



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:18 AM UTC

PDB ID : 5V5V / pdb_00005v5v
Title : Complex of NLGN2 with MDGA1 Ig1-Ig2
Authors : Gangwar, S.P.; Machius, M.; Rudenko, G.
Deposited on : 2017-03-15
Resolution : 4.11 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

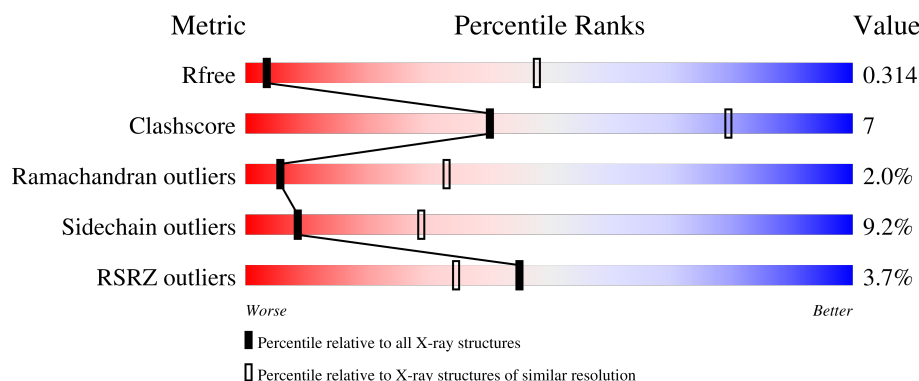
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.11 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	1249 (4.44-3.80)
Clashscore	190562	1031 (4.42-3.82)
Ramachandran outliers	187476	1211 (4.44-3.80)
Sidechain outliers	187428	1198 (4.44-3.80)
RSRZ outliers	180081	1246 (4.44-3.80)

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	582	0% 66% 21% • • 9%
1	B	582	2% 67% 20% • 9%
1	C	582	3% 68% 20% • 9%
1	D	582	4% 68% 20% • 9%
1	E	582	3% 67% 20% • 9%

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Mol	Chain	Length	Quality of chain
1	F	582	4% 68% 20% • 9%
2	G	230	5% 63% 14% •• 20%
2	H	230	3% 64% 13% •• 20%
2	I	230	7% 65% 13% • 20%
2	J	230	5% 64% 13% • 20%
2	K	230	6% 63% 15% • 20%
2	L	230	3% 65% 13% • 20%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 33540 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 Neuroligin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	0	0
			4130	2640	700	772	18			
1	B	527	Total	C	N	O	S	0	0	0
			4130	2640	700	772	18			
1	C	527	Total	C	N	O	S	0	0	0
			4130	2640	700	772	18			
1	D	527	Total	C	N	O	S	0	0	0
			4130	2640	700	772	18			
1	E	527	Total	C	N	O	S	0	0	0
			4130	2640	700	772	18			
1	F	527	Total	C	N	O	S	0	0	0
			4130	2640	700	772	18			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	ALA	-	expression tag	UNP Q62888
A	613	ALA	-	expression tag	UNP Q62888
A	614	SER	-	expression tag	UNP Q62888
A	615	THR	-	expression tag	UNP Q62888
A	616	SER	-	expression tag	UNP Q62888
A	617	HIS	-	expression tag	UNP Q62888
A	618	HIS	-	expression tag	UNP Q62888
A	619	HIS	-	expression tag	UNP Q62888
A	620	HIS	-	expression tag	UNP Q62888
A	621	HIS	-	expression tag	UNP Q62888
A	622	HIS	-	expression tag	UNP Q62888
B	41	ALA	-	expression tag	UNP Q62888
B	613	ALA	-	expression tag	UNP Q62888
B	614	SER	-	expression tag	UNP Q62888
B	615	THR	-	expression tag	UNP Q62888
B	616	SER	-	expression tag	UNP Q62888
B	617	HIS	-	expression tag	UNP Q62888

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Chain	Residue	Modelled	Actual	Comment	Reference
B	618	HIS	-	expression tag	UNP Q62888
B	619	HIS	-	expression tag	UNP Q62888
B	620	HIS	-	expression tag	UNP Q62888
B	621	HIS	-	expression tag	UNP Q62888
B	622	HIS	-	expression tag	UNP Q62888
C	41	ALA	-	expression tag	UNP Q62888
C	613	ALA	-	expression tag	UNP Q62888
C	614	SER	-	expression tag	UNP Q62888
C	615	THR	-	expression tag	UNP Q62888
C	616	SER	-	expression tag	UNP Q62888
C	617	HIS	-	expression tag	UNP Q62888
C	618	HIS	-	expression tag	UNP Q62888
C	619	HIS	-	expression tag	UNP Q62888
C	620	HIS	-	expression tag	UNP Q62888
C	621	HIS	-	expression tag	UNP Q62888
C	622	HIS	-	expression tag	UNP Q62888
D	41	ALA	-	expression tag	UNP Q62888
D	613	ALA	-	expression tag	UNP Q62888
D	614	SER	-	expression tag	UNP Q62888
D	615	THR	-	expression tag	UNP Q62888
D	616	SER	-	expression tag	UNP Q62888
D	617	HIS	-	expression tag	UNP Q62888
D	618	HIS	-	expression tag	UNP Q62888
D	619	HIS	-	expression tag	UNP Q62888
D	620	HIS	-	expression tag	UNP Q62888
D	621	HIS	-	expression tag	UNP Q62888
D	622	HIS	-	expression tag	UNP Q62888
E	41	ALA	-	expression tag	UNP Q62888
E	613	ALA	-	expression tag	UNP Q62888
E	614	SER	-	expression tag	UNP Q62888
E	615	THR	-	expression tag	UNP Q62888
E	616	SER	-	expression tag	UNP Q62888
E	617	HIS	-	expression tag	UNP Q62888
E	618	HIS	-	expression tag	UNP Q62888
E	619	HIS	-	expression tag	UNP Q62888
E	620	HIS	-	expression tag	UNP Q62888
E	621	HIS	-	expression tag	UNP Q62888
E	622	HIS	-	expression tag	UNP Q62888
F	41	ALA	-	expression tag	UNP Q62888
F	613	ALA	-	expression tag	UNP Q62888
F	614	SER	-	expression tag	UNP Q62888
F	615	THR	-	expression tag	UNP Q62888

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Chain	Residue	Modelled	Actual	Comment	Reference
F	616	SER	-	expression tag	UNP Q62888
F	617	HIS	-	expression tag	UNP Q62888
F	618	HIS	-	expression tag	UNP Q62888
F	619	HIS	-	expression tag	UNP Q62888
F	620	HIS	-	expression tag	UNP Q62888
F	621	HIS	-	expression tag	UNP Q62888
F	622	HIS	-	expression tag	UNP Q62888

- Molecule 2 is a protein called MAM domain-containing glycosylphosphatidylinositol anchor protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	184	Total	C	N	O	S	0	0	0
			1460	918	263	271	8			
2	H	184	Total	C	N	O	S	0	0	0
			1460	918	263	271	8			
2	I	184	Total	C	N	O	S	0	0	0
			1460	918	263	271	8			
2	J	184	Total	C	N	O	S	0	0	0
			1460	918	263	271	8			
2	K	184	Total	C	N	O	S	0	0	0
			1460	918	263	271	8			
2	L	184	Total	C	N	O	S	0	0	0
			1460	918	263	271	8			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	20	VAL	-	expression tag	UNP Q8NFP4
G	21	ASP	-	expression tag	UNP Q8NFP4
G	238	GLY	-	expression tag	UNP Q8NFP4
G	239	SER	-	expression tag	UNP Q8NFP4
G	240	ALA	-	expression tag	UNP Q8NFP4
G	241	SER	-	expression tag	UNP Q8NFP4
G	242	THR	-	expression tag	UNP Q8NFP4
G	243	SER	-	expression tag	UNP Q8NFP4
G	244	HIS	-	expression tag	UNP Q8NFP4
G	245	HIS	-	expression tag	UNP Q8NFP4
G	246	HIS	-	expression tag	UNP Q8NFP4
G	247	HIS	-	expression tag	UNP Q8NFP4
G	248	HIS	-	expression tag	UNP Q8NFP4
G	249	HIS	-	expression tag	UNP Q8NFP4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	20	VAL	-	expression tag	UNP Q8NFP4
H	21	ASP	-	expression tag	UNP Q8NFP4
H	238	GLY	-	expression tag	UNP Q8NFP4
H	239	SER	-	expression tag	UNP Q8NFP4
H	240	ALA	-	expression tag	UNP Q8NFP4
H	241	SER	-	expression tag	UNP Q8NFP4
H	242	THR	-	expression tag	UNP Q8NFP4
H	243	SER	-	expression tag	UNP Q8NFP4
H	244	HIS	-	expression tag	UNP Q8NFP4
H	245	HIS	-	expression tag	UNP Q8NFP4
H	246	HIS	-	expression tag	UNP Q8NFP4
H	247	HIS	-	expression tag	UNP Q8NFP4
H	248	HIS	-	expression tag	UNP Q8NFP4
H	249	HIS	-	expression tag	UNP Q8NFP4
I	20	VAL	-	expression tag	UNP Q8NFP4
I	21	ASP	-	expression tag	UNP Q8NFP4
I	238	GLY	-	expression tag	UNP Q8NFP4
I	239	SER	-	expression tag	UNP Q8NFP4
I	240	ALA	-	expression tag	UNP Q8NFP4
I	241	SER	-	expression tag	UNP Q8NFP4
I	242	THR	-	expression tag	UNP Q8NFP4
I	243	SER	-	expression tag	UNP Q8NFP4
I	244	HIS	-	expression tag	UNP Q8NFP4
I	245	HIS	-	expression tag	UNP Q8NFP4
I	246	HIS	-	expression tag	UNP Q8NFP4
I	247	HIS	-	expression tag	UNP Q8NFP4
I	248	HIS	-	expression tag	UNP Q8NFP4
I	249	HIS	-	expression tag	UNP Q8NFP4
J	20	VAL	-	expression tag	UNP Q8NFP4
J	21	ASP	-	expression tag	UNP Q8NFP4
J	238	GLY	-	expression tag	UNP Q8NFP4
J	239	SER	-	expression tag	UNP Q8NFP4
J	240	ALA	-	expression tag	UNP Q8NFP4
J	241	SER	-	expression tag	UNP Q8NFP4
J	242	THR	-	expression tag	UNP Q8NFP4
J	243	SER	-	expression tag	UNP Q8NFP4
J	244	HIS	-	expression tag	UNP Q8NFP4
J	245	HIS	-	expression tag	UNP Q8NFP4
J	246	HIS	-	expression tag	UNP Q8NFP4
J	247	HIS	-	expression tag	UNP Q8NFP4
J	248	HIS	-	expression tag	UNP Q8NFP4
J	249	HIS	-	expression tag	UNP Q8NFP4

