



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:38 PM UTC

PDB ID : 6YZ7 / pdb_00006yz7
Title : H11-D4, SARS-CoV-2 RBD, CR3022 ternary complex
Authors : Naismith, J.H.; Ren, J.; Zhou, D.; Zhao, Y.; Stuart, D.I.
Deposited on : 2020-05-06
Resolution : 3.30 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

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

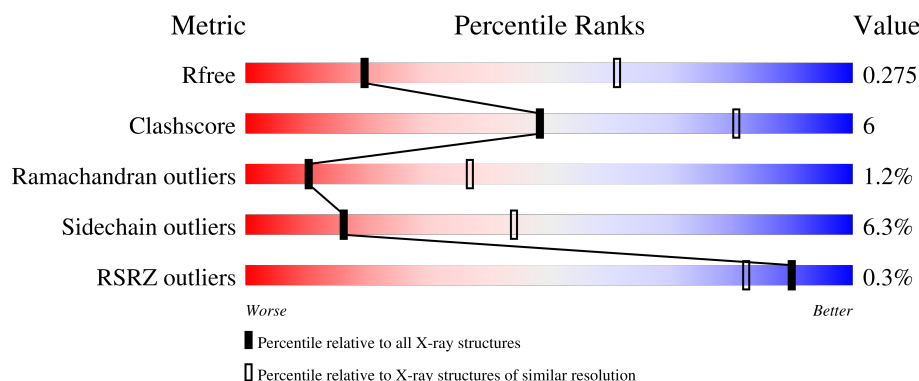
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	EEE	210	
2	BBB	229	
2	HHH	229	
3	CCC	220	

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Mol	Chain	Length	Quality of chain
3	LLL	220	81%18%•
4	DDD	134	% 74%19%• 5%
4	FFF	134	75%17%• 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11718 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	AAA	195	Total	C	N	O	S	0	0	0
			1545	991	258	288	8			
1	EEE	195	Total	C	N	O	S	0	0	0
			1545	991	258	288	8			

There are 14 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
EEE	533	LYS	-	expression tag	UNP P0DTC2
EEE	534	HIS	-	expression tag	UNP P0DTC2
EEE	535	HIS	-	expression tag	UNP P0DTC2
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

- Molecule 2 is a protein called Antibody Cr3022.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	BBB	216	Total	C	N	O	S	0	1	0
			1609	1023	261	317	8			
2	HHH	216	Total	C	N	O	S	0	1	0
			1609	1023	261	317	8			

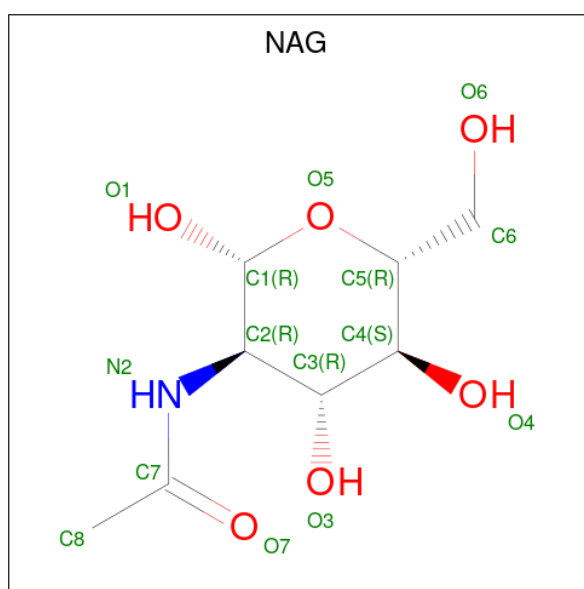
- Molecule 3 is a protein called Antibody light chain.

