



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:37 PM EDT

PDB ID : 4GZA / pdb_00004gza
Title : Complex of mouse Plexin A2 - Semaphorin 3A - Neuropilin-1
Authors : Janssen, B.J.C.; Malinauskas, T.; Siebold, C.; Jones, E.Y.
Deposited on : 2012-09-06
Resolution : 7.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

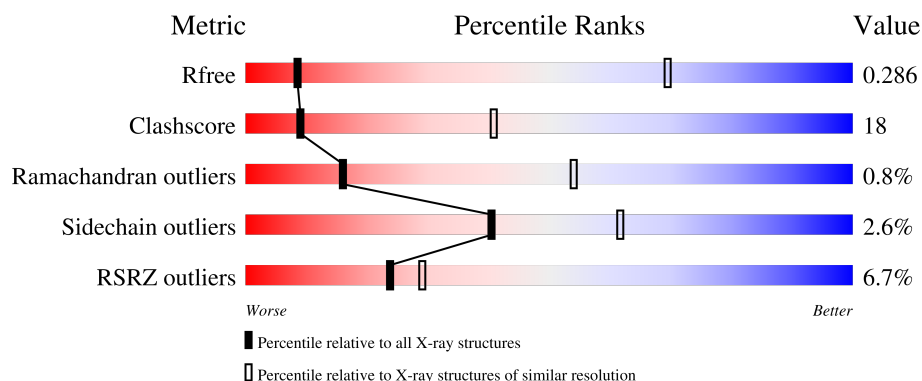
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1167 (10.00-4.00)
Clashscore	190562	1007 (9.70-4.04)
Ramachandran outliers	187476	1054 (10.00-4.00)
Sidechain outliers	187428	1017 (10.00-4.00)
RSRZ outliers	180081	1161 (10.00-4.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	681	7% 70% 25% • •
1	B	681	6% 72% 22% • •
1	C	681	7% 72% 23% • •
1	D	681	4% 72% 22% • •
1	E	681	7% 73% 22% • •

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Mol	Chain	Length	Quality of chain
1	F	681	8% 72% 23%
2	G	538	5% 42% 41% 6% 10%
3	H	577	% 17% 80%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 35655 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 Plexin-A2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	656	Total	C	N	O	S	0	0	0
			5138	3255	876	972	35			
1	B	656	Total	C	N	O	S	0	0	0
			5138	3255	876	972	35			
1	C	656	Total	C	N	O	S	0	0	0
			5138	3255	876	972	35			
1	D	656	Total	C	N	O	S	0	0	0
			5138	3255	876	972	35			
1	E	656	Total	C	N	O	S	0	0	0
			5138	3255	876	972	35			
1	F	656	Total	C	N	O	S	0	0	0
			5138	3255	876	972	35			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	32	GLU	-	expression tag	UNP P70207
A	704	GLY	-	expression tag	UNP P70207
A	705	THR	-	expression tag	UNP P70207
A	706	LYS	-	expression tag	UNP P70207
A	707	HIS	-	expression tag	UNP P70207
A	708	HIS	-	expression tag	UNP P70207
A	709	HIS	-	expression tag	UNP P70207
A	710	HIS	-	expression tag	UNP P70207
A	711	HIS	-	expression tag	UNP P70207
A	712	HIS	-	expression tag	UNP P70207
B	32	GLU	-	expression tag	UNP P70207
B	704	GLY	-	expression tag	UNP P70207
B	705	THR	-	expression tag	UNP P70207
B	706	LYS	-	expression tag	UNP P70207
B	707	HIS	-	expression tag	UNP P70207
B	708	HIS	-	expression tag	UNP P70207
B	709	HIS	-	expression tag	UNP P70207

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Chain	Residue	Modelled	Actual	Comment	Reference
B	710	HIS	-	expression tag	UNP P70207
B	711	HIS	-	expression tag	UNP P70207
B	712	HIS	-	expression tag	UNP P70207
C	32	GLU	-	expression tag	UNP P70207
C	704	GLY	-	expression tag	UNP P70207
C	705	THR	-	expression tag	UNP P70207
C	706	LYS	-	expression tag	UNP P70207
C	707	HIS	-	expression tag	UNP P70207
C	708	HIS	-	expression tag	UNP P70207
C	709	HIS	-	expression tag	UNP P70207
C	710	HIS	-	expression tag	UNP P70207
C	711	HIS	-	expression tag	UNP P70207
C	712	HIS	-	expression tag	UNP P70207
D	32	GLU	-	expression tag	UNP P70207
D	704	GLY	-	expression tag	UNP P70207
D	705	THR	-	expression tag	UNP P70207
D	706	LYS	-	expression tag	UNP P70207
D	707	HIS	-	expression tag	UNP P70207
D	708	HIS	-	expression tag	UNP P70207
D	709	HIS	-	expression tag	UNP P70207
D	710	HIS	-	expression tag	UNP P70207
D	711	HIS	-	expression tag	UNP P70207
D	712	HIS	-	expression tag	UNP P70207
E	32	GLU	-	expression tag	UNP P70207
E	704	GLY	-	expression tag	UNP P70207
E	705	THR	-	expression tag	UNP P70207
E	706	LYS	-	expression tag	UNP P70207
E	707	HIS	-	expression tag	UNP P70207
E	708	HIS	-	expression tag	UNP P70207
E	709	HIS	-	expression tag	UNP P70207
E	710	HIS	-	expression tag	UNP P70207
E	711	HIS	-	expression tag	UNP P70207
E	712	HIS	-	expression tag	UNP P70207
F	32	GLU	-	expression tag	UNP P70207
F	704	GLY	-	expression tag	UNP P70207
F	705	THR	-	expression tag	UNP P70207
F	706	LYS	-	expression tag	UNP P70207
F	707	HIS	-	expression tag	UNP P70207
F	708	HIS	-	expression tag	UNP P70207
F	709	HIS	-	expression tag	UNP P70207
F	710	HIS	-	expression tag	UNP P70207
F	711	HIS	-	expression tag	UNP P70207

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Chain	Residue	Modelled	Actual	Comment	Reference
F	712	HIS	-	expression tag	UNP P70207

- Molecule 2 is a protein called Semaphorin-3A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	484	Total	C	N	O	S	0	0	0
			3882	2474	669	720	19			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	18	GLU	-	expression tag	UNP O08665
G	19	THR	-	expression tag	UNP O08665
G	20	GLY	-	expression tag	UNP O08665
G	475	VAL	ILE	SEE REMARK 999	UNP O08665

- Molecule 3 is a protein called Neuropilin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	H	117	Total	C	N	O	S	0	0	0
			944	611	152	176	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	19	GLU	-	expression tag	UNP P97333
H	20	THR	-	expression tag	UNP P97333
H	21	GLY	-	expression tag	UNP P97333
H	587	ARG	-	expression tag	UNP P97333
H	588	THR	-	expression tag	UNP P97333
H	589	LYS	-	expression tag	UNP P97333
H	590	HIS	-	expression tag	UNP P97333
H	591	HIS	-	expression tag	UNP P97333
H	592	HIS	-	expression tag	UNP P97333
H	593	HIS	-	expression tag	UNP P97333
H	594	HIS	-	expression tag	UNP P97333
H	595	HIS	-	expression tag	UNP P97333

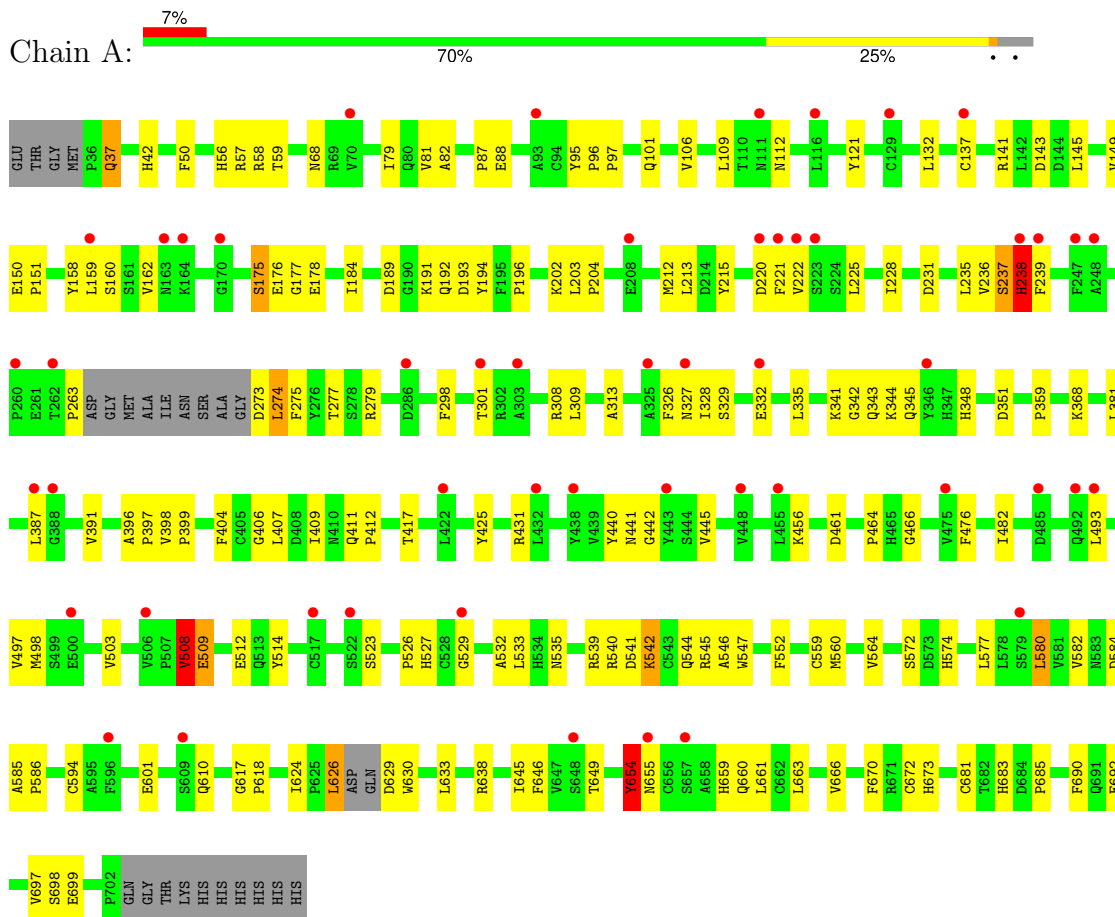
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total 1	Ca 1	0	0

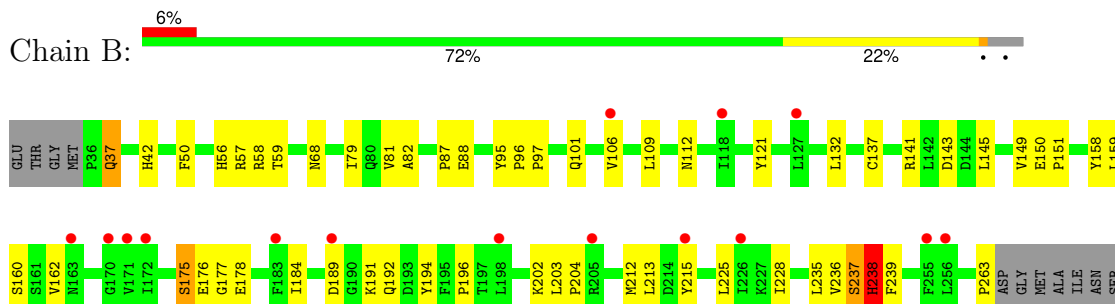
3 Residue-property plots

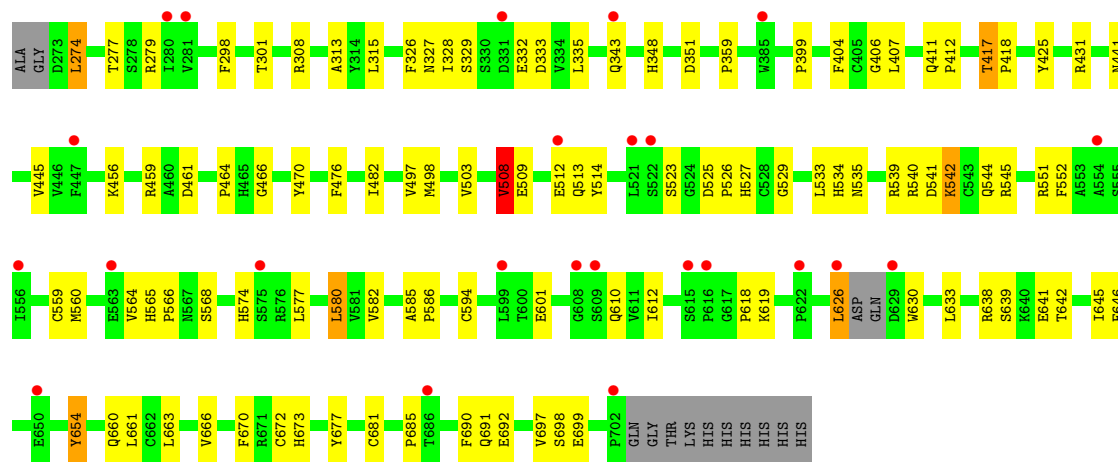
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Plexin-A2

