Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 01:52 am BST

PDB ID	:	6HC2
Title	:	Crystal structure of NuMA/LGN hetero-hexamers
Authors	:	Pasqualato, S.; Culurgioni, S.; Foadi, J.; Alfieri, A.; Mapelli, M.
Deposited on	:	2018-08-13
Resolution	:	4.31 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 following versions of software and data (see references ⓘ) were used in the production of this report:

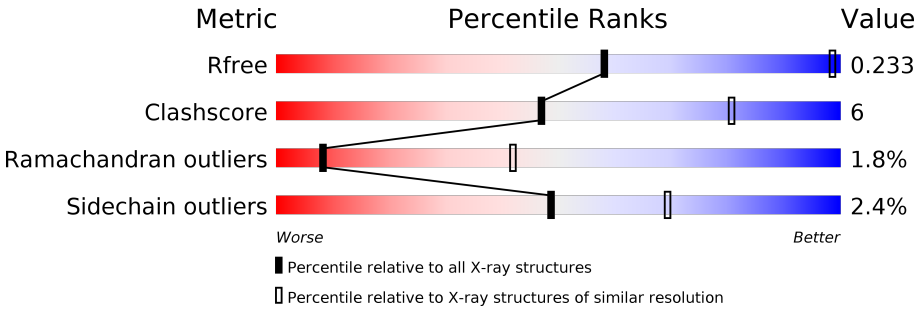
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 4.31 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}	130704	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)

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 on 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	367	79% 19% ••
1	C	367	86% 12% •
1	E	367	89% 9% •
1	G	367	91% 8% •
1	I	367	89% 11%
1	K	367	88% 11% •
1	M	367	90% 9% •

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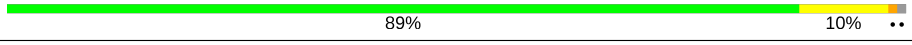
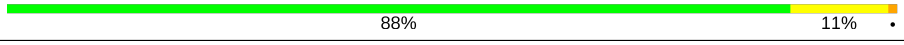
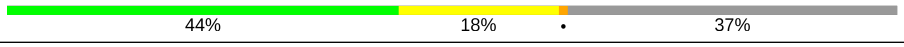
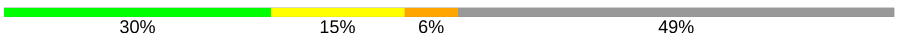
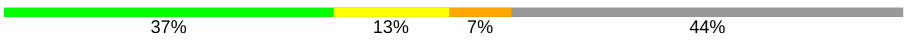
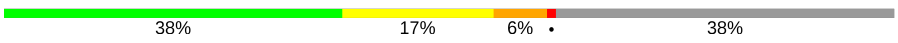
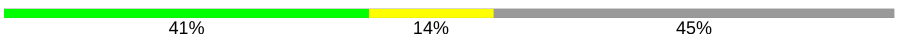
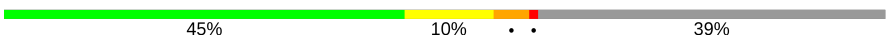
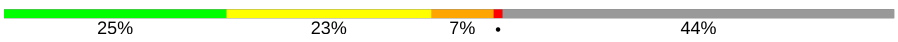
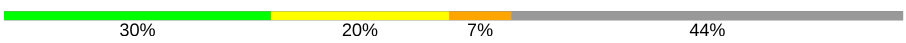
Mol	Chain	Length	Quality of chain
1	O	367	
1	Q	367	
1	S	367	
1	U	367	
1	W	367	
2	B	71	
2	D	71	
2	F	71	
2	H	71	
2	J	71	
2	L	71	
2	N	71	
2	P	71	
2	R	71	
2	T	71	
2	V	71	
2	X	71	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 37558 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 G-protein-signaling modulator 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2834	1778	497	548	11			
1	C	367	Total	C	N	O	S	0	0	0
			2847	1783	500	552	12			
1	E	366	Total	C	N	O	S	0	0	0
			2798	1750	494	545	9			
1	G	367	Total	C	N	O	S	0	0	0
			2815	1759	499	547	10			
1	I	367	Total	C	N	O	S	0	0	0
			2820	1768	497	546	9			
1	K	366	Total	C	N	O	S	0	0	0
			2828	1772	497	547	12			
1	M	366	Total	C	N	O	S	0	0	0
			2820	1767	499	544	10			
1	O	365	Total	C	N	O	S	0	0	0
			2821	1767	496	547	11			
1	Q	367	Total	C	N	O	S	0	0	0
			2831	1773	500	547	11			
1	S	362	Total	C	N	O	S	0	0	0
			2800	1753	496	541	10			
1	U	366	Total	C	N	O	S	0	0	0
			2823	1767	499	547	10			
1	W	366	Total	C	N	O	S	0	0	0
			2817	1763	499	545	10			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP P81274
A	2	PRO	-	expression tag	UNP P81274
A	3	LEU	-	expression tag	UNP P81274
A	4	GLY	-	expression tag	UNP P81274
A	5	SER	-	expression tag	UNP P81274

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Chain	Residue	Modelled	Actual	Comment	Reference
A	6	MET	-	expression tag	UNP P81274
C	1	GLY	-	expression tag	UNP P81274
C	2	PRO	-	expression tag	UNP P81274
C	3	LEU	-	expression tag	UNP P81274
C	4	GLY	-	expression tag	UNP P81274
C	5	SER	-	expression tag	UNP P81274
C	6	MET	-	expression tag	UNP P81274
E	1	GLY	-	expression tag	UNP P81274
E	2	PRO	-	expression tag	UNP P81274
E	3	LEU	-	expression tag	UNP P81274
E	4	GLY	-	expression tag	UNP P81274
E	5	SER	-	expression tag	UNP P81274
E	6	MET	-	expression tag	UNP P81274
G	1	GLY	-	expression tag	UNP P81274
G	2	PRO	-	expression tag	UNP P81274
G	3	LEU	-	expression tag	UNP P81274
G	4	GLY	-	expression tag	UNP P81274
G	5	SER	-	expression tag	UNP P81274
G	6	MET	-	expression tag	UNP P81274
I	1	GLY	-	expression tag	UNP P81274
I	2	PRO	-	expression tag	UNP P81274
I	3	LEU	-	expression tag	UNP P81274
I	4	GLY	-	expression tag	UNP P81274
I	5	SER	-	expression tag	UNP P81274
I	6	MET	-	expression tag	UNP P81274
K	1	GLY	-	expression tag	UNP P81274
K	2	PRO	-	expression tag	UNP P81274
K	3	LEU	-	expression tag	UNP P81274
K	4	GLY	-	expression tag	UNP P81274
K	5	SER	-	expression tag	UNP P81274
K	6	MET	-	expression tag	UNP P81274
M	1	GLY	-	expression tag	UNP P81274
M	2	PRO	-	expression tag	UNP P81274
M	3	LEU	-	expression tag	UNP P81274
M	4	GLY	-	expression tag	UNP P81274
M	5	SER	-	expression tag	UNP P81274
M	6	MET	-	expression tag	UNP P81274
O	1	GLY	-	expression tag	UNP P81274
O	2	PRO	-	expression tag	UNP P81274
O	3	LEU	-	expression tag	UNP P81274
O	4	GLY	-	expression tag	UNP P81274
O	5	SER	-	expression tag	UNP P81274

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Chain	Residue	Modelled	Actual	Comment	Reference
O	6	MET	-	expression tag	UNP P81274
Q	1	GLY	-	expression tag	UNP P81274
Q	2	PRO	-	expression tag	UNP P81274
Q	3	LEU	-	expression tag	UNP P81274
Q	4	GLY	-	expression tag	UNP P81274
Q	5	SER	-	expression tag	UNP P81274
Q	6	MET	-	expression tag	UNP P81274
S	1	GLY	-	expression tag	UNP P81274
S	2	PRO	-	expression tag	UNP P81274
S	3	LEU	-	expression tag	UNP P81274
S	4	GLY	-	expression tag	UNP P81274
S	5	SER	-	expression tag	UNP P81274
S	6	MET	-	expression tag	UNP P81274
U	1	GLY	-	expression tag	UNP P81274
U	2	PRO	-	expression tag	UNP P81274
U	3	LEU	-	expression tag	UNP P81274
U	4	GLY	-	expression tag	UNP P81274
U	5	SER	-	expression tag	UNP P81274
U	6	MET	-	expression tag	UNP P81274
W	1	GLY	-	expression tag	UNP P81274
W	2	PRO	-	expression tag	UNP P81274
W	3	LEU	-	expression tag	UNP P81274
W	4	GLY	-	expression tag	UNP P81274
W	5	SER	-	expression tag	UNP P81274
W	6	MET	-	expression tag	UNP P81274

- Molecule 2 is a protein called Nuclear mitotic apparatus protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	45	Total	C	N	O	S	0	0	0
			329	206	53	68	2			
2	D	36	Total	C	N	O	S	0	0	0
			280	177	44	57	2			
2	F	37	Total	C	N	O	S	0	0	0
			288	182	46	58	2			
2	H	36	Total	C	N	O	S	0	0	0
			284	180	44	58	2			
2	J	40	Total	C	N	O	S	0	0	0
			307	192	49	64	2			
2	L	44	Total	C	N	O	S	0	0	0
			341	210	58	71	2			
2	N	39	Total	C	N	O	S	0	0	0
			305	191	49	63	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	43	Total	C	N	O	S	0	0	0
			320	200	52	66	2			
2	R	40	Total	C	N	O	S	0	0	0
			312	195	50	65	2			
2	T	45	Total	C	N	O	S	0	0	0
			337	209	55	71	2			
2	V	39	Total	C	N	O	S	0	0	0
			301	187	49	63	2			
2	X	40	Total	C	N	O	S	0	0	0
			300	187	49	62	2			

There are 24 discrepancies between the modelled and reference sequences:

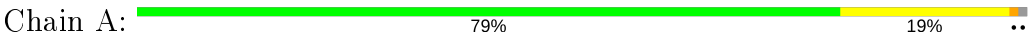
Chain	Residue	Modelled	Actual	Comment	Reference
B	1858	GLY	-	expression tag	UNP Q14980
B	1859	PRO	-	expression tag	UNP Q14980
D	1858	GLY	-	expression tag	UNP Q14980
D	1859	PRO	-	expression tag	UNP Q14980
F	1858	GLY	-	expression tag	UNP Q14980
F	1859	PRO	-	expression tag	UNP Q14980
H	1858	GLY	-	expression tag	UNP Q14980
H	1859	PRO	-	expression tag	UNP Q14980
J	1858	GLY	-	expression tag	UNP Q14980
J	1859	PRO	-	expression tag	UNP Q14980
L	1858	GLY	-	expression tag	UNP Q14980
L	1859	PRO	-	expression tag	UNP Q14980
N	1858	GLY	-	expression tag	UNP Q14980
N	1859	PRO	-	expression tag	UNP Q14980
P	1858	GLY	-	expression tag	UNP Q14980
P	1859	PRO	-	expression tag	UNP Q14980
R	1858	GLY	-	expression tag	UNP Q14980
R	1859	PRO	-	expression tag	UNP Q14980
T	1858	GLY	-	expression tag	UNP Q14980
T	1859	PRO	-	expression tag	UNP Q14980
V	1858	GLY	-	expression tag	UNP Q14980
V	1859	PRO	-	expression tag	UNP Q14980
X	1858	GLY	-	expression tag	UNP Q14980
X	1859	PRO	-	expression tag	UNP Q14980

3 Residue-property plots (i)

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. 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. 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.

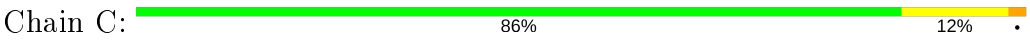
- Molecule 1: G-protein-signaling modulator 2

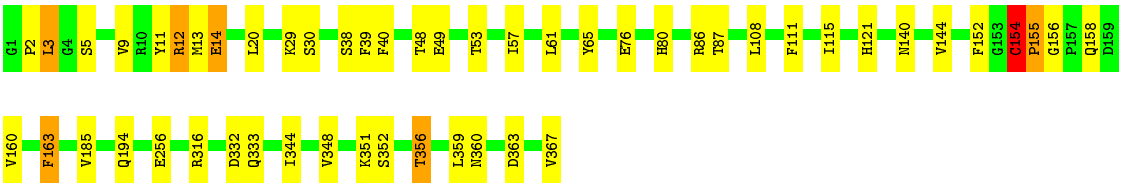
Chain A:



- Molecule 1: G-protein-signaling modulator 2

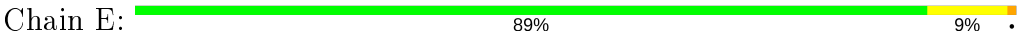
Chain C:

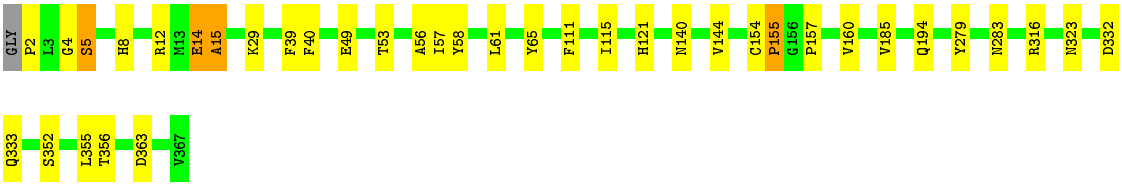




- Molecule 1: G-protein-signaling modulator 2

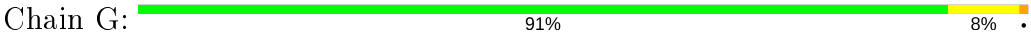
Chain E:

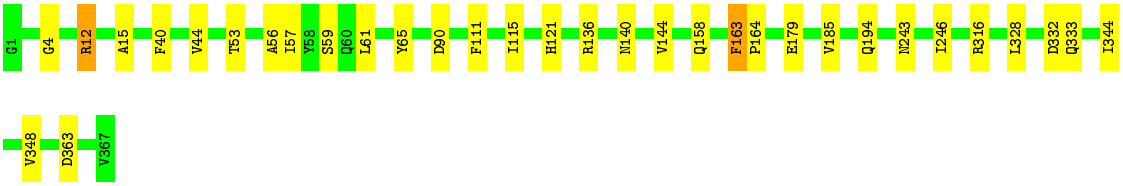




- Molecule 1: G-protein-signaling modulator 2

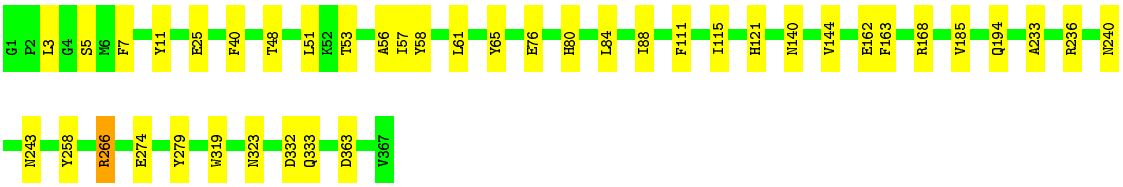
Chain G:





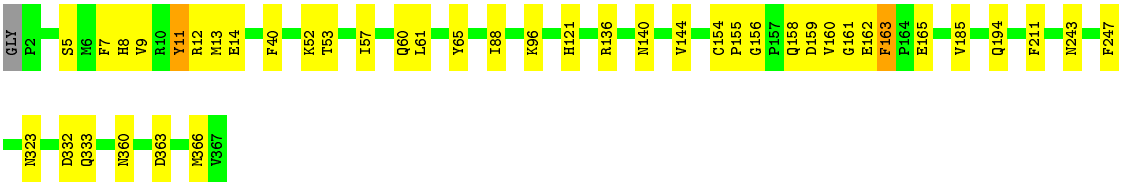
• Molecule 1: G-protein-signaling modulator 2

Chain I:



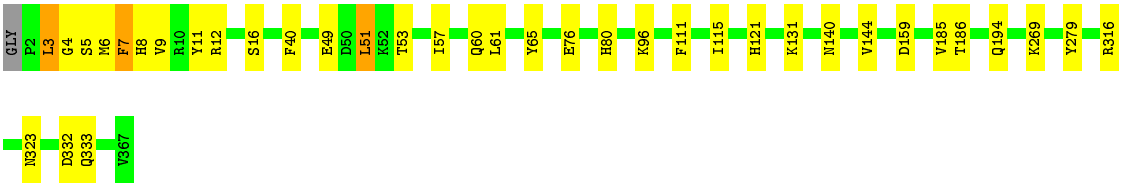
• Molecule 1: G-protein-signaling modulator 2

Chain K:



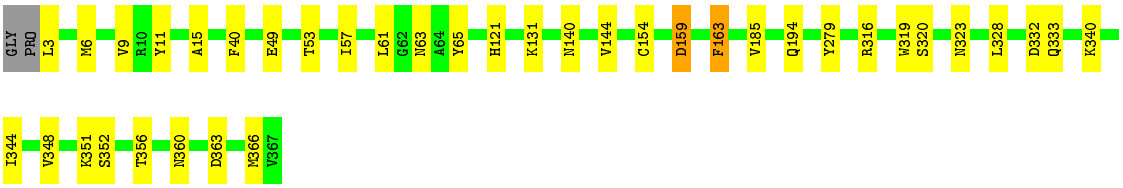
• Molecule 1: G-protein-signaling modulator 2

Chain M:



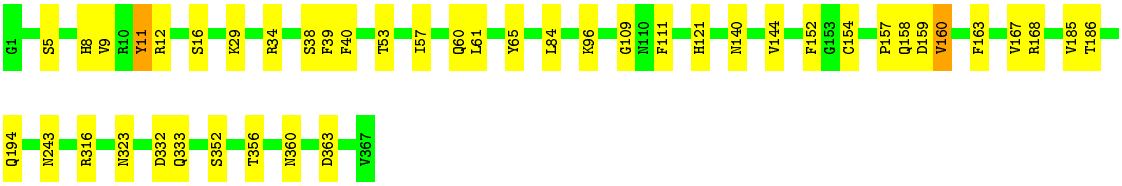
• Molecule 1: G-protein-signaling modulator 2

Chain O:



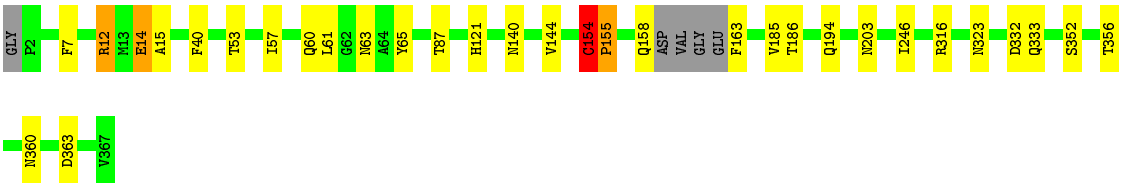
• Molecule 1: G-protein-signaling modulator 2

Chain Q:



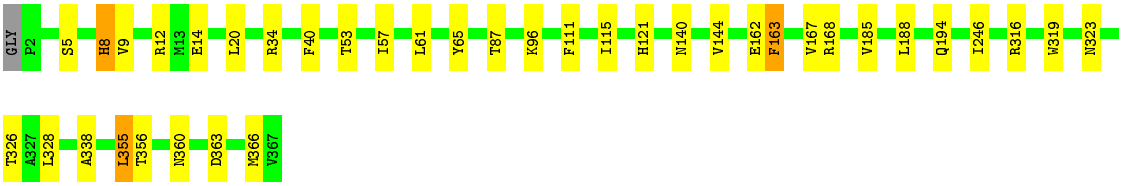
• Molecule 1: G-protein-signaling modulator 2

