wwPDB X-ray Structure Validation Summary Report (i)

Jan 9, 2024 – 02:04 AM EST

PDB ID	:	8FI9
Title	:	Crystal structure of SARS-CoV-2 receptor binding domain in complex with neutralizing antibody WRAIR-5001
Authors	:	Sankhala, R.S.; Jensen, J.L.; Joyce, M.G.
Deposited on	:	2022-12-15
Resolution	:	4.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

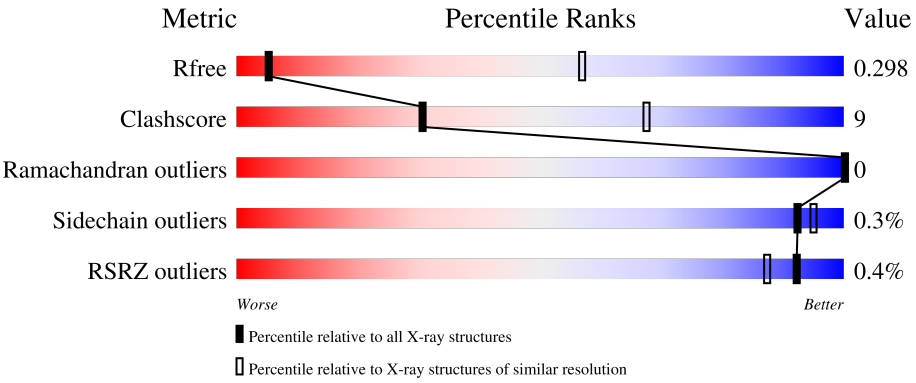
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 4.20 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	1005 (4.62-3.78)
Clashscore	141614	1044 (4.60-3.80)
Ramachandran outliers	138981	1000 (4.60-3.80)
Sidechain outliers	138945	1007 (4.62-3.78)
RSRZ outliers	127900	1063 (4.70-3.70)

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 >=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	205	68% 27%
1	C	205	75% 22%
1	K	205	72% 22% 5%
1	O	205	71% 25%
2	F	215	% 81% 17%

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Mol	Chain	Length	Quality of chain
2	I	215	39% 13% 49%
2	L	215	81% 19%
2	N	215	87% 13%
3	G	223	% 80% 19%
3	H	223	74% 25%
3	J	223	40% 12% 48%
3	Q	223	80% 19%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NAG	C	601	-	-	-	X
4	NAG	O	601	-	-	-	X
5	GOL	N	301	-	-	-	X
5	GOL	N	302	-	-	-	X
5	GOL	Q	301	-	-	-	X
5	GOL	Q	302	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 17945 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 protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	198	Total	C	N	O	S	0	0	0
			1563	1000	262	293	8			
1	C	198	Total	C	N	O	S	0	0	0
			1563	1000	262	293	8			
1	K	194	Total	C	N	O	S	0	0	0
			1536	985	256	287	8			
1	O	196	Total	C	N	O	S	0	0	0
			1551	995	258	290	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	528	GLY	-	expression tag	UNP P0DTC2
A	529	SER	-	expression tag	UNP P0DTC2
A	530	HIS	-	expression tag	UNP P0DTC2
A	531	HIS	-	expression tag	UNP P0DTC2
A	532	HIS	-	expression tag	UNP P0DTC2
A	533	HIS	-	expression tag	UNP P0DTC2
A	534	HIS	-	expression tag	UNP P0DTC2
A	535	HIS	-	expression tag	UNP P0DTC2
C	528	GLY	-	expression tag	UNP P0DTC2
C	529	SER	-	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
C	534	HIS	-	expression tag	UNP P0DTC2
C	535	HIS	-	expression tag	UNP P0DTC2
K	528	GLY	-	expression tag	UNP P0DTC2
K	529	SER	-	expression tag	UNP P0DTC2
K	530	HIS	-	expression tag	UNP P0DTC2
K	531	HIS	-	expression tag	UNP P0DTC2
K	532	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
K	533	HIS	-	expression tag	UNP P0DTC2
K	534	HIS	-	expression tag	UNP P0DTC2
K	535	HIS	-	expression tag	UNP P0DTC2
O	528	GLY	-	expression tag	UNP P0DTC2
O	529	SER	-	expression tag	UNP P0DTC2
O	530	HIS	-	expression tag	UNP P0DTC2
O	531	HIS	-	expression tag	UNP P0DTC2
O	532	HIS	-	expression tag	UNP P0DTC2
O	533	HIS	-	expression tag	UNP P0DTC2
O	534	HIS	-	expression tag	UNP P0DTC2
O	535	HIS	-	expression tag	UNP P0DTC2