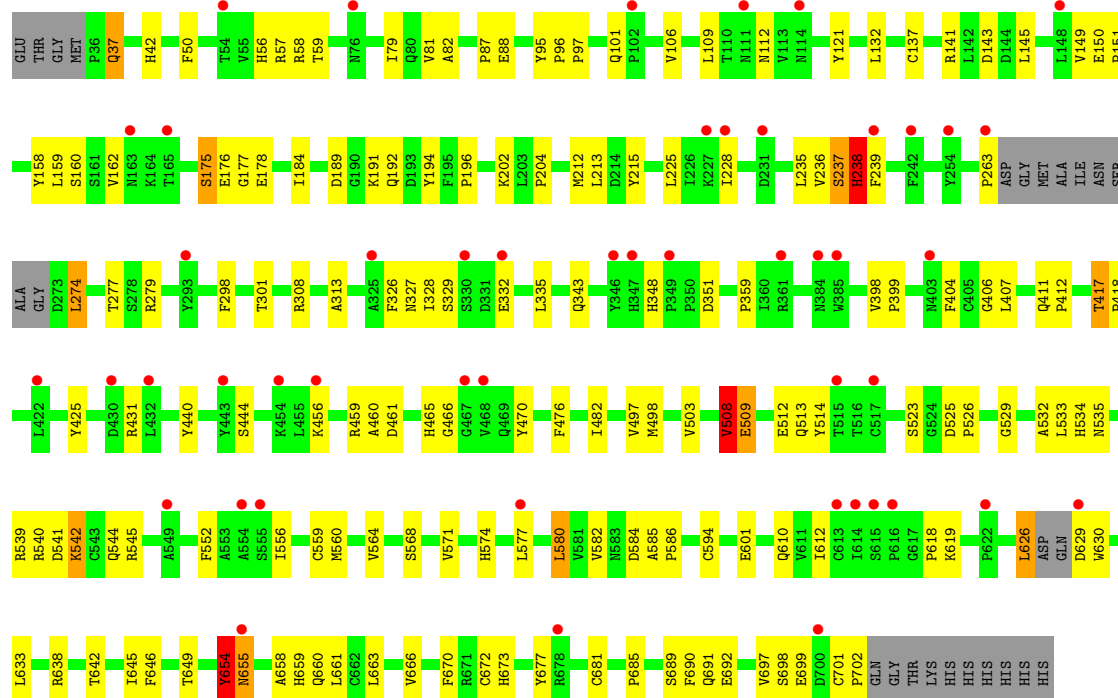


• Molecule 1: Plexin-A2

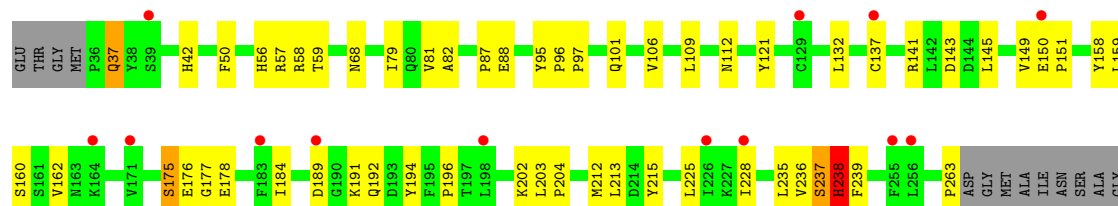


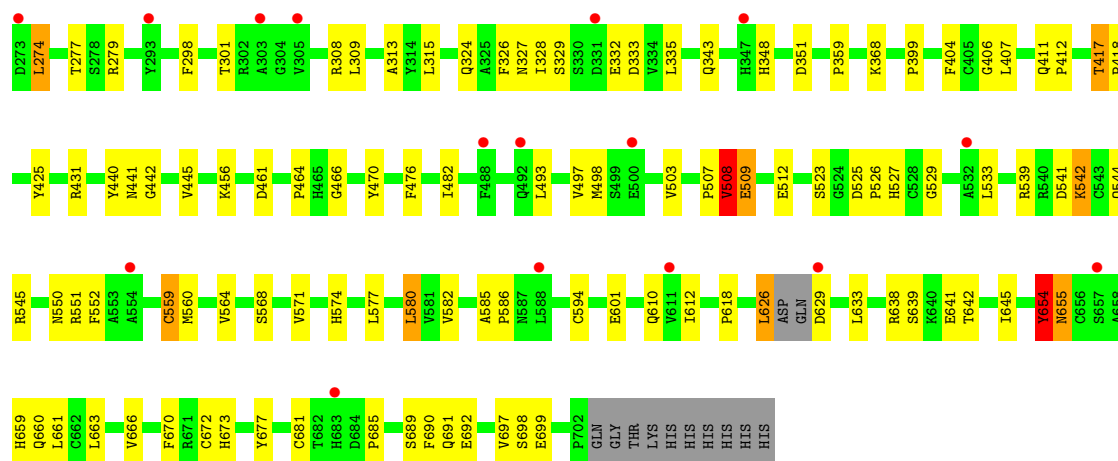


• Molecule 1: Plexin-A2

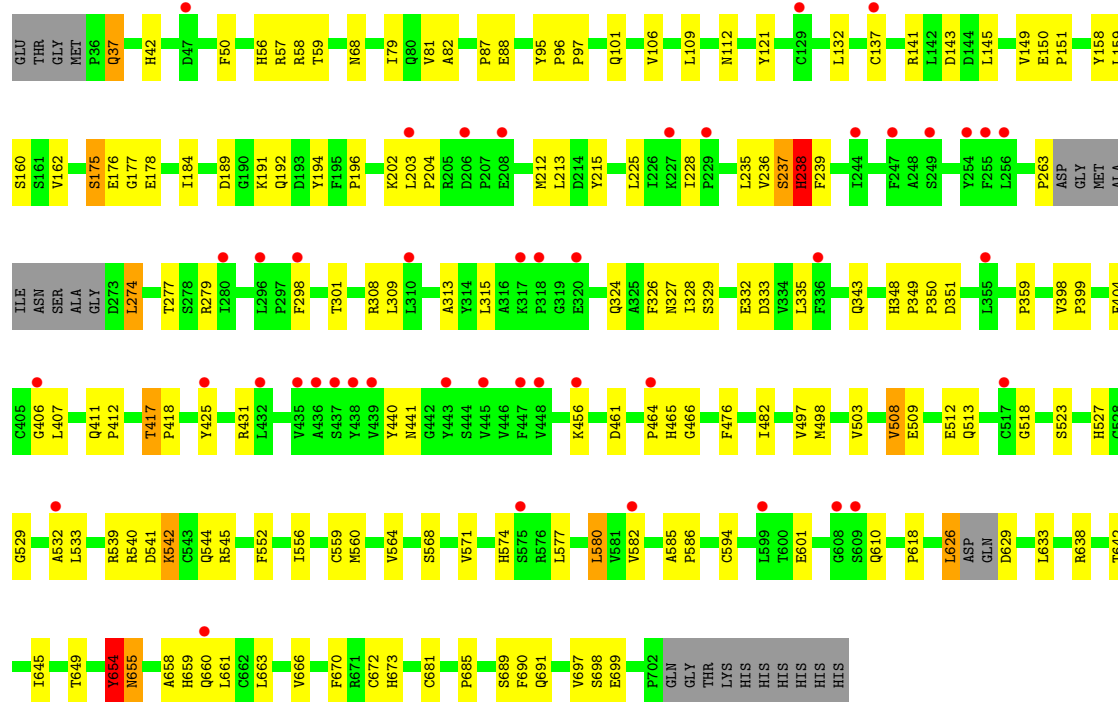


• Molecule 1: Plexin-A2

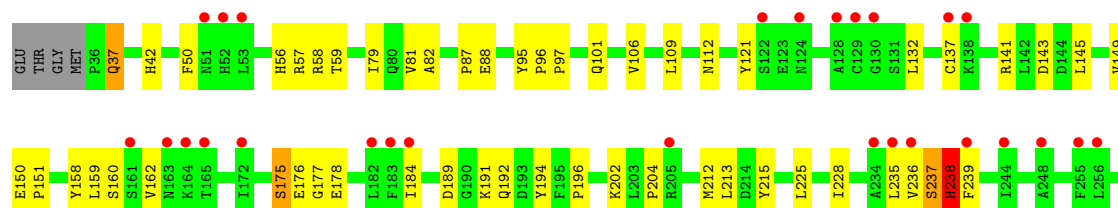


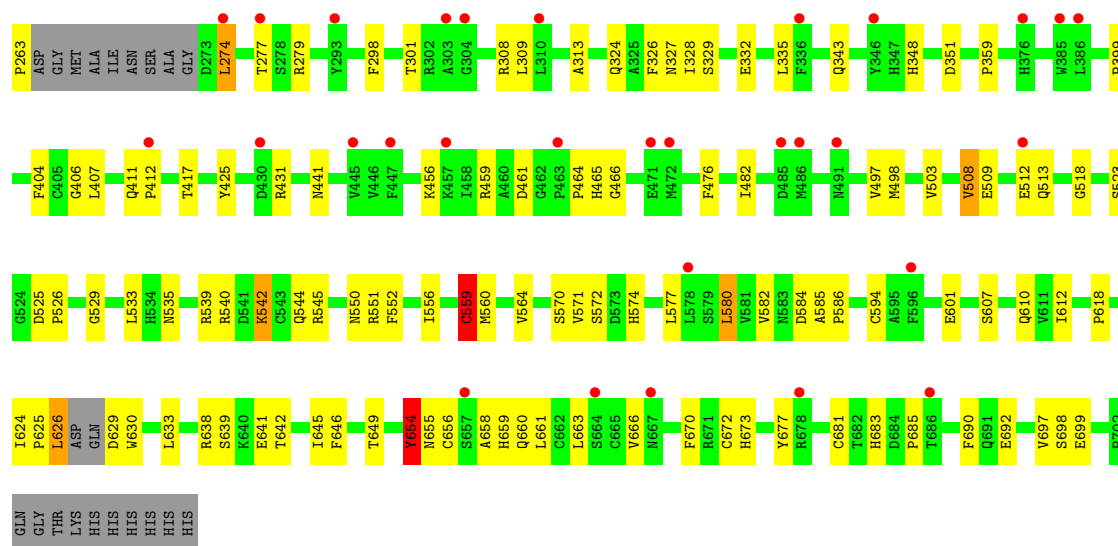


• Molecule 1: Plexin-A2

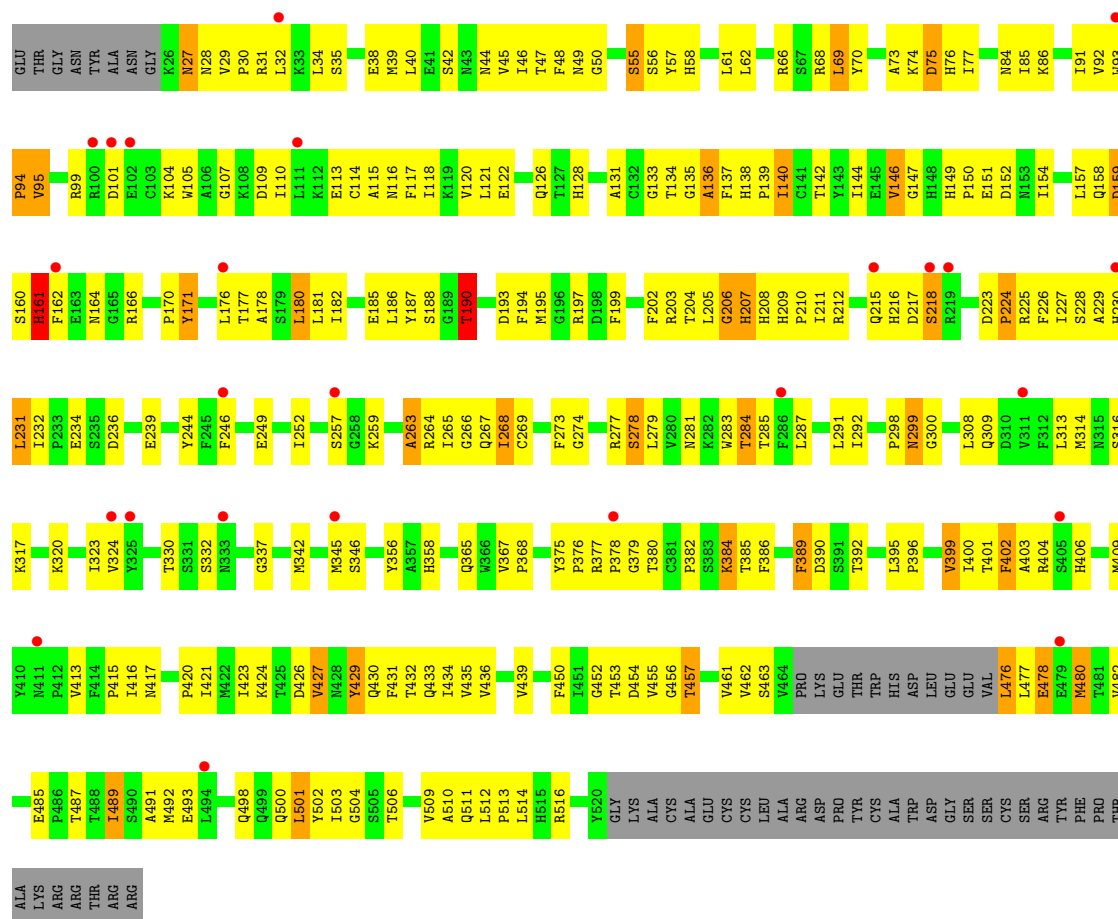


• Molecule 1: Plexin-A2

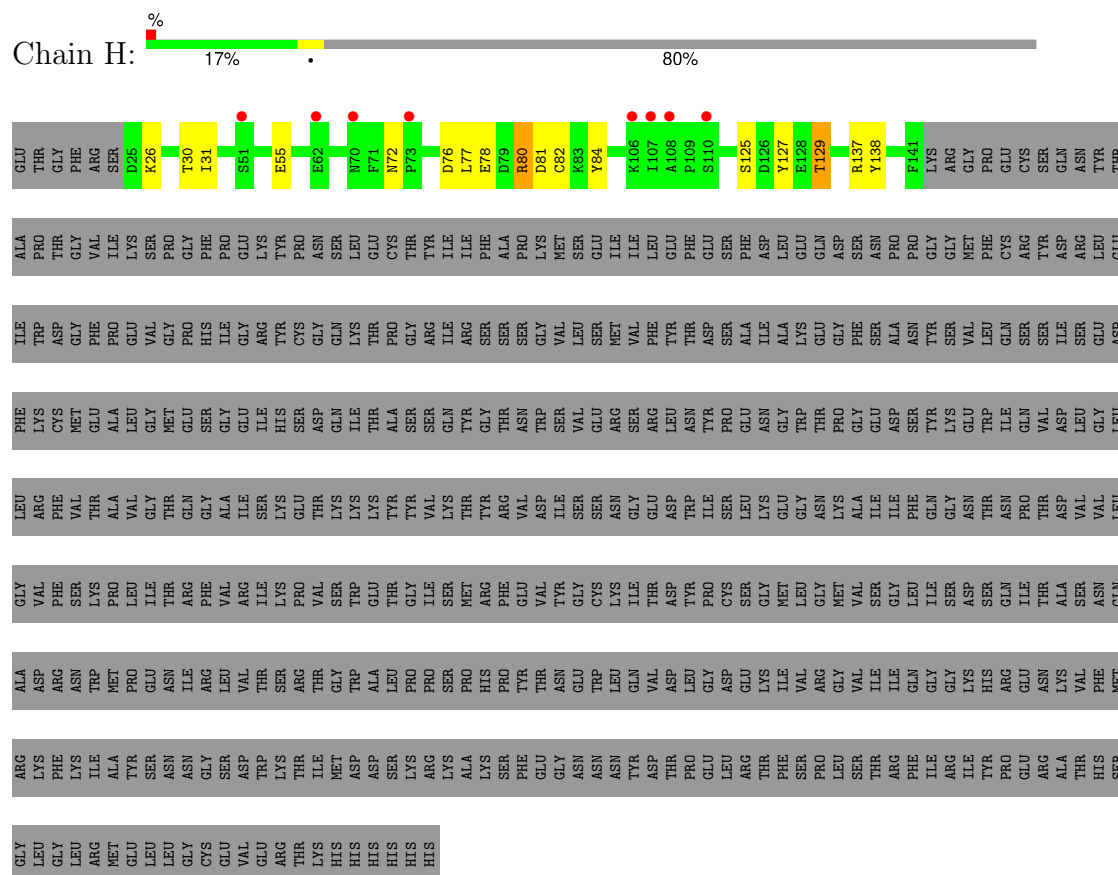




• Molecule 2: Semaphorin-3A



• Molecule 3: Neuropilin-1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	191.63Å 293.60Å 252.18Å 90.00° 106.38° 90.00°	Depositor
Resolution (Å)	125.51 – 7.00 125.51 – 7.00	Depositor EDS
% Data completeness (in resolution range)	95.6 (125.51-7.00) 95.5 (125.51-7.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 6.73Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.285 , 0.285 0.281 , 0.286	Depositor DCC
R_{free} test set	1022 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	293.7	Xtriage
Anisotropy	0.196	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 478.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.76	EDS
Total number of atoms	35655	wwPDB-VP
Average B, all atoms (Å ²)	323.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.77	6/5260 (0.1%)	0.79	14/7138 (0.2%)
1	B	0.41	7/5260 (0.1%)	0.87	12/7138 (0.2%)
1	C	0.62	8/5260 (0.2%)	1.00	10/7138 (0.1%)
1	D	0.69	7/5261 (0.1%)	0.98	13/7141 (0.2%)
1	E	0.40	6/5261 (0.1%)	1.07	15/7141 (0.2%)
1	F	0.50	6/5261 (0.1%)	0.87	16/7141 (0.2%)
2	G	0.61	0/3988	1.04	20/5411 (0.4%)
3	H	0.70	0/977	0.80	1/1325 (0.1%)
All	All	0.59	40/36528 (0.1%)	0.94	101/49573 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	2
1	D	0	2
1	E	0	1
1	F	0	2
2	G	0	2
3	H	0	1
All	All	0	12

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	508	VAL	C-N	46.75	1.91	1.33
1	C	508	VAL	C-N	-34.26	0.85	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	559	CYS	C-N	31.58	1.79	1.33
1	F	508	VAL	C-N	23.45	1.63	1.33
1	D	654	TYR	C-N	-20.15	1.05	1.33
1	D	508	VAL	C-N	-19.09	1.10	1.33
1	A	654	TYR	C-N	14.05	1.52	1.33
1	E	559	CYS	C-N	-11.02	1.19	1.33
1	B	508	VAL	C-N	9.93	1.47	1.33
1	C	654	TYR	C-N	-9.16	1.20	1.33
1	D	37	GLN	CD-OE1	5.40	1.33	1.23
1	A	37	GLN	CD-OE1	5.38	1.33	1.23
1	B	37	GLN	CD-OE1	5.37	1.33	1.23
1	A	42	HIS	ND1-CE1	5.34	1.37	1.32
1	B	42	HIS	ND1-CE1	5.33	1.37	1.32
1	E	37	GLN	CD-OE1	5.33	1.33	1.23
1	C	37	GLN	CD-OE1	5.30	1.33	1.23
1	F	37	GLN	CD-OE1	5.30	1.33	1.23
1	A	238	HIS	ND1-CE1	5.28	1.37	1.32
1	B	238	HIS	ND1-CE1	5.26	1.37	1.32
1	B	654	TYR	C-N	-5.26	1.26	1.33
1	C	42	HIS	ND1-CE1	5.25	1.37	1.32
1	C	238	HIS	ND1-CE1	5.25	1.37	1.32
1	E	42	HIS	ND1-CE1	5.22	1.37	1.32
1	B	101	GLN	CD-OE1	5.21	1.33	1.23
1	D	42	HIS	ND1-CE1	5.21	1.37	1.32
1	F	101	GLN	CD-OE1	5.20	1.33	1.23
1	C	101	GLN	CD-OE1	5.18	1.33	1.23
1	E	238	HIS	ND1-CE1	5.17	1.37	1.32
1	D	101	GLN	CD-OE1	5.16	1.33	1.23
1	F	238	HIS	ND1-CE1	5.16	1.37	1.32
1	D	238	HIS	ND1-CE1	5.15	1.37	1.32
1	E	101	GLN	CD-OE1	5.13	1.33	1.23
1	A	101	GLN	CD-OE1	5.10	1.33	1.23
1	B	513	GLN	CD-OE1	5.09	1.33	1.23
1	F	42	HIS	ND1-CE1	5.08	1.37	1.32
1	E	513	GLN	CD-OE1	5.08	1.33	1.23
1	C	513	GLN	CD-OE1	5.04	1.33	1.23
1	F	513	GLN	CD-OE1	5.01	1.33	1.23
1	C	42	HIS	CD2-NE2	-5.00	1.32	1.37

