



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2021 – 11:07 am BST

PDB ID : 7OAY  
Title : Nanobody F2 bound to RBD  
Authors : Naismith, J.H.; Mikolajek, H.  
Deposited on : 2021-04-20  
Resolution : 2.34 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

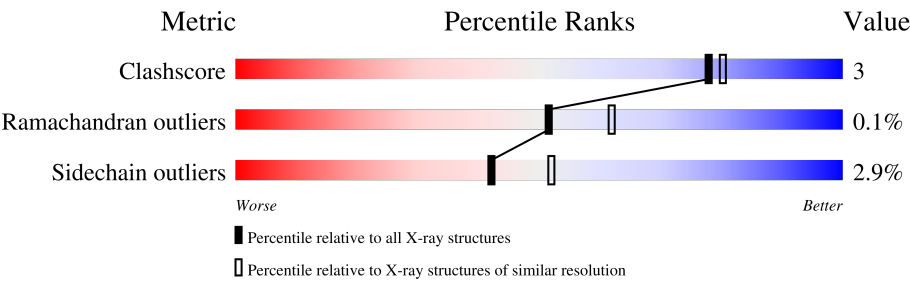
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.34 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))
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)

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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	AAA	210	<div><div>86%</div><div>8%</div><div>6%</div></div>
1	CCC	210	<div><div>84%</div><div>10%</div><div>6%</div></div>
1	EEE	210	<div><div>81%</div><div>10%</div><div>6%</div></div>
1	GGG	210	<div><div>84%</div><div>8%</div><div>7%</div></div>
1	III	210	<div><div>87%</div><div>7%</div><div>6%</div></div>
1	KKK	210	<div><div>86%</div><div>7%</div><div>6%</div></div>
2	BBB	132	<div><div>89%</div><div>5%</div><div>5%</div></div>
2	DDD	132	<div><div>92%</div><div>5%</div></div>

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Mol	Chain	Length	Quality of chain
2	FFF	132	<div><div></div><div>89%</div><div>5%6%</div></div>
2	HHH	132	<div><div></div><div>87%</div><div>8%5%</div></div>
2	JJJ	132	<div><div></div><div>89%</div><div>5%5%</div></div>
2	LLL	132	<div><div></div><div>91%</div><div>•5%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15699 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 Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	198	Total	C	N	O	S	0	0	0
			1568	1005	262	293	8			
1	CCC	198	Total	C	N	O	S	0	0	0
			1568	1005	262	293	8			
1	EEE	197	Total	C	N	O	S	0	0	0
			1560	1001	260	291	8			
1	GGG	196	Total	C	N	O	S	0	0	0
			1552	995	259	290	8			
1	III	198	Total	C	N	O	S	0	0	0
			1568	1005	262	293	8			
1	KKK	197	Total	C	N	O	S	0	0	0
			1560	1001	260	291	8			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	533	LYS	-	expression tag	UNP P0DTC2
AAA	534	HIS	-	expression tag	UNP P0DTC2
AAA	535	HIS	-	expression tag	UNP P0DTC2
AAA	536	HIS	-	expression tag	UNP P0DTC2
AAA	537	HIS	-	expression tag	UNP P0DTC2
AAA	538	HIS	-	expression tag	UNP P0DTC2
AAA	539	HIS	-	expression tag	UNP P0DTC2
CCC	533	LYS	-	expression tag	UNP P0DTC2
CCC	534	HIS	-	expression tag	UNP P0DTC2
CCC	535	HIS	-	expression tag	UNP P0DTC2
CCC	536	HIS	-	expression tag	UNP P0DTC2
CCC	537	HIS	-	expression tag	UNP P0DTC2
CCC	538	HIS	-	expression tag	UNP P0DTC2
CCC	539	HIS	-	expression tag	UNP P0DTC2
EEE	533	LYS	-	expression tag	UNP P0DTC2
EEE	534	HIS	-	expression tag	UNP P0DTC2
EEE	535	HIS	-	expression tag	UNP P0DTC2

