



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 04:30 PM GMT

PDB ID : 4F5C
Title : Crystal structure of the spike receptor binding domain of a porcine respiratory coronavirus in complex with the pig aminopeptidase N ectodomain
Authors : Santiago, C.; Reguera, J.; Gaurav, M.; Ordone, D.; Enjuanes, L.; Casasnovas, J.M.
Deposited on : 2012-05-13
Resolution : 3.20 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 (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

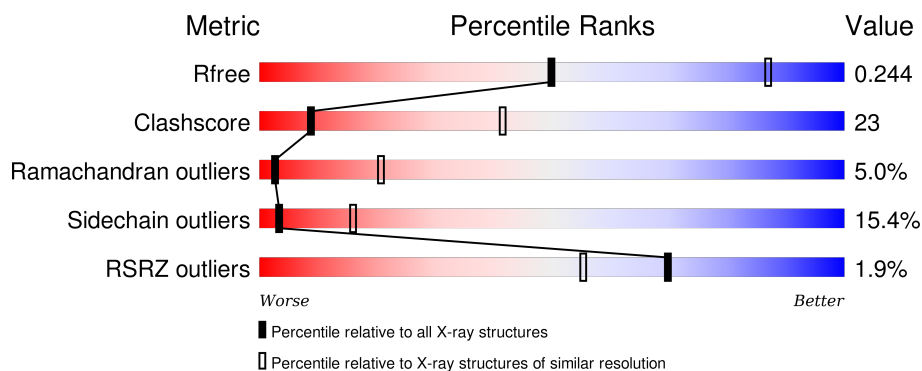
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	959	<div> <div>2%</div> <div>50% 33% 10% • 6%</div> </div>
1	B	959	<div> <div>2%</div> <div>52% 32% 10% • 6%</div> </div>
2	E	440	<div> <div>15% 12% 5% • 67%</div> </div>
2	F	440	<div> <div>2%</div> <div>15% 12% 5% 68%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17067 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	901	Total	C	N	O	S	0	0	0
			7245	4629	1208	1378	30			
1	B	900	Total	C	N	O	S	0	0	0
			7235	4623	1205	1377	30			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	TYR	-	EXPRESSION TAG	UNP P15145
A	20	PRO	-	EXPRESSION TAG	UNP P15145
A	21	TYR	-	EXPRESSION TAG	UNP P15145
A	22	ASP	-	EXPRESSION TAG	UNP P15145
A	23	VAL	-	EXPRESSION TAG	UNP P15145
A	24	PRO	-	EXPRESSION TAG	UNP P15145
A	25	ASP	-	EXPRESSION TAG	UNP P15145
A	26	TYR	-	EXPRESSION TAG	UNP P15145
A	27	ALA	-	EXPRESSION TAG	UNP P15145
A	28	GLY	-	EXPRESSION TAG	UNP P15145
A	29	ALA	-	EXPRESSION TAG	UNP P15145
A	30	GLN	-	EXPRESSION TAG	UNP P15145
A	31	PRO	-	EXPRESSION TAG	UNP P15145
A	32	ALA	-	EXPRESSION TAG	UNP P15145
A	33	ARG	-	EXPRESSION TAG	UNP P15145
A	34	SER	-	EXPRESSION TAG	UNP P15145
A	35	PRO	-	EXPRESSION TAG	UNP P15145
A	82	ASN	PHE	CONFLICT	UNP P15145
A	107	PHE	LEU	CONFLICT	UNP P15145
A	108	ILE	LEU	CONFLICT	UNP P15145
A	964	LEU	-	EXPRESSION TAG	UNP P15145
A	965	VAL	-	EXPRESSION TAG	UNP P15145
A	966	PRO	-	EXPRESSION TAG	UNP P15145
A	967	ARG	-	EXPRESSION TAG	UNP P15145
A	968	GLY	-	EXPRESSION TAG	UNP P15145