All (101) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	654	TYR	O-C-N	-53.52	51.41	122.59
1	D	654	TYR	O-C-N	-49.21	57.14	122.59
1	E	654	TYR	O-C-N	-41.76	72.32	123.27
1	E	654	TYR	CA-C-N	29.11	174.09	121.70
1	E	654	TYR	C-N-CA	29.11	174.09	121.70
1	B	654	TYR	CA-C-N	20.26	152.12	122.95
1	B	654	TYR	C-N-CA	20.26	152.12	122.95
1	B	654	TYR	O-C-N	-16.14	102.16	123.15
1	F	559	CYS	CA-C-N	-15.91	97.81	122.62
1	F	559	CYS	C-N-CA	-15.91	97.81	122.62
1	C	508	VAL	O-C-N	-15.70	102.95	122.57
1	A	654	TYR	O-C-N	-14.96	105.77	123.27
1	B	508	VAL	O-C-N	-14.87	103.98	122.57
1	E	559	CYS	O-C-N	14.03	140.01	122.89
1	F	508	VAL	O-C-N	-13.44	108.30	121.87
1	E	559	CYS	CA-C-N	-12.64	101.09	120.94
1	E	559	CYS	C-N-CA	-12.64	101.09	120.94
1	F	654	TYR	CA-C-N	-12.48	100.86	122.07
1	F	654	TYR	C-N-CA	-12.48	100.86	122.07
1	D	559	CYS	O-C-N	-11.87	106.45	122.36
1	F	508	VAL	CA-C-N	10.14	139.78	121.94
1	F	508	VAL	C-N-CA	10.14	139.78	121.94
1	E	508	VAL	O-C-N	9.71	131.68	121.87
1	D	508	VAL	CA-C-N	-9.67	100.92	121.81
1	D	508	VAL	C-N-CA	-9.67	100.92	121.81
2	G	402	PHE	N-CA-C	-9.48	98.44	110.19
1	F	559	CYS	O-C-N	-9.21	110.34	122.59
2	G	126	GLN	N-CA-C	-8.29	103.15	113.18
1	A	654	TYR	CA-C-N	7.38	134.12	122.17
1	A	654	TYR	C-N-CA	7.38	134.12	122.17
1	A	508	VAL	O-C-N	-7.23	113.25	122.22
2	G	399	VAL	N-CA-C	-6.67	104.67	110.74
1	F	238	HIS	CB-CG-CD2	-6.63	122.59	131.20
1	E	238	HIS	CB-CG-CD2	-6.60	122.62	131.20
1	A	238	HIS	CB-CG-CD2	-6.59	122.63	131.20
1	B	238	HIS	CB-CG-CD2	-6.58	122.65	131.20
1	D	42	HIS	CB-CG-CD2	-6.57	122.66	131.20
1	E	42	HIS	CB-CG-CD2	-6.56	122.67	131.20
1	C	238	HIS	CB-CG-CD2	-6.53	122.72	131.20
1	A	42	HIS	CB-CG-CD2	-6.52	122.73	131.20
1	B	42	HIS	CB-CG-CD2	-6.52	122.73	131.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	42	HIS	CB-CG-CD2	-6.51	122.73	131.20
1	C	42	HIS	CB-CG-CD2	-6.51	122.74	131.20
1	D	238	HIS	CB-CG-CD2	-6.48	122.77	131.20
2	G	171	TYR	N-CA-C	-6.37	105.63	113.41
2	G	193	ASP	N-CA-C	6.26	119.40	109.50
2	G	463	SER	N-CA-C	6.19	118.60	109.69
2	G	47	THR	N-CA-C	6.14	119.47	109.59
2	G	461	VAL	N-CA-C	6.07	117.51	108.46
2	G	284	THR	N-CA-C	-6.02	105.23	113.30
2	G	207	HIS	N-CA-C	5.90	123.36	110.80
2	G	346	SER	N-CA-C	-5.88	104.46	111.69
1	A	348	HIS	CA-C-N	5.83	123.92	119.66
1	A	348	HIS	C-N-CA	5.83	123.92	119.66
1	F	348	HIS	CA-C-N	5.80	123.90	119.66
1	F	348	HIS	C-N-CA	5.80	123.90	119.66
2	G	480	MET	N-CA-C	5.80	118.25	107.99
1	C	348	HIS	CA-C-N	5.78	123.88	119.66
1	C	348	HIS	C-N-CA	5.78	123.88	119.66
1	D	348	HIS	CA-C-N	5.76	123.87	119.66
1	D	348	HIS	C-N-CA	5.76	123.87	119.66
1	E	348	HIS	CA-C-N	5.73	123.84	119.66
1	E	348	HIS	C-N-CA	5.73	123.84	119.66
2	G	478	GLU	N-CA-C	5.72	117.82	108.55
1	B	348	HIS	CA-C-N	5.71	123.83	119.66
1	B	348	HIS	C-N-CA	5.71	123.83	119.66
1	A	238	HIS	CB-CG-ND1	5.69	131.23	122.70
1	F	238	HIS	CB-CG-ND1	5.68	131.23	122.70
1	B	238	HIS	CB-CG-ND1	5.68	131.22	122.70
1	E	238	HIS	CB-CG-ND1	5.67	131.21	122.70
1	C	238	HIS	CB-CG-ND1	5.66	131.20	122.70
2	G	263	ALA	N-CA-C	-5.66	102.65	110.35
1	A	617	GLY	CA-C-N	5.66	125.13	119.24
1	A	617	GLY	C-N-CA	5.66	125.13	119.24
2	G	136	ALA	N-CA-C	-5.66	103.60	111.52
1	D	238	HIS	CB-CG-ND1	5.65	131.18	122.70
1	D	42	HIS	CB-CG-ND1	5.64	131.16	122.70
1	F	42	HIS	CB-CG-ND1	5.63	131.15	122.70
1	C	42	HIS	CB-CG-ND1	5.62	131.13	122.70
1	E	42	HIS	CB-CG-ND1	5.59	131.09	122.70
1	A	42	HIS	CB-CG-ND1	5.59	131.08	122.70
1	B	42	HIS	CB-CG-ND1	5.57	131.05	122.70
2	G	489	ILE	N-CA-C	-5.52	101.56	108.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	128	HIS	N-CA-C	5.43	117.94	109.52
2	G	190	THR	CB-CA-C	-5.41	102.71	113.80
2	G	236	ASP	N-CA-C	-5.37	106.58	113.02
1	C	417	THR	CA-C-N	5.30	125.20	119.85
1	C	417	THR	C-N-CA	5.30	125.20	119.85
2	G	439	VAL	N-CA-C	5.25	115.66	107.99
1	D	417	THR	CA-C-N	5.19	125.09	119.85
1	D	417	THR	C-N-CA	5.19	125.09	119.85
1	E	417	THR	CA-C-N	5.18	125.08	119.85
1	E	417	THR	C-N-CA	5.18	125.08	119.85
1	F	417	THR	CA-C-N	5.15	125.05	119.85
1	F	417	THR	C-N-CA	5.15	125.05	119.85
3	H	129	THR	N-CA-C	5.14	121.76	110.80
1	B	417	THR	CA-C-N	5.14	125.04	119.85
1	B	417	THR	C-N-CA	5.14	125.04	119.85
1	A	417	THR	CA-C-N	5.11	125.01	119.85
1	A	417	THR	C-N-CA	5.11	125.01	119.85
1	D	508	VAL	O-C-N	5.02	128.84	122.57

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	654	TYR	Mainchain
1	B	508	VAL	Mainchain
1	C	508	VAL	Mainchain
1	C	654	TYR	Mainchain
1	D	508	VAL	Mainchain
1	D	654	TYR	Mainchain
1	E	654	TYR	Mainchain
1	F	559	CYS	Mainchain
1	F	654	TYR	Mainchain
2	G	429	TYR	Sidechain
2	G	57	TYR	Sidechain
3	H	80	ARG	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5138	0	4989	294	34
1	B	5138	0	4991	186	18
1	C	5138	0	4990	238	0
1	D	5138	0	4989	197	0
1	E	5138	0	4993	165	29
1	F	5138	0	4995	180	23
2	G	3882	0	3747	302	11
3	H	944	0	875	43	5
4	H	1	0	0	0	0
All	All	35655	0	34569	1291	63

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 18.

All (1291) 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:A:344:LYS:CD	3:H:80:ARG:HH11	1.00	1.58
1:A:344:LYS:HD3	3:H:80:ARG:CD	1.23	1.57
1:A:222:VAL:CG2	2:G:166:ARG:HH12	1.17	1.54
1:D:577:LEU:HD11	1:F:607:SER:CB	1.44	1.47
1:E:324:GLN:NE2	1:F:518:GLY:HA3	1.23	1.47
1:A:221:PHE:HZ	2:G:202:PHE:CE2	1.32	1.45
1:A:368:LYS:NZ	1:B:630:TRP:HZ2	1.09	1.44
1:E:324:GLN:NE2	1:F:518:GLY:CA	1.80	1.43
1:E:324:GLN:HE22	1:F:518:GLY:CA	1.30	1.43
1:A:546:ALA:HB1	1:C:690:PHE:CE2	1.52	1.42
1:A:409:ILE:HG23	2:G:194:PHE:CE2	1.53	1.41
1:A:409:ILE:CG2	2:G:194:PHE:HE2	1.31	1.41
1:A:96:PRO:HD3	2:G:277:ARG:NE	1.10	1.40
1:A:344:LYS:HD2	3:H:80:ARG:NH1	1.32	1.40
1:D:559:CYS:C	1:D:560:MET:N	1.79	1.38
1:C:568:SER:OG	1:C:670:PHE:HE1	1.06	1.37
1:A:221:PHE:CZ	2:G:202:PHE:CE2	2.14	1.34
1:A:344:LYS:CD	3:H:80:ARG:NH1	1.78	1.33
1:A:442:GLY:N	1:C:691:GLN:HE22	1.22	1.33
1:A:440:TYR:CZ	1:C:692:GLU:OE2	1.80	1.32
1:E:518:GLY:HA3	1:F:324:GLN:NE2	1.44	1.32
1:C:465:HIS:HE1	1:D:523:SER:O	0.99	1.31
1:B:691:GLN:OE1	1:D:442:GLY:N	1.63	1.31

