



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 27, 2026 – 04:52 PM UTC

PDB ID : 6QD6 / pdb_00006qd6
Title : Molecular scaffolds expand the nanobody toolkit for cryo-EM applications:
crystal structure of Mb-cHopQ-Nb207
Authors : Uchanski, T.; Masiulis, S.; Fischer, B.; Kalichuk, V.; Wohlkonig, A.; Zogg, T.;
Remaut, H.; Vranken, W.; Aricescu, A.R.; Pardon, E.; Steyaert, J.
Deposited on : 2018-12-31
Resolution : 2.84 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 ⓘ 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

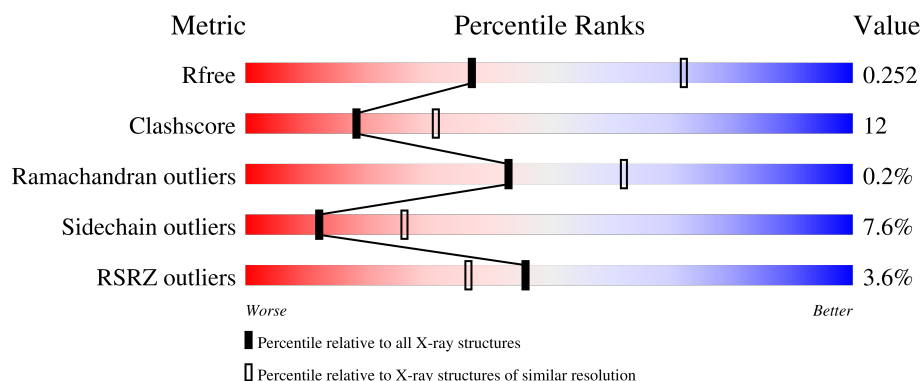
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

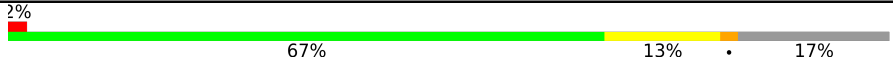
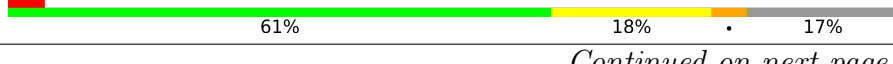
The reported resolution of this entry is 2.84 Å.

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	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	A	542	
1	B	542	
1	C	542	
1	D	542	
1	E	542	

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Mol	Chain	Length	Quality of chain
1	F	542	3% 62% 19% • 16%
1	G	542	% 62% 22% • 13%
1	H	542	4% 60% 12% • 26%
1	I	542	3% 60% 14% • 23%
1	J	542	4% 50% 17% • 30%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 33077 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 Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	448	Total	C	N	O	S	0	0	0
			3409	2107	603	686	13			
1	B	446	Total	C	N	O	S	0	0	0
			3372	2081	594	682	15			
1	C	431	Total	C	N	O	S	0	0	0
			3263	2015	573	660	15			
1	D	446	Total	C	N	O	S	0	0	0
			3384	2090	598	683	13			
1	E	451	Total	C	N	O	S	0	0	0
			3406	2103	599	689	15			
1	F	457	Total	C	N	O	S	0	0	0
			3465	2144	606	702	13			
1	G	469	Total	C	N	O	S	0	0	0
			3561	2197	626	723	15			
1	H	399	Total	C	N	O	S	0	0	0
			3015	1868	525	609	13			
1	I	419	Total	C	N	O	S	0	0	0
			3187	1976	558	640	13			
1	J	380	Total	C	N	O	S	0	0	0
			2900	1795	508	584	13			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		