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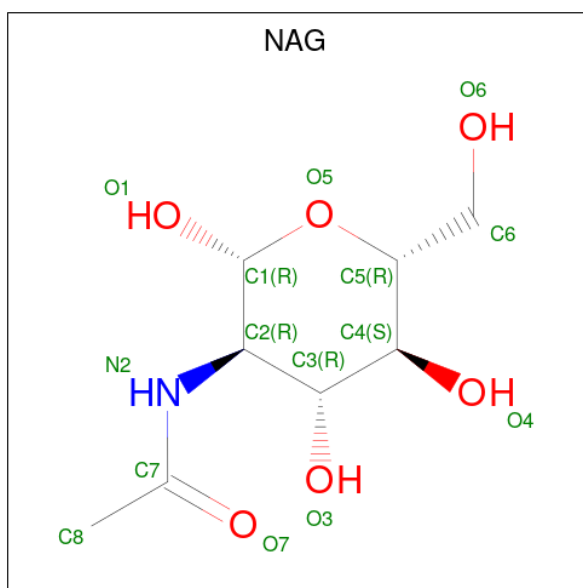
Chain	Residue	Modelled	Actual	Comment	Reference
EEE	536	HIS	-	expression tag	UNP P0DTC2
EEE	537	HIS	-	expression tag	UNP P0DTC2
EEE	538	HIS	-	expression tag	UNP P0DTC2
EEE	539	HIS	-	expression tag	UNP P0DTC2
GGG	533	LYS	-	expression tag	UNP P0DTC2
GGG	534	HIS	-	expression tag	UNP P0DTC2
GGG	535	HIS	-	expression tag	UNP P0DTC2
GGG	536	HIS	-	expression tag	UNP P0DTC2
GGG	537	HIS	-	expression tag	UNP P0DTC2
GGG	538	HIS	-	expression tag	UNP P0DTC2
GGG	539	HIS	-	expression tag	UNP P0DTC2
III	533	LYS	-	expression tag	UNP P0DTC2
III	534	HIS	-	expression tag	UNP P0DTC2
III	535	HIS	-	expression tag	UNP P0DTC2
III	536	HIS	-	expression tag	UNP P0DTC2
III	537	HIS	-	expression tag	UNP P0DTC2
III	538	HIS	-	expression tag	UNP P0DTC2
III	539	HIS	-	expression tag	UNP P0DTC2
KKK	533	LYS	-	expression tag	UNP P0DTC2
KKK	534	HIS	-	expression tag	UNP P0DTC2
KKK	535	HIS	-	expression tag	UNP P0DTC2
KKK	536	HIS	-	expression tag	UNP P0DTC2
KKK	537	HIS	-	expression tag	UNP P0DTC2
KKK	538	HIS	-	expression tag	UNP P0DTC2
KKK	539	HIS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called F2 nanobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	125	Total 987	C 624	N 171	O 188	S 4	0	0	0
2	DDD	125	Total 987	C 624	N 171	O 188	S 4	0	0	0
2	FFF	124	Total 981	C 621	N 170	O 186	S 4	0	0	0
2	HHH	125	Total 987	C 624	N 171	O 188	S 4	0	0	0
2	JJJ	125	Total 987	C 624	N 171	O 188	S 4	0	0	0
2	LLL	125	Total 987	C 624	N 171	O 188	S 4	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	AAA	1	Total	C	N	O	0	0
			14	8	1	5		
3	CCC	1	Total	C	N	O	0	0
			14	8	1	5		
3	EEE	1	Total	C	N	O	0	0
			14	8	1	5		
3	GGG	1	Total	C	N	O	0	0
			14	8	1	5		
3	III	1	Total	C	N	O	0	0
			14	8	1	5		
3	KKK	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	42	Total	O	0	0
			42	42		
4	BBB	20	Total	O	0	0
			20	20		
4	CCC	37	Total	O	0	0
			37	37		
4	DDD	11	Total	O	0	0
			11	11		
4	EEE	36	Total	O	0	0
			36	36		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	FFF	27	Total 27	O 27	0	0
4	GGG	37	Total 37	O 37	0	0
4	HHH	16	Total 16	O 16	0	0
4	III	16	Total 16	O 16	0	0
4	JJJ	15	Total 15	O 15	0	0
4	KKK	39	Total 39	O 39	0	0
4	LLL	27	Total 27	O 27	0	0

### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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. 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. 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.