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Chain	Residue	Modelled	Actual	Comment	Reference
A	969	SER	-	EXPRESSION TAG	UNP P15145
A	970	ASP	-	EXPRESSION TAG	UNP P15145
A	971	TYR	-	EXPRESSION TAG	UNP P15145
A	972	LYS	-	EXPRESSION TAG	UNP P15145
A	973	ASP	-	EXPRESSION TAG	UNP P15145
A	974	ASP	-	EXPRESSION TAG	UNP P15145
A	975	ASP	-	EXPRESSION TAG	UNP P15145
A	976	ASP	-	EXPRESSION TAG	UNP P15145
A	977	LYS	-	EXPRESSION TAG	UNP P15145
B	19	TYR	-	EXPRESSION TAG	UNP P15145
B	20	PRO	-	EXPRESSION TAG	UNP P15145
B	21	TYR	-	EXPRESSION TAG	UNP P15145
B	22	ASP	-	EXPRESSION TAG	UNP P15145
B	23	VAL	-	EXPRESSION TAG	UNP P15145
B	24	PRO	-	EXPRESSION TAG	UNP P15145
B	25	ASP	-	EXPRESSION TAG	UNP P15145
B	26	TYR	-	EXPRESSION TAG	UNP P15145
B	27	ALA	-	EXPRESSION TAG	UNP P15145
B	28	GLY	-	EXPRESSION TAG	UNP P15145
B	29	ALA	-	EXPRESSION TAG	UNP P15145
B	30	GLN	-	EXPRESSION TAG	UNP P15145
B	31	PRO	-	EXPRESSION TAG	UNP P15145
B	32	ALA	-	EXPRESSION TAG	UNP P15145
B	33	ARG	-	EXPRESSION TAG	UNP P15145
B	34	SER	-	EXPRESSION TAG	UNP P15145
B	35	PRO	-	EXPRESSION TAG	UNP P15145
B	82	ASN	PHE	CONFLICT	UNP P15145
B	107	PHE	LEU	CONFLICT	UNP P15145
B	108	ILE	LEU	CONFLICT	UNP P15145
B	964	LEU	-	EXPRESSION TAG	UNP P15145
B	965	VAL	-	EXPRESSION TAG	UNP P15145
B	966	PRO	-	EXPRESSION TAG	UNP P15145
B	967	ARG	-	EXPRESSION TAG	UNP P15145
B	968	GLY	-	EXPRESSION TAG	UNP P15145
B	969	SER	-	EXPRESSION TAG	UNP P15145
B	970	ASP	-	EXPRESSION TAG	UNP P15145
B	971	TYR	-	EXPRESSION TAG	UNP P15145
B	972	LYS	-	EXPRESSION TAG	UNP P15145
B	973	ASP	-	EXPRESSION TAG	UNP P15145
B	974	ASP	-	EXPRESSION TAG	UNP P15145
B	975	ASP	-	EXPRESSION TAG	UNP P15145
B	976	ASP	-	EXPRESSION TAG	UNP P15145

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Chain	Residue	Modelled	Actual	Comment	Reference
B	977	LYS	-	EXPRESSION TAG	UNP P15145

- Molecule 2 is a protein called PRCV spike protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	146	Total	C	N	O	S	0	0	0
			1138	722	192	216	8			
2	F	139	Total	C	N	O	S	0	0	0
			1079	688	179	204	8			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	409	ASP	GLU	CONFLICT	UNP Q84852
E	427	LEU	-	EXPRESSION TAG	UNP Q84852
E	428	VAL	-	EXPRESSION TAG	UNP Q84852
E	429	PRO	-	EXPRESSION TAG	UNP Q84852
E	430	ARG	-	EXPRESSION TAG	UNP Q84852
E	431	GLY	-	EXPRESSION TAG	UNP Q84852
E	432	SER	-	EXPRESSION TAG	UNP Q84852
E	433	ASP	-	EXPRESSION TAG	UNP Q84852
E	434	TYR	-	EXPRESSION TAG	UNP Q84852
E	435	LYS	-	EXPRESSION TAG	UNP Q84852
E	436	ASP	-	EXPRESSION TAG	UNP Q84852
E	437	ASP	-	EXPRESSION TAG	UNP Q84852
E	438	ASP	-	EXPRESSION TAG	UNP Q84852
E	439	ASP	-	EXPRESSION TAG	UNP Q84852
E	440	LYS	-	EXPRESSION TAG	UNP Q84852
F	409	ASP	GLU	CONFLICT	UNP Q84852
F	427	LEU	-	EXPRESSION TAG	UNP Q84852
F	428	VAL	-	EXPRESSION TAG	UNP Q84852
F	429	PRO	-	EXPRESSION TAG	UNP Q84852
F	430	ARG	-	EXPRESSION TAG	UNP Q84852
F	431	GLY	-	EXPRESSION TAG	UNP Q84852
F	432	SER	-	EXPRESSION TAG	UNP Q84852
F	433	ASP	-	EXPRESSION TAG	UNP Q84852
F	434	TYR	-	EXPRESSION TAG	UNP Q84852
F	435	LYS	-	EXPRESSION TAG	UNP Q84852
F	436	ASP	-	EXPRESSION TAG	UNP Q84852
F	437	ASP	-	EXPRESSION TAG	UNP Q84852
F	438	ASP	-	EXPRESSION TAG	UNP Q84852
F	439	ASP	-	EXPRESSION TAG	UNP Q84852