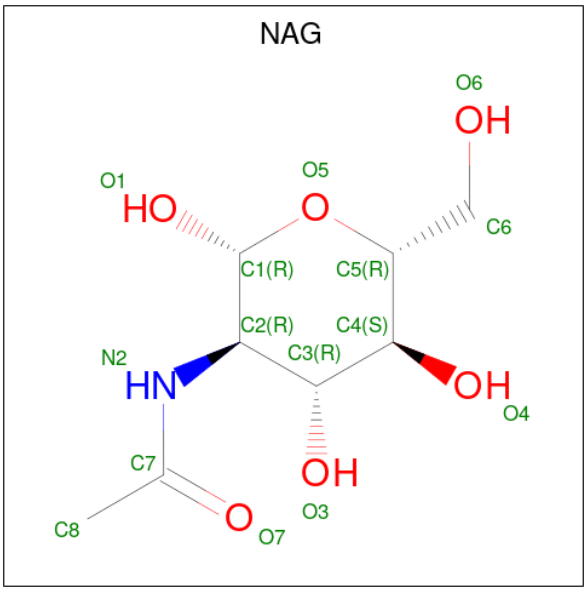
- Molecule 2 is a protein called WRAIR-5001 Fab Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	211	Total	C	N	O	S	0	0	0
			1590	993	270	323	4			
2	I	110	Total	C	N	O	S	0	0	0
			837	521	146	168	2			
2	L	215	Total	C	N	O	S	0	0	0
			1617	1007	274	331	5			
2	N	213	Total	C	N	O	S	0	0	0
			1604	1001	272	327	4			

- Molecule 3 is a protein called WRAIR-5001 Fab Heavy chain.

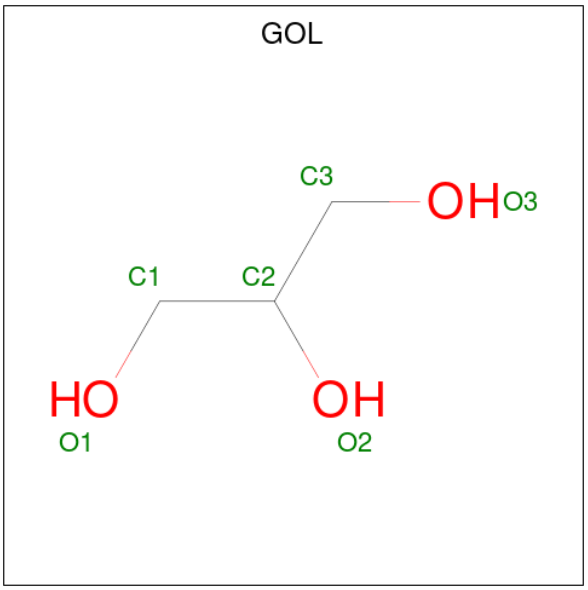
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	221	Total	C	N	O	S	0	0	0
			1679	1058	284	330	7			
3	H	222	Total	C	N	O	S	0	0	0
			1688	1063	286	332	7			
3	J	116	Total	C	N	O	S	0	0	0
			911	577	156	173	5			
3	Q	222	Total	C	N	O	S	0	0	0
			1686	1061	285	332	8			

- 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	A	1	Total C N O 14 8 1 5	0	0
4	C	1	Total C N O 14 8 1 5	0	0
4	K	1	Total C N O 14 8 1 5	0	0
4	O	1	Total C N O 14 8 1 5	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	H	1	Total C O 6 3 3	0	0
5	H	1	Total C O 6 3 3	0	0
5	J	1	Total C O 6 3 3	0	0
5	N	1	Total C O 6 3 3	0	0
5	N	1	Total C O 6 3 3	0	0
5	N	1	Total C O 6 3 3	0	0
5	O	1	Total C O 6 3 3	0	0
5	Q	1	Total C O 6 3 3	0	0
5	Q	1	Total C O 6 3 3	0	0
5	Q	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

