Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 11:05 PM EDT

PDB ID	:	7MMO
Title	:	LY-CoV1404 neutralizing antibody against SARS-CoV-2
Authors	:	Hendle, J.; Pustilnik, A.; Sauder, J.M.; Coleman, K.A.; Boyles, J.S.; Dickinson, C.D.
Deposited on	:	2021-04-30
Resolution	:	2.43 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:

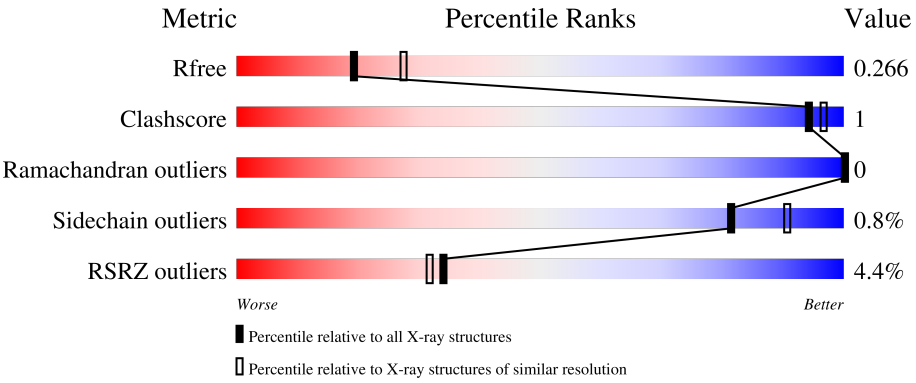
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.43 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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 <=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	223	2% 92% · 5%
1	D	223	% 90% · 7%
2	B	215	95% ·
2	E	215	95% 5%
3	C	205	7% 91% · 5%

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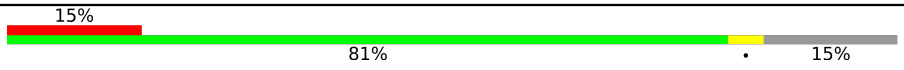
Mol	Chain	Length	Quality of chain
3	F	205	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9153 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 LY-CoV1404 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	1	0
			1580	1012	259	302	7			
1	D	208	Total	C	N	O	S	0	1	0
			1558	998	254	299	7			

- Molecule 2 is a protein called LY-CoV1404 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	1	0
			1585	981	262	335	7			
2	E	214	Total	C	N	O	S	0	1	0
			1584	983	262	332	7			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	194	Total	C	N	O	S	0	2	0
			1486	951	252	275	8			
3	F	175	Total	C	N	O	S	0	0	0
			1273	810	221	236	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	528	HIS	-	expression tag	UNP P0DTC2
C	529	HIS	-	expression tag	UNP P0DTC2
C	530	HIS	-	expression tag	UNP P0DTC2
C	531	HIS	-	expression tag	UNP P0DTC2
C	532	HIS	-	expression tag	UNP P0DTC2
C	533	HIS	-	expression tag	UNP P0DTC2
F	528	HIS	-	expression tag	UNP P0DTC2
F	529	HIS	-	expression tag	UNP P0DTC2

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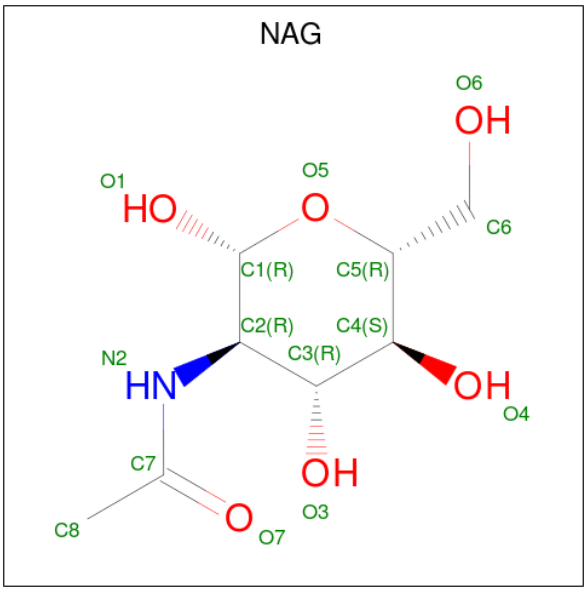
Chain	Residue	Modelled	Actual	Comment	Reference
F	530	HIS	-	expression tag	UNP P0DTC2
F	531	HIS	-	expression tag	UNP P0DTC2
F	532	HIS	-	expression tag	UNP P0DTC2
F	533	HIS	-	expression tag	UNP P0DTC2

