



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 02:48 PM UTC

PDB ID : 7ZFE / pdb_00007zfe
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 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	:	4-5-2 with Phenix2.0
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

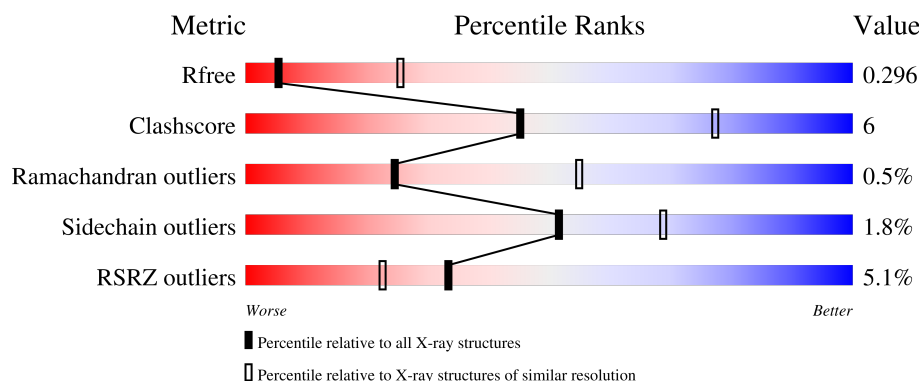
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (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 $\leq 5\%$. 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	W	131	
1	X	131	
1	Y	131	
1	Z	131	
2	A	202	

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Mol	Chain	Length	Quality of chain
2	B	202	4% 76% 14% 9%
2	C	202	7% 78% 12% 10%
2	E	202	4% 68% 16% 15%
3	F	221	4% 85% 11% ..
3	H	221	5% 85% 10% ..
3	J	221	5% 85% 11% ..
3	M	221	2% 81% 14% ..
4	G	216	4% 93% 6% .
4	K	216	5% 88% 11% .
4	L	216	5% 89% 9% .
4	N	216	6% 88% 11% .

2 Entry composition

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			

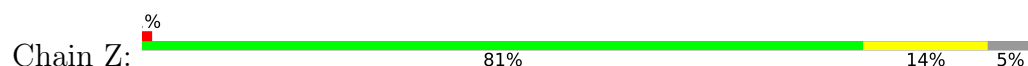
- Molecule 4 is a protein called Omi-32 light chain.

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			

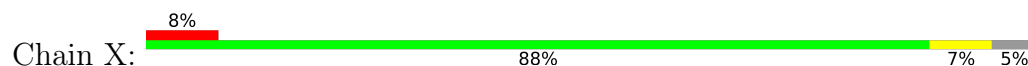
3 Residue-property plots [i](#)

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.

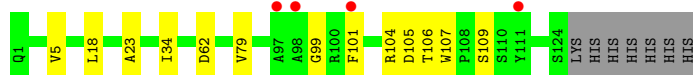
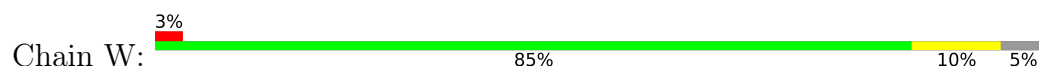
- Molecule 1: Nanobody C1



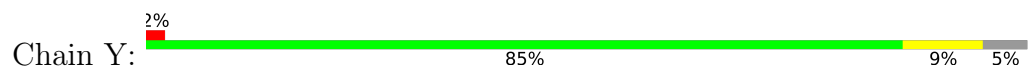
- Molecule 1: Nanobody C1



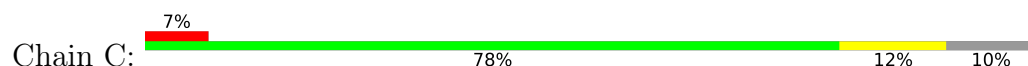
- Molecule 1: Nanobody C1

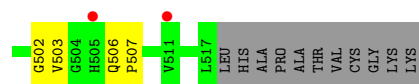


- Molecule 1: Nanobody C1

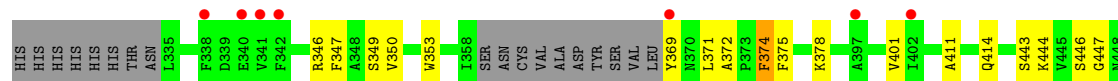


- Molecule 2: Spike protein S1

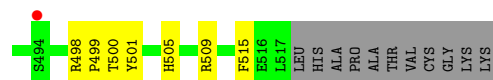
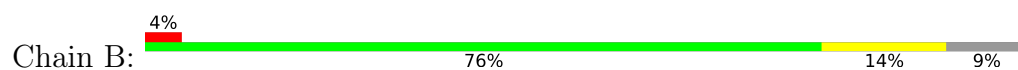