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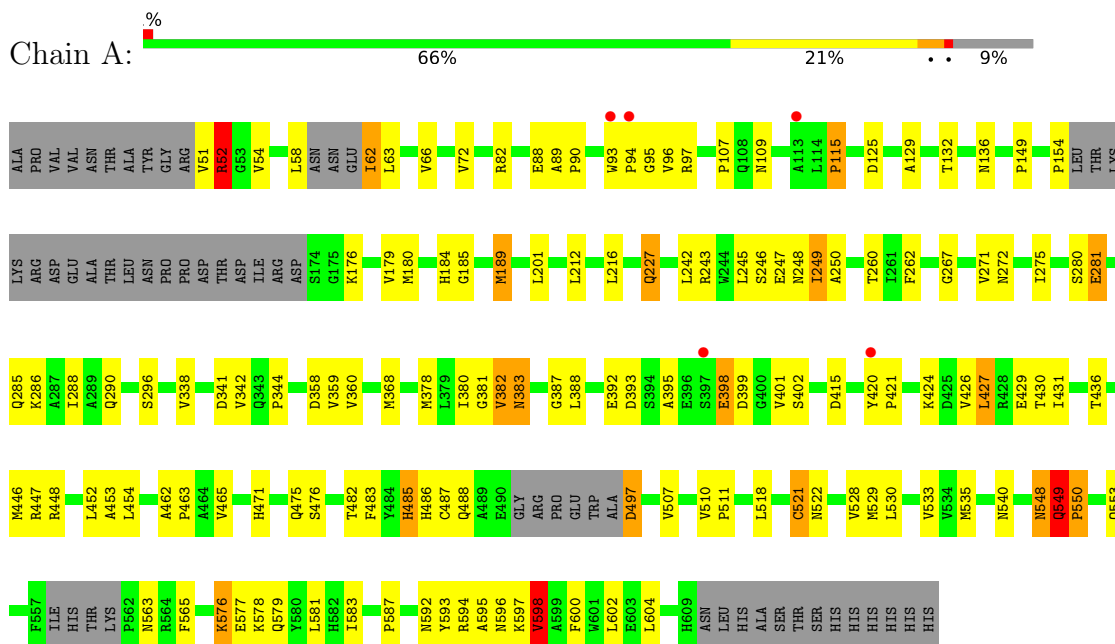
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Chain	Residue	Modelled	Actual	Comment	Reference
K	20	VAL	-	expression tag	UNP Q8NFP4
K	21	ASP	-	expression tag	UNP Q8NFP4
K	238	GLY	-	expression tag	UNP Q8NFP4
K	239	SER	-	expression tag	UNP Q8NFP4
K	240	ALA	-	expression tag	UNP Q8NFP4
K	241	SER	-	expression tag	UNP Q8NFP4
K	242	THR	-	expression tag	UNP Q8NFP4
K	243	SER	-	expression tag	UNP Q8NFP4
K	244	HIS	-	expression tag	UNP Q8NFP4
K	245	HIS	-	expression tag	UNP Q8NFP4
K	246	HIS	-	expression tag	UNP Q8NFP4
K	247	HIS	-	expression tag	UNP Q8NFP4
K	248	HIS	-	expression tag	UNP Q8NFP4
K	249	HIS	-	expression tag	UNP Q8NFP4
L	20	VAL	-	expression tag	UNP Q8NFP4
L	21	ASP	-	expression tag	UNP Q8NFP4
L	238	GLY	-	expression tag	UNP Q8NFP4
L	239	SER	-	expression tag	UNP Q8NFP4
L	240	ALA	-	expression tag	UNP Q8NFP4
L	241	SER	-	expression tag	UNP Q8NFP4
L	242	THR	-	expression tag	UNP Q8NFP4
L	243	SER	-	expression tag	UNP Q8NFP4
L	244	HIS	-	expression tag	UNP Q8NFP4
L	245	HIS	-	expression tag	UNP Q8NFP4
L	246	HIS	-	expression tag	UNP Q8NFP4
L	247	HIS	-	expression tag	UNP Q8NFP4
L	248	HIS	-	expression tag	UNP Q8NFP4
L	249	HIS	-	expression tag	UNP Q8NFP4

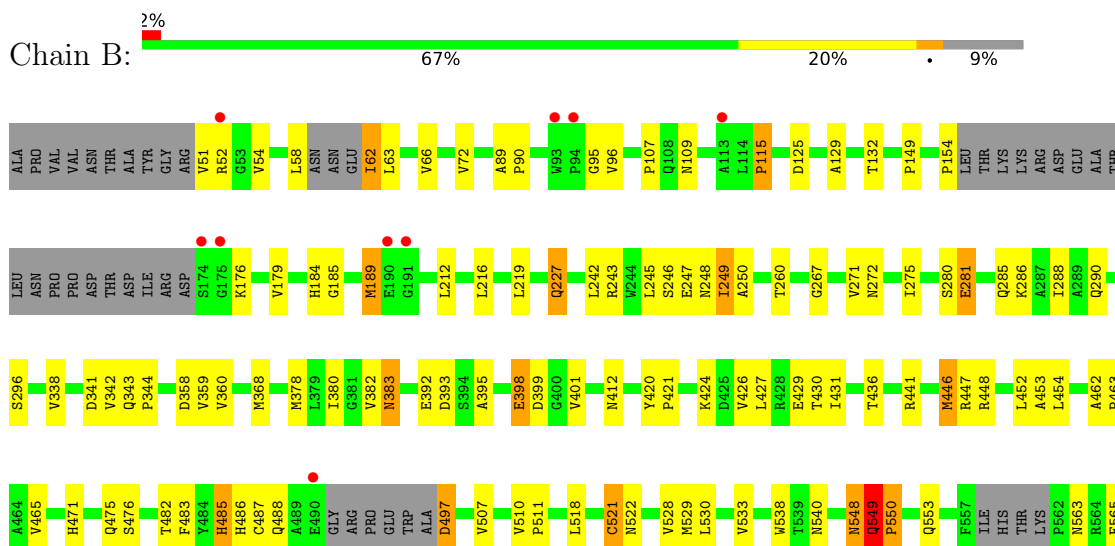
3 Residue-property plots

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: Neuroligin-2

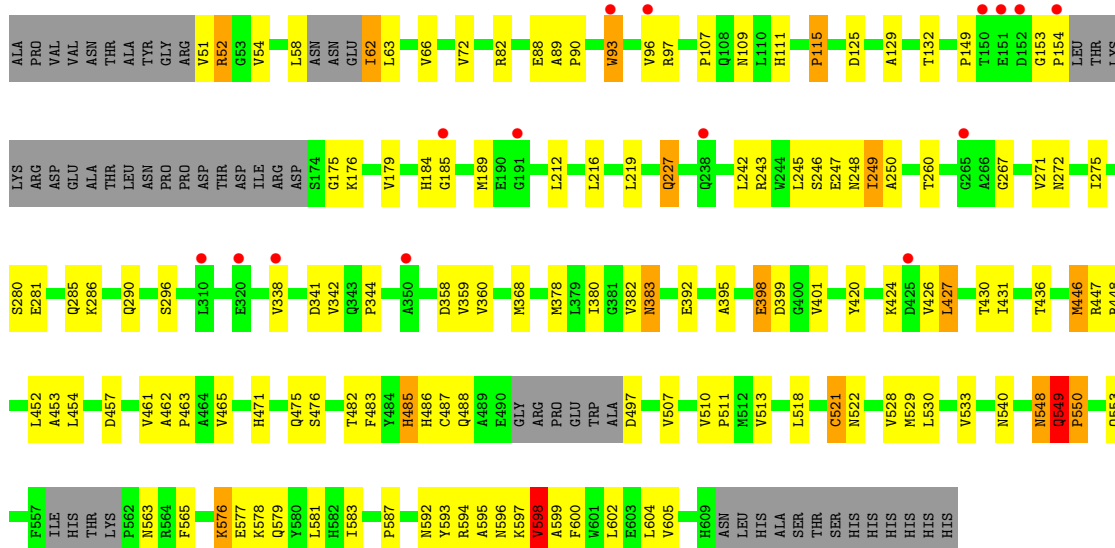


• Molecule 1: Neuroligin-2

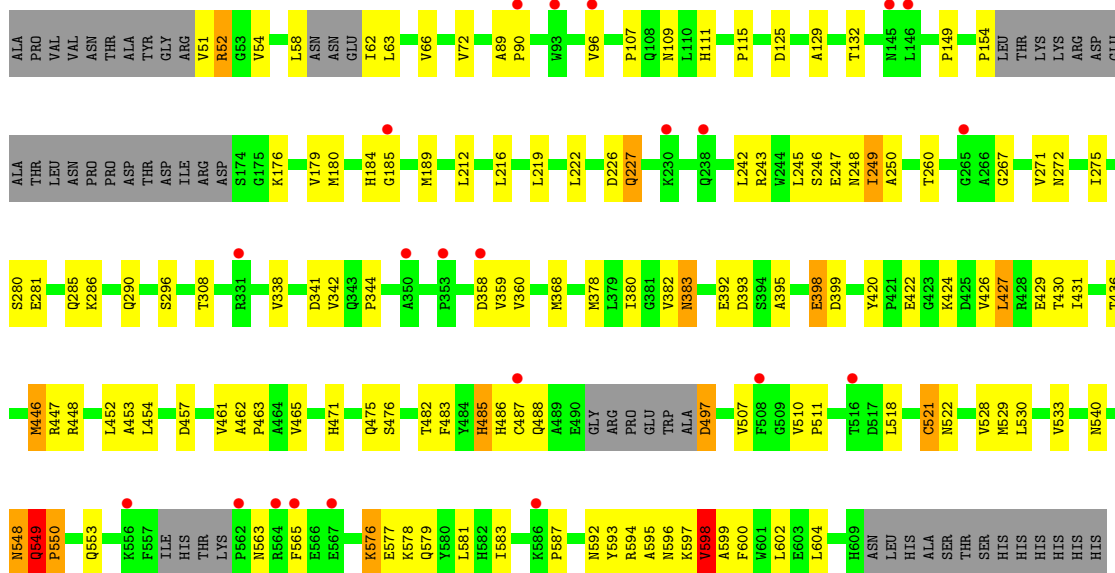


Chain C: 3% 68% 20% 9%

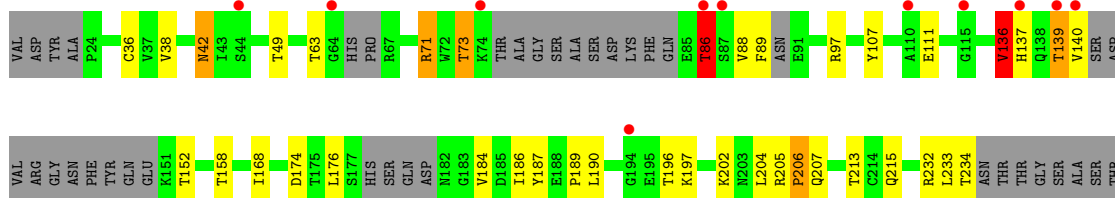




• Molecule 1: Neuroligin-2



• Molecule 2: MAM domain-containing glycosylphosphatidylinositol anchor protein 1



SER
HIS
HIS
HIS
HIS
HIS
HIS

- Molecule 2: MAM domain-containing glycosylphosphatidylinositol anchor protein 1



VAL ASP TYR ALA P24 C36 V37 V39 N42 T49 G64 G64 R67 R71 W72 W73 K74 THR ALA GLY SER ALA ASP LYS PHE GLN E85 T86 S87 V88 F89 E91 R97 Y107 E111 V136 H137 Q138 T139 V140 SER ASP VAL ARG GLY ASP PHE TYR

GLN GLU T152 T158 R166 F167 I168 D174 T175 L176 S177 HIS SER GLN ASP N182 G183 V184 D185 I186 Y187 E188 P189 G194 F195 T196 K197 K202 N203 L204 R205 P206 T213 C214 Q215 L233 T234 THR THR GLY SER SER THR SER HIS HIS HIS HIS HIS

HIS

- Molecule 2: MAM domain-containing glycosylphosphatidylinositol anchor protein 1



VAL ASP TYR ALA P24 C36 V37 V38 K39 N42 S53 T63 G64 HIS PRO R67 R71 W72 W73 K74 THR ALA GLY SER ALA ASP LYS PHE GLN E85 T86 S87 V88 F89 E91 Y107 E111 V116 M133 V136 Q138 T139 V140 SER ASP VAL ARG

GLY ASN PHE TYR GLU K151 T152 T158 V169 D174 T175 S177 HIS SER GLN ASP N182 G183 V184 D185 I186 Y187 E188 L190 T196 K197 K202 N203 L204 R205 P206 Q215 K227 L233 T234 THR THR GLY SER ALA THR THR THR HIS HIS HIS HIS HIS

HIS

- Molecule 2: MAM domain-containing glycosylphosphatidylinositol anchor protein 1



VAL ASP TYR ALA P24 A25 T29 V30 C36 V37 V38 N42 I43 S44 M57 G64 HIS PRO R67 P68 R71 W72 S177 T73 K74 THR ALA GLY SER ALA N182 G183 V184 D185 I186 Y187 E188 P189 T196 T196 S196 V88 F89 E91 T92 R97 T98 A99 Y107 T234 E111 V116 P117 A118

