



# Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2026 – 09:43 PM JST

PDB ID : 9V0O / pdb\_00009v0o  
Title : Crystal structure of nanobody Tnb494 with MERS-CoV RBD  
Authors : Wang, X.; Lin, Z.  
Deposited on : 2025-05-18  
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

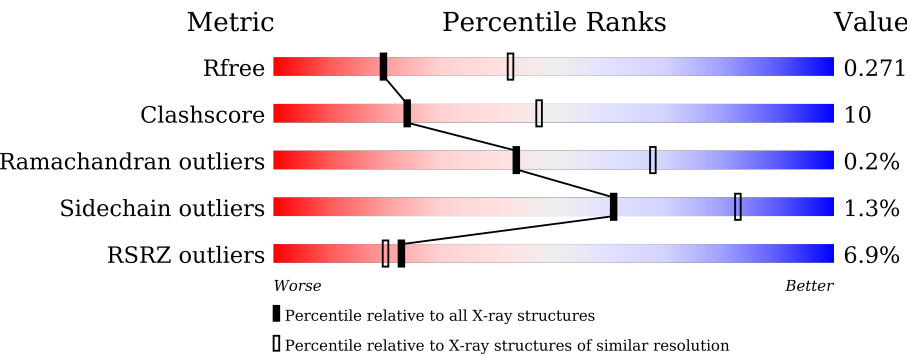
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal 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 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	A	125	<div><div>3%</div><div>78%</div><div>20%</div><div>.</div></div>
1	B	125	<div><div>10%</div><div>71%</div><div>23%</div><div>..</div></div>
1	E	125	<div><div>12%</div><div>70%</div><div>27%</div><div>.</div></div>
1	G	125	<div><div>14%</div><div>64%</div><div>33%</div><div>..</div></div>
2	C	211	<div><div>%</div><div>85%</div><div>14%</div><div></div></div>
2	D	211	<div><div>4%</div><div>86%</div><div>13%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	211	 6%76%23%
2	H	211	 10%77%23%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10421 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 nanobody Tnb494.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	125	Total	C	N	O	S	0	0	0
			958	597	163	194	4			
1	A	125	Total	C	N	O	S	0	0	0
			957	597	163	193	4			
1	E	125	Total	C	N	O	S	0	0	0
			958	597	163	194	4			
1	G	125	Total	C	N	O	S	0	0	0
			958	597	163	194	4			

- Molecule 2 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	211	Total	C	N	O	S	0	0	0
			1626	1036	259	320	11			
2	D	211	Total	C	N	O	S	0	0	0
			1630	1038	259	322	11			
2	F	211	Total	C	N	O	S	0	0	0
			1626	1036	259	320	11			
2	H	211	Total	C	N	O	S	0	0	0
			1626	1036	259	320	11			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		
3	H	1	Total	C	N	O	0	0
			14	8	1	5		

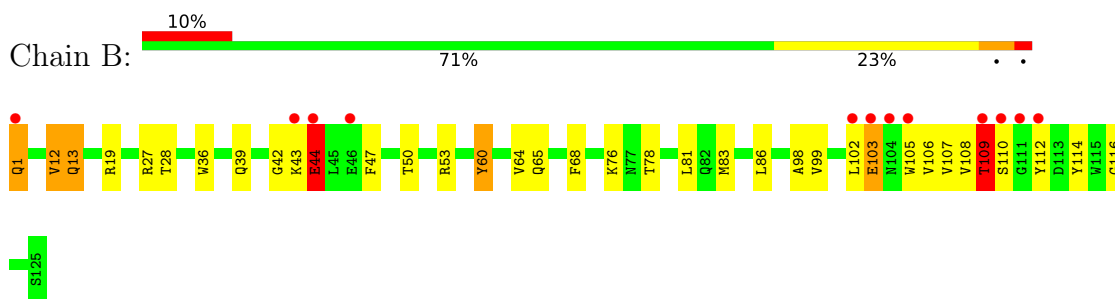
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	O	0	0
			1	1		
4	C	3	Total	O	0	0
			3	3		
4	A	1	Total	O	0	0
			1	1		
4	D	2	Total	O	0	0
			2	2		
4	E	3	Total	O	0	0
			3	3		
4	F	1	Total	O	0	0
			1	1		
4	H	1	Total	O	0	0
			1	1		

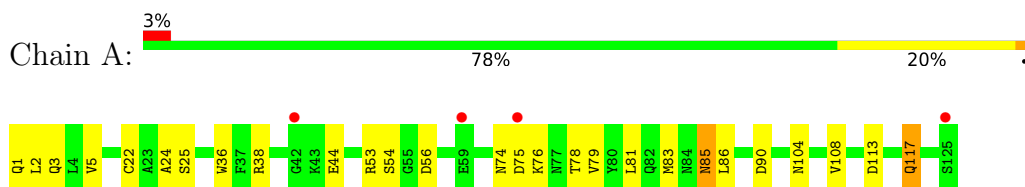
### 3 Residue-property plots

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.

