



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:02 AM UTC

PDB ID : 7OAY / pdb_00007oay
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.

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

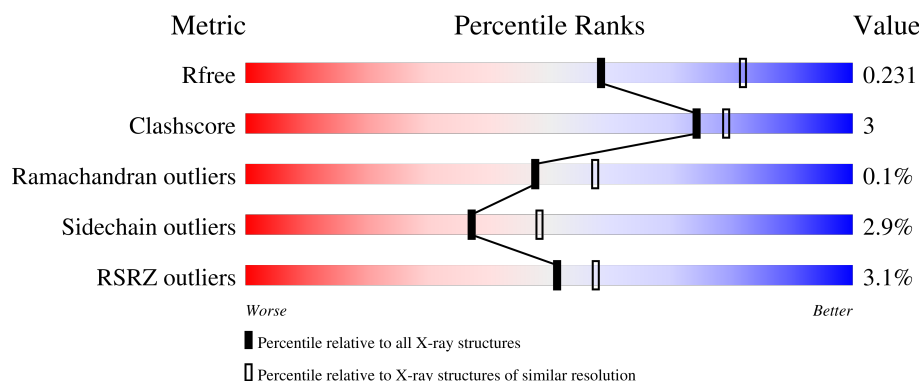
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

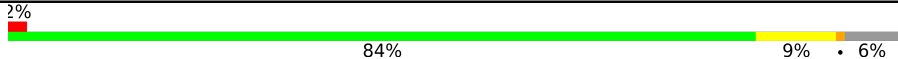
The reported resolution of this entry is 2.34 Å.

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))
R_{free}	180053	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (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 ≥ 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 $\leq 5\%$. 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	AAA	210	
1	CCC	210	
1	EEE	210	
1	GGG	210	
1	III	210	

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Mol	Chain	Length	Quality of chain
1	KKK	210	3% 86% 6% • 6%
2	BBB	132	2% 89% 6% 5%
2	DDD	132	2% 91% • 5%
2	FFF	132	2% 89% 5% 6%
2	HHH	132	3% 85% 10% 5%
2	JJJ	132	2% 88% 7% 5%
2	LLL	132	3% 89% 5% 5%

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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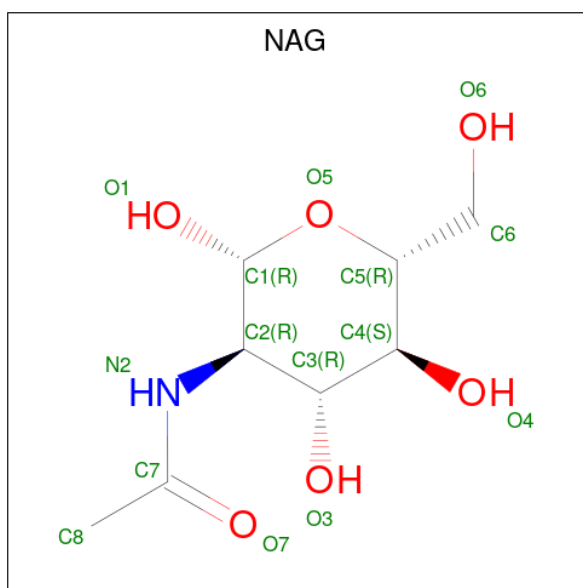
Chain	Residue	Modelled	Actual	Comment	Reference
EEE	536	HIS	-	expression tag	UNP P0DTC2
EEE	537	HIS	-	expression tag	UNP P0DTC2
EEE	538	HIS	-	expression tag	UNP P0DTC2
EEE	539	HIS	-	expression tag	UNP P0DTC2
GGG	533	LYS	-	expression tag	UNP P0DTC2
GGG	534	HIS	-	expression tag	UNP P0DTC2
GGG	535	HIS	-	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 (CCD ID: NAG) (formula:

C₈H₁₅NO₆).



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 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.

