



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 01:28 PM BST

PDB ID : 6YZ7
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 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) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

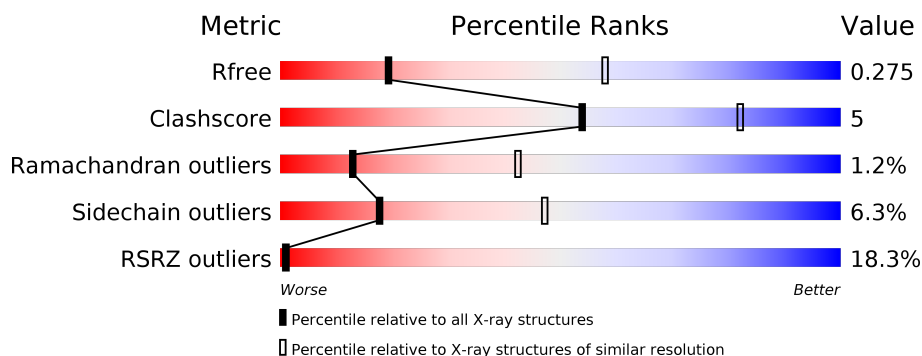
1 Overall quality at a glance

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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	<div> <div>19%</div> <div>79%</div> <div>12%</div> <div>7%</div> </div>
1	EEE	210	<div> <div>10%</div> <div>80%</div> <div>12%</div> <div>7%</div> </div>
2	BBB	229	<div> <div>14%</div> <div>82%</div> <div>11%</div> <div>6%</div> </div>
2	HHH	229	<div> <div>10%</div> <div>79%</div> <div>14%</div> <div>6%</div> </div>
3	CCC	220	<div> <div>11%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>
3	LLL	220	<div> <div>12%</div> <div>82%</div> <div>16%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
4	DDD	134	<div><div></div><div>70%</div><div></div><div>75%</div><div></div><div>18%</div><div></div><div>• 5%</div></div>
4	FFF	134	<div><div></div><div>12%</div><div></div><div>76%</div><div></div><div>16%</div><div></div><div>• 5%</div></div>

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			

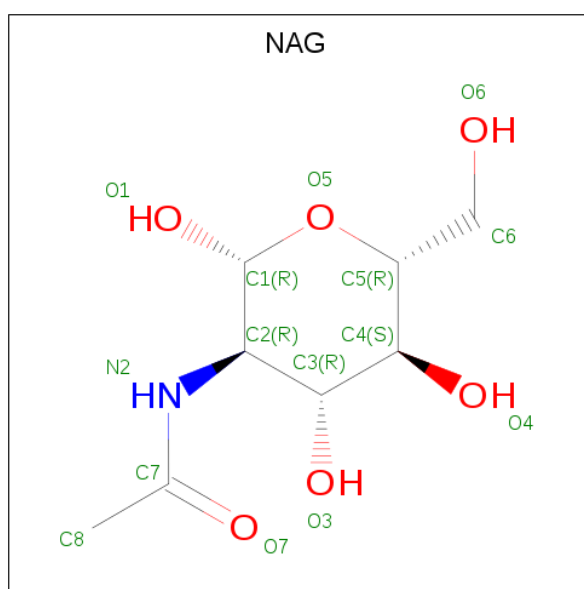
- Molecule 3 is a protein called Antibody light chain.

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 (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

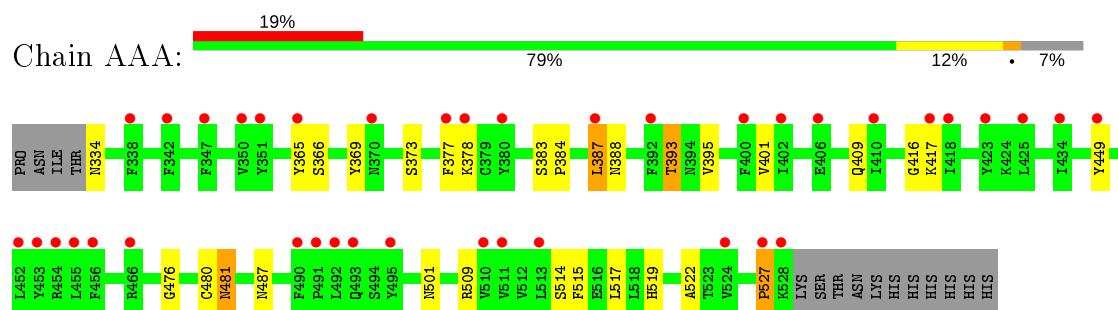


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	AAA	1	Total	C	N	O	0	0
			14	8	1	5		
5	EEE	1	Total	C	N	O	0	0
			14	8	1	5		

