Full wwPDB X-ray Structure Validation Report ⓘ

Jun 20, 2022 – 01:09 pm BST

PDB ID	:	7ZFE
Title	:	SARS-CoV-2 Omicron RBD in complex with Omi-32 Fab and nanobody C1
Authors	:	Zhou, D.; Huo, J.; Ren, J.; Stuart, D.I.
Deposited on	:	2022-04-01
Resolution	:	3.25 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:

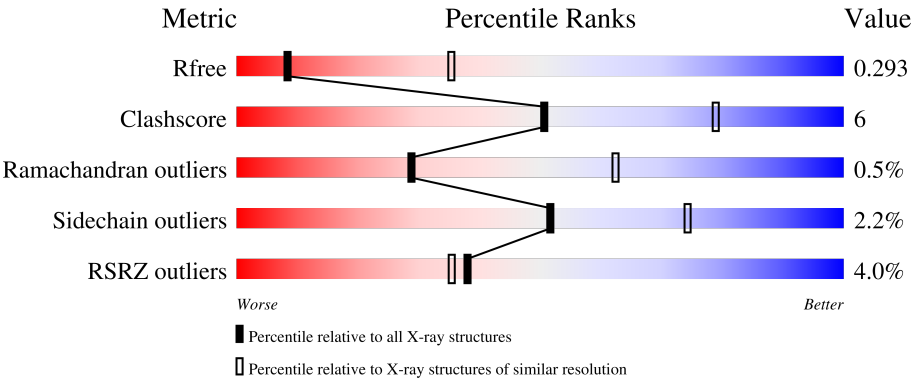
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.28.1

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 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	W	131	7% 85% 9% • 5%
1	X	131	4% 87% 8% 5%
1	Y	131	11% 85% 8% • 5%
1	Z	131	4% 81% 13% • 5%
2	A	202	11% 74% 16% • 9%

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Mol	Chain	Length	Quality of chain
2	B	202	2% 77% 13% 9%
2	C	202	5% 78% 11% 10%
2	E	202	2% 69% 15% 15%
3	F	221	4% 85% 11%
3	H	221	5% 85% 11%
3	J	221	3% 84% 12%
3	M	221	2% 81% 14%
4	G	216	2% 92% 7%
4	K	216	% 88% 11%
4	L	216	% 89% 9%
4	N	216	% 88% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 22839 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 C1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Z	124	Total	C	N	O	S	0	2	0
			973	612	167	190	4			
1	X	124	Total	C	N	O	S	0	2	0
			973	612	167	190	4			
1	W	124	Total	C	N	O	S	0	2	0
			973	612	167	190	4			
1	Y	124	Total	C	N	O	S	0	2	0
			973	612	167	190	4			

- Molecule 2 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	182	Total	C	N	O	S	0	0	0
			1476	953	248	268	7			
2	E	172	Total	C	N	O	S	0	0	0
			1403	908	237	252	6			
2	B	183	Total	C	N	O	S	0	0	0
			1484	959	249	269	7			
2	A	183	Total	C	N	O	S	0	0	0
			1484	959	249	269	7			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	327	HIS	-	expression tag	UNP P0DTC2
C	328	HIS	-	expression tag	UNP P0DTC2
C	329	HIS	-	expression tag	UNP P0DTC2
C	330	HIS	-	expression tag	UNP P0DTC2
C	331	HIS	-	expression tag	UNP P0DTC2
C	332	HIS	-	expression tag	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	LEU	SER	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	446	SER	GLY	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	493	ARG	GLN	variant	UNP P0DTC2
C	496	SER	GLY	variant	UNP P0DTC2
C	498	ARG	GLN	conflict	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	527	LYS	-	expression tag	UNP P0DTC2
C	528	LYS	-	expression tag	UNP P0DTC2
E	327	HIS	-	expression tag	UNP P0DTC2
E	328	HIS	-	expression tag	UNP P0DTC2
E	329	HIS	-	expression tag	UNP P0DTC2
E	330	HIS	-	expression tag	UNP P0DTC2
E	331	HIS	-	expression tag	UNP P0DTC2
E	332	HIS	-	expression tag	UNP P0DTC2
E	339	ASP	GLY	variant	UNP P0DTC2
E	371	LEU	SER	variant	UNP P0DTC2
E	373	PRO	SER	variant	UNP P0DTC2
E	375	PHE	SER	variant	UNP P0DTC2
E	417	ASN	LYS	variant	UNP P0DTC2
E	440	LYS	ASN	variant	UNP P0DTC2
E	446	SER	GLY	variant	UNP P0DTC2
E	477	ASN	SER	variant	UNP P0DTC2
E	478	LYS	THR	variant	UNP P0DTC2
E	484	ALA	GLU	variant	UNP P0DTC2
E	493	ARG	GLN	variant	UNP P0DTC2
E	496	SER	GLY	variant	UNP P0DTC2
E	498	ARG	GLN	conflict	UNP P0DTC2
E	501	TYR	ASN	variant	UNP P0DTC2
E	505	HIS	TYR	variant	UNP P0DTC2
E	527	LYS	-	expression tag	UNP P0DTC2
E	528	LYS	-	expression tag	UNP P0DTC2
B	327	HIS	-	expression tag	UNP P0DTC2
B	328	HIS	-	expression tag	UNP P0DTC2
B	329	HIS	-	expression tag	UNP P0DTC2
B	330	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	331	HIS	-	expression tag	UNP P0DTC2
B	332	HIS	-	expression tag	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	conflict	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	527	LYS	-	expression tag	UNP P0DTC2
B	528	LYS	-	expression tag	UNP P0DTC2
A	327	HIS	-	expression tag	UNP P0DTC2
A	328	HIS	-	expression tag	UNP P0DTC2
A	329	HIS	-	expression tag	UNP P0DTC2
A	330	HIS	-	expression tag	UNP P0DTC2
A	331	HIS	-	expression tag	UNP P0DTC2
A	332	HIS	-	expression tag	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2
A	496	SER	GLY	variant	UNP P0DTC2
A	498	ARG	GLN	conflict	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	527	LYS	-	expression tag	UNP P0DTC2
A	528	LYS	-	expression tag	UNP P0DTC2

- Molecule 3 is a protein called Omi-32 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	M	217	Total	C	N	O	S	0	0	0
			1627	1027	276	318	6			
3	J	217	Total	C	N	O	S	0	0	0
			1627	1027	276	318	6			
3	H	217	Total	C	N	O	S	0	0	0
			1623	1025	275	317	6			
3	F	217	Total	C	N	O	S	0	0	0
			1627	1027	276	318	6			

