



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 09:17 PM UTC

PDB ID : 8IVW / pdb_00008ivw
Title : Crystal structure of NRP2 in complex with aNRP2-10 Fab fragment
Authors : Geng, Y.; Zhai, L.
Deposited on : 2023-03-29
Resolution : 3.21 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

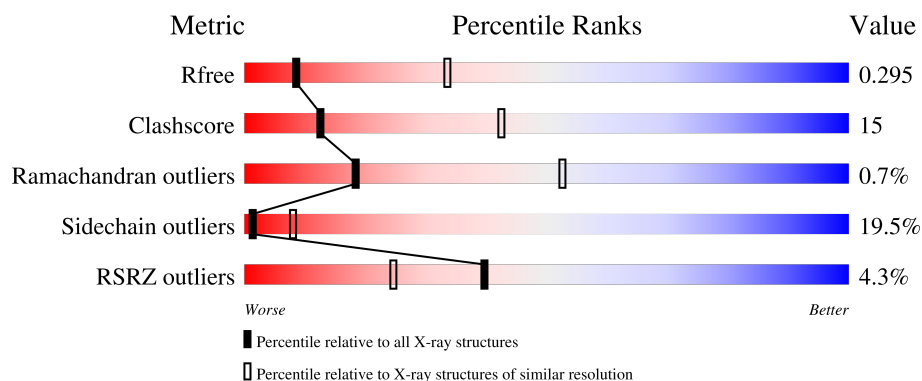
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	583	2% 50% 20% • 27%
1	D	583	2% 50% 18% • 28%
1	G	583	6% 45% 20% • 31%
1	J	583	4% 50% 17% 5% 27%
2	B	228	3% 61% 27% 7% • •

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Mol	Chain	Length	Quality of chain
2	E	228	4% 62% 25% 8%
2	H	228	3% 64% 24% 8%
2	K	228	3% 62% 25% 8%
3	C	215	5% 58% 35% 7%
3	F	215	5% 60% 33% 6%
3	I	215	3% 60% 34% 6%
3	L	215	4% 59% 34% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 26621 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 Neuropilin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	0	0
			3412	2169	594	632	17			
1	D	420	Total	C	N	O	S	0	0	0
			3337	2122	575	623	17			
1	G	402	Total	C	N	O	S	0	0	0
			3202	2030	557	599	16			
1	J	427	Total	C	N	O	S	0	0	0
			3410	2166	591	636	17			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	13	HIS	-	expression tag	UNP O60462
A	14	HIS	-	expression tag	UNP O60462
A	15	HIS	-	expression tag	UNP O60462
A	16	HIS	-	expression tag	UNP O60462
A	17	HIS	-	expression tag	UNP O60462
A	18	HIS	-	expression tag	UNP O60462
A	19	GLU	-	expression tag	UNP O60462
A	20	ASN	-	expression tag	UNP O60462
A	21	LEU	-	expression tag	UNP O60462
A	22	TYR	-	expression tag	UNP O60462
A	23	PHE	-	expression tag	UNP O60462
A	24	GLN	-	expression tag	UNP O60462
D	13	HIS	-	expression tag	UNP O60462
D	14	HIS	-	expression tag	UNP O60462
D	15	HIS	-	expression tag	UNP O60462
D	16	HIS	-	expression tag	UNP O60462
D	17	HIS	-	expression tag	UNP O60462
D	18	HIS	-	expression tag	UNP O60462
D	19	GLU	-	expression tag	UNP O60462
D	20	ASN	-	expression tag	UNP O60462
D	21	LEU	-	expression tag	UNP O60462