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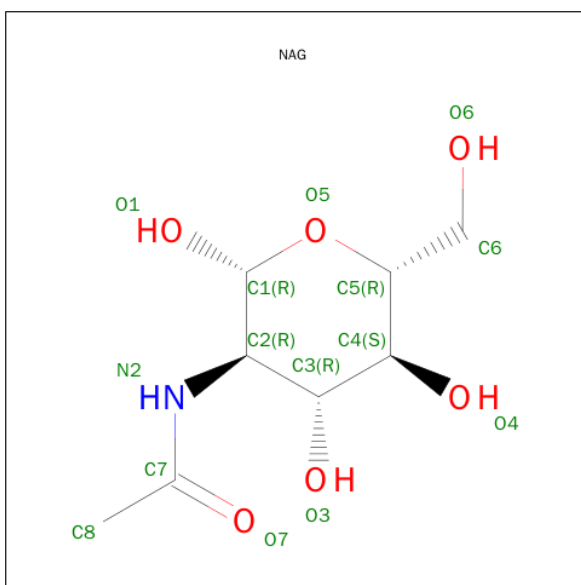
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Chain	Residue	Modelled	Actual	Comment	Reference
F	440	LYS	-	EXPRESSION TAG	UNP Q84852

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

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

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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		
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		
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		

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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		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

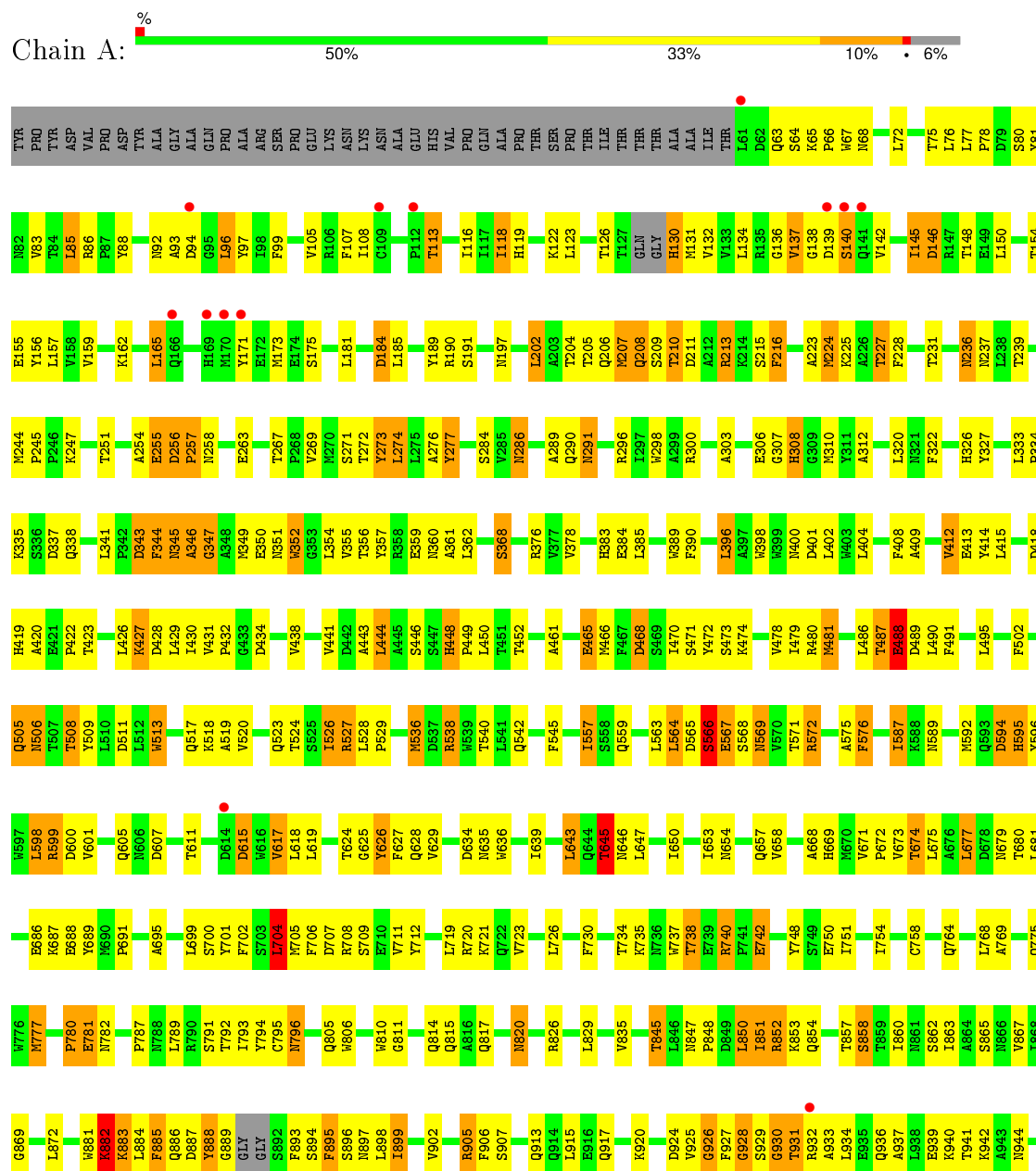
- Molecule 6 is water.