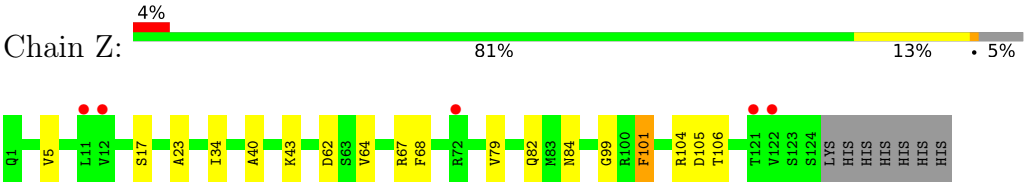
- Molecule 4 is a protein called Omi-32 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	N	216	Total	C	N	O	S	0	0	0
			1649	1028	284	331	6			
4	K	216	Total	C	N	O	S	0	0	0
			1649	1028	284	331	6			
4	L	216	Total	C	N	O	S	0	0	0
			1649	1028	284	331	6			
4	G	216	Total	C	N	O	S	0	0	0
			1649	1028	284	331	6			

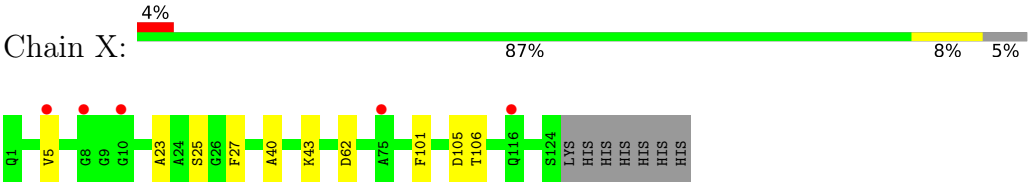
3 Residue-property plots (i)

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.