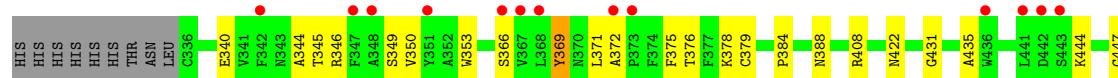
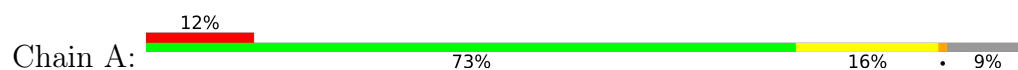
- Molecule 2: Spike protein S1



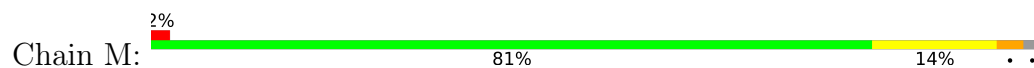
- Molecule 2: Spike protein S1



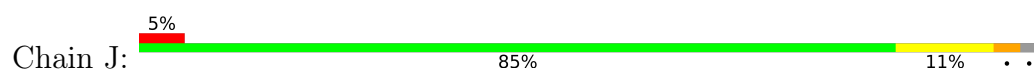
- Molecule 2: Spike protein S1

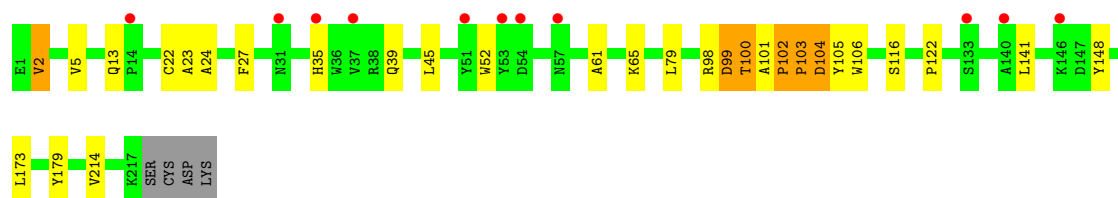


- Molecule 3: Omi-32 heavy chain

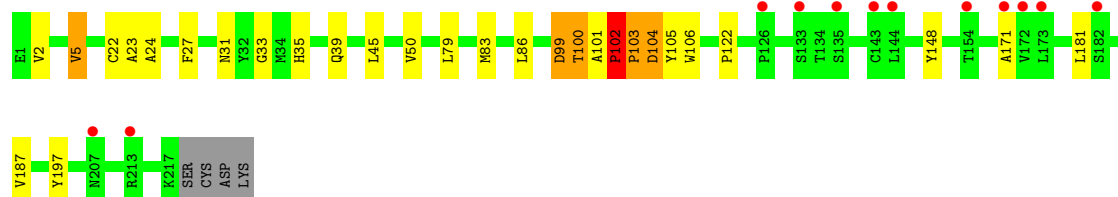
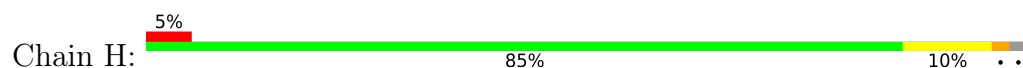


- Molecule 3: Omi-32 heavy chain

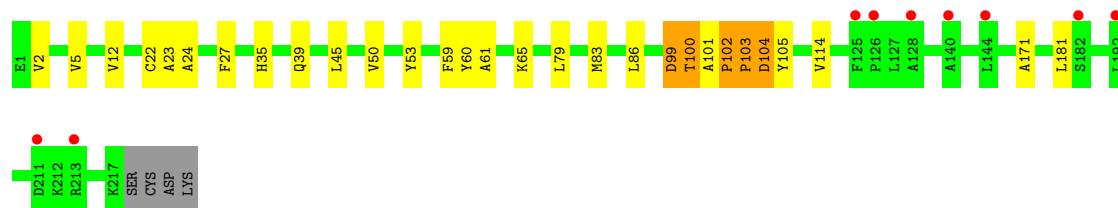
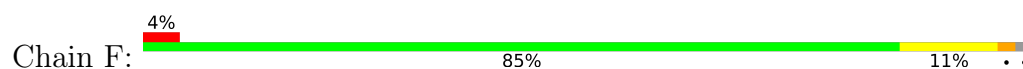