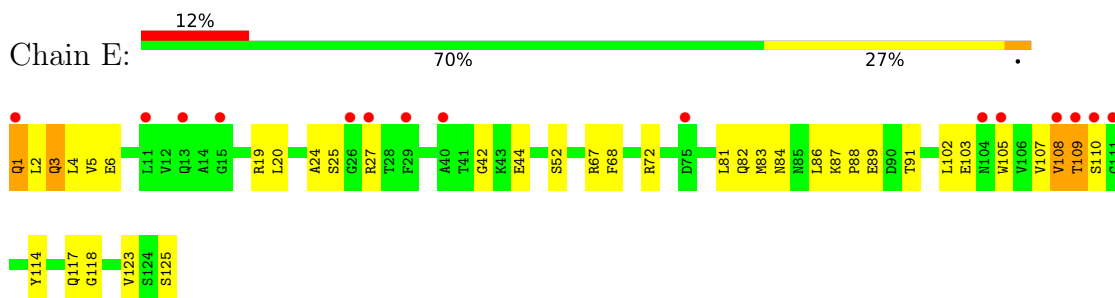
- Molecule 1: nanobody Tnb494



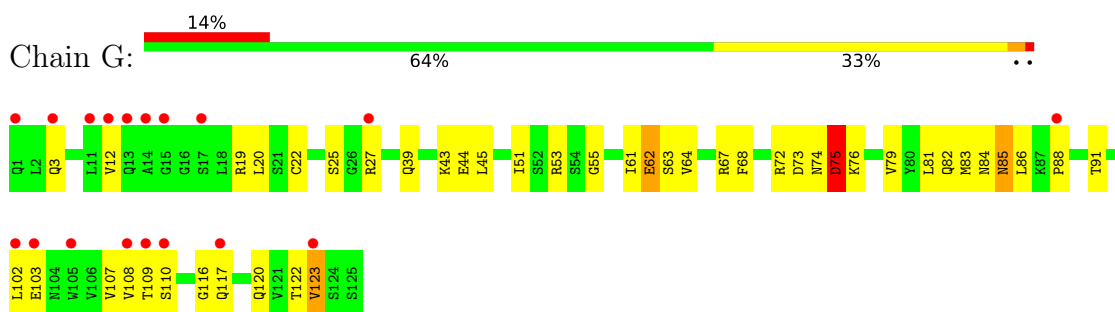
- Molecule 1: nanobody Tnb494



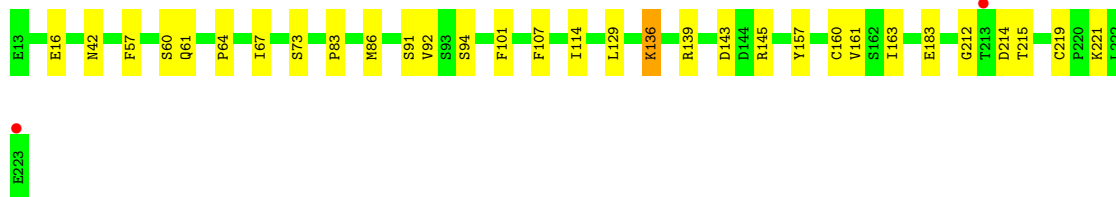
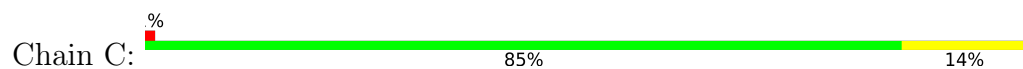
- Molecule 1: nanobody Tnb494



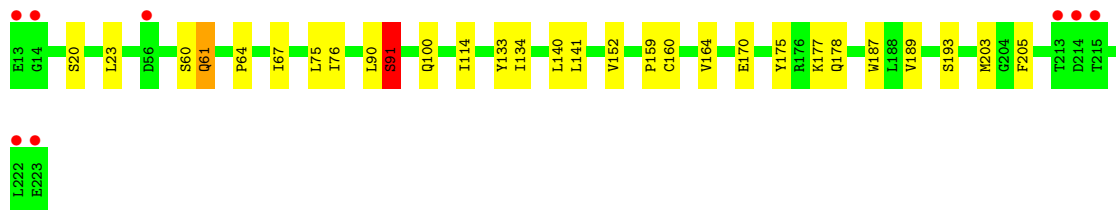
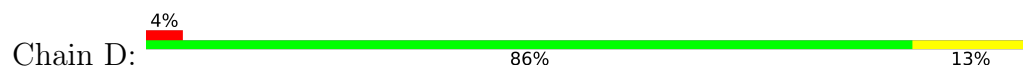
- Molecule 1: nanobody Tnb494



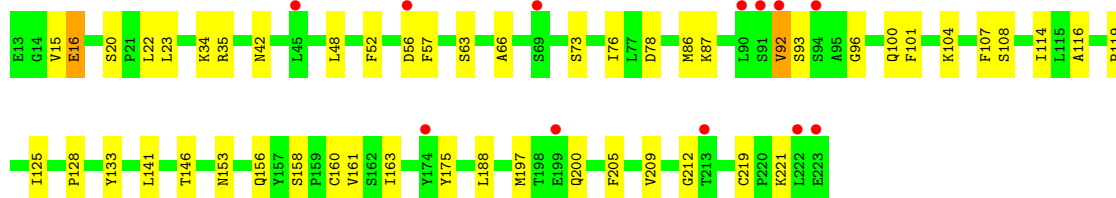
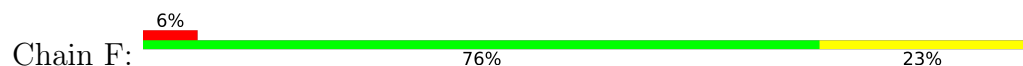
## ● Molecule 2: Spike glycoprotein



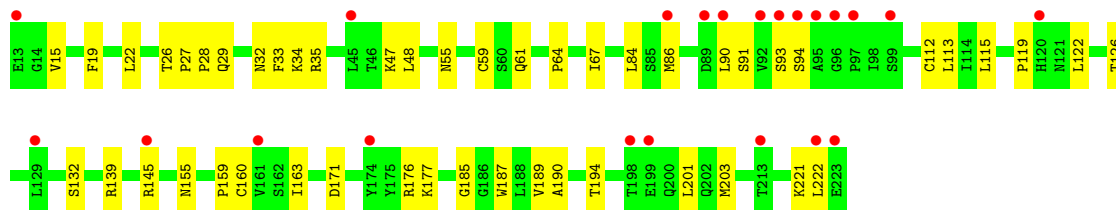
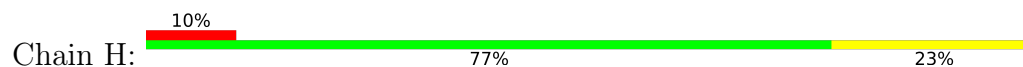
## ● Molecule 2: Spike glycoprotein