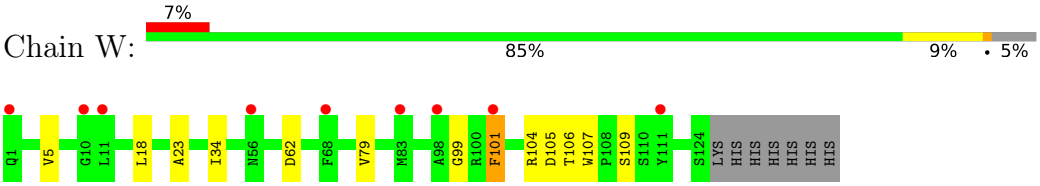
• Molecule 1: Nanobody C1



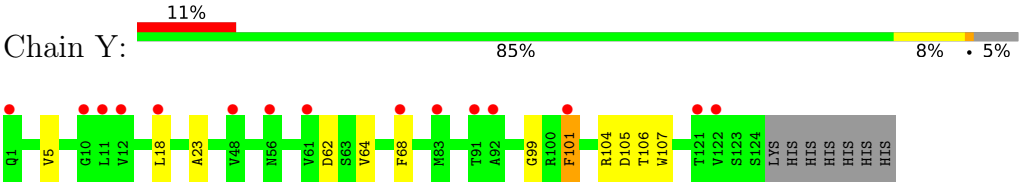
• Molecule 1: Nanobody C1



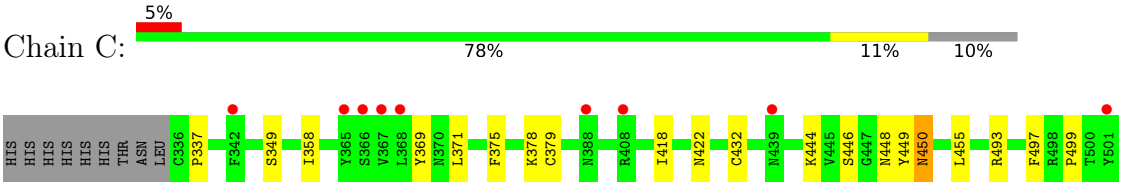
• Molecule 1: Nanobody C1

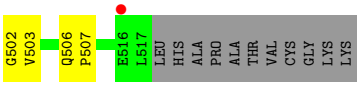


• Molecule 1: Nanobody C1

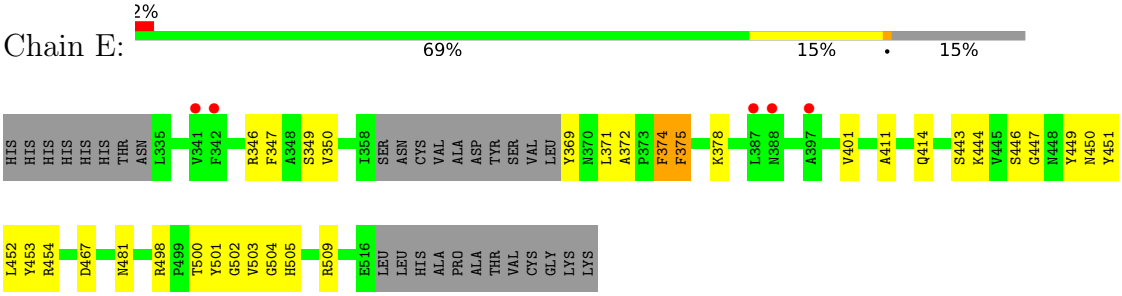


• Molecule 2: Spike protein S1

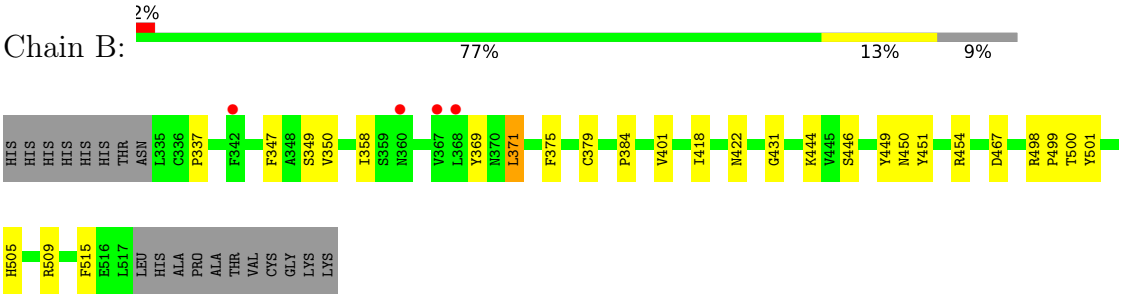




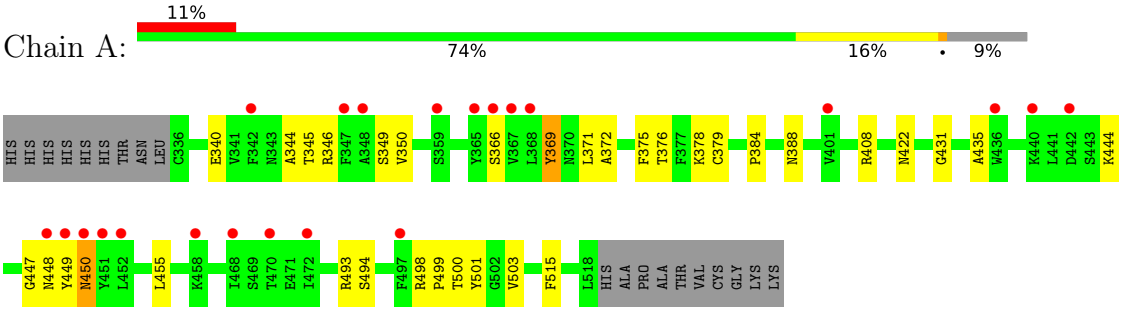
• Molecule 2: Spike protein S1



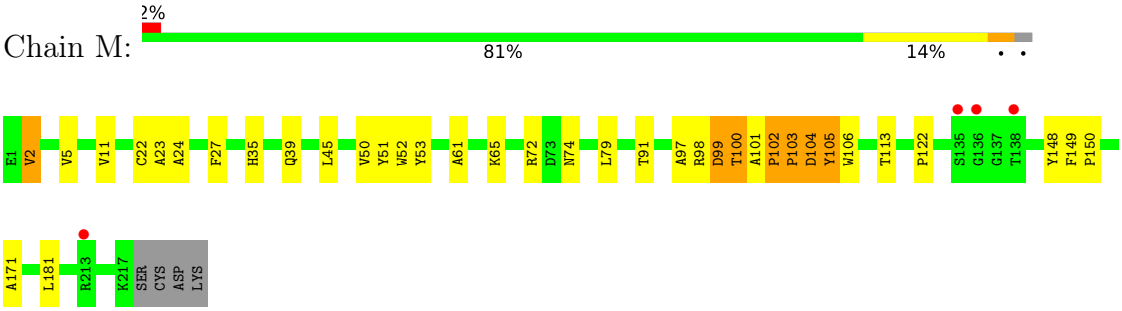
• Molecule 2: Spike protein S1



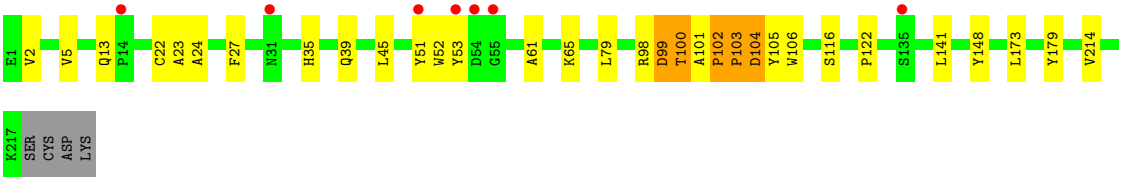
• Molecule 2: Spike protein S1



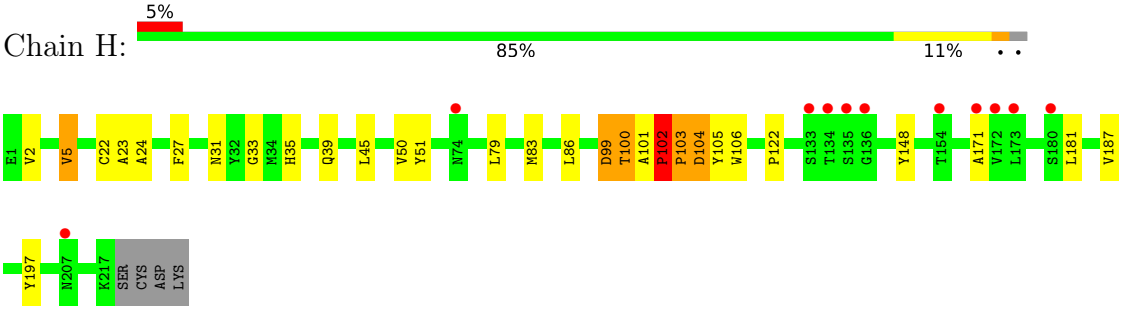
• Molecule 3: Omi-32 heavy chain



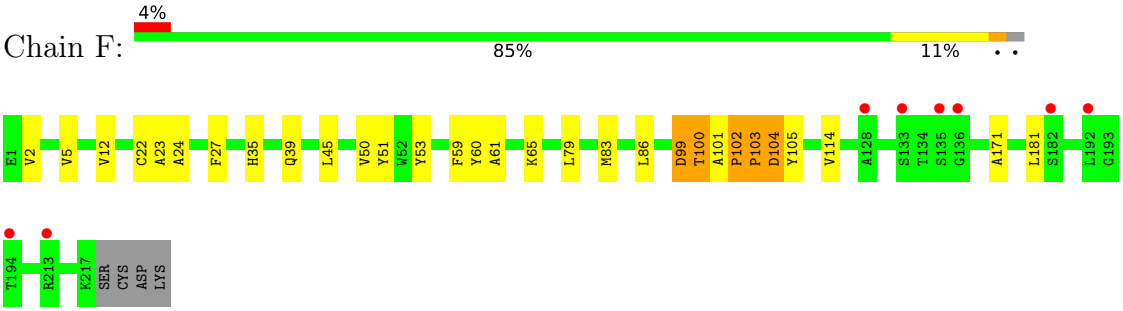
• Molecule 3: Omi-32 heavy chain



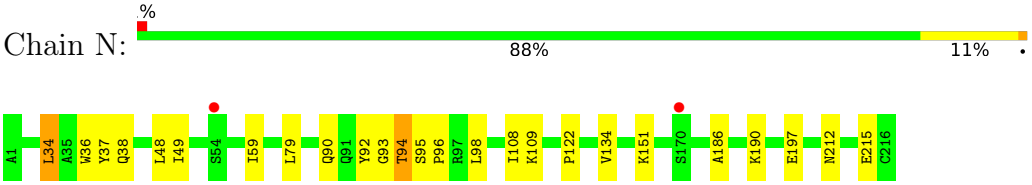
• Molecule 3: Omi-32 heavy chain



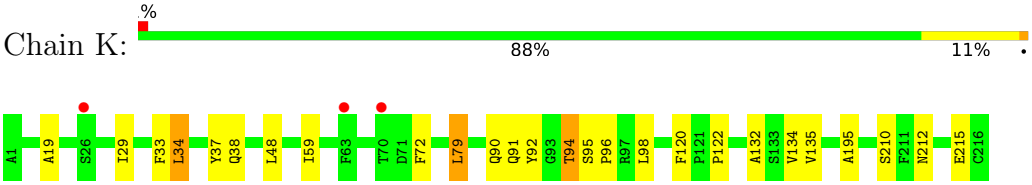
• Molecule 3: Omi-32 heavy chain



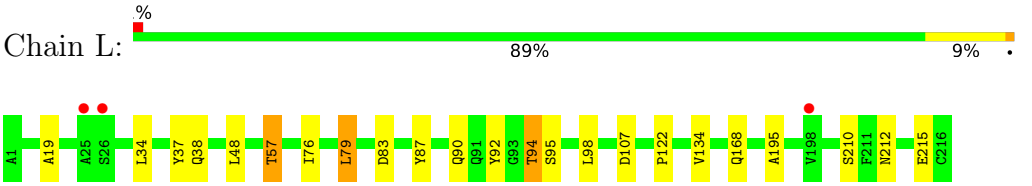
• Molecule 4: Omi-32 light chain



• Molecule 4: Omi-32 light chain

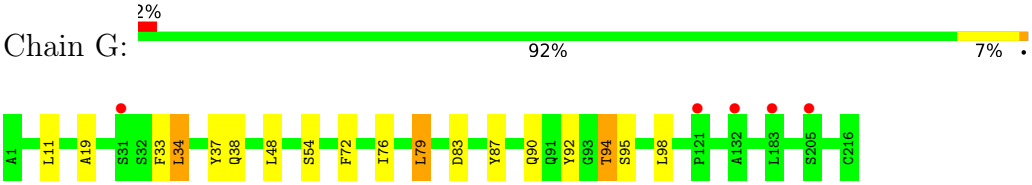


• Molecule 4: Omi-32 light chain



• Molecule 4: Omi-32 light chain

Chain G:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	98.49Å 159.91Å 133.27Å 90.00° 106.77° 90.00°	Depositor
Resolution (Å)	127.61 – 3.25 127.61 – 3.25	Depositor EDS
% Data completeness (in resolution range)	45.6 (127.61-3.25) 45.6 (127.61-3.25)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.237 , 0.293 0.236 , 0.293	Depositor DCC
R_{free} test set	1395 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	70.5	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	22839	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.31% 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