Note EDS was not executed.

- Molecule 1: Spike protein S1

Chain AAA:  86% 8% 6%



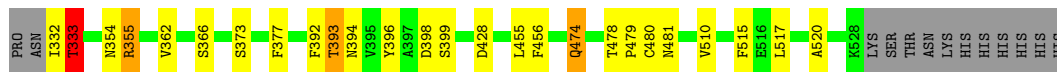
- Molecule 1: Spike protein S1

Chain CCC:  84% 10% 6%




- Molecule 1: Spike protein S1

Chain EEE:  81% 10% 6%




- Molecule 1: Spike protein S1

Chain GGG:  84% 8% 7%



- Molecule 1: Spike protein S1

Chain III:  87% 7% 6%



- Molecule 1: Spike protein S1



Chain KKK:  86% 7% • 6%



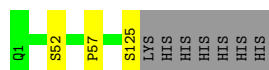
• Molecule 2: F2 nanobody

Chain BBB:  89% 5% 5%



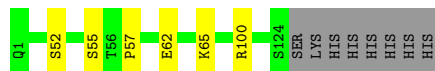
• Molecule 2: F2 nanobody

Chain DDD:  92% • 5%



• Molecule 2: F2 nanobody

Chain FFF:  89% 5% 6%



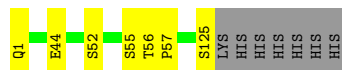
• Molecule 2: F2 nanobody

Chain HHH:  87% 8% 5%



• Molecule 2: F2 nanobody

Chain JJJ:  89% 5% 5%



• Molecule 2: F2 nanobody

Chain LLL:  91% • 5%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.42Å 108.42Å 165.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	93.89 – 2.34	Depositor
% Data completeness (in resolution range)	100.0 (93.89-2.34)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.192 , 0.228	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	15699	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	56.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	AAA	0.67	0/1612	0.87	3/2194 (0.1%)
1	CCC	0.69	0/1612	0.89	2/2194 (0.1%)
1	EEE	0.69	0/1604	0.87	2/2183 (0.1%)
1	GGG	0.68	0/1596	0.88	2/2172 (0.1%)
1	III	0.66	0/1612	0.86	3/2194 (0.1%)
1	KKK	0.67	0/1604	0.91	3/2183 (0.1%)
2	BBB	0.68	0/1012	0.85	0/1371
2	DDD	0.69	0/1012	0.84	0/1371
2	FFF	0.67	0/1006	0.86	1/1363 (0.1%)
2	HHH	0.69	0/1012	0.84	0/1371
2	JJJ	0.68	0/1012	0.85	0/1371
2	LLL	0.68	0/1012	0.83	0/1371
All	All	0.68	0/15706	0.87	16/21338 (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
2	BBB	0	1
2	FFF	0	1
2	HHH	0	1
2	JJJ	0	1
2	LLL	0	1
All	All	0	5

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	CCC	355	ARG	CB-CA-C	-8.47	93.47	110.40
1	EEE	355	ARG	CB-CA-C	-7.92	94.56	110.40
1	KKK	355	ARG	CB-CA-C	-7.90	94.60	110.40
1	AAA	355	ARG	CB-CA-C	-7.87	94.66	110.40
1	GGG	355	ARG	CG-CD-NE	-7.73	95.56	111.80
1	III	355	ARG	CB-CA-C	-7.68	95.04	110.40
1	GGG	355	ARG	CB-CA-C	-7.67	95.07	110.40
1	KKK	355	ARG	CG-CD-NE	-7.67	95.70	111.80
1	CCC	355	ARG	CG-CD-NE	-7.49	96.08	111.80
1	EEE	355	ARG	CG-CD-NE	-6.58	97.99	111.80
1	AAA	355	ARG	CG-CD-NE	-6.51	98.12	111.80
1	KKK	408	ARG	CG-CD-NE	-6.23	98.72	111.80
1	AAA	357	ARG	CG-CD-NE	-6.13	98.92	111.80
1	III	355	ARG	CG-CD-NE	-6.04	99.11	111.80
1	III	357	ARG	CG-CD-NE	-5.76	99.70	111.80
2	FFF	100	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	BBB	55	SER	Peptide
2	FFF	55	SER	Peptide
2	HHH	55	SER	Peptide
2	JJJ	55	SER	Peptide
2	LLL	55	SER	Peptide

