



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2017 – 10:25 PM EDT

PDB ID : 5V5V  
Title : Complex of NLGN2 with MDGA1 Ig1-Ig2  
Authors : Gangwar, S.P.; Machius, M.; Rudenko, G.  
Deposited on : unknown  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

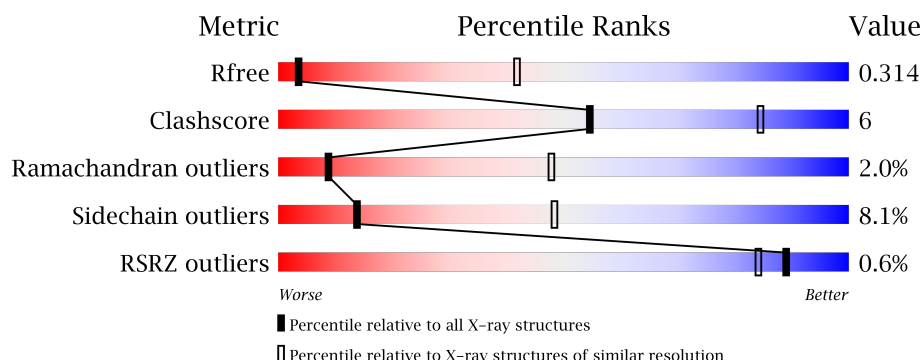
# 1 Overall quality at a glance

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))
$R_{free}$	100719	1156 (4.62-3.60)
Clashscore	112137	1003 (4.58-3.66)
Ramachandran outliers	110173	1012 (4.62-3.62)
Sidechain outliers	110143	1194 (4.62-3.60)
RSRZ outliers	101464	1168 (4.62-3.60)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	
1	B	582	
1	C	582	
1	D	582	
1	E	582	

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	582	
2	G	230	
2	H	230	
2	I	230	
2	J	230	
2	K	230	
2	L	230	

## 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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

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

*Continued on next page...*

*Continued from previous page...*

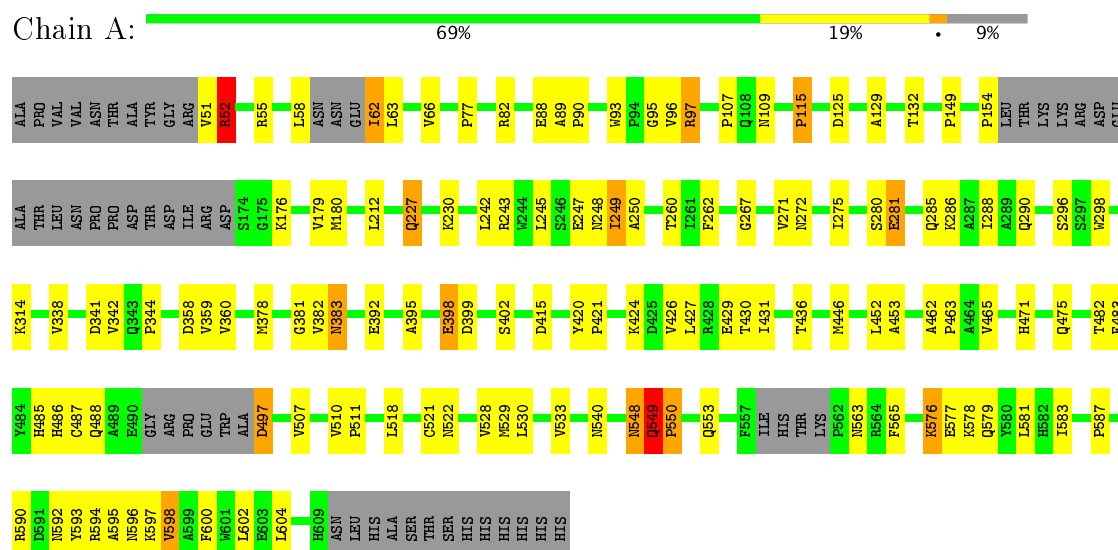
Chain	Residue	Modelled	Actual	Comment	Reference
K	20	VAL	-	expression tag	UNP Q8NFP4
K	21	ASP	-	expression tag	UNP Q8NFP4
K	238	GLY	-	expression tag	UNP Q8NFP4
K	239	SER	-	expression tag	UNP Q8NFP4
K	240	ALA	-	expression tag	UNP Q8NFP4
K	241	SER	-	expression tag	UNP Q8NFP4
K	242	THR	-	expression tag	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



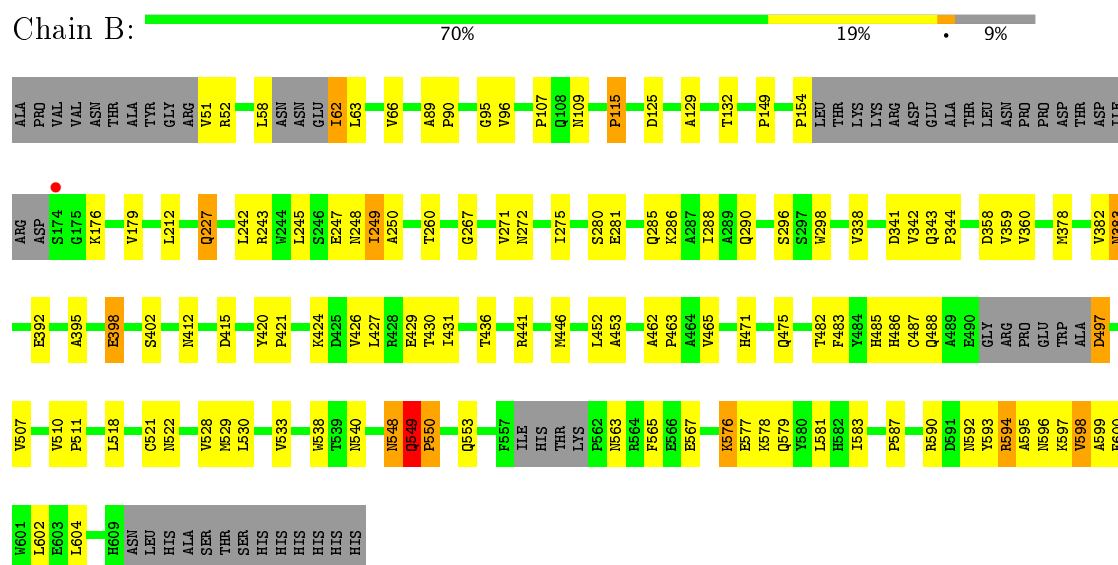
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