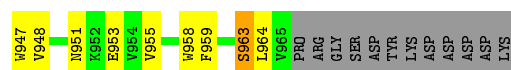
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total 2	O 2	0	0
6	B	2	Total 2	O 2	0	0

3 Residue-property plots

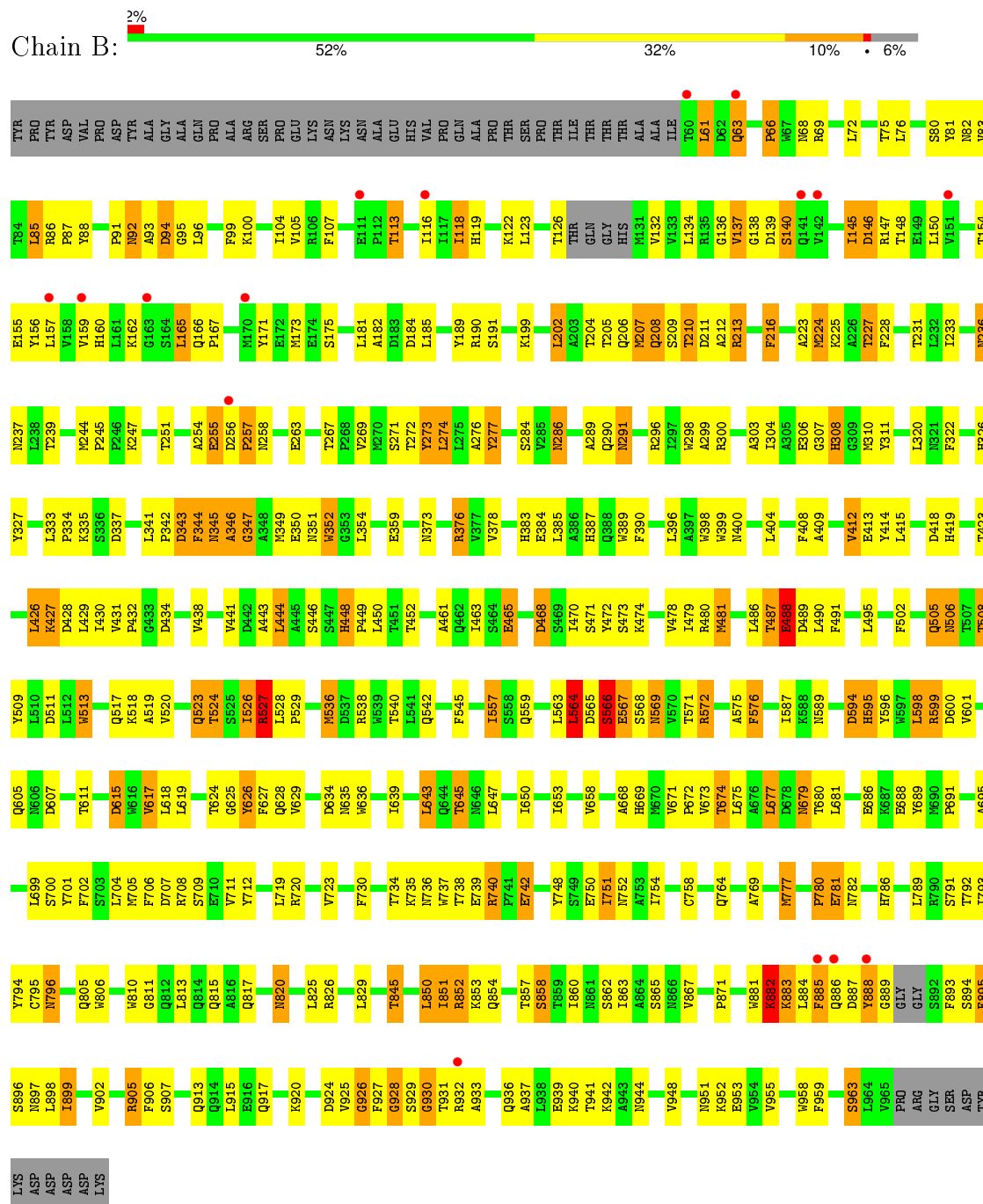
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