## ● Molecule 2: Spike glycoprotein



## ● Molecule 2: Spike glycoprotein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	83.89Å 141.53Å 153.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.65 – 2.70 76.65 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (76.65-2.70) 99.9 (76.65-2.70)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.55 (at 2.69Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, $R_{free}$	0.242 , 0.270 0.248 , 0.271	Depositor DCC
$R_{free}$ test set	2549 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	67.7	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	10421	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	A	0.64	0/974	1.05	3/1320 (0.2%)
1	B	0.77	1/975 (0.1%)	1.34	18/1320 (1.4%)
1	E	0.67	0/975	1.13	6/1320 (0.5%)
1	G	0.76	3/975 (0.3%)	1.32	16/1320 (1.2%)
2	C	0.52	0/1665	0.76	2/2273 (0.1%)
2	D	0.53	1/1669 (0.1%)	0.81	3/2278 (0.1%)
2	F	0.60	1/1665 (0.1%)	0.88	6/2273 (0.3%)
2	H	0.60	0/1665	0.86	2/2273 (0.1%)
All	All	0.62	6/10563 (0.1%)	0.99	56/14377 (0.4%)

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
1	A	0	1
1	B	0	1
1	E	0	1
1	G	0	4
2	H	0	1
All	All	0	8

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	87	LYS	CD-CE	7.18	1.74	1.52
1	G	123	VAL	CB-CG1	-5.67	1.33	1.52
1	G	123	VAL	CB-CG2	-5.43	1.34	1.52
2	D	61	GLN	C-N	5.33	1.36	1.33
1	G	85	ASN	CG-ND2	5.11	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	43	LYS	CE-NZ	5.08	1.64	1.49

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	THR	N-CA-C	-10.36	99.98	111.28
1	G	116	GLY	CA-C-N	-10.21	105.69	122.54
1	G	116	GLY	C-N-CA	-10.21	105.69	122.54
1	B	44	GLU	N-CA-C	9.47	124.82	110.14
1	A	1	GLN	N-CA-C	-9.41	84.65	111.00
1	E	1	GLN	CA-CB-CG	-9.10	95.89	114.10
1	G	76	LYS	CD-CE-NZ	8.94	140.51	111.90
1	B	12	VAL	CA-C-N	-8.90	107.27	122.67
1	B	12	VAL	C-N-CA	-8.90	107.27	122.67
1	E	44	GLU	CA-CB-CG	8.33	130.76	114.10
1	E	3	GLN	CB-CG-CD	-8.04	98.93	112.60
2	F	87	LYS	CD-CE-NZ	-7.08	89.23	111.90
1	G	85	ASN	CB-CA-C	-7.05	101.81	112.11
2	F	93	SER	N-CA-C	-6.85	103.81	111.28
1	B	65	GLN	CA-CB-CG	6.69	127.48	114.10
1	A	76	LYS	N-CA-C	-6.64	106.38	114.75
1	G	75	ASP	N-CA-C	-6.63	104.45	112.54
1	G	123	VAL	CA-C-N	-6.60	110.28	122.09
1	G	123	VAL	C-N-CA	-6.60	110.28	122.09
1	G	76	LYS	CB-CG-CD	6.55	126.37	111.30
1	G	76	LYS	N-CA-C	-6.52	104.56	113.30
2	F	16	GLU	CA-CB-CG	6.26	126.63	114.10
2	H	86	MET	CG-SD-CE	-6.07	87.54	100.90
2	D	91	SER	N-CA-C	6.05	123.68	110.80
1	E	3	GLN	CA-CB-CG	6.00	126.11	114.10
1	B	42	GLY	CA-C-N	-5.98	114.27	122.16
1	B	42	GLY	C-N-CA	-5.98	114.27	122.16
2	F	209	VAL	CA-C-N	-5.98	112.08	122.37
2	F	209	VAL	C-N-CA	-5.98	112.08	122.37
1	B	44	GLU	CG-CD-OE1	5.98	132.15	118.40
2	H	93	SER	N-CA-C	-5.98	104.63	113.72
1	B	116	GLY	CA-C-N	5.95	128.74	120.29
1	B	116	GLY	C-N-CA	5.95	128.74	120.29
1	A	85	ASN	CB-CA-C	-5.92	103.93	111.86
1	B	103	GLU	CA-C-N	-5.86	113.69	122.24
1	B	103	GLU	C-N-CA	-5.86	113.69	122.24
1	G	85	ASN	CA-C-N	-5.63	112.87	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	85	ASN	C-N-CA	-5.63	112.87	120.87
1	B	43	LYS	CD-CE-NZ	5.52	129.57	111.90
1	B	13	GLN	CB-CG-CD	-5.51	103.23	112.60
1	E	1	GLN	CB-CA-C	5.47	120.49	110.10
1	B	103	GLU	CA-CB-CG	5.46	125.03	114.10
2	D	134	ILE	CA-C-N	-5.41	113.65	122.26
2	D	134	ILE	C-N-CA	-5.41	113.65	122.26
1	G	76	LYS	CA-C-N	5.38	130.00	122.36
1	G	76	LYS	C-N-CA	5.38	130.00	122.36
1	E	89	GLU	CA-CB-CG	5.34	124.78	114.10
1	G	123	VAL	CA-CB-CG2	5.34	119.47	110.40
2	F	92	VAL	N-CA-C	-5.26	106.40	112.98
1	B	1	GLN	CB-CG-CD	5.24	121.51	112.60
2	C	16	GLU	N-CA-C	-5.18	102.08	110.32
1	B	1	GLN	CA-CB-CG	5.11	124.32	114.10
1	G	73	ASP	CA-C-N	5.08	127.09	120.28
1	G	73	ASP	C-N-CA	5.08	127.09	120.28
2	C	136	LYS	CB-CG-CD	5.03	122.86	111.30
1	B	44	GLU	CB-CA-C	-5.01	100.70	109.71

