



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 12:26 PM UTC

PDB ID : 6ZLR / pdb_00006zlr
Title : Soaking competent crystal form of the SARS-CoV-2 Receptor Binding Domain (RBD):CR3022 complex.
Authors : de Nicola, G.F.; Nichols, C.E.
Deposited on : 2020-07-01
Resolution : 3.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<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

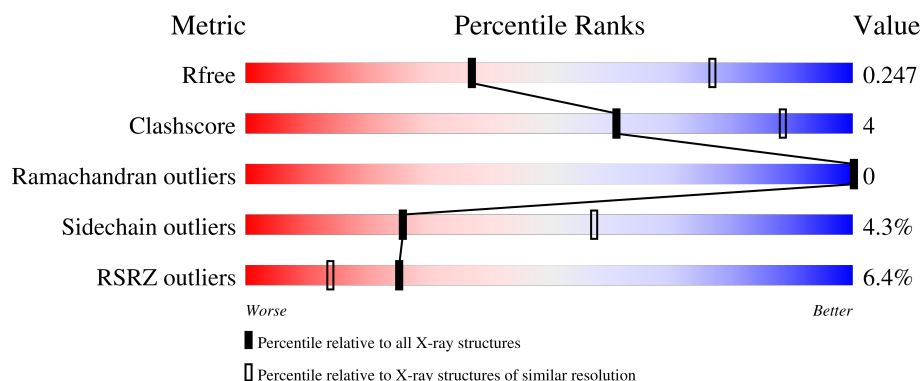
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 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	231	9% 75% 9% 15%
1	DDD	231	10% 77% 8% 15%
1	EEE	231	18% 77% 8% 15%
2	BBB	222	4% 83% 15% •
2	FFF	222	4% 85% 13% •

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Mol	Chain	Length	Quality of chain
2	HHH	222	3% 85% 14% .
3	CCC	221	2% 88% 10% ..
3	GGG	221	3% 90% 8% ..
3	LLL	221	% 89% 10% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14736 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 glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	EEE	196	Total	C	N	O	S	0	0	0
			1548	992	258	290	8			
1	AAA	196	Total	C	N	O	S	0	0	0
			1548	992	258	290	8			
1	DDD	196	Total	C	N	O	S	0	0	0
			1548	992	258	290	8			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
EEE	542	SER	-	expression tag	UNP P0DTC2
EEE	543	GLY	-	expression tag	UNP P0DTC2
EEE	544	HIS	-	expression tag	UNP P0DTC2
EEE	545	HIS	-	expression tag	UNP P0DTC2
EEE	546	HIS	-	expression tag	UNP P0DTC2
EEE	547	HIS	-	expression tag	UNP P0DTC2
EEE	548	HIS	-	expression tag	UNP P0DTC2
EEE	549	HIS	-	expression tag	UNP P0DTC2
AAA	542	SER	-	expression tag	UNP P0DTC2
AAA	543	GLY	-	expression tag	UNP P0DTC2
AAA	544	HIS	-	expression tag	UNP P0DTC2
AAA	545	HIS	-	expression tag	UNP P0DTC2
AAA	546	HIS	-	expression tag	UNP P0DTC2
AAA	547	HIS	-	expression tag	UNP P0DTC2
AAA	548	HIS	-	expression tag	UNP P0DTC2
AAA	549	HIS	-	expression tag	UNP P0DTC2
DDD	542	SER	-	expression tag	UNP P0DTC2
DDD	543	GLY	-	expression tag	UNP P0DTC2
DDD	544	HIS	-	expression tag	UNP P0DTC2
DDD	545	HIS	-	expression tag	UNP P0DTC2
DDD	546	HIS	-	expression tag	UNP P0DTC2
DDD	547	HIS	-	expression tag	UNP P0DTC2
DDD	548	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
DDD	549	HIS	-	expression tag	UNP P0DTC2