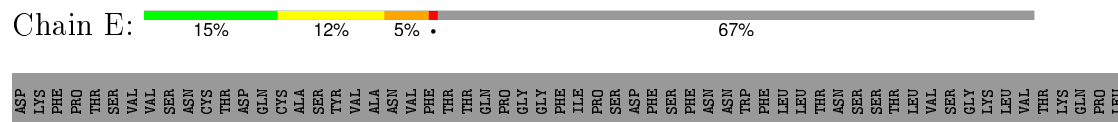




• Molecule 1: Aminopeptidase N



• Molecule 2: PRCV spike protein



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	220.86Å 87.94Å 176.91Å 90.00° 90.54° 90.00°	Depositor
Resolution (Å)	24.91 – 3.20 47.74 – 3.20	Depositor EDS
% Data completeness (in resolution range)	95.7 (24.91-3.20) 95.7 (47.74-3.20)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.201 , 0.245 0.202 , 0.244	Depositor DCC
R_{free} test set	2737 reflections (5.35%)	DCC
Wilson B-factor (Å ²)	85.3	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 68.3	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 54012 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17067	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.84% 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: 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	0.25	0/7431	0.56	13/10126 (0.1%)
1	B	0.25	0/7420	0.59	13/10111 (0.1%)
2	E	0.26	0/1160	0.52	1/1576 (0.1%)
2	F	0.23	0/1100	0.42	0/1494
All	All	0.25	0/17111	0.56	27/23307 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
2	E	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 27 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	527	ARG	NE-CZ-NH1	15.69	128.15	120.30
1	B	527	ARG	NE-CZ-NH2	-12.90	113.85	120.30
1	A	538	ARG	NE-CZ-NH1	-12.67	113.97	120.30
1	B	538	ARG	NE-CZ-NH2	-12.31	114.14	120.30
1	B	720	ARG	NE-CZ-NH1	-12.11	114.25	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	GLN	Peptide
1	B	208	GLN	Peptide
2	E	357	ASP	Peptide

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	7245	0	7006	328	0
1	B	7235	0	6998	319	2
2	E	1138	0	1126	80	2
2	F	1079	0	1065	70	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	126	0	117	0	0
4	B	154	0	143	7	0
5	A	28	0	25	0	0
5	E	28	0	25	0	0
5	F	28	0	25	0	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
All	All	17067	0	16530	788	2

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 23.

The worst 5 of 788 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)
2:E:324:THR:HG22	2:E:325:ASP:H	1.09	1.09
1:B:272:THR:O	1:B:274:LEU:N	1.87	1.07
1:A:272:THR:O	1:A:274:LEU:N	1.87	1.06
2:E:357:ASP:HB2	2:E:406:ARG:HH12	1.16	1.05
1:B:928:GLY:O	1:B:930:GLY:N	1.94	1.01

All (2) 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)
1:B:527:ARG:NH1	2:E:396:ASN:OD1[3_545]	1.91	0.29
1:B:527:ARG:NH1	2:E:396:ASN:CG[3_545]	2.05	0.15

