



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 09:51 AM 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 full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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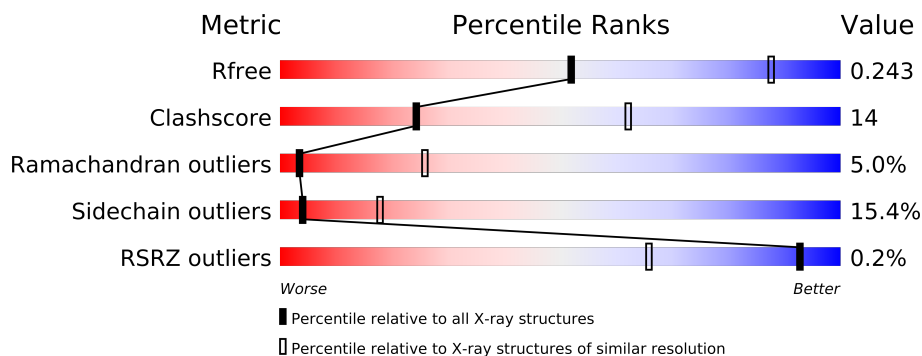
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	1824 (3.30-3.10)
Clashscore	79885	1078 (3.26-3.14)
Ramachandran outliers	78287	1059 (3.26-3.14)
Sidechain outliers	78261	1058 (3.26-3.14)
RSRZ outliers	66119	1825 (3.30-3.10)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	959	
1	B	959	
2	E	440	
2	F	440	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	NAG	A	1006	-	X
4	NAG	B	1009	-	X
4	NAG	B	1010	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17067 atoms, of which 0 are hydrogen and 0 are deuterium.

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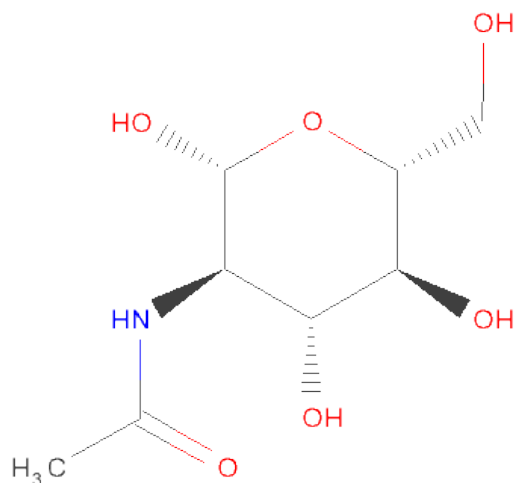
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Chain	Residue	Modelled	Actual	Comment	Reference
F	440	LYS	-	EXPRESSION TAG	UNP Q84852

- 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: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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		

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	TYR	-	EXPRESSION TAG	UNP P15145

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

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

- Molecule 6 is water.

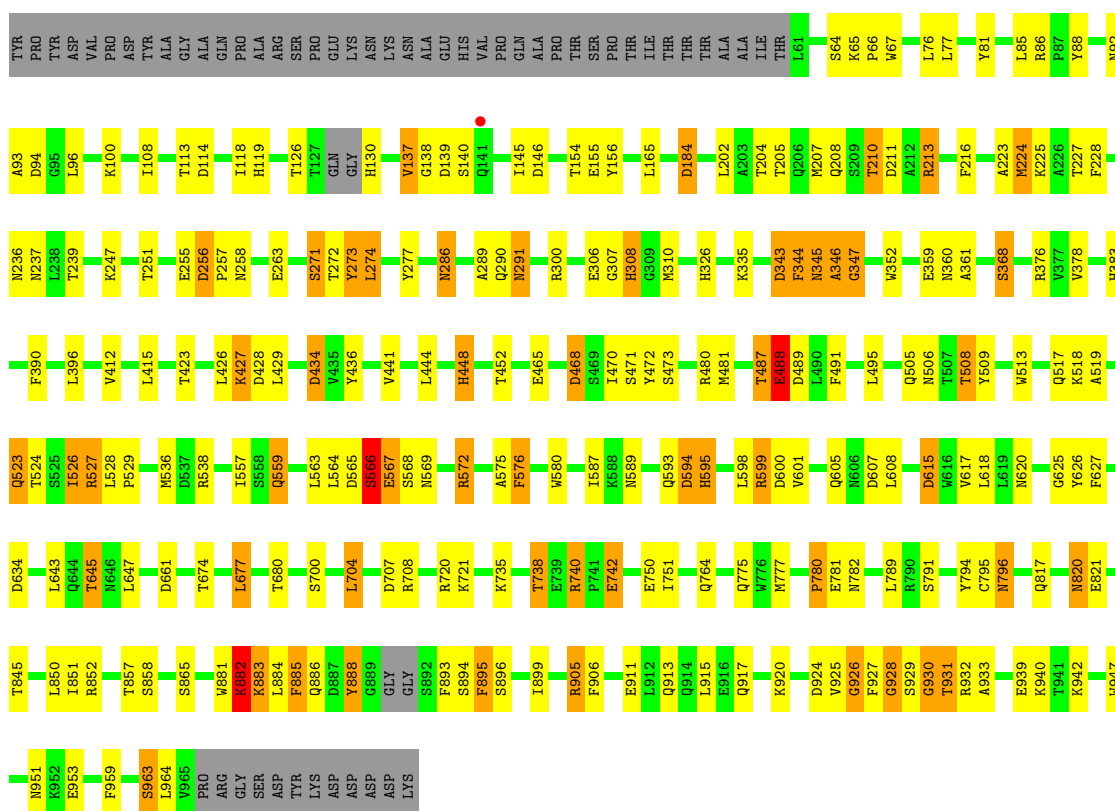
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total O 2 2	0	0
6	B	2	Total O 2 2	0	0