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	W	0.24	0/1004	0.50	0/1366
1	X	0.25	0/1004	0.50	0/1366
1	Y	0.24	0/1004	0.50	0/1366
1	Z	0.25	0/1004	0.50	0/1366
2	A	0.27	0/1528	0.50	0/2077
2	B	0.26	0/1528	0.49	0/2077
2	C	0.28	0/1520	0.50	0/2066
2	E	0.27	0/1445	0.53	0/1961
3	F	0.26	0/1670	0.50	0/2282
3	H	0.26	0/1666	0.51	0/2277
3	J	0.26	0/1670	0.51	0/2282
3	M	0.25	0/1670	0.50	0/2282
4	G	0.26	0/1684	0.51	0/2283
4	K	0.26	0/1684	0.52	0/2283
4	L	0.26	0/1684	0.51	0/2283
4	N	0.28	0/1684	0.52	0/2283
All	All	0.26	0/23449	0.51	0/31900

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
3	H	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
3	H	102	PRO	Peptide

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	W	973	0	922	10	0
1	X	973	0	922	4	0
1	Y	973	0	922	8	0
1	Z	973	0	922	10	0
2	A	1484	0	1417	24	0
2	B	1484	0	1417	22	0
2	C	1476	0	1406	17	0
2	E	1403	0	1339	22	0
3	F	1627	0	1563	19	0
3	H	1623	0	1557	24	0
3	J	1627	0	1563	25	0
3	M	1627	0	1563	32	0
4	G	1649	0	1609	15	0
4	K	1649	0	1609	20	0
4	L	1649	0	1609	16	0
4	N	1649	0	1609	21	0
All	All	22839	0	21949	253	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (253) 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:Z:105:ASP:HB2	2:E:378:LYS:HE2	1.55	0.89
3:J:13:GLN:HG2	3:J:116:SER:HA	1.61	0.82
3:F:104:ASP:OD1	3:F:104:ASP:N	2.13	0.82
3:H:104:ASP:OD1	3:H:104:ASP:N	2.14	0.81
2:C:378:LYS:HE2	1:Y:105:ASP:HB2	1.65	0.79
1:W:105:ASP:HB2	2:A:378:LYS:HE2	1.64	0.79
3:J:104:ASP:OD1	3:J:104:ASP:N	2.15	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:449:TYR:HB3	3:M:100:THR:HA	1.66	0.77
4:K:92:TYR:HD2	3:J:101:ALA:HB1	1.49	0.77
4:K:92:TYR:CD2	3:J:101:ALA:HB1	2.22	0.74
3:M:101:ALA:HB1	4:N:92:TYR:HD2	1.52	0.74
1:X:5:VAL:HB	1:X:23:ALA:HB3	1.68	0.74
1:Z:5:VAL:HB	1:Z:23:ALA:HB3	1.70	0.74
3:M:104:ASP:OD1	3:M:104:ASP:N	2.20	0.74
4:G:37:TYR:OH	4:G:90:GLN:OE1	2.05	0.73
3:M:101:ALA:HB1	4:N:92:TYR:CD2	2.27	0.70
2:E:449:TYR:HB3	3:H:100:THR:HA	1.74	0.69
2:C:444:LYS:HB2	2:C:499:PRO:HD3	1.75	0.68
4:L:37:TYR:OH	4:L:90:GLN:OE1	2.09	0.68
2:E:347:PHE:O	2:E:450:ASN:ND2	2.27	0.67
3:H:39:GLN:HB2	3:H:45:LEU:HD23	1.76	0.66
2:E:502:GLY:O	2:E:504:GLY:N	2.21	0.66
3:F:35:HIS:CE1	3:F:99:ASP:HA	2.32	0.64
3:F:39:GLN:HB2	3:F:45:LEU:HD23	1.80	0.64
4:N:151:LYS:NZ	4:N:197:GLU:OE1	2.30	0.63
1:Z:104:ARG:NH1	2:E:375:PHE:O	2.31	0.63
4:N:38:GLN:HB2	4:N:48:LEU:HD11	1.79	0.63
3:M:35:HIS:CE1	3:M:99:ASP:HA	2.34	0.63
4:K:37:TYR:OH	4:K:90:GLN:OE1	2.11	0.62
3:F:100:THR:HA	2:B:449:TYR:HB3	1.83	0.61
3:M:102:PRO:HB2	4:N:37:TYR:OH	2.01	0.61
4:K:90:GLN:HE21	4:K:98:LEU:HB3	1.66	0.60
3:J:24:ALA:HB1	3:J:27:PHE:HE1	1.66	0.60
4:K:38:GLN:HB2	4:K:48:LEU:HD11	1.84	0.60
3:F:5:VAL:HG23	3:F:23:ALA:HB3	1.84	0.60
3:F:60:TYR:HB2	3:F:65:LYS:HG2	1.84	0.59
3:M:24:ALA:HB1	3:M:27:PHE:HE1	1.66	0.59
3:J:35:HIS:CE1	3:J:99:ASP:HA	2.37	0.59
3:F:35:HIS:CE1	4:G:98:LEU:HD11	2.38	0.59
3:M:97:ALA:HB1	3:M:103:PRO:HB3	1.84	0.59
4:G:90:GLN:HE21	4:G:98:LEU:HB3	1.68	0.58
2:E:501:TYR:HB3	2:E:505:HIS:HB2	1.84	0.58
3:J:5:VAL:HG23	3:J:23:ALA:HB3	1.86	0.57
3:M:52:TRP:CZ2	4:N:96:PRO:HG3	2.40	0.56
1:W:109:SER:HB2	2:A:408:ARG:HD2	1.87	0.56
3:M:103:PRO:HB2	3:M:106:TRP:NE1	2.19	0.56
4:K:122:PRO:HD3	4:K:134:VAL:HG22	1.87	0.56
3:J:102:PRO:HB2	3:J:103:PRO:CD	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:346:ARG:NH2	2:A:448:ASN:OD1	2.38	0.56
3:F:102:PRO:HB2	3:F:103:PRO:CD	2.36	0.56
2:A:498:ARG:HG2	2:A:499:PRO:HD2	1.88	0.55
1:W:5:VAL:HB	1:W:23:ALA:HB3	1.88	0.55
2:E:498:ARG:HH21	2:E:500:THR:HB	1.71	0.55
2:C:449:TYR:CZ	3:M:101:ALA:HB3	2.41	0.55
3:M:2:VAL:HG21	3:M:98:ARG:HH21	1.72	0.55
4:L:90:GLN:HE22	4:L:98:LEU:HD13	1.71	0.55
1:Y:5:VAL:HB	1:Y:23:ALA:HB3	1.87	0.55
2:A:449:TYR:CZ	2:A:494:SER:HB2	2.43	0.54
3:M:103:PRO:HD2	4:N:37:TYR:OH	2.07	0.54
3:F:24:ALA:HB1	3:F:27:PHE:HE1	1.71	0.54
2:E:449:TYR:CB	3:H:100:THR:HA	2.38	0.53
4:K:19:ALA:HB2	4:K:79:LEU:HD21	1.90	0.53
3:H:102:PRO:HB2	3:H:103:PRO:CD	2.37	0.53
4:L:90:GLN:HE21	4:L:98:LEU:HB3	1.73	0.53
2:A:455:LEU:HD22	2:A:493:ARG:HG3	1.90	0.53
3:M:11:VAL:HG21	3:M:150:PRO:HG3	1.90	0.53
4:L:38:GLN:HB2	4:L:48:LEU:HD11	1.91	0.53
2:E:401:VAL:HB	2:E:451:TYR:CD1	2.44	0.53
2:B:498:ARG:HG2	2:B:501:TYR:CD2	2.43	0.53
3:M:122:PRO:HB3	3:M:148:TYR:HB3	1.91	0.53
4:G:90:GLN:HE22	4:G:98:LEU:HD13	1.75	0.52
3:M:99:ASP:O	3:M:101:ALA:N	2.42	0.52