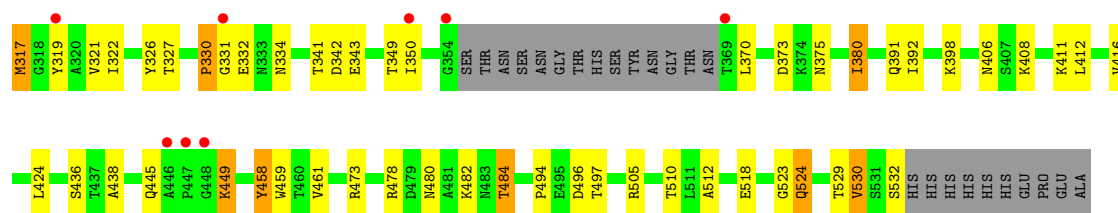
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	18	Total	O	0	0
			18	18		

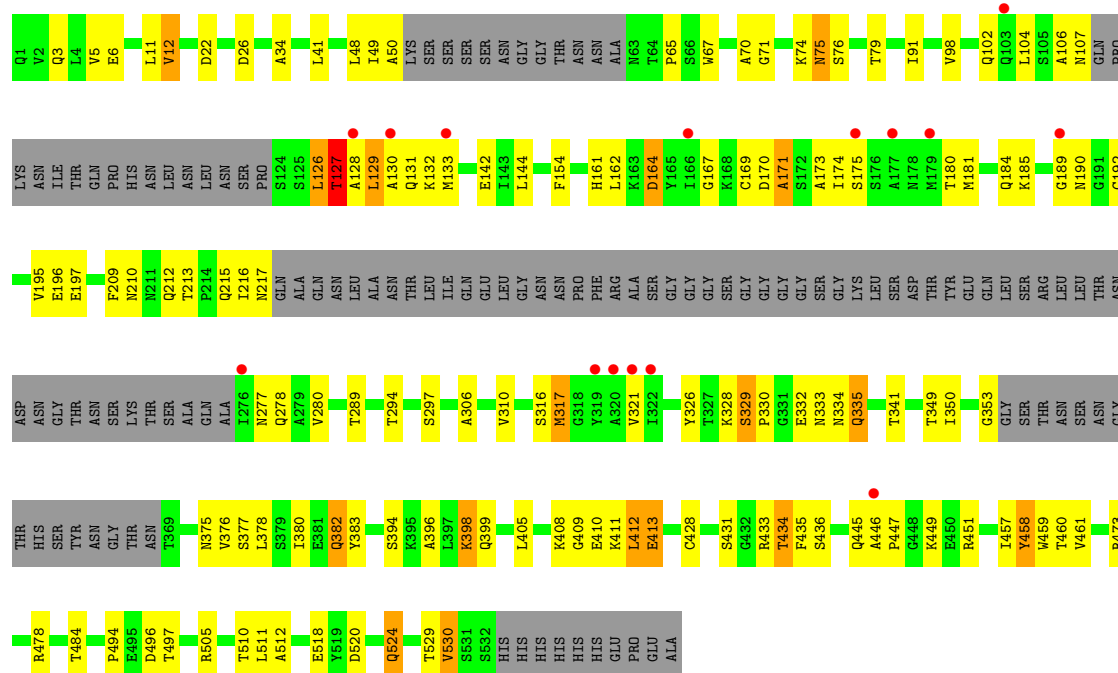
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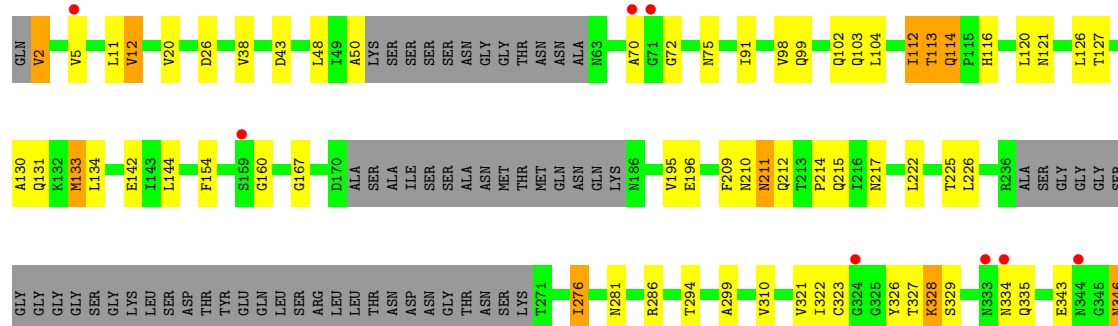
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	15	Total 15	O 15	0	0
3	C	11	Total 11	O 11	0	0
3	D	12	Total 12	O 12	0	0
3	E	8	Total 8	O 8	0	0
3	F	14	Total 14	O 14	0	0
3	G	14	Total 14	O 14	0	0
3	H	5	Total 5	O 5	0	0
3	I	12	Total 12	O 12	0	0
3	J	5	Total 5	O 5	0	0