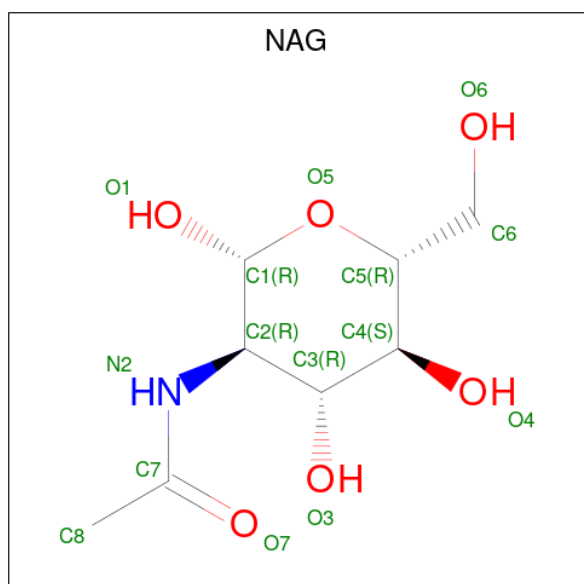
- Molecule 2 is a protein called CR3022 FAB HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	HHH	222	Total	C	N	O	S	0	0	0
			1647	1043	268	327	9			
2	BBB	222	Total	C	N	O	S	0	0	0
			1647	1043	268	327	9			
2	FFF	222	Total	C	N	O	S	0	0	0
			1647	1043	268	327	9			

- Molecule 3 is a protein called CR3022 FAB LIGHT CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	LLL	219	Total	C	N	O	S	0	0	0
			1703	1070	282	347	4			
3	CCC	219	Total	C	N	O	S	0	0	0
			1703	1070	282	347	4			
3	GGG	219	Total	C	N	O	S	0	0	0
			1703	1070	282	347	4			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

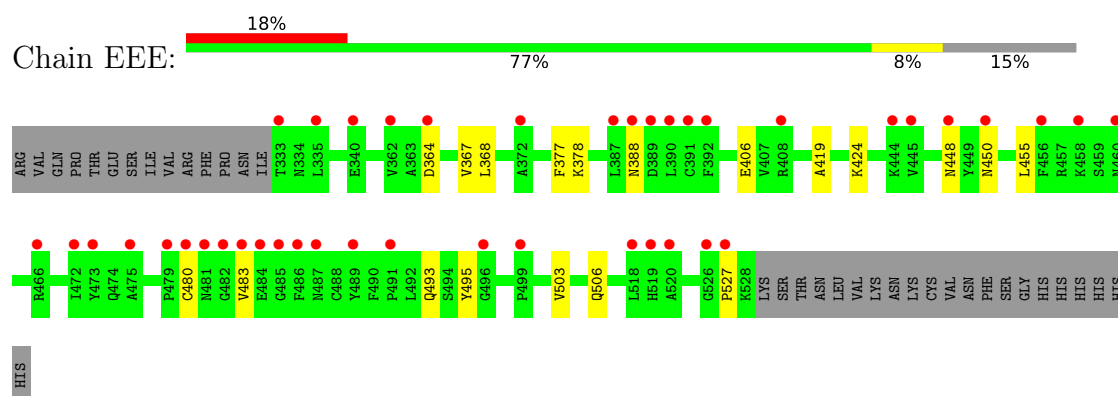


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	EEE	1	Total	C	N	O	0	0
			14	8	1	5		
4	AAA	1	Total	C	N	O	0	0
			14	8	1	5		
4	DDD	1	Total	C	N	O	0	0
			14	8	1	5		

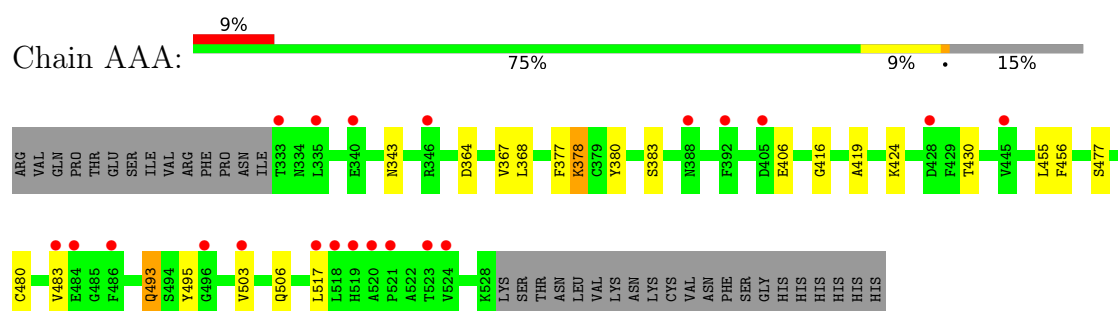
3 Residue-property plots [i](#)

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.