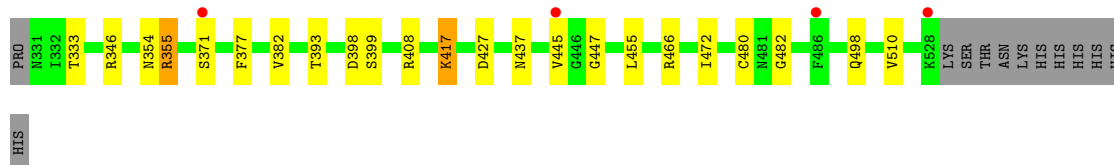
- Molecule 1: Spike protein S1

Chain AAA: 



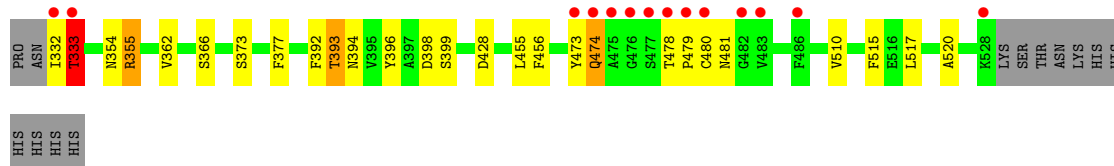
- Molecule 1: Spike protein S1

Chain CCC: 



- Molecule 1: Spike protein S1

Chain EEE: 



- Molecule 1: Spike protein S1

Chain GGG: 



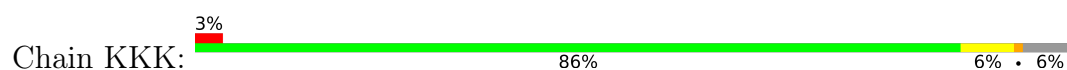
- Molecule 1: Spike protein S1

Chain III: 

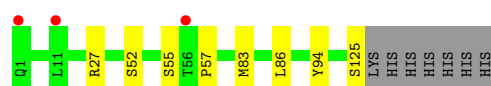




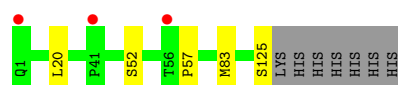
- Molecule 1: Spike protein S1



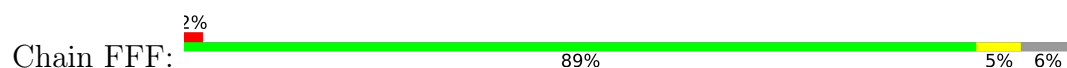
- Molecule 2: F2 nanobody



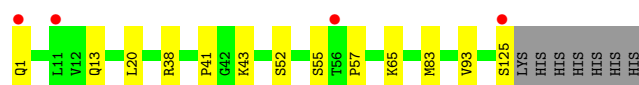
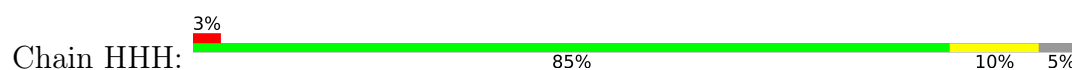
- Molecule 2: F2 nanobody



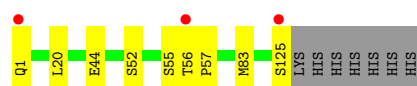
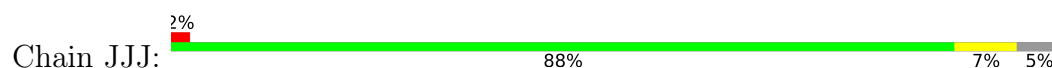
- Molecule 2: F2 nanobody