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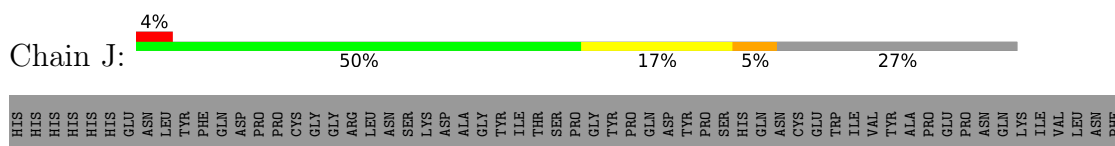
Chain	Residue	Modelled	Actual	Comment	Reference
D	22	TYR	-	expression tag	UNP O60462
D	23	PHE	-	expression tag	UNP O60462
D	24	GLN	-	expression tag	UNP O60462
G	13	HIS	-	expression tag	UNP O60462
G	14	HIS	-	expression tag	UNP O60462
G	15	HIS	-	expression tag	UNP O60462
G	16	HIS	-	expression tag	UNP O60462
G	17	HIS	-	expression tag	UNP O60462
G	18	HIS	-	expression tag	UNP O60462
G	19	GLU	-	expression tag	UNP O60462
G	20	ASN	-	expression tag	UNP O60462
G	21	LEU	-	expression tag	UNP O60462
G	22	TYR	-	expression tag	UNP O60462
G	23	PHE	-	expression tag	UNP O60462
G	24	GLN	-	expression tag	UNP O60462
J	13	HIS	-	expression tag	UNP O60462
J	14	HIS	-	expression tag	UNP O60462
J	15	HIS	-	expression tag	UNP O60462
J	16	HIS	-	expression tag	UNP O60462
J	17	HIS	-	expression tag	UNP O60462
J	18	HIS	-	expression tag	UNP O60462
J	19	GLU	-	expression tag	UNP O60462
J	20	ASN	-	expression tag	UNP O60462
J	21	LEU	-	expression tag	UNP O60462
J	22	TYR	-	expression tag	UNP O60462
J	23	PHE	-	expression tag	UNP O60462
J	24	GLN	-	expression tag	UNP O60462

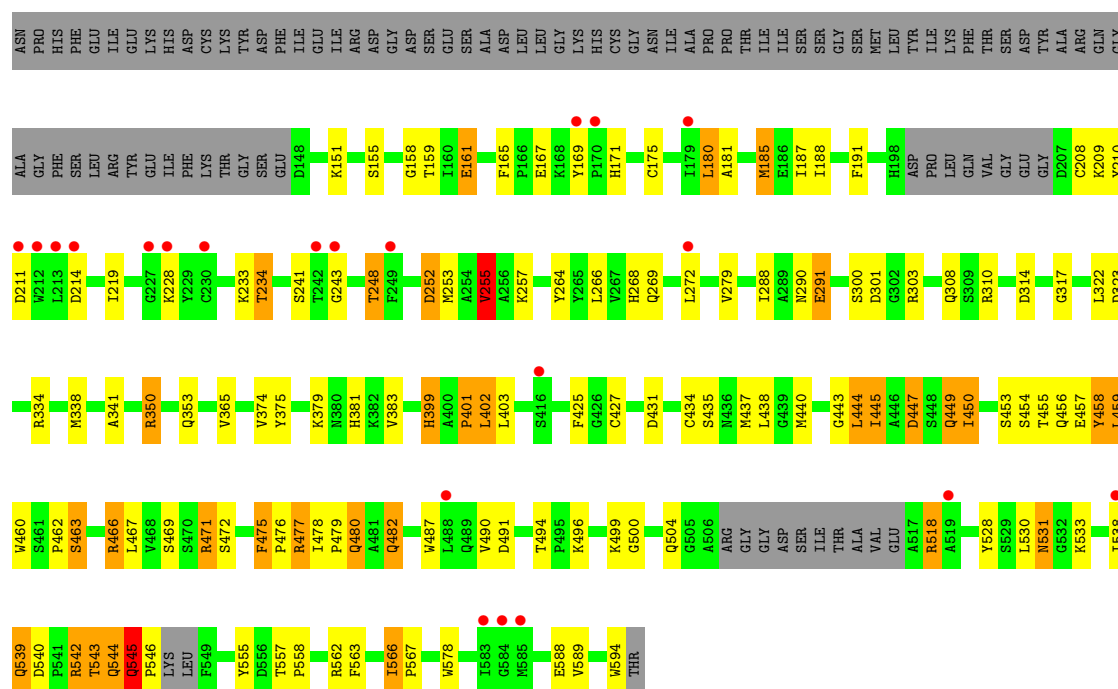
- Molecule 2 is a protein called Heavy chain of antibody 10V8 Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	219	Total	C	N	O	S	0	0	0
			1664	1053	273	331	7			
2	E	220	Total	C	N	O	S	0	0	0
			1668	1055	274	332	7			
2	H	220	Total	C	N	O	S	0	0	0
			1668	1055	274	332	7			
2	K	220	Total	C	N	O	S	0	0	0
			1668	1055	274	332	7			