Chain S:



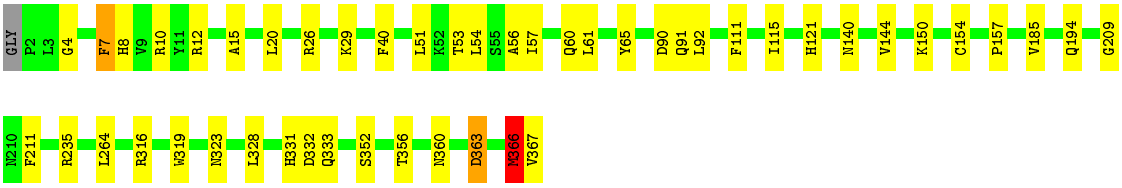
• Molecule 1: G-protein-signaling modulator 2

Chain U:



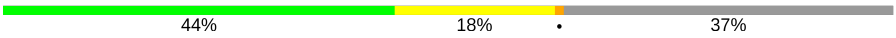
• Molecule 1: G-protein-signaling modulator 2

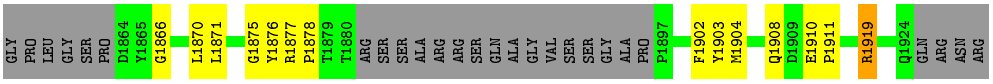
Chain W:



• Molecule 2: Nuclear mitotic apparatus protein 1

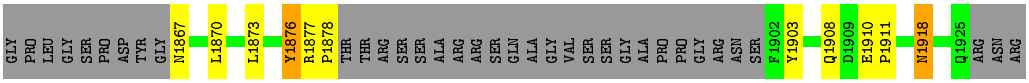
Chain B:





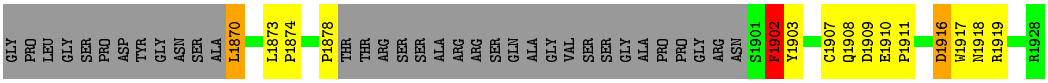
• Molecule 2: Nuclear mitotic apparatus protein 1

Chain D:



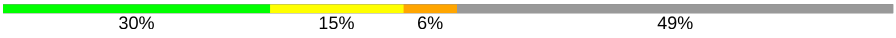
• Molecule 2: Nuclear mitotic apparatus protein 1

Chain F:



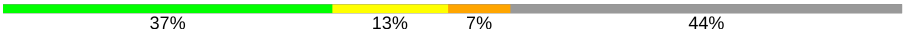
• Molecule 2: Nuclear mitotic apparatus protein 1

Chain H:



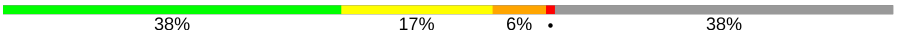
• Molecule 2: Nuclear mitotic apparatus protein 1

Chain J:



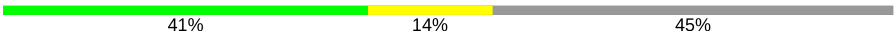
• Molecule 2: Nuclear mitotic apparatus protein 1

Chain L:



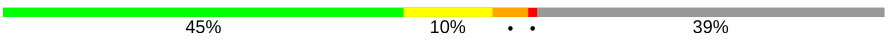
• Molecule 2: Nuclear mitotic apparatus protein 1

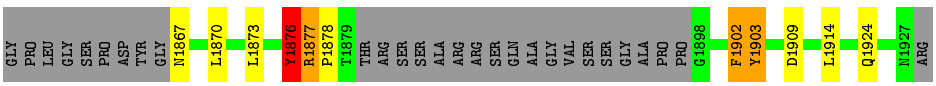
Chain N:



• Molecule 2: Nuclear mitotic apparatus protein 1

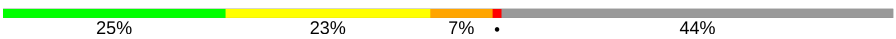
Chain P:

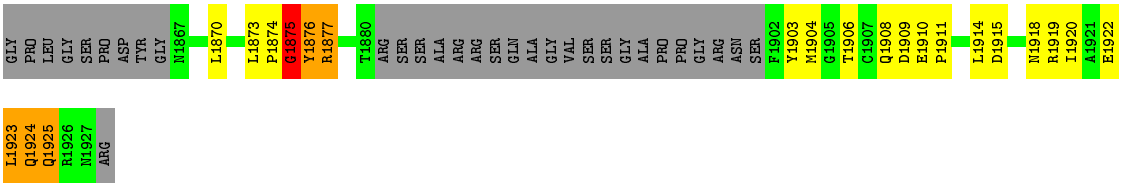




• Molecule 2: Nuclear mitotic apparatus protein 1

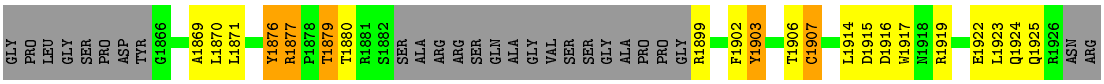
Chain R:





• Molecule 2: Nuclear mitotic apparatus protein 1

Chain T:

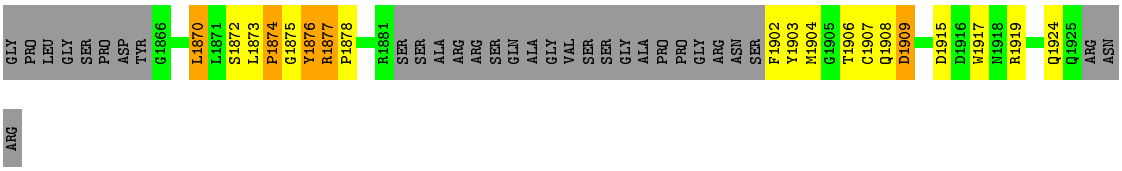


• Molecule 2: Nuclear mitotic apparatus protein 1

Chain V:

• Molecule 2: Nuclear mitotic apparatus protein 1

Chain X:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	153.94Å 153.94Å 732.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	150.65 – 4.31 183.24 – 4.31	Depositor EDS
% Data completeness (in resolution range)	99.8 (150.65-4.31) 95.8 (183.24-4.31)	Depositor EDS
R_{merge}	0.34	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.54 (at 4.30Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.182 , 0.234 0.182 , 0.233	Depositor DCC
R_{free} test set	3061 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	212.5	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 177.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	37558	wwPDB-VP
Average B, all atoms (Å^2)	241.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.31	0/2885	0.60	5/3892 (0.1%)
1	C	0.31	0/2898	0.57	4/3909 (0.1%)
1	E	0.29	0/2847	0.52	0/3845
1	G	0.30	0/2865	0.48	0/3868
1	I	0.30	0/2872	0.50	0/3881
1	K	0.30	0/2880	0.49	0/3887
1	M	0.30	0/2872	0.54	1/3877 (0.0%)
1	O	0.29	0/2872	0.48	0/3876
1	Q	0.30	0/2883	0.51	0/3892
1	S	0.31	0/2851	0.58	2/3847 (0.1%)
1	U	0.32	0/2874	0.53	1/3879 (0.0%)
1	W	0.30	0/2868	0.51	0/3871
2	B	0.46	0/336	0.81	0/458
2	D	0.42	0/286	0.82	0/389
2	F	0.35	0/294	0.85	0/400
2	H	0.44	0/290	0.83	0/395
2	J	0.47	0/313	0.88	2/426 (0.5%)
2	L	0.52	0/347	0.95	2/470 (0.4%)
2	N	0.37	0/311	0.78	0/423
2	P	0.44	0/326	0.98	3/444 (0.7%)
2	R	0.47	0/318	1.00	2/433 (0.5%)
2	T	0.40	0/343	0.88	0/467
2	V	0.32	0/306	0.82	0/415
2	X	0.42	0/306	0.82	1/417 (0.2%)
All	All	0.32	0/38243	0.57	23/51661 (0.0%)

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	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
1	E	0	1
1	I	0	1
1	O	0	1
1	Q	0	2
1	S	0	1
1	U	0	1
1	W	0	1
2	D	0	1
2	N	0	1
2	R	0	1
2	T	0	2
2	X	0	1
All	All	0	17

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	154	CYS	C-N-CD	-11.86	94.50	120.60
1	C	154	CYS	C-N-CD	-9.94	98.73	120.60
1	M	3	LEU	CB-CG-CD1	8.03	124.65	111.00
1	C	3	LEU	CB-CG-CD2	7.82	124.30	111.00
1	A	236	ARG	NE-CZ-NH2	-7.62	116.49	120.30
1	U	188	LEU	CB-CG-CD2	6.89	122.71	111.00
2	R	1914	LEU	CA-CB-CG	6.25	129.68	115.30
1	S	154	CYS	C-N-CA	6.24	148.20	122.00
1	A	75	LEU	CA-CB-CG	5.98	129.05	115.30
1	C	3	LEU	CA-CB-CG	5.95	128.98	115.30
2	J	1876	TYR	C-N-CA	5.94	136.55	121.70
2	L	1876	TYR	C-N-CA	5.92	136.49	121.70
2	P	1909	ASP	C-N-CA	5.79	136.17	121.70
2	P	1876	TYR	C-N-CA	5.53	135.52	121.70
2	J	1870	LEU	CA-CB-CG	5.51	127.97	115.30
1	A	236	ARG	NE-CZ-NH1	5.48	123.04	120.30
2	L	1870	LEU	CA-CB-CG	5.44	127.82	115.30
2	X	1909	ASP	C-N-CA	5.39	135.17	121.70
2	R	1875	GLY	N-CA-C	5.26	126.25	113.10
1	A	14	GLU	C-N-CA	5.19	134.66	121.70
1	C	356	THR	CA-CB-CG2	-5.17	105.16	112.40
1	A	263	LEU	CA-CB-CG	5.11	127.06	115.30
2	P	1903	TYR	N-CA-C	-5.06	97.35	111.00