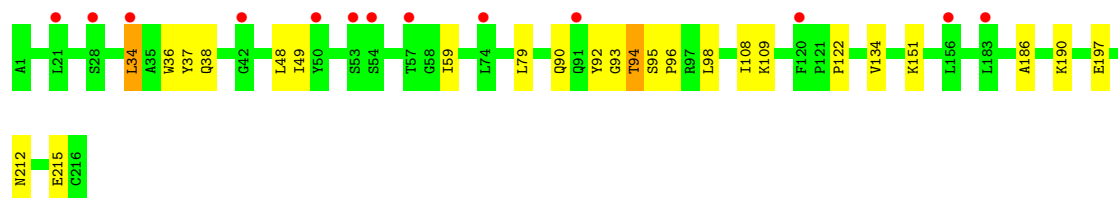
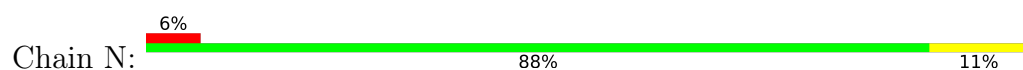
- Molecule 3: Omi-32 heavy chain



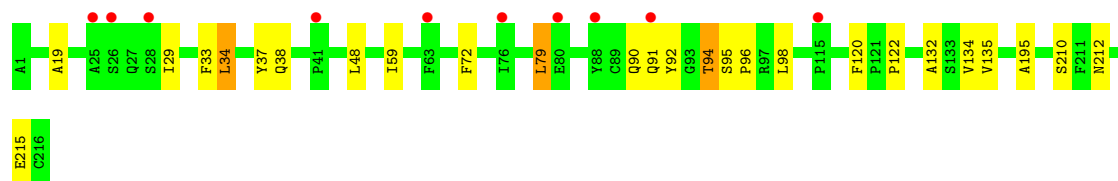
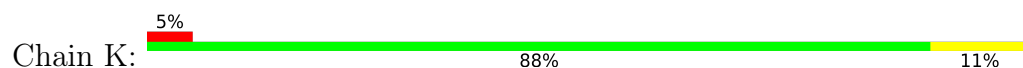
- Molecule 3: Omi-32 heavy chain