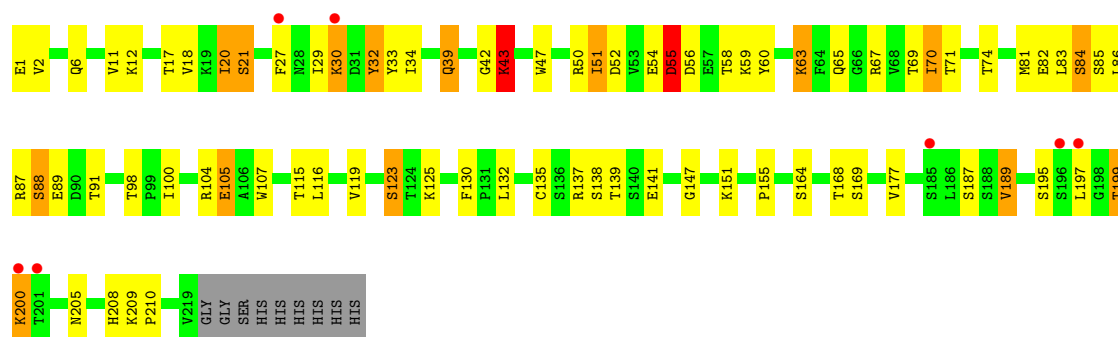
- Molecule 3 is a protein called Light chain of antibody 10V8 Fab fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	215	Total 1648	C 1029	N 277	O 336	S 6	0	0	0
3	F	215	Total 1648	C 1029	N 277	O 336	S 6	0	0	0
3	I	215	Total 1648	C 1029	N 277	O 336	S 6	0	0	0
3	L	215	Total 1648	C 1029	N 277	O 336	S 6	0	0	0