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	MET	Peptide
1	A	153	GLY	Peptide
1	C	154	CYS	Peptide
2	D	1876	TYR	Peptide
1	E	15	ALA	Peptide
1	I	162	GLU	Peptide
2	N	1905	GLY	Peptide
1	O	154	CYS	Peptide
1	Q	11	TYR	Peptide
1	Q	154	CYS	Peptide
2	R	1875	GLY	Peptide
1	S	154	CYS	Peptide
2	T	1879	THR	Peptide
2	T	1906	THR	Peptide
1	U	162	GLU	Peptide
1	W	366	MET	Peptide
2	X	1874	PRO	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	2834	0	2726	62	0
1	C	2847	0	2741	46	0
1	E	2798	0	2657	29	0
1	G	2815	0	2678	21	0
1	I	2820	0	2686	32	0
1	K	2828	0	2704	28	0
1	M	2820	0	2688	44	0
1	O	2821	0	2696	31	0
1	Q	2831	0	2707	34	0
1	S	2800	0	2671	31	0
1	U	2823	0	2696	44	0
1	W	2817	0	2685	51	0
2	B	329	0	282	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	280	0	246	8	0
2	F	288	0	248	13	0
2	H	284	0	255	10	0
2	J	307	0	271	22	0
2	L	341	0	300	16	0
2	N	305	0	269	6	0
2	P	320	0	272	10	0
2	R	312	0	276	17	0
2	T	337	0	290	14	0
2	V	301	0	260	15	0
2	X	300	0	258	12	0
All	All	37558	0	35562	453	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (453) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:4:GLY:H	1:M:6:MET:CE	1.07	1.55
1:M:3:LEU:HD22	1:M:6:MET:CE	1.34	1.54
1:M:4:GLY:N	1:M:6:MET:CE	1.92	1.29
1:M:4:GLY:H	1:M:6:MET:HE1	1.05	1.17
1:M:3:LEU:CD2	1:M:6:MET:CE	2.26	1.14
1:U:5:SER:HA	1:U:8:HIS:ND1	1.62	1.12
1:M:3:LEU:CD2	1:M:6:MET:HE2	1.80	1.10
2:V:1870:LEU:HD22	2:V:1876:TYR:CE1	1.87	1.08
1:M:4:GLY:H	1:M:6:MET:HE2	0.95	1.08
1:M:5:SER:N	1:M:6:MET:SD	2.27	1.07
2:V:1870:LEU:HD13	2:V:1876:TYR:CE2	1.89	1.07
1:M:3:LEU:HD22	1:M:6:MET:HE3	1.32	1.06
1:Q:9:VAL:HA	1:Q:12:ARG:HD2	1.37	1.05
2:V:1870:LEU:HD13	2:V:1876:TYR:CZ	1.95	1.01
1:M:4:GLY:N	1:M:6:MET:HE2	1.60	0.99
1:I:240:ASN:HD21	2:J:1908:GLN:HB2	1.26	0.98
1:A:236:ARG:HH22	2:B:1911:PRO:HD3	1.28	0.97
1:S:12:ARG:HB3	1:W:319:TRP:HE1	1.30	0.95
2:J:1902:PHE:CZ	2:J:1904:MET:HE3	2.03	0.94
2:L:1869:ALA:O	2:L:1872:SER:N	2.04	0.91
1:M:3:LEU:HD22	1:M:6:MET:HE2	0.90	0.90
2:V:1870:LEU:HD22	2:V:1876:TYR:CD1	2.06	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:5:SER:HA	1:U:8:HIS:CE1	2.07	0.90
1:M:3:LEU:CD2	1:M:6:MET:HE3	1.96	0.87
1:O:323:ASN:OD1	1:Q:12:ARG:HD3	1.76	0.84
1:A:76:GLU:HG2	1:A:80:HIS:HE1	1.41	0.84
1:C:367:VAL:HG22	1:E:2:PRO:HB2	1.60	0.83
1:A:367:VAL:HG21	1:C:2:PRO:HG3	1.61	0.82
2:J:1902:PHE:CZ	2:J:1904:MET:CE	2.62	0.82
1:K:158:GLN:OE1	1:K:163:PHE:HB3	1.79	0.82
1:M:4:GLY:CA	1:M:6:MET:SD	2.69	0.81
1:M:4:GLY:N	1:M:6:MET:HE1	1.73	0.81
1:U:163:PHE:HZ	1:U:168:ARG:H	1.28	0.80
2:J:1902:PHE:HZ	2:J:1904:MET:HE3	1.41	0.80
1:A:323:ASN:HB2	1:C:12:ARG:HH11	1.46	0.80
1:I:163:PHE:HE2	1:I:168:ARG:HB2	1.47	0.80
1:C:9:VAL:HA	1:C:12:ARG:HG3	1.65	0.79
1:Q:316:ARG:NH2	2:R:1903:TYR:OH	2.15	0.79
1:Q:152:PHE:HD2	1:Q:167:VAL:HG22	1.47	0.79
1:A:87:THR:HG21	2:F:1870:LEU:HB3	1.65	0.78
1:A:236:ARG:NH2	2:B:1911:PRO:HD3	1.98	0.78
1:A:236:ARG:NH2	2:B:1910:GLU:HA	1.99	0.77
1:O:319:TRP:O	1:O:323:ASN:ND2	2.18	0.76
1:S:323:ASN:OD1	1:U:12:ARG:NH1	2.18	0.76
1:S:12:ARG:HB3	1:W:319:TRP:NE1	2.00	0.75
1:A:319:TRP:NE1	1:C:12:ARG:O	2.18	0.75
1:A:118:CYS:SG	1:A:141:LEU:HG	2.27	0.74
1:U:319:TRP:HE1	1:W:12:ARG:HB3	1.51	0.73
2:J:1902:PHE:HZ	2:J:1904:MET:CE	2.01	0.73
1:A:76:GLU:HG2	1:A:80:HIS:CE1	2.24	0.72
1:O:279:TYR:HE2	2:P:1903:TYR:HB3	1.54	0.72
1:U:5:SER:CA	1:U:8:HIS:ND1	2.47	0.72
1:M:4:GLY:C	1:M:6:MET:SD	2.66	0.72
2:H:1916:ASP:O	2:H:1918:ASN:N	2.22	0.72
1:I:163:PHE:CE2	1:I:168:ARG:HB2	2.24	0.72
1:A:236:ARG:HH22	2:B:1911:PRO:CD	2.03	0.72
1:E:185:VAL:HG12	1:E:194:GLN:HG3	1.71	0.71
1:A:9:VAL:HG13	1:E:323:ASN:HB2	1.72	0.71
1:S:360:ASN:OD1	1:U:12:ARG:HG2	1.91	0.71
2:J:1876:TYR:HD1	2:J:1877:ARG:H	1.38	0.70
1:A:12:ARG:HH11	1:E:323:ASN:HB3	1.55	0.70
1:A:185:VAL:HG12	1:A:194:GLN:HG3	1.74	0.70
1:U:5:SER:HA	1:U:8:HIS:CG	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:51:LEU:HD13	1:I:88:ILE:HD13	1.73	0.70
1:U:360:ASN:ND2	1:W:12:ARG:HG2	2.07	0.69
1:S:12:ARG:HD2	1:W:323:ASN:ND2	2.07	0.69
1:S:185:VAL:HG12	1:S:194:GLN:HG3	1.74	0.69
1:M:185:VAL:HG12	1:M:194:GLN:HG3	1.72	0.69
1:C:2:PRO:HG2	1:C:5:SER:HB3	1.74	0.69
2:R:1870:LEU:HD22	2:R:1876:TYR:CD2	2.27	0.69
1:S:63:ASN:HB3	2:T:1914:LEU:HD21	1.73	0.69
1:W:60:GLN:HE21	2:X:1919:ARG:HB3	1.58	0.69
2:J:1876:TYR:HD1	2:J:1877:ARG:N	1.90	0.69
1:U:355:LEU:HD12	1:W:20:LEU:HD23	1.73	0.69
1:I:185:VAL:HG12	1:I:194:GLN:HG3	1.75	0.69
2:V:1876:TYR:CE2	1:W:51:LEU:HD21	2.27	0.69
2:D:1867:ASN:HA	2:D:1870:LEU:HD12	1.74	0.69
1:G:185:VAL:HG12	1:G:194:GLN:HG3	1.75	0.69
1:U:185:VAL:HG12	1:U:194:GLN:HG3	1.75	0.68
1:C:185:VAL:HG12	1:C:194:GLN:HG3	1.75	0.68
1:Q:185:VAL:HG12	1:Q:194:GLN:HG3	1.76	0.68
1:S:87:THR:HG21	2:X:1870:LEU:HD22	1.75	0.68
1:S:12:ARG:HD2	1:W:323:ASN:HD21	1.58	0.68
1:A:236:ARG:HH22	2:B:1910:GLU:HA	1.59	0.68
2:X:1873:LEU:O	2:X:1875:GLY:N	2.26	0.68
1:K:185:VAL:HG12	1:K:194:GLN:HG3	1.76	0.67
1:W:185:VAL:HG12	1:W:194:GLN:HG3	1.75	0.67
1:M:49:GLU:HA	2:R:1876:TYR:HD1	1.58	0.67
1:O:185:VAL:HG12	1:O:194:GLN:HG3	1.76	0.67
1:A:20:LEU:HD23	1:E:355:LEU:HD12	1.74	0.67
1:U:326:THR:HG21	1:W:8:HIS:HB2	1.78	0.66
1:C:352:SER:O	1:C:356:THR:HG23	1.95	0.66
1:A:90:ASP:O	1:A:93:GLY:N	2.29	0.66
1:M:8:HIS:O	1:M:12:ARG:HG3	1.95	0.66
1:E:316:ARG:HH21	2:F:1903:TYR:HB2	1.59	0.65
1:E:283:ASN:OD1	2:F:1902:PHE:HE2	1.79	0.65
1:I:25:GLU:OE1	2:J:1920:ILE:HG12	1.96	0.65
1:A:360:ASN:HD21	1:C:12:ARG:HG2	1.62	0.65
1:S:12:ARG:HG2	1:W:360:ASN:ND2	2.12	0.65
2:D:1878:PRO:HB3	1:E:49:GLU:OE2	1.97	0.64
2:L:1876:TYR:HD1	2:L:1877:ARG:N	1.94	0.64
1:M:12:ARG:HG2	1:Q:360:ASN:OD1	1.97	0.64
2:R:1876:TYR:CG	2:R:1877:ARG:N	2.66	0.64
1:O:351:LYS:HE3	1:Q:38:SER:HB3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:363:ASP:HB2	1:W:8:HIS:CE1	2.32	0.64
1:O:319:TRP:HE1	1:Q:12:ARG:HB3	1.64	0.63
1:A:9:VAL:HA	1:A:12:ARG:HG3	1.80	0.63
2:R:1870:LEU:HD22	2:R:1876:TYR:HD2	1.62	0.63
1:M:4:GLY:N	1:M:6:MET:SD	2.71	0.63
1:U:323:ASN:ND2	1:W:12:ARG:HD2	2.14	0.63
1:U:163:PHE:HZ	1:U:168:ARG:N	1.95	0.63
2:D:1873:LEU:HB3	1:E:58:TYR:OH	1.99	0.63
2:L:1876:TYR:HD1	2:L:1877:ARG:H	1.42	0.62
2:V:1870:LEU:CD2	2:V:1876:TYR:CD1	2.81	0.62
1:U:338:ALA:HB2	1:W:12:ARG:HH21	1.64	0.62
2:V:1873:LEU:HB3	2:V:1874:PRO:HD3	1.82	0.62
1:A:120:ARG:HA	1:A:123:ASP:OD1	2.00	0.62
1:U:163:PHE:CE2	1:U:168:ARG:HB2	2.35	0.61
1:S:12:ARG:NH1	1:W:323:ASN:OD1	2.33	0.61
1:U:163:PHE:CE1	1:U:167:VAL:HB	2.35	0.61
2:J:1902:PHE:CE2	2:J:1904:MET:HE2	2.36	0.61
1:E:29:LYS:NZ	2:F:1918:ASN:OD1	2.34	0.61
1:C:367:VAL:HG11	1:E:5:SER:HB2	1.81	0.61
1:M:4:GLY:CA	1:M:6:MET:CE	2.78	0.61
2:H:1873:LEU:O	2:H:1875:GLY:N	2.33	0.60
1:I:323:ASN:HB3	1:K:9:VAL:HG13	1.82	0.60
2:L:1876:TYR:CD1	2:L:1877:ARG:N	2.68	0.60
1:W:316:ARG:HH21	2:X:1903:TYR:HB2	1.66	0.60
1:A:360:ASN:ND2	1:C:12:ARG:HG2	2.16	0.60
1:U:360:ASN:CG	1:W:12:ARG:HG2	2.22	0.60
1:I:240:ASN:ND2	2:J:1908:GLN:HB2	2.09	0.59
1:M:323:ASN:HB3	1:O:9:VAL:HG13	1.84	0.59
2:J:1902:PHE:CE2	2:J:1904:MET:CE	2.86	0.59
2:V:1870:LEU:CD2	2:V:1876:TYR:CE1	2.77	0.59
1:W:366:MET:O	1:W:367:VAL:HG13	2.03	0.58
1:A:233:ALA:HA	1:A:236:ARG:HD3	1.85	0.58
2:L:1918:ASN:O	2:L:1922:GLU:HB2	2.03	0.58
1:M:323:ASN:HB3	1:O:9:VAL:HG22	1.84	0.58
2:B:1870:LEU:HD13	1:C:87:THR:HG21	1.83	0.58
2:P:1867:ASN:HA	2:P:1870:LEU:HD12	1.86	0.58
1:S:158:GLN:HG3	1:S:163:PHE:HZ	1.67	0.58
1:Q:152:PHE:CD2	1:Q:167:VAL:HG22	2.35	0.58
1:Q:186:THR:HG22	1:Q:194:GLN:NE2	2.18	0.58
2:R:1924:GLN:HG2	2:R:1925:GLN:OE1	2.04	0.58