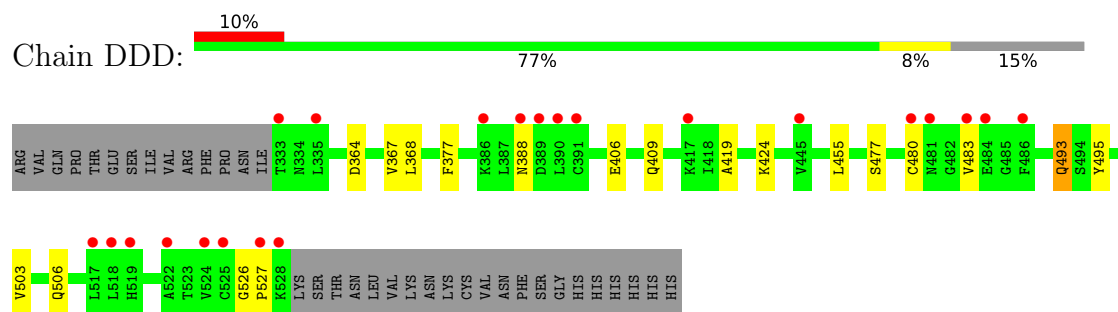
- Molecule 1: Spike glycoprotein



- Molecule 1: Spike glycoprotein

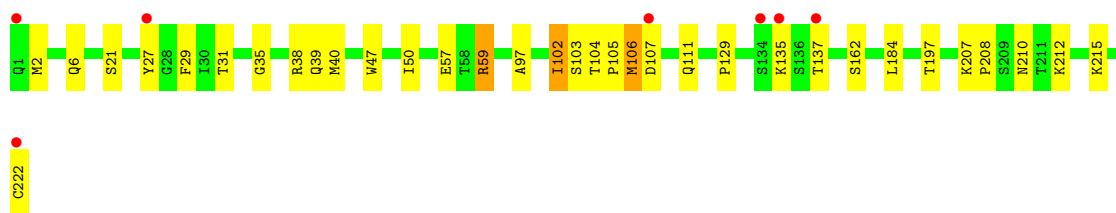


- Molecule 1: Spike glycoprotein

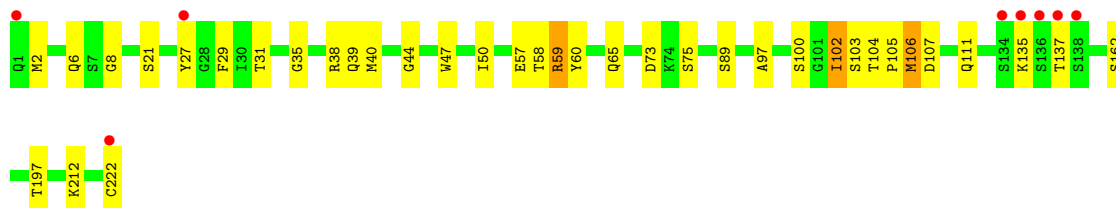


- Molecule 2: CR3022 FAB HEAVY CHAIN

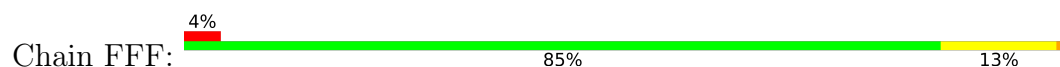




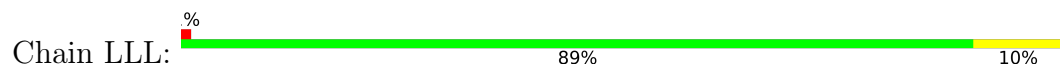
● Molecule 2: CR3022 FAB HEAVY CHAIN



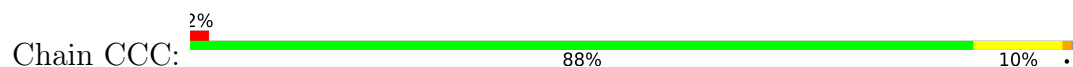
● Molecule 2: CR3022 FAB HEAVY CHAIN



● Molecule 3: CR3022 FAB LIGHT CHAIN



● Molecule 3: CR3022 FAB LIGHT CHAIN



● Molecule 3: CR3022 FAB LIGHT CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	207.13Å 207.13Å 199.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.03 – 3.10 68.03 – 3.10	Depositor EDS
% Data completeness (in resolution range)	90.5 (68.03-3.10) 90.5 (68.03-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.71 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.218 , 0.247 0.217 , 0.247	Depositor DCC
R_{free} test set	3669 reflections (4.64%)	wwPDB-VP
Wilson B-factor (Å ²)	52.5	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.000 for -h,-l,-k 0.001 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14736	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% 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	1.04	0/1592	1.38	1/2168 (0.0%)
1	DDD	1.04	0/1592	1.37	0/2168
1	EEE	1.02	0/1592	1.35	0/2168
