86	0
5	EDO	D	1028	4/4	0.95	0.15	-0.37	61,62,64,65	0
2	NAG	B	1005	14/15	0.91	0.15	-0.45	58,59,67,68	0
2	NAG	D	1004	14/15	0.95	0.14	-0.83	59,63,65,65	0
4	ZN	D	1026	1/1	0.99	0.10	-2.29	43,43,43,43	0
4	ZN	C	1134	1/1	1.00	0.09	-2.80	41,41,41,41	0
4	ZN	A	1023	1/1	0.99	0.09	-3.24	43,43,43,43	0
4	ZN	B	1022	1/1	0.99	0.09	-5.34	42,42,42,42	0
3	BMA	B	1016	11/12	0.49	0.46	-	105,108,114,116	0
3	BMA	B	1007	11/12	0.49	0.28	-	94,96,102,106	0
3	BMA	C	1103	11/12	0.63	0.60	-	134,138,146,147	0
2	NAG	D	1005	14/15	0.95	0.28	-	61,70,74,80	0
2	NAG	A	1015	14/15	0.79	0.38	-	97,107,115,116	0
3	BMA	C	1104	11/12	0.72	0.70	-	146,150,152,153	0
2	NAG	A	1013	14/15	0.83	0.45	-	100,105,112,115	0
2	NAG	A	1019	14/15	0.83	0.47	-	109,114,120,122	0
2	NAG	D	1024	14/15	0.73	0.66	-	126,131,135,136	0
3	BMA	A	1007	11/12	0.85	0.27	-	85,92,98,102	0
3	BMA	B	1008	11/12	0.82	0.35	-	99,102,107,108	0
3	BMA	A	1021	11/12	0.63	0.64	-	120,125,128,129	0
2	NAG	D	1014	14/15	0.68	0.51	-	115,122,129,133	0
3	BMA	C	1125	11/12	0.70	0.54	-	122,126,128,129	0
5	EDO	A	1036	4/4	0.76	0.24	-	73,74,76,77	0
5	EDO	A	1038	4/4	0.76	0.30	-	72,73,75,77	0
2	NAG	B	1014	14/15	0.80	0.27	-	87,89,94,95	0
2	NAG	D	1018	14/15	0.55	0.79	-	148,153,158,158	0
2	NAG	C	1128	14/15	0.70	0.33	-	114,122,126,127	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	B	1020	14/15	0.65	0.53	-	118,123,130,132	0
2	NAG	D	1022	14/15	0.51	0.52	-	115,120,124,125	0
2	NAG	B	1006	14/15	0.90	0.28	-	67,70,79,85	0
3	BMA	D	1009	11/12	0.78	0.44	-	115,117,121,122	0
3	BMA	D	1015	11/12	0.54	0.60	-	138,142,145,148	0
2	NAG	D	1020	14/15	0.87	0.33	-	94,97,101,102	0
3	BMA	C	1130	11/12	0.70	0.38	-	138,144,148,148	0
2	NAG	D	1016	14/15	0.73	0.38	-	85,97,99,102	0
3	BMA	A	1020	11/12	0.78	0.58	-	126,128,132,134	0
2	NAG	B	1021	14/15	0.80	0.46	-	129,142,145,148	0
2	NAG	A	1011	14/15	0.71	0.51	-	110,115,121,122	0
5	EDO	C	1138	4/4	0.76	0.39	-	77,78,79,79	0
2	NAG	B	1015	14/15	0.81	0.48	-	95,99,103,103	0
2	NAG	A	1002	14/15	0.91	0.32	-	80,88,95,102	0
2	NAG	D	1013	14/15	0.79	0.29	-	81,95,105,112	0
2	NAG	C	1115	14/15	0.82	0.51	-	99,109,115,118	0
3	BMA	A	1004	11/12	0.78	0.36	-	100,107,109,110	0
2	NAG	B	1002	14/15	0.82	0.32	-	99,105,115,124	0
3	BMA	A	1008	11/12	0.67	0.47	-	103,109,113,115	0
2	NAG	B	1019	14/15	0.72	0.34	-	100,107,113,116	0
2	NAG	D	1025	14/15	0.72	0.49	-	134,144,148,151	0
5	EDO	B	1024	4/4	0.93	0.18	-	60,61,64,67	0