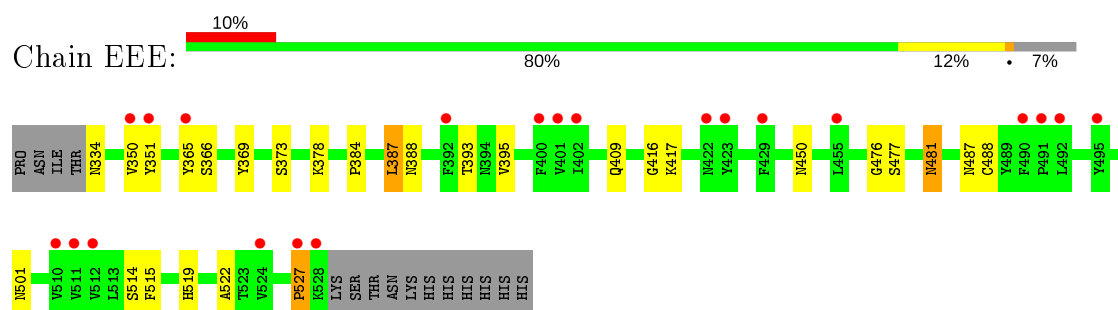
3 Residue-property plots [i](#)

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.

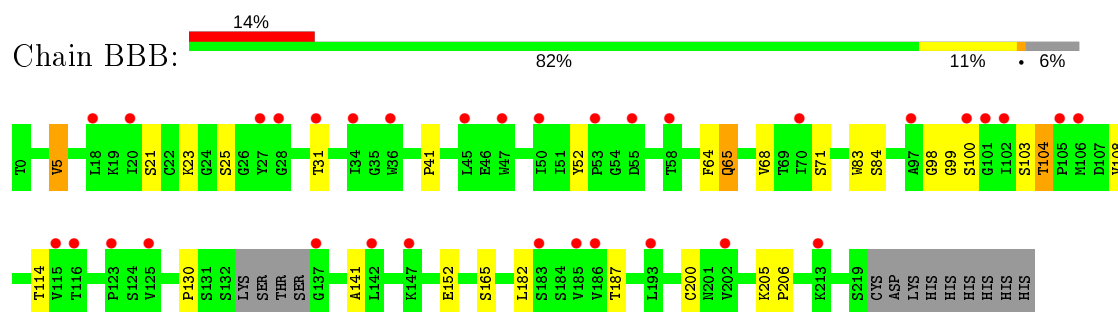
- Molecule 1: Spike glycoprotein



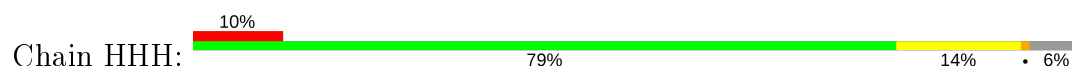
- Molecule 1: Spike glycoprotein

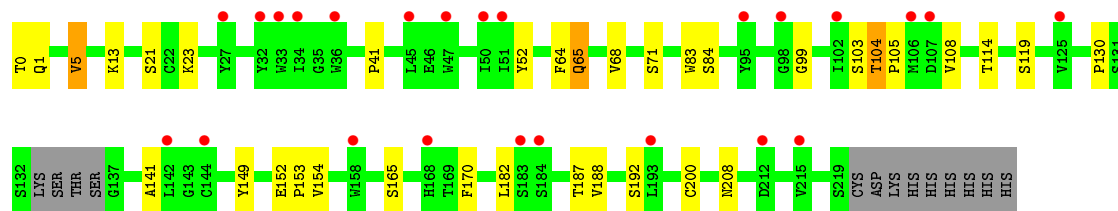


- Molecule 2: Antibody Cr3022

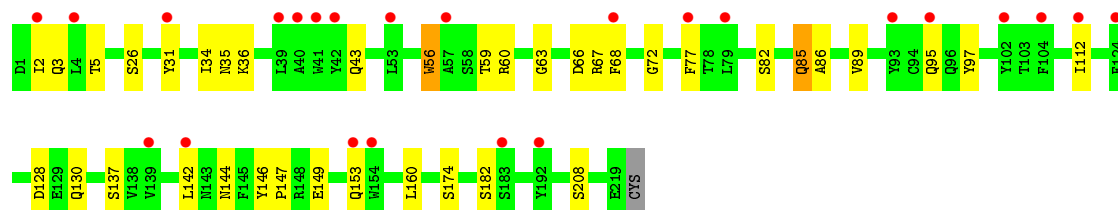