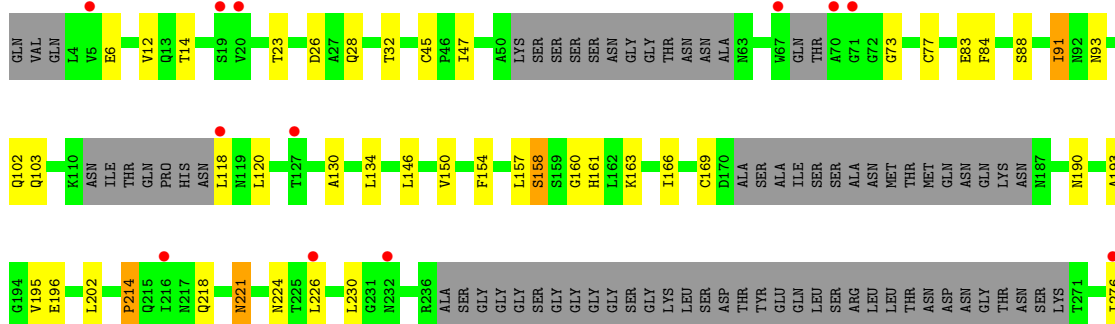
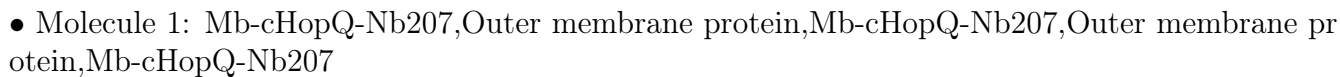
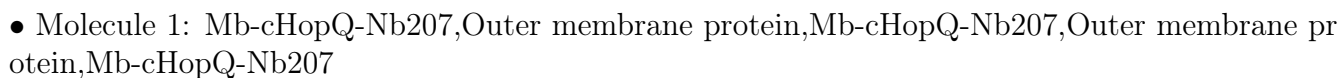


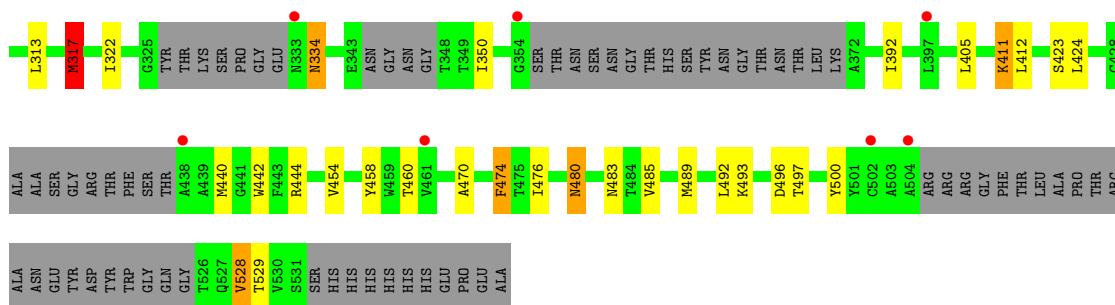
• Molecule 1: Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207