### 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.

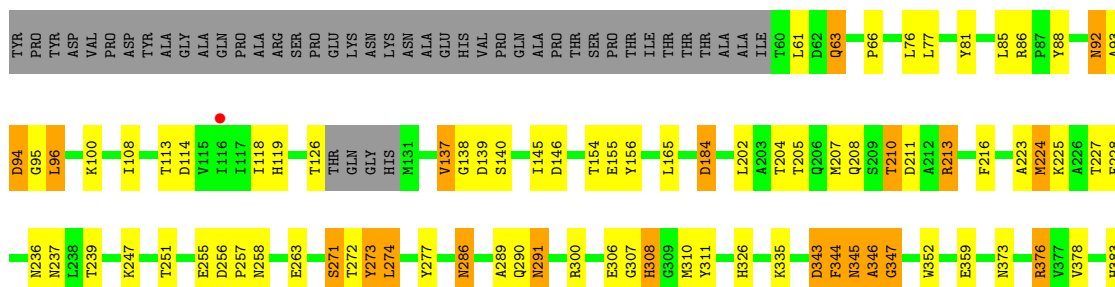
#### • Molecule 1: Aminopeptidase N

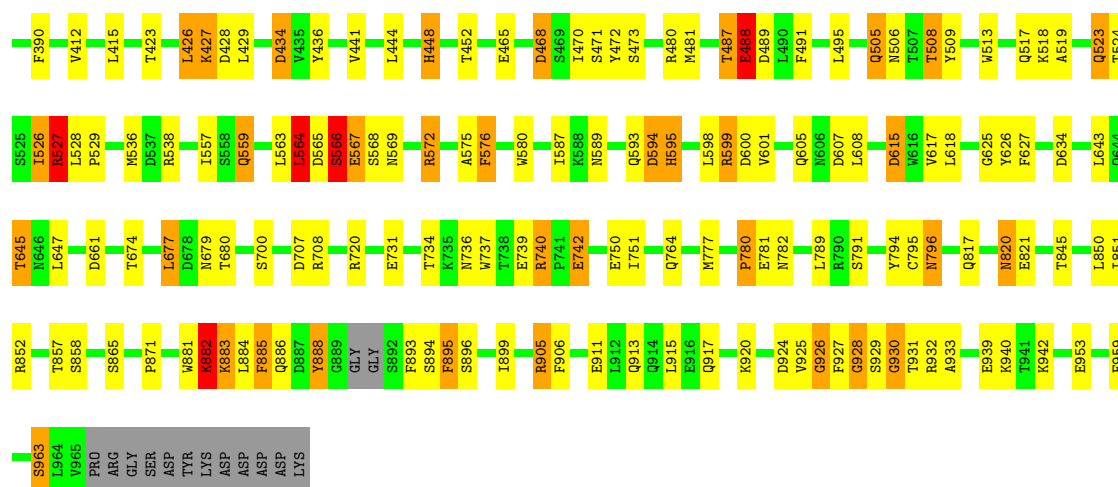
Chain A:



#### • Molecule 1: Aminopeptidase N

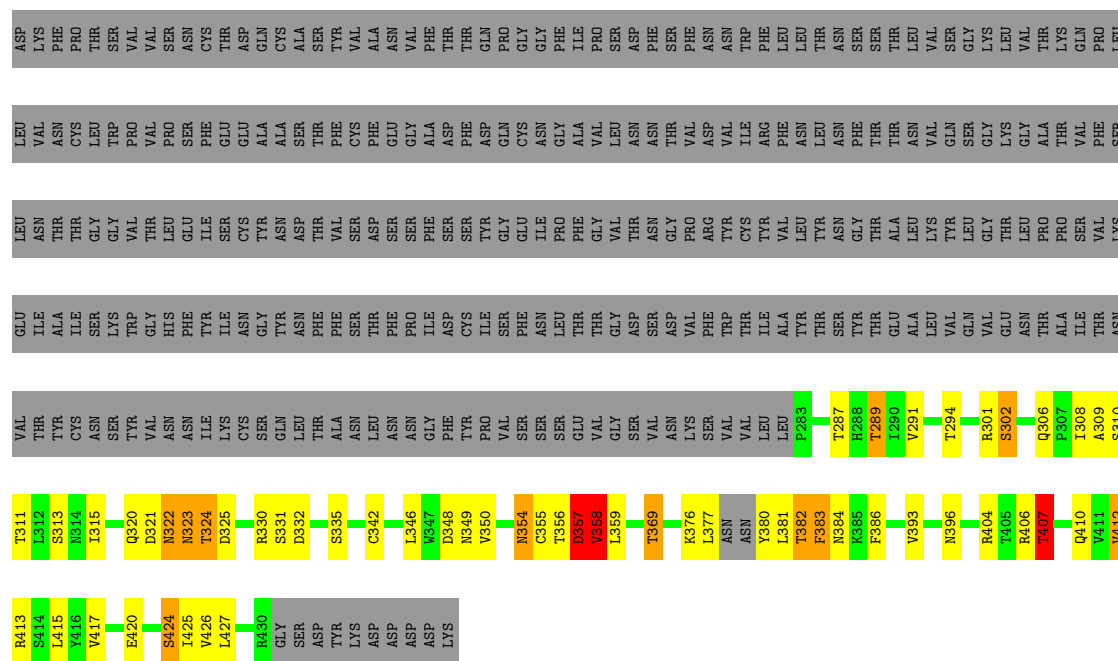
Chain B:





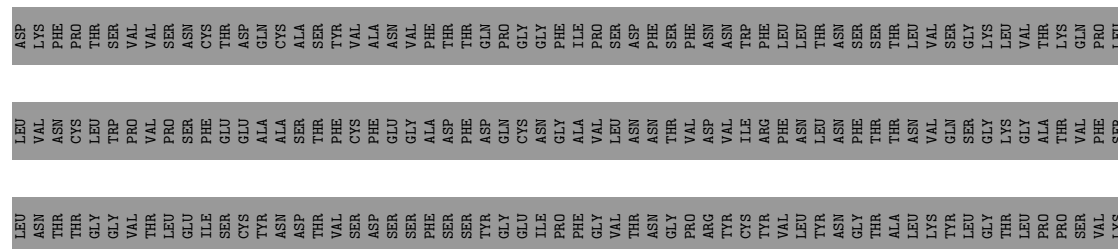
• Molecule 2: PRCV spike protein

Chain E:



• Molecule 2: PRCV spike protein

Chain F:



[illegible]

## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.201 , 0.245 0.201 , 0.243	Depositor DCC
$R_{free}$ test set	2737 reflections (5.08%)	DCC
Wilson B-factor (Å <sup>2</sup> )	85.3	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 55.0	EDS
Estimated twinning fraction	0.022 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, NAG

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.