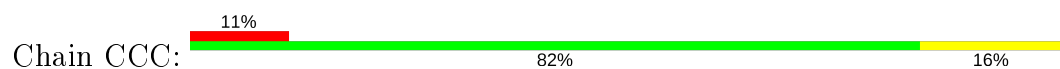


- Molecule 2: Antibody Cr3022

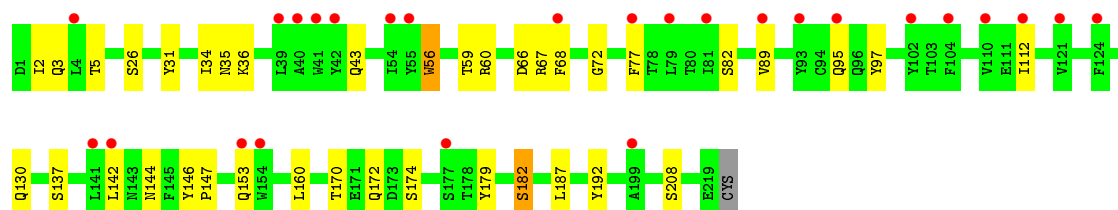
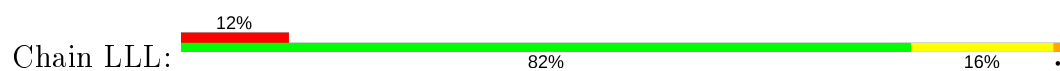




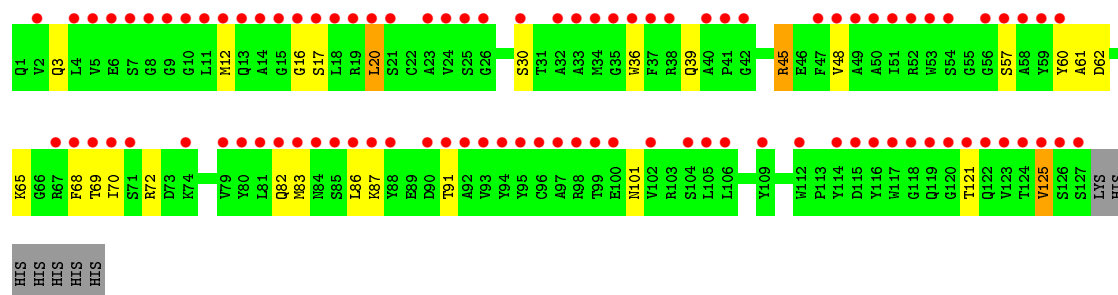
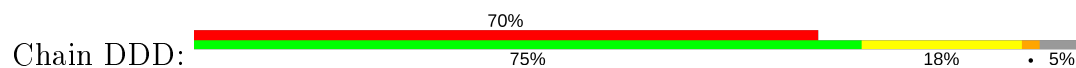
• Molecule 3: Antibody light chain



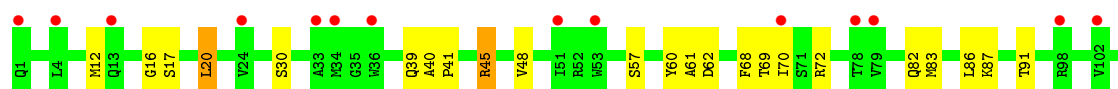
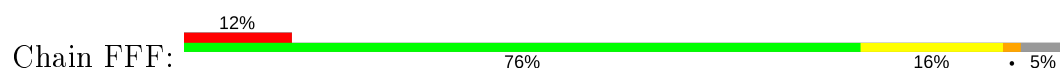
• Molecule 3: Antibody light chain