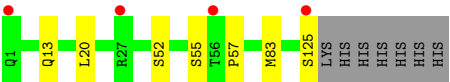
- Molecule 2: F2 nanobody



- Molecule 2: F2 nanobody



- Molecule 2: F2 nanobody



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	108.42Å 108.42Å 165.54Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	93.89 – 2.34 93.89 – 2.34	Depositor EDS
% Data completeness (in resolution range)	100.0 (93.89-2.34) 100.0 (93.89-2.34)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.192 , 0.228 0.198 , 0.231	Depositor DCC
R_{free} test set	4643 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	48.1	Xtriage
Anisotropy	0.016	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,l 0.029 for h,-h-k,-l 0.025 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15699	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.41% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0.99	1/1612 (0.1%)	1.29	6/2194 (0.3%)
1	CCC	1.02	0/1612	1.26	3/2194 (0.1%)
1	EEE	1.01	1/1604 (0.1%)	1.30	2/2183 (0.1%)
1	GGG	1.00	0/1596	1.28	2/2172 (0.1%)
1	III	0.97	0/1612	1.28	4/2194 (0.2%)
1	KKK	0.98	0/1604	1.31	5/2183 (0.2%)
2	BBB	0.98	0/1012	1.23	0/1371
2	DDD	0.98	0/1012	1.21	0/1371
2	FFF	0.95	0/1006	1.23	0/1363
2	HHH	0.99	0/1012	1.23	1/1371 (0.1%)
2	JJJ	0.99	0/1012	1.21	0/1371
2	LLL	0.98	0/1012	1.20	0/1371
All	All	0.99	2/15706 (0.0%)	1.26	23/21338 (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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	EEE	473	TYR	C-O	6.35	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	AAA	377	PHE	C-O	5.04	1.28	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EEE	355	ARG	CB-CA-C	-9.53	94.56	110.19
1	CCC	355	ARG	CB-CA-C	-9.39	93.47	109.72
1	KKK	355	ARG	CB-CA-C	-8.74	94.60	109.72
1	AAA	355	ARG	CB-CA-C	-8.70	94.66	109.72
1	III	355	ARG	CB-CA-C	-8.49	95.04	109.72
1	GGG	355	ARG	CB-CA-C	-8.47	95.07	109.72
1	GGG	355	ARG	CG-CD-NE	-7.47	95.56	112.00
1	KKK	355	ARG	CG-CD-NE	-7.41	95.70	112.00
1	CCC	355	ARG	CG-CD-NE	-7.24	96.08	112.00
1	AAA	519	HIS	CA-CB-CG	-6.44	107.36	113.80
1	EEE	355	ARG	CG-CD-NE	-6.37	97.99	112.00
1	AAA	355	ARG	CG-CD-NE	-6.31	98.12	112.00
1	KKK	408	ARG	CG-CD-NE	-6.04	98.72	112.00
1	AAA	357	ARG	CG-CD-NE	-5.95	98.92	112.00
2	HHH	41	PRO	CA-C-O	-5.89	110.67	119.86
1	III	355	ARG	CG-CD-NE	-5.86	99.11	112.00
1	AAA	445	VAL	CA-C-O	-5.70	115.02	120.95
1	III	357	ARG	CG-CD-NE	-5.59	99.70	112.00
1	KKK	332	ILE	CA-C-N	5.53	132.11	121.54
1	KKK	332	ILE	C-N-CA	5.53	132.11	121.54
1	III	416	GLY	CA-C-O	-5.50	117.88	122.33
1	AAA	416	GLY	CA-C-O	-5.29	118.05	122.33
1	CCC	445	VAL	CA-C-O	-5.26	115.58	121.05