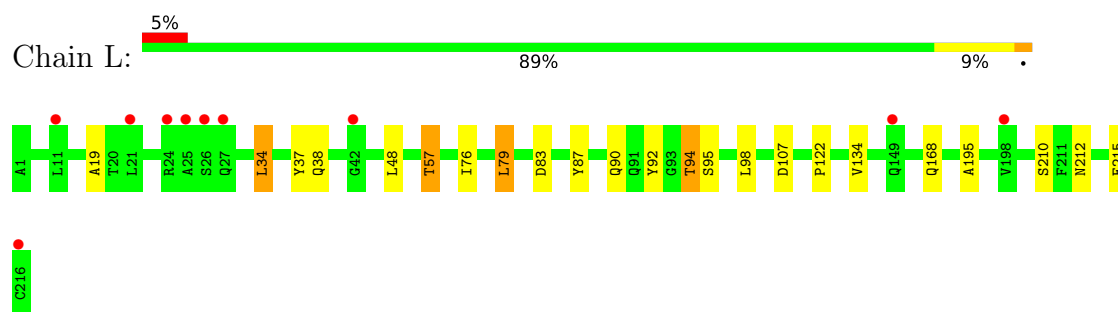
- Molecule 4: Omi-32 light chain



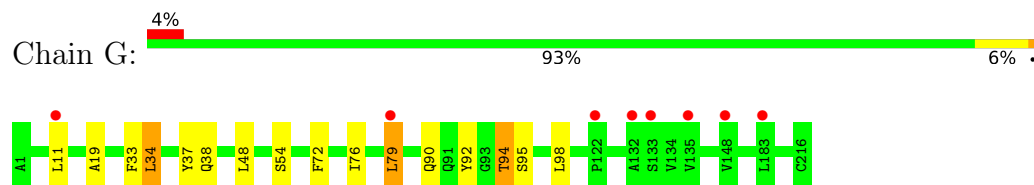
- Molecule 4: Omi-32 light chain



- Molecule 4: Omi-32 light chain



- Molecule 4: Omi-32 light chain



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.237 , 0.293 0.236 , 0.296	Depositor DCC
R_{free} test set	1396 reflections (2.25%)	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)	0.27 , 44.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.08	0/1004	0.26	0/1366
1	X	0.08	0/1004	0.27	0/1366
1	Y	0.10	0/1004	0.27	0/1366
1	Z	0.09	0/1004	0.26	0/1366
2	A	0.12	0/1528	0.30	0/2077
2	B	0.11	0/1528	0.29	0/2077
2	C	0.14	0/1520	0.30	0/2066
2	E	0.14	0/1445	0.34	0/1961
3	F	0.12	0/1670	0.31	0/2282
3	H	0.11	0/1666	0.31	0/2277
3	J	0.12	0/1670	0.33	0/2282
3	M	0.11	0/1670	0.33	0/2282
4	G	0.09	0/1684	0.29	0/2283
4	K	0.10	0/1684	0.30	0/2283
4	L	0.09	0/1684	0.29	0/2283
4	N	0.11	0/1684	0.30	0/2283
All	All	0.11	0/23449	0.30	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 ⓘ

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	25	0
2	B	1484	0	1417	23	0
2	C	1476	0	1406	18	0
2	E	1403	0	1339	24	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	34	0
4	G	1649	0	1609	15	0
4	K	1649	0	1609	22	0
4	L	1649	0	1609	17	0
4	N	1649	0	1609	21	0
All	All	22839	0	21949	262	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 (262) 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
4:N:34:LEU:C	4:N:92:TYR:HE1	2.22	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:105:ASP:OD1	1:Z:106:THR:N	2.48	0.47
2:E:349:SER:CB	2:E:452:LEU:H	2.28	0.46
3:H:33:GLY:C	3:H:99:ASP:HB3	2.40	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: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
3:M:33:GLY:C	3:M:99:ASP:HB3	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
2:B:353:TRP:H	2:B:353:TRP:CD1	2.36	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
4:K:34:LEU:C	4:K:92:TYR:HE1	2.28	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
2:E:353:TRP:CD1	2:E:353:TRP:H	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:103:PRO:HG2	3:J:106:TRP:CE2	2.55	0.42
4:L:34:LEU:C	4:L:92:TYR:HE1	2.28	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
3:M:35:HIS:CE1	4:N:98:LEU:HD11	2.55	0.42
4:K:90:GLN:CD	4:K:92:TYR:HB3	2.45	0.42
4:G:19:ALA:HB2	4:G:79:LEU:HD21	2.01	0.41
2:A:353:TRP:CD1	2:A:353:TRP:H	2.38	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:E:502:GLY:C	2:E:504:GLY:H	2.20	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
2:C:346:ARG:HG3	3:M:31:ASN:CG	2.46	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
4:G:34:LEU:C	4:G:92:TYR:HE1	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	21	51
2	C	180/202 (89%)	163 (91%)	17 (9%)	0	100	100
2	E	168/202 (83%)	154 (92%)	13 (8%)	1 (1%)	21	51
3	F	215/221 (97%)	202 (94%)	10 (5%)	3 (1%)	9	33
3	H	215/221 (97%)	203 (94%)	9 (4%)	3 (1%)	9	33
3	J	215/221 (97%)	203 (94%)	9 (4%)	3 (1%)	9	33
3	M	215/221 (97%)	203 (94%)	9 (4%)	3 (1%)	9	33
4	G	214/216 (99%)	205 (96%)	9 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	24	55

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	M	100	THR
3	M	102	PRO
2	E	503	VAL
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%)	104 (99%)	1 (1%)	68	75
1	X	105/110 (96%)	104 (99%)	1 (1%)	68	75
1	Y	105/110 (96%)	104 (99%)	1 (1%)	68	75
1	Z	105/110 (96%)	104 (99%)	1 (1%)	68	75
2	A	161/177 (91%)	156 (97%)	5 (3%)	35	59
2	B	161/177 (91%)	159 (99%)	2 (1%)	63	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	160/177 (90%)	156 (98%)	4 (2%)	42	63
2	E	151/177 (85%)	147 (97%)	4 (3%)	40	62
3	F	179/186 (96%)	176 (98%)	3 (2%)	53	69
3	H	178/186 (96%)	174 (98%)	4 (2%)	45	65
3	J	179/186 (96%)	176 (98%)	3 (2%)	53	69
3	M	179/186 (96%)	176 (98%)	3 (2%)	53	69
4	G	185/185 (100%)	182 (98%)	3 (2%)	55	70
4	K	185/185 (100%)	182 (98%)	3 (2%)	55	70
4	L	185/185 (100%)	181 (98%)	4 (2%)	45	65
4	N	185/185 (100%)	182 (98%)	3 (2%)	55	70
All	All	2508/2632 (95%)	2463 (98%)	45 (2%)	51	69