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

- Molecule 4 is a protein called Nanobody.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	DDD	127	Total	C	N	O	S	0	0	0
			988	621	173	189	5			
4	FFF	127	Total	C	N	O	S	0	0	0
			988	621	173	189	5			

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



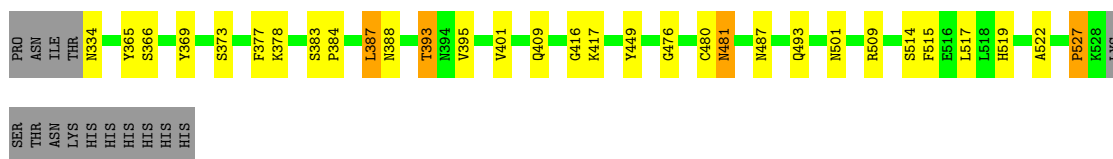
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	AAA	1	Total	C	N	O	0	0
			14	8	1	5		
5	EEE	1	Total	C	N	O	0	0
			14	8	1	5		

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.

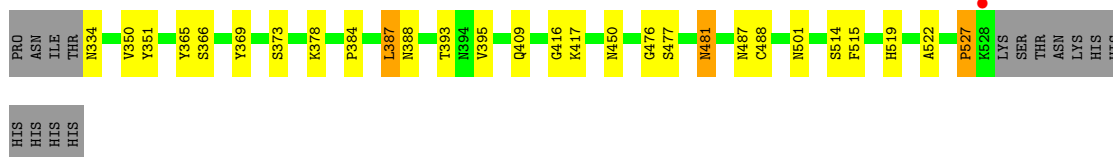
- Molecule 1: Spike glycoprotein

Chain AAA: 



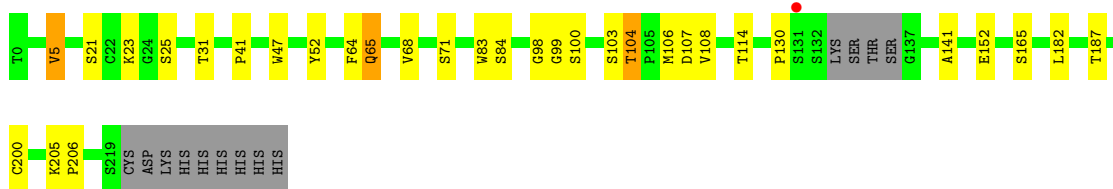
- Molecule 1: Spike glycoprotein

Chain EEE: 



- Molecule 2: Antibody Cr3022

Chain BBB: 



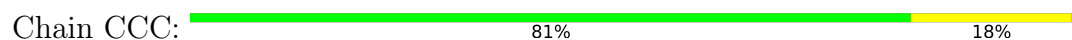
- Molecule 2: Antibody Cr3022

Chain HHH: 

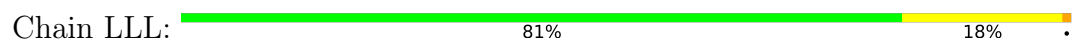




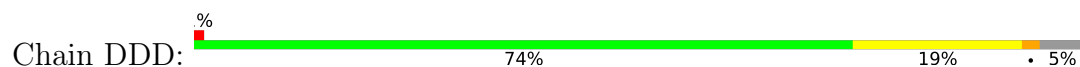
• Molecule 3: Antibody light chain



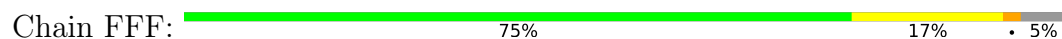
• Molecule 3: Antibody light chain



• Molecule 4: Nanobody



• Molecule 4: Nanobody



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	154.60Å 154.60Å 229.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	128.19 – 3.30 128.19 – 3.30	Depositor EDS
% Data completeness (in resolution range)	96.3 (128.19-3.30) 96.3 (128.19-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 3.33Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.238 , 0.269 0.242 , 0.275	Depositor DCC
R_{free} test set	2016 reflections (4.73%)	wwPDB-VP
Wilson B-factor (Å ²)	128.1	Xtrriage
Anisotropy	0.005	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 148.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11718	wwPDB-VP
Average B, all atoms (Å ²)	157.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.63 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.1168e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

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	1.00	0/1589	1.35	1/2162 (0.0%)
1	EEE	0.99	0/1589	1.32	0/2162
2	BBB	1.02	0/1654	1.31	1/2253 (0.0%)
2	HHH	1.01	0/1654	1.31	1/2253 (0.0%)
3	CCC	1.01	0/1741	1.33	5/2367 (0.2%)
3	LLL	1.00	0/1741	1.32	5/2367 (0.2%)
4	DDD	1.04	0/1010	1.37	1/1366 (0.1%)
4	FFF	1.00	0/1010	1.37	1/1366 (0.1%)
All	All	1.01	0/11988	1.33	15/16296 (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