All (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
1	B	376	ARG	NE-CZ-NH2	-11.88	114.36	120.30
1	B	720	ARG	NE-CZ-NH2	11.82	126.21	120.30
1	B	538	ARG	NE-CZ-NH1	11.71	126.16	120.30
1	A	538	ARG	NE-CZ-NH2	11.70	126.15	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	376	ARG	NE-CZ-NH1	11.58	126.09	120.30
1	A	376	ARG	NE-CZ-NH1	-11.56	114.52	120.30
1	A	720	ARG	NE-CZ-NH2	-11.28	114.66	120.30
1	A	376	ARG	NE-CZ-NH2	10.95	125.78	120.30
1	A	720	ARG	NE-CZ-NH1	10.57	125.59	120.30
1	A	527	ARG	NE-CZ-NH2	9.50	125.05	120.30
1	A	527	ARG	NE-CZ-NH1	-8.89	115.85	120.30
1	B	527	ARG	CD-NE-CZ	6.45	132.63	123.60
1	A	704	LEU	CA-CB-CG	6.41	130.04	115.30
1	B	538	ARG	CD-NE-CZ	6.24	132.34	123.60
1	A	538	ARG	CD-NE-CZ	5.97	131.96	123.60
1	B	720	ARG	CD-NE-CZ	5.83	131.76	123.60
1	B	376	ARG	CD-NE-CZ	5.82	131.75	123.60
1	A	376	ARG	CD-NE-CZ	5.68	131.56	123.60
1	A	720	ARG	CD-NE-CZ	5.62	131.47	123.60
2	E	357	ASP	N-CA-C	5.60	126.13	111.00
1	B	564	LEU	CA-CB-CG	5.57	128.10	115.30
1	A	527	ARG	CG-CD-NE	5.17	122.66	111.80

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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7245	0	0	96	0
1	B	7235	0	0	96	2
2	E	1138	0	0	27	2
2	F	1079	0	0	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	4	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	335	245	2

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 14.