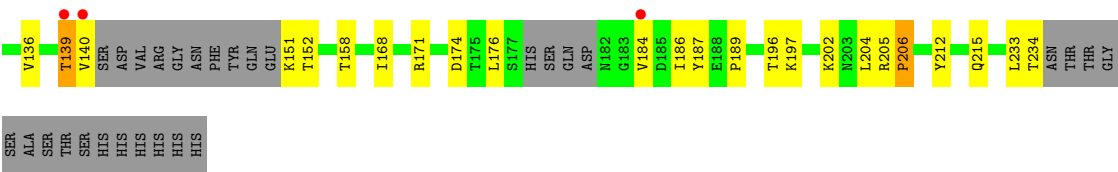
M133 V136 T139 V140 SER ASP VAL ARG GLY ASN PHE TYR GLN GLU K151 T152 T158 T158 I168 D174 T175 L176 S177 HIS SER GLN ASP N182 G183 V184 D185 I186 Y187 E188 P189 T196 T196 S196 V88 F89 E91 T92 R97 T98 A99 Y107 T234 E111 V116 P117 A118

ALA SER SER SER HIS HIS HIS HIS HIS

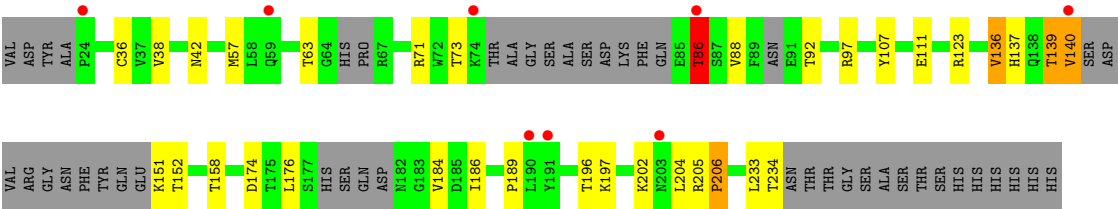
- Molecule 2: MAM domain-containing glycosylphosphatidylinositol anchor protein 1



VAL ASP TYR ALA P24 A27 A35 C36 V37 V38 N42 I43 S44 T49 M57 G64 HIS PRO R67 R71 W72 T73 K74 THR ALA GLY SER ALA N182 G183 V184 D185 I186 Y187 E188 P189 T196 T196 S196 V88 F89 E91 T92 R97 T98 A99 Y107 T234 E111 V116 P117 M133



● Molecule 2: MAM domain-containing glycosylphosphatidylinositol anchor protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	103.12Å 97.18Å 190.51Å 95.52° 80.97° 88.71°	Depositor
Resolution (Å)	49.77 – 4.11 49.77 – 4.11	Depositor EDS
% Data completeness (in resolution range)	81.3 (49.77-4.11) 81.5 (49.77-4.11)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.50 (at 4.14Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
R, R_{free}	0.289 , 0.319 0.287 , 0.314	Depositor DCC
R_{free} test set	2200 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å ²)	45.9	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 68.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	33540	wwPDB-VP
Average B, all atoms (Å ²)	114.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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	0.80	1/4240 (0.0%)	1.02	13/5769 (0.2%)
1	B	0.81	2/4240 (0.0%)	1.03	13/5769 (0.2%)
1	C	0.79	1/4240 (0.0%)	1.02	11/5769 (0.2%)
1	D	0.77	0/4240	1.00	14/5769 (0.2%)
1	E	0.77	0/4240	1.01	13/5769 (0.2%)
1	F	0.76	0/4240	1.00	10/5769 (0.2%)
2	G	1.04	3/1481 (0.2%)	0.99	7/2001 (0.3%)
2	H	1.05	3/1481 (0.2%)	0.99	7/2001 (0.3%)
2	I	0.99	4/1481 (0.3%)	0.97	5/2001 (0.2%)
2	J	1.00	4/1481 (0.3%)	0.98	6/2001 (0.3%)
2	K	1.02	4/1481 (0.3%)	0.97	7/2001 (0.3%)
2	L	1.00	4/1481 (0.3%)	0.98	4/2001 (0.2%)
All	All	0.85	26/34326 (0.1%)	1.01	110/46620 (0.2%)

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	A	0	4
1	B	0	4
1	C	0	6
1	D	0	4
1	E	0	5
1	F	0	4
2	G	0	1
All	All	0	28

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	567	GLU	N-CA	7.97	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	139	THR	CA-C	7.63	1.62	1.52
2	G	139	THR	CA-C	7.41	1.62	1.52
2	L	139	THR	CA-C	7.04	1.61	1.52
2	K	139	THR	CA-C	6.99	1.61	1.52
2	J	139	THR	CA-C	6.78	1.61	1.52
2	I	139	THR	CA-C	6.77	1.61	1.52
2	G	139	THR	N-CA	6.64	1.54	1.46
1	B	52	ARG	CA-C	6.54	1.60	1.52
1	C	51	VAL	C-N	6.23	1.41	1.33
2	J	38	VAL	CA-C	6.08	1.59	1.52
2	H	139	THR	N-CA	6.04	1.53	1.46
2	I	139	THR	N-CA	5.77	1.53	1.46
2	L	139	THR	N-CA	5.77	1.53	1.46
2	I	38	VAL	CA-C	5.72	1.59	1.52
2	K	139	THR	N-CA	5.65	1.53	1.46
1	A	52	ARG	CZ-NH2	5.46	1.40	1.33
2	K	38	VAL	CA-C	5.44	1.58	1.52
2	G	174	ASP	N-CA	5.42	1.52	1.46
2	L	140	VAL	N-CA	5.38	1.56	1.46
2	H	38	VAL	CA-CB	5.24	1.59	1.54
2	I	140	VAL	N-CA	5.22	1.56	1.46
2	J	139	THR	N-CA	5.21	1.52	1.46
2	J	86	THR	N-CA	5.11	1.52	1.46
2	L	38	VAL	CA-C	5.09	1.58	1.52
2	K	86	THR	N-CA	5.07	1.52	1.46

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	ARG	CA-CB-CG	9.40	132.90	114.10
1	B	485	HIS	N-CA-C	7.24	119.87	107.93
1	A	485	HIS	N-CA-C	7.20	119.81	107.93
1	C	485	HIS	N-CA-C	7.18	119.78	107.93
1	E	485	HIS	N-CA-C	7.10	119.84	107.49
1	F	485	HIS	N-CA-C	7.09	119.83	107.49
1	D	485	HIS	N-CA-C	7.07	119.60	107.93
2	J	174	ASP	N-CA-C	6.91	119.75	110.35
1	A	184	HIS	N-CA-C	6.80	117.21	108.24
2	K	174	ASP	N-CA-C	6.75	119.53	110.35
1	B	184	HIS	N-CA-C	6.70	117.08	108.24
1	D	184	HIS	N-CA-C	6.56	116.90	108.24
1	F	184	HIS	N-CA-C	6.40	116.69	108.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	399	ASP	N-CA-C	-6.38	105.46	113.18
1	D	399	ASP	N-CA-C	-6.37	105.47	113.18
2	K	38	VAL	N-CA-C	6.34	117.76	109.58
2	I	174	ASP	N-CA-C	6.33	118.96	110.35
1	A	549	GLN	CA-C-N	6.32	127.74	119.84
1	A	549	GLN	C-N-CA	6.32	127.74	119.84
1	C	549	GLN	CA-C-N	6.30	127.72	119.84
1	C	549	GLN	C-N-CA	6.30	127.72	119.84
1	C	399	ASP	N-CA-C	-6.29	105.56	113.18
1	E	184	HIS	N-CA-C	6.29	116.55	108.24
1	B	549	GLN	CA-C-N	6.27	127.67	119.84
1	B	549	GLN	C-N-CA	6.27	127.67	119.84
1	B	52	ARG	N-CA-CB	-6.25	101.21	111.66
1	E	549	GLN	CA-C-N	6.24	127.63	119.84
1	E	549	GLN	C-N-CA	6.24	127.63	119.84
1	C	184	HIS	N-CA-C	6.22	116.45	108.24
1	D	549	GLN	CA-C-N	6.19	127.58	119.84
1	D	549	GLN	C-N-CA	6.19	127.58	119.84
2	G	38	VAL	N-CA-C	6.17	117.54	109.58
2	J	38	VAL	N-CA-C	6.14	117.50	109.58
1	F	549	GLN	CA-C-N	6.11	127.47	119.84
1	F	549	GLN	C-N-CA	6.11	127.47	119.84
1	A	521	CYS	N-CA-C	6.08	119.07	110.50
1	B	399	ASP	N-CA-C	-6.07	105.37	112.89
1	B	185	GLY	N-CA-C	-6.06	104.08	111.35
1	A	399	ASP	N-CA-C	-6.03	105.41	112.89
1	C	185	GLY	N-CA-C	-6.01	104.14	111.35
1	E	185	GLY	N-CA-C	-5.94	104.22	111.35
1	B	521	CYS	N-CA-C	5.93	118.86	110.50
1	F	185	GLY	N-CA-C	-5.91	104.26	111.35
2	L	174	ASP	N-CA-C	5.89	118.36	110.35
2	L	42	ASN	N-CA-C	5.88	119.28	111.75
2	I	42	ASN	N-CA-C	5.86	119.25	111.75
1	F	399	ASP	N-CA-C	-5.83	105.66	112.89
2	J	42	ASN	N-CA-C	5.82	119.20	111.75
1	A	185	GLY	N-CA-C	-5.79	104.40	111.35
2	L	38	VAL	N-CA-C	5.79	117.05	109.58
2	K	42	ASN	N-CA-C	5.79	119.16	111.75
1	D	185	GLY	N-CA-C	-5.78	104.42	111.35
2	H	174	ASP	N-CA-C	5.75	118.17	110.35
1	F	521	CYS	N-CA-C	5.73	118.58	110.50
2	I	38	VAL	N-CA-C	5.73	116.97	109.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	521	CYS	N-CA-C	5.70	118.53	110.50
2	H	38	VAL	N-CA-C	5.64	117.75	109.63
1	C	54	VAL	N-CA-C	5.62	118.24	108.90
2	I	111	GLU	N-CA-C	5.59	117.49	108.32
2	H	187	TYR	N-CA-C	5.58	116.75	108.60
1	B	476	SER	N-CA-C	-5.56	103.06	110.07
1	E	521	CYS	N-CA-C	5.55	118.33	110.50
1	A	476	SER	N-CA-C	-5.54	103.08	110.07
1	C	521	CYS	N-CA-C	5.53	118.30	110.50
1	A	54	VAL	N-CA-C	5.50	118.04	108.90
2	J	187	TYR	N-CA-C	5.50	116.64	108.60
1	E	62	ILE	N-CA-C	5.50	126.39	111.00
1	F	54	VAL	N-CA-C	5.49	118.01	108.95
2	G	111	GLU	N-CA-C	5.47	117.29	108.32
1	B	54	VAL	N-CA-C	5.45	117.94	108.90
1	C	476	SER	N-CA-C	-5.43	103.22	110.07
2	G	187	TYR	N-CA-C	5.42	116.52	108.60
2	H	111	GLU	N-CA-C	5.42	117.21	108.32
2	J	111	GLU	N-CA-C	5.39	117.17	108.32
2	L	111	GLU	N-CA-C	5.39	117.16	108.32
1	E	476	SER	N-CA-C	-5.37	103.30	110.07
1	D	54	VAL	N-CA-C	5.37	117.81	108.90
2	K	111	GLU	N-CA-C	5.34	117.08	108.32
1	A	94	PRO	CA-C-N	5.33	126.30	121.82
1	A	94	PRO	C-N-CA	5.33	126.30	121.82
1	B	393	ASP	N-CA-C	5.30	116.74	111.07
1	D	393	ASP	N-CA-C	5.28	116.72	111.07
1	C	62	ILE	N-CA-C	5.26	125.72	111.00
1	F	393	ASP	N-CA-C	5.24	116.68	111.07
2	G	42	ASN	N-CA-C	5.23	119.14	112.34
1	F	476	SER	N-CA-C	-5.23	103.19	109.72
2	G	71	ARG	N-CA-C	5.23	115.96	107.23
2	K	187	TYR	N-CA-C	5.22	116.22	108.60
2	G	174	ASP	N-CA-C	5.22	117.45	110.35
1	D	62	ILE	N-CA-C	5.19	125.54	111.00
1	B	62	ILE	N-CA-C	5.19	125.53	111.00
1	E	54	VAL	N-CA-C	5.19	117.51	108.90
2	H	42	ASN	N-CA-C	5.18	119.07	112.34
2	G	73	THR	N-CA-C	5.17	116.27	108.46
2	H	71	ARG	N-CA-C	5.17	115.86	107.23
1	C	393	ASP	N-CA-C	5.16	116.59	111.07
1	A	393	ASP	N-CA-C	5.16	116.59	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	476	SER	N-CA-C	-5.15	103.17	109.65
1	E	605	VAL	CA-C-N	-5.13	114.38	119.56
1	E	605	VAL	C-N-CA	-5.13	114.38	119.56
1	A	62	ILE	N-CA-C	5.13	125.36	111.00
2	I	187	TYR	N-CA-C	5.13	116.08	108.60
2	H	73	THR	N-CA-C	5.12	116.19	108.46
2	J	71	ARG	N-CA-C	5.12	115.78	107.23
2	K	71	ARG	N-CA-C	5.09	115.73	107.23
1	D	605	VAL	CA-C-N	-5.06	114.44	119.56
1	D	605	VAL	C-N-CA	-5.06	114.44	119.56
2	K	73	THR	N-CA-C	5.05	116.08	108.46
1	D	56	ARG	N-CA-C	5.01	115.65	108.74
1	E	93	TRP	CA-CB-CG	5.01	123.11	113.60