• 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	154.60 Å 154.60 Å 229.31 Å 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 3.33 Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.238 , 0.269 0.242 , 0.275	Depositor DCC
R_{free} test set	1945 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	128.1	Xtriage
Anisotropy	0.005	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 129.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11718	wwPDB-VP
Average B, all atoms (Å ²)	157.0	wwPDB-VP

Xtriage'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

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	0.66	0/1589	0.79	0/2162
1	EEE	0.65	0/1589	0.80	0/2162
2	BBB	0.67	0/1654	0.79	0/2253
2	HHH	0.66	0/1654	0.81	0/2253
3	CCC	0.66	0/1741	0.80	0/2367
3	LLL	0.66	0/1741	0.80	0/2367
4	DDD	0.68	0/1010	0.81	0/1366
4	FFF	0.65	0/1010	0.82	0/1366
All	All	0.66	0/11988	0.80	0/16296

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.

There are no bond angle outliers.

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	10	0
2	HHH	1609	0	1585	16	0
3	CCC	1703	0	1649	14	0
3	LLL	1703	0	1649	16	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	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 5.

All (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)
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	0.96
4:FFF:60:TYR:OH	4:FFF:69:THR:C	2.02	0.96
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:17:SER:HA	4:DDD:86:LEU:HD11	1.74	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
4:DDD:60:TYR:HH	4:DDD:69:THR:C	1.92	0.66
1:EEE:365:TYR:CD2	1:EEE:387:LEU:HD13	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:FFF:60:TYR:HH	4:FFF:69:THR:C	1.90	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
4:DDD:60:TYR:HH	4:DDD:69:THR:CA	2.11	0.63
3:LLL:153:GLN:HG2	3:LLL:160:LEU:HD22	1.80	0.62
1:AAA:481:ASN:N	1:AAA:481:ASN:OD1	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
1:AAA:517:LEU:HB3	3:CCC:34:ILE:HG22	1.87	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
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:FFF:17:SER:CA	4:FFF:86:LEU:HD11	2.37	0.53
2:HHH:64:PHE:O	2:HHH:65:GLN:C	2.48	0.52
2:BBB:64:PHE:O	2:BBB:65:GLN:C	2.48	0.52
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:H	4:FFF:86:LEU:HD12	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:HD12	4:DDD:86:LEU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:BBB:5:VAL:HG22	2:BBB:23:LYS:HB3	1.96	0.47
1:EEE:450:ASN:HD21	4:FFF:30:SER:HB3	1.80	0.47
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:105:PRO:HD3	3:LLL:97:TYR:CE2	2.51	0.45
2:HHH:13:LYS:HE3	2:HHH:119:SER:HB3	1.97	0.45
4:DDD:48:VAL:O	4:DDD:61:ALA:CB	2.65	0.45
4:DDD:45:ARG:NE	4:DDD:45:ARG:O	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
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:NE	4:FFF:45:ARG:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:HHH:182:LEU:C	2:HHH:182:LEU:HD23	2.40	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
2:BBB:182:LEU:C	2:BBB:182:LEU:HD23	2.40	0.41
3:CCC:56:TRP:HD1	3:CCC:97:TYR:HH	1.64	0.41
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
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: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	0.41
4:FFF:40:ALA:HB1	4:FFF:41:PRO:HD2	2.03	0.41
4:FFF:12:MET:CE	4:FFF:16:GLY:HA3	2.51	0.40
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%)	29 61
1	EEE	193/210 (92%)	170 (88%)	22 (11%)	1 (0%)	29 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	BBB	213/229 (93%)	189 (89%)	21 (10%)	3 (1%)	11	38
2	HHH	213/229 (93%)	189 (89%)	21 (10%)	3 (1%)	11	38
3	CCC	217/220 (99%)	197 (91%)	14 (6%)	6 (3%)	5	25
3	LLL	217/220 (99%)	198 (91%)	15 (7%)	4 (2%)	8	35
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%)	13	42

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
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%)	17	46
1	EEE	168/183 (92%)	158 (94%)	10 (6%)	19	49
2	BBB	182/194 (94%)	170 (93%)	12 (7%)	16	46
2	HHH	182/194 (94%)	171 (94%)	11 (6%)	19	49
3	CCC	194/195 (100%)	183 (94%)	11 (6%)	20	51
3	LLL	194/195 (100%)	185 (95%)	9 (5%)	27	58
4	DDD	101/108 (94%)	91 (90%)	10 (10%)	8	28
4	FFF	101/108 (94%)	94 (93%)	7 (7%)	15	44
All	All	1290/1360 (95%)	1209 (94%)	81 (6%)	18	47