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	107	ASP	CA-CB-CG	6.21	118.81	112.60
3	CCC	107	GLY	CA-C-O	-6.20	117.95	122.23
2	HHH	107	ASP	CA-CB-CG	6.13	118.73	112.60
1	AAA	493	GLN	OE1-CD-NE2	5.72	128.32	122.60
3	LLL	107	GLY	CA-C-O	-5.53	118.42	122.23
4	FFF	120	GLY	CA-C-O	-5.48	117.53	122.57
3	LLL	65	PRO	CA-C-N	5.42	127.54	120.28
3	LLL	65	PRO	C-N-CA	5.42	127.54	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	CCC	173	ASP	CA-C-N	5.39	128.24	120.38
3	CCC	173	ASP	C-N-CA	5.39	128.24	120.38
4	DDD	120	GLY	CA-C-O	-5.27	117.72	122.57
3	LLL	173	ASP	CA-C-N	5.24	128.03	120.38
3	LLL	173	ASP	C-N-CA	5.24	128.03	120.38
3	CCC	65	PRO	CA-C-N	5.09	127.09	120.28
3	CCC	65	PRO	C-N-CA	5.09	127.09	120.28

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	BBB	98	GLY	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	1545	0	1465	15	0
1	EEE	1545	0	1465	13	0
2	BBB	1609	0	1585	12	0
2	HHH	1609	0	1585	17	0
3	CCC	1703	0	1649	15	0
3	LLL	1703	0	1649	17	0
4	DDD	988	0	951	24	0
4	FFF	988	0	951	24	0
5	AAA	14	0	13	0	0
5	EEE	14	0	13	0	0
All	All	11718	0	11326	127	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 6.