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	398	GLU	Peptide
1	A	446	MET	Peptide
1	A	475	GLN	Peptide
1	A	549	GLN	Peptide
1	B	398	GLU	Peptide
1	B	446	MET	Peptide
1	B	475	GLN	Peptide
1	B	549	GLN	Peptide
1	C	175	GLY	Peptide
1	C	398	GLU	Peptide
1	C	400	GLY	Peptide
1	C	446	MET	Peptide
1	C	475	GLN	Peptide
1	C	549	GLN	Peptide
1	D	398	GLU	Peptide
1	D	446	MET	Peptide
1	D	475	GLN	Peptide
1	D	549	GLN	Peptide
1	E	175	GLY	Peptide
1	E	398	GLU	Peptide
1	E	446	MET	Peptide
1	E	475	GLN	Peptide
1	E	549	GLN	Peptide
1	F	398	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	F	446	MET	Peptide
1	F	475	GLN	Peptide
1	F	549	GLN	Peptide
2	G	207	GLN	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	A	4130	0	3975	68	1
1	B	4130	0	3975	65	2
1	C	4130	0	3975	59	2
1	D	4130	0	3975	64	0
1	E	4130	0	3975	63	1
1	F	4130	0	3975	66	0
2	G	1460	0	1475	10	0
2	H	1460	0	1475	12	0
2	I	1460	0	1475	9	0
2	J	1460	0	1475	9	0
2	K	1460	0	1475	10	0
2	L	1460	0	1475	10	0
All	All	33540	0	32700	436	3

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 7.