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:LYS:NZ	3:H:84:TYR:CE1	1.97	1.31
1:A:222:VAL:HG23	2:G:166:ARG:NH1	1.47	1.30
1:E:654:TYR:CD2	1:E:670:PHE:CD1	2.19	1.30
1:A:546:ALA:HB1	1:C:690:PHE:CZ	1.67	1.29
1:A:546:ALA:CB	1:C:690:PHE:HE2	1.46	1.29
1:C:626:LEU:CD1	1:D:399:PRO:HG3	1.62	1.28
1:E:465:HIS:HE1	1:F:523:SER:O	1.11	1.28
1:A:508:VAL:C	1:A:509:GLU:N	1.91	1.28
1:A:546:ALA:CB	1:C:690:PHE:CE2	2.15	1.27
1:A:409:ILE:CG2	2:G:194:PHE:CE2	2.10	1.27
1:B:577:LEU:HD12	1:C:610:GLN:OE1	1.28	1.26
1:E:465:HIS:CE1	1:F:523:SER:O	1.86	1.26
1:A:222:VAL:CG2	2:G:166:ARG:NH1	1.96	1.26
1:A:368:LYS:NZ	1:B:630:TRP:CZ2	2.02	1.26
1:A:96:PRO:CD	2:G:277:ARG:NE	1.98	1.26
1:A:221:PHE:CZ	2:G:202:PHE:CZ	2.23	1.25
1:E:654:TYR:HB3	1:E:670:PHE:CE2	1.72	1.25
1:D:577:LEU:CD1	1:F:607:SER:HB2	1.67	1.23
1:C:465:HIS:CE1	1:D:523:SER:O	1.90	1.23
1:E:518:GLY:CA	1:F:324:GLN:NE2	2.02	1.23
1:A:344:LYS:CD	3:H:80:ARG:CD	2.18	1.21
1:C:508:VAL:C	1:C:509:GLU:CA	2.10	1.21
1:C:508:VAL:O	1:C:509:GLU:N	1.65	1.21
1:A:96:PRO:HD3	2:G:277:ARG:CZ	1.70	1.19
1:E:518:GLY:CA	1:F:324:GLN:HE22	1.55	1.19
1:F:624:ILE:HG13	1:F:655:ASN:HB2	1.23	1.17
1:A:344:LYS:CD	3:H:80:ARG:HD3	1.75	1.16
1:A:626:LEU:CD1	1:B:399:PRO:HG3	1.74	1.16
1:D:612:ILE:CD1	1:F:612:ILE:HD12	1.76	1.15
1:E:523:SER:O	1:F:465:HIS:HE1	1.27	1.14
1:F:630:TRP:HB3	1:F:670:PHE:CE2	1.82	1.13
1:A:344:LYS:CG	3:H:80:ARG:NH1	2.09	1.13
1:E:654:TYR:CE2	1:E:670:PHE:CD1	2.36	1.12
1:F:629:ASP:OD1	1:F:659:HIS:NE2	1.82	1.12
1:B:610:GLN:OE1	1:C:577:LEU:HD12	1.48	1.12
1:F:533:LEU:HB3	1:F:642:THR:HG21	1.18	1.12
1:A:222:VAL:HG21	2:G:166:ARG:HH12	1.08	1.11
1:A:273:ASP:HB3	3:H:80:ARG:CZ	1.79	1.11
1:A:341:LYS:NZ	3:H:84:TYR:HE1	1.39	1.11
1:D:690:PHE:CG	1:E:540:ARG:HD2	1.74	1.11
1:A:442:GLY:N	1:C:691:GLN:NE2	1.99	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:PRO:HD3	2:G:277:ARG:CD	1.80	1.10
1:A:626:LEU:HD12	1:B:399:PRO:HG3	1.19	1.10
1:B:577:LEU:CD1	1:C:610:GLN:OE1	2.00	1.09
1:B:610:GLN:OE1	1:C:577:LEU:CG	2.00	1.09
1:A:552:PHE:CD2	1:C:690:PHE:CE1	2.41	1.08
1:C:508:VAL:CA	1:C:509:GLU:N	2.16	1.08
1:E:518:GLY:HA2	1:F:324:GLN:HE22	1.10	1.07
1:C:630:TRP:HZ2	1:D:368:LYS:NZ	1.53	1.06
1:F:533:LEU:HB3	1:F:642:THR:CG2	1.85	1.06
1:E:654:TYR:CD2	1:E:670:PHE:CE1	2.42	1.06
1:B:691:GLN:OE1	1:D:441:ASN:C	1.96	1.06
1:C:523:SER:HA	1:D:464:PRO:HD2	1.38	1.06
1:A:344:LYS:HD3	3:H:80:ARG:HD2	1.37	1.05
1:D:690:PHE:CG	1:E:540:ARG:CD	2.37	1.05
1:A:192:GLN:HE22	2:G:404:ARG:NH2	1.53	1.05
1:A:341:LYS:NZ	3:H:84:TYR:CD1	2.24	1.05
1:A:440:TYR:CE1	1:C:692:GLU:OE2	2.08	1.05
1:B:610:GLN:OE1	1:C:577:LEU:CD1	2.04	1.05
1:D:677:TYR:CZ	1:E:541:ASP:HB3	1.91	1.04
1:A:222:VAL:HG23	2:G:166:ARG:HH12	0.92	1.04
1:D:692:GLU:OE2	1:E:440:TYR:CD1	2.11	1.03
1:A:344:LYS:NZ	3:H:78:GLU:OE2	1.92	1.03
1:E:523:SER:O	1:F:465:HIS:CE1	2.11	1.03
1:C:654:TYR:CE2	1:C:670:PHE:CD1	2.47	1.03
1:E:654:TYR:CG	1:E:670:PHE:CG	2.46	1.02
1:A:630:TRP:HB3	1:A:670:PHE:CE2	1.94	1.01
1:C:626:LEU:HD11	1:D:399:PRO:HG3	1.41	1.01
1:B:610:GLN:OE1	1:C:577:LEU:HB2	1.60	1.01
1:C:523:SER:HA	1:D:464:PRO:CD	1.91	1.00
1:E:654:TYR:CG	1:E:670:PHE:CD2	2.49	1.00
1:E:654:TYR:CB	1:E:670:PHE:CE2	2.44	1.00
2:G:273:PHE:H	2:G:392:THR:HG21	1.24	1.00
1:E:324:GLN:HE22	1:F:518:GLY:HA2	0.86	1.00
2:G:287:LEU:HD22	2:G:409:MET:CE	1.91	1.00
1:A:464:PRO:HG3	1:B:514:TYR:HE1	1.23	0.99
1:B:577:LEU:HD12	1:C:610:GLN:CD	1.86	0.99
1:B:610:GLN:CD	1:C:577:LEU:HD12	1.86	0.99
1:F:624:ILE:HG13	1:F:655:ASN:CB	1.93	0.99
1:A:654:TYR:HB3	1:A:670:PHE:CD2	1.97	0.98
1:E:654:TYR:CD2	1:E:670:PHE:CG	2.52	0.97
1:B:610:GLN:OE1	1:C:577:LEU:CB	2.13	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:691:GLN:HB3	1:D:441:ASN:HA	1.43	0.97
1:B:610:GLN:CD	1:C:577:LEU:HB2	1.91	0.96
1:A:344:LYS:HG2	3:H:80:ARG:NH1	1.80	0.96
1:E:654:TYR:CB	1:E:670:PHE:CD2	2.49	0.96
1:A:441:ASN:OD1	1:C:691:GLN:HB2	1.65	0.95
1:D:689:SER:HB3	1:E:540:ARG:HD3	1.47	0.95
1:A:344:LYS:HD3	3:H:80:ARG:HD3	0.98	0.95
1:A:546:ALA:HB3	1:C:690:PHE:HE2	1.31	0.95
1:C:508:VAL:C	1:C:509:GLU:N	0.85	0.95
1:C:559:CYS:C	1:C:560:MET:N	2.24	0.95
1:A:654:TYR:CD2	1:A:670:PHE:CD1	2.56	0.94
1:E:237:SER:HA	1:E:239:PHE:H	1.33	0.94
1:F:630:TRP:CB	1:F:670:PHE:CE2	2.50	0.94
1:A:237:SER:HA	1:A:239:PHE:H	1.33	0.94
1:A:344:LYS:HD3	3:H:80:ARG:NE	1.82	0.94
1:E:324:GLN:OE1	1:F:556:ILE:HD11	1.67	0.93
1:A:221:PHE:CE1	2:G:202:PHE:HZ	1.87	0.93
1:A:344:LYS:CG	3:H:80:ARG:HH11	1.78	0.93
1:C:630:TRP:CZ2	1:D:368:LYS:NZ	2.38	0.92
1:A:654:TYR:CB	1:A:670:PHE:CD2	2.52	0.92
1:A:626:LEU:CD1	1:B:399:PRO:CG	2.48	0.92
1:A:654:TYR:CG	1:A:670:PHE:CB	2.53	0.92
1:F:630:TRP:HB3	1:F:670:PHE:HE2	1.34	0.92
1:A:442:GLY:H	1:C:691:GLN:HE22	1.15	0.92
1:A:654:TYR:CG	1:A:670:PHE:CG	2.57	0.92
1:A:221:PHE:CE1	2:G:202:PHE:CZ	2.58	0.91
1:C:237:SER:HA	1:C:239:PHE:H	1.33	0.91
1:E:518:GLY:HA3	1:F:324:GLN:HE21	1.12	0.91
1:E:654:TYR:CE1	1:E:670:PHE:HB3	2.05	0.91
1:D:237:SER:HA	1:D:239:PHE:H	1.33	0.91
1:F:237:SER:HA	1:F:239:PHE:H	1.33	0.91
1:D:612:ILE:HD13	1:F:612:ILE:HD12	1.53	0.90
1:B:237:SER:HA	1:B:239:PHE:H	1.33	0.90
1:D:445:VAL:HG22	1:D:526:PRO:HG2	1.52	0.90
1:D:577:LEU:HD11	1:F:607:SER:HB2	0.92	0.90
1:B:610:GLN:NE2	1:C:577:LEU:HB2	1.85	0.90
1:A:552:PHE:CG	1:C:690:PHE:CZ	2.60	0.90
2:G:287:LEU:HD22	2:G:409:MET:HE1	1.52	0.89
1:A:221:PHE:CZ	2:G:202:PHE:HZ	1.87	0.89
1:B:654:TYR:CD2	1:B:670:PHE:CD1	2.60	0.89
1:A:409:ILE:HG22	2:G:194:PHE:HE2	1.33	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:612:ILE:CD1	1:F:612:ILE:CD1	2.49	0.89
1:A:345:GLN:OE1	3:H:127:TYR:OH	1.92	0.88
1:A:630:TRP:HB3	1:A:670:PHE:HE2	1.34	0.87
1:B:692:GLU:OE2	1:D:440:TYR:CD1	2.28	0.87
1:A:344:LYS:CD	3:H:80:ARG:CZ	2.52	0.87
1:A:654:TYR:CD2	1:A:670:PHE:HB3	2.09	0.87
1:A:464:PRO:CG	1:B:514:TYR:HE1	1.88	0.87
1:E:464:PRO:HD3	1:F:523:SER:HA	1.56	0.87
1:A:193:ASP:OD2	2:G:404:ARG:NH2	2.07	0.86
1:F:570:SER:HB2	1:F:683:HIS:CB	2.05	0.86
1:D:577:LEU:CD1	1:F:607:SER:CB	2.39	0.86
1:A:368:LYS:HZ2	1:B:630:TRP:HZ2	1.23	0.86
1:B:692:GLU:OE2	1:D:440:TYR:CG	2.29	0.86
1:A:221:PHE:CZ	2:G:202:PHE:HE2	1.69	0.86
1:A:464:PRO:HG3	1:B:514:TYR:CE1	2.10	0.85
1:C:440:TYR:HA	1:F:692:GLU:OE2	1.76	0.85
1:A:514:TYR:HE1	1:B:464:PRO:HG3	1.41	0.85
1:B:577:LEU:CG	1:C:610:GLN:OE1	2.23	0.85
1:A:654:TYR:CD2	1:A:670:PHE:CG	2.63	0.85
1:A:368:LYS:HZ3	1:B:630:TRP:HZ2	0.90	0.85
1:A:381:LEU:HD11	2:G:195:MET:HE1	1.59	0.85
1:A:508:VAL:CG1	1:A:527:HIS:NE2	2.38	0.85
1:D:568:SER:CB	1:D:670:PHE:CE1	2.60	0.85
1:A:445:VAL:HG22	1:A:526:PRO:HG2	1.57	0.84
1:B:691:GLN:OE1	1:D:442:GLY:CA	2.26	0.84
1:D:568:SER:CB	1:D:670:PHE:HE1	1.89	0.84
1:A:96:PRO:CD	2:G:277:ARG:CZ	2.48	0.84
1:F:629:ASP:CG	1:F:659:HIS:CE1	2.55	0.84
1:A:559:CYS:O	1:A:584:ASP:OD2	1.96	0.84
2:G:94:PRO:O	2:G:95:VAL:HB	1.77	0.83
1:D:612:ILE:HD13	1:F:612:ILE:CD1	2.09	0.83
1:A:192:GLN:HE22	2:G:404:ARG:HH21	1.25	0.83
1:D:571:VAL:HG22	1:D:655:ASN:HB2	1.60	0.83
1:B:677:TYR:CZ	1:D:541:ASP:HB3	2.15	0.82
1:A:409:ILE:HG22	2:G:194:PHE:CE2	2.07	0.82
2:G:32:LEU:HD22	2:G:34:LEU:HD21	1.61	0.82
1:C:532:ALA:HB1	1:C:560:MET:CE	2.10	0.82
1:A:552:PHE:CD2	1:C:690:PHE:HE1	1.92	0.81
1:B:445:VAL:HG22	1:B:526:PRO:HG2	1.61	0.81
1:A:552:PHE:CB	1:C:690:PHE:HZ	1.94	0.81
1:A:532:ALA:HB1	1:A:560:MET:CE	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:610:GLN:HE22	1:C:577:LEU:HB2	1.45	0.81
1:C:571:VAL:HG22	1:C:655:ASN:HB2	1.63	0.81
2:G:44:ASN:OD1	2:G:516:ARG:HG3	1.81	0.81
1:D:533:LEU:HB3	1:D:642:THR:HG21	1.61	0.80
1:A:391:VAL:HG21	2:G:197:ARG:NH1	1.96	0.80
1:C:571:VAL:CG2	1:C:655:ASN:HB2	2.12	0.80
1:A:192:GLN:NE2	2:G:404:ARG:NH2	2.29	0.79
1:A:654:TYR:CE2	1:A:670:PHE:HB3	2.17	0.79
1:C:568:SER:CB	1:C:670:PHE:HE1	1.96	0.79
1:A:552:PHE:CB	1:C:690:PHE:CZ	2.65	0.79
1:F:570:SER:CB	1:F:683:HIS:CG	2.65	0.79
1:A:540:ARG:CZ	1:C:690:PHE:HA	2.11	0.79
1:D:677:TYR:CE1	1:E:541:ASP:HB3	2.16	0.79
1:A:221:PHE:HZ	2:G:202:PHE:HE2	0.82	0.79
1:F:624:ILE:CG1	1:F:655:ASN:HB2	2.10	0.79
1:E:324:GLN:NE2	1:F:518:GLY:HA2	1.68	0.79
1:E:440:TYR:CE2	1:E:527:HIS:HA	2.19	0.78
2:G:273:PHE:N	2:G:392:THR:HG21	1.99	0.78
1:A:546:ALA:HB3	1:C:690:PHE:CE2	2.10	0.78
1:D:577:LEU:HD12	1:F:610:GLN:OE1	1.82	0.78
2:G:489:ILE:HG23	2:G:503:ILE:HG23	1.64	0.78
2:G:269:CYS:SG	2:G:285:THR:HG21	2.23	0.78
2:G:453:THR:HG21	2:G:455:VAL:HG12	1.66	0.78
1:A:222:VAL:HG21	2:G:166:ARG:NH1	1.78	0.78
1:D:551:ARG:NH1	1:D:641:GLU:OE2	2.14	0.78
1:E:464:PRO:CD	1:F:523:SER:HA	2.14	0.78
1:C:514:TYR:HE1	1:D:464:PRO:HG3	1.48	0.77
2:G:285:THR:O	2:G:285:THR:HG22	1.84	0.77
1:A:275:PHE:CE2	3:H:80:ARG:NE	2.45	0.77
1:A:441:ASN:OD1	1:C:691:GLN:CB	2.32	0.77
1:C:654:TYR:CG	1:C:670:PHE:CD2	2.72	0.77
1:A:391:VAL:HG21	2:G:197:ARG:CZ	2.14	0.77
1:B:690:PHE:HZ	1:D:552:PHE:CD2	2.03	0.77
1:C:654:TYR:CD2	1:C:670:PHE:CE2	2.73	0.77
2:G:152:ASP:HB2	2:G:154:ILE:HD11	1.65	0.77
1:C:568:SER:CB	1:C:670:PHE:CE1	2.68	0.77
1:C:654:TYR:CE2	1:C:670:PHE:CG	2.72	0.76
1:A:95:TYR:C	2:G:277:ARG:NH2	2.43	0.76
1:B:654:TYR:CD2	1:B:670:PHE:CG	2.73	0.76
1:B:654:TYR:HB3	1:B:670:PHE:CE2	2.19	0.76
1:E:324:GLN:HE21	1:F:518:GLY:HA3	0.94	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:215:GLN:HE21	2:G:216:HIS:CD2	2.03	0.76
1:B:551:ARG:HH12	1:B:641:GLU:CD	1.92	0.76
1:E:654:TYR:HD2	1:E:670:PHE:CE1	2.00	0.76
1:A:342:GLY:HA3	3:H:84:TYR:OH	1.86	0.76
1:E:654:TYR:CE1	1:E:670:PHE:CB	2.69	0.76
1:E:654:TYR:CZ	1:E:670:PHE:HB3	2.20	0.76
1:A:440:TYR:OH	1:C:692:GLU:OE2	2.02	0.76
1:A:221:PHE:HE1	2:G:212:ARG:HD2	1.50	0.75
1:A:552:PHE:CG	1:C:690:PHE:CE1	2.74	0.75
1:D:677:TYR:CZ	1:E:541:ASP:CB	2.69	0.75
1:A:654:TYR:CB	1:A:670:PHE:CG	2.70	0.75
1:B:551:ARG:NH1	1:B:641:GLU:OE2	2.14	0.75
1:B:577:LEU:HB2	1:C:610:GLN:OE1	1.86	0.75
2:G:402:PHE:O	2:G:403:ALA:HB3	1.86	0.75
1:C:626:LEU:HD13	1:D:399:PRO:HG3	1.65	0.75
1:A:387:LEU:HD22	2:G:197:ARG:HH12	1.52	0.74
1:C:540:ARG:HD2	1:F:690:PHE:CG	1.87	0.74
1:C:399:PRO:HG3	1:D:626:LEU:HD12	1.69	0.74