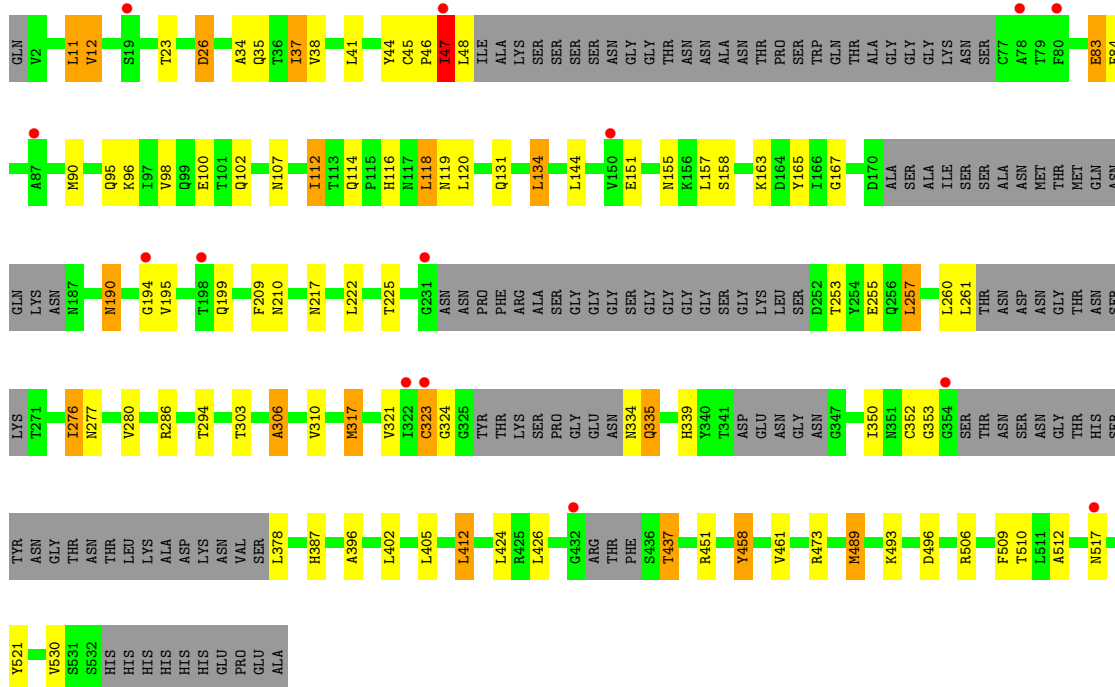
• Molecule 1: Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207