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 ⓘ

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	4	0
2	DDD	987	0	941	3	0
2	FFF	981	0	936	4	0
2	HHH	987	0	941	8	0
2	JJJ	987	0	941	7	0
2	LLL	987	0	941	4	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	94	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 (94) 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
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:GGG:482:GLY:C	4:GGG:702:HOH:O	2.49	0.55
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: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
2:LLL:20:LEU:HG	2:LLL:83:MET:HE2	1.95	0.49
1:EEE:474:GLN:OE1	1:EEE:480:CYS:SG	2.71	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HHH:20:LEU:HG	2:HHH:83:MET:HE2	1.94	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
2:BBB:83:MET:HE1	2:BBB:94:TYR:CZ	2.49	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
1:EEE:474:GLN:NE2	1:EEE:479:PRO:HA	2.30	0.47
2:DDD:20:LEU:HG	2:DDD:83:MET:HE2	1.97	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:CCC:437:ASN:CG	1:EEE:517:LEU:HD13	2.41	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
2:JJJ:20:LEU:HG	2:JJJ:83:MET:HE2	1.98	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
2:BBB:83:MET:HE2	2:BBB:86:LEU:HD21	1.99	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:FFF:52:SER:CB	2:FFF:57:PRO:HD2	2.44	0.43
2:FFF:20:LEU:HG	2:FFF:83:MET:HE2	2.00	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:EEE:392:PHE:CD1	1:EEE:515:PHE:HB3	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	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%)	24	26
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%)	24	26
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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	LLL	123/132 (93%)	118 (96%)	5 (4%)	0	100	100
All	All	1909/2052 (93%)	1833 (96%)	74 (4%)	2 (0%)	48	57

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%)	51	64
1	CCC	171/183 (93%)	163 (95%)	8 (5%)	23	30
1	EEE	170/183 (93%)	164 (96%)	6 (4%)	32	41
1	GGG	169/183 (92%)	161 (95%)	8 (5%)	23	30
1	III	171/183 (93%)	168 (98%)	3 (2%)	51	64
1	KKK	170/183 (93%)	162 (95%)	8 (5%)	23	30
2	BBB	102/109 (94%)	100 (98%)	2 (2%)	48	61
2	DDD	102/109 (94%)	101 (99%)	1 (1%)	68	79
2	FFF	101/109 (93%)	100 (99%)	1 (1%)	68	79
2	HHH	102/109 (94%)	98 (96%)	4 (4%)	28	37
2	JJJ	102/109 (94%)	100 (98%)	2 (2%)	48	61
2	LLL	102/109 (94%)	101 (99%)	1 (1%)	68	79
All	All	1633/1752 (93%)	1586 (97%)	47 (3%)	37	48

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

Mol	Chain	Res	Type
1	AAA	333	THR

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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	CCC	601	1	14,14,15	0.64	0	17,19,21	1.47	3 (17%)
3	NAG	EEE	601	1	14,14,15	0.41	0	17,19,21	1.18	0
3	NAG	KKK	601	1	14,14,15	1.01	1 (7%)	17,19,21	1.65	3 (17%)
3	NAG	GGG	601	1	14,14,15	0.81	0	17,19,21	1.98	4 (23%)
3	NAG	III	601	1	14,14,15	0.44	0	17,19,21	1.13	1 (5%)
3	NAG	AAA	601	1	14,14,15	0.55	0	17,19,21	0.80	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
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
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	AAA	601	1	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	KKK	601	NAG	C1-C2	2.05	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	GGG	601	NAG	C2-N2-C7	6.04	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	C3-C4-C5	3.12	115.89	110.23
3	GGG	601	NAG	C1-C2-N2	3.05	115.24	110.43
3	KKK	601	NAG	O5-C5-C6	2.43	112.39	107.66
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	-2.08	109.40	112.19
3	III	601	NAG	C1-O5-C5	2.07	114.96	112.19
3	CCC	601	NAG	C1-C2-N2	2.06	113.69	110.43