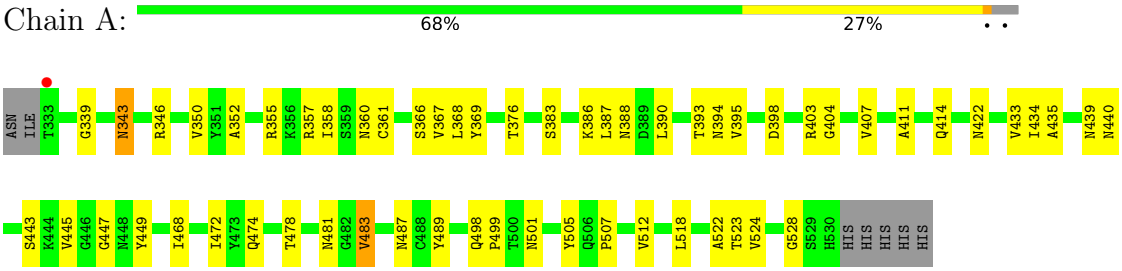
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	4	Total O 4 4	0	0

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.

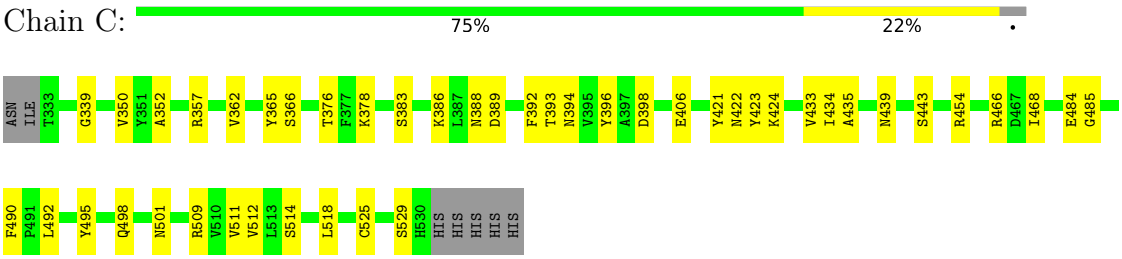
• Molecule 1: Spike protein S1

Chain A:



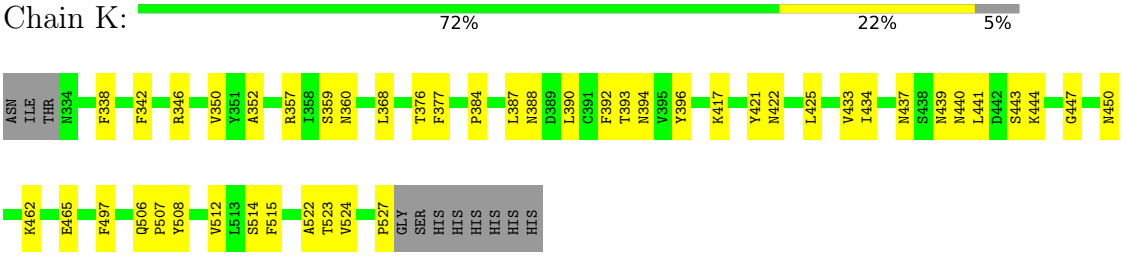
• Molecule 1: Spike protein S1

Chain C:



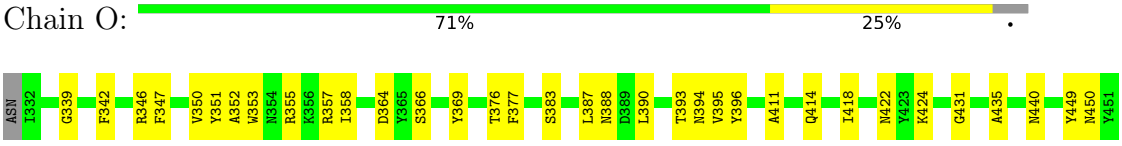
• Molecule 1: Spike protein S1

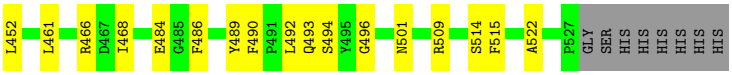
Chain K:



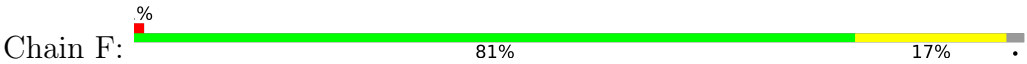
• Molecule 1: Spike protein S1

Chain O:

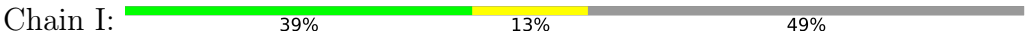


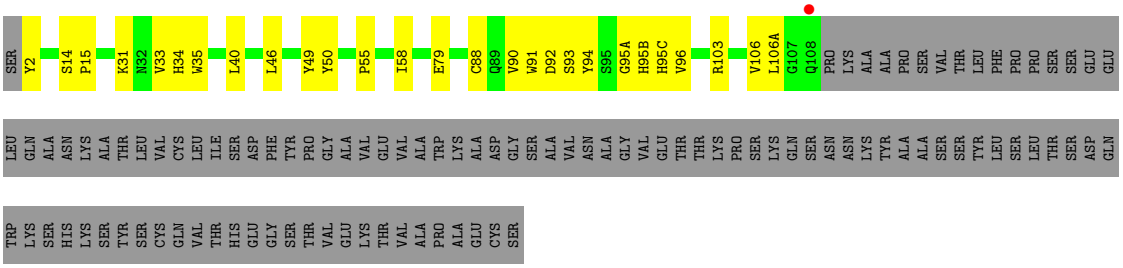


• Molecule 2: WRAIR-5001 Fab Light chain

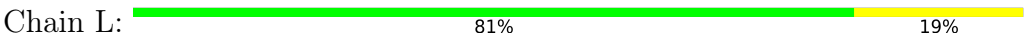


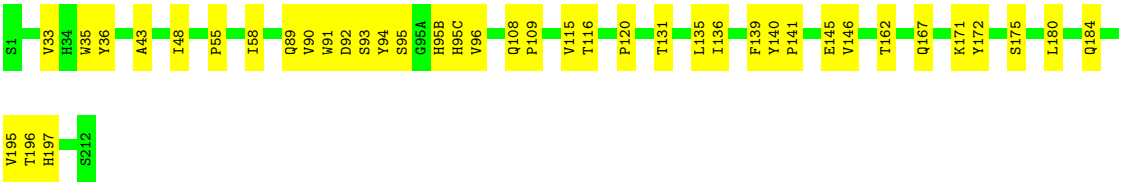
• Molecule 2: WRAIR-5001 Fab Light chain



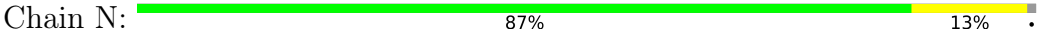


• Molecule 2: WRAIR-5001 Fab Light chain

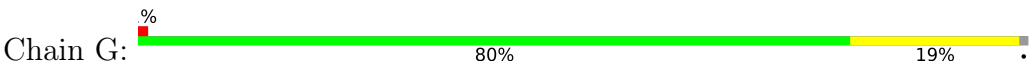


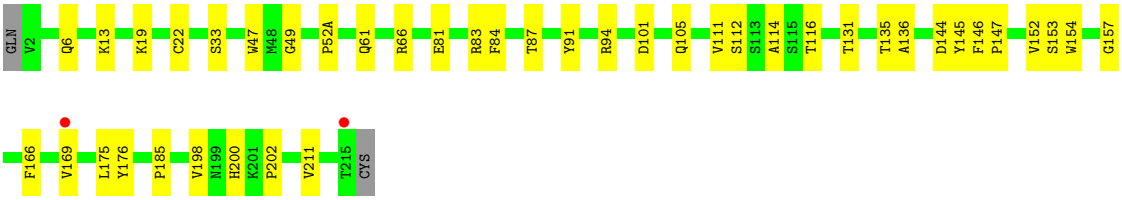


• Molecule 2: WRAIR-5001 Fab Light chain



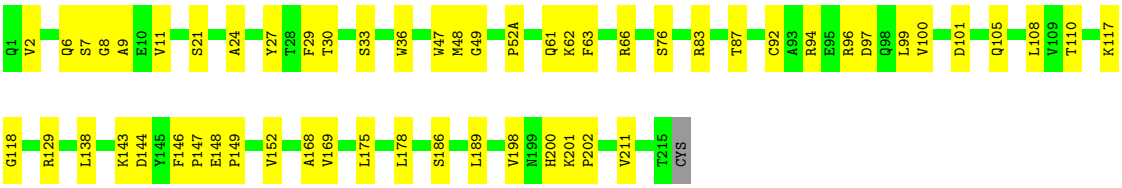
• Molecule 3: WRAIR-5001 Fab Heavy chain