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



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

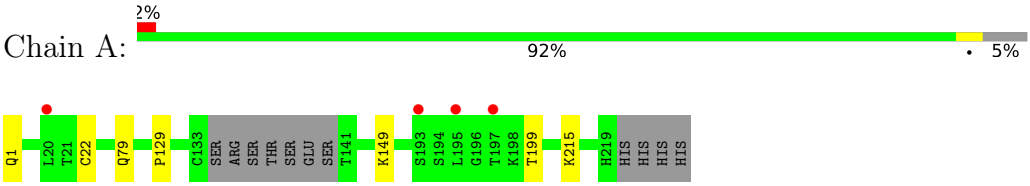
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	12	Total O 12 12	0	0
5	B	24	Total O 24 24	0	0
5	C	7	Total O 8 8	0	1
5	D	8	Total O 8 8	0	0
5	E	19	Total O 19 19	0	0
5	F	2	Total O 2 2	0	0

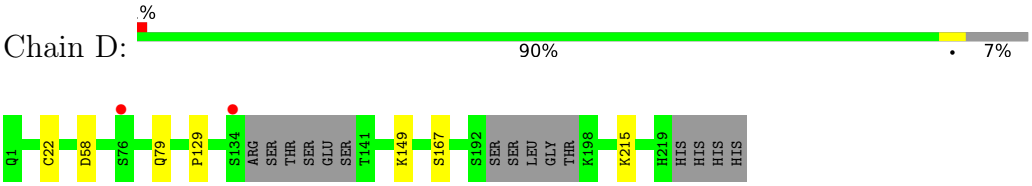
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

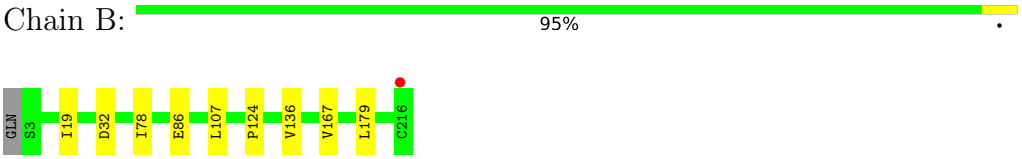
• Molecule 1: LY-CoV1404 Fab heavy chain



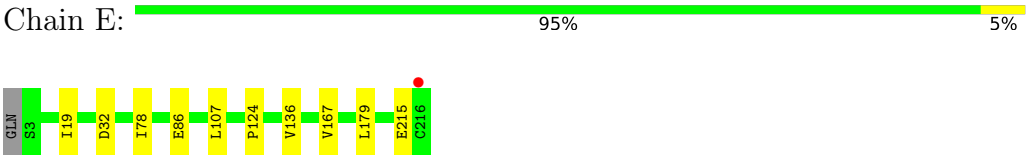
• Molecule 1: LY-CoV1404 Fab heavy chain



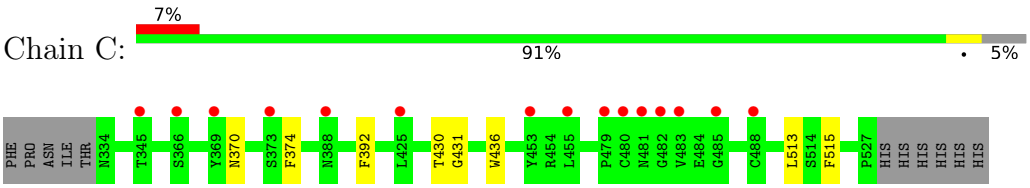
• Molecule 2: LY-CoV1404 Fab light chain



• Molecule 2: LY-CoV1404 Fab light chain

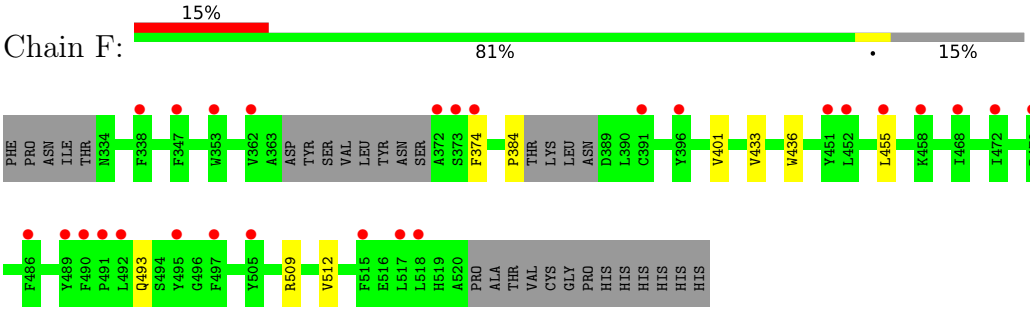


• Molecule 3: Spike protein S1



• Molecule 3: Spike protein S1

Chain F:


15%
81%
15%
PHE PRO ASN ILE THR N334 F338 F347 W353 V362 A363 ASP TYR SER VAL LEU TYR ASN SER A372 S373 F374 P384 THR LYS LEU ASN D389 L390 C391 Y396 V401 V433 W436 Y451 L452 L455 K458 I468 I472 P479 C480 N481 G482 V483
F486 Y489 F490 P491 L492 Q493 S494 Y495 G496 F497 Y505 R509 V512 F515 E516 L517 L518 H519 A520 PRO ALA THR VAL CYS GLY PRO HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	73.09Å 107.69Å 190.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	93.75 – 2.43 93.75 – 2.43	Depositor EDS
% Data completeness (in resolution range)	99.5 (93.75-2.43) 99.5 (93.75-2.43)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.21 (at 2.42Å)	Xtriage
Refinement program	BUSTER 2.11.7 (18-SEP-2020)	Depositor
R, R_{free}	0.226 , 0.253 0.239 , 0.266	Depositor DCC
R_{free} test set	2788 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	55.6	Xtriage
Anisotropy	0.003	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 39.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	9153	wwPDB-VP
Average B, all atoms (Å^2)	58.0	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 23.23 % 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 4.8631e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, PCA

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	0.39	0/1617	0.59	0/2219
1	D	0.38	0/1593	0.58	0/2183
2	B	0.40	0/1619	0.60	0/2203
2	E	0.39	0/1618	0.60	0/2201
3	C	0.35	0/1534	0.50	0/2093
3	F	0.29	0/1306	0.47	0/1784
All	All	0.37	0/9287	0.56	0/12683

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1580	0	1522	2	0
1	D	1558	0	1515	2	0
2	B	1585	0	1484	4	0
2	E	1584	0	1479	4	0
3	C	1486	0	1346	7	0
3	F	1273	0	1074	7	0
4	C	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	12	0	0	0	0
5	B	24	0	0	0	0
5	C	8	0	0	0	0
5	D	8	0	0	0	0
5	E	19	0	0	0	0
5	F	2	0	0	0	0
All	All	9153	0	8433	23	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 1.

All (23) 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)
3:C:370:ASN:HA	3:F:384:PRO:HG2	1.34	1.04
3:C:370:ASN:HA	3:F:384:PRO:CG	2.23	0.57
3:C:374:PHE:HA	3:C:436:TRP:HB3	1.89	0.54
3:F:433:VAL:HG22	3:F:512:VAL:HG13	1.88	0.54
3:F:455:LEU:HD22	3:F:493:GLN:HG3	1.90	0.53
2:E:19:ILE:HD11	2:E:78:ILE:HD12	1.90	0.53
2:B:124:PRO:HD3	2:B:136:VAL:HG22	1.93	0.51
2:E:124:PRO:HD3	2:E:136:VAL:HG22	1.93	0.49
3:C:430:THR:HG22	3:C:515:PHE:HB2	1.95	0.49
2:B:19:ILE:HD11	2:B:78:ILE:HD12	1.96	0.48
3:C:431:GLY:HA3	3:C:513:LEU:O	2.14	0.47
2:B:167:VAL:HG22	2:B:179:LEU:HD12	1.97	0.45
1:D:129:PRO:HD3	1:D:215:LYS:HE2	1.99	0.45
2:E:167:VAL:HG22	2:E:179:LEU:HD12	1.99	0.45
1:A:129:PRO:HD3	1:A:215:LYS:HE2	1.97	0.44
3:F:374:PHE:HA	3:F:436:TRP:HB3	2.02	0.42
2:E:86:GLU:HG3	2:E:107:LEU:O	2.20	0.42
2:B:86:GLU:HG3	2:B:107:LEU:O	2.20	0.41
3:F:401:VAL:HG22	3:F:509:ARG:HG2	2.02	0.41
3:C:392:PHE:CE2	3:C:515:PHE:HB3	2.55	0.41
1:A:22:CYS:O	1:A:79:GLN:HA	2.21	0.41
1:D:22:CYS:O	1:D:79:GLN:HA	2.21	0.40
3:C:370:ASN:CA	3:F:384:PRO:HG2	2.26	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	A	209/223 (94%)	205 (98%)	4 (2%)	0	100	100
1	D	203/223 (91%)	198 (98%)	5 (2%)	0	100	100
2	B	213/215 (99%)	210 (99%)	3 (1%)	0	100	100
2	E	213/215 (99%)	210 (99%)	3 (1%)	0	100	100
3	C	194/205 (95%)	187 (96%)	7 (4%)	0	100	100
3	F	169/205 (82%)	158 (94%)	11 (6%)	0	100	100
All	All	1201/1286 (93%)	1168 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	173/198 (87%)	171 (99%)	2 (1%)	71	84
1	D	174/198 (88%)	171 (98%)	3 (2%)	60	77
2	B	176/184 (96%)	175 (99%)	1 (1%)	86	93
2	E	173/184 (94%)	171 (99%)	2 (1%)	71	84
3	C	149/178 (84%)	149 (100%)	0	100	100
3	F	112/178 (63%)	112 (100%)	0	100	100
All	All	957/1120 (85%)	949 (99%)	8 (1%)	81	91