All (245) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:272:THR:O	1:A:274:LEU:N	1.87	1.07
1:B:272:THR:O	1:B:274:LEU:N	1.87	1.07
1:B:928:GLY:O	1:B:930:GLY:N	1.94	1.01
1:A:928:GLY:O	1:A:930:GLY:N	1.94	0.99
2:F:357:ASP:O	2:F:406:ARG:NH2	2.02	0.91
2:F:341:THR:OG1	2:F:342:CYS:N	2.09	0.84
1:A:930:GLY:O	1:A:932:ARG:N	2.11	0.83
2:E:320:GLN:O	2:E:322:ASN:N	2.11	0.83
1:B:930:GLY:O	1:B:932:ARG:N	2.11	0.83
1:A:86:ARG:NH1	1:A:88:TYR:OH	2.11	0.83
1:B:707:ASP:OD2	1:B:905:ARG:NH1	2.14	0.81
1:B:505:GLN:OE1	4:B:1011:NAG:O6	1.99	0.81
1:B:426:LEU:O	1:B:428:ASP:N	2.15	0.80
1:A:426:LEU:O	1:A:428:ASP:N	2.14	0.80
1:A:707:ASP:OD2	1:A:905:ARG:NH1	2.15	0.79
2:E:384:ASN:OD1	2:E:424:SER:OG	2.01	0.79
2:E:322:ASN:CG	2:E:323:ASN:N	2.36	0.78
1:B:86:ARG:NH1	1:B:88:TYR:OH	2.16	0.78
2:F:283:PRO:O	2:F:285:PHE:N	2.19	0.76
1:B:959:PHE:O	1:B:963:SER:OG	2.06	0.74
1:A:306:GLU:O	1:A:308:HIS:N	2.22	0.73
1:B:306:GLU:O	1:B:308:HIS:N	2.22	0.73
1:A:959:PHE:O	1:A:963:SER:OG	2.07	0.72
1:A:326:HIS:O	1:A:326:HIS:ND1	2.23	0.72
1:B:326:HIS:ND1	1:B:326:HIS:O	2.22	0.72
2:F:384:ASN:OD1	2:F:424:SER:OG	2.09	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:735:LYS:O	1:A:738:THR:OG1	2.11	0.68
1:B:256:ASP:O	1:B:258:ASN:N	2.27	0.68
1:B:930:GLY:O	1:B:933:ALA:N	2.27	0.68
1:A:780:PRO:O	1:A:782:ASN:N	2.27	0.67
2:E:324:THR:CG2	2:E:325:ASP:N	2.57	0.67
1:B:780:PRO:O	1:B:782:ASN:N	2.28	0.67
1:A:930:GLY:O	1:A:933:ALA:N	2.28	0.67
1:B:599:ARG:O	1:B:601:VAL:N	2.27	0.67
1:A:300:ARG:NH2	1:A:359:GLU:OE1	2.28	0.66
1:A:599:ARG:O	1:A:601:VAL:N	2.28	0.66
1:B:210:THR:OG1	1:B:211:ASP:N	2.30	0.65
2:E:382:THR:C	2:E:383:PHE:CD1	2.70	0.65
1:A:775:GLN:OE1	2:E:301:ARG:NH1	2.30	0.64
1:A:92:ASN:CG	1:A:93:ALA:N	2.51	0.64
1:B:764:GLN:N	1:B:764:GLN:OE1	2.31	0.64
1:A:210:THR:OG1	1:A:211:ASP:N	2.30	0.64
2:E:309:ALA:N	2:E:410:GLN:OE1	2.30	0.63
1:A:740:ARG:NH1	1:A:750:GLU:OE2	2.31	0.63
1:A:154:THR:O	1:A:156:TYR:N	2.32	0.63
1:A:893:PHE:O	1:A:893:PHE:CD1	2.52	0.63
1:A:764:GLN:N	1:A:764:GLN:OE1	2.32	0.63
1:A:589:ASN:ND2	1:A:615:ASP:OD1	2.32	0.63
1:B:154:THR:O	1:B:156:TYR:N	2.31	0.63
2:E:322:ASN:OD1	2:E:323:ASN:N	2.31	0.62
2:F:300:LYS:NZ	2:F:349:ASN:OD1	2.31	0.62
1:B:589:ASN:ND2	1:B:615:ASP:OD1	2.33	0.62
1:A:256:ASP:O	1:A:258:ASN:N	2.33	0.62
1:B:289:ALA:O	1:B:291:ASN:N	2.32	0.62
2:E:380:TYR:O	2:E:380:TYR:CD2	2.53	0.62
1:B:820:ASN:N	1:B:820:ASN:OD1	2.33	0.61
2:E:383:PHE:CD1	2:E:383:PHE:N	2.65	0.61
1:B:92:ASN:O	1:B:95:GLY:N	2.33	0.61
1:B:300:ARG:NH2	1:B:359:GLU:OE1	2.33	0.61
1:A:565:ASP:O	1:A:567:GLU:N	2.33	0.61
1:A:820:ASN:N	1:A:820:ASN:OD1	2.34	0.61
1:A:289:ALA:O	1:A:291:ASN:N	2.34	0.60
1:B:734:THR:OG1	1:B:739:GLU:O	2.20	0.60
1:B:448:HIS:CB	1:B:572:ARG:NH1	2.64	0.60
1:A:247:LYS:N	1:A:263:GLU:O	2.35	0.60
1:B:565:ASP:O	1:B:567:GLU:N	2.34	0.59
1:B:247:LYS:N	1:B:263:GLU:O	2.34	0.59
1:B:742:GLU:N	1:B:742:GLU:CD	2.55	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:928:GLY:C	1:B:930:GLY:N	2.55	0.58
2:E:354:ASN:OD1	2:E:354:ASN:N	2.35	0.58
1:B:237:ASN:O	1:B:237:ASN:OD1	2.22	0.58
4:B:1008:NAG:O6	2:F:306:GLN:NE2	2.37	0.57
1:A:928:GLY:C	1:A:930:GLY:N	2.55	0.57
1:B:893:PHE:CD1	1:B:893:PHE:O	2.57	0.57
2:F:383:PHE:CE2	2:F:386:PHE:CD2	2.93	0.57
2:E:357:ASP:CB	2:E:406:ARG:NH1	2.69	0.56
1:A:448:HIS:CB	1:A:572:ARG:NH1	2.69	0.55
1:A:488:GLU:O	1:A:491:PHE:N	2.40	0.55
1:A:721:LYS:NZ	1:A:964:LEU:O	2.40	0.55
1:B:488:GLU:O	1:B:491:PHE:N	2.41	0.54
2:F:369:THR:OG1	2:F:369:THR:O	2.26	0.54
1:B:625:GLY:O	1:B:627:PHE:N	2.41	0.54
1:A:92:ASN:OD1	1:A:93:ALA:N	2.40	0.54
1:B:742:GLU:N	1:B:742:GLU:OE1	2.41	0.54
1:B:86:ARG:N	1:B:100:LYS:O	2.41	0.54
1:B:119:HIS:ND1	1:B:213:ARG:CZ	2.70	0.54
1:A:742:GLU:N	1:A:742:GLU:CD	2.61	0.53
1:B:677:LEU:O	1:B:680:THR:OG1	2.27	0.53
1:B:575:ALA:O	1:B:576:PHE:CB	2.57	0.53
1:B:559:GLN:OE1	1:B:580:TRP:N	2.42	0.53
1:A:119:HIS:ND1	1:A:213:ARG:CZ	2.72	0.53
1:A:559:GLN:OE1	1:A:580:TRP:N	2.42	0.53
1:A:426:LEU:O	1:A:429:LEU:N	2.43	0.52
1:B:346:ALA:O	1:B:347:GLY:C	2.48	0.52
2:F:302:SER:N	2:F:306:GLN:O	2.43	0.52
1:A:677:LEU:O	1:A:680:THR:OG1	2.28	0.52
1:A:65:LYS:O	1:A:67:TRP:N	2.42	0.52
1:A:625:GLY:O	1:A:627:PHE:N	2.43	0.52
1:B:780:PRO:C	1:B:782:ASN:N	2.64	0.51
1:B:708:ARG:NH2	1:B:911:GLU:OE1	2.44	0.51
2:F:283:PRO:C	2:F:285:PHE:N	2.62	0.51
1:A:780:PRO:C	1:A:782:ASN:N	2.64	0.51
2:E:348:ASP:O	2:E:350:VAL:N	2.44	0.51
2:F:301:ARG:NH2	2:F:357:ASP:OD1	2.44	0.50
1:B:426:LEU:O	1:B:429:LEU:N	2.44	0.50
2:E:383:PHE:CE2	2:E:386:PHE:CD2	2.99	0.50
1:A:925:VAL:O	1:A:926:GLY:O	2.29	0.50
1:B:885:PHE:CD2	1:B:895:PHE:CE2	2.98	0.50
1:A:184:ASP:OD1	1:A:184:ASP:N	2.44	0.50
1:A:708:ARG:NH2	1:A:911:GLU:OE1	2.45	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:575:ALA:O	1:A:576:PHE:CB	2.59	0.50
2:F:382:THR:O	2:F:383:PHE:CD1	2.65	0.49
1:A:272:THR:C	1:A:274:LEU:N	2.64	0.49
1:B:343:ASP:OD1	1:B:343:ASP:C	2.51	0.49
1:B:925:VAL:O	1:B:926:GLY:O	2.29	0.49
1:A:523:GLN:OE1	1:A:526:ILE:N	2.45	0.49
1:A:343:ASP:OD1	1:A:343:ASP:C	2.50	0.49
1:A:448:HIS:NE2	1:A:468:ASP:OD2	2.46	0.49
1:A:360:ASN:OD1	1:A:360:ASN:C	2.50	0.49
2:F:392:PRO:O	2:F:394:GLY:N	2.46	0.49
1:A:86:ARG:N	1:A:100:LYS:O	2.45	0.49
2:E:426:VAL:CG1	2:E:427:LEU:N	2.75	0.49