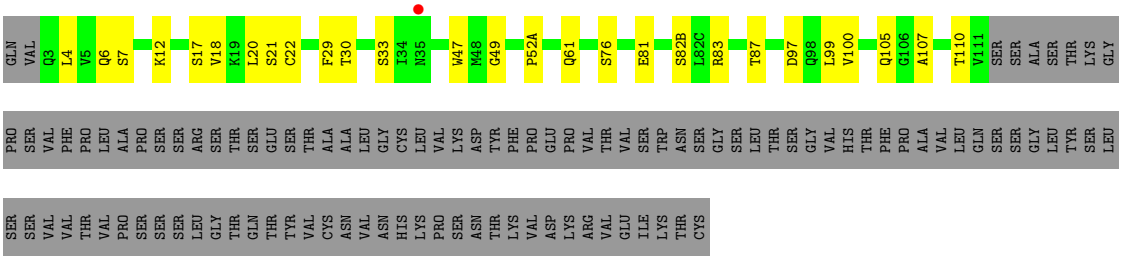
• Molecule 3: WRAIR-5001 Fab Heavy chain

Chain H:



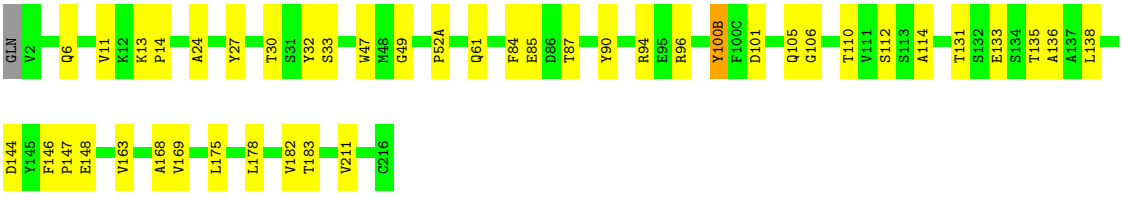
• Molecule 3: WRAIR-5001 Fab Heavy chain

Chain J:



• Molecule 3: WRAIR-5001 Fab Heavy chain

Chain Q:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	141.51Å 115.56Å 142.17Å 90.00° 111.97° 90.00°	Depositor
Resolution (Å)	19.99 – 4.20 19.99 – 4.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (19.99-4.20) 99.9 (19.99-4.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.92 (at 4.21Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.252 , 0.296 0.254 , 0.298	Depositor DCC
R_{free} test set	1550 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	173.4	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 138.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Estimated twinning fraction	0.077 for l,-k,h	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	17945	wwPDB-VP
Average B, all atoms (Å^2)	210.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

[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: GOL, 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	0.33	0/1608	0.52	0/2189
1	C	0.28	0/1608	0.51	0/2189
1	K	0.27	0/1580	0.50	0/2151
1	O	0.28	0/1595	0.50	0/2172
2	F	0.26	0/1629	0.49	0/2223
2	I	0.26	0/857	0.51	0/1168
2	L	0.27	0/1656	0.52	0/2258
2	N	0.26	0/1643	0.49	0/2242
3	G	0.27	0/1719	0.53	0/2344
3	H	0.29	0/1728	0.53	0/2356
3	J	0.26	0/933	0.52	0/1267
3	Q	0.27	0/1726	0.53	0/2352
All	All	0.28	0/18282	0.51	0/24911

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	1563	0	1474	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1563	0	1474	27	0
1	K	1536	0	1452	29	0
1	O	1551	0	1470	36	0
2	F	1590	0	1521	24	0
2	I	837	0	786	20	0
2	L	1617	0	1542	27	0
2	N	1604	0	1532	25	0
3	G	1679	0	1644	34	0
3	H	1688	0	1655	43	0
3	J	911	0	877	18	0
3	Q	1686	0	1651	30	0
4	A	14	0	13	3	0
4	C	14	0	13	1	0
4	K	14	0	13	4	0
4	O	14	0	13	2	0
5	H	12	0	16	0	0
5	J	6	0	8	0	0
5	N	18	0	24	0	0
5	O	6	0	8	0	0
5	Q	18	0	24	0	0
6	H	4	0	0	1	0
All	All	17945	0	17210	324	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 9.