## 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	AAA	1568	0	1489	9	0
1	CCC	1568	0	1489	11	0
1	EEE	1560	0	1483	22	0
1	GGG	1552	0	1472	13	0
1	III	1568	0	1489	10	0
1	KKK	1560	0	1483	6	0
2	BBB	987	0	941	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	DDD	987	0	941	2	0
2	FFF	981	0	936	3	0
2	HHH	987	0	941	7	0
2	JJJ	987	0	941	6	0
2	LLL	987	0	941	3	0
3	AAA	14	0	13	0	0
3	CCC	14	0	13	0	0
3	EEE	14	0	13	0	0
3	GGG	14	0	13	2	0
3	III	14	0	13	0	0
3	KKK	14	0	13	1	0
4	AAA	42	0	0	1	0
4	BBB	20	0	0	0	0
4	CCC	37	0	0	4	0
4	DDD	11	0	0	0	0
4	EEE	36	0	0	7	0
4	FFF	27	0	0	1	0
4	GGG	37	0	0	8	0
4	HHH	16	0	0	0	0
4	III	16	0	0	2	0
4	JJJ	15	0	0	4	0
4	KKK	39	0	0	4	0
4	LLL	27	0	0	1	0
All	All	15699	0	14624	88	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (88) 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:GGG:389:ASP:OD1	1:GGG:528:LYS:HD2	1.69	0.93
2:HHH:43:LYS:HG2	1:III:477:SER:HB2	1.53	0.91
1:EEE:455:LEU:HB3	4:EEE:702:HOH:O	1.71	0.89
2:HHH:43:LYS:HG2	1:III:477:SER:CB	2.02	0.88
1:AAA:486:PHE:CE1	1:AAA:487:ASN:OD1	2.33	0.81
1:EEE:481:ASN:O	4:EEE:701:HOH:O	1.99	0.79
2:LLL:13:GLN:HG2	4:LLL:202:HOH:O	1.86	0.75
1:CCC:480:CYS:HB2	4:CCC:736:HOH:O	1.86	0.75
1:CCC:382:VAL:HG12	4:CCC:726:HOH:O	1.87	0.74
1:GGG:345:THR:HB	4:GGG:728:HOH:O	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:LLL:52:SER:HB3	2:LLL:57:PRO:HD2	1.70	0.73
1:EEE:456:PHE:CD2	4:EEE:702:HOH:O	2.42	0.72
2:BBB:52:SER:HB3	2:BBB:57:PRO:HD2	1.72	0.71
1:EEE:393:THR:CG2	1:EEE:520:ALA:HB3	2.21	0.71
2:JJJ:52:SER:HB3	2:JJJ:57:PRO:HD2	1.72	0.71
2:HHH:52:SER:HB3	2:HHH:57:PRO:HD2	1.73	0.70
2:FFF:52:SER:HB3	2:FFF:57:PRO:HD2	1.74	0.69
1:AAA:357:ARG:NH1	1:AAA:394:ASN:OD1	2.27	0.68
2:DDD:52:SER:HB3	2:DDD:57:PRO:HD2	1.77	0.67
1:GGG:472:ILE:HG13	4:GGG:702:HOH:O	1.95	0.66
1:GGG:371:SER:HB3	4:GGG:701:HOH:O	1.96	0.65
1:EEE:479:PRO:HA	4:EEE:706:HOH:O	1.96	0.64