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	85	ASN	Sidechain
1	B	44	GLU	Sidechain
1	E	42	GLY	Peptide
1	G	62	GLU	Sidechain
1	G	74	ASN	Sidechain
1	G	75	ASP	Peptide
1	G	85	ASN	Sidechain
2	H	91	SER	Mainchain

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	957	0	914	19	0
1	B	958	0	914	43	1
1	E	958	0	914	29	0
1	G	958	0	914	31	1
2	C	1626	0	1584	20	0
2	D	1630	0	1586	21	0
2	F	1626	0	1584	32	0
2	H	1626	0	1584	28	0
3	C	14	0	13	1	0
3	D	28	0	26	0	0
3	F	14	0	13	1	0
3	H	14	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	1	0
4	C	3	0	0	0	0
4	D	2	0	0	0	0
4	E	3	0	0	0	0
4	F	1	0	0	0	0
4	H	1	0	0	0	0
All	All	10421	0	10059	207	1

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 10.

All (207) 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:E:102:LEU:HD22	1:E:105:TRP:HE1	1.25	0.96
1:B:44:GLU:OE1	1:B:44:GLU:HA	1.64	0.96
2:F:108:SER:HA	2:H:145:ARG:HE	1.28	0.96
1:B:105:TRP:CZ2	2:C:161:VAL:HG12	2.09	0.87
1:B:103:GLU:HG2	1:B:105:TRP:HZ3	1.40	0.86
1:G:91:THR:OG1	1:G:123:VAL:HG12	1.77	0.84
1:G:3:GLN:HB2	1:G:25:SER:HB3	1.57	0.83
1:B:103:GLU:HG2	1:B:105:TRP:CZ3	2.15	0.81
2:H:119:PRO:HD2	2:H:122:LEU:HD12	1.61	0.81
2:D:141:LEU:HD22	1:E:3:GLN:HG2	1.63	0.80
1:E:6:GLU:OE2	1:E:118:GLY:N	2.16	0.77
1:E:91:THR:HG22	1:E:123:VAL:H	1.50	0.77
1:B:19:ARG:NH2	4:B:201:HOH:O	2.14	0.76
1:G:88:PRO:HA	1:G:123:VAL:HG11	1.67	0.75
1:G:64:VAL:HB	1:G:68:PHE:CD2	2.22	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:103:GLU:HG3	1:E:105:TRP:CZ3	2.23	0.74
1:B:102:LEU:HA	1:B:105:TRP:CH2	2.22	0.73
2:F:153:ASN:HB2	2:F:156:GLN:HG3	1.69	0.73
1:B:102:LEU:HD22	1:B:105:TRP:CZ2	2.25	0.72
1:B:53:ARG:HH11	1:B:103:GLU:HA	1.58	0.69
1:E:102:LEU:HD22	1:E:105:TRP:NE1	2.06	0.69
1:A:44:GLU:HB2	1:E:27:ARG:HH12	1.55	0.69
1:G:68:PHE:HD1	1:G:83:MET:HA	1.58	0.68
2:F:108:SER:HA	2:H:145:ARG:NE	2.05	0.68
1:B:39:GLN:NE2	1:B:44:GLU:OE1	2.27	0.68
1:B:44:GLU:OE1	1:B:44:GLU:CA	2.42	0.68
1:E:102:LEU:HA	1:E:105:TRP:CZ2	2.30	0.67
1:E:83:MET:HE3	1:E:86:LEU:HD21	1.78	0.66
2:H:19:PHE:CD2	2:H:48:LEU:HD22	2.31	0.65
1:A:44:GLU:HB2	1:E:27:ARG:NH1	2.10	0.65
2:F:128:PRO:HG2	2:F:197:MET:HE3	1.78	0.65
1:G:64:VAL:HB	1:G:68:PHE:HD2	1.59	0.65
1:B:28:THR:HG21	2:D:193:SER:OG	1.96	0.65
1:G:63:SER:O	1:G:67:ARG:NH1	2.29	0.64
2:D:20:SER:HA	2:D:23:LEU:HD12	1.79	0.64
1:E:3:GLN:O	1:E:4:LEU:HD23	1.96	0.64
1:E:52:SER:O	1:E:72:ARG:NH1	2.32	0.62
2:F:158:SER:O	2:F:161:VAL:HG22	2.00	0.62
1:A:74:ASN:O	1:A:75:ASP:HB2	1.98	0.62
1:G:12:VAL:HG11	1:G:86:LEU:HD22	1.81	0.61
1:G:110:SER:HB3	2:H:159:PRO:HB3	1.82	0.61
1:E:2:LEU:HD11	1:E:24:ALA:HB1	1.82	0.60
2:C:57:PHE:CD1	2:C:114:ILE:HG12	2.37	0.60
2:F:23:LEU:HD13	2:F:125:ILE:HD11	1.84	0.59
2:F:35:ARG:HG2	2:F:78:ASP:OD1	2.02	0.59
2:F:221:LYS:HG2	3:F:301:NAG:H83	1.83	0.59
1:B:53:ARG:NH1	1:B:103:GLU:HA	2.17	0.59
1:G:67:ARG:HB3	1:G:84:ASN:O	2.03	0.59
2:H:26:THR:OG1	2:H:126:THR:HG23	2.03	0.59
2:F:101:PHE:O	2:F:158:SER:HB2	2.01	0.59
1:B:12:VAL:HG11	1:B:86:LEU:HD12	1.85	0.59
1:B:108:VAL:HG23	1:B:109:THR:H	1.68	0.58
1:G:43:LYS:HD3	1:G:44:GLU:H	1.68	0.58
1:G:53:ARG:HA	1:G:72:ARG:HH12	1.68	0.58
1:G:88:PRO:HA	1:G:123:VAL:CG1	2.33	0.58
1:B:102:LEU:HD22	1:B:105:TRP:HZ2	1.66	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:53:ARG:HA	1:G:72:ARG:NH1	2.19	0.57