The worst 5 of 324 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:Q:96:ARG:HD3	3:Q:100(B):TYR:OH	1.77	0.84
2:N:188:HIS:HD1	2:N:191:TYR:HH	1.28	0.80
1:C:352:ALA:HB1	2:F:93:SER:HB2	1.61	0.80
2:N:37:GLN:HG2	2:N:47:VAL:HG13	1.62	0.80
2:F:162:THR:HB	3:G:169:VAL:HG22	1.64	0.79

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	196/205 (96%)	190 (97%)	6 (3%)	0	100	100
1	C	196/205 (96%)	187 (95%)	9 (5%)	0	100	100
1	K	192/205 (94%)	185 (96%)	7 (4%)	0	100	100
1	O	194/205 (95%)	189 (97%)	5 (3%)	0	100	100
2	F	209/215 (97%)	199 (95%)	10 (5%)	0	100	100
2	I	108/215 (50%)	103 (95%)	5 (5%)	0	100	100
2	L	213/215 (99%)	201 (94%)	12 (6%)	0	100	100
2	N	211/215 (98%)	202 (96%)	9 (4%)	0	100	100
3	G	219/223 (98%)	211 (96%)	8 (4%)	0	100	100
3	H	220/223 (99%)	210 (96%)	10 (4%)	0	100	100
3	J	114/223 (51%)	113 (99%)	1 (1%)	0	100	100
3	Q	220/223 (99%)	213 (97%)	7 (3%)	0	100	100
All	All	2292/2572 (89%)	2203 (96%)	89 (4%)	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	170/177 (96%)	166 (98%)	4 (2%)	49	69
1	C	170/177 (96%)	170 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	K	167/177 (94%)	167 (100%)	0	100	100
1	O	169/177 (96%)	169 (100%)	0	100	100
2	F	175/178 (98%)	175 (100%)	0	100	100
2	I	90/178 (51%)	90 (100%)	0	100	100
2	L	178/178 (100%)	178 (100%)	0	100	100
2	N	176/178 (99%)	176 (100%)	0	100	100
3	G	191/193 (99%)	191 (100%)	0	100	100
3	H	192/193 (100%)	192 (100%)	0	100	100
3	J	97/193 (50%)	97 (100%)	0	100	100
3	Q	192/193 (100%)	191 (100%)	1 (0%)	88	93
All	All	1967/2192 (90%)	1962 (100%)	5 (0%)	92	95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	343	ASN
1	A	478	THR
1	A	481	ASN
1	A	483	VAL
3	Q	100(B)	TYR

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

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

14 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	A	601	1	14,14,15	0.27	0	17,19,21	1.01	2 (11%)
5	GOL	Q	303	-	5,5,5	0.93	0	5,5,5	0.98	0
5	GOL	N	303	-	5,5,5	0.93	0	5,5,5	0.97	0
5	GOL	O	602	-	5,5,5	0.93	0	5,5,5	0.97	0
5	GOL	J	301	-	5,5,5	0.90	0	5,5,5	0.98	0
4	NAG	O	601	1	14,14,15	0.33	0	17,19,21	0.68	0
5	GOL	H	302	-	5,5,5	0.93	0	5,5,5	0.97	0
5	GOL	N	302	-	5,5,5	0.90	0	5,5,5	0.99	0
5	GOL	Q	302	-	5,5,5	0.93	0	5,5,5	1.00	0
5	GOL	Q	301	-	5,5,5	0.92	0	5,5,5	0.99	0
5	GOL	N	301	-	5,5,5	0.92	0	5,5,5	0.98	0
5	GOL	H	301	-	5,5,5	0.92	0	5,5,5	0.99	0
4	NAG	C	601	1	14,14,15	0.34	0	17,19,21	0.76	0
4	NAG	K	601	1	14,14,15	0.33	0	17,19,21	0.69	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
4	NAG	A	601	1	-	3/6/23/26	0/1/1/1
5	GOL	Q	303	-	-	0/4/4/4	-
5	GOL	N	303	-	-	0/4/4/4	-
5	GOL	O	602	-	-	0/4/4/4	-
5	GOL	J	301	-	-	2/4/4/4	-
4	NAG	O	601	1	-	3/6/23/26	0/1/1/1
5	GOL	H	302	-	-	0/4/4/4	-
5	GOL	N	302	-	-	0/4/4/4	-
5	GOL	Q	302	-	-	0/4/4/4	-
5	GOL	Q	301	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	N	301	-	-	0/4/4/4	-
5	GOL	H	301	-	-	0/4/4/4	-
4	NAG	C	601	1	-	4/6/23/26	0/1/1/1
4	NAG	K	601	1	-	4/6/23/26	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(^{o})	Ideal(^{o})
4	A	601	NAG	O5-C1-C2	2.26	114.86	111.29
4	A	601	NAG	C1-O5-C5	2.25	115.25	112.19