2	BBB	1.02	2/1689 (0.1%)	1.39	11/2299 (0.5%)
2	FFF	1.01	0/1689	1.39	11/2299 (0.5%)
2	HHH	1.01	0/1689	1.40	11/2299 (0.5%)
3	CCC	1.00	0/1741	1.30	3/2367 (0.1%)
3	GGG	0.98	0/1741	1.29	2/2367 (0.1%)
3	LLL	1.00	0/1741	1.30	1/2367 (0.0%)
All	All	1.01	2/15066 (0.0%)	1.35	40/20502 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	44	GLY	C-O	5.08	1.28	1.23
2	BBB	8	GLY	C-O	5.06	1.29	1.23

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	102	ILE	N-CA-C	-7.77	97.39	108.58
2	FFF	102	ILE	N-CA-C	-7.33	98.03	108.58
2	HHH	102	ILE	N-CA-C	-7.15	98.29	108.58
2	BBB	137	THR	CA-C-N	6.32	128.74	120.28
2	BBB	137	THR	C-N-CA	6.32	128.74	120.28

There are no chirality outliers.

There are no planarity outliers.

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	1548	0	1462	18	0
1	DDD	1548	0	1460	8	0
1	EEE	1548	0	1461	9	0
2	BBB	1647	0	1623	25	0
2	FFF	1647	0	1623	20	0
2	HHH	1647	0	1623	21	0
3	CCC	1703	0	1649	18	0
3	GGG	1703	0	1649	13	0
3	LLL	1703	0	1649	14	0
4	AAA	14	0	13	4	0
4	DDD	14	0	13	0	0
4	EEE	14	0	13	1	0
All	All	14736	0	14238	122	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 4.

The worst 5 of 122 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:AAA:343:ASN:HD21	4:AAA:601:NAG:C1	1.31	1.38
1:AAA:343:ASN:ND2	4:AAA:601:NAG:C1	1.93	1.29
2:FFF:39:GLN:HE22	3:GGG:44:GLN:HE22	1.02	0.94
2:BBB:39:GLN:HE22	3:CCC:44:GLN:HE22	1.11	0.93
2:HHH:39:GLN:HE22	3:LLL:44:GLN:HE22	1.21	0.89