All (436) 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)
2:L:158:THR:HG22	2:L:196:THR:HG22	1.50	0.93
2:I:158:THR:HG22	2:I:196:THR:HG22	1.51	0.93
2:K:158:THR:HG22	2:K:196:THR:HG22	1.50	0.92
2:J:158:THR:HG22	2:J:196:THR:HG22	1.50	0.91
2:H:158:THR:HG22	2:H:196:THR:HG22	1.50	0.89
2:G:158:THR:HG22	2:G:196:THR:HG22	1.52	0.89
2:I:140:VAL:HG22	2:I:151:LYS:HE3	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:565:PHE:CE1	1:D:587:PRO:HB3	2.26	0.70
2:G:42:ASN:HD21	1:B:227:GLN:HG2	1.56	0.70
1:F:565:PHE:CE1	1:F:587:PRO:HB3	2.28	0.68
2:J:57:MET:HE3	2:J:92:THR:HG21	1.74	0.68
2:L:140:VAL:HG22	2:L:151:LYS:HE3	1.77	0.67
1:A:565:PHE:CE1	1:A:587:PRO:HB3	2.30	0.67
1:B:565:PHE:CE1	1:B:587:PRO:HB3	2.29	0.67
1:C:565:PHE:CE1	1:C:587:PRO:HB3	2.31	0.65
1:D:89:ALA:HB1	1:D:90:PRO:CD	2.26	0.65
1:F:89:ALA:HB1	1:F:90:PRO:CD	2.26	0.65
1:C:89:ALA:HB1	1:C:90:PRO:CD	2.26	0.65
1:E:565:PHE:CE1	1:E:587:PRO:HB3	2.30	0.65
1:B:89:ALA:HB1	1:B:90:PRO:CD	2.27	0.65
1:E:89:ALA:HB1	1:E:90:PRO:CD	2.26	0.65
1:D:427:LEU:O	1:D:431:ILE:HG23	1.98	0.64
1:A:427:LEU:O	1:A:431:ILE:HG23	1.98	0.64
1:A:89:ALA:HB1	1:A:90:PRO:CD	2.27	0.64
1:B:427:LEU:O	1:B:431:ILE:HG23	1.98	0.63
1:C:427:LEU:O	1:C:431:ILE:HG23	1.98	0.63
1:F:427:LEU:O	1:F:431:ILE:HG23	1.98	0.63
1:E:427:LEU:O	1:E:431:ILE:HG23	1.98	0.63
2:G:158:THR:HG22	2:G:196:THR:CG2	2.30	0.61
1:A:89:ALA:HB1	1:A:90:PRO:HD2	1.83	0.60
1:B:89:ALA:HB1	1:B:90:PRO:HD2	1.83	0.60
1:E:392:GLU:HA	1:E:395:ALA:HB2	1.83	0.60
1:A:392:GLU:HA	1:A:395:ALA:HB2	1.84	0.60
2:L:57:MET:HE3	2:L:92:THR:HG21	1.84	0.60
1:E:89:ALA:HB1	1:E:90:PRO:HD2	1.83	0.60
1:A:272:ASN:HA	1:A:275:ILE:HD12	1.84	0.60
1:A:227:GLN:HG2	2:H:42:ASN:HD21	1.67	0.59
1:C:272:ASN:HA	1:C:275:ILE:HD12	1.84	0.59
1:E:272:ASN:HA	1:E:275:ILE:HD12	1.84	0.59
1:F:272:ASN:HA	1:F:275:ILE:HD12	1.84	0.59
1:C:392:GLU:HA	1:C:395:ALA:HB2	1.84	0.59
1:F:89:ALA:HB1	1:F:90:PRO:HD2	1.84	0.59
1:B:272:ASN:HA	1:B:275:ILE:HD12	1.84	0.59
1:D:89:ALA:HB1	1:D:90:PRO:HD2	1.84	0.58
1:C:89:ALA:HB1	1:C:90:PRO:HD2	1.83	0.58
1:D:272:ASN:HA	1:D:275:ILE:HD12	1.84	0.58
1:D:392:GLU:HA	1:D:395:ALA:HB2	1.85	0.58
1:B:392:GLU:HA	1:B:395:ALA:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:392:GLU:HA	1:F:395:ALA:HB2	1.84	0.58
1:F:226:ASP:HA	2:J:42:ASN:ND2	2.18	0.57
2:J:158:THR:HG22	2:J:196:THR:CG2	2.31	0.57
1:B:129:ALA:O	1:B:132:THR:HG22	2.05	0.57
1:F:129:ALA:O	1:F:132:THR:HG22	2.05	0.56
2:K:57:MET:HE3	2:K:92:THR:HG21	1.87	0.56
1:E:129:ALA:O	1:E:132:THR:HG22	2.05	0.56
1:F:533:VAL:HG23	1:F:553:GLN:CD	2.32	0.55
1:D:129:ALA:O	1:D:132:THR:HG22	2.05	0.55
1:A:129:ALA:O	1:A:132:THR:HG22	2.05	0.55
1:D:533:VAL:HG23	1:D:553:GLN:CD	2.32	0.55
1:A:462:ALA:HB3	1:A:463:PRO:CD	2.37	0.55
2:H:158:THR:HG22	2:H:196:THR:CG2	2.30	0.55
1:C:129:ALA:O	1:C:132:THR:HG22	2.05	0.55
1:B:533:VAL:HG23	1:B:553:GLN:CD	2.32	0.55
1:B:462:ALA:HB3	1:B:463:PRO:CD	2.37	0.54
1:B:598:VAL:HG13	1:B:602:LEU:HD12	1.89	0.54
1:C:462:ALA:HB3	1:C:463:PRO:CD	2.38	0.54
1:C:533:VAL:HG23	1:C:553:GLN:CD	2.33	0.54
1:A:533:VAL:HG23	1:A:553:GLN:CD	2.32	0.54
2:L:158:THR:HG22	2:L:196:THR:CG2	2.30	0.54
1:D:462:ALA:HB3	1:D:463:PRO:CD	2.37	0.54
1:E:462:ALA:HB3	1:E:463:PRO:CD	2.38	0.54
1:E:533:VAL:HG23	1:E:553:GLN:CD	2.33	0.54
1:D:548:ASN:C	1:D:548:ASN:HD22	2.16	0.54
1:F:453:ALA:HB1	1:F:594:ARG:HH22	1.73	0.54
2:I:152:THR:HG22	2:I:202:LYS:O	2.08	0.53
2:G:152:THR:HG22	2:G:202:LYS:O	2.08	0.53
1:D:497:ASP:OD1	1:D:497:ASP:N	2.41	0.53
1:F:462:ALA:HB3	1:F:463:PRO:CD	2.38	0.53
2:L:152:THR:HG22	2:L:202:LYS:O	2.09	0.53
2:J:152:THR:HG22	2:J:202:LYS:O	2.09	0.53
2:K:152:THR:HG22	2:K:202:LYS:O	2.09	0.53
1:A:548:ASN:C	1:A:548:ASN:HD22	2.17	0.53
1:E:548:ASN:C	1:E:548:ASN:HD22	2.17	0.53
1:D:533:VAL:HG21	1:D:565:PHE:CD1	2.44	0.53
1:F:578:LYS:HB2	1:F:592:ASN:HA	1.91	0.53
1:C:548:ASN:C	1:C:548:ASN:HD22	2.17	0.52
2:I:158:THR:HG22	2:I:196:THR:CG2	2.32	0.52
2:G:71:ARG:HD3	2:G:86:THR:HG21	1.91	0.52
1:C:598:VAL:HG13	1:C:602:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:453:ALA:HB1	1:D:594:ARG:HH22	1.74	0.52
1:F:533:VAL:HG21	1:F:565:PHE:CD1	2.44	0.52
2:H:140:VAL:HG12	2:H:140:VAL:O	2.09	0.52
2:I:71:ARG:HD3	2:I:86:THR:HG21	1.91	0.52
2:H:71:ARG:HD3	2:H:86:THR:HG21	1.91	0.52
1:C:578:LYS:HB2	1:C:592:ASN:HA	1.92	0.52
2:H:152:THR:HG22	2:H:202:LYS:O	2.08	0.52
1:A:267:GLY:O	1:A:271:VAL:HG23	2.10	0.52
1:B:267:GLY:O	1:B:271:VAL:HG23	2.10	0.52
1:B:548:ASN:C	1:B:548:ASN:HD22	2.17	0.52
1:C:533:VAL:HG21	1:C:565:PHE:CD1	2.45	0.52
1:D:378:MET:HE2	1:D:380:ILE:HD11	1.91	0.52
2:K:158:THR:HG22	2:K:196:THR:CG2	2.32	0.52
1:D:267:GLY:O	1:D:271:VAL:HG23	2.10	0.51
1:F:548:ASN:C	1:F:548:ASN:HD22	2.17	0.51
1:E:378:MET:HE2	1:E:380:ILE:HD11	1.93	0.51
1:A:58:LEU:O	1:A:58:LEU:HD23	2.10	0.51
1:B:533:VAL:HG21	1:B:565:PHE:CD1	2.45	0.51
1:F:497:ASP:OD1	1:F:497:ASP:N	2.43	0.51
1:A:548:ASN:HD22	1:A:549:GLN:N	2.08	0.51
1:B:245:LEU:CD2	1:B:249:ILE:HD13	2.40	0.51
1:E:578:LYS:HB2	1:E:592:ASN:HA	1.92	0.51
1:C:267:GLY:O	1:C:271:VAL:HG23	2.10	0.51
1:E:267:GLY:O	1:E:271:VAL:HG23	2.10	0.51
1:E:533:VAL:HG21	1:E:565:PHE:CD1	2.45	0.51
1:B:58:LEU:HD23	1:B:58:LEU:O	2.11	0.51
1:B:548:ASN:HD22	1:B:549:GLN:N	2.08	0.51
1:F:598:VAL:HG13	1:F:602:LEU:HD12	1.92	0.51
1:A:245:LEU:CD2	1:A:249:ILE:HD13	2.41	0.51
1:B:378:MET:HE2	1:B:380:ILE:HD11	1.92	0.51
1:D:260:THR:HG23	1:D:286:LYS:HB2	1.93	0.51
1:F:260:THR:HG23	1:F:286:LYS:HB2	1.93	0.51
2:J:71:ARG:HD3	2:J:86:THR:HG21	1.93	0.51
1:A:429:GLU:OE1	2:G:190:LEU:N	2.44	0.51
1:F:378:MET:HE2	1:F:380:ILE:HD11	1.92	0.51
1:F:548:ASN:HD22	1:F:549:GLN:N	2.08	0.51
1:A:598:VAL:HG13	1:A:602:LEU:HD12	1.91	0.50
1:D:487:CYS:O	1:D:521:CYS:HB3	2.11	0.50
1:B:578:LYS:HB2	1:B:592:ASN:HA	1.93	0.50
1:E:453:ALA:HB1	1:E:594:ARG:HH22	1.76	0.50
1:E:497:ASP:N	1:E:497:ASP:OD1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:429:GLU:OE1	2:I:190:LEU:N	2.44	0.50
1:A:533:VAL:HG21	1:A:565:PHE:CD1	2.46	0.50
1:D:245:LEU:CD2	1:D:249:ILE:HD13	2.42	0.50
1:E:548:ASN:HD22	1:E:549:GLN:N	2.08	0.50
1:C:378:MET:HE2	1:C:380:ILE:HD11	1.94	0.50
1:D:578:LYS:HB2	1:D:592:ASN:HA	1.94	0.50
1:E:245:LEU:CD2	1:E:249:ILE:HD13	2.42	0.50
1:F:267:GLY:O	1:F:271:VAL:HG23	2.10	0.50
2:K:71:ARG:HD3	2:K:86:THR:HG21	1.94	0.50
1:A:378:MET:HE2	1:A:380:ILE:HD11	1.93	0.50
1:F:58:LEU:O	1:F:58:LEU:HD23	2.11	0.50
1:A:487:CYS:O	1:A:521:CYS:HB3	2.12	0.50
1:A:497:ASP:OD1	1:A:497:ASP:N	2.44	0.50
1:C:548:ASN:HD22	1:C:549:GLN:N	2.08	0.50
1:D:548:ASN:HD22	1:D:549:GLN:N	2.09	0.50
1:F:245:LEU:CD2	1:F:249:ILE:HD13	2.42	0.50
1:C:453:ALA:HB1	1:C:594:ARG:HH22	1.77	0.50
1:E:540:ASN:ND2	1:E:549:GLN:O	2.45	0.50
2:L:71:ARG:HD3	2:L:86:THR:HG21	1.93	0.50
1:A:540:ASN:ND2	1:A:549:GLN:O	2.45	0.50
1:C:260:THR:HG23	1:C:286:LYS:HB2	1.94	0.49
1:C:540:ASN:ND2	1:C:549:GLN:O	2.45	0.49
1:B:540:ASN:ND2	1:B:549:GLN:O	2.45	0.49
1:E:260:THR:HG23	1:E:286:LYS:HB2	1.94	0.49
1:E:431:ILE:HG22	1:E:600:PHE:CZ	2.48	0.49
1:E:598:VAL:HG13	1:E:602:LEU:HD12	1.94	0.49
1:B:487:CYS:O	1:B:521:CYS:HB3	2.13	0.49
1:D:58:LEU:HD23	1:D:58:LEU:O	2.12	0.49
1:D:540:ASN:ND2	1:D:549:GLN:O	2.45	0.49
1:B:359:VAL:HG23	1:B:360:VAL:HG23	1.94	0.49
1:C:66:VAL:HA	1:C:149:PRO:HA	1.95	0.49
1:C:359:VAL:HG23	1:C:360:VAL:HG23	1.95	0.49
1:D:431:ILE:HG22	1:D:600:PHE:CZ	2.48	0.49
1:E:359:VAL:HG23	1:E:360:VAL:HG23	1.94	0.49
1:F:540:ASN:ND2	1:F:549:GLN:O	2.45	0.49
1:C:245:LEU:CD2	1:C:249:ILE:HD13	2.42	0.49
1:C:487:CYS:O	1:C:521:CYS:HB3	2.13	0.49
1:D:359:VAL:HG23	1:D:360:VAL:HG23	1.94	0.49
1:E:487:CYS:O	1:E:521:CYS:HB3	2.12	0.49
1:A:577:GLU:O	1:A:579:GLN:N	2.46	0.49
1:C:431:ILE:HG22	1:C:600:PHE:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:577:GLU:O	1:E:579:GLN:N	2.46	0.49
1:A:260:THR:HG23	1:A:286:LYS:HB2	1.93	0.49
1:A:359:VAL:HG23	1:A:360:VAL:HG23	1.94	0.49
1:A:578:LYS:HB2	1:A:592:ASN:HA	1.94	0.49
2:K:140:VAL:O	2:K:140:VAL:HG12	2.13	0.49
1:A:431:ILE:HG22	1:A:600:PHE:CZ	2.48	0.48
1:C:497:ASP:OD1	1:C:497:ASP:N	2.45	0.48
1:E:66:VAL:HA	1:E:149:PRO:HA	1.95	0.48
1:B:431:ILE:HG22	1:B:600:PHE:CZ	2.48	0.48
1:E:227:GLN:HA	1:E:227:GLN:HE21	1.78	0.48
1:F:553:GLN:O	1:F:563:ASN:ND2	2.47	0.48
1:B:553:GLN:O	1:B:563:ASN:ND2	2.47	0.48
1:B:577:GLU:O	1:B:579:GLN:N	2.46	0.48
1:D:227:GLN:HA	1:D:227:GLN:HE21	1.78	0.48
1:F:227:GLN:HE21	1:F:227:GLN:HA	1.77	0.48
1:B:66:VAL:HA	1:B:149:PRO:HA	1.96	0.48
1:E:553:GLN:O	1:E:563:ASN:ND2	2.46	0.48
2:H:205:ARG:O	2:H:206:PRO:C	2.57	0.48
1:A:553:GLN:O	1:A:563:ASN:ND2	2.47	0.48
2:K:205:ARG:O	2:K:206:PRO:C	2.57	0.48
1:A:66:VAL:HA	1:A:149:PRO:HA	1.96	0.48
1:B:497:ASP:N	1:B:497:ASP:OD1	2.47	0.48
1:F:431:ILE:HG22	1:F:600:PHE:CZ	2.48	0.48
1:F:66:VAL:HA	1:F:149:PRO:HA	1.95	0.48
1:F:359:VAL:HG23	1:F:360:VAL:HG23	1.94	0.48
2:L:140:VAL:HG12	2:L:140:VAL:O	2.12	0.48
1:B:260:THR:HG23	1:B:286:LYS:HB2	1.94	0.48
1:D:553:GLN:O	1:D:563:ASN:ND2	2.46	0.48
1:D:592:ASN:HB3	1:D:595:ALA:HB2	1.96	0.48
1:D:598:VAL:HG13	1:D:602:LEU:HD12	1.94	0.48
1:A:453:ALA:HB1	1:A:594:ARG:HH22	1.79	0.48
1:D:66:VAL:HA	1:D:149:PRO:HA	1.95	0.48
1:F:577:GLU:O	1:F:579:GLN:N	2.46	0.47
1:A:227:GLN:HE21	1:A:227:GLN:HA	1.79	0.47
1:C:227:GLN:HA	1:C:227:GLN:HE21	1.78	0.47
1:C:362:ASP:OD1	2:L:123:ARG:NH2	2.48	0.47
1:C:530:LEU:HA	1:C:533:VAL:HG12	1.96	0.47
1:F:487:CYS:O	1:F:521:CYS:HB3	2.13	0.47
2:J:205:ARG:O	2:J:206:PRO:C	2.57	0.47
2:G:140:VAL:HG12	2:G:140:VAL:O	2.14	0.47
1:C:553:GLN:O	1:C:563:ASN:ND2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:577:GLU:O	1:D:579:GLN:N	2.46	0.47
1:E:248:ASN:O	1:E:250:ALA:N	2.48	0.47