1:U:319:TRP:NE1	1:W:12:ARG:HB3	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:163:PHE:HE1	1:U:167:VAL:HB	1.67	0.57
1:W:331:HIS:CD2	1:W:367:VAL:HG23	2.38	0.57
2:R:1870:LEU:CD2	2:R:1876:TYR:CD2	2.87	0.57
1:M:279:TYR:CE2	2:N:1903:TYR:HD1	2.22	0.57
1:A:323:ASN:HB2	1:C:12:ARG:HD3	1.87	0.56
1:C:53:THR:O	1:C:57:ILE:HG12	2.05	0.56
1:A:75:LEU:HD12	1:A:104:THR:HG22	1.88	0.56
1:I:51:LEU:HD22	1:I:88:ILE:HG21	1.86	0.56
1:G:12:ARG:HD3	1:K:323:ASN:HB2	1.87	0.56
1:Q:352:SER:O	1:Q:356:THR:HG23	2.06	0.56
1:W:29:LYS:HE2	2:X:1917:TRP:O	2.05	0.56
2:L:1866:GLY:HA3	2:L:1871:LEU:HD12	1.87	0.56
2:N:1870:LEU:HD13	2:N:1876:TYR:H	1.71	0.56
1:W:53:THR:O	1:W:57:ILE:HG12	2.06	0.56
1:Q:53:THR:O	1:Q:57:ILE:HG12	2.05	0.56
1:A:121:HIS:CD2	1:A:137:ALA:HB2	2.40	0.56
1:U:363:ASP:HB2	1:W:8:HIS:HE1	1.71	0.56
1:E:53:THR:O	1:E:57:ILE:HG12	2.06	0.55
2:X:1906:THR:HG22	2:X:1907:CYS:H	1.71	0.55
1:K:53:THR:O	1:K:57:ILE:HG12	2.05	0.55
1:O:53:THR:O	1:O:57:ILE:HG12	2.06	0.55
1:I:56:ALA:HB1	2:J:1920:ILE:HG22	1.89	0.55
2:J:1876:TYR:CD1	2:J:1877:ARG:N	2.67	0.55
1:Q:186:THR:HG22	1:Q:194:GLN:HE21	1.70	0.55
1:S:12:ARG:HG2	1:W:360:ASN:HD21	1.70	0.55
1:C:154:CYS:N	1:C:155:PRO:O	2.39	0.55
2:T:1869:ALA:HB2	1:U:87:THR:HG21	1.89	0.55
1:U:53:THR:O	1:U:57:ILE:HG12	2.06	0.55
1:A:53:THR:O	1:A:57:ILE:HG12	2.06	0.55
2:J:1902:PHE:CZ	2:J:1904:MET:HE2	2.41	0.55
1:I:53:THR:O	1:I:57:ILE:HG12	2.08	0.54
2:V:1923:LEU:O	2:V:1925:GLN:N	2.35	0.54
1:G:158:GLN:HG3	1:G:163:PHE:CE1	2.43	0.54
1:O:351:LYS:HD2	1:Q:39:PHE:CE1	2.41	0.54
1:I:76:GLU:O	1:I:80:HIS:ND1	2.40	0.54
1:A:311:ARG:HG2	1:A:347:GLU:OE2	2.07	0.54
1:A:49:GLU:HB3	2:F:1878:PRO:HA	1.88	0.54
2:R:1873:LEU:O	2:R:1875:GLY:N	2.40	0.54
1:A:356:THR:HG21	1:C:14:GLU:HA	1.89	0.54
1:M:76:GLU:O	1:M:80:HIS:ND1	2.41	0.54
2:V:1873:LEU:HB3	2:V:1874:PRO:CD	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:186:THR:HG22	1:S:194:GLN:NE2	2.22	0.53
2:R:1870:LEU:CD2	2:R:1876:TYR:HD2	2.21	0.53
1:A:76:GLU:O	1:A:80:HIS:ND1	2.42	0.53
1:A:16:SER:OG	1:A:19:GLU:HB2	2.08	0.53
1:Q:29:LYS:NZ	2:R:1918:ASN:OD1	2.42	0.53
2:H:1874:PRO:HG2	1:I:58:TYR:CE1	2.43	0.53
1:G:53:THR:O	1:G:57:ILE:HG12	2.08	0.53
1:C:76:GLU:O	1:C:80:HIS:ND1	2.42	0.52
1:M:186:THR:HG22	1:M:194:GLN:NE2	2.24	0.52
1:U:319:TRP:CD1	1:W:12:ARG:HD3	2.44	0.52
2:X:1876:TYR:CG	2:X:1877:ARG:N	2.76	0.52
1:G:44:VAL:HG13	2:L:1874:PRO:HB2	1.90	0.52
1:A:60:GLN:HE21	2:B:1919:ARG:HB3	1.74	0.52
1:M:4:GLY:HA3	1:M:6:MET:SD	2.48	0.52
1:I:56:ALA:HA	2:J:1919:ARG:HH11	1.74	0.52
1:M:53:THR:O	1:M:57:ILE:HG13	2.10	0.52
1:A:75:LEU:HD12	1:A:104:THR:CG2	2.39	0.52
1:C:256:GLU:OE1	1:G:90:ASP:HA	2.10	0.52
1:S:7:PHE:HB3	1:W:363:ASP:OD2	2.10	0.52
1:S:61:LEU:HD22	1:S:65:TYR:CE2	2.46	0.51
1:A:323:ASN:OD1	1:C:9:VAL:HG13	2.11	0.51
1:I:363:ASP:OD2	1:K:7:PHE:HB2	2.11	0.51
1:E:352:SER:O	1:E:356:THR:HG23	2.10	0.51
1:U:246:ILE:HG21	2:V:1902:PHE:HE2	1.76	0.51
1:I:319:TRP:HZ2	1:K:13:MET:HG2	1.76	0.51
1:Q:160:VAL:HG13	1:Q:163:PHE:CE2	2.46	0.51
1:S:352:SER:O	1:S:356:THR:HG23	2.11	0.51
1:A:351:LYS:HD2	1:C:39:PHE:CE1	2.46	0.51
1:K:96:LYS:NZ	1:K:136:ARG:HH12	2.07	0.51
1:Q:9:VAL:HA	1:Q:12:ARG:CD	2.25	0.51
1:Q:61:LEU:HD22	1:Q:65:TYR:CE2	2.46	0.51
1:I:319:TRP:HE1	1:K:12:ARG:CB	2.24	0.51
1:S:53:THR:O	1:S:57:ILE:HG13	2.11	0.51
1:E:56:ALA:HA	2:F:1919:ARG:HH11	1.76	0.51
1:U:323:ASN:HD21	1:W:12:ARG:HD2	1.74	0.51
1:C:61:LEU:HD22	1:C:65:TYR:CE2	2.46	0.51
1:G:246:ILE:HG21	2:H:1904:MET:HG2	1.93	0.51
1:K:247:PHE:HE1	2:L:1902:PHE:CE1	2.29	0.50
2:V:1873:LEU:CB	2:V:1874:PRO:HD3	2.41	0.50
1:A:61:LEU:HD22	1:A:65:TYR:CE2	2.47	0.50
1:M:9:VAL:HG13	1:Q:323:ASN:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:THR:HG21	1:E:14:GLU:HA	1.94	0.50
1:U:9:VAL:HA	1:U:12:ARG:HG3	1.94	0.50
2:B:1871:LEU:HD23	2:B:1876:TYR:CE2	2.47	0.50
1:I:61:LEU:HD22	1:I:65:TYR:CE2	2.47	0.50
1:K:61:LEU:HD22	1:K:65:TYR:CE2	2.47	0.50
1:U:319:TRP:HD1	1:W:12:ARG:HD3	1.76	0.50
1:U:360:ASN:OD1	1:W:12:ARG:HG2	2.12	0.50
1:U:61:LEU:HD22	1:U:65:TYR:CE2	2.47	0.50
1:A:335:MET:O	1:A:339:GLU:HG3	2.12	0.49
1:A:140:ASN:O	1:A:144:VAL:HG23	2.12	0.49
1:O:61:LEU:HD22	1:O:65:TYR:CE2	2.47	0.49
1:M:12:ARG:NE	1:Q:323:ASN:HB3	2.27	0.49
1:A:86:ARG:HG3	1:A:94:GLU:OE1	2.12	0.49
1:U:360:ASN:HD21	1:W:12:ARG:HG2	1.75	0.49
1:W:61:LEU:HD22	1:W:65:TYR:CE2	2.48	0.49
1:E:154:CYS:N	1:E:155:PRO:HD2	2.28	0.49
1:G:61:LEU:HD22	1:G:65:TYR:CE2	2.48	0.49
1:I:56:ALA:CB	2:J:1920:ILE:HG22	2.43	0.49
1:M:140:ASN:O	1:M:144:VAL:HG23	2.12	0.49
1:Q:5:SER:HA	1:Q:8:HIS:CD2	2.47	0.49
2:T:1876:TYR:CG	2:T:1877:ARG:N	2.80	0.49
2:V:1870:LEU:CD1	2:V:1876:TYR:CE2	2.80	0.49
2:F:1916:ASP:O	2:F:1918:ASN:N	2.37	0.49
1:W:4:GLY:HA2	1:W:7:PHE:CD1	2.47	0.49
1:E:61:LEU:HD22	1:E:65:TYR:CE2	2.48	0.49
1:Q:332:ASP:OD1	1:Q:333:GLN:N	2.45	0.49
2:R:1920:ILE:HG22	2:R:1923:LEU:HD11	1.94	0.49
1:A:262:LEU:HG	1:A:266:ARG:HD2	1.95	0.48
1:A:12:ARG:HD3	1:E:323:ASN:CB	2.44	0.48
1:C:356:THR:CG2	1:E:14:GLU:HA	2.43	0.48
1:G:243:ASN:ND2	2:H:1906:THR:O	2.46	0.48
2:H:1876:TYR:HB2	1:I:48:THR:O	2.14	0.48
1:M:61:LEU:HD22	1:M:65:TYR:CE2	2.48	0.48
1:O:323:ASN:OD1	1:Q:12:ARG:NH1	2.45	0.48
1:O:40:PHE:HB3	1:O:61:LEU:HG	1.96	0.48
1:Q:158:GLN:HA	1:Q:159:ASP:HA	1.56	0.48
2:X:1870:LEU:C	2:X:1872:SER:H	2.17	0.48
1:O:3:LEU:HB3	1:O:6:MET:HG3	1.95	0.48
1:E:279:TYR:CE2	2:F:1903:TYR:HD2	2.32	0.48
2:R:1922:GLU:O	2:R:1924:GLN:N	2.46	0.48
1:A:355:LEU:HD12	1:C:20:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:51:LEU:H	1:M:51:LEU:HD23	1.78	0.47
1:I:3:LEU:C	1:I:5:SER:H	2.17	0.47
1:O:159:ASP:HB2	1:O:163:PHE:CE1	2.49	0.47
1:W:209:GLY:HA2	1:W:211:PHE:CE2	2.49	0.47
1:I:279:TYR:HE2	2:J:1903:TYR:HD2	1.62	0.47
1:K:247:PHE:HE1	2:L:1902:PHE:HE1	1.62	0.47
1:Q:60:GLN:HE21	2:R:1919:ARG:HB3	1.80	0.47
1:I:243:ASN:ND2	1:I:258:TYR:OH	2.43	0.47
2:T:1924:GLN:H	2:T:1925:GLN:HA	1.79	0.47
1:S:323:ASN:OD1	1:U:12:ARG:HD3	2.13	0.47
1:S:352:SER:HA	1:U:20:LEU:HD21	1.96	0.47
1:A:359:LEU:HD13	1:C:11:TYR:CE1	2.49	0.47
2:F:1907:CYS:O	2:F:1908:GLN:HB2	2.14	0.47
1:M:269:LYS:HE2	1:M:269:LYS:HB3	1.72	0.47
1:O:140:ASN:O	1:O:144:VAL:HG23	2.15	0.47
1:S:40:PHE:HB3	1:S:61:LEU:HG	1.96	0.47
2:J:1920:ILE:HG13	2:J:1921:ALA:N	2.29	0.47
1:A:40:PHE:HB3	1:A:61:LEU:HG	1.97	0.46
2:L:1867:ASN:O	2:L:1870:LEU:HB3	2.15	0.46
2:T:1879:THR:HG22	2:T:1880:THR:N	2.30	0.46
1:A:87:THR:CG2	2:F:1870:LEU:HB3	2.41	0.46
1:I:140:ASN:O	1:I:144:VAL:HG23	2.15	0.46
1:O:351:LYS:HE3	1:Q:38:SER:CB	2.44	0.46
1:S:140:ASN:O	1:S:144:VAL:HG23	2.15	0.46
1:K:140:ASN:O	1:K:144:VAL:HG23	2.16	0.46
1:C:360:ASN:OD1	1:E:12:ARG:HA	2.16	0.46
1:K:40:PHE:HB3	1:K:61:LEU:HG	1.98	0.46
1:O:320:SER:HA	1:O:323:ASN:HD22	1.80	0.46
2:P:1873:LEU:CD1	1:Q:84:LEU:HB2	2.45	0.46
1:M:12:ARG:HE	1:Q:323:ASN:HB3	1.81	0.46
1:K:52:LYS:HE2	2:L:1923:LEU:HG	1.98	0.46
1:M:7:PHE:CZ	1:M:11:TYR:HD2	2.34	0.46
1:Q:40:PHE:HB3	1:Q:61:LEU:HG	1.98	0.46
1:E:140:ASN:O	1:E:144:VAL:HG23	2.15	0.46
2:T:1915:ASP:O	2:T:1917:TRP:N	2.45	0.46
1:C:140:ASN:O	1:C:144:VAL:HG23	2.15	0.46
1:W:140:ASN:O	1:W:144:VAL:HG23	2.15	0.46
2:H:1873:LEU:HD13	1:I:84:LEU:HB2	1.98	0.46
2:L:1869:ALA:O	2:L:1870:LEU:C	2.54	0.46
1:M:316:ARG:HH21	2:N:1903:TYR:HB2	1.81	0.46
2:T:1879:THR:HG22	2:T:1880:THR:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:319:TRP:O	1:I:323:ASN:ND2	2.49	0.45
2:B:1871:LEU:HA	2:B:1876:TYR:HE2	1.80	0.45
1:K:156:GLY:O	1:K:158:GLN:HG3	2.16	0.45
1:S:12:ARG:HG2	1:W:360:ASN:CG	2.36	0.45