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	149	LYS
1	A	199	THR
2	B	32	ASP
1	D	58	ASP
1	D	149	LYS
1	D	167	SER
2	E	32	ASP
2	E	215	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	$\#\|Z\| > 2$
1	PCA	A	1	1	7,8,9	1.16	1 (14%)	9,10,12	1.26	1 (11%)
1	PCA	D	1	1	7,8,9	0.73	0	9,10,12	0.80	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	A	1	1	-	0/0/11/13	0/1/1/1
1	PCA	D	1	1	-	0/0/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	CD-N	2.06	1.39	1.34

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	PCA	OE-CD-CG	-2.00	123.27	126.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	C	601	3	14,14,15	0.26	0	17,19,21	0.59	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
4	NAG	C	601	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	601	NAG	O5-C1-C2	-2.35	107.58	111.29

There are no chirality outliers.

There are no torsion outliers.

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

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^{th} 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	A	211/223 (94%)	0.20	4 (1%) 66 64	36, 52, 70, 89	0
1	D	207/223 (92%)	0.22	2 (0%) 82 80	39, 54, 71, 85	0
2	B	214/215 (99%)	0.06	1 (0%) 91 89	33, 48, 60, 74	0
2	E	214/215 (99%)	0.07	1 (0%) 91 89	37, 50, 63, 79	0
3	C	194/205 (94%)	0.47	15 (7%) 13 11	42, 64, 103, 111	0
3	F	175/205 (85%)	1.06	31 (17%) 1 1	57, 92, 119, 121	0
All	All	1215/1286 (94%)	0.32	54 (4%) 34 32	33, 54, 105, 121	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	482	GLY	5.8
3	F	491	PRO	5.7
3	F	486	PHE	5.6
3	F	481	ASN	5.1
3	F	479	PRO	4.4
3	F	480	CYS	4.4
2	B	216	CYS	4.2
3	F	495	TYR	4.0
1	A	193	SER	3.8
3	F	373	SER	3.7
3	C	388	ASN	3.7
3	C	488	CYS	3.7
3	F	505	TYR	3.4
2	E	216	CYS	3.4
3	C	480	CYS	3.3
3	C	369	TYR	3.2
3	C	481	ASN	3.1
3	F	472	ILE	3.0
3	F	455	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
3	F	483	VAL	2.9
3	F	391	CYS	2.9
3	F	515	PHE	2.9
3	F	347	PHE	2.9
3	F	517	LEU	2.8
3	C	483	VAL	2.6
3	F	490	PHE	2.5
3	F	492	LEU	2.5
3	F	338	PHE	2.5
3	F	374	PHE	2.5
3	C	453	TYR	2.4
3	F	372	ALA	2.4
3	F	458	LYS	2.3
1	D	76	SER	2.3
3	F	452	LEU	2.3
1	A	195	LEU	2.3
3	F	518	LEU	2.3
3	F	482	GLY	2.3
3	C	373	SER	2.3
3	C	485	GLY	2.2
1	A	197	THR	2.2
3	C	366	SER	2.2
3	F	489	TYR	2.2
1	D	134	SER	2.2
3	F	362	VAL	2.2
3	F	497	PHE	2.2
3	F	396	TYR	2.2
3	C	479	PRO	2.2
3	C	345	THR	2.1
3	C	425	LEU	2.1
3	F	468	ILE	2.1
3	C	455	LEU	2.1
3	F	353	TRP	2.1
1	A	20	LEU	2.0
3	F	451	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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^{th} 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
1	PCA	A	1	8/9	0.87	0.19	64,66,68,73	0
1	PCA	D	1	8/9	0.89	0.15	62,63,65,67	0

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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NAG	C	601	14/15	0.68	0.35	71,72,72,72	14

6.5 Other polymers (i)

There are no such residues in this entry.