1:B:184:ASP:N	1:B:184:ASP:OD1	2.45	0.49
1:B:223:ALA:O	1:B:225:LYS:N	2.46	0.49
1:A:881:TRP:CZ2	1:A:927:PHE:CD1	3.01	0.49
1:A:346:ALA:O	1:A:347:GLY:C	2.51	0.49
1:B:204:THR:CG2	1:B:205:THR:N	2.76	0.49
2:E:383:PHE:CD2	2:E:386:PHE:CD2	3.00	0.48
1:A:426:LEU:O	1:A:427:LYS:C	2.52	0.48
1:A:517:GLN:O	1:A:519:ALA:N	2.46	0.48
1:B:888:TYR:CB	1:B:893:PHE:CE2	2.96	0.48
1:A:204:THR:CG2	1:A:205:THR:N	2.76	0.48
1:B:448:HIS:NE2	1:B:468:ASP:OD2	2.46	0.48
2:E:406:ARG:O	2:E:407:THR:CG2	2.62	0.48
1:B:237:ASN:C	1:B:237:ASN:OD1	2.51	0.48
1:A:77:LEU:O	1:A:108:ILE:N	2.47	0.48
1:A:888:TYR:CB	1:A:893:PHE:CE2	2.97	0.47
1:B:523:GLN:OE1	1:B:526:ILE:N	2.47	0.47
1:A:223:ALA:O	1:A:225:LYS:N	2.46	0.47
1:A:865:SER:O	1:A:905:ARG:NH2	2.47	0.47
2:F:289:THR:OG1	2:F:331:SER:OG	2.32	0.47
2:E:302:SER:N	2:E:306:GLN:O	2.48	0.47
1:B:426:LEU:O	1:B:427:LYS:C	2.52	0.47
1:B:865:SER:O	1:B:905:ARG:NH2	2.48	0.47
1:A:487:THR:O	1:A:488:GLU:C	2.53	0.47
1:A:885:PHE:CD2	1:A:895:PHE:CE2	3.02	0.47
1:A:857:THR:CG2	1:A:893:PHE:CE1	2.98	0.47
2:E:289:THR:OG1	2:E:331:SER:OG	2.33	0.47
2:F:354:ASN:OD1	2:F:354:ASN:N	2.48	0.47
1:B:517:GLN:O	1:B:519:ALA:N	2.48	0.47
2:F:356:THR:O	2:F:357:ASP:C	2.53	0.47
1:B:487:THR:O	1:B:488:GLU:C	2.53	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:373:ASN:OD1	1:B:376:ARG:NH2	2.48	0.46
1:A:383:HIS:C	1:A:383:HIS:CD2	2.89	0.46
1:A:436:TYR:OH	1:A:661:ASP:OD2	2.34	0.46
1:A:594:ASP:O	1:A:595:HIS:CB	2.63	0.46
2:E:369:THR:O	2:E:369:THR:OG1	2.34	0.46
1:B:885:PHE:CZ	1:B:927:PHE:O	2.69	0.46
2:F:341:THR:O	2:F:342:CYS:CB	2.62	0.46
2:E:357:ASP:C	2:E:359:LEU:N	2.69	0.46
1:B:92:ASN:O	1:B:94:ASP:N	2.48	0.46
1:A:742:GLU:OE1	1:A:742:GLU:N	2.49	0.46
2:F:288:HIS:C	2:F:288:HIS:CD2	2.88	0.46
1:B:594:ASP:O	1:B:595:HIS:CB	2.64	0.46
1:B:882:LYS:O	1:B:883:LYS:C	2.54	0.46
2:F:374:PHE:N	2:F:374:PHE:CD1	2.82	0.45
1:B:881:TRP:CZ2	1:B:927:PHE:CD1	3.04	0.45
1:B:448:HIS:CA	1:B:572:ARG:NH1	2.80	0.45
1:B:576:PHE:CD2	1:B:576:PHE:N	2.84	0.45
1:A:885:PHE:CZ	1:A:927:PHE:O	2.69	0.45
2:F:383:PHE:CD2	2:F:386:PHE:CD2	3.04	0.45
1:A:576:PHE:CD2	1:A:576:PHE:N	2.83	0.45
1:B:63:GLN:NE2	1:B:63:GLN:O	2.50	0.45
1:B:436:TYR:OH	1:B:661:ASP:OD2	2.35	0.45
1:A:565:ASP:O	1:A:566:SER:C	2.55	0.45
1:B:894:SER:O	1:B:896:SER:N	2.50	0.45
1:B:917:GLN:O	1:B:920:LYS:N	2.50	0.45
1:B:92:ASN:N	1:B:96:LEU:O	2.50	0.44
1:B:343:ASP:O	1:B:344:PHE:C	2.55	0.44
1:A:237:ASN:OD1	1:A:237:ASN:C	2.55	0.44
1:A:882:LYS:O	1:A:883:LYS:C	2.55	0.44
1:A:917:GLN:O	1:A:920:LYS:N	2.50	0.44
1:A:343:ASP:O	1:A:344:PHE:C	2.55	0.44
1:B:888:TYR:CD1	1:B:893:PHE:CE2	3.05	0.44
1:B:731:GLU:OE2	2:F:304:TYR:OH	2.34	0.44
1:B:740:ARG:NH1	1:B:750:GLU:OE2	2.50	0.44
1:B:272:THR:C	1:B:274:LEU:N	2.64	0.44
1:A:360:ASN:OD1	1:A:361:ALA:N	2.51	0.44
1:A:81:TYR:CD1	1:A:228:PHE:CE1	3.05	0.44
1:B:565:ASP:O	1:B:566:SER:C	2.56	0.43
1:B:383:HIS:CD2	1:B:383:HIS:C	2.91	0.43
2:F:295:ILE:CD1	2:F:363:ALA:CB	2.96	0.43
2:F:301:ARG:NH2	2:F:357:ASP:OD2	2.52	0.43
1:A:470:ILE:C	1:A:472:TYR:N	2.72	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:517:GLN:C	1:A:519:ALA:N	2.71	0.43
2:F:382:THR:C	2:F:383:PHE:CD1	2.91	0.43
2:E:406:ARG:O	2:E:407:THR:CB	2.67	0.43
1:B:434:ASP:OD2	1:B:473:SER:OG	2.37	0.43
1:A:271:SER:O	1:A:272:THR:OG1	2.36	0.43
1:A:930:GLY:O	1:A:931:THR:C	2.57	0.43
1:B:857:THR:CG2	1:B:893:PHE:CE1	3.01	0.43
1:A:593:GLN:NE2	1:A:608:LEU:O	2.52	0.43
1:B:286:ASN:O	1:B:286:ASN:ND2	2.52	0.43
1:A:740:ARG:NH1	1:A:750:GLU:CD	2.72	0.43
1:B:63:GLN:CD	1:B:63:GLN:N	2.72	0.43
2:E:357:ASP:O	2:E:358:VAL:CG1	2.66	0.43
1:B:564:LEU:N	1:B:564:LEU:CD2	2.82	0.43
2:E:287:THR:N	2:E:332:ASP:OD2	2.52	0.42
1:B:794:TYR:OH	1:B:821:GLU:OE2	2.38	0.42
1:B:271:SER:O	1:B:272:THR:OG1	2.37	0.42
1:A:256:ASP:C	1:A:258:ASN:N	2.72	0.42
1:B:593:GLN:NE2	1:B:608:LEU:O	2.52	0.42
1:A:434:ASP:OD2	1:A:473:SER:OG	2.37	0.42
4:B:1008:NAG:H2	4:B:1008:NAG:H83	1.86	0.42
1:B:736:ASN:C	1:B:737:TRP:CD1	2.93	0.42
1:A:894:SER:O	1:A:896:SER:N	2.53	0.42
1:B:707:ASP:CG	1:B:905:ARG:NH1	2.73	0.42
1:B:470:ILE:C	1:B:472:TYR:N	2.72	0.42
1:A:286:ASN:ND2	1:A:286:ASN:O	2.53	0.42
1:A:470:ILE:O	1:A:472:TYR:N	2.53	0.41
1:B:508:THR:OG1	1:B:509:TYR:N	2.53	0.41
1:A:707:ASP:CG	1:A:905:ARG:NH1	2.72	0.41
2:E:381:LEU:CB	2:E:383:PHE:CE1	3.03	0.41
1:A:448:HIS:CA	1:A:572:ARG:NH1	2.84	0.41
1:B:517:GLN:C	1:B:519:ALA:N	2.71	0.41
1:A:508:THR:OG1	1:A:509:TYR:N	2.53	0.41
1:A:794:TYR:OH	1:A:821:GLU:OE2	2.38	0.41
1:A:620:ASN:ND2	1:A:625:GLY:O	2.53	0.41
2:E:393:VAL:O	2:E:393:VAL:CG2	2.68	0.41
1:B:906:PHE:CD1	1:B:906:PHE:N	2.87	0.41
1:B:81:TYR:CD1	1:B:228:PHE:CE1	3.08	0.41
1:B:311:TYR:CD1	4:B:1009:NAG:O7	2.74	0.41
2:E:310:SER:O	2:E:412:VAL:CG1	2.68	0.41
2:F:357:ASP:C	2:F:406:ARG:NH2	2.71	0.41
1:A:114:ASP:OD1	1:A:114:ASP:N	2.54	0.41
1:B:114:ASP:N	1:B:114:ASP:OD1	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:906:PHE:N	1:A:906:PHE:CD1	2.87	0.41
2:F:283:PRO:CA	2:F:286:LEU:O	2.69	0.41
1:B:77:LEU:O	1:B:108:ILE:N	2.53	0.41
1:B:470:ILE:O	1:B:472:TYR:N	2.54	0.40
1:A:794:TYR:O	1:A:796:ASN:N	2.54	0.40
1:A:947:TRP:O	1:A:951:ASN:ND2	2.54	0.40
1:B:794:TYR:O	1:B:796:ASN:N	2.53	0.40
2:F:357:ASP:CG	2:F:358:VAL:N	2.74	0.40
1:A:888:TYR:CD1	1:A:893:PHE:CE2	3.09	0.40