1:B:99:VAL:HB	1:B:112:TYR:CD1	2.39	0.57
2:D:178:GLN:HG2	2:D:187:TRP:CZ3	2.39	0.57
2:D:60:SER:OG	2:D:61:GLN:OE1	2.18	0.57
1:E:67:ARG:HB3	1:E:84:ASN:O	2.05	0.57
1:G:102:LEU:HD11	1:G:107:VAL:HG22	1.85	0.57
2:C:101:PHE:CE2	2:C:136:LYS:HA	2.41	0.56
1:G:68:PHE:CD1	1:G:83:MET:HA	2.39	0.55
2:F:96:GLY:O	2:F:100:GLN:HG3	2.07	0.55
1:B:50:THR:HG23	1:B:106:VAL:CG2	2.36	0.55
1:B:50:THR:HG23	1:B:106:VAL:HG22	1.89	0.55
1:E:88:PRO:HA	1:E:123:VAL:CG2	2.36	0.55
2:D:114:ILE:HB	2:D:205:PHE:HB2	1.88	0.54
2:F:22:LEU:HD11	2:F:205:PHE:HE2	1.72	0.54
2:F:119:PRO:HA	2:F:200:GLN:HE22	1.72	0.54
1:B:1:GLN:HG2	1:B:114:TYR:CE1	2.43	0.53
1:E:107:VAL:HB	1:E:110:SER:HB3	1.90	0.53
2:F:20:SER:O	2:F:23:LEU:N	2.41	0.53
2:F:15:VAL:HG22	2:F:16:GLU:O	2.09	0.53
2:C:214:ASP:OD1	2:C:215:THR:N	2.42	0.53
1:B:1:GLN:HG2	1:B:114:TYR:OH	2.08	0.53
1:B:83:MET:HB3	1:B:86:LEU:HD21	1.90	0.53
1:B:28:THR:HG21	2:D:193:SER:CB	2.38	0.52
1:B:76:LYS:O	1:B:78:THR:HG23	2.09	0.52
2:H:29:GLN:HG3	2:H:132:SER:HB2	1.89	0.52
1:G:62:GLU:O	1:G:64:VAL:N	2.42	0.52
1:G:110:SER:CB	2:H:159:PRO:HB3	2.40	0.52
1:B:50:THR:CG2	1:B:106:VAL:HG22	2.40	0.52
2:F:104:LYS:HE2	2:F:107:PHE:CE2	2.45	0.52
1:B:53:ARG:NH1	1:B:102:LEU:O	2.41	0.52
1:B:105:TRP:CD1	1:B:106:VAL:N	2.78	0.52
1:E:1:GLN:N	1:E:114:TYR:CZ	2.77	0.51
1:B:98:ALA:C	1:B:112:TYR:HD1	2.18	0.51
2:D:64:PRO:O	2:D:67:ILE:HG22	2.10	0.51
1:A:108:VAL:CG2	2:D:159:PRO:HA	2.41	0.51
2:H:90:LEU:HG	2:H:113:LEU:HD22	1.91	0.51
2:F:73:SER:HB2	2:F:212:GLY:N	2.26	0.50
1:G:61:ILE:HG13	1:G:64:VAL:HG22	1.94	0.50
2:H:171:ASP:HB2	2:H:194:THR:HG22	1.92	0.50
2:F:34:LYS:O	2:F:78:ASP:HA	2.11	0.50
1:G:3:GLN:CB	1:G:25:SER:HB3	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:28:PRO:HG3	2:H:34:LYS:HB2	1.94	0.50
1:A:36:TRP:NE1	1:A:81:LEU:HB2	2.27	0.50
2:C:101:PHE:CD2	2:C:136:LYS:HA	2.47	0.49
1:G:19:ARG:NH1	1:G:82:GLN:OE1	2.45	0.49
2:F:73:SER:HB2	2:F:212:GLY:H	1.78	0.49
2:F:86:MET:HE1	2:F:133:TYR:CZ	2.47	0.49
2:C:160:CYS:O	2:C:163:ILE:HG12	2.13	0.49
2:H:22:LEU:HD11	2:H:48:LEU:HD11	1.94	0.49
2:H:176:ARG:HG2	2:H:187:TRP:CE3	2.47	0.49
1:A:83:MET:HB3	1:A:86:LEU:HD11	1.95	0.49
1:B:60:TYR:CD1	1:B:60:TYR:N	2.81	0.49
1:A:5:VAL:O	1:A:22:CYS:HA	2.13	0.49
1:B:36:TRP:CG	1:B:81:LEU:HD22	2.48	0.49
2:C:60:SER:O	2:C:61:GLN:HB2	2.12	0.48
1:G:62:GLU:O	1:G:63:SER:C	2.54	0.48
1:B:60:TYR:N	1:B:60:TYR:HD1	2.11	0.48
1:E:88:PRO:HG3	1:E:125:SER:HB2	1.95	0.48
2:F:22:LEU:HD11	2:F:205:PHE:CE2	2.49	0.48
1:G:39:GLN:HB2	1:G:45:LEU:HD12	1.96	0.48
1:B:27:ARG:HH12	2:D:170:GLU:HG2	1.78	0.48
2:H:64:PRO:O	2:H:67:ILE:HG22	2.14	0.48
1:A:53:ARG:HB2	1:A:104:ASN:HB2	1.96	0.48
2:C:42:ASN:HA	2:C:219:CYS:O	2.14	0.48
2:H:55:ASN:ND2	2:H:84:LEU:HD21	2.29	0.48
1:B:105:TRP:CZ2	2:C:161:VAL:CG1	2.92	0.47
2:H:176:ARG:HG3	2:H:189:VAL:HG12	1.96	0.47
1:E:88:PRO:O	1:E:91:THR:HG23	2.14	0.47
2:C:139:ARG:NH1	2:C:183:GLU:O	2.37	0.47
1:E:68:PHE:HA	1:E:82:GLN:O	2.15	0.47
1:B:103:GLU:N	1:B:105:TRP:CZ3	2.66	0.46
2:F:104:LYS:HE2	2:F:107:PHE:HE2	1.78	0.46
2:H:163:ILE:HG21	2:H:177:LYS:HB2	1.96	0.46
1:A:3:GLN:HG2	1:A:25:SER:OG	2.14	0.46
2:F:160:CYS:SG	2:F:188:LEU:HD21	2.55	0.46
1:A:3:GLN:O	1:A:3:GLN:HG3	2.14	0.46
2:F:56:ASP:OD1	2:F:57:PHE:N	2.49	0.46