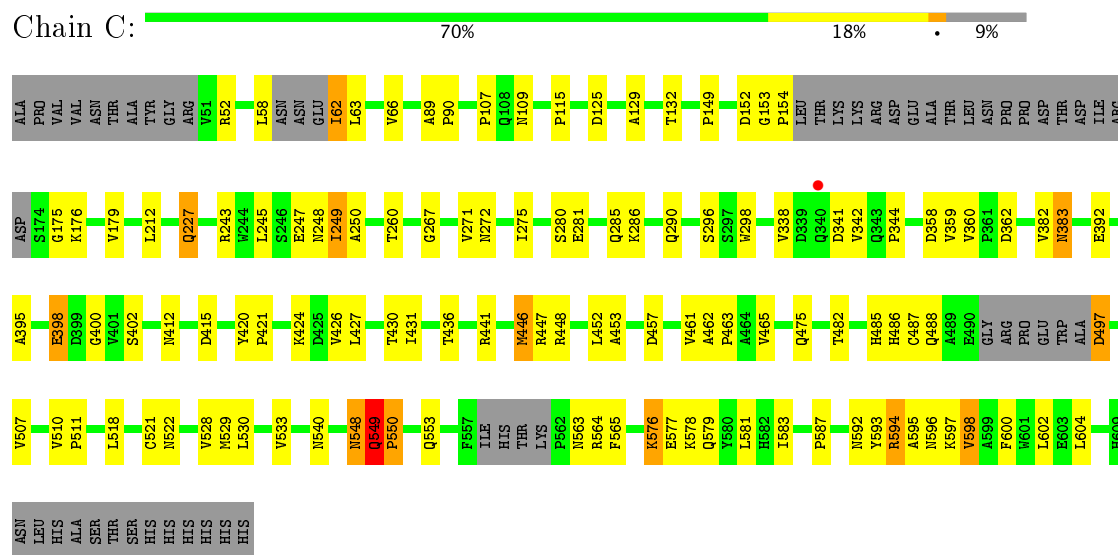
#### • Molecule 1: Neuroligin-2



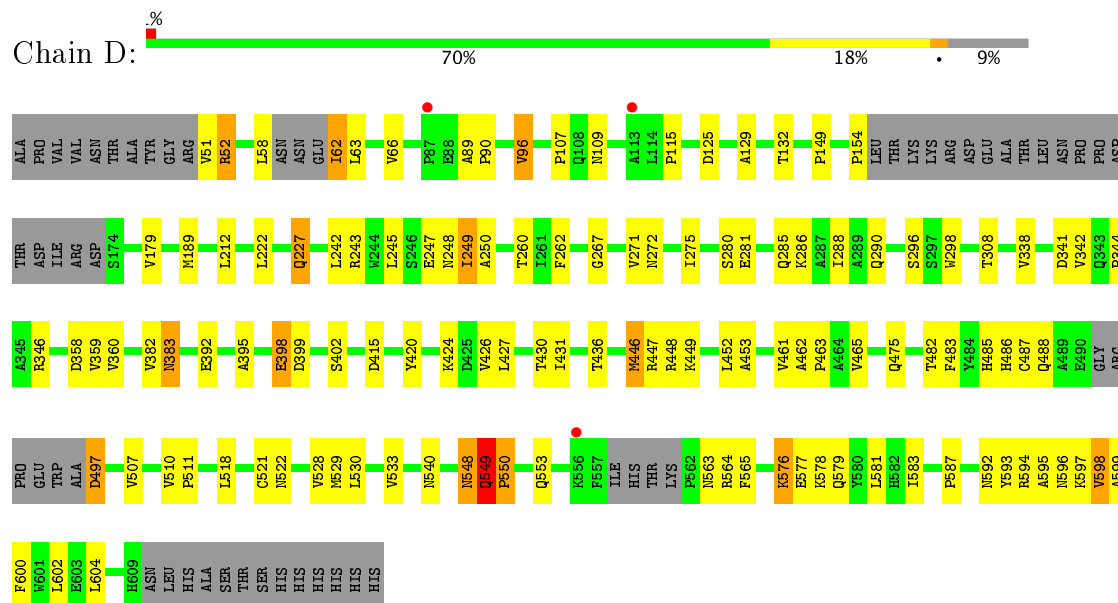
#### • Molecule 1: Neuroligin-2



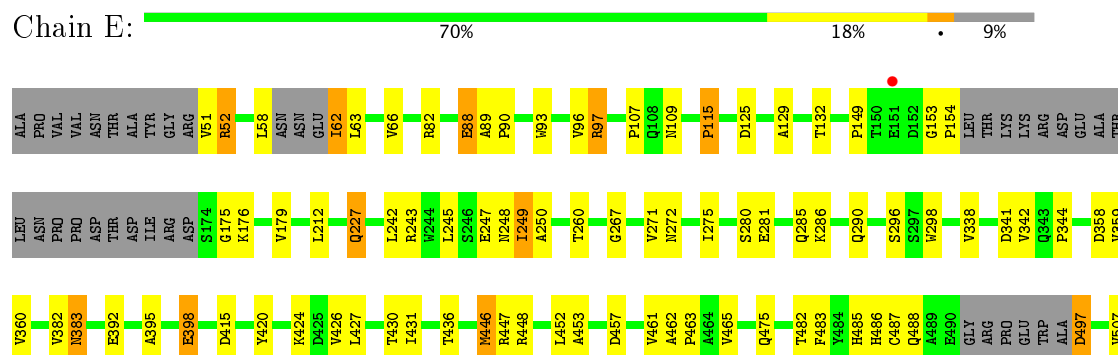
#### • Molecule 1: Neuroligin-2

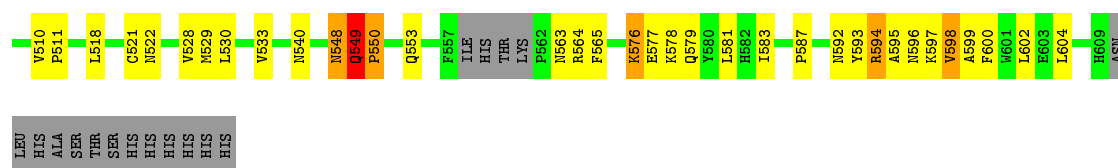


- Molecule 1: Neuroligin-2

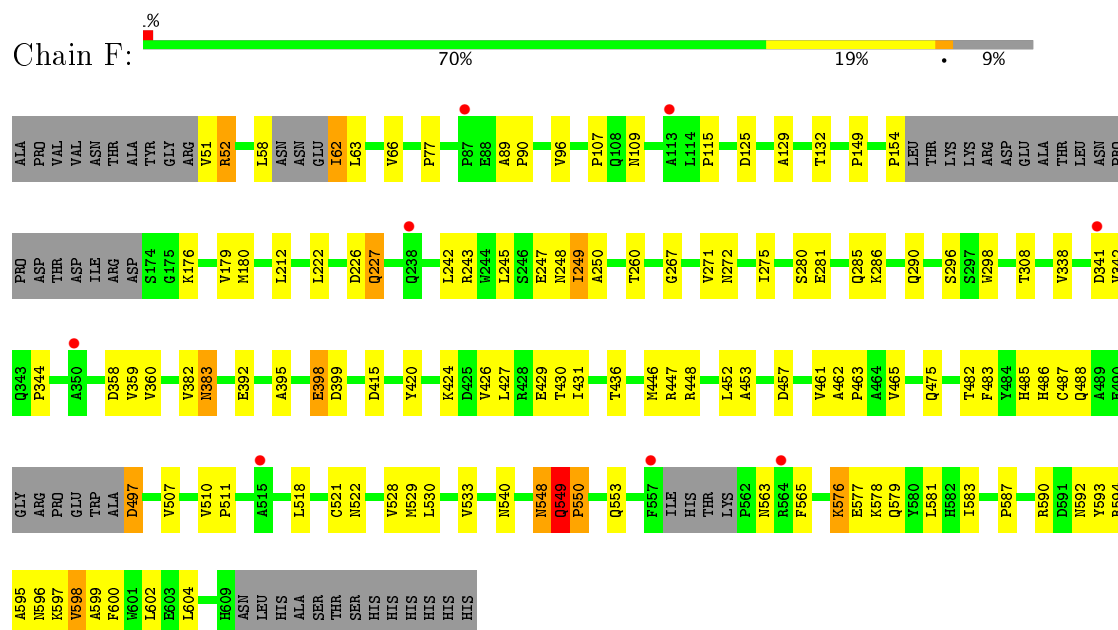


- Molecule 1: Neuroligin-2

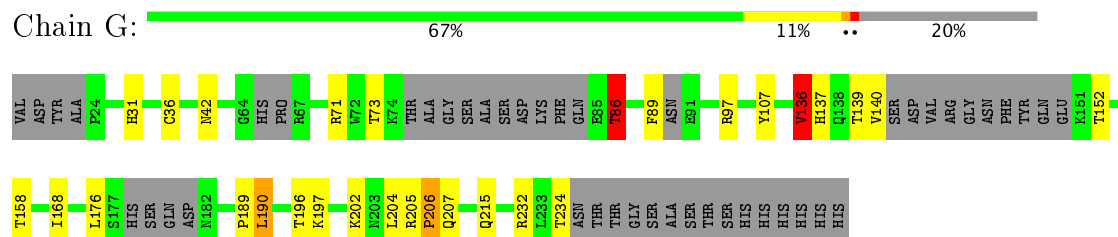




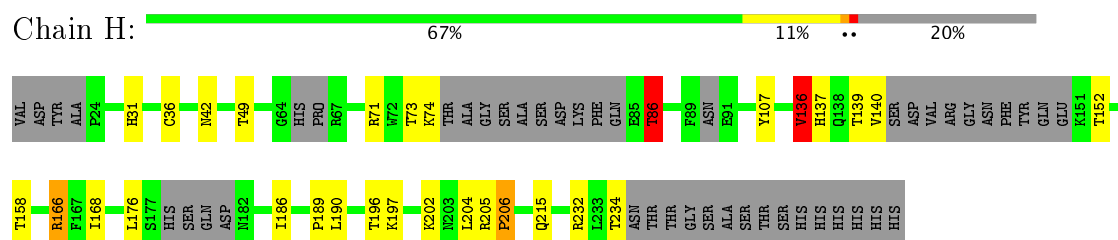
• Molecule 1: Neuroligin-2



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

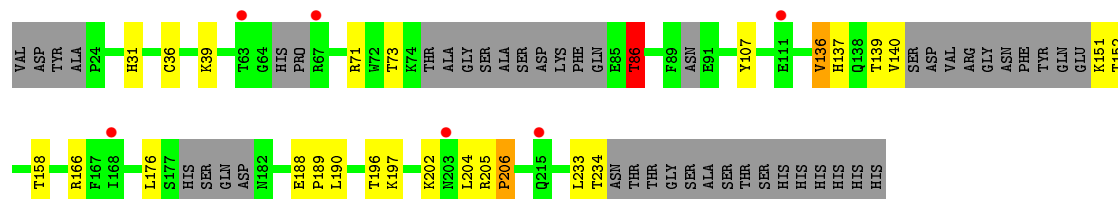


• Molecule 2: MAM domain-containing glycosylphosphatidylinositol anchor protein 1

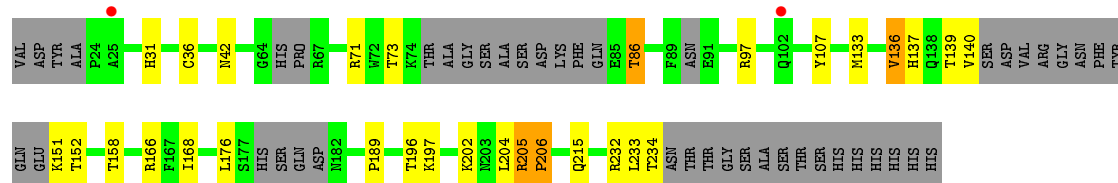


• Molecule 2: MAM domain-containing glycosylphosphatidylinositol anchor protein 1

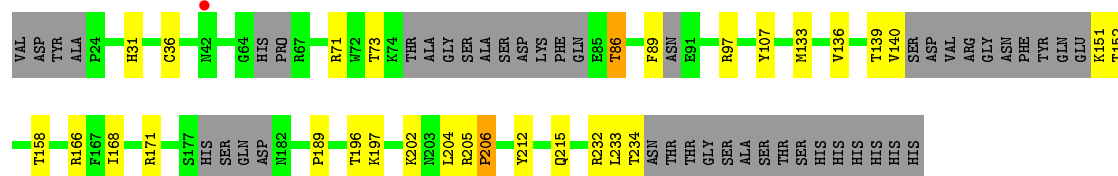




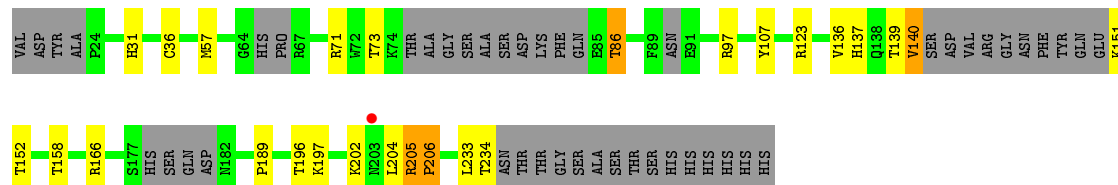
- Molecule 2: MAM domain-containing glycosylphosphatidylinositol anchor protein 1



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



- 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, $\alpha$ , $\beta$ , $\gamma$	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) 81.3 (49.77-4.11)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	2198 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	45.9	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 40.