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	Distance(Å)	Clash(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

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	895/959 (93%)	766 (86%)	84 (9%)	45 (5%)	3	26
1	B	894/959 (93%)	768 (86%)	82 (9%)	44 (5%)	3	26
2	E	142/440 (32%)	111 (78%)	22 (16%)	9 (6%)	2	18
2	F	133/440 (30%)	107 (80%)	20 (15%)	6 (4%)	4	29
All	All	2064/2798 (74%)	1752 (85%)	208 (10%)	104 (5%)	3	26

All (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

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Mol	Chain	Res	Type
1	A	344	PHE
1	A	427	LYS
1	A	488	GLU
1	A	566	SER
1	A	595	HIS
1	A	781	GLU
1	A	884	LEU
1	A	929	SER
1	A	931	THR
1	B	146	ASP
1	B	155	GLU
1	B	273	TYR
1	B	290	GLN
1	B	344	PHE
1	B	427	LYS
1	B	488	GLU
1	B	566	SER
1	B	781	GLU
1	B	884	LEU
1	B	929	SER
1	B	931	THR
2	E	321	ASP
2	E	324	THR
2	E	349	ASN
2	E	356	THR
2	E	358	VAL
2	F	284	SER
2	F	342	CYS
2	F	357	ASP
2	F	393	VAL
1	A	137	VAL
1	A	138	GLY
1	A	307	GLY
1	A	345	ASN
1	A	347	GLY
1	A	368	SER
1	A	487	THR
1	A	518	LYS
1	A	600	ASP
1	A	645	THR
1	A	882	LYS
1	A	888	TYR

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Mol	Chain	Res	Type
1	A	895	PHE
1	A	926	GLY
1	A	930	GLY
1	B	93	ALA
1	B	137	VAL
1	B	138	GLY
1	B	307	GLY
1	B	345	ASN
1	B	347	GLY
1	B	471	SER
1	B	487	THR
1	B	518	LYS
1	B	595	HIS
1	B	600	ASP
1	B	645	THR
1	B	882	LYS
1	B	888	TYR
1	B	895	PHE
1	B	926	GLY
1	B	930	GLY
2	E	322	ASN
2	E	407	THR
1	A	64	SER
1	A	224	MET
1	A	257	PRO
1	A	291	ASN
1	A	471	SER
1	A	529	PRO
1	A	626	TYR
1	A	795	CYS
1	B	224	MET
1	B	257	PRO
1	B	291	ASN
1	B	346	ALA
1	B	529	PRO
1	B	795	CYS
2	E	342	CYS
1	A	346	ALA
1	A	489	ASP
1	A	780	PRO
1	A	928	GLY
1	B	210	THR

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Mol	Chain	Res	Type
1	B	489	ASP
1	B	572	ARG
1	B	626	TYR
1	B	780	PRO
1	B	883	LYS
2	F	285	PHE
2	F	395	ALA
1	A	66	PRO
1	A	210	THR
1	A	572	ARG
1	A	576	PHE
1	A	883	LYS
1	B	576	PHE
1	B	928	GLY
2	E	355	CYS
1	B	66	PRO

### 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	799/845 (95%)	682 (85%)	117 (15%)	5	21
1	B	798/845 (94%)	681 (85%)	117 (15%)	4	21
2	E	132/393 (34%)	104 (79%)	28 (21%)	1	8
2	F	125/393 (32%)	102 (82%)	23 (18%)	2	11
All	All	1854/2476 (75%)	1569 (85%)	285 (15%)	4	18

All (285) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	LEU
1	A	85	LEU
1	A	94	ASP
1	A	96	LEU
1	A	113	THR
1	A	118	ILE

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Mol	Chain	Res	Type
1	A	126	THR
1	A	130	HIS
1	A	137	VAL
1	A	139	ASP
1	A	140	SER
1	A	145	ILE
1	A	165	LEU
1	A	184	ASP
1	A	202	LEU
1	A	207	MET
1	A	213	ARG
1	A	216	PHE
1	A	224	MET
1	A	227	THR
1	A	236	ASN
1	A	239	THR
1	A	251	THR
1	A	255	GLU
1	A	256	ASP
1	A	271	SER
1	A	273	TYR
1	A	274	LEU
1	A	277	TYR
1	A	286	ASN
1	A	308	HIS
1	A	310	MET
1	A	335	LYS
1	A	343	ASP
1	A	345	ASN
1	A	352	TRP
1	A	368	SER
1	A	378	VAL
1	A	390	PHE
1	A	396	LEU
1	A	412	VAL
1	A	415	LEU
1	A	423	THR
1	A	434	ASP
1	A	441	VAL
1	A	444	LEU
1	A	448	HIS
1	A	452	THR

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Mol	Chain	Res	Type
1	A	465	GLU
1	A	468	ASP
1	A	480	ARG
1	A	481	MET
1	A	488	GLU
1	A	495	LEU
1	A	505	GLN
1	A	506	ASN
1	A	508	THR
1	A	513	TRP
1	A	523	GLN
1	A	524	THR
1	A	526	ILE
1	A	527	ARG
1	A	528	LEU
1	A	536	MET
1	A	557	ILE
1	A	559	GLN
1	A	563	LEU
1	A	564	LEU
1	A	566	SER
1	A	567	GLU
1	A	568	SER
1	A	569	ASN
1	A	587	ILE
1	A	594	ASP
1	A	598	LEU
1	A	599	ARG
1	A	605	GLN
1	A	607	ASP
1	A	615	ASP
1	A	617	VAL
1	A	618	LEU
1	A	634	ASP
1	A	643	LEU
1	A	645	THR
1	A	647	LEU
1	A	674	THR
1	A	677	LEU
1	A	700	SER
1	A	704	LEU
1	A	738	THR