2:F:163:ILE:HD12	2:F:175:TYR:HB2	1.98	0.46
2:D:61:GLN:HG2	2:H:61:GLN:OE1	2.15	0.46
2:C:221:LYS:O	3:C:301:NAG:H82	2.14	0.46
2:H:139:ARG:NH1	2:H:185:GLY:O	2.48	0.46
2:H:47:LYS:HD2	2:H:47:LYS:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:22:CYS:HB3	1:G:79:VAL:CG1	2.46	0.46
1:B:1:GLN:HG2	1:B:114:TYR:CZ	2.51	0.45
2:F:42:ASN:HA	2:F:219:CYS:O	2.16	0.45
1:A:36:TRP:CD1	1:A:81:LEU:HB2	2.51	0.45
1:A:22:CYS:HB3	1:A:79:VAL:CG1	2.46	0.45
1:B:12:VAL:HG22	1:B:13:GLN:N	2.32	0.45
2:F:128:PRO:HG2	2:F:197:MET:CE	2.46	0.45
2:H:90:LEU:HD23	2:H:115:LEU:HD21	1.98	0.45
1:G:81:LEU:HD23	1:G:83:MET:HE2	1.98	0.45
2:F:22:LEU:HD23	2:F:48:LEU:HD11	1.99	0.45
2:C:91:SER:HB3	2:C:94:SER:HB3	1.99	0.44
1:A:38:ARG:NH1	1:A:90:ASP:OD1	2.46	0.44
2:H:19:PHE:HD2	2:H:48:LEU:HD22	1.78	0.44
1:A:22:CYS:O	1:A:78:THR:HA	2.16	0.44
2:C:64:PRO:O	2:C:67:ILE:HG22	2.18	0.44
1:E:3:GLN:O	1:E:24:ALA:HA	2.18	0.44
1:G:51:ILE:HD11	1:G:55:GLY:HA2	1.99	0.44
2:H:35:ARG:HH12	2:H:155:ASN:ND2	2.16	0.44
2:C:83:PRO:HG2	2:C:86:MET:HB2	2.00	0.44
2:D:203:MET:HE2	2:D:205:PHE:CE1	2.53	0.44
1:G:120:GLN:HG3	1:G:122:THR:HG23	1.99	0.44
1:B:105:TRP:HB2	2:C:157:TYR:CE2	2.53	0.43
2:C:73:SER:HB2	2:C:212:GLY:CA	2.48	0.43
2:D:160:CYS:O	2:D:164:VAL:HG23	2.18	0.43
2:D:140:LEU:HD12	2:D:140:LEU:HA	1.74	0.43
1:B:47:PHE:CZ	1:B:108:VAL:HG12	2.54	0.43
2:F:63:SER:OG	2:F:66:ALA:N	2.45	0.43
1:G:12:VAL:CG1	1:G:86:LEU:HD22	2.48	0.43
2:H:160:CYS:SG	2:H:190:ALA:HB2	2.59	0.43
2:D:178:GLN:HG2	2:D:187:TRP:CE3	2.54	0.43
2:F:52:PHE:HB3	2:F:116:ALA:HB1	2.01	0.43
2:F:141:LEU:HD12	2:F:146:THR:OG1	2.19	0.43
2:C:129:LEU:HD12	2:C:129:LEU:HA	1.85	0.43
1:E:5:VAL:HA	1:E:117:GLN:HE22	1.84	0.43
1:E:67:ARG:NH1	1:E:87:LYS:HG3	2.33	0.43
1:E:86:LEU:HB3	1:E:123:VAL:HG11	2.01	0.43
1:A:54:SER:OG	1:A:56:ASP:HB2	2.19	0.42
1:E:20:LEU:HB2	1:E:81:LEU:HB3	2.00	0.42
1:G:20:LEU:HG	1:G:83:MET:HE3	2.01	0.42
2:D:133:TYR:CE1	2:D:193:SER:HB2	2.55	0.42
1:E:87:LYS:O	1:E:123:VAL:HG21	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:75:ASP:OD1	1:G:75:ASP:N	2.51	0.42
1:B:105:TRP:CD1	1:B:105:TRP:C	2.96	0.42
2:H:203:MET:HE2	2:H:203:MET:HB3	1.90	0.42
1:B:12:VAL:HG22	1:B:13:GLN:H	1.85	0.41
1:B:110:SER:OG	1:B:112:TYR:CD2	2.73	0.41
1:E:117:GLN:H	1:E:117:GLN:CD	2.28	0.41
2:F:114:ILE:HB	2:F:205:PHE:HB2	2.02	0.41
2:C:143:ASP:OD2	2:C:145:ARG:HB2	2.20	0.41
2:D:90:LEU:O	2:D:91:SER:O	2.38	0.41
2:F:35:ARG:NH2	2:F:76:ILE:HG21	2.34	0.41
2:D:175:TYR:O	2:D:189:VAL:HA	2.20	0.41
2:D:100:GLN:O	2:D:152:VAL:HG12	2.21	0.41
1:E:108:VAL:HG13	1:E:109:THR:H	1.84	0.41
1:B:64:VAL:HB	1:B:68:PHE:CG	2.56	0.41
1:B:108:VAL:HG23	1:B:109:THR:N	2.36	0.41
1:A:22:CYS:HB3	1:A:79:VAL:HG13	2.01	0.41
1:E:19:ARG:HB2	1:E:82:GLN:HE22	1.86	0.41
1:A:2:LEU:HD11	1:A:24:ALA:HB1	2.03	0.41
2:D:75:LEU:HD23	2:D:76:ILE:N	2.36	0.41
1:G:62:GLU:C	1:G:64:VAL:H	2.28	0.41
1:B:107:VAL:HB	1:B:110:SER:HA	2.03	0.40
2:C:92:VAL:HG12	2:C:107:PHE:CE1	2.56	0.40
2:H:27:PRO:HG2	2:H:201:LEU:HD21	2.02	0.40
1:A:117:GLN:H	1:A:117:GLN:HG3	1.37	0.40
2:H:59:CYS:HA	2:H:112:CYS:HA	2.02	0.40
1:A:113:ASP:OD1	2:D:177:LYS:HD2	2.22	0.40
2:C:73:SER:HB2	2:C:212:GLY:HA3	2.02	0.40
2:H:32:ASN:O	2:H:33:PHE:C	2.65	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:GLU:OE2	1:G:27:ARG:NE[3_555]	2.01	0.19