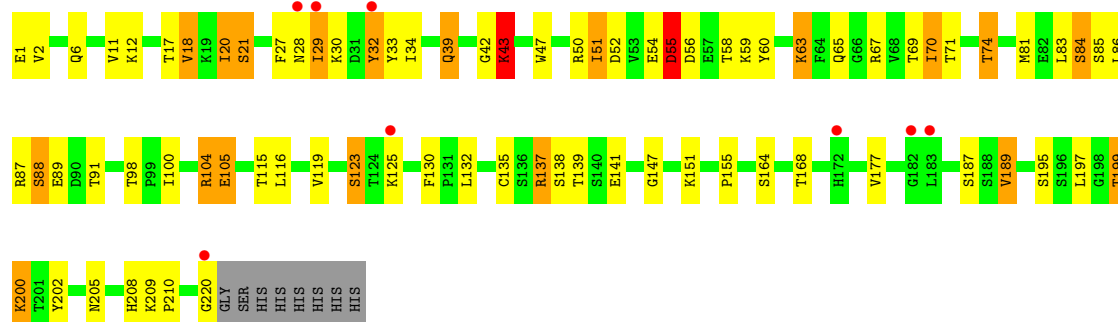




- Molecule 2: Heavy chain of antibody 10V8 Fab fragment

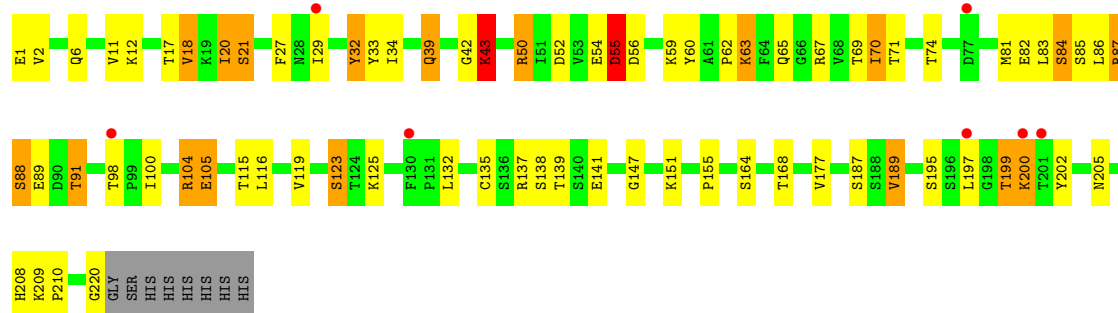


- Molecule 2: Heavy chain of antibody 10V8 Fab fragment



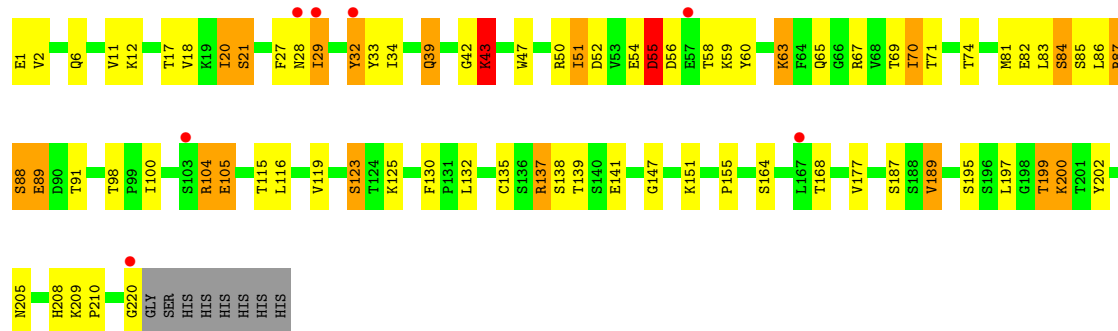
- Molecule 2: Heavy chain of antibody 10V8 Fab fragment

Chain H: 



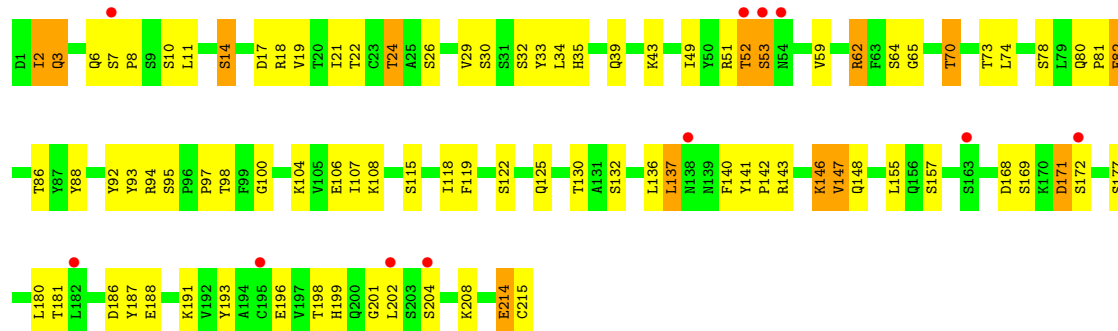
- Molecule 2: Heavy chain of antibody 10V8 Fab fragment

Chain K: 



- Molecule 3: Light chain of antibody 10V8 Fab fragment

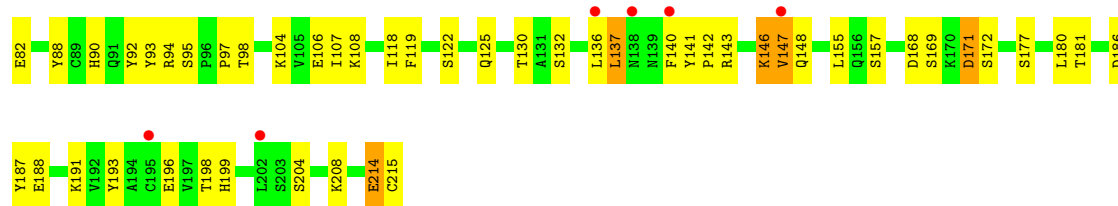
Chain C: 



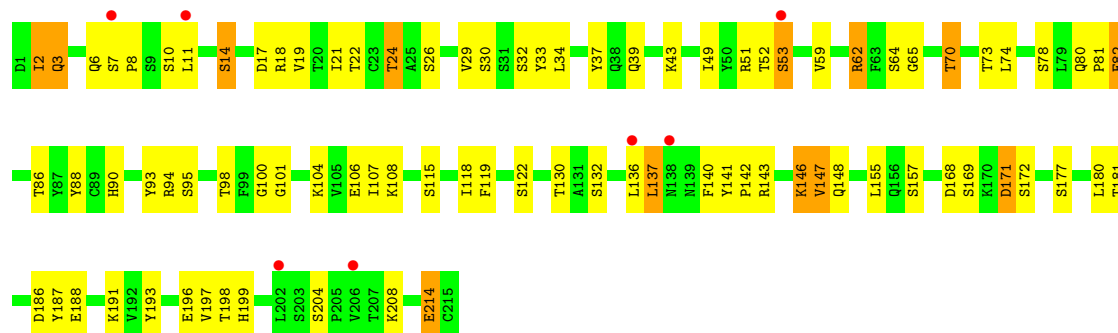
- Molecule 3: Light chain of antibody 10V8 Fab fragment