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	895/959 (93%)	766 (86%)	84 (9%)	45 (5%)	3	21
1	B	894/959 (93%)	768 (86%)	82 (9%)	44 (5%)	3	22
2	E	142/440 (32%)	111 (78%)	22 (16%)	9 (6%)	2	13
2	F	133/440 (30%)	107 (80%)	20 (15%)	6 (4%)	3	24
All	All	2064/2798 (74%)	1752 (85%)	208 (10%)	104 (5%)	3	21

5 of 104 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	146	ASP
1	A	155	GLU
1	A	273	TYR
1	A	290	GLN
1	A	344	PHE

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	799/845 (95%)	682 (85%)	117 (15%)	4	19
1	B	798/845 (94%)	681 (85%)	117 (15%)	4	18
2	E	132/393 (34%)	104 (79%)	28 (21%)	1	7
2	F	125/393 (32%)	102 (82%)	23 (18%)	2	10
All	All	1854/2476 (75%)	1569 (85%)	285 (15%)	3	16

5 of 285 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	139	ASP
1	B	426	LEU
2	F	289	THR
1	B	184	ASP
1	B	273	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	951	ASN
1	B	951	ASN
1	B	640	GLN
1	A	679	ASN
1	B	679	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

6 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	$\# Z > 2$
5	NAG	A	1008	1,5	14,14,15	0.60	0	15,19,21	0.94	1 (6%)
5	NAG	A	1009	5	14,14,15	0.69	0	15,19,21	0.77	0
5	NAG	E	501	2,5	14,14,15	0.60	0	15,19,21	1.10	1 (6%)
5	NAG	E	502	5	14,14,15	0.47	0	15,19,21	1.17	1 (6%)
5	NAG	F	501	2,5	14,14,15	0.64	0	15,19,21	1.03	2 (13%)
5	NAG	F	502	5	14,14,15	0.45	0	15,19,21	1.15	1 (6%)

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	1008	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1009	5	-	0/6/23/26	0/1/1/1
5	NAG	E	501	2,5	-	0/6/23/26	0/1/1/1
5	NAG	E	502	5	-	0/6/23/26	0/1/1/1
5	NAG	F	501	2,5	-	0/6/23/26	0/1/1/1
5	NAG	F	502	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	501	NAG	C2-N2-C7	-2.09	120.35	123.04
5	A	1008	NAG	C4-C3-C2	2.28	114.77	111.23
5	F	501	NAG	C3-C4-C5	2.54	114.63	110.20
5	E	501	NAG	C3-C4-C5	2.99	115.41	110.20
5	F	502	NAG	C1-O5-C5	3.57	116.77	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry ⓘ

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 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	1002	1	14,14,15	0.51	0	15,19,21	0.74	0
4	NAG	A	1003	1	14,14,15	0.40	0	15,19,21	0.97	0
4	NAG	A	1004	1	14,14,15	0.46	0	15,19,21	1.33	1 (6%)
4	NAG	A	1005	1	14,14,15	0.49	0	15,19,21	0.89	1 (6%)
4	NAG	A	1006	1	14,14,15	0.50	0	15,19,21	0.56	0
4	NAG	A	1007	1	14,14,15	0.55	0	15,19,21	0.65	0
4	NAG	A	1010	1	14,14,15	0.48	0	15,19,21	0.92	1 (6%)
4	NAG	A	1011	1	14,14,15	0.52	0	15,19,21	0.85	0
4	NAG	A	1012	1	14,14,15	0.47	0	15,19,21	0.96	1 (6%)
4	NAG	B	1002	1	14,14,15	0.42	0	15,19,21	1.28	2 (13%)
4	NAG	B	1003	1	14,14,15	0.46	0	15,19,21	1.31	2 (13%)
4	NAG	B	1004	1	14,14,15	0.49	0	15,19,21	0.86	1 (6%)
4	NAG	B	1005	1	14,14,15	0.69	0	15,19,21	0.70	0
4	NAG	B	1006	1	14,14,15	0.55	0	15,19,21	0.56	0
4	NAG	B	1007	1	14,14,15	0.68	0	15,19,21	1.00	1 (6%)
4	NAG	B	1008	1	14,14,15	0.42	0	15,19,21	1.29	1 (6%)
4	NAG	B	1009	1	14,14,15	0.63	0	15,19,21	0.92	1 (6%)
4	NAG	B	1010	1	14,14,15	0.42	0	15,19,21	1.15	3 (20%)
4	NAG	B	1011	1	14,14,15	0.49	0	15,19,21	1.07	2 (13%)
4	NAG	B	1012	1	14,14,15	0.53	0	15,19,21	0.94	1 (6%)