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Z	62	ASP
2	C	369	TYR
2	C	446	SER
2	C	448	ASN
2	C	450	ASN
3	M	2	VAL
3	M	99	ASP
3	M	104	ASP
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	W	62	ASP
2	E	369	TYR
2	E	374	PHE
2	E	446	SER
2	E	453	TYR
3	J	2	VAL
3	J	99	ASP
3	J	104	ASP

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Mol	Chain	Res	Type
3	H	2	VAL
3	H	5	VAL
3	H	99	ASP
3	H	104	ASP
4	L	34	LEU
4	L	57	THR
4	L	79	LEU
4	L	94	THR
3	F	2	VAL
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	Z	82	GLN
2	C	437	ASN
2	C	448	ASN
2	C	450	ASN
2	C	481	ASN
4	N	191	HIS
4	K	191	HIS
1	W	82	GLN
2	E	414	GLN
3	J	35	HIS
4	L	162	GLN
3	F	31	ASN
3	F	35	HIS
4	G	139	ASN
4	G	162	GLN
4	G	212	ASN

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Mol	Chain	Res	Type
2	B	448	ASN
2	B	481	ASN
2	A	394	ASN
2	A	481	ASN
1	Y	77	ASN
1	Y	82	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](#)

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	W	124/131 (94%)	0.26	4 (3%)	50	34	63, 101, 138, 162	2 (1%)
1	X	124/131 (94%)	0.41	10 (8%)	18	14	59, 98, 138, 165	2 (1%)
1	Y	124/131 (94%)	0.42	2 (1%)	70	52	78, 121, 163, 195	2 (1%)
1	Z	124/131 (94%)	0.15	1 (0%)	82	68	57, 98, 139, 168	2 (1%)
2	A	183/202 (90%)	0.78	25 (13%)	6	6	85, 119, 197, 272	0
2	B	183/202 (90%)	0.36	8 (4%)	39	25	52, 87, 152, 210	0
2	C	182/202 (90%)	0.63	14 (7%)	19	14	77, 115, 189, 253	0
2	E	172/202 (85%)	0.47	9 (5%)	33	22	53, 83, 143, 195	0
3	F	217/221 (98%)	0.18	9 (4%)	41	27	52, 79, 125, 190	0
3	H	217/221 (98%)	0.29	12 (5%)	30	21	53, 86, 143, 242	0
3	J	217/221 (98%)	0.32	11 (5%)	33	22	51, 99, 148, 200	0
3	M	217/221 (98%)	0.08	5 (2%)	61	41	52, 84, 128, 172	0
4	G	216/216 (100%)	0.27	8 (3%)	45	30	57, 83, 135, 198	0
4	K	216/216 (100%)	0.31	10 (4%)	37	25	53, 85, 130, 192	0
4	L	216/216 (100%)	0.32	10 (4%)	37	25	57, 90, 141, 182	0
4	N	216/216 (100%)	0.30	13 (6%)	27	19	64, 88, 129, 193	0
All	All	2948/3080 (95%)	0.34	151 (5%)	33	22	51, 93, 154, 272	8 (0%)

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	G	132	ALA	6.3
2	C	367	VAL	6.0
2	A	367	VAL	5.4
3	H	171	ALA	5.2
2	E	342	PHE	5.0