2	NAG	C	1117	14/15	0.85	0.34	-	94,100,106,107	0
2	NAG	C	1119	14/15	0.65	0.74	-	139,156,163,163	0
3	BMA	C	1109	11/12	0.88	0.42	-	95,103,106,108	0
5	EDO	B	1023	4/4	0.80	0.30	-	65,66,69,70	0
3	BMA	C	1131	11/12	0.72	0.25	-	134,143,145,146	0
3	BMA	C	1108	11/12	0.73	0.43	-	103,105,114,114	0
2	NAG	D	1017	14/15	0.74	0.44	-	131,138,145,147	0
3	BMA	B	1003	11/12	0.74	0.42	-	129,131,133,137	0
2	NAG	A	1017	14/15	0.83	0.37	-	87,94,99,101	0
3	BMA	D	1007	11/12	0.80	0.51	-	107,113,116,117	0
2	NAG	C	1127	14/15	0.79	0.47	-	123,127,133,135	0
3	BMA	A	1009	11/12	0.58	0.34	-	98,100,102,102	0
2	NAG	D	1023	14/15	0.75	0.38	-	128,131,133,134	0
2	NAG	C	1102	14/15	0.74	0.58	-	126,131,133,133	0
3	BMA	C	1132	11/12	0.59	0.56	-	133,143,147,148	0
2	NAG	B	1018	14/15	0.78	0.34	-	80,87,99,102	0
3	BMA	C	1116	11/12	0.38	0.56	-	123,126,129,132	0
2	NAG	C	1121	14/15	0.81	0.24	-	88,94,104,112	0
5	EDO	D	1030	4/4	0.76	0.36	-	65,68,71,72	0
3	BMA	C	1124	11/12	0.70	0.65	-	131,138,142,143	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	EDO	A	1025	4/4	0.89	0.35	-	63,65,67,68	0
3	BMA	C	1122	11/12	0.70	0.52	-	121,129,136,138	0
3	BMA	C	1133	11/12	0.66	0.44	-	138,141,145,145	0
3	BMA	C	1113	11/12	0.65	0.57	-	127,134,137,138	0
3	BMA	D	1012	11/12	0.76	0.43	-	103,107,110,113	0
3	BMA	A	1003	11/12	0.71	0.40	-	106,108,111,114	0
3	BMA	A	1014	11/12	0.47	0.57	-	120,127,130,133	0
2	NAG	A	1006	14/15	0.94	0.26	-	63,71,74,80	0
3	BMA	B	1009	11/12	0.44	0.47	-	104,108,110,111	0
5	EDO	C	1137	4/4	0.85	0.33	-	75,75,76,76	0
3	BMA	C	1123	11/12	0.64	0.67	-	138,140,141,142	0
3	BMA	C	1107	11/12	0.81	0.29	-	85,92,98,99	0
3	BMA	D	1008	11/12	0.90	0.32	-	104,106,109,112	0
3	BMA	D	1003	11/12	0.75	0.69	-	131,136,139,141	0
2	NAG	B	1011	14/15	0.85	0.45	-	112,116,121,122	0
2	NAG	C	1111	14/15	0.91	0.20	-	86,91,97,104	0
3	BMA	B	1004	11/12	0.65	0.42	-	132,138,143,143	0
2	NAG	A	1022	14/15	0.62	0.61	-	136,139,145,147	0
2	NAG	C	1118	14/15	0.60	0.58	-	149,151,153,156	0
3	BMA	D	1006	11/12	0.84	0.30	-	87,94,100,103	0
2	NAG	B	1013	14/15	0.75	0.55	-	108,121,126,126	0
5	EDO	B	1029	4/4	0.81	0.19	-	68,70,70,71	0
2	NAG	C	1129	14/15	0.86	0.50	-	124,128,135,135	0
2	NAG	D	1021	14/15	0.82	0.29	-	103,108,115,117	0
2	NAG	C	1106	14/15	0.95	0.27	-	59,64,72,78	0
3	BMA	C	1112	11/12	0.70	0.38	-	113,124,129,131	0
2	NAG	D	1002	14/15	0.76	0.47	-	121,128,134,134	0

6.5 Other polymers [i](#)

There are no such residues in this entry.