1:KKK:528:LYS:HA	4:KKK:722:HOH:O	1.99	0.62
1:KKK:519:HIS:HB3	4:KKK:724:HOH:O	2.01	0.61
1:CCC:417:LYS:HD3	1:CCC:455:LEU:HD12	1.83	0.60
2:HHH:43:LYS:HG2	1:III:477:SER:HB3	1.83	0.58
2:JJJ:44:GLU:HG2	4:JJJ:212:HOH:O	2.04	0.58
1:CCC:417:LYS:HE3	4:CCC:735:HOH:O	2.03	0.57
1:EEE:332:ILE:HG23	1:EEE:362:VAL:HG22	1.89	0.54
1:EEE:479:PRO:HD2	4:EEE:735:HOH:O	2.06	0.54
1:EEE:478:THR:HA	4:EEE:735:HOH:O	2.07	0.54
1:III:440:ASN:HB2	4:III:713:HOH:O	2.09	0.53
2:FFF:62:GLU:HG2	4:FFF:225:HOH:O	2.08	0.53
1:EEE:393:THR:HG21	1:EEE:520:ALA:HB3	1.90	0.53
1:GGG:374:PHE:N	4:GGG:701:HOH:O	2.39	0.51
1:AAA:428:ASP:OD2	1:EEE:373:SER:HB2	2.10	0.51
1:GGG:367:VAL:HG21	3:GGG:601:NAG:H82	1.92	0.51
1:GGG:482:GLY:C	4:GGG:702:HOH:O	2.49	0.50
1:KKK:339:GLY:HA2	3:KKK:601:NAG:H83	1.93	0.50
1:AAA:477:SER:HB3	4:AAA:736:HOH:O	2.11	0.49
1:EEE:474:GLN:OE1	1:EEE:480:CYS:SG	2.71	0.49
1:AAA:354:ASN:O	1:AAA:398:ASP:HA	2.13	0.48
2:DDD:52:SER:CB	2:DDD:57:PRO:HD2	2.43	0.48
1:III:471:GLU:HG2	4:III:715:HOH:O	2.14	0.48
1:CCC:447:GLY:HA2	1:CCC:498:GLN:HG2	1.95	0.48
1:EEE:354:ASN:O	1:EEE:398:ASP:HA	2.12	0.48
1:GGG:354:ASN:O	1:GGG:398:ASP:HA	2.12	0.48
1:GGG:472:ILE:CG1	4:GGG:702:HOH:O	2.57	0.48
1:EEE:393:THR:HG23	1:EEE:520:ALA:HB3	1.93	0.48
1:III:354:ASN:O	1:III:398:ASP:HA	2.13	0.48
2:LLL:52:SER:CB	2:LLL:57:PRO:HD2	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:474:GLN:NE2	1:EEE:479:PRO:HA	2.30	0.47
2:HHH:43:LYS:CG	1:III:477:SER:HB3	2.46	0.47
2:HHH:52:SER:CB	2:HHH:57:PRO:HD2	2.43	0.46
1:CCC:371:SER:HB3	1:EEE:428:ASP:OD2	2.15	0.46
1:AAA:394:ASN:ND2	1:AAA:396:TYR:CE2	2.84	0.46
1:CCC:472:ILE:HD12	1:CCC:482:GLY:HA2	1.96	0.46
1:CCC:354:ASN:O	1:CCC:398:ASP:HA	2.15	0.45
1:EEE:479:PRO:CD	4:EEE:735:HOH:O	2.63	0.45
2:JJJ:44:GLU:CG	4:JJJ:212:HOH:O	2.62	0.45
1:KKK:354:ASN:O	1:KKK:398:ASP:HA	2.15	0.45
1:EEE:394:ASN:ND2	1:EEE:396:TYR:CE2	2.86	0.44