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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	0.61	1/4240 (0.0%)	0.78	7/5769 (0.1%)
1	B	0.62	0/4240	0.80	7/5769 (0.1%)
1	C	0.60	0/4240	0.79	4/5769 (0.1%)
1	D	0.58	0/4240	0.76	3/5769 (0.1%)
1	E	0.58	0/4240	0.78	4/5769 (0.1%)
1	F	0.58	0/4240	0.76	3/5769 (0.1%)
2	G	0.72	0/1481	0.83	1/2001 (0.0%)
2	H	0.72	0/1481	0.83	2/2001 (0.1%)
2	I	0.68	0/1481	0.78	0/2001
2	J	0.69	0/1481	0.81	1/2001 (0.0%)
2	K	0.69	0/1481	0.79	0/2001
2	L	0.69	1/1481 (0.1%)	0.81	2/2001 (0.1%)
All	All	0.62	2/34326 (0.0%)	0.79	34/46620 (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	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 (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	52	ARG	CZ-NH2	5.76	1.40	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	140	VAL	N-CA	5.06	1.56	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	52	ARG	CA-CB-CG	8.87	132.90	113.40
2	H	166	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	B	549	GLN	C-N-CD	-6.11	107.16	120.60
1	E	549	GLN	C-N-CD	-6.07	107.25	120.60
1	D	549	GLN	C-N-CD	-6.04	107.31	120.60
1	C	549	GLN	C-N-CD	-6.03	107.33	120.60
1	A	549	GLN	C-N-CD	-6.01	107.37	120.60
1	F	549	GLN	C-N-CD	-6.00	107.40	120.60
2	J	205	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	E	62	ILE	N-CA-C	5.70	126.39	111.00
1	B	590	ARG	NE-CZ-NH2	-5.65	117.48	120.30
1	A	97	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	E	97	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	C	62	ILE	N-CA-C	5.45	125.72	111.00
2	L	57	MET	CG-SD-CE	5.41	108.85	100.20
1	C	441	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	D	62	ILE	N-CA-C	5.38	125.54	111.00
2	L	205	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	B	62	ILE	N-CA-C	5.38	125.53	111.00
1	A	62	ILE	N-CA-C	5.32	125.36	111.00
1	F	590	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	52	ARG	N-CA-CB	-5.21	101.21	110.60
1	F	62	ILE	N-CA-C	5.16	124.92	111.00
1	A	314	LYS	CD-CE-NZ	5.14	123.52	111.70
1	E	594	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	A	590	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	C	594	ARG	NE-CZ-NH2	-5.11	117.75	120.30
2	G	190	LEU	CA-CB-CG	5.10	127.04	115.30
2	H	166	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	B	567	GLU	OE1-CD-OE2	-5.06	117.22	123.30
1	A	55	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	590	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	594	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	D	346	ARG	NE-CZ-NH1	5.02	122.81	120.30