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Mol	Chain	Res	Type	RSRZ
2	C	368	LEU	4.9
4	N	91	GLN	4.7
2	A	347	PHE	4.7
3	J	54	ASP	4.7
2	A	497	PHE	4.6
2	B	367	VAL	4.5
2	A	342	PHE	4.5
4	L	26	SER	4.4
4	L	25	ALA	4.4
2	A	368	LEU	4.2
2	B	410	ILE	4.2
2	B	368	LEU	4.2
4	K	91	GLN	4.1
2	E	397	ALA	4.1
3	H	172	VAL	4.0
2	A	449	TYR	4.0
4	L	27	GLN	4.0
2	A	436	TRP	3.9
3	H	207	ASN	3.9
2	E	341	VAL	3.9
3	H	173	LEU	3.8
2	B	341	VAL	3.7
3	J	53	TYR	3.6
2	E	402	ILE	3.6
3	J	35	HIS	3.6
2	A	450	ASN	3.5
1	X	5	VAL	3.5
4	N	183	LEU	3.5
4	N	54	SER	3.5
4	N	21	LEU	3.5
1	W	101	PHE	3.4
1	X	75	ALA	3.3
4	K	26	SER	3.3
2	A	451	TYR	3.3
2	C	494	SER	3.3
2	A	348	ALA	3.3
3	M	135	SER	3.2
2	E	513	LEU	3.2
2	C	342	PHE	3.2
4	K	80	GLU	3.1
3	F	126	PRO	3.1
3	F	144	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	A	452	LEU	3.0
2	A	448	ASN	3.0
2	B	342	PHE	3.0
4	K	63	PHE	3.0
4	N	53	SER	3.0
3	J	37	VAL	3.0
2	E	338	PHE	2.9
2	C	449	TYR	2.9
3	J	31	ASN	2.9
4	N	50	TYR	2.9
4	L	198	VAL	2.8
3	F	182	SER	2.8
3	J	14	PRO	2.8
4	L	24	ARG	2.8
3	J	51	TYR	2.8
4	G	122	PRO	2.8
2	A	442	ASP	2.7
3	F	140	ALA	2.7
3	H	126	PRO	2.7
2	E	340	GLU	2.7
2	C	468	ILE	2.7
1	X	116	GLN	2.7
4	L	149	GLN	2.7
1	X	109	SER	2.7
3	F	128	ALA	2.6
1	X	20	LEU	2.6
3	M	211	ASP	2.6
3	F	211	ASP	2.6
3	H	213	ARG	2.5
2	C	338	PHE	2.5
2	B	494	SER	2.5
4	L	11	LEU	2.5
1	W	98	ALA	2.5
4	N	34	LEU	2.5
3	H	182	SER	2.5
2	B	338	PHE	2.5
1	W	111	TYR	2.5
2	E	450	ASN	2.4
2	B	408	ARG	2.4
3	J	57	ASN	2.4
2	C	341	VAL	2.4
3	H	154	THR	2.4

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Mol	Chain	Res	Type	RSRZ
3	F	192	LEU	2.4
1	Y	48	VAL	2.4
1	X	117	GLY	2.4
2	A	443	SER	2.4
3	H	135	SER	2.4
3	J	140	ALA	2.3
4	G	11	LEU	2.3
2	A	509	ARG	2.3
1	X	8	GLY	2.3
2	A	441	LEU	2.3
4	G	183	LEU	2.3
2	C	511	VAL	2.3
3	H	133	SER	2.3
1	Z	11[A]	LEU	2.3
1	X	18	LEU	2.3
4	L	21	LEU	2.3
3	M	100	THR	2.2
2	E	369	TYR	2.2
2	A	366	SER	2.2
4	K	28	SER	2.2
4	K	76	ILE	2.2
2	C	497	PHE	2.2
1	X	124	SER	2.2
4	G	133	SER	2.2
3	H	144	LEU	2.2
2	C	423	TYR	2.2
2	A	518	LEU	2.2
4	K	25	ALA	2.2
3	H	143	CYS	2.2
2	A	456	PHE	2.2
4	G	135	VAL	2.1
4	G	79	LEU	2.1
4	N	42	GLY	2.1
3	F	125	PHE	2.1
2	C	436	TRP	2.1
4	N	57	THR	2.1
1	Y	3	GLN	2.1
1	W	97	ALA	2.1
2	C	447	GLY	2.1
4	K	41	PRO	2.1
4	N	120	PHE	2.1
4	L	216	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
4	K	88	TYR	2.1
2	A	475	ALA	2.1
4	K	115	PRO	2.1
2	C	505	HIS	2.1
3	M	35	HIS	2.1
4	N	74	LEU	2.1
2	A	351	TYR	2.1
4	L	42	GLY	2.1
2	A	373	PRO	2.1
2	A	458	LYS	2.1
4	G	148	VAL	2.0
4	N	156	LEU	2.0
3	M	3	GLN	2.0
2	A	513	LEU	2.0
3	F	213	ARG	2.0
3	J	133	SER	2.0
4	N	28	SER	2.0
1	X	36	TRP	2.0
2	A	372	ALA	2.0
3	J	146	LYS	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 oligosaccharides 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.