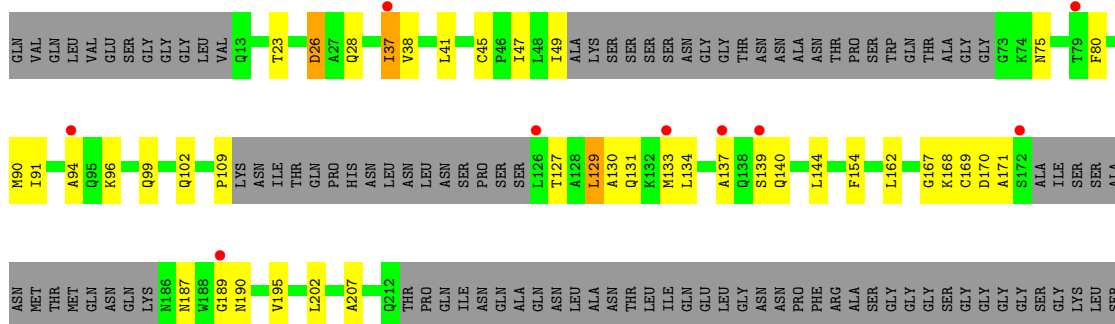


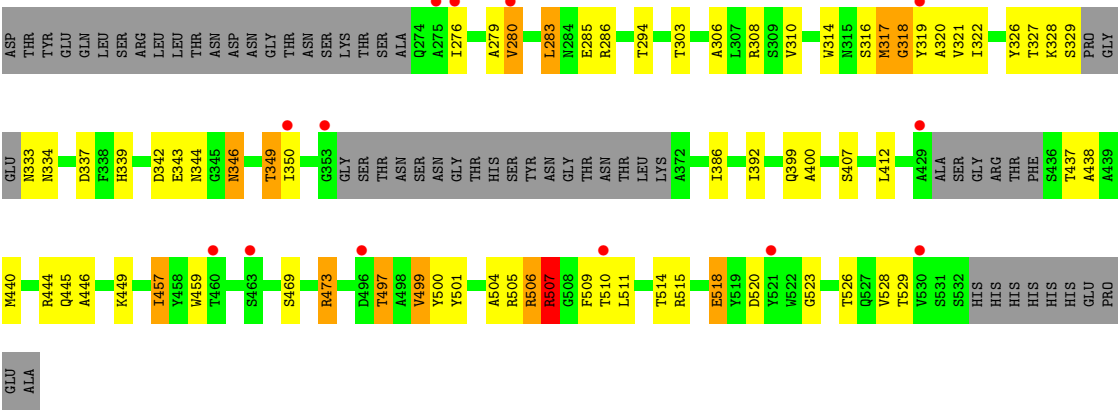


- Molecule 1: Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207



- Molecule 1: Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207,Outer membrane protein,Mb-cHopQ-Nb207





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.17Å 92.92Å 244.22Å 92.05° 96.93° 112.15°	Depositor
Resolution (Å)	41.45 – 2.84 41.45 – 2.84	Depositor EDS
% Data completeness (in resolution range)	95.5 (41.45-2.84) 95.6 (41.45-2.84)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 2.86Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.204 , 0.239 0.226 , 0.252	Depositor DCC
R_{free} test set	6538 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	82.3	Xtriage
Anisotropy	0.101	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 98.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.039 for h,-h-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	33077	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section:
CL

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	0.84	1/3461 (0.0%)	1.39	19/4690 (0.4%)
1	B	0.88	1/3419 (0.0%)	1.40	24/4625 (0.5%)
1	C	0.89	0/3310	1.44	30/4479 (0.7%)
1	D	0.86	1/3432 (0.0%)	1.39	23/4647 (0.5%)
1	E	0.86	0/3453	1.37	24/4676 (0.5%)
1	F	0.89	4/3514 (0.1%)	1.41	27/4760 (0.6%)
1	G	0.83	0/3610	1.39	15/4887 (0.3%)
1	H	0.82	0/3051	1.39	13/4124 (0.3%)
1	I	0.83	2/3229 (0.1%)	1.40	35/4369 (0.8%)
1	J	0.89	1/2939 (0.0%)	1.40	27/3971 (0.7%)
All	All	0.86	10/33418 (0.0%)	1.40	237/45228 (0.5%)

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	489	MET	SD-CE	-6.99	1.62	1.79
1	F	317	MET	CA-C	6.75	1.61	1.52
1	F	317	MET	N-CA	-5.98	1.36	1.45
1	J	170	ASP	CA-C	5.88	1.59	1.52
1	F	489	MET	SD-CE	-5.63	1.65	1.79

The worst 5 of 237 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	191	GLY	N-CA-C	10.55	124.74	112.50
1	D	70	ALA	N-CA-C	10.40	122.20	111.07
1	G	431	SER	N-CA-C	10.28	122.57	111.36
1	C	127	THR	N-CA-C	-9.94	100.43	111.07
1	E	333	ASN	N-CA-C	9.13	121.59	110.91

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	3409	0	3318	66	0
1	B	3372	0	3291	67	0
1	C	3263	0	3181	80	0
1	D	3384	0	3298	48	0
1	E	3406	0	3329	100	0
1	F	3465	0	3388	87	0
1	G	3561	0	3477	127	0
1	H	3015	0	2948	58	0
1	I	3187	0	3118	60	0
1	J	2900	0	2817	105	0
2	A	1	0	0	0	0
3	A	18	0	0	0	0
3	B	15	0	0	0	0
3	C	11	0	0	0	0
3	D	12	0	0	1	0
3	E	8	0	0	3	0
3	F	14	0	0	0	0
3	G	14	0	0	0	0
3	H	5	0	0	0	0
3	I	12	0	0	2	0
3	J	5	0	0	0	0
All	All	33077	0	32165	788	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 12.