1:A:163:PHE:HE2	1:A:168:ARG:HD3	1.80	0.45
1:A:262:LEU:HD11	1:A:266:ARG:HH11	1.81	0.45
1:W:91:GLN:HG3	1:W:92:LEU:H	1.81	0.45
2:L:1869:ALA:O	2:L:1871:LEU:N	2.49	0.45
1:M:60:GLN:HE21	2:N:1919:ARG:HB3	1.82	0.45
1:S:203:ASN:OD1	2:T:1907:CYS:HB2	2.17	0.45
1:E:40:PHE:HB3	1:E:61:LEU:HG	1.98	0.45
1:O:328:LEU:HD23	1:O:328:LEU:HA	1.85	0.45
2:R:1920:ILE:HA	2:R:1923:LEU:HD21	1.99	0.45
1:S:154:CYS:HB3	1:S:155:PRO:HD2	1.99	0.45
2:B:1903:TYR:CG	2:B:1904:MET:N	2.85	0.45
1:G:140:ASN:O	1:G:144:VAL:HG23	2.17	0.45
1:U:140:ASN:O	1:U:144:VAL:HG23	2.16	0.45
2:X:1876:TYR:CD1	2:X:1877:ARG:N	2.83	0.45
1:Q:140:ASN:O	1:Q:144:VAL:HG23	2.16	0.45
2:V:1874:PRO:HG3	1:W:54:LEU:HD11	1.99	0.45
2:J:1902:PHE:CE2	2:J:1904:MET:HG2	2.51	0.45
1:G:332:ASP:OD1	1:G:333:GLN:N	2.51	0.44
1:S:14:GLU:O	1:W:356:THR:HG21	2.17	0.44
1:U:316:ARG:HD3	1:U:316:ARG:HA	1.71	0.44
1:A:96:LYS:HA	1:A:96:LYS:HD3	1.83	0.44
1:I:40:PHE:HB3	1:I:61:LEU:HG	1.99	0.44
1:O:279:TYR:CE2	2:P:1903:TYR:HB3	2.44	0.44
1:S:60:GLN:HE21	2:T:1919:ARG:HB3	1.82	0.44
1:W:40:PHE:HB3	1:W:61:LEU:HG	1.98	0.44
1:G:12:ARG:HG2	1:K:360:ASN:OD1	2.17	0.44
1:M:40:PHE:HB3	1:M:61:LEU:HG	1.99	0.44
2:N:1877:ARG:O	1:O:49:GLU:HG2	2.16	0.44
1:S:186:THR:HG22	1:S:194:GLN:HE21	1.82	0.44
1:C:40:PHE:HB3	1:C:61:LEU:HG	1.98	0.44
1:O:159:ASP:HB2	1:O:163:PHE:HE1	1.81	0.44
2:T:1922:GLU:O	2:T:1923:LEU:HD12	2.17	0.44
1:I:51:LEU:HD12	1:I:51:LEU:C	2.38	0.44
1:K:161:GLY:O	1:K:162:GLU:HB3	2.18	0.44
1:S:332:ASP:OD1	1:S:333:GLN:N	2.51	0.44
1:K:332:ASP:OD1	1:K:333:GLN:N	2.50	0.44
2:R:1910:GLU:HA	2:R:1911:PRO:HD3	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:328:LEU:HD23	1:U:328:LEU:HA	1.85	0.44
1:A:352:SER:O	1:A:356:THR:HG23	2.17	0.44
1:C:332:ASP:OD1	1:C:333:GLN:N	2.51	0.44
1:K:88:ILE:HA	1:M:131:LYS:HG3	1.99	0.44
1:M:332:ASP:OD1	1:M:333:GLN:N	2.51	0.44
1:U:5:SER:CA	1:U:8:HIS:CE1	2.77	0.44
1:W:332:ASP:OD1	1:W:333:GLN:N	2.51	0.44
1:W:8:HIS:C	1:W:10:ARG:H	2.20	0.44
1:A:367:VAL:HG21	1:C:2:PRO:CG	2.41	0.43
1:S:316:ARG:HH21	2:T:1903:TYR:HB3	1.83	0.43
1:U:356:THR:CG2	1:W:15:ALA:HB2	2.48	0.43
2:B:1878:PRO:HB3	1:C:49:GLU:HB3	2.00	0.43
1:C:316:ARG:HH21	2:D:1903:TYR:HB2	1.82	0.43
2:J:1910:GLU:HA	2:J:1911:PRO:HD3	1.89	0.43
2:P:1876:TYR:HD1	2:P:1877:ARG:N	2.15	0.43
1:A:12:ARG:NH1	1:E:323:ASN:HB3	2.29	0.43
1:Q:109:GLY:HA2	1:Q:111:PHE:CE2	2.52	0.43
1:I:332:ASP:OD1	1:I:333:GLN:N	2.50	0.43
1:A:332:ASP:OD1	1:A:333:GLN:N	2.51	0.43
1:C:29:LYS:HD2	2:D:1918:ASN:ND2	2.34	0.43
1:E:332:ASP:OD1	1:E:333:GLN:N	2.52	0.43
1:W:150:LYS:NZ	2:X:1909:ASP:OD2	2.52	0.43
2:F:1873:LEU:HA	2:F:1874:PRO:HD3	1.82	0.43
1:G:40:PHE:HB3	1:G:61:LEU:HG	2.00	0.43
1:O:332:ASP:OD1	1:O:333:GLN:N	2.51	0.43
1:A:73:LYS:HD3	1:A:73:LYS:HA	1.71	0.43
1:C:111:PHE:O	1:C:115:ILE:HG12	2.18	0.43
1:A:128:LEU:HD23	1:A:128:LEU:HA	1.82	0.43
1:I:233:ALA:HA	1:I:236:ARG:HG2	2.00	0.43
1:O:63:ASN:HB3	2:P:1914:LEU:HD21	2.01	0.43
2:T:1870:LEU:HB3	2:T:1871:LEU:H	1.70	0.43
1:O:3:LEU:HD22	1:O:6:MET:HG3	2.01	0.43
1:G:53:THR:O	1:G:56:ALA:HB3	2.19	0.43
1:K:159:ASP:CB	1:K:211:PHE:HZ	2.31	0.43
1:U:40:PHE:HB3	1:U:61:LEU:HG	2.00	0.43
1:O:360:ASN:OD1	1:Q:12:ARG:HG2	2.19	0.42
2:B:1876:TYR:HA	1:C:48:THR:O	2.19	0.42
1:G:59:SER:HB3	2:H:1919:ARG:HH12	1.84	0.42
1:M:111:PHE:O	1:M:115:ILE:HG12	2.19	0.42
1:A:87:THR:HG21	2:F:1870:LEU:CB	2.45	0.42
2:L:1871:LEU:HD23	2:L:1871:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:356:THR:HG21	1:E:14:GLU:CA	2.49	0.42
1:I:266:ARG:NH1	1:I:274:GLU:OE1	2.50	0.42
2:J:1914:LEU:HD12	2:J:1914:LEU:HA	1.91	0.42
1:W:56:ALA:HA	2:X:1919:ARG:HE	1.84	0.42
1:C:108:LEU:HA	1:C:108:LEU:HD23	1.72	0.42
2:H:1924:GLN:HB3	2:H:1925:GLN:H	1.53	0.42
1:A:323:ASN:CB	1:C:12:ARG:HD3	2.49	0.42
1:U:323:ASN:CG	1:W:12:ARG:HD2	2.39	0.42
2:J:1902:PHE:HE2	2:J:1904:MET:HE2	1.83	0.42
1:K:5:SER:O	1:K:5:SER:OG	2.38	0.42
1:K:61:LEU:HD23	1:K:61:LEU:HA	1.93	0.42
1:Q:243:ASN:ND2	2:R:1906:THR:O	2.52	0.42
1:W:235:ARG:HB2	1:W:264:LEU:HD23	2.02	0.42
1:C:156:GLY:O	1:C:158:GLN:HG3	2.19	0.42
2:F:1910:GLU:HA	2:F:1911:PRO:HD3	1.80	0.42
2:V:1915:ASP:O	2:V:1917:TRP:N	2.51	0.42
1:A:129:ASN:CG	1:A:129:ASN:O	2.58	0.42
1:A:328:LEU:HD23	1:A:328:LEU:HA	1.86	0.42
1:C:29:LYS:HD2	2:D:1918:ASN:HD21	1.85	0.42
1:C:359:LEU:HA	1:C:359:LEU:HD23	1.80	0.41
1:W:352:SER:O	1:W:356:THR:HG23	2.19	0.41
1:E:61:LEU:HD23	1:E:61:LEU:HA	1.94	0.41
2:H:1875:GLY:O	2:H:1876:TYR:HB3	2.20	0.41
2:P:1867:ASN:CA	2:P:1870:LEU:HD12	2.49	0.41
1:A:351:LYS:HE3	1:C:38:SER:HB3	2.02	0.41
1:C:351:LYS:HD2	1:E:39:PHE:CE1	2.56	0.41
1:M:49:GLU:HA	2:R:1876:TYR:CD1	2.48	0.41
2:N:1873:LEU:HA	2:N:1874:PRO:HD3	1.85	0.41
2:X:1906:THR:HG22	2:X:1907:CYS:N	2.34	0.41
1:G:158:GLN:HG3	1:G:163:PHE:HE1	1.83	0.41
2:P:1902:PHE:HD1	2:P:1903:TYR:H	1.67	0.41
1:A:61:LEU:HD23	1:A:61:LEU:HA	1.95	0.41
1:K:60:GLN:HE21	2:L:1919:ARG:HB3	1.86	0.41
1:O:352:SER:O	1:O:356:THR:HG23	2.20	0.41
1:M:323:ASN:CB	1:O:9:VAL:HG13	2.50	0.41
1:G:111:PHE:O	1:G:115:ILE:HG12	2.21	0.41
1:G:328:LEU:HD23	1:G:328:LEU:HA	1.85	0.41
1:K:154:CYS:HB2	1:K:155:PRO:HD3	2.02	0.41
1:O:316:ARG:HH21	2:P:1903:TYR:HB2	1.84	0.41
1:W:111:PHE:O	1:W:115:ILE:HG12	2.20	0.41
1:G:4:GLY:HA3	1:K:366:MET:SD	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:ARG:NH1	1:C:12:ARG:HB3	2.36	0.41
1:E:111:PHE:O	1:E:115:ILE:HG12	2.21	0.41
1:A:111:PHE:O	1:A:115:ILE:HG12	2.21	0.41
1:G:158:GLN:HG3	1:G:163:PHE:CZ	2.56	0.41
1:I:111:PHE:O	1:I:115:ILE:HG12	2.21	0.41
1:A:14:GLU:HB3	1:A:15:ALA:H	1.53	0.40
1:S:246:ILE:HG21	2:T:1902:PHE:HE2	1.86	0.40
1:C:344:ILE:O	1:C:348:VAL:HG22	2.21	0.40
1:K:243:ASN:ND2	2:L:1906:THR:O	2.54	0.40
1:O:360:ASN:HD21	1:Q:12:ARG:HG2	1.87	0.40
2:P:1877:ARG:HA	2:P:1878:PRO:HD3	1.95	0.40
2:T:1899:ARG:N	1:U:14:GLU:OE2	2.54	0.40
1:U:163:PHE:CZ	1:U:168:ARG:HB2	2.56	0.40
1:C:316:ARG:NH2	2:D:1903:TYR:HB2	2.36	0.40
2:D:1910:GLU:HA	2:D:1911:PRO:HD3	1.83	0.40
1:O:344:ILE:O	1:O:348:VAL:HG22	2.22	0.40
1:U:111:PHE:O	1:U:115:ILE:HG12	2.21	0.40
1:W:4:GLY:HA2	1:W:7:PHE:HD1	1.84	0.40
1:G:344:ILE:O	1:G:348:VAL:HG22	2.22	0.40
1:K:7:PHE:HB3	1:K:11:TYR:CD2	2.57	0.40
1:W:328:LEU:HD23	1:W:328:LEU:HA	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	363/367 (99%)	352 (97%)	6 (2%)	5 (1%)	11 47
1	C	365/367 (100%)	352 (96%)	7 (2%)	6 (2%)	9 45
1	E	364/367 (99%)	349 (96%)	8 (2%)	7 (2%)	8 41
1	G	365/367 (100%)	346 (95%)	17 (5%)	2 (0%)	29 68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	I	365/367 (100%)	352 (96%)	13 (4%)	0	100 100
1	K	364/367 (99%)	351 (96%)	10 (3%)	3 (1%)	19 60
1	M	364/367 (99%)	351 (96%)	10 (3%)	3 (1%)	19 60
1	O	363/367 (99%)	350 (96%)	12 (3%)	1 (0%)	41 76
1	Q	365/367 (100%)	352 (96%)	10 (3%)	3 (1%)	19 60
1	S	358/367 (98%)	345 (96%)	9 (2%)	4 (1%)	14 52
1	U	364/367 (99%)	351 (96%)	12 (3%)	1 (0%)	41 76
1	W	364/367 (99%)	347 (95%)	14 (4%)	3 (1%)	19 60
2	B	41/71 (58%)	25 (61%)	11 (27%)	5 (12%)	0 5
2	D	32/71 (45%)	24 (75%)	6 (19%)	2 (6%)	1 19
2	F	33/71 (46%)	22 (67%)	8 (24%)	3 (9%)	1 12
2	H	32/71 (45%)	21 (66%)	4 (12%)	7 (22%)	0 1
2	J	36/71 (51%)	25 (69%)	7 (19%)	4 (11%)	0 8
2	L	40/71 (56%)	26 (65%)	10 (25%)	4 (10%)	0 10
2	N	35/71 (49%)	19 (54%)	14 (40%)	2 (6%)	1 20
2	P	39/71 (55%)	24 (62%)	13 (33%)	2 (5%)	2 22
2	R	36/71 (51%)	19 (53%)	12 (33%)	5 (14%)	0 4
2	T	41/71 (58%)	27 (66%)	11 (27%)	3 (7%)	1 16
2	V	35/71 (49%)	22 (63%)	10 (29%)	3 (9%)	1 13
2	X	36/71 (51%)	21 (58%)	9 (25%)	6 (17%)	0 3
All	All	4800/5256 (91%)	4473 (93%)	243 (5%)	84 (2%)	8 42