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
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 [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	4130	0	3975	60	1
1	B	4130	0	3975	58	2
1	C	4130	0	3975	54	2
1	D	4130	0	3975	60	0
1	E	4130	0	3975	58	1
1	F	4130	0	3975	61	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	9	0
2	L	1460	0	1475	9	0
All	All	33540	0	32700	400	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 6.

All (400) 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
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: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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
1:E:129:ALA:O	1:E:132:THR:HG22	2.05	0.56
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: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: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
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: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
1:D:497:ASP:N	1:D:497:ASP:OD1	2.41	0.53
1:F:462:ALA:HB3	1:F:463:PRO:CD	2.38	0.53
2:G:152:THR:HG22	2:G:202:LYS:O	2.08	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:H:140:VAL:O	2:H:140:VAL:HG12	2.09	0.53
2:I:158:THR:HG22	2:I:196:THR:CG2	2.32	0.52
1:C:598:VAL:HG13	1:C:602:LEU:HD12	1.91	0.52
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:G:71:ARG:HD3	2:G:86:THR:HG21	1.91	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:C:533:VAL:HG21	1:C:565:PHE:CD1	2.45	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:A:58:LEU:HD23	1:A:58:LEU:O	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:548:ASN:HD22	1:B:549:GLN:N	2.08	0.51
1:B:58:LEU:O	1:B:58:LEU:HD23	2.11	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: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:548:ASN:HD22	1:F:549:GLN:N	2.08	0.51
1:F:533:VAL:HG23	1:F:553:GLN:CD	2.32	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:578:LYS:HB2	1:B:592:ASN:HA	1.93	0.50
1:D:533:VAL:HG23	1:D:553:GLN:CD	2.32	0.50
1:E:497:ASP:N	1:E:497:ASP:OD1	2.44	0.50
1:E:453:ALA:HB1	1:E:594:ARG:HH22	1.76	0.50
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: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: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:B:533:VAL:HG23	1:B:553:GLN:CD	2.32	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:C:533:VAL:HG23	1:C:553:GLN:CD	2.33	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:A:533:VAL:HG23	1:A:553:GLN:CD	2.32	0.49
1:B:487:CYS:O	1:B:521:CYS:HB3	2.13	0.49
1:D:540:ASN:ND2	1:D:549:GLN:O	2.45	0.49
1:D:58:LEU:HD23	1:D:58:LEU:O	2.12	0.49
1:E:533:VAL:HG23	1:E:553:GLN:CD	2.33	0.49
1:B:359:VAL:HG23	1:B:360:VAL:HG23	1.94	0.49
1:C:359:VAL:HG23	1:C:360:VAL:HG23	1.95	0.49
1:C:66:VAL:HA	1:C:149:PRO:HA	1.95	0.49
1:D:431:ILE:HG22	1:D:600:PHE:CZ	2.48	0.49
1:D:548:ASN:HD22	1:D:548:ASN:C	2.16	0.49
1:E:359:VAL:HG23	1:E:360:VAL:HG23	1.94	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HG12	2:K:140:VAL:O	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:HE21	1:E:227:GLN:HA	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:A:548:ASN:C	1:A:548:ASN:HD22	2.17	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
1:A:553:GLN:O	1:A:563:ASN:ND2	2.47	0.48
1:E:548:ASN:C	1:E:548:ASN:HD22	2.17	0.48
1:A:66:VAL:HA	1:A:149:PRO:HA	1.96	0.48
1:B:497:ASP:OD1	1:B:497:ASP:N	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:O	2:L:140:VAL:HG12	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:C:548:ASN:C	1:C:548:ASN:HD22	2.17	0.47
1:F:577:GLU:O	1:F:579:GLN:N	2.46	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLN:HA	1:A:227:GLN:HE21	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
1:C:553:GLN:O	1:C:563:ASN:ND2	2.47	0.47
1:D:577:GLU:O	1:D:579:GLN:N	2.46	0.47
2:G:140:VAL:O	2:G:140:VAL:HG12	2.14	0.47
1:E:248:ASN:O	1:E:250:ALA:N	2.48	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
1:B:227:GLN:HA	1:B:227:GLN:HE21	1.80	0.47
1:D:248:ASN:O	1:D:250:ALA:N	2.48	0.47
1:B:548:ASN:HD22	1:B:548:ASN:C	2.17	0.47
1:C:577:GLU:O	1:C:579:GLN:N	2.46	0.47
1:F:248:ASN:O	1:F:250:ALA:N	2.48	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:F:548:ASN:HD22	1:F:548:ASN:C	2.17	0.47
1:A:592:ASN:HB3	1:A:595:ALA:HB2	1.96	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:58:LEU:HD23	1:C:58:LEU:O	2.15	0.46
1:A:248:ASN:O	1:A:250:ALA:N	2.48	0.46
1:B:426:VAL:O	1:B:430:THR:HG22	2.16	0.46
2:J:140:VAL:HG12	2:J:140:VAL:O	2.15	0.46
1:D:383:ASN:OD1	1:D:383:ASN:N	2.49	0.46
1:C:383:ASN:OD1	1:C:383:ASN:N	2.49	0.46
1:C:426:VAL:O	1:C:430:THR:HG22	2.16	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:E:107:PRO:HB2	1:E:338:VAL:HG11	1.98	0.46
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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:533:VAL:HG23	1:E:553:GLN:NE2	2.32	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: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: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
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: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:E:382:VAL:O	1:E:482:THR:HA	2.17	0.44
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:F:107:PRO:HB2	1:F:338:VAL:HG11	1.98	0.44
1:F:383:ASN:OD1	1:F:383:ASN:N	2.49	0.44
1:A:383:ASN:N	1:A:383:ASN:OD1	2.49	0.43
1:A:382:VAL:O	1:A:482:THR:HA	2.18	0.43
1:A:533:VAL:HG23	1:A:553:GLN: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: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:B:383:ASN:OD1	1:B:383:ASN:N	2.49	0.43
2:H:205:ARG:O	2:H:206:PRO:C	2.57	0.43
2:K:205:ARG:O	2:K:206:PRO:C	2.57	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