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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

Some 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 [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	0.32	0	17,19,21	1.03	1 (5%)
5	NAG	AAA	601	1	14,14,15	0.36	0	17,19,21	1.08	2 (11%)

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 (3) 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	-2.59	107.21	111.29
5	AAA	601	NAG	O5-C5-C6	2.10	110.50	107.20

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

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	1.08	39 (20%) 1 1	130, 167, 212, 245	0
1	EEE	195/210 (92%)	0.90	21 (10%) 5 5	114, 135, 182, 226	0
2	BBB	216/229 (94%)	0.90	33 (15%) 2 2	111, 150, 183, 206	0
2	HHH	216/229 (94%)	0.91	24 (11%) 5 5	99, 134, 193, 216	0
3	CCC	219/220 (99%)	0.90	24 (10%) 5 5	113, 148, 174, 200	0
3	LLL	219/220 (99%)	0.91	26 (11%) 4 4	104, 143, 172, 197	0
4	DDD	127/134 (94%)	3.96	94 (74%) 0 0	214, 271, 304, 315	0
4	FFF	127/134 (94%)	1.04	16 (12%) 3 3	117, 140, 171, 207	0
All	All	1514/1586 (95%)	1.19	277 (18%) 1 1	99, 148, 267, 315	0

All (277) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	DDD	35	GLY	15.8
4	DDD	33	ALA	14.0
4	DDD	34	MET	13.9
4	DDD	81	LEU	12.3
4	DDD	97	ALA	12.3
4	DDD	10	GLY	11.2
4	DDD	8	GLY	10.3
4	DDD	18	LEU	9.1
4	DDD	20	LEU	8.8
4	DDD	9	GLY	8.6
4	DDD	49	ALA	8.1
4	DDD	51	ILE	7.8
4	DDD	94	TYR	7.7
4	DDD	70	ILE	7.7
4	DDD	21	SER	7.6
4	DDD	123	VAL	7.2

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Mol	Chain	Res	Type	RSRZ
4	DDD	99	THR	6.9
4	DDD	90	ASP	6.4
4	DDD	13	GLN	6.3
4	DDD	109	TYR	6.0
4	DDD	84	ASN	6.0
4	DDD	83	MET	6.0
1	AAA	455	LEU	5.9
4	DDD	119	GLN	5.8
4	DDD	69	THR	5.8
4	DDD	115	ASP	5.7
4	DDD	24	VAL	5.7
4	DDD	50	ALA	5.6
4	DDD	126	SER	5.6
1	AAA	528	LYS	5.6
4	DDD	79	VAL	5.6
4	DDD	58	ALA	5.6
4	DDD	15	GLY	5.6
4	DDD	36	TRP	5.5
4	DDD	106	LEU	5.5
4	DDD	116	TYR	5.4
4	DDD	82	GLN	5.3
1	AAA	492	LEU	5.2
4	DDD	16	GLY	5.2
4	DDD	7	SER	5.2
4	DDD	117	TRP	5.1
4	DDD	47	PHE	5.0
4	DDD	26	GLY	5.0
4	DDD	118	GLY	5.0
1	EEE	527	PRO	4.9
4	DDD	11	LEU	4.8
4	DDD	104	SER	4.7
4	DDD	98	ARG	4.7
1	AAA	491	PRO	4.6
1	AAA	392	PHE	4.6
1	EEE	528	LYS	4.4
4	DDD	114	TYR	4.3
4	DDD	124	THR	4.3
4	DDD	12	MET	4.2
4	DDD	67	ARG	4.2
4	DDD	37	PHE	4.1
1	AAA	350	VAL	4.1
4	DDD	80	TYR	4.1