All (127) 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)
4:DDD:60:TYR:OH	4:DDD:70:ILE:N	1.68	1.26
4:FFF:60:TYR:OH	4:FFF:70:ILE:N	1.69	1.23
4:DDD:60:TYR:OH	4:DDD:69:THR:CA	1.94	1.15
4:FFF:60:TYR:OH	4:FFF:69:THR:CA	1.94	1.14
4:FFF:60:TYR:OH	4:FFF:69:THR:HA	1.47	1.13
4:DDD:60:TYR:OH	4:DDD:69:THR:HA	1.48	1.13
4:DDD:60:TYR:OH	4:DDD:69:THR:C	2.02	1.01
4:FFF:60:TYR:OH	4:FFF:69:THR:C	2.02	1.00
4:FFF:60:TYR:HH	4:FFF:70:ILE:N	1.60	0.91
4:DDD:60:TYR:HH	4:DDD:70:ILE:N	1.69	0.90
3:CCC:85:GLN:HE21	3:CCC:85:GLN:HA	1.48	0.78
3:LLL:34:ILE:O	3:LLL:36:LYS:N	2.23	0.72
4:DDD:60:TYR:HH	4:DDD:69:THR:C	1.92	0.70
4:DDD:17:SER:HA	4:DDD:86:LEU:HD11	1.74	0.69
4:FFF:60:TYR:HH	4:FFF:69:THR:C	1.90	0.69
3:CCC:34:ILE:O	3:CCC:36:LYS:N	2.26	0.69
4:FFF:17:SER:HA	4:FFF:86:LEU:HD11	1.75	0.69
1:EEE:365:TYR:CD2	1:EEE:387:LEU:HD13	2.30	0.66
2:HHH:152:GLU:HB2	2:HHH:153:PRO:HA	1.77	0.66
4:DDD:60:TYR:CZ	4:DDD:69:THR:HA	2.31	0.65
3:CCC:153:GLN:HG2	3:CCC:160:LEU:HD22	1.80	0.64
4:FFF:60:TYR:CZ	4:FFF:69:THR:HA	2.31	0.64
3:LLL:153:GLN:HG2	3:LLL:160:LEU:HD22	1.80	0.62
2:BBB:47:TRP:CD1	2:BBB:106:MET:HE1	2.35	0.61
1:AAA:481:ASN:N	1:AAA:481:ASN:OD1	2.34	0.61
2:HHH:47:TRP:CD1	2:HHH:106:MET:HE1	2.34	0.61
4:DDD:87:LYS:O	4:DDD:125:VAL:HG21	1.99	0.61
4:FFF:87:LYS:O	4:FFF:125:VAL:HG21	2.00	0.61
1:EEE:481:ASN:OD1	1:EEE:481:ASN:N	2.35	0.59
1:AAA:365:TYR:CD1	1:AAA:387:LEU:HD13	2.39	0.58
4:FFF:60:TYR:CE1	4:FFF:70:ILE:HG22	2.39	0.57
4:DDD:60:TYR:CE1	4:DDD:70:ILE:HG22	2.40	0.57
2:HHH:64:PHE:O	2:HHH:65:GLN:C	2.48	0.57
2:BBB:64:PHE:O	2:BBB:65:GLN:C	2.48	0.57
1:AAA:517:LEU:HB3	3:CCC:34:ILE:HG22	1.87	0.56
3:LLL:56:TRP:CD1	3:LLL:97:TYR:HH	2.23	0.56
3:LLL:67:ARG:HB2	3:LLL:82:SER:O	2.05	0.56
1:EEE:384:PRO:HA	1:EEE:387:LEU:HG	1.87	0.56
4:DDD:20:LEU:HD12	4:DDD:83:MET:SD	2.46	0.55
4:FFF:20:LEU:HD12	4:FFF:83:MET:SD	2.47	0.54
1:AAA:384:PRO:HA	1:AAA:387:LEU:HG	1.90	0.54
3:CCC:67:ARG:HB2	3:CCC:82:SER:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:CCC:56:TRP:CD1	3:CCC:97:TYR:HH	2.26	0.54
1:EEE:395:VAL:HG22	1:EEE:515:PHE:CD1	2.44	0.53
1:AAA:395:VAL:HG22	1:AAA:515:PHE:CD1	2.44	0.53
4:DDD:60:TYR:HH	4:DDD:69:THR:CA	2.11	0.53
4:FFF:17:SER:CA	4:FFF:86:LEU:HD11	2.37	0.53
1:AAA:449:TYR:HB3	4:DDD:101:ASN:HA	1.92	0.52
1:AAA:378:LYS:HG3	2:BBB:52:TYR:CE2	2.45	0.52
4:DDD:17:SER:CA	4:DDD:86:LEU:HD11	2.38	0.51
4:FFF:39:GLN:HB2	4:FFF:45:ARG:HB2	1.93	0.50
2:BBB:205:LYS:HB2	2:BBB:206:PRO:HD3	1.94	0.49
1:AAA:384:PRO:HD2	2:BBB:100:SER:O	2.12	0.49
4:FFF:86:LEU:HD12	4:FFF:86:LEU:H	1.77	0.49
2:BBB:99:GLY:HA3	2:BBB:104:THR:CG2	2.43	0.49
3:LLL:72:GLY:HA3	3:LLL:77:PHE:CD1	2.47	0.48
4:DDD:86:LEU:H	4:DDD:86:LEU:HD12	1.76	0.48
2:BBB:130:PRO:HB3	2:BBB:141:ALA:O	2.14	0.48
3:CCC:72:GLY:HA3	3:CCC:77:PHE:CD1	2.50	0.47
4:FFF:16:GLY:O	4:FFF:86:LEU:HD12	2.13	0.47
2:HHH:149:TYR:CE1	2:HHH:154:VAL:HG23	2.49	0.47
1:AAA:476:GLY:H	1:AAA:487:ASN:HB3	1.78	0.47
2:BBB:5:VAL:HG22	2:BBB:23:LYS:HB3	1.96	0.47
2:HHH:182:LEU:C	2:HHH:182:LEU:HD23	2.40	0.47
1:EEE:450:ASN:HD21	4:FFF:30:SER:HB3	1.80	0.47
2:BBB:182:LEU:C	2:BBB:182:LEU:HD23	2.40	0.46
4:DDD:20:LEU:CD1	4:DDD:83:MET:SD	3.03	0.46
4:FFF:68:PHE:HA	4:FFF:82:GLN:O	2.16	0.46
4:DDD:68:PHE:HA	4:DDD:82:GLN:O	2.16	0.46