3:J:2:VAL:HG21	3:J:98:ARG:NH2	2.24	0.52
3:H:5:VAL:HG23	3:H:23:ALA:HB3	1.92	0.52
3:H:171:ALA:HA	3:H:181:LEU:HB3	1.91	0.52
3:H:24:ALA:HB1	3:H:27:PHE:HE1	1.74	0.52
2:B:498:ARG:HE	2:B:500:THR:HB	1.75	0.52
3:M:91:THR:HG23	3:M:113:THR:HA	1.90	0.52
4:N:90:GLN:NE2	4:N:98:LEU:HD13	2.25	0.52
4:L:212:ASN:HB2	4:L:215:GLU:HG3	1.92	0.52
4:K:90:GLN:HE22	4:K:98:LEU:HD13	1.74	0.52
1:Z:99:GLY:HA3	1:Z:101:PHE:CZ	2.45	0.51
2:C:449:TYR:OH	4:N:93:GLY:HA2	2.09	0.51
4:L:19:ALA:HB2	4:L:79:LEU:HD21	1.92	0.51
3:M:39:GLN:HB2	3:M:45:LEU:HD23	1.92	0.51
2:B:379:CYS:SG	2:B:384:PRO:HG3	2.50	0.51
4:G:94:THR:HG23	4:G:95:SER:H	1.75	0.51
2:C:375:PHE:O	1:Y:104:ARG:NH1	2.44	0.50
4:N:212:ASN:HB2	4:N:215:GLU:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:345:THR:O	2:A:346:ARG:HD3	2.12	0.50
2:A:349:SER:OG	2:A:450:ASN:O	2.30	0.50
4:L:19:ALA:HB3	4:L:76:ILE:HB	1.94	0.50
2:B:501:TYR:HB3	2:B:505:HIS:HB2	1.94	0.50
3:H:35:HIS:CD2	3:H:99:ASP:HB2	2.46	0.49
2:A:376:THR:HB	2:A:435:ALA:HB3	1.94	0.49
4:G:38:GLN:HB2	4:G:48:LEU:HD11	1.94	0.49
4:N:122:PRO:HD3	4:N:134:VAL:HG22	1.94	0.49
3:J:100:THR:HG21	2:A:447:GLY:O	2.13	0.49
2:C:455:LEU:HD22	2:C:493:ARG:HG3	1.95	0.49
3:J:39:GLN:HB2	3:J:45:LEU:HD23	1.95	0.49
3:H:35:HIS:CD2	3:H:50:VAL:HG23	2.47	0.49
3:M:35:HIS:NE2	3:M:103:PRO:HG3	2.28	0.49
2:E:346:ARG:HG3	3:H:31:ASN:HB3	1.93	0.49
4:K:94:THR:HG23	4:K:95:SER:H	1.78	0.49
4:L:90:GLN:NE2	4:L:98:LEU:HD13	2.28	0.49
4:G:90:GLN:NE2	4:G:98:LEU:HD13	2.27	0.48
2:B:349:SER:OG	2:B:450:ASN:O	2.30	0.48
4:N:48:LEU:HD23	4:N:59:ILE:HD12	1.95	0.48
2:A:340:GLU:O	2:A:344:ALA:HB2	2.13	0.48
2:C:449:TYR:CE2	3:M:101:ALA:HB3	2.49	0.48
1:Z:40:ALA:HB3	1:Z:43:LYS:HB2	1.95	0.48
2:C:337:PRO:HD2	2:C:358:ILE:HG23	1.94	0.48
2:C:379:CYS:HA	2:C:432:CYS:HA	1.95	0.48
3:H:101:ALA:HB1	4:L:92:TYR:CD2	2.48	0.48
3:M:171:ALA:HA	3:M:181:LEU:HB3	1.96	0.48
3:J:102:PRO:HB2	3:J:103:PRO:HD3	1.96	0.48
3:J:122:PRO:HB3	3:J:148:TYR:HB3	1.95	0.48
2:B:350:VAL:HG22	2:B:422:ASN:HB3	1.96	0.48
2:B:418:ILE:HA	2:B:422:ASN:HD22	1.79	0.47
3:H:171:ALA:HB2	3:H:181:LEU:HD23	1.96	0.47
4:N:36:TRP:HB2	4:N:49:ILE:HB	1.96	0.47
3:J:22:CYS:HB3	3:J:79:LEU:HB3	1.95	0.47
3:J:61:ALA:O	3:J:65:LYS:HG3	2.14	0.47
2:C:418:ILE:HA	2:C:422:ASN:HD22	1.79	0.47
1:W:105:ASP:OD1	1:W:106:THR:N	2.48	0.47
2:B:449:TYR:CG	2:B:449:TYR:O	2.67	0.47
3:F:104:ASP:HB2	3:F:105:TYR:CD2	2.50	0.47
3:M:104:ASP:HB2	3:M:105:TYR:CD1	2.50	0.47
2:E:350:VAL:HG12	2:E:452:LEU:O	2.15	0.47
1:Z:105:ASP:OD1	1:Z:106:THR:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:349:SER:CB	2:E:452:LEU:H	2.28	0.46
4:L:195:ALA:HB2	4:L:210:SER:HB3	1.96	0.46
3:J:101:ALA:HB3	2:A:449:TYR:CD1	2.50	0.46
1:Z:34:ILE:HG13	1:Z:79:VAL:HG21	1.97	0.46
4:K:29:ILE:HD13	4:K:91:GLN:HG3	1.97	0.46
1:X:40:ALA:HB3	1:X:43:LYS:HB2	1.96	0.46
1:Z:67:ARG:HB3	1:Z:84:ASN:O	2.14	0.46
3:J:100:THR:O	3:J:100:THR:HG22	2.15	0.46
3:J:103:PRO:HG2	3:J:106:TRP:NE1	2.31	0.46
3:J:104:ASP:HB2	3:J:105:TYR:CD1	2.50	0.46
2:B:444:LYS:HB2	2:B:499:PRO:HD3	1.97	0.46
1:W:34:ILE:HG13	1:W:79:VAL:HG21	1.98	0.46
4:G:54:SER:OG	2:B:498:ARG:NH1	2.49	0.46
4:L:107:ASP:HB2	4:L:168:GLN:OE1	2.16	0.45
2:A:346:ARG:HD3	2:A:346:ARG:HA	1.57	0.45
2:A:379:CYS:SG	2:A:384:PRO:HG3	2.56	0.45
2:C:449:TYR:CD1	2:C:449:TYR:O	2.69	0.45
4:K:34:LEU:HD22	4:K:72:PHE:CD2	2.51	0.45
3:H:122:PRO:HB3	3:H:148:TYR:HB3	1.98	0.45
2:E:411:ALA:HB3	2:E:414:GLN:HG3	1.98	0.45
4:G:83:ASP:O	4:G:87:TYR:OH	2.26	0.45
4:K:33:PHE:HB3	4:K:92:TYR:O	2.17	0.45
3:F:50:VAL:HG12	3:F:59:PHE:HB2	1.99	0.45
3:F:101:ALA:HB1	4:G:92:TYR:CD2	2.51	0.45
4:N:94:THR:HG23	4:N:95:SER:H	1.81	0.45
3:F:61:ALA:O	3:F:65:LYS:HG3	2.16	0.45
3:H:104:ASP:HB2	3:H:105:TYR:CD2	2.52	0.45
1:Y:18:LEU:HD12	1:Y:18:LEU:HA	1.88	0.45
4:N:90:GLN:HE22	4:N:98:LEU:HD13	1.82	0.44
4:K:48:LEU:HD23	4:K:59:ILE:HD12	2.00	0.44
3:H:22:CYS:HB3	3:H:79:LEU:HB3	1.97	0.44
4:L:94:THR:HG23	4:L:95:SER:H	1.81	0.44
4:K:122:PRO:HG3	4:K:132:ALA:HB1	1.99	0.44
2:B:371:LEU:HD23	2:B:371:LEU:HA	1.85	0.44
2:C:371:LEU:HD23	2:C:371:LEU:HA	1.85	0.44
3:F:35:HIS:HB3	3:F:50:VAL:HG23	1.99	0.44
2:B:401:VAL:HB	2:B:451:TYR:CD1	2.53	0.44
1:Z:17[B]:SER:OG	1:Z:82:GLN:NE2	2.51	0.44
2:C:349:SER:OG	2:C:450:ASN:O	2.36	0.44
3:M:61:ALA:O	3:M:65:LYS:HG3	2.18	0.43
2:E:444:LYS:HE2	4:L:57:THR:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:498:ARG:NE	2:B:500:THR:HB	2.33	0.43