2:G:453:THR:CG2	2:G:455:VAL:HG12	2.17	0.74
1:D:577:LEU:CD1	1:F:610:GLN:OE1	2.34	0.74
1:D:690:PHE:HE2	1:E:540:ARG:C	1.52	0.74
1:A:654:TYR:CG	1:A:670:PHE:HB3	2.20	0.74
1:A:654:TYR:HB3	1:A:670:PHE:CE2	2.22	0.74
1:A:441:ASN:C	1:C:691:GLN:NE2	2.39	0.74
1:D:571:VAL:CG2	1:D:655:ASN:HB2	2.17	0.74
1:E:556:ILE:HD11	1:F:324:GLN:OE1	1.86	0.74
2:G:287:LEU:HB3	2:G:409:MET:HE3	1.69	0.74
1:D:568:SER:HB2	1:D:670:PHE:CE1	2.22	0.74
1:B:610:GLN:OE1	1:C:577:LEU:HG	1.87	0.74
1:C:399:PRO:HG3	1:D:626:LEU:CD1	2.18	0.74
1:A:441:ASN:OD1	1:C:691:GLN:OE1	2.04	0.73
1:A:344:LYS:HD3	3:H:80:ARG:CZ	2.13	0.73
1:D:507:PRO:C	1:D:509:GLU:N	2.42	0.73
1:E:544:GLN:HG2	1:E:545:ARG:HG2	1.71	0.73
1:A:368:LYS:HZ1	1:B:630:TRP:HZ2	1.34	0.73
1:B:544:GLN:HG2	1:B:545:ARG:HG2	1.71	0.73
1:F:544:GLN:HG2	1:F:545:ARG:HG2	1.71	0.73
1:C:654:TYR:CD2	1:C:670:PHE:CZ	2.77	0.72
1:D:544:GLN:HG2	1:D:545:ARG:HG2	1.71	0.72
1:B:677:TYR:CE1	1:D:541:ASP:HB3	2.24	0.72
1:A:544:GLN:HG2	1:A:545:ARG:HG2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:PRO:CD	2:G:277:ARG:CD	2.58	0.72
1:A:96:PRO:CD	2:G:277:ARG:HE	1.98	0.72
1:A:399:PRO:HG3	1:B:626:LEU:CD1	2.20	0.72
1:D:577:LEU:HB2	1:F:610:GLN:OE1	1.90	0.72
1:A:192:GLN:NE2	2:G:404:ARG:HH21	1.88	0.72
1:A:464:PRO:CG	1:B:514:TYR:CE1	2.72	0.72
2:G:501:LEU:HD22	2:G:503:ILE:CD1	2.19	0.72
1:A:95:TYR:C	2:G:277:ARG:CZ	2.63	0.71
2:G:453:THR:HG22	2:G:455:VAL:H	1.54	0.71
1:A:654:TYR:HB3	1:A:670:PHE:CG	2.25	0.71
1:C:544:GLN:HG2	1:C:545:ARG:HG2	1.71	0.71
2:G:498:GLN:O	2:G:500:GLN:HG2	1.90	0.71
2:G:502:TYR:C	2:G:503:ILE:HD12	2.16	0.71
1:C:630:TRP:HZ2	1:D:368:LYS:HZ1	1.37	0.71
1:D:612:ILE:HD12	1:F:612:ILE:HD12	1.69	0.71
2:G:170:PRO:HD3	2:G:190:THR:HG21	1.71	0.71
2:G:186:LEU:HB2	2:G:205:LEU:HD22	1.71	0.71
1:A:560:MET:HE2	1:A:586:PRO:HD3	1.73	0.71
1:D:560:MET:HE2	1:D:586:PRO:HD3	1.73	0.71
1:C:560:MET:HE2	1:C:586:PRO:HD3	1.73	0.71
1:F:560:MET:HE2	1:F:586:PRO:HD3	1.73	0.71
1:A:342:GLY:CA	3:H:84:TYR:OH	2.39	0.70
1:D:577:LEU:HD11	1:F:607:SER:OG	1.89	0.70
1:F:697:VAL:HG12	1:F:699:GLU:H	1.57	0.70
1:A:654:TYR:CD1	1:A:670:PHE:CB	2.74	0.70
1:A:697:VAL:HG12	1:A:699:GLU:H	1.56	0.70
1:E:560:MET:HE2	1:E:586:PRO:HD3	1.73	0.70
1:B:560:MET:HE2	1:B:586:PRO:HD3	1.73	0.70
1:C:697:VAL:HG12	1:C:699:GLU:H	1.56	0.70
1:A:344:LYS:HD2	3:H:80:ARG:HH11	0.54	0.70
1:A:532:ALA:HB1	1:A:560:MET:HE3	1.73	0.70
1:B:692:GLU:OE2	1:D:441:ASN:N	2.24	0.70
1:B:697:VAL:HG12	1:B:699:GLU:H	1.56	0.70
1:D:677:TYR:CE1	1:E:541:ASP:CB	2.74	0.70
1:A:654:TYR:CD2	1:A:670:PHE:CB	2.71	0.70
1:C:654:TYR:CD2	1:C:670:PHE:CD2	2.79	0.70
1:D:697:VAL:HG12	1:D:699:GLU:H	1.56	0.70
1:A:344:LYS:CD	3:H:80:ARG:HD2	2.05	0.70
2:G:452:GLY:CA	2:G:492:MET:HE1	2.22	0.70
1:A:535:ASN:HB2	1:A:646:PHE:HA	1.73	0.70
1:C:523:SER:HA	1:D:464:PRO:HD3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:654:TYR:CD1	1:E:670:PHE:CG	2.79	0.70
1:A:96:PRO:CG	2:G:277:ARG:HE	2.05	0.69
2:G:116:ASN:HA	2:G:134:THR:O	1.91	0.69
1:C:508:VAL:O	1:C:509:GLU:CA	2.27	0.69
1:F:533:LEU:O	1:F:642:THR:OG1	2.04	0.69
1:A:95:TYR:O	2:G:277:ARG:NH1	2.25	0.69
1:F:629:ASP:OD1	1:F:659:HIS:CE1	2.45	0.69
2:G:273:PHE:H	2:G:392:THR:CG2	2.01	0.69
1:A:273:ASP:CB	3:H:80:ARG:CZ	2.67	0.69
1:F:533:LEU:CB	1:F:642:THR:HG21	2.10	0.69
1:E:697:VAL:HG12	1:E:699:GLU:H	1.57	0.69
1:B:577:LEU:HB2	1:C:610:GLN:HE22	1.57	0.69
2:G:226:PHE:O	2:G:227:ILE:HD12	1.93	0.69
1:A:237:SER:HA	1:A:239:PHE:N	2.08	0.69
1:A:96:PRO:HG3	2:G:277:ARG:HE	1.57	0.69
1:B:237:SER:HA	1:B:239:PHE:N	2.08	0.68
1:E:654:TYR:CD1	1:E:670:PHE:CB	2.76	0.68
1:D:568:SER:OG	1:D:670:PHE:CE1	2.46	0.68
2:G:420:PRO:HG3	2:G:423:ILE:HD11	1.75	0.68
1:E:79:ILE:HD11	1:E:82:ALA:HB2	1.76	0.68
1:F:79:ILE:HD11	1:F:82:ALA:HB2	1.76	0.68
1:B:691:GLN:CD	1:D:442:GLY:N	2.51	0.68
1:C:237:SER:HA	1:C:239:PHE:N	2.07	0.68
1:F:630:TRP:CG	1:F:670:PHE:HE2	2.12	0.68
1:C:626:LEU:HD12	1:D:399:PRO:HG3	1.69	0.68
2:G:330:THR:HG22	2:G:332:SER:H	1.57	0.68
1:A:273:ASP:HB3	3:H:80:ARG:NH1	2.09	0.68
1:A:572:SER:HB2	1:A:683:HIS:CE1	2.28	0.68
1:B:79:ILE:HD11	1:B:82:ALA:HB2	1.75	0.68
1:E:564:VAL:HG22	1:E:580:LEU:HD13	1.76	0.68
1:A:541:ASP:HB3	1:C:677:TYR:OH	1.94	0.68
1:C:630:TRP:HZ2	1:D:368:LYS:HZ2	1.38	0.68
1:C:534:HIS:CD2	1:C:642:THR:HB	2.28	0.67
1:E:532:ALA:HB1	1:E:560:MET:HE3	1.77	0.67
1:A:96:PRO:CG	2:G:277:ARG:NE	2.57	0.67
1:F:237:SER:HA	1:F:239:PHE:N	2.08	0.67
1:B:564:VAL:HG22	1:B:580:LEU:HD13	1.76	0.67
1:B:577:LEU:HB2	1:C:610:GLN:NE2	2.09	0.67
1:D:237:SER:HA	1:D:239:PHE:N	2.08	0.67
1:E:654:TYR:HB3	1:E:670:PHE:CZ	2.29	0.67
1:D:79:ILE:HD11	1:D:82:ALA:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ILE:HD11	1:A:82:ALA:HB2	1.76	0.67
1:C:79:ILE:HD11	1:C:82:ALA:HB2	1.75	0.67
1:C:564:VAL:HG22	1:C:580:LEU:HD13	1.76	0.67
1:C:666:VAL:HG11	1:C:698:SER:N	2.10	0.67
1:D:666:VAL:HG11	1:D:698:SER:N	2.10	0.67
1:E:629:ASP:OD1	1:E:659:HIS:CE1	2.47	0.67
1:F:564:VAL:HG22	1:F:580:LEU:HD13	1.76	0.67
2:G:30:PRO:HG3	2:G:476:LEU:HD13	1.75	0.67
1:B:666:VAL:HG11	1:B:698:SER:N	2.10	0.67
1:F:666:VAL:HG11	1:F:698:SER:N	2.10	0.67
1:A:523:SER:HA	1:B:464:PRO:HD2	1.78	0.66
1:F:570:SER:CB	1:F:683:HIS:CB	2.72	0.66
2:G:274:GLY:O	2:G:392:THR:HG23	1.94	0.66
2:G:516:ARG:HA	2:G:516:ARG:NE	2.10	0.66
1:F:533:LEU:HD13	1:F:642:THR:HG23	1.77	0.66
1:A:399:PRO:HG3	1:B:626:LEU:HD11	1.76	0.66
1:B:654:TYR:CG	1:B:670:PHE:CG	2.83	0.66
1:C:654:TYR:CE2	1:C:670:PHE:CE1	2.84	0.66
1:D:533:LEU:HD22	1:D:639:SER:HB2	1.78	0.66
1:E:666:VAL:HG11	1:E:698:SER:N	2.10	0.66
1:F:570:SER:HB2	1:F:683:HIS:HB2	1.76	0.66
1:D:564:VAL:HG22	1:D:580:LEU:HD13	1.76	0.66
1:E:523:SER:HA	1:F:464:PRO:HD3	1.75	0.66
1:A:552:PHE:HB2	1:C:690:PHE:HZ	1.59	0.66
1:B:577:LEU:CB	1:C:610:GLN:OE1	2.43	0.66
1:C:626:LEU:HD11	1:D:399:PRO:CG	2.23	0.66
2:G:180:LEU:HD11	2:G:182:ILE:HD13	1.78	0.66
1:A:666:VAL:HG11	1:A:698:SER:N	2.10	0.66
1:A:564:VAL:HG22	1:A:580:LEU:HD13	1.76	0.66
1:E:237:SER:HA	1:E:239:PHE:N	2.07	0.66
1:F:571:VAL:HG22	1:F:655:ASN:HA	1.78	0.66
1:D:533:LEU:HB3	1:D:642:THR:CG2	2.27	0.65
2:G:56:SER:HA	2:G:506:THR:HG22	1.77	0.65
1:B:654:TYR:HB3	1:B:670:PHE:CD2	2.31	0.65
1:D:568:SER:HG	1:D:670:PHE:HD1	1.39	0.65
2:G:404:ARG:HH11	2:G:404:ARG:HG2	1.62	0.65
1:F:630:TRP:CG	1:F:670:PHE:CE2	2.85	0.65
1:A:95:TYR:O	2:G:277:ARG:CZ	2.44	0.65
1:B:577:LEU:HB2	1:C:610:GLN:CD	2.22	0.65
1:F:630:TRP:CB	1:F:670:PHE:HE2	1.97	0.65
2:G:95:VAL:HG23	2:G:116:ASN:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:SER:HA	1:B:464:PRO:CD	2.28	0.64
1:E:88:GLU:HB2	1:E:132:LEU:HD21	1.79	0.64
1:E:629:ASP:CG	1:E:659:HIS:CE1	2.75	0.64
1:C:514:TYR:CE1	1:D:464:PRO:HG3	2.31	0.64
1:D:691:GLN:HB3	1:E:441:ASN:HA	1.78	0.64
1:D:88:GLU:HB2	1:D:132:LEU:HD21	1.79	0.64
1:F:88:GLU:HB2	1:F:132:LEU:HD21	1.79	0.64
1:A:88:GLU:HB2	1:A:132:LEU:HD21	1.79	0.64
1:C:532:ALA:HB1	1:C:560:MET:HE2	1.77	0.64
1:F:551:ARG:NH1	1:F:641:GLU:OE2	2.31	0.64
1:B:660:GLN:HB2	2:G:105:TRP:HE1	1.63	0.64
2:G:226:PHE:C	2:G:227:ILE:HD12	2.22	0.64
1:A:192:GLN:HE22	2:G:404:ARG:HH22	1.44	0.64
1:B:559:CYS:C	1:B:560:MET:N	2.56	0.64
1:E:533:LEU:HB3	1:E:642:THR:HG21	1.79	0.64
2:G:85:ILE:HG12	2:G:511:GLN:HE21	1.63	0.64
1:A:442:GLY:H	1:C:691:GLN:NE2	1.79	0.64
1:B:654:TYR:CB	1:B:670:PHE:CD2	2.80	0.64
1:A:654:TYR:CZ	1:A:670:PHE:HB3	2.33	0.63
1:C:88:GLU:HB2	1:C:132:LEU:HD21	1.79	0.63
2:G:452:GLY:HA3	2:G:492:MET:HE1	1.79	0.63
1:E:568:SER:HB2	1:E:670:PHE:HE1	1.63	0.63
1:E:654:TYR:HB2	1:E:670:PHE:CD2	2.32	0.63
2:G:478:GLU:CD	2:G:480:MET:HE2	2.22	0.63
1:E:568:SER:CB	1:E:670:PHE:HE1	2.11	0.63
1:A:508:VAL:HG13	1:A:527:HIS:NE2	2.14	0.63
1:B:677:TYR:OH	1:D:541:ASP:HB3	1.99	0.63
2:G:48:PHE:CE2	2:G:50:GLY:HA2	2.33	0.63
2:G:209:HIS:HD2	2:G:210:PRO:O	1.82	0.63
2:G:218:SER:HB2	2:G:252:ILE:HD11	1.80	0.63
2:G:317:LYS:HE2	2:G:317:LYS:HA	1.79	0.63
1:A:344:LYS:HZ2	3:H:80:ARG:HD2	1.64	0.63
1:B:534:HIS:NE2	1:B:642:THR:HB	2.14	0.63
1:C:654:TYR:CD2	1:C:670:PHE:CE1	2.87	0.63
2:G:85:ILE:H	2:G:511:GLN:HE22	1.46	0.63
1:F:629:ASP:CG	1:F:659:HIS:NE2	2.54	0.62
2:G:203:ARG:NH2	2:G:273:PHE:CE2	2.65	0.62
1:A:344:LYS:HG2	3:H:80:ARG:CZ	2.29	0.62
1:D:274:LEU:HD12	1:D:274:LEU:H	1.64	0.62
1:A:654:TYR:CD1	1:A:670:PHE:HB2	2.34	0.62
1:B:88:GLU:HB2	1:B:132:LEU:HD21	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:629:ASP:OD1	1:C:659:HIS:CE1	2.53	0.62
1:D:568:SER:OG	1:D:670:PHE:CD1	2.51	0.62
1:D:654:TYR:CD2	1:D:670:PHE:CG	2.88	0.62
1:E:50:PHE:HB3	1:E:498:MET:HE2	1.82	0.62
2:G:396:PRO:HG2	2:G:399:VAL:HG12	1.81	0.62
1:A:50:PHE:HB3	1:A:498:MET:HE2	1.82	0.62
1:A:630:TRP:CB	1:A:670:PHE:CE2	2.77	0.62
1:B:690:PHE:CZ	1:D:552:PHE:CD2	2.87	0.62
1:C:654:TYR:CZ	1:C:670:PHE:CG	2.88	0.62
1:F:274:LEU:HD12	1:F:274:LEU:H	1.64	0.62
1:A:552:PHE:HD2	1:C:690:PHE:HE1	1.43	0.62
1:D:50:PHE:HB3	1:D:498:MET:HE2	1.82	0.62
2:G:249:GLU:OE2	2:G:264:ARG:CD	2.47	0.62
1:A:654:TYR:CD1	1:A:670:PHE:HB3	2.34	0.61
1:B:508:VAL:CG1	1:B:527:HIS:NE2	2.63	0.61
2:G:154:ILE:HD12	2:G:154:ILE:H	1.65	0.61
1:F:572:SER:HB2	1:F:683:HIS:CE1	2.35	0.61
2:G:118:ILE:HD12	2:G:118:ILE:N	2.16	0.61
1:C:534:HIS:CE1	1:C:642:THR:HG22	2.35	0.61
1:A:442:GLY:CA	1:C:691:GLN:HE22	2.10	0.61
1:C:50:PHE:HB3	1:C:498:MET:HE2	1.82	0.61
2:G:164:ASN:HD22	2:G:166:ARG:H	1.47	0.61
1:A:222:VAL:HG21	2:G:166:ARG:CZ	2.30	0.61
1:A:546:ALA:HB1	1:C:690:PHE:HZ	1.53	0.61
1:B:274:LEU:H	1:B:274:LEU:HD12	1.64	0.61
2:G:285:THR:HG23	2:G:379:GLY:HA2	1.82	0.61
1:B:50:PHE:HB3	1:B:498:MET:HE2	1.82	0.61
1:C:274:LEU:HD12	1:C:274:LEU:H	1.64	0.61
2:G:427:VAL:HG21	2:G:429:TYR:OH	2.00	0.61
1:A:396:ALA:CB	2:G:107:GLY:HA3	2.31	0.61
1:D:191:LYS:HB3	1:D:194:TYR:HB2	1.83	0.61
1:D:654:TYR:HB3	1:D:670:PHE:CE2	2.35	0.61
1:E:274:LEU:H	1:E:274:LEU:HD12	1.64	0.61
1:A:274:LEU:HD12	1:A:274:LEU:H	1.64	0.61
2:G:85:ILE:H	2:G:511:GLN:NE2	1.99	0.61
1:A:547:TRP:HA	1:C:689:SER:CB	2.31	0.60
1:C:459:ARG:HG3	1:C:526:PRO:HG3	1.82	0.60
1:E:191:LYS:HB3	1:E:194:TYR:HB2	1.83	0.60
1:D:692:GLU:OE2	1:E:440:TYR:CG	2.55	0.60