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:205:ARG:O	2:J:206:PRO:C	2.57	0.43
1:A:107:PRO:HB2	1:A:338:VAL:HG11	2.00	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
2:I:205:ARG:O	2:I:206:PRO:C	2.57	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:482:THR:HG21	1:E:593:TYR:CE1	2.55	0.42
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: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:F:597:LYS:O	1:F:598:VAL:C	2.58	0.42
2:G:205:ARG:O	2:G:206:PRO:C	2.57	0.42
2:L:205:ARG:O	2:L:206:PRO:C	2.57	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:A:482:THR:HG21	1:A:593:TYR:CE1	2.55	0.42
1:B:597:LYS:O	1:B:598:VAL:C	2.58	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:447:ARG:O	1:D:448:ARG:C	2.58	0.42
1:D:597:LYS:O	1:D:598:VAL:C	2.58	0.42
1:D:431:ILE:HG22	1:D:600:PHE:CE2	2.55	0.42
1:E:528:VAL:O	1:E:529:MET:C	2.58	0.42
1:F:483:PHE:HA	1:F:583:ILE:HB	2.02	0.42

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:ARG:NE	1:A:88:GLU:OE2	2.49	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
2:G:136:VAL:O	2:G:137:HIS:HB2	2.20	0.42
1:A:290:GLN:OE1	1:A:507:VAL:HG21	2.20	0.41
1:C:462:ALA:O	1:C:463:PRO:C	2.58	0.41
1:D:222:LEU:HD11	1:D:308:THR:HG23	2.02	0.41
1:D:528:VAL:O	1:D:529:MET:C	2.58	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
1:F:528:VAL:O	1:F:529:MET:C	2.58	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
1:C:592:ASN:HB3	1:C:595:ALA:HB2	2.02	0.41
1:D:462:ALA:O	1:D:463:PRO:C	2.58	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: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:C:528:VAL:O	1:C:529:MET:C	2.58	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:597:LYS:O	1:E:598:VAL:C	2.58	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:290:GLN:OE1	1:F:507:VAL:HG21	2.20	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:C:597:LYS:O	1:C:598:VAL:C	2.58	0.41
1:D:290:GLN:OE1	1:D:507:VAL:HG21	2.21	0.41
2:G:168:ILE:HB	2:G:215:GLN:HB3	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:446:MET:SD	1:D:449:LYS:HE3	2.61	0.41
1:D:51:VAL:HG12	1:D:52:ARG:N	2.35	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:447:ARG:O	1:C:448:ARG:C	2.59	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:D:179:VAL:O	1:D:260:THR:N	2.51	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:E:462:ALA:O	1:E:463:PRO:C	2.58	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:F:180:MET:HA	1:F:260:THR:O	2.21	0.41
1:F:447:ARG:O	1:F:448:ARG:C	2.59	0.41
1:A:462:ALA:O	1:A:463:PRO:C	2.59	0.40
1:A:51:VAL:HG12	1:A:52:ARG:N	2.36	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
1:D:262:PHE:CB	1:D:288:ILE:HB	2.51	0.40
1:D:96:VAL:O	1:D:96:VAL:HG13	2.22	0.40
1:F:549:GLN:HB3	1:F:550:PRO:HD2	2.03	0.40
1:B:528:VAL:O	1:B:529:MET:C	2.58	0.40
1:E:483:PHE:HA	1:E:583:ILE:HB	2.02	0.40
1:F:462:ALA:O	1:F:463:PRO:C	2.58	0.40
1:A:528:VAL:O	1:A:529:MET:C	2.58	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:J:136:VAL:O	2:J:137:HIS:HB2	2.21	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:A:597:LYS:O	1:A:598:VAL:C	2.58	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:E:447:ARG:O	1:E:448:ARG:C	2.58	0.40
1:A:180:MET:HA	1:A:260:THR:O	2.21	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