2:I:205:ARG:O	2:I:206:PRO:C	2.57	0.47
1:B:248:ASN:O	1:B:250:ALA:N	2.48	0.47
1:E:58:LEU:HD23	1:E:58:LEU:O	2.14	0.47
2:G:205:ARG:O	2:G:206:PRO:C	2.57	0.47
1:B:227:GLN:HE21	1:B:227:GLN:HA	1.80	0.47
1:C:577:GLU:O	1:C:579:GLN:N	2.46	0.47
1:D:248:ASN:O	1:D:250:ALA:N	2.48	0.47
1:F:248:ASN:O	1:F:250:ALA:N	2.48	0.47
1:F:597:LYS:O	1:F:598:VAL:C	2.58	0.47
1:B:107:PRO:HB2	1:B:338:VAL:HG11	1.97	0.47
1:C:248:ASN:O	1:C:250:ALA:N	2.48	0.47
1:E:530:LEU:HA	1:E:533:VAL:HG12	1.97	0.47
1:B:453:ALA:HB1	1:B:594:ARG:HH22	1.79	0.47
1:B:597:LYS:O	1:B:598:VAL:C	2.58	0.47
2:L:205:ARG:O	2:L:206:PRO:C	2.57	0.47
1:A:592:ASN:HB3	1:A:595:ALA:HB2	1.96	0.46
1:D:447:ARG:O	1:D:448:ARG:C	2.58	0.46
1:D:597:LYS:O	1:D:598:VAL:C	2.58	0.46
1:E:528:VAL:O	1:E:529:MET:C	2.58	0.46
1:A:426:VAL:O	1:A:430:THR:HG22	2.15	0.46
1:B:530:LEU:HA	1:B:533:VAL:HG12	1.97	0.46
1:C:462:ALA:O	1:C:463:PRO:C	2.58	0.46
1:C:58:LEU:HD23	1:C:58:LEU:O	2.15	0.46
1:D:528:VAL:O	1:D:529:MET:C	2.58	0.46
1:A:248:ASN:O	1:A:250:ALA:N	2.48	0.46
1:E:597:LYS:O	1:E:598:VAL:C	2.58	0.46
1:F:528:VAL:O	1:F:529:MET:C	2.58	0.46
1:B:426:VAL:O	1:B:430:THR:HG22	2.16	0.46
1:C:528:VAL:O	1:C:529:MET:C	2.58	0.46
2:J:140:VAL:HG12	2:J:140:VAL:O	2.15	0.46
1:C:597:LYS:O	1:C:598:VAL:C	2.58	0.46
1:D:383:ASN:OD1	1:D:383:ASN:N	2.49	0.46
1:C:383:ASN:N	1:C:383:ASN:OD1	2.49	0.46
1:C:426:VAL:O	1:C:430:THR:HG22	2.16	0.46
1:D:462:ALA:O	1:D:463:PRO:C	2.58	0.46
1:F:426:VAL:O	1:F:430:THR:HG22	2.16	0.46
1:A:530:LEU:HA	1:A:533:VAL:HG12	1.97	0.46
1:C:447:ARG:O	1:C:448:ARG:C	2.59	0.46
1:E:107:PRO:HB2	1:E:338:VAL:HG11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:510:VAL:N	1:E:511:PRO:CD	2.79	0.46
1:B:510:VAL:N	1:B:511:PRO:CD	2.80	0.45
1:C:510:VAL:N	1:C:511:PRO:CD	2.79	0.45
1:D:426:VAL:O	1:D:430:THR:HG22	2.16	0.45
1:D:533:VAL:HG23	1:D:553:GLN:NE2	2.31	0.45
1:C:533:VAL:HG23	1:C:553:GLN:NE2	2.32	0.45
1:E:383:ASN:OD1	1:E:383:ASN:N	2.49	0.45
2:I:140:VAL:HG12	2:I:140:VAL:O	2.16	0.45
1:D:530:LEU:HA	1:D:533:VAL:HG12	1.98	0.45
1:F:447:ARG:O	1:F:448:ARG:C	2.59	0.45
1:A:462:ALA:O	1:A:463:PRO:C	2.59	0.45
1:B:528:VAL:O	1:B:529:MET:C	2.58	0.45
1:E:533:VAL:HG23	1:E:553:GLN:NE2	2.32	0.45
1:F:462:ALA:O	1:F:463:PRO:C	2.58	0.45
1:F:565:PHE:CE1	1:F:587:PRO:CB	2.99	0.45
1:B:429:GLU:OE1	2:H:190:LEU:N	2.50	0.45
1:D:565:PHE:CE1	1:D:587:PRO:CB	2.99	0.45
1:F:530:LEU:HA	1:F:533:VAL:HG12	1.98	0.45
1:A:528:VAL:O	1:A:529:MET:C	2.58	0.45
1:A:597:LYS:O	1:A:598:VAL:C	2.58	0.45
1:B:533:VAL:HG23	1:B:553:GLN:NE2	2.32	0.45
1:E:426:VAL:O	1:E:430:THR:HG22	2.16	0.45
1:E:447:ARG:O	1:E:448:ARG:C	2.58	0.45
1:E:462:ALA:O	1:E:463:PRO:C	2.58	0.45
1:F:510:VAL:N	1:F:511:PRO:CD	2.80	0.45
1:F:592:ASN:HB3	1:F:595:ALA:HB2	1.99	0.45
1:C:382:VAL:O	1:C:482:THR:HA	2.17	0.45
1:F:189:MET:C	1:F:216:LEU:HD23	2.42	0.45
2:L:136:VAL:O	2:L:137:HIS:HB2	2.17	0.45
1:A:510:VAL:N	1:A:511:PRO:CD	2.80	0.45
1:F:533:VAL:HG23	1:F:553:GLN:NE2	2.31	0.45
1:B:592:ASN:HB3	1:B:595:ALA:HB2	1.98	0.44
1:C:189:MET:C	1:C:216:LEU:HD23	2.42	0.44
1:E:189:MET:C	1:E:216:LEU:HD23	2.42	0.44
1:F:424:LYS:O	1:F:427:LEU:N	2.51	0.44
1:C:424:LYS:O	1:C:427:LEU:N	2.51	0.44
1:D:382:VAL:O	1:D:482:THR:HA	2.18	0.44
1:D:510:VAL:N	1:D:511:PRO:CD	2.80	0.44
1:B:382:VAL:O	1:B:482:THR:HA	2.17	0.44
1:B:447:ARG:O	1:B:448:ARG:C	2.58	0.44
1:E:382:VAL:O	1:E:482:THR:HA	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:592:ASN:HB3	1:E:595:ALA:HB2	2.00	0.44
1:B:581:LEU:CD2	1:B:583:ILE:HD13	2.48	0.44
1:D:189:MET:C	1:D:216:LEU:HD23	2.43	0.44
1:F:107:PRO:HB2	1:F:338:VAL:HG11	1.98	0.44
1:B:189:MET:C	1:B:216:LEU:HD23	2.42	0.44
1:F:368:MET:HE2	1:F:471:HIS:NE2	2.33	0.44
1:F:383:ASN:N	1:F:383:ASN:OD1	2.49	0.44
1:A:382:VAL:O	1:A:482:THR:HA	2.18	0.43
1:A:383:ASN:OD1	1:A:383:ASN:N	2.49	0.43
1:A:447:ARG:O	1:A:448:ARG:C	2.59	0.43
1:A:533:VAL:HG23	1:A:553:GLN:NE2	2.33	0.43
1:E:368:MET:HE2	1:E:471:HIS:NE2	2.33	0.43
1:B:179:VAL:O	1:B:260:THR:N	2.51	0.43
1:B:424:LYS:O	1:B:427:LEU:N	2.51	0.43
1:B:462:ALA:O	1:B:463:PRO:C	2.59	0.43
1:C:63:LEU:HA	1:C:154:PRO:CD	2.49	0.43
1:D:107:PRO:HB2	1:D:338:VAL:HG11	1.99	0.43
1:A:179:VAL:O	1:A:260:THR:N	2.51	0.43
1:A:368:MET:HE2	1:A:471:HIS:NE2	2.33	0.43
1:B:383:ASN:OD1	1:B:383:ASN:N	2.49	0.43
1:D:368:MET:HE2	1:D:471:HIS:NE2	2.33	0.43
1:A:424:LYS:O	1:A:427:LEU:N	2.51	0.43
1:D:424:LYS:O	1:D:427:LEU:N	2.51	0.43
1:F:382:VAL:O	1:F:482:THR:HA	2.17	0.43
1:F:382:VAL:HG11	1:F:461:VAL:HG22	2.00	0.43
1:A:107:PRO:HB2	1:A:338:VAL:HG11	2.00	0.43
1:A:189:MET:C	1:A:216:LEU:HD23	2.43	0.43
1:B:368:MET:HE2	1:B:471:HIS:NE2	2.33	0.43
1:E:424:LYS:O	1:E:427:LEU:N	2.51	0.43
2:I:136:VAL:O	2:I:137:HIS:HB2	2.19	0.43
1:E:63:LEU:HA	1:E:154:PRO:CD	2.48	0.43
1:F:51:VAL:HG12	1:F:52:ARG:N	2.33	0.43
1:B:243:ARG:O	1:B:247:GLU:N	2.52	0.43
1:A:581:LEU:CD2	1:A:583:ILE:HD13	2.49	0.42
1:C:107:PRO:HB2	1:C:338:VAL:HG11	2.00	0.42
1:D:382:VAL:HG11	1:D:461:VAL:HG22	2.00	0.42
1:A:243:ARG:O	1:A:247:GLU:N	2.52	0.42
1:C:179:VAL:O	1:C:260:THR:N	2.51	0.42
1:E:243:ARG:O	1:E:247:GLU:N	2.52	0.42
1:E:245:LEU:O	1:E:246:SER:C	2.63	0.42
1:E:482:THR:HG21	1:E:593:TYR:CE1	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:581:LEU:CD2	1:F:583:ILE:HD13	2.48	0.42
1:F:243:ARG:O	1:F:247:GLU:N	2.52	0.42
1:A:245:LEU:O	1:A:246:SER:C	2.63	0.42
1:E:382:VAL:HG11	1:E:461:VAL:HG22	2.01	0.42
1:E:565:PHE:CE1	1:E:587:PRO:CB	3.01	0.42
1:B:245:LEU:O	1:B:246:SER:C	2.62	0.42
1:C:245:LEU:O	1:C:246:SER:C	2.63	0.42
1:B:290:GLN:OE1	1:B:507:VAL:HG21	2.19	0.42
1:B:593:TYR:CE2	1:B:594:ARG:HG3	2.55	0.42
1:D:593:TYR:CE2	1:D:594:ARG:HG3	2.54	0.42
1:A:93:TRP:HB2	1:A:97:ARG:HD2	2.02	0.42
1:B:482:THR:HG21	1:B:593:TYR:CE1	2.55	0.42
1:C:243:ARG:O	1:C:247:GLU:N	2.52	0.42
1:C:565:PHE:CE1	1:C:587:PRO:CB	3.02	0.42
1:D:245:LEU:O	1:D:246:SER:C	2.63	0.42
1:A:482:THR:HG21	1:A:593:TYR:CE1	2.55	0.42
1:C:368:MET:HE2	1:C:471:HIS:NE2	2.35	0.42
1:C:482:THR:HG21	1:C:593:TYR:CE1	2.54	0.42
1:E:581:LEU:CD2	1:E:583:ILE:HD13	2.49	0.42
2:H:168:ILE:HB	2:H:215:GLN:HB3	2.02	0.42
1:A:593:TYR:CE2	1:A:594:ARG:HG3	2.54	0.42
1:D:243:ARG:O	1:D:247:GLU:N	2.52	0.42
1:D:431:ILE:HG22	1:D:600:PHE:CE2	2.55	0.42
1:F:483:PHE:HA	1:F:583:ILE:HB	2.02	0.42
1:A:82:ARG:NE	1:A:88:GLU:OE2	2.49	0.42
2:G:136:VAL:O	2:G:137:HIS:HB2	2.20	0.42
1:B:63:LEU:HA	1:B:154:PRO:CD	2.49	0.42
1:B:565:PHE:CE1	1:B:587:PRO:CB	3.00	0.42
1:D:63:LEU:HA	1:D:154:PRO:CD	2.50	0.42
1:E:290:GLN:OE1	1:E:507:VAL:HG21	2.19	0.42
1:F:179:VAL:O	1:F:260:THR:N	2.51	0.42
1:F:453:ALA:O	1:F:454:LEU:C	2.63	0.42
1:A:290:GLN:OE1	1:A:507:VAL:HG21	2.20	0.41
1:D:222:LEU:HD11	1:D:308:THR:HG23	2.02	0.41
1:A:63:LEU:HA	1:A:154:PRO:CD	2.50	0.41
1:A:549:GLN:HB3	1:A:550:PRO:HD2	2.02	0.41
1:D:482:THR:HG21	1:D:593:TYR:CE1	2.55	0.41
1:B:245:LEU:HD22	1:B:249:ILE:HD13	2.02	0.41
1:D:549:GLN:HB3	1:D:550:PRO:HD2	2.02	0.41
2:H:74:LYS:O	2:H:74:LYS:HG2	2.21	0.41
1:B:431:ILE:HG22	1:B:600:PHE:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:592:ASN:HB3	1:C:595:ALA:HB2	2.02	0.41
1:D:581:LEU:CD2	1:D:583:ILE:HD13	2.50	0.41
1:D:598:VAL:HG12	1:D:599:ALA:N	2.36	0.41
1:E:549:GLN:HB3	1:E:550:PRO:HD2	2.02	0.41
1:F:593:TYR:CE2	1:F:594:ARG:HG3	2.55	0.41
1:F:598:VAL:HG12	1:F:599:ALA:N	2.36	0.41
1:A:453:ALA:O	1:A:454:LEU:C	2.64	0.41
1:A:483:PHE:HA	1:A:583:ILE:HB	2.03	0.41
1:C:290:GLN:OE1	1:C:507:VAL:HG21	2.20	0.41
1:E:51:VAL:HG12	1:E:52:ARG:N	2.36	0.41
1:E:593:TYR:CE2	1:E:594:ARG:HG3	2.56	0.41
1:E:598:VAL:HG12	1:E:599:ALA:N	2.36	0.41
1:F:63:LEU:HA	1:F:154:PRO:CD	2.50	0.41
1:F:222:LEU:HD11	1:F:308:THR:HG23	2.01	0.41
1:F:245:LEU:O	1:F:246:SER:C	2.63	0.41
1:F:290:GLN:OE1	1:F:507:VAL:HG21	2.20	0.41
2:G:168:ILE:HB	2:G:215:GLN:HB3	2.03	0.41
1:B:453:ALA:O	1:B:454:LEU:C	2.63	0.41
1:B:483:PHE:HA	1:B:583:ILE:HB	2.03	0.41
1:C:581:LEU:CD2	1:C:583:ILE:HD13	2.50	0.41
1:D:290:GLN:OE1	1:D:507:VAL:HG21	2.21	0.41
1:D:51:VAL:HG12	1:D:52:ARG:N	2.35	0.41
1:D:446:MET:SD	1:D:449:LYS:HE3	2.61	0.41
1:E:82:ARG:NE	1:E:88:GLU:OE2	2.50	0.41
1:F:482:THR:HG21	1:F:593:TYR:CE1	2.55	0.41
1:A:381:GLY:O	1:A:382:VAL:HG23	2.21	0.41
1:C:549:GLN:HB3	1:C:550:PRO:HD2	2.02	0.41
1:F:431:ILE:HG22	1:F:600:PHE:CE2	2.56	0.41
2:K:168:ILE:HB	2:K:215:GLN:HB3	2.03	0.41
1:A:565:PHE:CE1	1:A:587:PRO:CB	3.01	0.41
1:C:457:ASP:OD2	1:C:594:ARG:NH2	2.54	0.41
1:D:179:VAL:O	1:D:260:THR:N	2.51	0.41
2:J:168:ILE:HB	2:J:215:GLN:HB3	2.03	0.41
1:B:288:ILE:HD13	1:B:538:TRP:CD1	2.56	0.41
1:E:93:TRP:HB2	1:E:97:ARG:HD2	2.02	0.41
1:E:453:ALA:O	1:E:454:LEU:C	2.63	0.41
1:F:180:MET:HA	1:F:260:THR:O	2.21	0.41
1:A:51:VAL:HG12	1:A:52:ARG:N	2.36	0.40
1:A:387:GLY:O	1:A:388:LEU:C	2.64	0.40
1:B:412:ASN:OD1	2:H:152:THR:HG21	2.21	0.40
1:B:598:VAL:HG12	1:B:599:ALA:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:453:ALA:O	1:C:454:LEU:C	2.63	0.40
1:D:96:VAL:HG13	1:D:96:VAL:O	2.22	0.40
1:D:262:PHE:CB	1:D:288:ILE:HB	2.51	0.40
1:F:549:GLN:HB3	1:F:550:PRO:HD2	2.03	0.40
1:E:483:PHE:HA	1:E:583:ILE:HB	2.02	0.40
1:B:378:MET:SD	1:B:471:HIS:CG	3.14	0.40
1:D:483:PHE:HA	1:D:583:ILE:HB	2.03	0.40
2:K:171:ARG:HD3	2:K:212:TYR:CE1	2.56	0.40
1:A:378:MET:SD	1:A:471:HIS:CG	3.14	0.40
1:C:382:VAL:HG11	1:C:461:VAL:HG22	2.02	0.40
1:E:179:VAL:O	1:E:260:THR:N	2.51	0.40
1:A:180:MET:HA	1:A:260:THR:O	2.21	0.40
1:A:201:LEU:HA	1:A:535:MET:HE3	2.04	0.40
1:A:262:PHE:CB	1:A:288:ILE:HB	2.52	0.40
1:B:549:GLN:HB3	1:B:550:PRO:HD2	2.04	0.40
1:C:412:ASN:OD1	2:K:152:THR:HG21	2.22	0.40
1:E:457:ASP:OD2	1:E:594:ARG:NH2	2.55	0.40
1:F:457:ASP:OD2	1:F:594:ARG:NH2	2.54	0.40
2:H:136:VAL:O	2:H:137:HIS:HB2	2.21	0.40