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	15	ALA
1	C	14	GLU
1	C	155	PRO
1	E	8	HIS
1	E	157	PRO
1	G	15	ALA
1	G	164	PRO
2	H	1874	PRO
2	H	1876	TYR

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Mol	Chain	Res	Type
2	H	1917	TRP
1	K	165	GLU
1	O	15	ALA
2	R	1923	LEU
1	S	15	ALA
1	S	154	CYS
1	S	155	PRO
2	T	1916	ASP
2	V	1873	LEU
2	V	1924	GLN
1	W	366	MET
1	A	4	GLY
2	B	1875	GLY
1	C	163	PHE
1	E	4	GLY
2	H	1924	GLN
2	J	1877	ARG
2	J	1908	GLN
2	L	1877	ARG
1	M	7	PHE
2	N	1908	GLN
2	P	1924	GLN
1	U	8	HIS
2	V	1925	GLN
2	X	1915	ASP
1	A	159	ASP
2	B	1877	ARG
2	B	1902	PHE
2	B	1908	GLN
1	C	13	MET
2	D	1908	GLN
1	E	14	GLU
1	E	15	ALA
2	F	1902	PHE
2	F	1916	ASP
2	H	1908	GLN
1	K	14	GLU
2	L	1870	LEU
2	L	1911	PRO
2	R	1908	GLN
2	R	1915	ASP
1	W	157	PRO