1:III:394:ASN:ND2	1:III:396:TYR:CE2	2.85	0.44
2:JJJ:56:THR:HB	4:JJJ:207:HOH:O	2.18	0.44
1:III:392:PHE:CD1	1:III:515:PHE:HB3	2.52	0.44
1:KKK:332:ILE:HG12	4:KKK:730:HOH:O	2.17	0.43
1:CCC:466:ARG:HD2	4:CCC:734:HOH:O	2.19	0.43
1:GGG:417:LYS:HA	1:GGG:417:LYS:HD3	1.88	0.43
2:BBB:68:PHE:CZ	2:BBB:83:MET:HE2	2.54	0.43
2:FFF:52:SER:CB	2:FFF:57:PRO:HD2	2.44	0.43
1:AAA:392:PHE:CD1	1:AAA:515:PHE:HB3	2.53	0.42
1:GGG:367:VAL:HG21	3:GGG:601:NAG:C8	2.48	0.42
2:BBB:52:SER:CB	2:BBB:57:PRO:HD2	2.44	0.42
1:CCC:399:SER:HA	1:CCC:510:VAL:O	2.20	0.42
1:EEE:332:ILE:HG23	1:EEE:362:VAL:CG2	2.50	0.42
1:CCC:437:ASN:CG	1:EEE:517:LEU:HD13	2.41	0.41
1:EEE:392:PHE:CD1	1:EEE:515:PHE:HB3	2.55	0.41
2:JJJ:44:GLU:HB2	4:JJJ:212:HOH:O	2.20	0.41
2:HHH:38:ARG:HA	2:HHH:93:VAL:O	2.20	0.41
2:JJJ:52:SER:CB	2:JJJ:57:PRO:HD2	2.44	0.41
1:AAA:472:ILE:HD12	1:AAA:484:GLU:HG2	2.02	0.41
1:III:399:SER:HA	1:III:510:VAL:O	2.21	0.41
1:GGG:371:SER:CB	4:GGG:701:HOH:O	2.62	0.41
1:AAA:399:SER:HA	1:AAA:510:VAL:O	2.21	0.41
1:EEE:399:SER:HA	1:EEE:510:VAL:O	2.20	0.40
1:KKK:505:TYR:HE1	4:KKK:717:HOH:O	2.04	0.40
1:GGG:373:SER:N	4:GGG:701:HOH:O	2.55	0.40
1:EEE:332:ILE:O	1:EEE:333:THR:HG23	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	196/210 (93%)	188 (96%)	8 (4%)	0	100	100
1	CCC	196/210 (93%)	190 (97%)	6 (3%)	0	100	100
1	EEE	195/210 (93%)	186 (95%)	8 (4%)	1 (0%)	29	31
1	GGG	194/210 (92%)	187 (96%)	7 (4%)	0	100	100
1	III	196/210 (93%)	189 (96%)	7 (4%)	0	100	100
1	KKK	195/210 (93%)	187 (96%)	7 (4%)	1 (0%)	29	31
2	BBB	123/132 (93%)	118 (96%)	5 (4%)	0	100	100
2	DDD	123/132 (93%)	118 (96%)	5 (4%)	0	100	100
2	FFF	122/132 (92%)	117 (96%)	5 (4%)	0	100	100
2	HHH	123/132 (93%)	117 (95%)	6 (5%)	0	100	100
2	JJJ	123/132 (93%)	118 (96%)	5 (4%)	0	100	100
2	LLL	123/132 (93%)	118 (96%)	5 (4%)	0	100	100
All	All	1909/2052 (93%)	1833 (96%)	74 (4%)	2 (0%)	51	62