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Mol	Chain	Res	Type	RSRZ
3	CCC	39	LEU	4.1
4	DDD	86	LEU	4.0
4	DDD	102	VAL	4.0
1	AAA	527	PRO	4.0
4	DDD	57	SER	3.9
4	DDD	122	GLN	3.9
4	DDD	59	TYR	3.9
3	CCC	42	TYR	3.9
4	DDD	60	TYR	3.8
4	DDD	127	SER	3.8
3	LLL	41	TRP	3.7
1	EEE	351	TYR	3.7
4	DDD	68	PHE	3.7
4	DDD	125	VAL	3.7
4	DDD	4	LEU	3.6
3	CCC	104	PHE	3.6
4	DDD	85	SER	3.6
1	EEE	492	LEU	3.6
4	FFF	33	ALA	3.6
4	DDD	6	GLU	3.5
2	BBB	47	TRP	3.4
4	DDD	121	THR	3.4
4	DDD	38	ARG	3.3
1	AAA	351	TYR	3.3
4	DDD	32	ALA	3.3
4	DDD	2	VAL	3.3
4	DDD	42	GLY	3.3
4	DDD	96	CYS	3.3
4	DDD	48	VAL	3.3
4	DDD	105	LEU	3.3
4	DDD	41	PRO	3.3
3	CCC	95	GLN	3.2
2	HHH	142	LEU	3.2
3	CCC	41	TRP	3.1
3	CCC	53	LEU	3.1
1	AAA	378	LYS	3.1
3	LLL	42	TYR	3.1
4	FFF	36	TRP	3.1
2	BBB	193	LEU	3.1
1	AAA	493	GLN	3.0
1	AAA	490	PHE	3.0
2	BBB	183	SER	3.0