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	194/231 (84%)	185 (95%)	9 (5%)	0	100	100
1	DDD	194/231 (84%)	185 (95%)	9 (5%)	0	100	100
1	EEE	194/231 (84%)	185 (95%)	9 (5%)	0	100	100
2	BBB	220/222 (99%)	214 (97%)	6 (3%)	0	100	100
2	FFF	220/222 (99%)	212 (96%)	8 (4%)	0	100	100
2	HHH	220/222 (99%)	215 (98%)	5 (2%)	0	100	100
3	CCC	217/221 (98%)	206 (95%)	11 (5%)	0	100	100
3	GGG	217/221 (98%)	207 (95%)	10 (5%)	0	100	100
3	LLL	217/221 (98%)	206 (95%)	11 (5%)	0	100	100
All	All	1893/2022 (94%)	1815 (96%)	78 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	168/203 (83%)	161 (96%)	7 (4%)	26	58
1	DDD	168/203 (83%)	162 (96%)	6 (4%)	31	62
1	EEE	168/203 (83%)	164 (98%)	4 (2%)	43	69
2	BBB	187/187 (100%)	179 (96%)	8 (4%)	26	57
2	FFF	187/187 (100%)	179 (96%)	8 (4%)	26	57
2	HHH	187/187 (100%)	179 (96%)	8 (4%)	26	57
3	CCC	194/196 (99%)	184 (95%)	10 (5%)	21	51
3	GGG	194/196 (99%)	184 (95%)	10 (5%)	21	51
3	LLL	194/196 (99%)	184 (95%)	10 (5%)	21	51
All	All	1647/1758 (94%)	1576 (96%)	71 (4%)	26	57

5 of 71 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	FFF	135	LYS
2	FFF	212	LYS
3	GGG	87	GLU
1	AAA	378	LYS
1	AAA	377	PHE

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
4	NAG	AAA	601	-	14,14,15	0.69	0	17,19,21	1.10	0
4	NAG	DDD	601	1	14,14,15	0.66	0	17,19,21	1.94	4 (23%)
4	NAG	EEE	601	1	14,14,15	0.81	0	17,19,21	1.88	5 (29%)

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	AAA	601	-	-	2/6/23/26	0/1/1/1
4	NAG	DDD	601	1	-	2/6/23/26	0/1/1/1
4	NAG	EEE	601	1	-	4/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	DDD	601	NAG	C1-O5-C5	4.93	118.80	112.19
4	EEE	601	NAG	C1-O5-C5	-4.27	106.47	112.19
4	DDD	601	NAG	O5-C1-C2	4.04	117.54	111.29
4	EEE	601	NAG	O5-C5-C6	-3.08	101.67	107.66
4	EEE	601	NAG	C3-C4-C5	3.04	115.74	110.23

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	EEE	601	NAG	C8-C7-N2-C2
4	EEE	601	NAG	O7-C7-N2-C2
4	AAA	601	NAG	C8-C7-N2-C2
4	AAA	601	NAG	O7-C7-N2-C2
4	DDD	601	NAG	C8-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	AAA	601	NAG	4	0
4	EEE	601	NAG	1	0

5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	196/231 (84%)	0.73	21 (10%) 11 6	36, 65, 120, 143	0
1	DDD	196/231 (84%)	0.52	22 (11%) 10 5	33, 61, 116, 153	0
1	EEE	196/231 (84%)	1.10	42 (21%) 2 1	39, 95, 142, 165	0
2	BBB	222/222 (100%)	0.10	8 (3%) 46 26	27, 47, 79, 143	0
2	FFF	222/222 (100%)	-0.01	9 (4%) 41 23	28, 48, 82, 203	0
2	HHH	222/222 (100%)	-0.04	7 (3%) 50 30	26, 45, 88, 161	0
3	CCC	219/221 (99%)	0.02	5 (2%) 61 39	31, 51, 76, 98	0
3	GGG	219/221 (99%)	0.09	7 (3%) 50 30	33, 56, 90, 103	0
3	LLL	219/221 (99%)	0.05	2 (0%) 81 63	32, 54, 79, 115	0
All	All	1911/2022 (94%)	0.26	123 (6%) 25 14	26, 54, 114, 203	0

The worst 5 of 123 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	FFF	222	CYS	6.1
2	FFF	137	THR	5.2
1	AAA	484	GLU	4.9
1	AAA	518	LEU	4.6
1	EEE	483	VAL	4.6

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(Å ²)	Q<0.9
4	NAG	DDD	601	14/15	0.74	0.16	76,107,112,112	0
4	NAG	AAA	601	14/15	0.77	0.17	80,110,124,124	0
4	NAG	EEE	601	14/15	0.77	0.16	77,128,145,155	0

6.5 Other polymers [i](#)

There are no such residues in this entry.