## 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	A	123/125 (98%)	119 (97%)	4 (3%)	0	100	100
1	B	123/125 (98%)	117 (95%)	6 (5%)	0	100	100
1	E	123/125 (98%)	119 (97%)	3 (2%)	1 (1%)	16	37
1	G	123/125 (98%)	118 (96%)	5 (4%)	0	100	100
2	C	209/211 (99%)	203 (97%)	6 (3%)	0	100	100
2	D	209/211 (99%)	196 (94%)	12 (6%)	1 (0%)	24	48
2	F	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
2	H	209/211 (99%)	201 (96%)	8 (4%)	0	100	100
All	All	1328/1344 (99%)	1274 (96%)	52 (4%)	2 (0%)	43	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	91	SER
1	E	108	VAL

### 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	A	102/102 (100%)	101 (99%)	1 (1%)	68	86
1	B	102/102 (100%)	99 (97%)	3 (3%)	37	67
1	E	102/102 (100%)	100 (98%)	2 (2%)	48	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	102/102 (100%)	98 (96%)	4 (4%)	28	57
2	C	191/192 (100%)	191 (100%)	0	100	100
2	D	192/192 (100%)	192 (100%)	0	100	100
2	F	191/192 (100%)	190 (100%)	1 (0%)	81	92
2	H	191/192 (100%)	187 (98%)	4 (2%)	47	75
All	All	1173/1176 (100%)	1158 (99%)	15 (1%)	61	83

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	44	GLU
1	B	60	TYR
1	B	109	THR
1	A	117	GLN
1	E	25	SER
1	E	109	THR
2	F	92	VAL
1	G	103	GLU
1	G	108	VAL
1	G	109	THR
1	G	117	GLN
2	H	15	VAL
2	H	94	SER
2	H	221	LYS
2	H	222	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	3	GLN
1	B	77	ASN
1	B	104	ASN
2	C	105	GLN
2	C	150	GLN
2	C	153	ASN
2	D	70	ASN
2	D	100	GLN
2	D	156	GLN
1	E	74	ASN

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Mol	Chain	Res	Type
1	E	117	GLN
2	F	55	ASN
2	F	120	HIS
2	F	200	GLN
1	G	77	ASN
2	H	42	ASN
2	H	70	ASN
2	H	150	GLN