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1003	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1004	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1005	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1006	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1007	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1010	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1011	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1012	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1002	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1003	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1004	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1005	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1006	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1007	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1008	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1009	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1010	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1011	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1012	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1003	NAG	C2-N2-C7	-2.83	119.41	123.04
4	B	1010	NAG	C2-N2-C7	-2.54	119.77	123.04
4	B	1011	NAG	C2-N2-C7	-2.53	119.78	123.04
4	B	1002	NAG	C2-N2-C7	-2.13	120.30	123.04
4	B	1012	NAG	C2-N2-C7	-2.13	120.30	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1008	NAG	2	0
4	B	1009	NAG	3	0
4	B	1011	NAG	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 ⓘ

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	901/959 (93%)	-0.05	13 (1%) 78 65	50, 84, 143, 186	0
1	B	900/959 (93%)	-0.05	16 (1%) 71 58	48, 86, 154, 203	0
2	E	146/440 (33%)	0.06	2 (1%) 78 65	66, 96, 148, 188	0
2	F	139/440 (31%)	0.62	8 (5%) 26 15	75, 127, 162, 185	0
All	All	2086/2798 (74%)	0.00	39 (1%) 70 55	48, 88, 153, 203	0

The worst 5 of 39 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	419	TYR	4.8
1	A	141	GLN	4.0
1	A	94	ASP	3.3
1	A	166	GLN	3.3
1	B	141	GLN	3.3

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

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

6.3 Carbohydrates ⓘ

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	NAG	E	501	14/15	0.95	0.31	0.29	88,117,142,149	0
5	NAG	F	501	14/15	0.94	0.32	-0.17	97,120,144,146	0
5	NAG	A	1008	14/15	0.93	0.19	-0.62	65,95,112,120	0
5	NAG	A	1009	14/15	0.89	0.23	-	104,125,171,174	0
5	NAG	F	502	14/15	0.85	0.39	-	144,150,156,159	0
5	NAG	E	502	14/15	0.87	0.23	-	126,140,146,149	0

6.4 Ligands ⓘ

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
4	NAG	B	1002	14/15	0.83	0.38	1.35	107,137,154,158	0
4	NAG	B	1008	14/15	0.89	0.26	1.26	73,97,115,119	0
4	NAG	A	1004	14/15	0.79	0.30	1.14	125,149,160,160	0
4	NAG	A	1007	14/15	0.87	0.23	1.09	92,117,143,146	0
4	NAG	B	1011	14/15	0.79	0.24	0.64	114,128,147,148	0
4	NAG	B	1007	14/15	0.83	0.26	0.34	90,99,133,141	0
4	NAG	A	1002	14/15	0.87	0.24	0.23	107,119,135,139	0
4	NAG	A	1012	14/15	0.87	0.22	0.08	58,80,99,100	0
3	ZN	B	1001	1/1	0.97	0.17	-0.23	83,83,83,83	0
4	NAG	A	1003	14/15	0.90	0.19	-0.34	51,79,92,96	0
4	NAG	B	1003	14/15	0.86	0.19	-0.50	75,88,102,106	0
4	NAG	A	1011	14/15	0.84	0.20	-0.71	84,95,117,134	0
3	ZN	A	1001	1/1	0.99	0.18	-0.76	75,75,75,75	0
4	NAG	B	1012	14/15	0.93	0.14	-1.41	74,87,113,124	0
4	NAG	B	1005	14/15	0.87	0.22	-	123,148,157,159	0
4	NAG	A	1010	14/15	0.91	0.17	-	106,121,131,137	0
4	NAG	B	1009	14/15	0.86	0.38	-	125,143,149,155	0
4	NAG	B	1010	14/15	0.87	0.28	-	127,145,159,164	0
4	NAG	B	1004	14/15	0.63	0.44	-	130,164,186,189	0
4	NAG	A	1005	14/15	0.87	0.22	-	135,142,162,163	0
4	NAG	A	1006	14/15	0.86	0.42	-	138,158,186,192	0
4	NAG	B	1006	14/15	0.93	0.25	-	117,129,135,140	0

6.5 Other polymers [i](#)

There are no such residues in this entry.