2:A:376:THR:N	2:A:435:ALA:O	2.50	0.43
1:W:104:ARG:NH1	2:A:375:PHE:O	2.50	0.43
2:B:347:PHE:CE1	2:B:509:ARG:HD3	2.53	0.43
2:B:401:VAL:HG22	2:B:509:ARG:HG2	2.00	0.43
4:N:186:ALA:O	4:N:190:LYS:HG3	2.18	0.43
2:E:481:ASN:O	2:E:481:ASN:ND2	2.51	0.43
4:N:34:LEU:C	4:N:92:TYR:HE1	2.22	0.43
4:G:34:LEU:HD13	4:G:72:PHE:CD1	2.52	0.43
2:A:350:VAL:HG22	2:A:422:ASN:HB3	2.01	0.43
2:E:371:LEU:HB3	2:E:372:ALA:H	1.75	0.43
3:J:173:LEU:HD13	3:J:179:TYR:CZ	2.54	0.43
3:H:102:PRO:HB2	3:H:103:PRO:HD3	2.00	0.43
2:A:366:SER:HA	2:A:369:TYR:HB2	2.01	0.43
1:Y:105:ASP:OD1	1:Y:106:THR:N	2.52	0.43
1:X:105:ASP:OD1	1:X:106:THR:N	2.52	0.43
3:H:103:PRO:HG2	3:H:106:TRP:NE1	2.34	0.43
2:B:431:GLY:HA2	2:B:515:PHE:HD2	1.82	0.43
4:G:19:ALA:HB3	4:G:76:ILE:HB	2.00	0.43
3:M:101:ALA:HA	3:M:102:PRO:O	2.19	0.42
4:N:90:GLN:HE21	4:N:98:LEU:HB3	1.84	0.42
1:Z:64:VAL:HB	1:Z:68:PHE:CG	2.54	0.42
4:K:212:ASN:HB2	4:K:215:GLU:HG3	2.00	0.42
3:J:2:VAL:HG21	3:J:98:ARG:HH21	1.82	0.42
3:F:83:MET:HB3	3:F:86:LEU:HD21	2.00	0.42
2:C:503:VAL:HG12	1:Y:107:TRP:CH2	2.55	0.42
4:L:83:ASP:O	4:L:87:TYR:OH	2.23	0.42
1:W:99:GLY:HA3	1:W:101:PHE:CZ	2.53	0.42
2:E:454:ARG:NH2	2:E:467:ASP:O	2.48	0.42
2:A:371:LEU:HD23	2:A:371:LEU:HA	1.89	0.42
3:M:72:ARG:NE	3:M:74:ASN:OD1	2.50	0.42
2:E:498:ARG:HB2	2:E:501:TYR:CE2	2.54	0.42
2:B:350:VAL:HG21	2:B:418:ILE:HG23	2.00	0.42
2:B:371:LEU:HD13	2:B:375:PHE:HB3	2.02	0.42
3:M:149:PHE:HA	3:M:150:PRO:HA	1.89	0.42
3:H:187:VAL:HG11	3:H:197:TYR:CE1	2.55	0.42
1:Y:99:GLY:HA3	1:Y:101:PHE:CZ	2.55	0.42
3:J:103:PRO:HG2	3:J:106:TRP:CE2	2.55	0.42
3:H:33:GLY:C	3:H:99:ASP:HB3	2.40	0.42
2:B:337:PRO:HD2	2:B:358:ILE:HG23	2.02	0.42
3:M:2:VAL:HG21	3:M:98:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:M:35:HIS:CE1	4:N:98:LEU:HD11	2.55	0.42
4:G:19:ALA:HB2	4:G:79:LEU:HD21	2.01	0.41
3:M:5:VAL:HG23	3:M:23:ALA:HB3	2.02	0.41
1:Y:64:VAL:HB	1:Y:68:PHE:CG	2.54	0.41
4:K:195:ALA:HB2	4:K:210:SER:HB3	2.01	0.41
1:X:25:SER:O	1:X:27:PHE:N	2.47	0.41
3:J:141:LEU:HB2	3:J:214:VAL:HG11	2.03	0.41
3:M:171:ALA:HB2	3:M:181:LEU:HD23	2.02	0.41
1:W:18:LEU:HD12	1:W:18:LEU:HA	1.88	0.41
4:K:96:PRO:HG3	3:J:52:TRP:CZ2	2.56	0.41
1:W:104:ARG:NH2	2:A:372:ALA:O	2.53	0.41
3:M:35:HIS:HB3	3:M:50:VAL:HG23	2.03	0.41
4:K:34:LEU:HD13	4:K:72:PHE:CD1	2.55	0.41
4:K:120:PHE:HB2	4:K:135:VAL:HB	2.03	0.41
3:H:83:MET:HB3	3:H:86:LEU:HD21	2.02	0.41
2:E:401:VAL:HG22	2:E:509:ARG:HA	2.02	0.41
2:E:401:VAL:HG22	2:E:509:ARG:HG2	2.03	0.41
2:E:443:SER:O	2:E:447:GLY:N	2.50	0.41
2:B:454:ARG:NH2	2:B:467:ASP:O	2.46	0.41
2:A:444:LYS:HB2	2:A:499:PRO:HD3	2.03	0.41
4:N:212:ASN:HB2	4:N:215:GLU:CG	2.50	0.41
4:K:79:LEU:HD13	4:K:79:LEU:HA	1.88	0.41
3:F:53:TYR:HE2	2:B:450:ASN:HD21	1.68	0.41
2:C:497:PHE:CE2	2:C:507:PRO:HB3	2.56	0.40
3:H:103:PRO:HG2	3:H:106:TRP:CE2	2.56	0.40
3:F:22:CYS:HB3	3:F:79:LEU:HB3	2.03	0.40
3:F:171:ALA:HA	3:F:181:LEU:HB3	2.03	0.40
4:G:11:LEU:HD12	4:G:11:LEU:HA	1.94	0.40
2:A:449:TYR:OH	2:A:494:SER:HB2	2.20	0.40
3:M:22:CYS:HB3	3:M:79:LEU:HB3	2.03	0.40
1:W:107:TRP:CH2	2:A:503:VAL:HG12	2.57	0.40
3:H:35:HIS:NE2	3:H:99:ASP:HB2	2.36	0.40
2:C:502:GLY:O	2:C:506:GLN:HG3	2.21	0.40
2:E:372:ALA:HB3	2:E:374:PHE:CE1	2.56	0.40
3:J:99:ASP:O	3:J:101:ALA:N	2.54	0.40
3:H:101:ALA:HB1	4:L:92:TYR:CE2	2.56	0.40
4:G:33:PHE:HB3	4:G:92:TYR:O	2.21	0.40
2:A:431:GLY:HA2	2:A:515:PHE:HD2	1.87	0.40
4:N:108:ILE:HG22	4:N:109:LYS:N	2.36	0.40
4:L:122:PRO:HD3	4:L:134:VAL:HG22	2.04	0.40
3:F:12:VAL:O	3:F:114:VAL:HA	2.21	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	W	124/131 (95%)	120 (97%)	4 (3%)	0	100	100
1	X	124/131 (95%)	120 (97%)	4 (3%)	0	100	100
1	Y	124/131 (95%)	120 (97%)	4 (3%)	0	100	100
1	Z	124/131 (95%)	120 (97%)	4 (3%)	0	100	100
2	A	181/202 (90%)	163 (90%)	18 (10%)	0	100	100
2	B	181/202 (90%)	166 (92%)	14 (8%)	1 (1%)	25	59
2	C	180/202 (89%)	163 (91%)	17 (9%)	0	100	100
2	E	168/202 (83%)	154 (92%)	13 (8%)	1 (1%)	25	59
3	F	215/221 (97%)	202 (94%)	10 (5%)	3 (1%)	11	40
3	H	215/221 (97%)	203 (94%)	9 (4%)	3 (1%)	11	40
3	J	215/221 (97%)	203 (94%)	9 (4%)	3 (1%)	11	40
3	M	215/221 (97%)	203 (94%)	9 (4%)	3 (1%)	11	40
4	G	214/216 (99%)	205 (96%)	9 (4%)	0	100	100
4	K	214/216 (99%)	205 (96%)	9 (4%)	0	100	100
4	L	214/216 (99%)	205 (96%)	9 (4%)	0	100	100
4	N	214/216 (99%)	205 (96%)	9 (4%)	0	100	100
All	All	2922/3080 (95%)	2757 (94%)	151 (5%)	14 (0%)	29	62