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Mol	Chain	Res	Type
2	X	1878	PRO
2	X	1908	GLN
2	D	1877	ARG
1	E	160	VAL
2	H	1877	ARG
1	K	160	VAL
2	L	1874	PRO
2	N	1926	ARG
2	P	1877	ARG
1	Q	157	PRO
1	Q	160	VAL
2	R	1877	ARG
2	T	1876	TYR
2	T	1877	ARG
2	X	1876	TYR
1	C	152	PHE
1	C	160	VAL
2	F	1917	TRP
2	J	1874	PRO
2	J	1921	ALA
1	Q	16	SER
1	S	14	GLU
2	X	1877	ARG
1	E	155	PRO
1	M	16	SER
1	M	159	ASP
2	R	1874	PRO
1	W	154	CYS
2	X	1874	PRO
2	B	1866	GLY
2	H	1878	PRO
1	A	154	CYS

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	285/291 (98%)	276 (97%)	9 (3%)	39 62
1	C	287/291 (99%)	280 (98%)	7 (2%)	49 69
1	E	275/291 (94%)	272 (99%)	3 (1%)	73 85
1	G	278/291 (96%)	271 (98%)	7 (2%)	47 68
1	I	279/291 (96%)	275 (99%)	4 (1%)	67 81
1	K	283/291 (97%)	278 (98%)	5 (2%)	59 77
1	M	279/291 (96%)	276 (99%)	3 (1%)	73 85
1	O	282/291 (97%)	274 (97%)	8 (3%)	43 65
1	Q	282/291 (97%)	276 (98%)	6 (2%)	53 72
1	S	279/291 (96%)	276 (99%)	3 (1%)	73 85
1	U	281/291 (97%)	275 (98%)	6 (2%)	53 72
1	W	279/291 (96%)	273 (98%)	6 (2%)	52 71
2	B	32/58 (55%)	31 (97%)	1 (3%)	40 63
2	D	29/58 (50%)	27 (93%)	2 (7%)	15 42
2	F	29/58 (50%)	26 (90%)	3 (10%)	7 27
2	H	30/58 (52%)	29 (97%)	1 (3%)	38 62
2	J	32/58 (55%)	31 (97%)	1 (3%)	40 63
2	L	35/58 (60%)	33 (94%)	2 (6%)	20 48
2	N	32/58 (55%)	32 (100%)	0	100 100
2	P	31/58 (53%)	29 (94%)	2 (6%)	17 44
2	R	33/58 (57%)	28 (85%)	5 (15%)	3 16
2	T	34/58 (59%)	32 (94%)	2 (6%)	19 47
2	V	31/58 (53%)	31 (100%)	0	100 100
2	X	30/58 (52%)	26 (87%)	4 (13%)	4 20
All	All	3747/4188 (90%)	3657 (98%)	90 (2%)	49 69

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	TYR
1	A	17	CYS
1	A	29	LYS
1	A	34	ARG
1	A	90	ASP
1	A	123	ASP

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Mol	Chain	Res	Type
1	A	127	GLU
1	A	228	PHE
1	A	363	ASP
2	B	1919	ARG
1	C	3	LEU
1	C	12	ARG
1	C	30	SER
1	C	86	ARG
1	C	121	HIS
1	C	163	PHE
1	C	363	ASP
2	D	1876	TYR
2	D	1918	ASN
1	E	5	SER
1	E	121	HIS
1	E	363	ASP
2	F	1870	LEU
2	F	1902	PHE
2	F	1909	ASP
1	G	12	ARG
1	G	121	HIS
1	G	136	ARG
1	G	163	PHE
1	G	179	GLU
1	G	316	ARG
1	G	363	ASP
2	H	1916	ASP
1	I	7	PHE
1	I	11	TYR
1	I	121	HIS
1	I	266	ARG
2	J	1904	MET
1	K	8	HIS
1	K	11	TYR
1	K	121	HIS
1	K	163	PHE
1	K	363	ASP
2	L	1902	PHE
2	L	1904	MET
1	M	51	LEU
1	M	96	LYS
1	M	121	HIS

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Mol	Chain	Res	Type
1	O	11	TYR
1	O	121	HIS
1	O	131	LYS
1	O	159	ASP
1	O	163	PHE
1	O	340	LYS
1	O	363	ASP
1	O	366	MET
2	P	1876	TYR
2	P	1902	PHE
1	Q	11	TYR
1	Q	34	ARG
1	Q	96	LYS
1	Q	121	HIS
1	Q	168	ARG
1	Q	363	ASP
2	R	1876	TYR
2	R	1904	MET
2	R	1909	ASP
2	R	1924	GLN
2	R	1925	GLN
1	S	12	ARG
1	S	121	HIS
1	S	363	ASP
2	T	1903	TYR
2	T	1907	CYS
1	U	34	ARG
1	U	96	LYS
1	U	121	HIS
1	U	163	PHE
1	U	355	LEU
1	U	366	MET
1	W	7	PHE
1	W	26	ARG
1	W	90	ASP
1	W	121	HIS
1	W	363	ASP
1	W	366	MET
2	X	1870	LEU
2	X	1902	PHE
2	X	1904	MET
2	X	1924	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	360	ASN
2	F	1908	GLN
1	G	323	ASN
2	H	1908	GLN
1	I	240	ASN
1	I	243	ASN
1	I	360	ASN
1	M	203	ASN
2	P	1924	GLN
1	S	8	HIS
1	S	205	HIS
1	U	8	HIS
1	W	8	HIS
1	W	60	GLN
1	W	331	HIS

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.