2:HHH:130:PRO:HB3	2:HHH:141:ALA:O	2.16	0.46
2:BBB:68:VAL:HG12	2:BBB:83:TRP:CD1	2.50	0.46
4:DDD:16:GLY:O	4:DDD:86:LEU:HD12	2.16	0.46
2:HHH:188:VAL:CG1	2:HHH:192:SER:HB2	2.46	0.46
4:DDD:39:GLN:HB2	4:DDD:45:ARG:HB2	1.99	0.45
1:AAA:366:SER:HA	1:AAA:369:TYR:CZ	2.52	0.45
3:CCC:89:VAL:CG2	3:CCC:112:ILE:HG12	2.46	0.45
2:HHH:13:LYS:HE3	2:HHH:119:SER:HB3	1.97	0.45
2:HHH:105:PRO:HD3	3:LLL:97:TYR:CE2	2.51	0.45
4:DDD:48:VAL:O	4:DDD:61:ALA:CB	2.65	0.45
4:DDD:45:ARG:O	4:DDD:45:ARG:NE	2.48	0.45
2:HHH:5:VAL:HG22	2:HHH:23:LYS:HB3	1.98	0.45
1:EEE:476:GLY:H	1:EEE:487:ASN:HB3	1.81	0.45
4:FFF:20:LEU:CD1	4:FFF:83:MET:SD	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:LLL:130:GLN:HE22	3:LLL:137:SER:CB	2.29	0.45
1:EEE:393:THR:HA	1:EEE:522:ALA:HA	1.98	0.45
3:CCC:130:GLN:HE22	3:CCC:137:SER:CB	2.30	0.44
4:FFF:48:VAL:O	4:FFF:61:ALA:CB	2.65	0.44
4:FFF:60:TYR:HH	4:FFF:69:THR:CA	2.16	0.44
3:LLL:56:TRP:HD1	3:LLL:97:TYR:HH	1.62	0.44
1:AAA:393:THR:HA	1:AAA:522:ALA:HA	1.98	0.44
1:AAA:409:GLN:HE22	1:AAA:416:GLY:HA3	1.83	0.44
4:DDD:12:MET:CE	4:DDD:16:GLY:HA3	2.48	0.44
1:AAA:401:VAL:HG22	1:AAA:509:ARG:HG2	2.00	0.43
2:HHH:68:VAL:HG12	2:HHH:83:TRP:CD1	2.53	0.43
4:DDD:91:THR:OG1	4:DDD:125:VAL:HG23	2.19	0.43
3:LLL:89:VAL:CG2	3:LLL:112:ILE:HG12	2.49	0.43
1:EEE:388:ASN:HB2	1:EEE:527:PRO:HD2	2.01	0.43
4:FFF:91:THR:OG1	4:FFF:125:VAL:HG23	2.18	0.43
1:EEE:365:TYR:CD2	1:EEE:387:LEU:CD1	3.01	0.43
4:FFF:45:ARG:O	4:FFF:45:ARG:NE	2.49	0.43
2:HHH:188:VAL:CG1	2:HHH:192:SER:CB	2.97	0.42
3:LLL:146:TYR:CG	3:LLL:147:PRO:HA	2.54	0.42
4:DDD:36:TRP:O	4:DDD:48:VAL:HB	2.20	0.42
3:CCC:146:TYR:CG	3:CCC:147:PRO:HA	2.54	0.42
1:EEE:366:SER:HA	1:EEE:369:TYR:CZ	2.53	0.42
3:LLL:2:ILE:HG22	3:LLL:3:GLN:N	2.34	0.42
1:AAA:388:ASN:HB2	1:AAA:527:PRO:HD2	2.01	0.42
3:LLL:182:SER:O	3:LLL:182:SER:OG	2.36	0.42
1:EEE:378:LYS:HG3	2:HHH:52:TYR:CE2	2.55	0.42
2:HHH:99:GLY:HA3	2:HHH:104:THR:CG2	2.48	0.42
3:LLL:142:LEU:HD12	3:LLL:142:LEU:N	2.35	0.42
3:CCC:60:ARG:HD3	3:CCC:68:PHE:O	2.21	0.41
3:LLL:60:ARG:HD3	3:LLL:68:PHE:O	2.20	0.41
1:AAA:377:PHE:CD1	2:BBB:31:THR:HG22	2.56	0.41
2:BBB:47:TRP:NE1	2:BBB:106:MET:HE1	2.35	0.41
3:CCC:142:LEU:HD12	3:CCC:142:LEU:N	2.34	0.41
3:CCC:63:GLY:HA3	2:HHH:1:GLN:HA	2.01	0.41
1:EEE:409:GLN:HE22	1:EEE:416:GLY:HA3	1.84	0.41
3:CCC:56:TRP:HD1	3:CCC:97:TYR:HH	1.65	0.41
4:FFF:40:ALA:HB1	4:FFF:41:PRO:HD2	2.03	0.41
3:LLL:172:GLN:HG3	3:LLL:179:TYR:CE1	2.56	0.41
3:LLL:187:LEU:HD11	3:LLL:192:TYR:HA	2.03	0.41
3:CCC:2:ILE:HG22	3:CCC:3:GLN:N	2.36	0.40
4:FFF:12:MET:CE	4:FFF:16:GLY:HA3	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:350:VAL:HG13	1:EEE:351:TYR:N	2.36	0.40
2:HHH:0:THR:OG1	2:HHH:1:GLN:N	2.55	0.40
2:HHH:170:PHE:CE1	3:LLL:170:THR:HG23	2.56	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	193/210 (92%)	169 (88%)	23 (12%)	1 (0%)	24	55
1	EEE	193/210 (92%)	170 (88%)	22 (11%)	1 (0%)	24	55
2	BBB	213/229 (93%)	189 (89%)	21 (10%)	3 (1%)	9	33
2	HHH	213/229 (93%)	189 (89%)	21 (10%)	3 (1%)	9	33
3	CCC	217/220 (99%)	197 (91%)	14 (6%)	6 (3%)	4	21
3	LLL	217/220 (99%)	198 (91%)	15 (7%)	4 (2%)	6	29
4	DDD	125/134 (93%)	116 (93%)	9 (7%)	0	100	100
4	FFF	125/134 (93%)	116 (93%)	9 (7%)	0	100	100
All	All	1496/1586 (94%)	1344 (90%)	134 (9%)	18 (1%)	10	37