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	100	THR
3	M	102	PRO
2	E	503	VAL

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Mol	Chain	Res	Type
3	J	102	PRO
3	J	103	PRO
3	H	102	PRO
3	H	103	PRO
3	F	102	PRO
3	F	103	PRO
3	J	100	THR
3	H	100	THR
3	F	100	THR
2	B	371	LEU
3	M	103	PRO

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	W	105/110 (96%)	103 (98%)	2 (2%)	57	76
1	X	105/110 (96%)	103 (98%)	2 (2%)	57	76
1	Y	105/110 (96%)	103 (98%)	2 (2%)	57	76
1	Z	105/110 (96%)	103 (98%)	2 (2%)	57	76
2	A	161/177 (91%)	156 (97%)	5 (3%)	40	67
2	B	161/177 (91%)	159 (99%)	2 (1%)	71	83
2	C	160/177 (90%)	156 (98%)	4 (2%)	47	71
2	E	151/177 (85%)	146 (97%)	5 (3%)	38	65
3	F	179/186 (96%)	175 (98%)	4 (2%)	52	74
3	H	178/186 (96%)	173 (97%)	5 (3%)	43	69
3	J	179/186 (96%)	175 (98%)	4 (2%)	52	74
3	M	179/186 (96%)	173 (97%)	6 (3%)	37	64
4	G	185/185 (100%)	182 (98%)	3 (2%)	62	79
4	K	185/185 (100%)	182 (98%)	3 (2%)	62	79
4	L	185/185 (100%)	181 (98%)	4 (2%)	52	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	N	185/185 (100%)	182 (98%)	3 (2%)	62 79
All	All	2508/2632 (95%)	2452 (98%)	56 (2%)	52 74