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Mol	Chain	Res	Type
1	A	740	ARG
1	A	742	GLU
1	A	751	ILE
1	A	777	MET
1	A	789	LEU
1	A	791	SER
1	A	796	ASN
1	A	817	GLN
1	A	820	ASN
1	A	845	THR
1	A	850	LEU
1	A	851	ILE
1	A	852	ARG
1	A	858	SER
1	A	882	LYS
1	A	885	PHE
1	A	886	GLN
1	A	899	ILE
1	A	905	ARG
1	A	913	GLN
1	A	915	LEU
1	A	924	ASP
1	A	939	GLU
1	A	940	LYS
1	A	942	LYS
1	A	953	GLU
1	A	963	SER
1	B	61	LEU
1	B	63	GLN
1	B	76	LEU
1	B	85	LEU
1	B	92	ASN
1	B	94	ASP
1	B	96	LEU
1	B	113	THR
1	B	118	ILE
1	B	126	THR
1	B	137	VAL
1	B	139	ASP
1	B	140	SER
1	B	145	ILE
1	B	165	LEU

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Mol	Chain	Res	Type
1	B	184	ASP
1	B	202	LEU
1	B	207	MET
1	B	213	ARG
1	B	216	PHE
1	B	224	MET
1	B	227	THR
1	B	236	ASN
1	B	239	THR
1	B	251	THR
1	B	255	GLU
1	B	271	SER
1	B	273	TYR
1	B	274	LEU
1	B	277	TYR
1	B	286	ASN
1	B	308	HIS
1	B	310	MET
1	B	335	LYS
1	B	343	ASP
1	B	345	ASN
1	B	352	TRP
1	B	378	VAL
1	B	390	PHE
1	B	412	VAL
1	B	415	LEU
1	B	423	THR
1	B	426	LEU
1	B	434	ASP
1	B	441	VAL
1	B	444	LEU
1	B	448	HIS
1	B	452	THR
1	B	465	GLU
1	B	468	ASP
1	B	480	ARG
1	B	481	MET
1	B	488	GLU
1	B	495	LEU
1	B	505	GLN
1	B	506	ASN
1	B	508	THR

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Mol	Chain	Res	Type
1	B	513	TRP
1	B	523	GLN
1	B	524	THR
1	B	526	ILE
1	B	527	ARG
1	B	528	LEU
1	B	536	MET
1	B	557	ILE
1	B	559	GLN
1	B	563	LEU
1	B	564	LEU
1	B	566	SER
1	B	567	GLU
1	B	568	SER
1	B	569	ASN
1	B	587	ILE
1	B	594	ASP
1	B	598	LEU
1	B	599	ARG
1	B	605	GLN
1	B	607	ASP
1	B	615	ASP
1	B	617	VAL
1	B	618	LEU
1	B	634	ASP
1	B	643	LEU
1	B	645	THR
1	B	647	LEU
1	B	674	THR
1	B	677	LEU
1	B	679	ASN
1	B	700	SER
1	B	740	ARG
1	B	742	GLU
1	B	751	ILE
1	B	777	MET
1	B	789	LEU
1	B	791	SER
1	B	796	ASN
1	B	817	GLN
1	B	820	ASN
1	B	845	THR

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Mol	Chain	Res	Type
1	B	850	LEU
1	B	851	ILE
1	B	852	ARG
1	B	858	SER
1	B	871	PRO
1	B	882	LYS
1	B	885	PHE
1	B	886	GLN
1	B	899	ILE
1	B	905	ARG
1	B	913	GLN
1	B	915	LEU
1	B	924	ASP
1	B	939	GLU
1	B	940	LYS
1	B	942	LYS
1	B	953	GLU
1	B	963	SER
2	E	289	THR
2	E	291	VAL
2	E	294	THR
2	E	302	SER
2	E	308	ILE
2	E	311	THR
2	E	313	SER
2	E	315	ILE
2	E	323	ASN
2	E	330	ARG
2	E	335	SER
2	E	346	LEU
2	E	354	ASN
2	E	358	VAL
2	E	369	THR
2	E	376	LYS
2	E	377	LEU
2	E	382	THR
2	E	383	PHE
2	E	404	ARG
2	E	407	THR
2	E	412	VAL
2	E	413	ARG
2	E	415	LEU

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Mol	Chain	Res	Type
2	E	417	VAL
2	E	420	GLU
2	E	424	SER
2	E	425	ILE
2	F	286	LEU
2	F	289	THR
2	F	291	VAL
2	F	294	THR
2	F	308	ILE
2	F	311	THR
2	F	313	SER
2	F	315	ILE
2	F	335	SER
2	F	341	THR
2	F	346	LEU
2	F	354	ASN
2	F	367	THR
2	F	369	THR
2	F	404	ARG
2	F	405	THR
2	F	406	ARG
2	F	412	VAL
2	F	413	ARG
2	F	415	LEU
2	F	417	VAL
2	F	420	GLU
2	F	424	SER