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	BBB	165	SER
3	CCC	35	ASN
3	LLL	35	ASN
1	AAA	527	PRO
2	BBB	65	GLN
1	EEE	527	PRO
2	HHH	65	GLN

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Mol	Chain	Res	Type
2	HHH	165	SER
3	CCC	56	TRP
3	CCC	144	ASN
3	LLL	144	ASN
3	CCC	208	SER
3	LLL	56	TRP
3	LLL	208	SER
3	CCC	86	ALA
3	CCC	149	GLU
2	HHH	41	PRO
2	BBB	41	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	AAA	168/183 (92%)	157 (94%)	11 (6%)	15	43
1	EEE	168/183 (92%)	158 (94%)	10 (6%)	17	46
2	BBB	182/194 (94%)	170 (93%)	12 (7%)	15	43
2	HHH	182/194 (94%)	171 (94%)	11 (6%)	17	46
3	CCC	194/195 (100%)	183 (94%)	11 (6%)	18	47
3	LLL	194/195 (100%)	185 (95%)	9 (5%)	24	53
4	DDD	101/108 (94%)	91 (90%)	10 (10%)	7	27
4	FFF	101/108 (94%)	94 (93%)	7 (7%)	14	41
All	All	1290/1360 (95%)	1209 (94%)	81 (6%)	16	44

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	334	ASN
1	AAA	373	SER
1	AAA	383	SER
1	AAA	387	LEU