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	515/582 (88%)	433 (84%)	72 (14%)	10 (2%)	9	49
1	B	515/582 (88%)	435 (84%)	70 (14%)	10 (2%)	9	49
1	C	515/582 (88%)	434 (84%)	72 (14%)	9 (2%)	11	51
1	D	515/582 (88%)	434 (84%)	72 (14%)	9 (2%)	11	51
1	E	515/582 (88%)	436 (85%)	70 (14%)	9 (2%)	11	51
1	F	515/582 (88%)	434 (84%)	72 (14%)	9 (2%)	11	51
2	G	172/230 (75%)	144 (84%)	23 (13%)	5 (3%)	5	40
2	H	172/230 (75%)	144 (84%)	23 (13%)	5 (3%)	5	40
2	I	172/230 (75%)	145 (84%)	23 (13%)	4 (2%)	7	45
2	J	172/230 (75%)	143 (83%)	25 (14%)	4 (2%)	7	45
2	K	172/230 (75%)	145 (84%)	23 (13%)	4 (2%)	7	45

Continued on next page...

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	172/230 (75%)	143 (83%)	25 (14%)	4 (2%)	7	45
All	All	4122/4872 (85%)	3470 (84%)	570 (14%)	82 (2%)	9	48

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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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
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

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
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%)	401 (91%)	38 (9%)	12	45
1	B	439/487 (90%)	404 (92%)	35 (8%)	14	49
1	C	439/487 (90%)	405 (92%)	34 (8%)	15	51
1	D	439/487 (90%)	404 (92%)	35 (8%)	14	49
1	E	439/487 (90%)	403 (92%)	36 (8%)	13	47
1	F	439/487 (90%)	405 (92%)	34 (8%)	15	51
2	G	163/202 (81%)	150 (92%)	13 (8%)	14	49
2	H	163/202 (81%)	149 (91%)	14 (9%)	12	46
2	I	163/202 (81%)	149 (91%)	14 (9%)	12	46
2	J	163/202 (81%)	148 (91%)	15 (9%)	11	42
2	K	163/202 (81%)	148 (91%)	15 (9%)	11	42
2	L	163/202 (81%)	153 (94%)	10 (6%)	22	59
All	All	3612/4134 (87%)	3319 (92%)	293 (8%)	14	48

All (293) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	62	ILE
1	A	77	PRO
1	A	109	ASN
1	A	115	PRO
1	A	125	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	176	LYS
1	A	212	LEU
1	A	227	GLN
1	A	230	LYS
1	A	242	LEU
1	A	280	SER
1	A	281	GLU
1	A	285	GLN
1	A	296	SER
1	A	298	TRP
1	A	341	ASP
1	A	342	VAL
1	A	358	ASP
1	A	383	ASN
1	A	398	GLU
1	A	399	ASP
1	A	402	SER
1	A	415	ASP
1	A	420	TYR
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
1	A	518	LEU
1	A	548	ASN
1	A	549	GLN
1	A	576	LYS
1	A	596	ASN
1	A	604	LEU
2	G	31	HIS
2	G	36	CYS
2	G	73	THR
2	G	86	THR
2	G	89	PHE
2	G	97	ARG
2	G	107	TYR
2	G	136	VAL
2	G	139	THR
2	G	176	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	G	197	LYS
2	G	232	ARG
2	G	234	THR
1	B	62	ILE
1	B	109	ASN
1	B	115	PRO
1	B	125	ASP
1	B	176	LYS
1	B	212	LEU
1	B	227	GLN
1	B	242	LEU
1	B	280	SER
1	B	285	GLN
1	B	296	SER
1	B	298	TRP
1	B	341	ASP
1	B	342	VAL
1	B	343	GLN
1	B	358	ASP
1	B	383	ASN
1	B	398	GLU
1	B	402	SER
1	B	415	ASP
1	B	420	TYR
1	B	436	THR
1	B	441	ARG
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	604	LEU
1	C	52	ARG
1	C	62	ILE
1	C	109	ASN
1	C	125	ASP