All (3) 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)
1:B:95:GLY:CA	1:C:153:GLY:O[1_655]	1.81	0.39
1:A:95:GLY:CA	1:E:153:GLY:O[1_456]	2.01	0.19
1:B:51:VAL:N	1:C:152:ASP:OD1[1_655]	2.13	0.07

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	515/582 (88%)	433 (84%)	72 (14%)	10 (2%)	6	34
1	B	515/582 (88%)	435 (84%)	70 (14%)	10 (2%)	6	34
1	C	515/582 (88%)	434 (84%)	72 (14%)	9 (2%)	7	36
1	D	515/582 (88%)	434 (84%)	72 (14%)	9 (2%)	7	36
1	E	515/582 (88%)	436 (85%)	70 (14%)	9 (2%)	7	36
1	F	515/582 (88%)	434 (84%)	72 (14%)	9 (2%)	7	36
2	G	172/230 (75%)	144 (84%)	23 (13%)	5 (3%)	3	26
2	H	172/230 (75%)	144 (84%)	23 (13%)	5 (3%)	3	26
2	I	172/230 (75%)	145 (84%)	23 (13%)	4 (2%)	5	30
2	J	172/230 (75%)	143 (83%)	25 (14%)	4 (2%)	5	30
2	K	172/230 (75%)	145 (84%)	23 (13%)	4 (2%)	5	30
2	L	172/230 (75%)	143 (83%)	25 (14%)	4 (2%)	5	30
All	All	4122/4872 (85%)	3470 (84%)	570 (14%)	82 (2%)	6	33

All (82) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	550	PRO
1	B	550	PRO
1	C	550	PRO
1	D	550	PRO
1	E	550	PRO
1	F	550	PRO
1	A	115	PRO
1	A	576	LYS
2	G	86	THR
1	B	115	PRO
1	B	522	ASN
1	B	576	LYS
1	C	115	PRO
1	C	522	ASN
1	C	576	LYS
1	D	115	PRO
1	D	522	ASN
1	D	576	LYS
1	E	115	PRO
1	E	522	ASN
1	E	576	LYS
1	F	115	PRO

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Mol	Chain	Res	Type
1	F	522	ASN
1	F	576	LYS
2	H	86	THR
2	I	86	THR
2	J	86	THR
2	K	86	THR
2	L	86	THR
1	A	249	ILE
1	A	522	ASN
1	B	249	ILE
1	C	249	ILE
1	D	249	ILE
1	E	249	ILE
1	F	249	ILE
1	A	281	GLU
2	G	204	LEU
1	D	281	GLU
1	E	281	GLU
1	F	281	GLU
2	H	204	LEU
2	I	204	LEU
2	K	204	LEU
2	L	204	LEU
2	G	189	PRO
2	G	206	PRO
1	B	281	GLU
1	C	281	GLU
2	H	189	PRO
2	I	189	PRO
2	I	206	PRO
2	J	189	PRO
2	J	204	LEU
2	K	189	PRO
2	L	189	PRO
2	J	206	PRO
2	K	206	PRO
2	L	206	PRO
2	H	206	PRO
1	F	344	PRO
1	B	96	VAL
1	B	344	PRO
1	C	344	PRO

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Mol	Chain	Res	Type
1	D	344	PRO
1	F	96	VAL
1	A	96	VAL
1	A	344	PRO
1	A	598	VAL
2	G	136	VAL
1	B	598	VAL
1	C	598	VAL
1	D	598	VAL
1	E	96	VAL
1	E	344	PRO
1	E	598	VAL
1	F	598	VAL
2	H	136	VAL
1	D	96	VAL
1	B	421	PRO
1	A	421	PRO
1	C	421	PRO

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	439/487 (90%)	398 (91%)	41 (9%)	8	28
1	B	439/487 (90%)	400 (91%)	39 (9%)	9	30
1	C	439/487 (90%)	401 (91%)	38 (9%)	9	31
1	D	439/487 (90%)	403 (92%)	36 (8%)	10	33
1	E	439/487 (90%)	401 (91%)	38 (9%)	9	31
1	F	439/487 (90%)	402 (92%)	37 (8%)	10	32
2	G	163/202 (81%)	144 (88%)	19 (12%)	5	21
2	H	163/202 (81%)	146 (90%)	17 (10%)	7	24
2	I	163/202 (81%)	146 (90%)	17 (10%)	7	24
2	J	163/202 (81%)	146 (90%)	17 (10%)	7	24

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	163/202 (81%)	145 (89%)	18 (11%)	6	23
2	L	163/202 (81%)	148 (91%)	15 (9%)	8	29
All	All	3612/4134 (87%)	3280 (91%)	332 (9%)	8	29

All (332) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	62	ILE
1	A	72	VAL
1	A	109	ASN
1	A	115	PRO
1	A	125	ASP
1	A	136	ASN
1	A	176	LYS
1	A	189	MET
1	A	212	LEU
1	A	227	GLN
1	A	242	LEU
1	A	280	SER
1	A	281	GLU
1	A	285	GLN
1	A	296	SER
1	A	341	ASP
1	A	342	VAL
1	A	358	ASP
1	A	382	VAL
1	A	383	ASN
1	A	398	GLU
1	A	401	VAL
1	A	402	SER
1	A	415	ASP
1	A	420	TYR
1	A	427	LEU
1	A	436	THR
1	A	452	LEU
1	A	465	VAL
1	A	485	HIS
1	A	486	HIS
1	A	488	GLN
1	A	497	ASP

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Mol	Chain	Res	Type
1	A	518	LEU
1	A	548	ASN
1	A	549	GLN
1	A	576	LYS
1	A	596	ASN
1	A	598	VAL
1	A	604	LEU
2	G	36	CYS
2	G	49	THR
2	G	63	THR
2	G	73	THR
2	G	86	THR
2	G	88	VAL
2	G	89	PHE
2	G	97	ARG
2	G	107	TYR
2	G	136	VAL
2	G	139	THR
2	G	176	LEU
2	G	184	VAL
2	G	186	ILE
2	G	197	LYS
2	G	213	THR
2	G	232	ARG
2	G	233	LEU
2	G	234	THR
1	B	62	ILE
1	B	72	VAL
1	B	109	ASN
1	B	115	PRO
1	B	125	ASP
1	B	176	LYS
1	B	189	MET
1	B	212	LEU
1	B	219	LEU
1	B	227	GLN
1	B	242	LEU
1	B	280	SER
1	B	281	GLU
1	B	285	GLN
1	B	296	SER
1	B	341	ASP

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Mol	Chain	Res	Type
1	B	342	VAL
1	B	343	GLN
1	B	358	ASP
1	B	383	ASN
1	B	398	GLU
1	B	401	VAL
1	B	420	TYR
1	B	436	THR
1	B	441	ARG
1	B	446	MET
1	B	452	LEU
1	B	465	VAL
1	B	485	HIS
1	B	486	HIS
1	B	488	GLN
1	B	497	ASP
1	B	518	LEU
1	B	548	ASN
1	B	549	GLN
1	B	576	LYS
1	B	596	ASN
1	B	598	VAL
1	B	604	LEU
1	C	52	ARG
1	C	62	ILE
1	C	72	VAL
1	C	109	ASN
1	C	111	HIS
1	C	125	ASP
1	C	176	LYS
1	C	212	LEU
1	C	219	LEU
1	C	227	GLN
1	C	242	LEU
1	C	280	SER
1	C	285	GLN
1	C	296	SER
1	C	341	ASP
1	C	342	VAL
1	C	358	ASP
1	C	383	ASN
1	C	398	GLU

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Mol	Chain	Res	Type
1	C	401	VAL
1	C	420	TYR
1	C	427	LEU
1	C	436	THR
1	C	446	MET
1	C	452	LEU
1	C	465	VAL
1	C	485	HIS
1	C	486	HIS
1	C	488	GLN
1	C	497	ASP
1	C	513	VAL
1	C	518	LEU
1	C	548	ASN
1	C	549	GLN
1	C	576	LYS
1	C	596	ASN
1	C	598	VAL
1	C	604	LEU
1	D	52	ARG
1	D	62	ILE
1	D	72	VAL
1	D	109	ASN
1	D	125	ASP
1	D	189	MET
1	D	212	LEU
1	D	219	LEU
1	D	227	GLN
1	D	242	LEU
1	D	280	SER
1	D	285	GLN
1	D	296	SER
1	D	341	ASP
1	D	342	VAL
1	D	343	GLN
1	D	358	ASP
1	D	383	ASN
1	D	398	GLU
1	D	401	VAL
1	D	420	TYR
1	D	436	THR
1	D	452	LEU

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Mol	Chain	Res	Type
1	D	465	VAL
1	D	485	HIS
1	D	486	HIS
1	D	488	GLN
1	D	497	ASP
1	D	518	LEU
1	D	548	ASN
1	D	549	GLN
1	D	564	ARG
1	D	576	LYS
1	D	596	ASN
1	D	598	VAL
1	D	604	LEU
1	E	52	ARG
1	E	62	ILE
1	E	72	VAL
1	E	109	ASN
1	E	111	HIS
1	E	115	PRO
1	E	125	ASP
1	E	176	LYS
1	E	212	LEU
1	E	219	LEU
1	E	227	GLN
1	E	242	LEU
1	E	280	SER
1	E	285	GLN
1	E	296	SER
1	E	341	ASP
1	E	342	VAL
1	E	358	ASP
1	E	383	ASN
1	E	398	GLU
1	E	401	VAL
1	E	420	TYR
1	E	427	LEU
1	E	436	THR
1	E	446	MET
1	E	452	LEU
1	E	465	VAL
1	E	485	HIS
1	E	486	HIS