### 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](#)

5 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	F	301	2	14,14,15	0.99	1 (7%)	17,19,21	1.46	1 (5%)
3	NAG	C	301	2	14,14,15	1.39	2 (14%)	17,19,21	1.16	1 (5%)
3	NAG	D	302	2	14,14,15	0.37	0	17,19,21	1.45	1 (5%)
3	NAG	H	301	2	14,14,15	0.24	0	17,19,21	1.02	0
3	NAG	D	301	2	14,14,15	0.91	1 (7%)	17,19,21	0.65	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	F	301	2	-	1/6/23/26	0/1/1/1
3	NAG	C	301	2	-	1/6/23/26	0/1/1/1
3	NAG	D	302	2	-	3/6/23/26	0/1/1/1
3	NAG	H	301	2	-	3/6/23/26	0/1/1/1
3	NAG	D	301	2	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	301	NAG	O5-C1	4.68	1.51	1.43
3	F	301	NAG	O5-C1	3.33	1.49	1.43
3	D	301	NAG	O5-C1	3.16	1.48	1.43
3	C	301	NAG	C1-C2	2.04	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	302	NAG	C1-O5-C5	5.02	118.99	112.19
3	F	301	NAG	C1-O5-C5	5.00	118.97	112.19
3	C	301	NAG	C1-O5-C5	4.19	117.88	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	302	NAG	C8-C7-N2-C2
3	D	302	NAG	O7-C7-N2-C2
3	H	301	NAG	O7-C7-N2-C2
3	H	301	NAG	C8-C7-N2-C2
3	D	301	NAG	O5-C5-C6-O6
3	D	301	NAG	C4-C5-C6-O6
3	C	301	NAG	O5-C5-C6-O6
3	D	302	NAG	O5-C5-C6-O6
3	H	301	NAG	C3-C2-N2-C7
3	F	301	NAG	C3-C2-N2-C7

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	301	NAG	1	0
3	C	301	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	125/125 (100%)	0.35	4 (3%)	50	46	30, 62, 80, 89	0
1	B	125/125 (100%)	0.48	12 (9%)	13	11	41, 59, 90, 99	0
1	E	125/125 (100%)	0.93	15 (12%)	9	7	30, 82, 106, 124	0
1	G	125/125 (100%)	1.10	18 (14%)	6	5	58, 82, 107, 113	0
2	C	211/211 (100%)	0.11	2 (0%)	81	80	41, 54, 84, 111	0
2	D	211/211 (100%)	0.22	8 (3%)	44	40	30, 55, 80, 97	0
2	F	211/211 (100%)	0.78	12 (5%)	29	26	30, 73, 106, 127	0
2	H	211/211 (100%)	0.81	22 (10%)	11	10	30, 71, 102, 112	0
All	All	1344/1344 (100%)	0.57	93 (6%)	23	20	30, 66, 99, 127	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	105	TRP	7.9
1	G	105	TRP	7.4
2	H	13	GLU	7.1
2	D	14	GLY	7.0
2	D	214	ASP	6.8
1	E	105	TRP	6.8
2	D	223	GLU	6.2
2	F	91	SER	6.1
2	H	93	SER	5.8
2	D	213	THR	5.8
1	E	109	THR	5.7
2	D	13	GLU	5.5
2	D	215	THR	5.4
1	B	110	SER	5.3
1	A	75	ASP	4.7
2	H	94	SER	4.7

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Mol	Chain	Res	Type	RSRZ
2	H	96	GLY	4.7
2	H	199	GLU	4.7
2	F	94	SER	4.7
2	F	92	VAL	4.7
2	H	92	VAL	4.4
2	H	223	GLU	4.3
1	E	26	GLY	4.2
1	G	109	THR	3.9
1	E	110	SER	3.9
1	E	13	GLN	3.7
1	E	27	ARG	3.6
1	B	112	TYR	3.6
1	G	13	GLN	3.6
2	H	95	ALA	3.6
1	G	110	SER	3.6
1	B	109	THR	3.5
2	F	199	GLU	3.5
2	F	222	LEU	3.4
2	F	213	THR	3.4
1	G	11	LEU	3.2
2	H	213	THR	3.2
1	G	27	ARG	3.2
1	G	88	PRO	3.2
1	G	117	GLN	3.2
1	E	11	LEU	3.1
1	B	44	GLU	3.1
1	E	104	ASN	3.1
2	F	90	LEU	3.0
1	B	46	GLU	3.0
1	E	108	VAL	3.0
1	B	104	ASN	2.9
2	H	86	MET	2.9
1	E	111	GLY	2.9
1	G	12	VAL	2.9
1	E	75	ASP	2.9
2	H	90	LEU	2.9
1	G	103	GLU	2.9
2	H	145	ARG	2.8
1	E	1	GLN	2.8
1	E	40	ALA	2.7
1	G	108	VAL	2.7
1	G	3	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
2	F	56	ASP	2.7
1	A	125	SER	2.6
1	G	14	ALA	2.6
2	H	99	SER	2.5
2	D	56	ASP	2.5
1	G	17	SER	2.5
2	H	97	PRO	2.5
2	F	69	SER	2.5
2	C	223	GLU	2.5
1	B	102	LEU	2.4
2	D	222	LEU	2.4
1	B	43	LYS	2.4
1	A	42	GLY	2.4
2	H	161	VAL	2.4
2	H	198	THR	2.3
1	B	103	GLU	2.3
2	C	213	THR	2.3
2	H	174	TYR	2.3
1	A	59	GLU	2.3
2	H	89	ASP	2.3
2	H	120	HIS	2.2
1	B	1	GLN	2.2
1	G	102	LEU	2.2
1	G	15	GLY	2.2
1	G	1	GLN	2.1
2	H	129	LEU	2.1
2	H	222	LEU	2.1
1	B	111	GLY	2.1
1	G	123	VAL	2.1
2	F	223	GLU	2.1
2	F	174	TYR	2.1
1	E	15	GLY	2.1
1	E	29	PHE	2.1
2	H	45	LEU	2.0
2	F	45	LEU	2.0

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

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, 95<sup>th</sup> 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	F	301	14/15	0.55	0.17	97,105,108,109	0
3	NAG	D	302	14/15	0.56	0.15	95,102,108,112	0
3	NAG	H	301	14/15	0.65	0.18	95,98,108,108	0
3	NAG	C	301	14/15	0.82	0.12	73,79,83,85	0
3	NAG	D	301	14/15	0.85	0.13	81,87,93,96	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.