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 chains 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	12,14,15	0.79	1 (8%)	15,19,21	1.34	3 (20%)
5	NAG	A	1009	5	12,14,15	0.79	1 (8%)	15,19,21	1.15	2 (13%)
5	NAG	E	501	2,5	12,14,15	0.73	0	15,19,21	1.22	2 (13%)
5	NAG	E	502	5	12,14,15	0.62	0	15,19,21	0.64	0
5	NAG	F	501	2,5	12,14,15	0.78	1 (8%)	15,19,21	1.12	1 (6%)
5	NAG	F	502	5	12,14,15	0.60	0	15,19,21	0.76	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
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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1008	NAG	O5-C5	-2.34	1.41	1.45
5	F	501	NAG	O5-C5	-2.15	1.41	1.45
5	A	1009	NAG	O5-C5	-2.10	1.41	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1008	NAG	O5-C5-C6	3.15	110.29	106.98
5	E	501	NAG	C3-C4-C5	2.92	115.41	110.20
5	A	1009	NAG	O5-C5-C4	-2.72	107.20	110.65
5	A	1008	NAG	O5-C5-C4	-2.52	107.45	110.65
5	F	501	NAG	C3-C4-C5	2.48	114.63	110.20
5	A	1009	NAG	C3-C2-N2	-2.41	108.09	111.76
5	E	501	NAG	O5-C5-C4	2.23	113.49	110.65
5	A	1008	NAG	C3-C2-N2	-2.20	108.42	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	12,14,15	0.68	0	15,19,21	1.32	2 (13%)
4	NAG	A	1003	1	12,14,15	0.54	0	15,19,21	0.99	1 (6%)
4	NAG	A	1004	1	12,14,15	0.66	0	15,19,21	0.68	0
4	NAG	A	1005	1	12,14,15	0.59	0	15,19,21	0.77	0
4	NAG	A	1006	1	12,14,15	0.64	0	15,19,21	0.76	1 (6%)
4	NAG	A	1007	1	12,14,15	0.73	1 (8%)	15,19,21	1.11	1 (6%)
4	NAG	A	1010	1	12,14,15	0.70	0	15,19,21	0.87	1 (6%)
4	NAG	A	1011	1	12,14,15	0.69	1 (8%)	15,19,21	0.87	0
4	NAG	A	1012	1	12,14,15	0.65	0	15,19,21	0.71	0
4	NAG	B	1002	1	12,14,15	0.59	0	15,19,21	1.11	1 (6%)
4	NAG	B	1003	1	12,14,15	0.62	0	15,19,21	1.01	2 (13%)
4	NAG	B	1004	1	12,14,15	0.66	0	15,19,21	1.10	1 (6%)
4	NAG	B	1005	1	12,14,15	0.82	1 (8%)	15,19,21	1.27	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	B	1006	1	12,14,15	0.71	1 (8%)	15,19,21	0.64	0
4	NAG	B	1007	1	12,14,15	0.82	1 (8%)	15,19,21	1.12	2 (13%)
4	NAG	B	1008	1	12,14,15	0.58	0	15,19,21	0.99	1 (6%)
4	NAG	B	1009	1	12,14,15	0.72	1 (8%)	15,19,21	0.73	0
4	NAG	B	1010	1	12,14,15	0.56	0	15,19,21	0.99	1 (6%)
4	NAG	B	1011	1	12,14,15	0.65	0	15,19,21	0.85	0
4	NAG	B	1012	1	12,14,15	0.70	0	15,19,21	1.25	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
4	NAG	A	1002	1	-	0/6/23/26	0/1/1/1
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

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1007	NAG	O5-C5	-2.55	1.40	1.45
4	B	1005	NAG	O5-C5	-2.53	1.40	1.45
4	B	1009	NAG	O5-C5	-2.28	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1007	NAG	O5-C5	-2.15	1.41	1.45
4	B	1006	NAG	O5-C5	-2.14	1.41	1.45
4	A	1011	NAG	O5-C5	-2.11	1.41	1.45

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1005	NAG	O5-C5-C4	-3.98	105.60	110.65
4	A	1002	NAG	O5-C5-C6	3.74	110.91	106.98
4	B	1012	NAG	O5-C5-C6	3.21	110.35	106.98
4	B	1004	NAG	O5-C5-C6	3.13	110.26	106.98
4	A	1007	NAG	O5-C5-C6	2.96	110.09	106.98
4	A	1003	NAG	O5-C5-C6	2.65	109.76	106.98
4	B	1007	NAG	O5-C5-C6	-2.36	104.50	106.98
4	B	1012	NAG	C3-C2-N2	-2.36	108.17	111.76
4	B	1002	NAG	O5-C5-C4	2.35	113.63	110.65
4	A	1002	NAG	C3-C2-N2	-2.28	108.28	111.76
4	B	1007	NAG	C3-C2-N2	-2.20	108.41	111.76
4	B	1003	NAG	C2-N2-C7	-2.19	119.41	123.09
4	A	1006	NAG	O5-C5-C6	2.17	109.26	106.98
4	B	1008	NAG	O5-C5-C4	2.16	113.39	110.65
4	A	1010	NAG	O5-C5-C6	2.07	109.16	106.98
4	B	1010	NAG	O5-C5-C6	2.03	109.11	106.98
4	B	1003	NAG	O5-C5-C6	2.01	109.09	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	901/959 (93%)	-0.10	1 (0%) 93 74	50, 84, 143, 186	0
1	B	900/959 (93%)	-0.11	1 (0%) 93 74	48, 86, 154, 203	0
2	E	146/440 (33%)	-0.00	0 100 100	66, 96, 148, 188	0
2	F	139/440 (31%)	0.27	3 (2%) 59 14	75, 127, 162, 185	0
All	All	2086/2798 (74%)	-0.07	5 (0%) 93 66	48, 88, 153, 203	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	419	TYR	2.8
1	A	141	GLN	2.3
1	B	116	ILE	2.3
2	F	353	ARG	2.2
2	F	388	LEU	2.0

### 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, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	NAG	F	502	14/15	0.36	2.45	144,150,156,159	0
5	NAG	E	501	14/15	0.32	0.44	88,117,142,149	0
5	NAG	F	501	14/15	0.27	-0.49	97,120,144,146	0
5	NAG	A	1008	14/15	0.18	-0.79	65,95,112,120	0
5	NAG	E	502	14/15	0.27	-1.89	126,140,146,149	0
5	NAG	A	1009	14/15	0.22	-	104,125,171,174	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, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	A	1006	14/15	0.46	9.08	138,158,186,192	0
4	NAG	B	1010	14/15	0.24	6.08	127,145,159,164	0
4	NAG	B	1009	14/15	0.38	4.81	125,143,149,155	0
4	NAG	B	1004	14/15	0.44	1.56	130,164,186,189	0
4	NAG	A	1004	14/15	0.30	1.44	125,149,160,160	0
4	NAG	A	1007	14/15	0.22	1.40	92,117,143,146	0
4	NAG	B	1002	14/15	0.34	1.33	107,137,154,158	0
4	NAG	B	1008	14/15	0.23	1.02	73,97,115,119	0
4	NAG	A	1012	14/15	0.27	0.82	58,80,99,100	0
4	NAG	A	1002	14/15	0.25	0.53	107,119,135,139	0
4	NAG	B	1006	14/15	0.27	0.44	117,129,135,140	0
4	NAG	B	1007	14/15	0.23	0.41	90,99,133,141	0
4	NAG	A	1010	14/15	0.17	0.38	106,121,131,137	0
4	NAG	B	1011	14/15	0.23	0.36	114,128,147,148	0
4	NAG	A	1005	14/15	0.21	0.11	135,142,162,163	0
4	NAG	B	1005	14/15	0.22	-0.23	123,148,157,159	0
3	ZN	B	1001	1/1	0.17	-0.31	83,83,83,83	0
4	NAG	A	1003	14/15	0.18	-0.44	51,79,92,96	0
4	NAG	A	1011	14/15	0.19	-0.57	84,95,117,134	0
4	NAG	B	1003	14/15	0.17	-0.57	75,88,102,106	0
3	ZN	A	1001	1/1	0.18	-0.66	75,75,75,75	0
4	NAG	B	1012	14/15	0.14	-1.31	74,87,113,124	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.