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Mol	Chain	Res	Type
1	E	488	GLN
1	E	513	VAL
1	E	518	LEU
1	E	548	ASN
1	E	549	GLN
1	E	576	LYS
1	E	596	ASN
1	E	598	VAL
1	E	604	LEU
1	F	52	ARG
1	F	62	ILE
1	F	72	VAL
1	F	109	ASN
1	F	111	HIS
1	F	125	ASP
1	F	176	LYS
1	F	212	LEU
1	F	219	LEU
1	F	227	GLN
1	F	242	LEU
1	F	280	SER
1	F	285	GLN
1	F	296	SER
1	F	341	ASP
1	F	342	VAL
1	F	358	ASP
1	F	383	ASN
1	F	398	GLU
1	F	420	TYR
1	F	422	GLU
1	F	427	LEU
1	F	436	THR
1	F	446	MET
1	F	452	LEU
1	F	465	VAL
1	F	485	HIS
1	F	486	HIS
1	F	488	GLN
1	F	497	ASP
1	F	518	LEU
1	F	548	ASN
1	F	549	GLN

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Mol	Chain	Res	Type
1	F	576	LYS
1	F	596	ASN
1	F	598	VAL
1	F	604	LEU
2	H	36	CYS
2	H	49	THR
2	H	73	THR
2	H	86	THR
2	H	88	VAL
2	H	97	ARG
2	H	107	TYR
2	H	136	VAL
2	H	139	THR
2	H	166	ARG
2	H	176	LEU
2	H	184	VAL
2	H	186	ILE
2	H	197	LYS
2	H	213	THR
2	H	233	LEU
2	H	234	THR
2	I	36	CYS
2	I	39	LYS
2	I	73	THR
2	I	86	THR
2	I	88	VAL
2	I	107	TYR
2	I	133	MET
2	I	136	VAL
2	I	139	THR
2	I	176	LEU
2	I	184	VAL
2	I	186	ILE
2	I	188	GLU
2	I	197	LYS
2	I	227	LYS
2	I	233	LEU
2	I	234	THR
2	J	36	CYS
2	J	73	THR
2	J	86	THR
2	J	88	VAL

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Mol	Chain	Res	Type
2	J	97	ARG
2	J	107	TYR
2	J	133	MET
2	J	136	VAL
2	J	139	THR
2	J	151	LYS
2	J	176	LEU
2	J	184	VAL
2	J	186	ILE
2	J	197	LYS
2	J	232	ARG
2	J	233	LEU
2	J	234	THR
2	K	36	CYS
2	K	49	THR
2	K	73	THR
2	K	86	THR
2	K	88	VAL
2	K	89	PHE
2	K	97	ARG
2	K	107	TYR
2	K	133	MET
2	K	136	VAL
2	K	139	THR
2	K	151	LYS
2	K	176	LEU
2	K	184	VAL
2	K	186	ILE
2	K	197	LYS
2	K	233	LEU
2	K	234	THR
2	L	36	CYS
2	L	63	THR
2	L	73	THR
2	L	86	THR
2	L	88	VAL
2	L	97	ARG
2	L	107	TYR
2	L	136	VAL
2	L	139	THR
2	L	176	LEU
2	L	184	VAL

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Mol	Chain	Res	Type
2	L	186	ILE
2	L	197	LYS
2	L	233	LEU
2	L	234	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	ASN
1	A	227	GLN
1	A	248	ASN
1	A	458	HIS
1	A	459	GLN
1	A	549	GLN
1	A	563	ASN
1	A	592	ASN
2	G	42	ASN
1	B	126	ASN
1	B	145	ASN
1	B	227	GLN
1	B	248	ASN
1	B	458	HIS
1	B	549	GLN
1	B	563	ASN
1	C	68	GLN
1	C	126	ASN
1	C	145	ASN
1	C	227	GLN
1	C	248	ASN
1	C	458	HIS
1	C	548	ASN
1	C	592	ASN
1	D	145	ASN
1	D	227	GLN
1	D	248	ASN
1	D	458	HIS
1	D	459	GLN
1	D	549	GLN
1	D	563	ASN
1	E	85	GLN
1	E	145	ASN
1	E	227	GLN

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Mol	Chain	Res	Type
1	E	248	ASN
1	E	303	GLN
1	E	458	HIS
1	E	548	ASN
1	E	563	ASN
1	E	592	ASN
1	F	126	ASN
1	F	145	ASN
1	F	227	GLN
1	F	248	ASN
1	F	458	HIS
1	F	548	ASN
1	F	549	GLN
1	F	563	ASN
2	H	42	ASN
2	I	220	ASN
2	J	42	ASN
2	J	59	GLN
2	J	220	ASN
2	K	59	GLN
2	K	220	ASN
2	L	59	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1
1	C	1
1	D	1
1	F	1
1	B	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	246:SER	C	247:GLU	N	2.87
1	C	246:SER	C	247:GLU	N	2.87
1	D	246:SER	C	247:GLU	N	2.87
1	F	246:SER	C	247:GLU	N	2.87
1	B	246:SER	C	247:GLU	N	2.86
1	E	246:SER	C	247:GLU	N	2.86

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	A	527/582 (90%)	0.28	5 (0%) 81 65	42, 77, 133, 178	0
1	B	527/582 (90%)	0.40	9 (1%) 69 52	42, 78, 134, 183	0
1	C	527/582 (90%)	0.56	17 (3%) 50 38	54, 99, 193, 254	0
1	D	527/582 (90%)	0.60	24 (4%) 37 30	69, 126, 215, 262	0
1	E	527/582 (90%)	0.50	15 (2%) 55 41	65, 108, 182, 251	0
1	F	527/582 (90%)	0.71	22 (4%) 40 32	89, 143, 221, 257	0
2	G	184/230 (80%)	0.68	11 (5%) 27 25	68, 94, 118, 130	0
2	H	184/230 (80%)	0.63	8 (4%) 40 32	67, 96, 121, 129	0
2	I	184/230 (80%)	0.92	15 (8%) 17 19	138, 156, 171, 185	0
2	J	184/230 (80%)	0.91	11 (5%) 27 25	122, 139, 159, 181	0
2	K	184/230 (80%)	0.85	13 (7%) 22 21	105, 124, 143, 161	0
2	L	184/230 (80%)	0.69	8 (4%) 40 32	121, 140, 161, 171	0
All	All	4266/4872 (87%)	0.58	158 (3%) 45 35	42, 112, 186, 262	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	238	GLN	4.9
2	H	140	VAL	4.8
1	F	508	PHE	4.7
1	C	190	GLU	4.4
2	G	140	VAL	4.3
1	C	154	PRO	4.1
2	J	25	ALA	3.9
1	C	151	GLU	3.8
1	D	565	PHE	3.7
1	F	565	PHE	3.7
2	G	86	THR	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	154	PRO	3.6
1	D	567	GLU	3.6
1	F	567	GLU	3.6
1	C	340	GLN	3.6
1	B	174	SER	3.5
1	E	151	GLU	3.5
1	F	353	PRO	3.4
1	F	562	PRO	3.4
1	A	94	PRO	3.3
2	I	64	GLY	3.3
2	J	116	VAL	3.3
1	F	564	ARG	3.3
2	H	139	THR	3.3
1	C	254	GLY	3.2
2	L	140	VAL	3.2
1	D	556	LYS	3.2
1	D	564	ARG	3.2
2	J	44	SER	3.1
2	H	86	THR	3.1
1	F	146	LEU	3.1
1	D	562	PRO	3.1
1	D	190	GLU	3.1
2	I	116	VAL	3.0
1	F	265	GLY	3.0
2	G	194	GLY	3.0
2	L	191	TYR	3.0
2	I	140	VAL	3.0
1	E	185	GLY	2.9
2	H	74	LYS	2.9
1	F	145	ASN	2.9
2	L	203	ASN	2.9
1	C	51	VAL	2.9
1	D	93	TRP	2.8
1	D	87	PRO	2.8
1	C	150	THR	2.8
1	B	94	PRO	2.8
2	I	190	LEU	2.7
2	G	139	THR	2.7
1	F	96	VAL	2.7
2	J	38	VAL	2.7
1	B	191	GLY	2.7
2	G	115	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	350	ALA	2.6
2	K	38	VAL	2.6
1	D	145	ASN	2.6
1	C	238	GLN	2.6
2	I	37	VAL	2.6
1	B	93	TRP	2.6
1	A	113	ALA	2.6
1	D	602	LEU	2.5
1	F	331	ARG	2.5
2	K	44	SER	2.5
1	C	311	LEU	2.5
1	B	190	GLU	2.5
2	G	44	SER	2.5
1	D	557	PHE	2.5
1	F	358	ASP	2.5
2	K	140	VAL	2.5
1	D	345	ALA	2.5
2	G	74	LYS	2.5
1	F	90	PRO	2.5
1	C	93	TRP	2.5
1	B	113	ALA	2.5
2	J	29	ILE	2.4
2	H	64	GLY	2.4
1	D	108	GLN	2.4
2	H	195	GLU	2.4
1	E	152	ASP	2.4
1	E	93	TRP	2.4
2	I	169	TRP	2.4
1	F	516	THR	2.4
1	C	96	VAL	2.4
1	F	185	GLY	2.4
2	K	64	GLY	2.4
2	L	86	THR	2.4
1	F	556	LYS	2.4
2	L	74	LYS	2.4
2	G	64	GLY	2.4
2	K	27	ALA	2.4
2	I	215	GLN	2.4
2	L	24	PRO	2.4
1	E	320	GLU	2.4
2	I	91	GLU	2.4
2	K	139	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	244	TRP	2.3
1	D	566	GLU	2.3
2	G	110	ALA	2.3
2	J	30	VAL	2.3
2	G	137	HIS	2.3
1	C	152	ASP	2.3
1	E	191	GLY	2.3
1	D	230	LYS	2.3
1	F	487	CYS	2.3
1	D	154	PRO	2.3
1	E	265	GLY	2.3
2	I	53	GLY	2.3
1	B	52	ARG	2.3
2	L	59	GLN	2.3
2	I	24	PRO	2.2
2	K	24	PRO	2.2
2	K	99	ALA	2.2
1	E	150	THR	2.2
2	K	37	VAL	2.2
1	B	490	GLU	2.2
1	D	555	THR	2.2
1	A	397	SER	2.2
1	D	235	LEU	2.2
1	B	175	GLY	2.2
2	H	87	SER	2.2
1	A	420	TYR	2.2
2	I	203	ASN	2.2
1	F	586	LYS	2.2
2	L	190	LEU	2.2
1	E	96	VAL	2.2
2	G	87	SER	2.2
2	K	74	LYS	2.1
1	F	93	TRP	2.1
2	J	99	ALA	2.1
1	D	563	ASN	2.1
2	I	63	THR	2.1
1	E	238	GLN	2.1
1	A	93	TRP	2.1
1	C	62	ILE	2.1
1	E	338	VAL	2.1
2	J	37	VAL	2.1
1	C	567	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	84	PHE	2.1
2	I	89	PHE	2.1
2	J	68	PRO	2.1
2	J	98	ILE	2.1
1	D	545	GLY	2.1
1	F	230	LYS	2.1
2	K	116	VAL	2.1
2	I	39	LYS	2.1
1	D	73	PRO	2.1
2	K	184	VAL	2.1
1	E	310	LEU	2.0
1	D	442	ASP	2.0
1	D	554	ASP	2.0
1	E	350	ALA	2.0
2	H	194	GLY	2.0
1	C	248	ASN	2.0
2	J	118	ALA	2.0
2	K	35	ALA	2.0
1	E	425	ASP	2.0
1	C	512	MET	2.0
2	I	67	ARG	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.