The worst 5 of 788 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:J:326:TYR:CD1	1:J:329:SER:HB3	1.50	1.46
1:F:45:CYS:SG	1:F:77:CYS:CB	2.23	1.27
1:J:326:TYR:CG	1:J:329:SER:HB3	1.70	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:CYS:SG	1:A:77:CYS:SG	1.45	1.24
1:F:45:CYS:CB	1:F:77:CYS:SG	2.25	1.23

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	436/542 (80%)	417 (96%)	19 (4%)	0	100	100
1	B	432/542 (80%)	412 (95%)	19 (4%)	1 (0%)	43	62
1	C	421/542 (78%)	398 (94%)	21 (5%)	2 (0%)	24	43
1	D	432/542 (80%)	417 (96%)	15 (4%)	0	100	100
1	E	439/542 (81%)	422 (96%)	17 (4%)	0	100	100
1	F	443/542 (82%)	424 (96%)	18 (4%)	1 (0%)	43	62
1	G	457/542 (84%)	441 (96%)	15 (3%)	1 (0%)	43	62
1	H	377/542 (70%)	364 (97%)	12 (3%)	1 (0%)	36	55
1	I	401/542 (74%)	388 (97%)	12 (3%)	1 (0%)	43	62
1	J	364/542 (67%)	350 (96%)	14 (4%)	0	100	100
All	All	4202/5420 (78%)	4033 (96%)	162 (4%)	7 (0%)	43	62

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	161	HIS
1	I	47	ILE
1	C	75	ASN
1	F	333	ASN
1	G	507	ARG

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	366/438 (84%)	346 (94%)	20 (6%)	19	40
1	B	361/438 (82%)	330 (91%)	31 (9%)	10	21
1	C	349/438 (80%)	314 (90%)	35 (10%)	7	16
1	D	364/438 (83%)	336 (92%)	28 (8%)	12	26
1	E	365/438 (83%)	336 (92%)	29 (8%)	11	25
1	F	373/438 (85%)	349 (94%)	24 (6%)	16	33
1	G	384/438 (88%)	352 (92%)	32 (8%)	10	23
1	H	325/438 (74%)	305 (94%)	20 (6%)	16	34
1	I	342/438 (78%)	314 (92%)	28 (8%)	10	23
1	J	309/438 (70%)	287 (93%)	22 (7%)	13	29
All	All	3538/4380 (81%)	3269 (92%)	269 (8%)	12	26

5 of 269 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	210	ASN
1	I	317	MET
1	J	346	ASN
1	D	196	GLU
1	D	116	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 150 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	103	GLN
1	J	281	ASN
1	H	232	ASN
1	I	187	ASN
1	D	155	ASN

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](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	A	448/542 (82%)	0.16	11 (2%)	58	49	56, 89, 132, 163	0
1	B	446/542 (82%)	0.21	25 (5%)	30	23	47, 89, 149, 197	0
1	C	431/542 (79%)	0.23	15 (3%)	47	37	46, 88, 138, 186	0
1	D	446/542 (82%)	0.16	10 (2%)	62	53	54, 89, 135, 160	0
1	E	451/542 (83%)	0.34	19 (4%)	40	32	61, 103, 160, 179	0
1	F	457/542 (84%)	0.22	16 (3%)	47	37	55, 88, 130, 157	0
1	G	469/542 (86%)	0.21	6 (1%)	75	69	59, 95, 144, 178	0
1	H	399/542 (73%)	0.39	19 (4%)	35	29	76, 110, 152, 175	0
1	I	419/542 (77%)	0.34	14 (3%)	49	39	63, 107, 151, 183	0
1	J	380/542 (70%)	0.44	22 (5%)	29	22	69, 110, 152, 184	0
All	All	4346/5420 (80%)	0.27	157 (3%)	46	37	46, 97, 146, 197	0

The worst 5 of 157 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	319	TYR	6.8
1	J	133	MET	4.8
1	G	506	ARG	4.6
1	J	496	ASP	4.5
1	B	316	SER	4.4

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](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	A	601	1/1	0.92	0.11	91,91,91,91	0

6.5 Other polymers [i](#)

There are no such residues in this entry.