Chain F: 

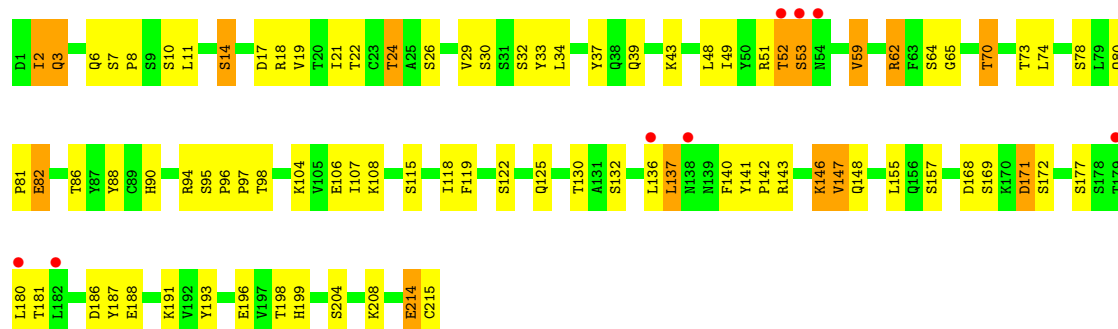




● Molecule 3: Light chain of antibody 10V8 Fab fragment



● Molecule 3: Light chain of antibody 10V8 Fab fragment



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.42Å 225.16Å 143.00Å 90.00° 91.30° 90.00°	Depositor
Resolution (Å)	49.65 – 3.21 49.65 – 3.21	Depositor EDS
% Data completeness (in resolution range)	90.6 (49.65-3.21) 90.6 (49.65-3.21)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.248 , 0.294 0.249 , 0.295	Depositor DCC
R_{free} test set	3309 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	59.5	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 69.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.117 for h,-k,-l	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	26621	wwPDB-VP
Average B, all atoms (Å ²)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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	A	0.59	0/3503	1.01	4/4755 (0.1%)
1	D	0.59	0/3426	0.99	5/4654 (0.1%)
1	G	0.59	0/3283	1.01	1/4452 (0.0%)
1	J	0.59	0/3502	1.01	6/4757 (0.1%)
2	B	0.56	0/1705	1.00	1/2326 (0.0%)
2	E	0.56	0/1709	1.01	1/2331 (0.0%)
2	H	0.56	0/1709	1.01	1/2331 (0.0%)
2	K	0.56	0/1709	1.01	1/2331 (0.0%)
3	C	0.61	0/1686	1.07	1/2289 (0.0%)
3	F	0.60	0/1686	1.07	1/2289 (0.0%)
3	I	0.62	0/1686	1.08	0/2289
3	L	0.61	0/1686	1.07	1/2289 (0.0%)
All	All	0.59	0/27290	1.02	23/37093 (0.1%)

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
1	D	0	1
2	B	0	1
2	E	0	1
2	H	0	1
2	K	0	1
3	F	0	1
All	All	0	6

There are no bond length outliers.

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	55	ASP	CA-CB-CG	6.21	118.81	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	482	GLN	CA-C-N	6.07	126.03	119.78
1	J	482	GLN	C-N-CA	6.07	126.03	119.78
2	E	55	ASP	CA-CB-CG	6.02	118.62	112.60
2	B	55	ASP	CA-CB-CG	5.82	118.42	112.60

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	123	SER	Peptide
1	D	542	ARG	Sidechain
2	E	123	SER	Peptide
3	F	18	ARG	Sidechain
2	H	123	SER	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	A	3412	0	3313	93	0
1	D	3337	0	3230	97	0
1	G	3202	0	3088	101	1
1	J	3410	0	3297	141	0
2	B	1664	0	1627	55	0
2	E	1668	0	1630	54	1
2	H	1668	0	1630	55	0
2	K	1668	0	1630	62	0
3	C	1648	0	1595	54	0
3	F	1648	0	1595	52	0
3	I	1648	0	1595	58	0
3	L	1648	0	1595	59	0
All	All	26621	0	25825	804	1

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 15.