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	KKK	333	THR
1	EEE	333	THR

### 5.3.2 Protein sidechains

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

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



Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AAA	171/183 (93%)	168 (98%)	3 (2%)	59	70
1	CCC	171/183 (93%)	163 (95%)	8 (5%)	26	33
1	EEE	170/183 (93%)	164 (96%)	6 (4%)	36	45
1	GGG	169/183 (92%)	161 (95%)	8 (5%)	26	33
1	III	171/183 (93%)	168 (98%)	3 (2%)	59	70
1	KKK	170/183 (93%)	162 (95%)	8 (5%)	26	33
2	BBB	102/109 (94%)	100 (98%)	2 (2%)	55	66
2	DDD	102/109 (94%)	101 (99%)	1 (1%)	76	85
2	FFF	101/109 (93%)	100 (99%)	1 (1%)	76	85
2	HHH	102/109 (94%)	98 (96%)	4 (4%)	32	41
2	JJJ	102/109 (94%)	100 (98%)	2 (2%)	55	66
2	LLL	102/109 (94%)	101 (99%)	1 (1%)	76	85
All	All	1633/1752 (93%)	1586 (97%)	47 (3%)	42	52

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	333	THR
1	AAA	355	ARG
1	AAA	377	PHE
2	BBB	27	ARG
2	BBB	125	SER
1	CCC	333	THR
1	CCC	346	ARG
1	CCC	355	ARG
1	CCC	377	PHE
1	CCC	393	THR
1	CCC	408	ARG
1	CCC	417	LYS
1	CCC	427	ASP
2	DDD	125	SER
1	EEE	333	THR
1	EEE	355	ARG
1	EEE	366	SER
1	EEE	377	PHE
1	EEE	393	THR
1	EEE	474	GLN
2	FFF	65	LYS
1	GGG	333	THR

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Mol	Chain	Res	Type
1	GGG	346	ARG
1	GGG	355	ARG
1	GGG	377	PHE
1	GGG	427	ASP
1	GGG	462	LYS
1	GGG	494	SER
1	GGG	528	LYS
2	HHH	1	GLN
2	HHH	13	GLN
2	HHH	65	LYS
2	HHH	125	SER
1	III	355	ARG
1	III	377	PHE
1	III	408	ARG
2	JJJ	1	GLN
2	JJJ	125	SER
1	KKK	346	ARG
1	KKK	355	ARG
1	KKK	377	PHE
1	KKK	393	THR
1	KKK	424	LYS
1	KKK	462	LYS
1	KKK	477	SER
1	KKK	519	HIS
2	LLL	125	SER

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

6 ligands 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
3	NAG	AAA	601	1	14,14,15	0.55	0	17,19,21	0.79	0
3	NAG	GGG	601	1	14,14,15	0.79	0	17,19,21	1.92	4 (23%)
3	NAG	III	601	1	14,14,15	0.44	0	17,19,21	1.14	1 (5%)
3	NAG	CCC	601	1	14,14,15	0.62	0	17,19,21	1.46	2 (11%)
3	NAG	EEE	601	1	14,14,15	0.39	0	17,19,21	1.15	0
3	NAG	KKK	601	1	14,14,15	0.98	0	17,19,21	1.74	3 (17%)

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
3	NAG	AAA	601	1	-	0/6/23/26	0/1/1/1
3	NAG	GGG	601	1	-	1/6/23/26	0/1/1/1
3	NAG	III	601	1	-	2/6/23/26	0/1/1/1
3	NAG	CCC	601	1	-	0/6/23/26	0/1/1/1
3	NAG	EEE	601	1	-	0/6/23/26	0/1/1/1
3	NAG	KKK	601	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	GGG	601	NAG	C2-N2-C7	5.69	131.00	122.90
3	KKK	601	NAG	C4-C3-C2	3.95	116.81	111.02
3	CCC	601	NAG	C4-C3-C2	3.71	116.45	111.02
3	KKK	601	NAG	O5-C5-C6	3.30	112.39	107.20
3	KKK	601	NAG	C3-C4-C5	3.17	115.89	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	GGG	601	NAG	C1-C2-N2	2.78	115.24	110.49
3	GGG	601	NAG	O5-C5-C4	-2.41	104.97	110.83
3	GGG	601	NAG	C4-C3-C2	2.25	114.31	111.02
3	CCC	601	NAG	C1-O5-C5	-2.06	109.40	112.19
3	III	601	NAG	C1-O5-C5	2.04	114.96	112.19

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	GGG	601	NAG	C1-C2-N2-C7
3	III	601	NAG	O5-C5-C6-O6
3	III	601	NAG	C4-C5-C6-O6
3	KKK	601	NAG	C1-C2-N2-C7
3	KKK	601	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	GGG	601	NAG	2	0
3	KKK	601	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.