1:C:654:TYR:CD2	1:C:670:PHE:CG	2.89	0.60
1:F:50:PHE:HB3	1:F:498:MET:HE2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:164:ASN:ND2	2:G:166:ARG:H	1.98	0.60
2:G:268:ILE:HD13	2:G:283:TRP:CD2	2.35	0.60
2:G:453:THR:HG22	2:G:455:VAL:N	2.15	0.60
1:A:464:PRO:HD2	1:B:523:SER:HA	1.82	0.60
1:F:191:LYS:HB3	1:F:194:TYR:HB2	1.83	0.60
1:A:397:PRO:HD2	2:G:107:GLY:HA2	1.83	0.60
1:A:398:VAL:HG22	2:G:105:TRP:O	2.00	0.60
1:D:508:VAL:CG1	1:D:527:HIS:NE2	2.65	0.60
1:F:654:TYR:HB3	1:F:670:PHE:CD2	2.37	0.60
1:B:191:LYS:HB3	1:B:194:TYR:HB2	1.83	0.60
1:A:191:LYS:HB3	1:A:194:TYR:HB2	1.83	0.60
1:A:273:ASP:HB3	3:H:80:ARG:NE	2.14	0.60
2:G:66:ARG:HA	2:G:150:PRO:CB	2.32	0.60
1:F:654:TYR:CD2	1:F:670:PHE:HB3	2.36	0.60
2:G:154:ILE:HD12	2:G:154:ILE:N	2.17	0.60
1:C:535:ASN:CG	1:C:646:PHE:HA	2.27	0.60
1:F:626:LEU:HD21	1:F:658:ALA:O	2.01	0.60
2:G:501:LEU:HD22	2:G:503:ILE:HD11	1.84	0.60
2:G:66:ARG:HA	2:G:150:PRO:HB3	1.84	0.59
2:G:105:TRP:HA	2:G:105:TRP:CE3	2.36	0.59
1:B:663:LEU:HD23	1:B:698:SER:HB2	1.84	0.59
1:C:626:LEU:CD1	1:D:399:PRO:CG	2.58	0.59
1:D:692:GLU:OE2	1:E:440:TYR:HA	2.02	0.59
2:G:209:HIS:CD2	2:G:210:PRO:O	2.56	0.59
2:G:313:LEU:HD22	2:G:324:VAL:HG22	1.83	0.59
1:C:191:LYS:HB3	1:C:194:TYR:HB2	1.83	0.59
1:C:663:LEU:HD23	1:C:698:SER:HB2	1.84	0.59
1:E:654:TYR:CD2	1:E:670:PHE:CZ	2.90	0.59
1:E:663:LEU:HD23	1:E:698:SER:HB2	1.84	0.59
1:F:663:LEU:HD23	1:F:698:SER:HB2	1.84	0.59
1:A:663:LEU:HD23	1:A:698:SER:HB2	1.84	0.59
1:B:533:LEU:HD22	1:B:639:SER:HB2	1.84	0.59
2:G:367:VAL:HG13	2:G:368:PRO:HD2	1.85	0.59
2:G:48:PHE:CZ	2:G:50:GLY:HA2	2.37	0.59
2:G:176:LEU:O	2:G:190:THR:HG23	2.03	0.59
1:A:341:LYS:NZ	3:H:84:TYR:HD1	1.93	0.59
1:D:97:PRO:HG2	1:D:158:TYR:CE1	2.38	0.59
1:D:663:LEU:HD23	1:D:698:SER:HB2	1.84	0.59
2:G:249:GLU:OE2	2:G:264:ARG:HD2	2.03	0.59
1:C:654:TYR:CZ	1:C:670:PHE:HB3	2.38	0.58
1:E:629:ASP:OD1	1:E:659:HIS:NE2	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:46:ILE:O	2:G:85:ILE:HD11	2.03	0.58
1:F:97:PRO:HG2	1:F:158:TYR:CE1	2.38	0.58
1:A:97:PRO:HG2	1:A:158:TYR:CE1	2.38	0.58
1:A:654:TYR:HB2	1:A:670:PHE:CD2	2.35	0.58
1:E:97:PRO:HG2	1:E:158:TYR:CE1	2.38	0.58
1:E:532:ALA:HB1	1:E:560:MET:CE	2.33	0.58
2:G:404:ARG:HG2	2:G:404:ARG:NH1	2.18	0.58
1:B:690:PHE:CZ	1:D:552:PHE:CE2	2.92	0.58
1:C:571:VAL:HG22	1:C:655:ASN:CB	2.32	0.58
1:E:523:SER:HA	1:F:464:PRO:CD	2.32	0.58
2:G:186:LEU:O	2:G:203:ARG:HA	2.04	0.58
2:G:493:GLU:O	2:G:501:LEU:HD23	2.04	0.58
1:C:97:PRO:HG2	1:C:158:TYR:CE1	2.38	0.58
1:C:541:ASP:HB3	1:F:677:TYR:CZ	2.39	0.58
2:G:178:ALA:O	2:G:188:SER:HA	2.03	0.58
1:A:341:LYS:HZ2	3:H:84:TYR:HE1	0.67	0.58
1:A:547:TRP:HA	1:C:689:SER:HB3	1.85	0.58
1:C:508:VAL:C	1:C:509:GLU:CB	2.77	0.58
1:C:654:TYR:CG	1:C:670:PHE:CE2	2.91	0.58
1:F:626:LEU:HD22	1:F:658:ALA:HB1	1.85	0.58
2:G:70:TYR:OH	2:G:146:VAL:HG21	2.04	0.58
2:G:501:LEU:HD22	2:G:503:ILE:HD12	1.86	0.58
2:G:140:ILE:HD13	2:G:140:ILE:H	1.68	0.58
1:F:533:LEU:HD22	1:F:639:SER:OG	2.03	0.58
2:G:287:LEU:HD22	2:G:409:MET:HE2	1.83	0.58
1:B:97:PRO:HG2	1:B:158:TYR:CE1	2.38	0.57
1:D:175:SER:OG	1:D:178:GLU:HG2	2.04	0.57
1:A:175:SER:OG	1:A:178:GLU:HG2	2.05	0.57
1:C:654:TYR:CD2	1:C:670:PHE:CD1	2.93	0.57
1:A:552:PHE:HB3	1:C:690:PHE:CE1	2.40	0.57
1:C:629:ASP:HA	1:C:658:ALA:HB1	1.86	0.57
1:A:231:ASP:CG	2:G:217:ASP:HA	2.30	0.57
2:G:435:VAL:HG23	2:G:450:PHE:HB2	1.87	0.57
1:B:175:SER:OG	1:B:178:GLU:HG2	2.04	0.57
1:E:407:LEU:O	1:E:411:GLN:HG2	2.05	0.57
1:D:533:LEU:HD22	1:D:639:SER:CB	2.35	0.57
1:F:175:SER:OG	1:F:178:GLU:HG2	2.04	0.57
2:G:187:TYR:CE2	2:G:203:ARG:HD3	2.40	0.57
2:G:309:GLN:OE1	2:G:309:GLN:HA	2.05	0.57
1:B:407:LEU:O	1:B:411:GLN:HG2	2.05	0.57
1:C:425:TYR:OH	1:C:456:LYS:HE2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:120:VAL:O	2:G:131:ALA:HA	2.04	0.57
1:C:465:HIS:NE2	1:D:470:TYR:HA	2.20	0.57
1:D:407:LEU:O	1:D:411:GLN:HG2	2.05	0.57
1:D:577:LEU:CB	1:F:610:GLN:OE1	2.52	0.57
2:G:170:PRO:HD3	2:G:177:THR:OG1	2.05	0.57
2:G:265:ILE:HB	2:G:291:LEU:HD11	1.87	0.57
1:A:559:CYS:O	1:A:584:ASP:CG	2.48	0.56
1:B:612:ILE:HG13	1:C:577:LEU:HD13	1.86	0.56
1:C:175:SER:OG	1:C:178:GLU:HG2	2.05	0.56
1:E:175:SER:OG	1:E:178:GLU:HG2	2.05	0.56
2:G:135:GLY:H	2:G:139:PRO:HA	1.68	0.56
1:A:407:LEU:O	1:A:411:GLN:HG2	2.05	0.56
1:F:529:GLY:HA3	1:F:552:PHE:CZ	2.40	0.56
1:A:222:VAL:HG21	2:G:166:ARG:HH22	1.70	0.56
1:A:654:TYR:HD2	1:A:670:PHE:CD1	2.16	0.56
1:C:407:LEU:O	1:C:411:GLN:HG2	2.05	0.56
1:C:529:GLY:HA3	1:C:552:PHE:CZ	2.40	0.56
1:D:529:GLY:HA3	1:D:552:PHE:CZ	2.40	0.56
1:F:407:LEU:O	1:F:411:GLN:HG2	2.05	0.56
1:A:629:ASP:OD1	1:A:659:HIS:NE2	2.38	0.56
1:C:470:TYR:CE1	1:C:525:ASP:CG	2.84	0.56
1:E:571:VAL:HG21	1:E:655:ASN:HB2	1.88	0.56
1:F:425:TYR:OH	1:F:456:LYS:HE2	2.05	0.56
1:A:514:TYR:CE1	1:B:464:PRO:HG3	2.30	0.56
1:E:529:GLY:HA3	1:E:552:PHE:CZ	2.41	0.56
2:G:457:THR:H	2:G:489:ILE:HD11	1.70	0.56
1:E:425:TYR:OH	1:E:456:LYS:HE2	2.05	0.56
1:F:570:SER:OG	1:F:683:HIS:CG	2.59	0.56
1:A:425:TYR:OH	1:A:456:LYS:HE2	2.05	0.56
1:B:529:GLY:HA3	1:B:552:PHE:CZ	2.40	0.56
1:E:626:LEU:HD21	1:E:658:ALA:O	2.05	0.56
1:F:535:ASN:OD1	1:F:646:PHE:HA	2.05	0.56
1:F:570:SER:HB2	1:F:683:HIS:HB3	1.86	0.56
1:E:568:SER:HB2	1:E:670:PHE:CE1	2.40	0.56
2:G:227:ILE:O	2:G:228:SER:HB3	2.04	0.56
1:A:274:LEU:O	3:H:80:ARG:NH2	2.13	0.56
1:B:425:TYR:OH	1:B:456:LYS:HE2	2.05	0.56
1:D:235:LEU:HG	1:D:236:VAL:HG23	1.88	0.56
2:G:285:THR:O	2:G:285:THR:CG2	2.52	0.56
1:A:344:LYS:CE	3:H:80:ARG:HD3	2.35	0.55
1:A:398:VAL:CG2	2:G:105:TRP:O	2.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:568:SER:OG	1:C:670:PHE:CE1	1.98	0.55
2:G:149:HIS:C	2:G:151:GLU:H	2.13	0.55
1:C:235:LEU:HG	1:C:236:VAL:HG23	1.88	0.55
2:G:45:VAL:HG11	2:G:482:VAL:HG13	1.88	0.55
2:G:402:PHE:O	2:G:403:ALA:CB	2.52	0.55
1:A:654:TYR:CE1	1:A:670:PHE:HB3	2.42	0.55
2:G:104:LYS:HD2	2:G:110:ILE:HD11	1.87	0.55
1:A:222:VAL:HG21	2:G:166:ARG:NH2	2.22	0.55
1:A:529:GLY:HA3	1:A:552:PHE:CZ	2.41	0.55
1:E:235:LEU:HG	1:E:236:VAL:HG23	1.88	0.55
2:G:420:PRO:CG	2:G:423:ILE:HD11	2.37	0.55
2:G:426:ASP:N	2:G:426:ASP:OD1	2.40	0.55
1:A:221:PHE:CE1	2:G:212:ARG:HD2	2.36	0.55
1:C:571:VAL:HG21	1:C:655:ASN:HB2	1.88	0.55
1:D:425:TYR:OH	1:D:456:LYS:HE2	2.05	0.55
1:F:533:LEU:HD22	1:F:639:SER:CB	2.37	0.55
2:G:389:PHE:HD1	2:G:389:PHE:H	1.53	0.55
2:G:249:GLU:OE2	2:G:264:ARG:HD3	2.07	0.55
1:A:235:LEU:HG	1:A:236:VAL:HG23	1.88	0.55
1:C:574:HIS:ND1	1:C:618:PRO:HD3	2.22	0.55
1:E:629:ASP:CG	1:E:659:HIS:HE1	2.14	0.55
1:A:552:PHE:CG	1:C:690:PHE:HZ	2.13	0.54
1:D:689:SER:HB3	1:E:540:ARG:CD	2.31	0.54
1:E:574:HIS:ND1	1:E:618:PRO:HD3	2.22	0.54
1:F:574:HIS:ND1	1:F:618:PRO:HD3	2.23	0.54
1:A:220:ASP:OD2	2:G:209:HIS:NE2	2.40	0.54
1:A:221:PHE:HE1	2:G:212:ARG:CD	2.20	0.54
1:A:532:ALA:HB1	1:A:560:MET:HE2	1.88	0.54
1:B:235:LEU:HG	1:B:236:VAL:HG23	1.88	0.54
1:B:574:HIS:ND1	1:B:618:PRO:HD3	2.22	0.54
1:F:235:LEU:HG	1:F:236:VAL:HG23	1.89	0.54
2:G:30:PRO:HG3	2:G:476:LEU:CD1	2.37	0.54
2:G:378:PRO:HG3	2:G:399:VAL:HG23	1.87	0.54
1:B:610:GLN:CD	1:C:577:LEU:CD1	2.68	0.54
1:D:574:HIS:ND1	1:D:618:PRO:HD3	2.22	0.54
2:G:32:LEU:HB2	2:G:478:GLU:HB3	1.89	0.54
1:A:87:PRO:HB2	1:A:109:LEU:HD11	1.90	0.54
1:B:551:ARG:NH1	1:B:641:GLU:CD	2.62	0.54
1:D:571:VAL:HG22	1:D:655:ASN:CB	2.34	0.54
1:E:399:PRO:HG3	1:F:626:LEU:HD11	1.90	0.54
2:G:401:THR:O	2:G:404:ARG:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:95:TYR:HA	1:B:96:PRO:C	2.33	0.54
1:D:551:ARG:HH12	1:D:641:GLU:CD	2.13	0.54
1:D:612:ILE:HD11	1:F:612:ILE:CD1	2.38	0.54
2:G:384:LYS:NZ	2:G:384:LYS:HB3	2.23	0.54
1:D:87:PRO:HB2	1:D:109:LEU:HD11	1.90	0.53
1:A:660:GLN:C	1:A:661:LEU:HD12	2.34	0.53
1:B:87:PRO:HB2	1:B:109:LEU:HD11	1.90	0.53
1:C:534:HIS:CE1	1:C:642:THR:CG2	2.92	0.53
1:E:95:TYR:HA	1:E:96:PRO:C	2.33	0.53
2:G:31:ARG:N	2:G:31:ARG:HD2	2.23	0.53
2:G:199:PHE:CZ	2:G:225:ARG:NH1	2.76	0.53
1:D:95:TYR:HA	1:D:96:PRO:C	2.33	0.53
2:G:279:LEU:HD12	2:G:400:ILE:HG23	1.90	0.53
1:A:344:LYS:NZ	3:H:80:ARG:HD2	2.23	0.53
1:B:535:ASN:HB2	1:B:646:PHE:HA	1.90	0.53
1:D:660:GLN:C	1:D:661:LEU:HD12	2.34	0.53
2:G:134:THR:HG23	2:G:171:TYR:O	2.08	0.53
1:A:574:HIS:ND1	1:A:618:PRO:HD3	2.22	0.53
2:G:93:TRP:CH2	2:G:142:THR:HG22	2.43	0.53
2:G:218:SER:HB2	2:G:252:ILE:CD1	2.39	0.53
1:C:95:TYR:HA	1:C:96:PRO:C	2.33	0.53
1:B:534:HIS:CD2	1:B:642:THR:HB	2.44	0.53
1:E:87:PRO:HB2	1:E:109:LEU:HD11	1.90	0.53
1:E:660:GLN:C	1:E:661:LEU:HD12	2.34	0.53
1:C:508:VAL:CG1	1:C:539:ARG:NH2	2.72	0.53
2:G:56:SER:CA	2:G:506:THR:HG22	2.38	0.53
2:G:267:GLN:O	2:G:268:ILE:HG13	2.09	0.53
1:F:87:PRO:HB2	1:F:109:LEU:HD11	1.90	0.53
2:G:204:THR:O	2:G:205:LEU:HB2	2.09	0.53
1:A:95:TYR:HA	1:A:96:PRO:C	2.33	0.53
1:C:660:GLN:C	1:C:661:LEU:HD12	2.34	0.53
1:A:552:PHE:CB	1:C:690:PHE:CE1	2.92	0.52
1:C:87:PRO:HB2	1:C:109:LEU:HD11	1.90	0.52
1:C:459:ARG:CG	1:C:526:PRO:HG3	2.39	0.52
1:F:660:GLN:C	1:F:661:LEU:HD12	2.34	0.52
1:A:327:ASN:CG	1:A:327:ASN:O	2.52	0.52
1:C:535:ASN:HB2	1:C:646:PHE:HA	1.92	0.52
1:D:507:PRO:O	1:D:509:GLU:N	2.42	0.52
1:F:533:LEU:HD11	1:F:641:GLU:OE1	2.09	0.52
1:A:540:ARG:NH1	1:C:689:SER:O	2.42	0.52
1:C:568:SER:HB2	1:C:670:PHE:CE1	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:327:ASN:O	1:E:327:ASN:CG	2.52	0.52
2:G:161:HIS:O	2:G:162:PHE:HB2	2.08	0.52
1:C:459:ARG:CD	1:C:526:PRO:HG3	2.39	0.52
2:G:427:VAL:HG13	2:G:429:TYR:CD2	2.44	0.52
2:G:39:MET:HE3	2:G:45:VAL:HG13	1.91	0.52
1:F:95:TYR:HA	1:F:96:PRO:C	2.33	0.52
2:G:35:SER:OG	2:G:38:GLU:HG3	2.09	0.52
2:G:453:THR:H	2:G:489:ILE:HD12	1.75	0.52
1:A:552:PHE:HD2	1:C:690:PHE:CE1	2.17	0.52
1:B:660:GLN:C	1:B:661:LEU:HD12	2.34	0.52
1:B:327:ASN:CG	1:B:327:ASN:O	2.52	0.52
1:C:308:ARG:HB2	1:C:343:GLN:HG2	1.92	0.52
1:D:235:LEU:HD21	1:D:263:PRO:HG2	1.92	0.52
1:A:96:PRO:N	2:G:277:ARG:CZ	2.72	0.52
1:A:308:ARG:HB2	1:A:343:GLN:HG2	1.92	0.52
1:C:654:TYR:CZ	1:C:670:PHE:CB	2.93	0.52
1:F:235:LEU:HD21	1:F:263:PRO:HG2	1.92	0.52
1:A:274:LEU:HD12	1:A:274:LEU:N	2.25	0.51