The worst 5 of 804 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:185:MET:HE1	1:J:268:HIS:CD2	1.61	1.35
1:G:443:GLY:HA2	1:G:466:ARG:NH1	1.44	1.31
1:J:449:GLN:NE2	1:J:491:ASP:O	1.71	1.24
1:J:272:LEU:CD1	1:J:279:VAL:HG21	1.69	1.20
1:A:272:LEU:CD1	1:A:279:VAL:HG21	1.71	1.17

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:27:PHE:O	1:G:531:ASN:OD1[2_546]	1.96	0.24

5.3 Torsion angles

5.3.1 Protein backbone

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	418/583 (72%)	393 (94%)	23 (6%)	2 (0%)	24	59
1	D	412/583 (71%)	390 (95%)	20 (5%)	2 (0%)	24	59
1	G	388/583 (67%)	365 (94%)	18 (5%)	5 (1%)	9	40
1	J	419/583 (72%)	391 (93%)	23 (6%)	5 (1%)	10	42
2	B	217/228 (95%)	199 (92%)	16 (7%)	2 (1%)	14	47
2	E	218/228 (96%)	200 (92%)	16 (7%)	2 (1%)	14	47
2	H	218/228 (96%)	200 (92%)	16 (7%)	2 (1%)	14	47
2	K	218/228 (96%)	201 (92%)	15 (7%)	2 (1%)	14	47
3	C	213/215 (99%)	204 (96%)	9 (4%)	0	100	100
3	F	213/215 (99%)	204 (96%)	9 (4%)	0	100	100
3	I	213/215 (99%)	204 (96%)	9 (4%)	0	100	100
3	L	213/215 (99%)	204 (96%)	9 (4%)	0	100	100
All	All	3360/4104 (82%)	3155 (94%)	183 (5%)	22 (1%)	18	52

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	29	ILE
2	B	43	LYS
2	E	29	ILE
1	G	545	GLN
2	H	29	ILE

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	372/506 (74%)	322 (87%)	50 (13%)	4	19
1	D	363/506 (72%)	320 (88%)	43 (12%)	5	23
1	G	350/506 (69%)	302 (86%)	48 (14%)	3	18
1	J	372/506 (74%)	318 (86%)	54 (14%)	3	16
2	B	187/194 (96%)	141 (75%)	46 (25%)	1	3
2	E	187/194 (96%)	141 (75%)	46 (25%)	1	3
2	H	187/194 (96%)	141 (75%)	46 (25%)	1	3
2	K	187/194 (96%)	142 (76%)	45 (24%)	1	4
3	C	190/190 (100%)	140 (74%)	50 (26%)	0	3
3	F	190/190 (100%)	141 (74%)	49 (26%)	0	3
3	I	190/190 (100%)	140 (74%)	50 (26%)	0	3
3	L	190/190 (100%)	140 (74%)	50 (26%)	0	3
All	All	2965/3560 (83%)	2388 (80%)	577 (20%)	1	8

5 of 577 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	458	TYR
3	L	198	THR
1	J	539	GLN
1	J	455	THR

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Mol	Chain	Res	Type
2	K	177	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 68 such sidechains are listed below:

Mol	Chain	Res	Type
1	J	531	ASN
1	J	545	GLN
3	L	3	GLN
2	E	3	GLN
1	D	569	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 [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	426/583 (73%)	0.32	14 (3%) 49 30	37, 79, 167, 239	0
1	D	420/583 (72%)	0.37	9 (2%) 63 43	39, 110, 168, 220	0
1	G	402/583 (68%)	0.74	37 (9%) 14 9	42, 114, 196, 269	0
1	J	427/583 (73%)	0.52	21 (4%) 35 22	38, 111, 174, 256	0
2	B	219/228 (96%)	0.43	7 (3%) 50 31	35, 72, 122, 168	0
2	E	220/228 (96%)	0.40	8 (3%) 46 28	36, 74, 131, 198	0
2	H	220/228 (96%)	0.34	7 (3%) 50 31	34, 67, 124, 166	0
2	K	220/228 (96%)	0.38	7 (3%) 50 31	34, 70, 124, 161	0
3	C	215/215 (100%)	0.49	11 (5%) 33 21	28, 61, 135, 169	0
3	F	215/215 (100%)	0.43	10 (4%) 36 23	29, 62, 140, 159	0
3	I	215/215 (100%)	0.38	7 (3%) 49 30	29, 57, 122, 158	0
3	L	215/215 (100%)	0.36	8 (3%) 45 28	28, 65, 132, 152	0
All	All	3414/4104 (83%)	0.44	146 (4%) 40 24	28, 82, 160, 269	0

The worst 5 of 146 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	584	GLY	5.4
3	F	53	SER	4.7
1	G	573	VAL	4.5
3	I	138	ASN	4.5
3	I	53	SER	4.1

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.