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Mol	Chain	Res	Type	RSRZ
4	FFF	34	MET	3.0
2	BBB	102	ILE	3.0
3	LLL	40	ALA	3.0
1	AAA	400	PHE	3.0
1	EEE	400	PHE	3.0
1	AAA	418	ILE	3.0
1	AAA	423	TYR	2.9
2	HHH	106	MET	2.9
4	DDD	88	TYR	2.9
4	DDD	40	ALA	2.9
3	CCC	102	TYR	2.9
1	AAA	410	ILE	2.9
1	AAA	406	GLU	2.9
4	DDD	54	SER	2.9
3	LLL	95	GLN	2.9
4	DDD	52	ARG	2.9
1	AAA	387	LEU	2.9
3	LLL	102	TYR	2.8
3	LLL	124	PHE	2.8
4	FFF	51	ILE	2.8
2	HHH	184	SER	2.8
4	DDD	91	THR	2.8
1	AAA	365	TYR	2.8
1	AAA	342	PHE	2.8
4	FFF	123	VAL	2.8
2	HHH	47	TRP	2.7
3	LLL	104	PHE	2.7
1	AAA	434	ILE	2.7
4	DDD	14	ALA	2.7
4	FFF	109	TYR	2.7
1	AAA	453	TYR	2.7
1	EEE	510	VAL	2.7
3	LLL	112	ILE	2.7
4	DDD	112	TRP	2.7
3	LLL	81	ILE	2.7
3	CCC	139	VAL	2.6
2	HHH	45	LEU	2.6
3	LLL	68	PHE	2.6
4	DDD	100	GLU	2.6
3	LLL	77	PHE	2.6
4	DDD	95	TYR	2.6
4	DDD	53	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	AAA	338	PHE	2.6
1	EEE	350	VAL	2.6
4	DDD	120	GLY	2.6
1	AAA	425	LEU	2.6
2	HHH	212	ASP	2.6
2	BBB	34	ILE	2.6
3	LLL	54	ILE	2.5
4	DDD	74	LYS	2.5
3	CCC	112	ILE	2.5
3	CCC	31	TYR	2.5
4	DDD	17	SER	2.5
3	CCC	57	ALA	2.5
1	AAA	452	LEU	2.5
2	BBB	186	VAL	2.5
1	AAA	495	TYR	2.5
1	EEE	524	VAL	2.5
3	CCC	93	TYR	2.5
3	CCC	142	LEU	2.5
4	FFF	79	VAL	2.5
2	BBB	45	LEU	2.4
4	DDD	25	SER	2.4
4	DDD	92	ALA	2.4
1	EEE	422	ASN	2.4
1	AAA	377	PHE	2.4
1	AAA	456	PHE	2.4
2	HHH	27	TYR	2.4
1	AAA	524	VAL	2.4
4	FFF	4	LEU	2.4
3	CCC	68	PHE	2.4
3	CCC	77	PHE	2.4
3	LLL	142	LEU	2.4
4	DDD	87	LYS	2.4
1	AAA	370	ASN	2.4
3	LLL	39	LEU	2.4
3	LLL	79	LEU	2.4
4	DDD	56	GLY	2.4
2	HHH	107	ASP	2.3
4	DDD	5	VAL	2.3
2	BBB	100	SER	2.3
4	DDD	30	SER	2.3
1	EEE	401	VAL	2.3
3	CCC	40	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
4	DDD	19	ARG	2.3
4	FFF	13	GLN	2.3
2	BBB	20	ILE	2.3
2	BBB	123	PRO	2.3
1	EEE	495	TYR	2.3
1	EEE	491	PRO	2.3
2	HHH	102	ILE	2.3
1	AAA	513	LEU	2.3
1	AAA	347	PHE	2.3
1	AAA	449	TYR	2.3
2	HHH	125	VAL	2.3
3	LLL	154	TRP	2.3
4	FFF	24	VAL	2.3
2	BBB	28	GLY	2.3
1	AAA	454	ARG	2.3
1	EEE	423	TYR	2.3
2	HHH	183	SER	2.3
3	LLL	89	VAL	2.3
3	CCC	153	GLN	2.2
4	FFF	102	VAL	2.2
1	EEE	512	VAL	2.2
2	HHH	33	TRP	2.2
1	AAA	466	ARG	2.2
2	BBB	185	VAL	2.2
3	CCC	4	LEU	2.2
2	HHH	98	GLY	2.2
1	EEE	455	LEU	2.2
4	FFF	1	GLN	2.2
2	HHH	51	ILE	2.2
4	DDD	93	VAL	2.2
4	FFF	78	THR	2.2
2	BBB	125	VAL	2.2
1	EEE	490	PHE	2.2
1	EEE	392	PHE	2.2
1	AAA	510	VAL	2.2
2	BBB	50	ILE	2.2
3	CCC	79	LEU	2.2
1	EEE	429	PHE	2.2
1	EEE	402	ILE	2.2
2	BBB	55	ASP	2.2
1	AAA	380	TYR	2.1
2	BBB	27	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
3	CCC	192	TYR	2.1
4	DDD	71	SER	2.1
2	HHH	144	CYS	2.1
3	CCC	154	TRP	2.1
1	AAA	402	ILE	2.1
3	LLL	110	VAL	2.1
2	BBB	70	ILE	2.1
2	HHH	34	ILE	2.1
4	FFF	98	ARG	2.1
3	LLL	153	GLN	2.1
2	BBB	105	PRO	2.1
2	BBB	137	GLY	2.1
4	DDD	23	ALA	2.1
1	AAA	511	VAL	2.1
4	FFF	70	ILE	2.1
2	BBB	101	GLY	2.1
3	LLL	141	LEU	2.1
2	HHH	95	TYR	2.1
2	BBB	202	VAL	2.1
3	CCC	2	ILE	2.1
2	BBB	18	LEU	2.1
2	BBB	213	LYS	2.1
3	CCC	183	SER	2.1
2	HHH	50	ILE	2.1
3	LLL	121	VAL	2.1
2	BBB	142	LEU	2.1
1	EEE	365	TYR	2.1
3	LLL	55	TYR	2.1
3	CCC	124	PHE	2.1
2	HHH	32	TYR	2.1
3	LLL	93	TYR	2.1
1	AAA	417	LYS	2.1
3	LLL	4	LEU	2.1
1	EEE	511	VAL	2.1
2	HHH	168	HIS	2.1
2	BBB	97	ALA	2.1
3	LLL	177	SER	2.1
2	BBB	36	TRP	2.0
2	BBB	106	MET	2.1
2	HHH	158	TRP	2.0
2	BBB	31	THR	2.0
2	BBB	147	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
2	HHH	215	VAL	2.0
2	BBB	53	PRO	2.0
2	HHH	193	LEU	2.0
3	LLL	199	ALA	2.0
2	BBB	116	THR	2.0
2	HHH	36	TRP	2.0
4	FFF	53	TRP	2.0
2	BBB	58	THR	2.0
2	BBB	115	VAL	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 monosaccharides 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	0.85	0.28	162,172,176,179	0
5	NAG	EEE	601	14/15	0.89	0.30	140,150,156,157	0

6.5 Other polymers [i](#)

There are no such residues in this entry.