1:B:610:GLN:CG	1:C:577:LEU:HD12	2.40	0.51
1:D:274:LEU:HD12	1:D:274:LEU:N	2.25	0.51
1:A:547:TRP:HA	1:C:689:SER:OG	2.09	0.51
1:C:559:CYS:O	1:C:584:ASP:OD2	2.27	0.51
1:B:176:GLU:HG3	1:B:177:GLY:N	2.26	0.51
1:E:235:LEU:HD21	1:E:263:PRO:HG2	1.93	0.51
1:F:274:LEU:HD12	1:F:274:LEU:N	2.25	0.51
1:F:327:ASN:CG	1:F:327:ASN:O	2.52	0.51
1:A:344:LYS:CE	3:H:80:ARG:CD	2.88	0.51
1:C:274:LEU:HD12	1:C:274:LEU:N	2.26	0.51
1:D:176:GLU:HG3	1:D:177:GLY:N	2.26	0.51
1:D:677:TYR:CE1	1:E:541:ASP:HB2	2.45	0.51
1:E:308:ARG:HB2	1:E:343:GLN:HG2	1.92	0.51
2:G:46:ILE:HD12	2:G:511:GLN:NE2	2.26	0.51
2:G:46:ILE:HB	2:G:511:GLN:HB3	1.91	0.51
2:G:66:ARG:O	2:G:68:ARG:HG3	2.11	0.51
1:A:235:LEU:HD21	1:A:263:PRO:HG2	1.93	0.51
1:A:176:GLU:HG3	1:A:177:GLY:N	2.26	0.51
1:C:176:GLU:HG3	1:C:177:GLY:N	2.26	0.51
1:C:327:ASN:CG	1:C:327:ASN:O	2.52	0.51
1:B:308:ARG:HB2	1:B:343:GLN:HG2	1.92	0.51
1:D:308:ARG:HB2	1:D:343:GLN:HG2	1.92	0.51
1:D:327:ASN:CG	1:D:327:ASN:O	2.52	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:461:ASP:O	1:E:466:GLY:O	2.29	0.51
2:G:274:GLY:HA2	2:G:284:THR:HG23	1.93	0.51
1:A:624:ILE:HG13	1:A:655:ASN:HB2	1.93	0.51
1:E:176:GLU:HG3	1:E:177:GLY:N	2.26	0.51
1:E:274:LEU:HD12	1:E:274:LEU:N	2.25	0.51
1:A:461:ASP:O	1:A:466:GLY:O	2.29	0.51
1:F:308:ARG:HB2	1:F:343:GLN:HG2	1.92	0.51
1:B:612:ILE:CD1	1:C:577:LEU:HD13	2.40	0.51
1:C:235:LEU:HD21	1:C:263:PRO:HG2	1.93	0.51
1:D:574:HIS:CE1	1:D:618:PRO:HD3	2.46	0.51
1:B:574:HIS:CE1	1:B:618:PRO:HD3	2.46	0.50
1:B:690:PHE:HZ	1:D:552:PHE:CE2	2.28	0.50
1:E:654:TYR:CE2	1:E:670:PHE:HD1	2.17	0.50
2:G:455:VAL:HG13	2:G:455:VAL:O	2.10	0.50
1:A:626:LEU:HD11	1:B:399:PRO:CG	2.38	0.50
1:F:570:SER:OG	1:F:683:HIS:ND1	2.44	0.50
2:G:462:VAL:CG2	2:G:477:LEU:HD11	2.41	0.50
2:G:234:GLU:O	2:G:320:LYS:HD3	2.12	0.50
2:G:503:ILE:HD12	2:G:503:ILE:N	2.25	0.50
1:A:221:PHE:CE1	2:G:202:PHE:CE2	2.88	0.50
1:B:274:LEU:HD12	1:B:274:LEU:N	2.25	0.50
2:G:109:ASP:HB3	2:G:113:GLU:HG3	1.93	0.50
1:A:275:PHE:CD2	3:H:80:ARG:NE	2.78	0.50
1:B:235:LEU:HD21	1:B:263:PRO:HG2	1.93	0.50
1:D:508:VAL:HG13	1:D:527:HIS:CE1	2.46	0.50
1:F:176:GLU:HG3	1:F:177:GLY:N	2.26	0.50
1:F:574:HIS:CE1	1:F:618:PRO:HD3	2.46	0.50
1:A:514:TYR:HE1	1:B:464:PRO:CG	2.20	0.50
1:A:539:ARG:HD2	1:A:542:LYS:NZ	2.27	0.50
1:A:552:PHE:HB3	1:C:690:PHE:CZ	2.44	0.50
1:B:461:ASP:O	1:B:466:GLY:O	2.29	0.50
1:E:574:HIS:CE1	1:E:618:PRO:HD3	2.46	0.50
1:F:539:ARG:HD2	1:F:542:LYS:NZ	2.27	0.50
1:B:654:TYR:CZ	1:B:670:PHE:HB3	2.46	0.50
1:D:654:TYR:CG	1:D:670:PHE:CD2	3.00	0.50
1:E:518:GLY:HA2	1:F:324:GLN:NE2	1.87	0.50
1:F:630:TRP:CB	1:F:670:PHE:CZ	2.93	0.50
2:G:140:ILE:HD13	2:G:140:ILE:N	2.27	0.50
1:C:574:HIS:CE1	1:C:618:PRO:HD3	2.46	0.50
1:A:574:HIS:CE1	1:A:618:PRO:HD3	2.46	0.50
2:G:491:ALA:HB3	2:G:504:GLY:HA3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:VAL:CG1	1:A:527:HIS:HE2	2.23	0.49
1:D:461:ASP:O	1:D:466:GLY:O	2.29	0.49
1:A:399:PRO:HG3	1:B:626:LEU:HD13	1.94	0.49
2:G:313:LEU:CD2	2:G:324:VAL:HG22	2.42	0.49
1:A:508:VAL:HG13	1:A:527:HIS:CE1	2.48	0.49
1:C:539:ARG:HD2	1:C:542:LYS:NZ	2.27	0.49
1:D:673:HIS:CD2	1:D:685:PRO:HG3	2.48	0.49
1:F:461:ASP:O	1:F:466:GLY:O	2.29	0.49
2:G:157:LEU:HD13	2:G:157:LEU:O	2.13	0.49
1:E:137:CYS:SG	1:E:159:LEU:HD11	2.53	0.49
1:F:411:GLN:HA	1:F:412:PRO:C	2.38	0.49
2:G:69:LEU:HD13	2:G:69:LEU:O	2.12	0.49
2:G:178:ALA:HB1	2:G:228:SER:HA	1.94	0.49
2:G:202:PHE:CZ	2:G:212:ARG:HD2	2.48	0.49
1:A:508:VAL:CG1	1:A:527:HIS:CD2	2.96	0.49
1:B:237:SER:OG	1:B:238:HIS:HA	2.13	0.49
1:C:508:VAL:O	1:C:509:GLU:HA	2.11	0.49
1:E:539:ARG:HD2	1:E:542:LYS:NZ	2.27	0.49
2:G:453:THR:HG22	2:G:455:VAL:HG12	1.93	0.49
2:G:512:LEU:HD23	2:G:512:LEU:C	2.38	0.49
1:A:673:HIS:CD2	1:A:685:PRO:HG3	2.48	0.49
1:C:137:CYS:SG	1:C:159:LEU:HD11	2.53	0.49
1:C:461:ASP:O	1:C:466:GLY:O	2.29	0.49
2:G:118:ILE:N	2:G:118:ILE:CD1	2.76	0.49
1:D:445:VAL:CG2	1:D:526:PRO:HG2	2.33	0.49
1:E:673:HIS:CD2	1:E:685:PRO:HG3	2.48	0.49
2:G:399:VAL:HG13	2:G:400:ILE:H	1.77	0.49
1:A:464:PRO:CD	1:B:523:SER:HA	2.42	0.49
1:B:411:GLN:HA	1:B:412:PRO:C	2.38	0.49
1:D:411:GLN:HA	1:D:412:PRO:C	2.38	0.49
1:F:137:CYS:SG	1:F:159:LEU:HD11	2.53	0.49
2:G:206:GLY:O	2:G:208:HIS:N	2.41	0.49
1:B:137:CYS:SG	1:B:159:LEU:HD11	2.53	0.49
1:B:560:MET:CE	1:B:586:PRO:HD3	2.43	0.49
1:C:629:ASP:CG	1:C:659:HIS:CE1	2.91	0.49
1:D:137:CYS:SG	1:D:159:LEU:HD11	2.53	0.49
1:E:411:GLN:HA	1:E:412:PRO:C	2.38	0.49
1:C:673:HIS:CD2	1:C:685:PRO:HG3	2.48	0.48
1:F:50:PHE:CE2	1:F:503:VAL:HG23	2.48	0.48
1:C:514:TYR:HE1	1:D:464:PRO:CG	2.22	0.48
1:D:539:ARG:HD2	1:D:542:LYS:NZ	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:237:SER:OG	1:E:238:HIS:HA	2.13	0.48
2:G:429:TYR:O	2:G:430:GLN:HG3	2.14	0.48
1:A:50:PHE:CE2	1:A:503:VAL:HG23	2.48	0.48
1:A:411:GLN:HA	1:A:412:PRO:C	2.38	0.48
1:B:539:ARG:HD2	1:B:542:LYS:NZ	2.27	0.48
1:D:690:PHE:HE2	1:E:541:ASP:N	2.06	0.48
1:F:237:SER:OG	1:F:238:HIS:HA	2.13	0.48
1:F:570:SER:HG	1:F:683:HIS:CG	2.31	0.48
1:B:673:HIS:CD2	1:B:685:PRO:HG3	2.48	0.48
1:D:50:PHE:CE2	1:D:503:VAL:HG23	2.48	0.48
1:E:560:MET:CE	1:E:586:PRO:HD3	2.43	0.48
1:F:673:HIS:CD2	1:F:685:PRO:HG3	2.48	0.48
2:G:170:PRO:CD	2:G:190:THR:HG21	2.42	0.48
1:C:237:SER:OG	1:C:238:HIS:HA	2.13	0.48
1:E:351:ASP:HA	1:E:431:ARG:HB2	1.96	0.48
1:E:568:SER:HG	1:E:670:PHE:HE1	1.60	0.48
1:A:137:CYS:SG	1:A:159:LEU:HD11	2.53	0.48
1:C:411:GLN:HA	1:C:412:PRO:C	2.38	0.48
1:D:237:SER:OG	1:D:238:HIS:HA	2.13	0.48
2:G:433:GLN:HB2	2:G:492:MET:HE3	1.95	0.48
1:A:237:SER:OG	1:A:238:HIS:HA	2.13	0.48
1:B:508:VAL:HB	1:B:539:ARG:NH2	2.28	0.48
1:D:417:THR:HA	1:D:418:PRO:HD3	1.74	0.48
1:F:535:ASN:CG	1:F:645:ILE:O	2.57	0.48
1:F:559:CYS:HB3	1:F:560:MET:H	1.31	0.48
1:C:654:TYR:CE1	1:C:670:PHE:CB	2.96	0.48
1:E:50:PHE:CE2	1:E:503:VAL:HG23	2.48	0.48
2:G:427:VAL:HG11	2:G:429:TYR:CE1	2.48	0.48
1:A:326:PHE:CG	1:A:359:PRO:HG3	2.49	0.48
1:A:445:VAL:CG2	1:A:526:PRO:HG2	2.36	0.48
1:B:50:PHE:CE2	1:B:503:VAL:HG23	2.48	0.48
1:B:691:GLN:CB	1:D:441:ASN:HA	2.31	0.48
1:C:50:PHE:CE2	1:C:503:VAL:HG23	2.48	0.48
1:C:326:PHE:CG	1:C:359:PRO:HG3	2.49	0.48
1:B:141:ARG:HD2	1:B:143:ASP:OD1	2.14	0.47
1:E:141:ARG:HD2	1:E:143:ASP:OD1	2.14	0.47
1:F:594:CYS:O	1:F:601:GLU:HA	2.14	0.47
1:E:326:PHE:CG	1:E:359:PRO:HG3	2.49	0.47
1:F:533:LEU:CD1	1:F:641:GLU:CD	2.87	0.47
1:F:351:ASP:HA	1:F:431:ARG:HB2	1.96	0.47
2:G:211:ILE:CD1	2:G:281:ASN:HA	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:285:THR:HG23	2:G:379:GLY:CA	2.44	0.47
1:A:594:CYS:O	1:A:601:GLU:HA	2.14	0.47
2:G:84:ASN:C	2:G:86:LYS:H	2.22	0.47
2:G:263:ALA:O	2:G:264:ARG:HG2	2.15	0.47
1:A:141:ARG:HD2	1:A:143:ASP:OD1	2.15	0.47
1:F:141:ARG:HD2	1:F:143:ASP:OD1	2.15	0.47
2:G:453:THR:CG2	2:G:454:ASP:N	2.78	0.47
1:D:351:ASP:HA	1:D:431:ARG:HB2	1.96	0.47
1:D:470:TYR:CE1	1:D:525:ASP:CG	2.92	0.47
1:D:654:TYR:CD2	1:D:670:PHE:CD1	3.02	0.47
2:G:246:PHE:CZ	2:G:265:ILE:HD12	2.49	0.47
2:G:427:VAL:CG1	2:G:429:TYR:H	2.27	0.47
1:C:594:CYS:O	1:C:601:GLU:HA	2.14	0.47
1:E:654:TYR:CD1	1:E:670:PHE:HB2	2.49	0.47
2:G:287:LEU:HD11	2:G:379:GLY:HA3	1.96	0.47
2:G:377:ARG:O	2:G:380:THR:HB	2.14	0.47
1:A:508:VAL:CG1	1:A:527:HIS:CE1	2.97	0.47
1:F:326:PHE:CG	1:F:359:PRO:HG3	2.49	0.47
1:B:508:VAL:HG13	1:B:527:HIS:NE2	2.29	0.47
1:B:638:ARG:HB2	1:B:645:ILE:HD13	1.97	0.47
1:D:141:ARG:HD2	1:D:143:ASP:OD1	2.14	0.47
1:D:594:CYS:O	1:D:601:GLU:HA	2.14	0.47
2:G:482:VAL:HG12	2:G:510:ALA:HB1	1.97	0.47
2:G:509:VAL:HG12	2:G:510:ALA:N	2.30	0.47
1:A:409:ILE:CG2	2:G:194:PHE:CD2	2.89	0.47
1:B:594:CYS:O	1:B:601:GLU:HA	2.14	0.47
1:F:459:ARG:HD3	1:F:526:PRO:HG3	1.97	0.47
2:G:160:SER:HB3	2:G:161:HIS:CE1	2.49	0.47
1:A:476:PHE:CE2	1:A:482:ILE:HD13	2.51	0.46
1:C:417:THR:HA	1:C:418:PRO:HD3	1.74	0.46
1:C:560:MET:CE	1:C:586:PRO:HD3	2.43	0.46
1:E:594:CYS:O	1:E:601:GLU:HA	2.14	0.46
1:F:533:LEU:HD13	1:F:641:GLU:HB3	1.96	0.46
1:F:570:SER:HB3	1:F:683:HIS:CG	2.49	0.46
2:G:92:VAL:HG12	2:G:94:PRO:HD3	1.97	0.46
1:A:508:VAL:HG11	1:A:527:HIS:NE2	2.27	0.46
1:B:326:PHE:CG	1:B:359:PRO:HG3	2.49	0.46
1:C:351:ASP:HA	1:C:431:ARG:HB2	1.96	0.46
1:A:630:TRP:CB	1:A:670:PHE:CZ	2.98	0.46
1:B:159:LEU:HD13	1:B:184:ILE:HD13	1.98	0.46
1:C:141:ARG:HD2	1:C:143:ASP:OD1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:539:ARG:HB2	1:C:542:LYS:HD3	1.97	0.46
1:D:326:PHE:CG	1:D:359:PRO:HG3	2.49	0.46
1:F:533:LEU:HB3	1:F:642:THR:HG23	1.86	0.46
1:F:654:TYR:CG	1:F:670:PHE:CB	2.98	0.46
1:A:96:PRO:N	2:G:277:ARG:NH2	2.62	0.46
1:B:328:ILE:HB	1:B:332:GLU:OE1	2.16	0.46
1:B:654:TYR:CE2	1:B:670:PHE:HB3	2.50	0.46
1:C:328:ILE:HB	1:C:332:GLU:OE1	2.16	0.46
1:D:577:LEU:HD11	1:F:607:SER:HB3	1.75	0.46
1:F:159:LEU:HD13	1:F:184:ILE:HD13	1.98	0.46
2:G:164:ASN:ND2	2:G:166:ARG:HG3	2.31	0.46
2:G:358:HIS:CD2	2:G:406:HIS:HE1	2.33	0.46
1:A:638:ARG:HB2	1:A:645:ILE:HD13	1.97	0.46
1:D:638:ARG:HB2	1:D:645:ILE:HD13	1.97	0.46
1:E:476:PHE:CE2	1:E:482:ILE:HD13	2.51	0.46
1:F:81:VAL:HG11	1:F:145:LEU:HB2	1.98	0.46
1:A:464:PRO:HG2	1:B:514:TYR:CE1	2.51	0.46
1:B:81:VAL:HG11	1:B:145:LEU:HB2	1.98	0.46
1:B:351:ASP:HA	1:B:431:ARG:HB2	1.96	0.46
1:B:539:ARG:HB2	1:B:542:LYS:HD3	1.97	0.46
1:D:203:LEU:HD23	1:D:203:LEU:HA	1.83	0.46
1:D:476:PHE:CE2	1:D:482:ILE:HD13	2.51	0.46
1:E:277:THR:HG22	1:E:279:ARG:HG3	1.98	0.46
1:E:539:ARG:HB2	1:E:542:LYS:HD3	1.97	0.46
1:F:476:PHE:CE2	1:F:482:ILE:HD13	2.51	0.46
1:F:533:LEU:CD1	1:F:641:GLU:OE1	2.64	0.46
2:G:121:LEU:C	2:G:122:GLU:HG2	2.40	0.46
1:A:159:LEU:HD13	1:A:184:ILE:HD13	1.98	0.46
1:A:539:ARG:HB2	1:A:542:LYS:HD3	1.97	0.46
1:D:328:ILE:HB	1:D:332:GLU:OE1	2.16	0.46
1:F:539:ARG:HB2	1:F:542:LYS:HD3	1.97	0.46
1:F:672:CYS:HB3	1:F:681:CYS:SG	2.56	0.46
2:G:115:ALA:HB3	2:G:117:PHE:CE1	2.50	0.46
1:B:476:PHE:CE2	1:B:482:ILE:HD13	2.51	0.46
1:D:539:ARG:HB2	1:D:542:LYS:HD3	1.97	0.46
1:D:691:GLN:CB	1:E:441:ASN:HA	2.43	0.46
2:G:134:THR:O	2:G:136:ALA:N	2.43	0.46
1:A:351:ASP:HA	1:A:431:ARG:HB2	1.96	0.46
1:D:550:ASN:HB2	1:D:586:PRO:HA	1.97	0.46