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Mol	Chain	Res	Type
1	AAA	393	THR
1	AAA	417	LYS
1	AAA	480	CYS
1	AAA	481	ASN
1	AAA	501	ASN
1	AAA	514	SER
1	AAA	519	HIS
2	BBB	5	VAL
2	BBB	21	SER
2	BBB	25	SER
2	BBB	71	SER
2	BBB	84	SER
2	BBB	103	SER
2	BBB	104	THR
2	BBB	108	VAL
2	BBB	114	THR
2	BBB	152	GLU
2	BBB	187	THR
2	BBB	200	CYS
3	CCC	5	THR
3	CCC	26	SER
3	CCC	31	TYR
3	CCC	43	GLN
3	CCC	59	THR
3	CCC	66	ASP
3	CCC	85	GLN
3	CCC	95	GLN
3	CCC	128	ASP
3	CCC	174	SER
3	CCC	182	SER
4	DDD	3	GLN
4	DDD	20	LEU
4	DDD	30	SER
4	DDD	45	ARG
4	DDD	57	SER
4	DDD	62	ASP
4	DDD	65	LYS
4	DDD	72	ARG
4	DDD	121	THR
4	DDD	125	VAL
1	EEE	334	ASN
1	EEE	373	SER

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Mol	Chain	Res	Type
1	EEE	387	LEU
1	EEE	417	LYS
1	EEE	477	SER
1	EEE	481	ASN
1	EEE	488	CYS
1	EEE	501	ASN
1	EEE	514	SER
1	EEE	519	HIS
4	FFF	20	LEU
4	FFF	45	ARG
4	FFF	57	SER
4	FFF	62	ASP
4	FFF	72	ARG
4	FFF	121	THR
4	FFF	125	VAL
2	HHH	5	VAL
2	HHH	21	SER
2	HHH	71	SER
2	HHH	84	SER
2	HHH	103	SER
2	HHH	104	THR
2	HHH	108	VAL
2	HHH	114	THR
2	HHH	187	THR
2	HHH	200	CYS
2	HHH	208	ASN
3	LLL	5	THR
3	LLL	26	SER
3	LLL	31	TYR
3	LLL	43	GLN
3	LLL	59	THR
3	LLL	66	ASP
3	LLL	95	GLN
3	LLL	174	SER
3	LLL	182	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 [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](#)

2 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	$\# Z > 2$
5	NAG	EEE	601	1	14,14,15	0.31	0	17,19,21	1.04	1 (5%)
5	NAG	AAA	601	1	14,14,15	0.35	0	17,19,21	1.04	1 (5%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	EEE	601	NAG	C4-C3-C2	-2.98	106.65	111.02
5	AAA	601	NAG	O5-C1-C2	-2.64	107.21	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	AAA	601	NAG	O5-C5-C6-O6
5	AAA	601	NAG	C4-C5-C6-O6
5	EEE	601	NAG	O5-C5-C6-O6
5	EEE	601	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	195/210 (92%)	-0.38	0 100 100	130, 167, 212, 245	0
1	EEE	195/210 (92%)	-0.44	1 (0%) 87 76	114, 135, 182, 226	0
2	BBB	216/229 (94%)	-0.47	1 (0%) 87 76	111, 150, 183, 206	1 (0%)
2	HHH	216/229 (94%)	-0.41	2 (0%) 81 65	99, 134, 193, 216	1 (0%)
3	CCC	219/220 (99%)	-0.48	0 100 100	113, 148, 174, 200	0
3	LLL	219/220 (99%)	-0.48	0 100 100	104, 143, 172, 197	0
4	DDD	127/134 (94%)	-0.02	1 (0%) 82 68	214, 271, 304, 315	0
4	FFF	127/134 (94%)	-0.35	0 100 100	117, 140, 171, 207	0
All	All	1514/1586 (95%)	-0.40	5 (0%) 90 82	99, 148, 267, 315	2 (0%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	BBB	131[A]	SER	2.4
1	EEE	528	LYS	2.2
2	HHH	132	SER	2.2
4	DDD	35	GLY	2.2
2	HHH	131[A]	SER	2.2

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
5	NAG	AAA	601	14/15	0.82	0.09	162,172,176,179	0
5	NAG	EEE	601	14/15	0.93	0.07	140,150,156,157	0

6.5 Other polymers [i](#)

There are no such residues in this entry.