There are no chirality outliers.

5 of 16 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	NAG	C8-C7-N2-C2
4	A	601	NAG	O7-C7-N2-C2
4	C	601	NAG	C8-C7-N2-C2
4	C	601	NAG	O7-C7-N2-C2
4	K	601	NAG	C3-C2-N2-C7

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	601	NAG	3	0
4	O	601	NAG	2	0
4	C	601	NAG	1	0
4	K	601	NAG	4	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^{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	198/205 (96%)	-0.34	1 (0%) 91 86	132, 173, 238, 266	0
1	C	198/205 (96%)	-0.30	0 100 100	161, 194, 257, 285	0
1	K	194/205 (94%)	-0.29	0 100 100	197, 228, 262, 275	0
1	O	196/205 (95%)	-0.27	0 100 100	172, 207, 255, 293	0
2	F	211/215 (98%)	-0.08	3 (1%) 75 65	216, 253, 337, 364	0
2	I	110/215 (51%)	-0.43	1 (0%) 84 77	168, 194, 227, 245	0
2	L	215/215 (100%)	-0.38	0 100 100	156, 183, 227, 241	0
2	N	213/215 (99%)	-0.36	1 (0%) 91 86	180, 222, 271, 290	0
3	G	221/223 (99%)	-0.15	2 (0%) 84 77	203, 227, 251, 270	0
3	H	222/223 (99%)	-0.43	0 100 100	151, 177, 224, 248	0
3	J	116/223 (52%)	-0.23	1 (0%) 84 77	207, 246, 279, 305	0
3	Q	222/223 (99%)	-0.46	0 100 100	172, 198, 234, 257	0
All	All	2316/2572 (90%)	-0.31	9 (0%) 92 87	132, 210, 271, 364	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	158	GLY	3.3
2	I	108	GLN	2.9
2	F	199	GLY	2.6
1	A	333	THR	2.5
2	N	106(A)	LEU	2.4

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 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
5	GOL	Q	301	6/6	0.50	0.70	229,229,229,229	0
5	GOL	N	302	6/6	0.53	0.84	229,229,229,229	0
5	GOL	N	301	6/6	0.64	0.42	229,229,229,229	0
4	NAG	O	601	14/15	0.75	0.45	229,229,229,229	0
4	NAG	C	601	14/15	0.76	0.41	229,229,229,229	0
5	GOL	Q	303	6/6	0.78	0.27	229,229,229,229	0
5	GOL	N	303	6/6	0.80	0.33	229,229,229,229	0
5	GOL	Q	302	6/6	0.80	0.50	229,229,229,229	0
5	GOL	O	602	6/6	0.80	0.59	229,229,229,229	0
5	GOL	H	301	6/6	0.81	0.27	229,229,229,229	0
4	NAG	K	601	14/15	0.81	0.35	229,229,229,229	0
4	NAG	A	601	14/15	0.82	0.70	229,229,229,229	0
5	GOL	J	301	6/6	0.86	0.68	229,229,229,229	0
5	GOL	H	302	6/6	0.87	0.23	229,229,229,229	0

6.5 Other polymers (i)

There are no such residues in this entry.