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Z	62	ASP
1	Z	101	PHE
2	C	369	TYR
2	C	446	SER
2	C	448	ASN
2	C	450	ASN
3	M	2	VAL
3	M	51	TYR
3	M	53	TYR
3	M	99	ASP
3	M	104	ASP
3	M	105	TYR
4	N	34	LEU
4	N	79	LEU
4	N	94	THR
4	K	34	LEU
4	K	79	LEU
4	K	94	THR
1	X	62	ASP
1	X	101	PHE
1	W	62	ASP
1	W	101	PHE
2	E	369	TYR
2	E	374	PHE
2	E	375	PHE
2	E	446	SER
2	E	453	TYR
3	J	51	TYR
3	J	53	TYR
3	J	99	ASP
3	J	104	ASP
3	H	2	VAL
3	H	5	VAL
3	H	51	TYR
3	H	99	ASP
3	H	104	ASP

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Mol	Chain	Res	Type
4	L	34	LEU
4	L	57	THR
4	L	79	LEU
4	L	94	THR
3	F	2	VAL
3	F	51	TYR
3	F	99	ASP
3	F	104	ASP
4	G	34	LEU
4	G	79	LEU
4	G	94	THR
2	B	369	TYR
2	B	446	SER
2	A	369	TYR
2	A	388	ASN
2	A	450	ASN
2	A	500	THR
2	A	501	TYR
1	Y	62	ASP
1	Y	101	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	Z	82	GLN
3	M	31	ASN
3	J	35	HIS
3	F	31	ASN
3	F	35	HIS

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)

There are no ligands in this entry.

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	W	124/131 (94%)	0.37	9 (7%) 15 14	64, 102, 138, 162	0
1	X	124/131 (94%)	0.20	5 (4%) 38 35	59, 100, 138, 165	0
1	Y	124/131 (94%)	0.93	15 (12%) 4 4	78, 122, 164, 195	0
1	Z	124/131 (94%)	-0.04	5 (4%) 38 35	57, 98, 140, 168	0
2	A	183/202 (90%)	0.78	22 (12%) 4 4	85, 119, 197, 272	0
2	B	183/202 (90%)	0.10	4 (2%) 62 59	52, 87, 152, 210	0
2	C	182/202 (90%)	0.61	10 (5%) 25 23	77, 115, 189, 253	0
2	E	172/202 (85%)	0.06	5 (2%) 51 50	53, 83, 143, 195	0
3	F	217/221 (98%)	0.15	8 (3%) 41 38	52, 79, 125, 190	0
3	H	217/221 (98%)	0.05	11 (5%) 28 26	53, 86, 143, 242	0
3	J	217/221 (98%)	0.08	7 (3%) 47 45	51, 99, 148, 200	0
3	M	217/221 (98%)	-0.08	4 (1%) 68 65	52, 84, 128, 172	0
4	G	216/216 (100%)	0.04	5 (2%) 60 58	57, 83, 135, 198	0
4	K	216/216 (100%)	0.07	3 (1%) 75 74	53, 85, 130, 192	0
4	L	216/216 (100%)	-0.13	3 (1%) 75 74	57, 90, 141, 182	0
4	N	216/216 (100%)	-0.01	2 (0%) 84 84	64, 88, 129, 193	0
All	All	2948/3080 (95%)	0.17	118 (4%) 38 35	51, 93, 154, 272	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	366	SER	11.6
2	A	367	VAL	11.3
2	C	367	VAL	10.4
3	H	135	SER	9.8
2	B	367	VAL	8.9

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Mol	Chain	Res	Type	RSRZ
2	C	366	SER	7.5
2	C	368	LEU	6.1
3	H	133	SER	6.0
1	Y	10	GLY	5.7
2	A	347	PHE	5.4
2	A	368	LEU	5.2
3	H	136	GLY	4.9
1	Y	11[A]	LEU	4.6
1	W	10	GLY	4.5
2	B	368	LEU	4.3
3	F	133	SER	4.1
1	Y	122	VAL	4.0
2	B	360	ASN	4.0
1	W	101	PHE	3.9
2	C	516	GLU	3.9
2	E	342	PHE	3.9
2	A	449	TYR	3.9
3	J	54	ASP	3.8
4	K	26	SER	3.7
3	H	171	ALA	3.6
3	H	172	VAL	3.6
2	A	451	TYR	3.6
2	A	450	ASN	3.6
4	G	132	ALA	3.6
1	Y	1	GLN	3.5
2	A	458	LYS	3.5
3	F	135	SER	3.5
1	Y	121	THR	3.5
2	A	342	PHE	3.4
3	J	135	SER	3.4
2	C	365	TYR	3.3
3	J	53	TYR	3.3
1	X	116	GLN	3.3
1	W	98	ALA	3.2
3	H	134	THR	3.2
3	M	135	SER	3.2
1	Z	121	THR	3.2
3	F	136	GLY	3.2
1	Y	91	THR	3.1
1	Y	101	PHE	3.1
3	F	194	THR	3.1
1	Y	83	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	Y	18	LEU	3.0
1	X	75	ALA	2.9
2	A	365	TYR	2.8
3	H	207	ASN	2.8
2	A	452	LEU	2.8
2	A	359	SER	2.8
3	J	51	TYR	2.8
1	Z	12	VAL	2.7
3	H	173	LEU	2.7
3	F	192	LEU	2.7
1	X	5	VAL	2.7
1	W	1	GLN	2.6
3	J	55	GLY	2.6
1	Z	122	VAL	2.6
1	X	8	GLY	2.6
1	Y	12	VAL	2.6
3	H	154	THR	2.6
2	A	472	ILE	2.6
3	M	136	GLY	2.5
1	Z	11[A]	LEU	2.5
1	Y	68	PHE	2.5
4	L	26	SER	2.5
3	F	128	ALA	2.5
2	A	348	ALA	2.5
1	Y	56	ASN	2.4
2	C	388	ASN	2.4
1	Y	92	ALA	2.4
3	M	138	THR	2.4
4	G	121	PRO	2.4
4	L	198	VAL	2.4
1	W	111	TYR	2.4
2	E	397	ALA	2.3
4	G	205	SER	2.3
3	J	14	PRO	2.3
1	X	10	GLY	2.3
2	E	388	ASN	2.3
3	F	213	ARG	2.3
4	N	54	SER	2.3
2	A	470	THR	2.3
4	G	31	SER	2.3
4	L	25	ALA	2.3
2	A	442	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
4	K	63	PHE	2.3
2	A	497	PHE	2.2
2	A	436	TRP	2.2
2	B	342	PHE	2.2
1	W	56	ASN	2.2
1	Z	72	ARG	2.2
3	H	180	SER	2.2
3	H	74	ASN	2.2
3	F	182	SER	2.1
4	G	183	LEU	2.1
2	A	440	LYS	2.1
1	W	83	MET	2.1
3	M	213	ARG	2.1
2	C	501	TYR	2.1
1	Y	48	VAL	2.1
2	E	341	VAL	2.1
2	E	387	LEU	2.1
3	J	31	ASN	2.1
4	N	170	SER	2.1
1	W	68	PHE	2.1
2	C	342	PHE	2.1
4	K	70	THR	2.1
2	A	401	VAL	2.1
2	A	448	ASN	2.0
1	Y	61	VAL	2.0
1	W	11[A]	LEU	2.0
2	C	408	ARG	2.0
2	A	468	ILE	2.0
2	C	439	ASN	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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.