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	C4-C5-C6-O6
3	III	601	NAG	O5-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	KKK	601	NAG	1	0
3	GGG	601	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	AAA	198/210 (94%)	0.01	4 (2%) 65 70	35, 49, 95, 111	0
1	CCC	198/210 (94%)	0.06	4 (2%) 65 70	36, 51, 86, 103	0
1	EEE	197/210 (93%)	0.27	14 (7%) 22 26	37, 51, 116, 148	0
1	GGG	196/210 (93%)	0.01	4 (2%) 65 70	36, 50, 83, 100	0
1	III	198/210 (94%)	0.36	8 (4%) 42 48	40, 64, 103, 122	0
1	KKK	197/210 (93%)	0.19	6 (3%) 52 59	38, 56, 86, 111	0
2	BBB	125/132 (94%)	-0.00	3 (2%) 59 65	38, 51, 84, 103	0
2	DDD	125/132 (94%)	0.10	3 (2%) 59 65	40, 55, 89, 104	0
2	FFF	124/132 (93%)	-0.08	3 (2%) 59 65	36, 46, 74, 85	0
2	HHH	125/132 (94%)	0.11	4 (3%) 50 57	41, 54, 85, 101	0
2	JJJ	125/132 (94%)	0.14	3 (2%) 59 65	39, 55, 86, 96	0
2	LLL	125/132 (94%)	-0.14	4 (3%) 50 57	35, 47, 75, 82	0
All	All	1933/2052 (94%)	0.10	60 (3%) 51 58	35, 53, 89, 148	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	EEE	486	PHE	4.2
1	EEE	332	ILE	4.2
1	KKK	332	ILE	4.1
1	KKK	486	PHE	4.0
1	AAA	332	ILE	3.8
1	EEE	482	GLY	3.7
1	GGG	486	PHE	3.7
1	GGG	333	THR	3.7
2	FFF	56	THR	3.7
1	GGG	528	LYS	3.5
2	DDD	1	GLN	3.4

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Mol	Chain	Res	Type	RSRZ
1	AAA	486	PHE	3.4
2	HHH	56	THR	3.4
1	EEE	476	GLY	3.3
2	JJJ	56	THR	3.2
1	EEE	483	VAL	3.1
2	DDD	56	THR	3.1
1	EEE	333	THR	3.0
1	EEE	478	THR	3.0
1	CCC	486	PHE	3.0
1	CCC	445	VAL	2.9
1	EEE	479	PRO	2.9
1	III	372	ALA	2.9
1	EEE	475	ALA	2.8
1	KKK	519	HIS	2.8
2	BBB	56	THR	2.8
2	FFF	11	LEU	2.8
2	LLL	1	GLN	2.7
2	LLL	56	THR	2.7
1	CCC	371	SER	2.6
1	AAA	482	GLY	2.5
1	III	483	VAL	2.5
1	KKK	445	VAL	2.5
2	JJJ	1	GLN	2.5
1	EEE	477	SER	2.4
2	DDD	41	PRO	2.4
1	III	445	VAL	2.4
1	EEE	473	TYR	2.4
1	III	528	LYS	2.4
2	HHH	125	SER	2.4
1	AAA	483	VAL	2.4
2	HHH	11	LEU	2.3
2	FFF	27	ARG	2.3
1	CCC	528	LYS	2.3
1	EEE	480	CYS	2.2
1	EEE	474	GLN	2.2
1	EEE	528	LYS	2.2
2	BBB	11	LEU	2.2
2	LLL	125	SER	2.2
1	III	479	PRO	2.2
2	LLL	27	ARG	2.1
1	III	332	ILE	2.1
2	BBB	1	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	JJJ	125	SER	2.1
2	HHH	1	GLN	2.1
1	GGG	483	VAL	2.1
1	KKK	528	LYS	2.0
1	III	478	THR	2.0
1	III	475	ALA	2.0
1	KKK	517	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors($\text{\AA}^2$)	Q<0.9
3	NAG	GGG	601	14/15	0.56	0.17	76,86,94,95	0
3	NAG	KKK	601	14/15	0.79	0.15	72,84,88,89	0
3	NAG	III	601	14/15	0.83	0.12	72,80,89,96	0
3	NAG	AAA	601	14/15	0.96	0.06	44,46,49,53	0
3	NAG	CCC	601	14/15	0.96	0.06	48,53,57,58	0
3	NAG	EEE	601	14/15	0.96	0.06	44,50,57,58	0

6.5 Other polymers [i](#)

There are no such residues in this entry.