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	176	LYS
1	C	212	LEU
1	C	227	GLN
1	C	280	SER
1	C	285	GLN
1	C	296	SER
1	C	298	TRP
1	C	341	ASP
1	C	342	VAL
1	C	358	ASP
1	C	383	ASN
1	C	398	GLU
1	C	402	SER
1	C	415	ASP
1	C	420	TYR
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	518	LEU
1	C	548	ASN
1	C	549	GLN
1	C	564	ARG
1	C	576	LYS
1	C	596	ASN
1	C	604	LEU
1	D	52	ARG
1	D	62	ILE
1	D	109	ASN
1	D	125	ASP
1	D	189	MET
1	D	212	LEU
1	D	227	GLN
1	D	242	LEU
1	D	280	SER
1	D	285	GLN
1	D	296	SER
1	D	298	TRP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	341	ASP
1	D	342	VAL
1	D	358	ASP
1	D	383	ASN
1	D	398	GLU
1	D	399	ASP
1	D	402	SER
1	D	415	ASP
1	D	420	TYR
1	D	436	THR
1	D	452	LEU
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	604	LEU
1	E	52	ARG
1	E	62	ILE
1	E	88	GLU
1	E	109	ASN
1	E	115	PRO
1	E	125	ASP
1	E	176	LYS
1	E	212	LEU
1	E	227	GLN
1	E	242	LEU
1	E	280	SER
1	E	285	GLN
1	E	296	SER
1	E	298	TRP
1	E	341	ASP
1	E	342	VAL
1	E	358	ASP
1	E	383	ASN
1	E	398	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	415	ASP
1	E	420	TYR
1	E	436	THR
1	E	446	MET
1	E	452	LEU
1	E	465	VAL
1	E	485	HIS
1	E	486	HIS
1	E	488	GLN
1	E	497	ASP
1	E	518	LEU
1	E	548	ASN
1	E	549	GLN
1	E	564	ARG
1	E	576	LYS
1	E	596	ASN
1	E	604	LEU
1	F	52	ARG
1	F	62	ILE
1	F	77	PRO
1	F	109	ASN
1	F	125	ASP
1	F	176	LYS
1	F	212	LEU
1	F	227	GLN
1	F	242	LEU
1	F	280	SER
1	F	285	GLN
1	F	296	SER
1	F	298	TRP
1	F	341	ASP
1	F	342	VAL
1	F	358	ASP
1	F	383	ASN
1	F	398	GLU
1	F	399	ASP
1	F	415	ASP
1	F	420	TYR
1	F	436	THR
1	F	452	LEU
1	F	465	VAL
1	F	485	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	F	486	HIS
1	F	488	GLN
1	F	497	ASP
1	F	518	LEU
1	F	548	ASN
1	F	549	GLN
1	F	576	LYS
1	F	596	ASN
1	F	604	LEU
2	H	31	HIS
2	H	36	CYS
2	H	49	THR
2	H	73	THR
2	H	86	THR
2	H	107	TYR
2	H	136	VAL
2	H	139	THR
2	H	166	ARG
2	H	176	LEU
2	H	186	ILE
2	H	197	LYS
2	H	232	ARG
2	H	234	THR
2	I	31	HIS
2	I	36	CYS
2	I	39	LYS
2	I	73	THR
2	I	86	THR
2	I	107	TYR
2	I	136	VAL
2	I	139	THR
2	I	166	ARG
2	I	176	LEU
2	I	188	GLU
2	I	197	LYS
2	I	233	LEU
2	I	234	THR
2	J	31	HIS
2	J	36	CYS
2	J	73	THR
2	J	97	ARG
2	J	107	TYR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	J	133	MET
2	J	136	VAL
2	J	139	THR
2	J	151	LYS
2	J	166	ARG
2	J	176	LEU
2	J	197	LYS
2	J	232	ARG
2	J	233	LEU
2	J	234	THR
2	K	31	HIS
2	K	36	CYS
2	K	73	THR
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	166	ARG
2	K	197	LYS
2	K	232	ARG
2	K	233	LEU
2	K	234	THR
2	L	31	HIS
2	L	36	CYS
2	L	73	THR
2	L	97	ARG
2	L	107	TYR
2	L	139	THR
2	L	166	ARG
2	L	197	LYS
2	L	233	LEU
2	L	234	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	GLN
1	A	458	HIS
1	A	488	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	549	GLN
1	A	592	ASN
2	G	42	ASN
1	B	227	GLN
1	B	458	HIS
1	B	488	GLN
1	B	592	ASN
1	C	227	GLN
1	C	458	HIS
1	C	488	GLN
1	C	592	ASN
1	D	227	GLN
1	D	458	HIS
1	D	488	GLN
1	D	549	GLN
1	D	592	ASN
1	E	227	GLN
1	E	458	HIS
1	E	488	GLN
1	E	592	ASN
1	F	227	GLN
1	F	458	HIS
1	F	488	GLN
2	H	42	ASN
2	J	42	ASN
2	J	59	GLN
2	K	42	ASN
2	K	59	GLN
2	L	42	ASN
2	L	59	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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	D	1
1	E	1
1	B	1
1	C	1
1	A	1
1	F	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	527/582 (90%)	-0.38	0 100 100	42, 77, 133, 178	0
1	B	527/582 (90%)	-0.35	1 (0%) 94 93	42, 78, 134, 183	0
1	C	527/582 (90%)	-0.28	1 (0%) 94 93	54, 99, 193, 254	0
1	D	527/582 (90%)	-0.24	3 (0%) 89 84	69, 126, 215, 262	0
1	E	527/582 (90%)	-0.21	1 (0%) 94 93	65, 108, 182, 251	0
1	F	527/582 (90%)	-0.05	8 (1%) 74 64	89, 143, 221, 257	0
2	G	184/230 (80%)	-0.21	0 100 100	68, 94, 118, 130	0
2	H	184/230 (80%)	-0.22	0 100 100	67, 96, 121, 129	0
2	I	184/230 (80%)	0.37	6 (3%) 47 37	138, 156, 171, 185	0
2	J	184/230 (80%)	0.09	2 (1%) 80 72	122, 139, 159, 181	0
2	K	184/230 (80%)	0.09	1 (0%) 90 86	105, 124, 143, 161	0
2	L	184/230 (80%)	0.07	1 (0%) 90 86	121, 140, 161, 171	0
All	All	4266/4872 (87%)	-0.18	24 (0%) 89 84	42, 112, 186, 262	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	J	25	ALA	3.3
2	L	203	ASN	2.9
1	C	340	GLN	2.9
1	F	564	ARG	2.8
2	I	215	GLN	2.8
2	I	203	ASN	2.7
2	I	111	GLU	2.6
1	F	87	PRO	2.6
1	B	174	SER	2.6
2	K	42	ASN	2.5
1	F	557	PHE	2.3

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	F	238	GLN	2.2
1	E	151	GLU	2.2
1	F	350	ALA	2.2
1	D	556	LYS	2.2
2	I	63	THR	2.2
2	I	67	ARG	2.2
2	I	168	ILE	2.1
1	F	341	ASP	2.1
1	F	113	ALA	2.1
1	F	515	ALA	2.1
1	D	87	PRO	2.1
2	J	102	GLN	2.1
1	D	113	ALA	2.1

## 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 carbohydrates 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.