1:E:329:SER:HB3	1:E:332:GLU:HG3	1.98	0.46
1:F:638:ARG:HB2	1:F:645:ILE:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:180:LEU:HD11	2:G:182:ILE:CD1	2.46	0.46
1:A:112:ASN:HB2	1:A:132:LEU:HD22	1.98	0.46
1:B:329:SER:HB3	1:B:332:GLU:HG3	1.98	0.46
1:C:81:VAL:HG11	1:C:145:LEU:HB2	1.98	0.46
1:D:81:VAL:HG11	1:D:145:LEU:HB2	1.98	0.46
1:D:329:SER:HB3	1:D:332:GLU:HG3	1.98	0.46
1:E:654:TYR:CG	1:E:670:PHE:CE2	2.92	0.46
2:G:323:ILE:HD12	2:G:323:ILE:N	2.31	0.46
2:G:342:MET:HG3	2:G:421:ILE:CG1	2.46	0.46
1:B:112:ASN:HB2	1:B:132:LEU:HD22	1.98	0.45
1:B:470:TYR:CE1	1:B:525:ASP:CG	2.94	0.45
1:C:277:THR:HG22	1:C:279:ARG:HG3	1.98	0.45
1:C:638:ARG:HB2	1:C:645:ILE:HD13	1.97	0.45
1:F:277:THR:HG22	1:F:279:ARG:HG3	1.98	0.45
1:F:559:CYS:O	1:F:584:ASP:HB2	2.16	0.45
2:G:432:THR:CG2	2:G:454:ASP:HB3	2.46	0.45
1:A:274:LEU:O	3:H:80:ARG:CZ	2.63	0.45
1:C:112:ASN:HB2	1:C:132:LEU:HD22	1.98	0.45
1:C:329:SER:HB3	1:C:332:GLU:HG3	1.98	0.45
1:C:654:TYR:HB3	1:C:670:PHE:CE2	2.50	0.45
1:C:672:CYS:HB3	1:C:681:CYS:SG	2.56	0.45
1:E:626:LEU:C	1:F:399:PRO:HA	2.40	0.45
2:G:180:LEU:HD13	2:G:180:LEU:C	2.41	0.45
1:A:231:ASP:OD2	2:G:218:SER:N	2.45	0.45
1:A:342:GLY:HA2	3:H:84:TYR:OH	2.16	0.45
1:B:660:GLN:HB2	2:G:105:TRP:NE1	2.31	0.45
1:C:476:PHE:CE2	1:C:482:ILE:HD13	2.51	0.45
1:C:514:TYR:CE1	1:D:464:PRO:CG	2.98	0.45
1:D:560:MET:CE	1:D:586:PRO:HD3	2.43	0.45
1:E:328:ILE:HB	1:E:332:GLU:OE1	2.16	0.45
1:B:533:LEU:HD23	1:B:533:LEU:HA	1.84	0.45
1:B:672:CYS:HB3	1:B:681:CYS:SG	2.56	0.45
1:D:508:VAL:HB	1:D:539:ARG:NH2	2.32	0.45
1:E:638:ARG:HB2	1:E:645:ILE:HD13	1.97	0.45
2:G:62:LEU:C	2:G:62:LEU:HD13	2.41	0.45
2:G:110:ILE:HA	2:G:114:CYS:HB2	1.98	0.45
2:G:375:TYR:HA	2:G:376:PRO:C	2.42	0.45
2:G:399:VAL:HG13	2:G:400:ILE:N	2.32	0.45
1:A:328:ILE:HB	1:A:332:GLU:OE1	2.16	0.45
1:A:533:LEU:HD23	1:A:533:LEU:HA	1.84	0.45
1:D:112:ASN:HB2	1:D:132:LEU:HD22	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:508:VAL:CG1	1:D:527:HIS:CD2	3.00	0.45
1:A:277:THR:HG22	1:A:279:ARG:HG3	1.98	0.45
1:B:568:SER:HB2	1:B:670:PHE:CE1	2.51	0.45
1:B:577:LEU:HD13	1:C:612:ILE:CD1	2.45	0.45
1:B:612:ILE:HD13	1:C:612:ILE:HD13	1.97	0.45
1:D:159:LEU:HD13	1:D:184:ILE:HD13	1.98	0.45
2:G:512:LEU:HD23	2:G:513:PRO:O	2.17	0.45
1:A:672:CYS:HB3	1:A:681:CYS:SG	2.56	0.45
1:B:630:TRP:HB3	1:B:670:PHE:HE2	1.81	0.45
1:B:661:LEU:HD11	2:G:105:TRP:CD1	2.52	0.45
1:E:159:LEU:HD13	1:E:184:ILE:HD13	1.98	0.45
1:F:328:ILE:HB	1:F:332:GLU:OE1	2.16	0.45
2:G:263:ALA:C	2:G:264:ARG:HG2	2.42	0.45
1:B:612:ILE:HD12	1:C:612:ILE:HG21	1.99	0.45
1:D:677:TYR:CE2	1:E:541:ASP:HB3	2.45	0.45
2:G:160:SER:O	2:G:161:HIS:C	2.60	0.45
2:G:239:GLU:OE1	2:G:384:LYS:HG3	2.17	0.45
1:D:277:THR:HG22	1:D:279:ARG:HG3	1.98	0.45
1:F:560:MET:CE	1:F:586:PRO:HD3	2.43	0.45
2:G:27:ASN:ND2	2:G:28:ASN:H	2.14	0.45
2:G:77:ILE:CD1	2:G:144:ILE:HD11	2.47	0.45
2:G:152:ASP:HB2	2:G:154:ILE:CD1	2.40	0.45
2:G:427:VAL:HG13	2:G:429:TYR:CE2	2.52	0.45
1:A:162:VAL:CG2	1:A:189:ASP:HB2	2.47	0.45
1:A:329:SER:HB3	1:A:332:GLU:HG3	1.98	0.45
1:B:661:LEU:HD11	2:G:105:TRP:HD1	1.82	0.45
1:C:159:LEU:HD13	1:C:184:ILE:HD13	1.98	0.45
1:C:571:VAL:CG2	1:C:655:ASN:CB	2.89	0.45
1:E:81:VAL:HG11	1:E:145:LEU:HB2	1.98	0.45
2:G:105:TRP:HA	2:G:105:TRP:HE3	1.80	0.45
1:A:547:TRP:HB3	1:C:677:TYR:HB3	2.00	0.44
1:F:570:SER:CB	1:F:683:HIS:HB3	2.45	0.44
2:G:91:ILE:HD13	2:G:157:LEU:HB2	1.98	0.44
2:G:95:VAL:HG13	2:G:99:ARG:HB3	1.99	0.44
2:G:502:TYR:CD1	2:G:502:TYR:N	2.85	0.44
1:B:162:VAL:CG2	1:B:189:ASP:HB2	2.47	0.44
1:C:535:ASN:CB	1:C:646:PHE:HA	2.47	0.44
1:E:112:ASN:HB2	1:E:132:LEU:HD22	1.98	0.44
1:E:672:CYS:HB3	1:E:681:CYS:SG	2.56	0.44
1:A:81:VAL:HG11	1:A:145:LEU:HB2	1.98	0.44
1:B:277:THR:HG22	1:B:279:ARG:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:612:ILE:CG1	1:C:577:LEU:HD13	2.47	0.44
1:D:672:CYS:HB3	1:D:681:CYS:SG	2.56	0.44
1:E:417:THR:HA	1:E:418:PRO:HD3	1.74	0.44
1:E:533:LEU:HD23	1:E:533:LEU:HA	1.84	0.44
1:E:533:LEU:HD13	1:E:642:THR:HG23	2.00	0.44
2:G:181:LEU:HD23	2:G:181:LEU:C	2.42	0.44
2:G:277:ARG:O	2:G:278:SER:O	2.35	0.44
1:F:329:SER:HB3	1:F:332:GLU:HG3	1.98	0.44
1:C:162:VAL:CG2	1:C:189:ASP:HB2	2.48	0.44
1:F:112:ASN:HB2	1:F:132:LEU:HD22	1.98	0.44
1:F:162:VAL:CG2	1:F:189:ASP:HB2	2.47	0.44
1:F:654:TYR:HB3	1:F:670:PHE:CG	2.52	0.44
3:H:80:ARG:O	3:H:82:CYS:N	2.51	0.44
1:F:482:ILE:HG23	1:F:497:VAL:HG13	2.00	0.44
1:A:409:ILE:HG21	2:G:194:PHE:HE2	1.57	0.44
1:E:162:VAL:CG2	1:E:189:ASP:HB2	2.48	0.44
2:G:478:GLU:CG	2:G:480:MET:HE2	2.48	0.44
1:A:231:ASP:OD1	2:G:217:ASP:HA	2.18	0.44
1:B:630:TRP:HB3	1:B:670:PHE:CE2	2.53	0.44
1:C:149:VAL:HG22	1:C:150:GLU:N	2.33	0.44
1:C:191:LYS:HD2	1:C:191:LYS:N	2.33	0.44
1:C:482:ILE:HG23	1:C:497:VAL:HG13	2.00	0.44
1:D:525:ASP:HA	1:D:526:PRO:HD3	1.86	0.44
1:D:551:ARG:NH1	1:D:641:GLU:CD	2.74	0.44
2:G:66:ARG:HA	2:G:150:PRO:HB2	1.98	0.44
2:G:149:HIS:HB2	2:G:152:ASP:OD2	2.17	0.44
1:A:225:LEU:C	1:A:225:LEU:HD12	2.43	0.44
1:A:523:SER:HA	1:B:464:PRO:HD3	1.99	0.44
1:B:191:LYS:N	1:B:191:LYS:HD2	2.33	0.44
1:C:459:ARG:HG3	1:C:526:PRO:CG	2.47	0.44
1:D:149:VAL:HG22	1:D:150:GLU:N	2.33	0.44
1:D:690:PHE:CE2	1:E:541:ASP:N	2.85	0.44
1:F:149:VAL:HG22	1:F:150:GLU:N	2.33	0.44
1:F:225:LEU:C	1:F:225:LEU:HD12	2.43	0.44
2:G:287:LEU:HD11	2:G:378:PRO:O	2.17	0.44
2:G:382:PRO:HA	2:G:389:PHE:CZ	2.53	0.44
1:A:396:ALA:HB2	2:G:107:GLY:HA3	1.98	0.43
1:A:547:TRP:CA	1:C:689:SER:OG	2.66	0.43
1:C:313:ALA:HB1	1:C:335:LEU:HD11	2.00	0.43
1:D:508:VAL:HG13	1:D:527:HIS:NE2	2.33	0.43
1:E:149:VAL:HG22	1:E:150:GLU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:191:LYS:HD2	1:E:191:LYS:N	2.33	0.43
1:F:654:TYR:CD1	1:F:656:CYS:SG	3.11	0.43
1:B:313:ALA:HB1	1:B:335:LEU:HD11	2.00	0.43
1:C:539:ARG:HD2	1:C:542:LYS:HZ2	1.83	0.43
1:E:57:ARG:HG2	1:E:121:TYR:CE1	2.53	0.43
1:F:629:ASP:CG	1:F:659:HIS:HE1	2.16	0.43
2:G:181:LEU:HA	2:G:185:GLU:O	2.17	0.43
1:A:191:LYS:HD2	1:A:191:LYS:N	2.33	0.43
1:B:525:ASP:HA	1:B:526:PRO:HD3	1.85	0.43
1:D:629:ASP:OD1	1:D:659:HIS:CE1	2.71	0.43
1:F:191:LYS:HD2	1:F:191:LYS:N	2.33	0.43
2:G:492:MET:HG3	2:G:501:LEU:HD21	2.01	0.43
1:B:482:ILE:HG23	1:B:497:VAL:HG13	2.00	0.43
1:D:482:ILE:HG23	1:D:497:VAL:HG13	2.00	0.43
1:A:273:ASP:CB	3:H:80:ARG:NE	2.79	0.43
1:A:560:MET:CE	1:A:586:PRO:HD3	2.43	0.43
1:B:202:LYS:C	1:B:204:PRO:HD3	2.44	0.43
1:D:313:ALA:HB1	1:D:335:LEU:HD11	2.00	0.43
1:A:149:VAL:HG22	1:A:150:GLU:N	2.33	0.43
1:A:202:LYS:C	1:A:204:PRO:HD3	2.44	0.43
1:B:149:VAL:HG22	1:B:150:GLU:N	2.33	0.43
1:B:225:LEU:HD12	1:B:225:LEU:C	2.43	0.43
1:D:56:HIS:HB3	1:D:59:THR:OG1	2.19	0.43
1:F:56:HIS:HB3	1:F:59:THR:OG1	2.19	0.43
1:F:57:ARG:HG2	1:F:121:TYR:CE1	2.54	0.43
2:G:285:THR:HG23	2:G:379:GLY:C	2.43	0.43
2:G:292:ILE:O	2:G:415:PRO:HD3	2.18	0.43
3:H:76:ASP:O	3:H:77:LEU:HD23	2.19	0.43
1:A:313:ALA:HB1	1:A:335:LEU:HD11	2.00	0.43
1:D:162:VAL:CG2	1:D:189:ASP:HB2	2.47	0.43
2:G:75:ASP:HB3	2:G:94:PRO:HB3	2.01	0.43
2:G:118:ILE:HA	2:G:133:GLY:CA	2.49	0.43
2:G:356:TYR:OH	2:G:377:ARG:NH1	2.51	0.43
1:A:96:PRO:HD3	2:G:277:ARG:HD3	1.88	0.43
1:D:191:LYS:N	1:D:191:LYS:HD2	2.33	0.43
1:D:225:LEU:HD12	1:D:225:LEU:C	2.44	0.43
1:E:225:LEU:C	1:E:225:LEU:HD12	2.44	0.43
2:G:375:TYR:CD1	2:G:376:PRO:HA	2.54	0.43
1:D:57:ARG:HG2	1:D:121:TYR:CE1	2.54	0.43
1:E:56:HIS:HB3	1:E:59:THR:OG1	2.19	0.43
2:G:287:LEU:CD2	2:G:409:MET:CE	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:ILE:HG23	1:A:497:VAL:HG13	2.00	0.43
1:B:417:THR:HA	1:B:418:PRO:HD3	1.74	0.43
1:C:57:ARG:HG2	1:C:121:TYR:CE1	2.53	0.43
1:C:532:ALA:HB1	1:C:560:MET:HE3	1.95	0.43
1:E:196:PRO:HG3	1:E:215:TYR:OH	2.19	0.43
2:G:503:ILE:CD1	2:G:503:ILE:N	2.82	0.43
1:A:57:ARG:HG2	1:A:121:TYR:CE1	2.54	0.42
1:B:533:LEU:HB3	1:B:642:THR:HG21	2.01	0.42
1:C:654:TYR:HD2	1:C:670:PHE:CZ	2.34	0.42
2:G:137:PHE:CD2	2:G:171:TYR:HB3	2.53	0.42
2:G:149:HIS:C	2:G:151:GLU:N	2.76	0.42
1:A:151:PRO:HG2	1:A:213:LEU:HD12	2.02	0.42
1:C:225:LEU:C	1:C:225:LEU:HD12	2.44	0.42
1:D:196:PRO:HG3	1:D:215:TYR:OH	2.19	0.42
1:D:654:TYR:CD2	1:D:670:PHE:CD2	3.07	0.42
2:G:182:ILE:CD1	2:G:231:LEU:HG	2.48	0.42
2:G:229:ALA:HA	2:G:244:TYR:O	2.19	0.42
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.84	0.42
1:C:701:CYS:HA	1:C:702:PRO:HD3	1.89	0.42
1:E:192:GLN:HG3	1:E:228:ILE:O	2.19	0.42
2:G:431:PHE:N	2:G:431:PHE:CD1	2.83	0.42
1:A:56:HIS:HB3	1:A:59:THR:OG1	2.19	0.42
1:B:57:ARG:HG2	1:B:121:TYR:CE1	2.54	0.42
1:D:192:GLN:HG3	1:D:228:ILE:O	2.19	0.42
1:D:202:LYS:C	1:D:204:PRO:HD3	2.44	0.42
1:D:610:GLN:HE22	1:F:577:LEU:HB3	1.84	0.42
1:E:202:LYS:C	1:E:204:PRO:HD3	2.44	0.42
2:G:203:ARG:NH2	2:G:273:PHE:CZ	2.87	0.42
2:G:208:HIS:ND1	2:G:209:HIS:N	2.68	0.42
2:G:401:THR:C	2:G:402:PHE:O	2.58	0.42
1:B:192:GLN:HG3	1:B:228:ILE:O	2.19	0.42
1:B:619:LYS:HA	1:B:619:LYS:HD3	1.91	0.42
1:F:204:PRO:HD2	1:F:212:MET:SD	2.60	0.42
1:C:482:ILE:HD12	1:C:497:VAL:HG11	2.02	0.42
1:D:571:VAL:HG21	1:D:655:ASN:HB2	2.00	0.42
1:E:654:TYR:CE2	1:E:670:PHE:CG	2.91	0.42
1:F:313:ALA:HB1	1:F:335:LEU:HD11	2.00	0.42
1:A:196:PRO:HG3	1:A:215:TYR:OH	2.19	0.42
1:B:56:HIS:HB3	1:B:59:THR:OG1	2.19	0.42
1:C:56:HIS:HB3	1:C:59:THR:OG1	2.19	0.42
1:C:202:LYS:C	1:C:204:PRO:HD3	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:619:LYS:HA	1:C:619:LYS:HD3	1.91	0.42
1:D:151:PRO:HG2	1:D:213:LEU:HD12	2.01	0.42
1:F:57:ARG:HG3	1:F:58:ARG:HG3	2.02	0.42
1:F:309:LEU:HD23	1:F:309:LEU:HA	1.89	0.42
1:F:476:PHE:HE2	1:F:482:ILE:HD13	1.85	0.42
1:F:482:ILE:HD12	1:F:497:VAL:HG11	2.02	0.42
1:A:204:PRO:HD2	1:A:212:MET:SD	2.60	0.42
1:C:192:GLN:HG3	1:C:228:ILE:O	2.20	0.42
1:C:204:PRO:HD2	1:C:212:MET:SD	2.60	0.42
1:E:37:GLN:OE1	1:E:37:GLN:HA	2.20	0.42
1:E:482:ILE:HG23	1:E:497:VAL:HG13	2.00	0.42
1:E:482:ILE:HD12	1:E:497:VAL:HG11	2.02	0.42
1:F:624:ILE:HG13	1:F:655:ASN:HB3	1.91	0.42
2:G:55:SER:O	2:G:73:ALA:HB1	2.19	0.42
1:A:57:ARG:HG3	1:A:58:ARG:HG3	2.02	0.42
1:B:577:LEU:HD13	1:C:612:ILE:HD11	2.02	0.42
1:B:691:GLN:HE22	1:D:442:GLY:HA2	1.85	0.42
1:C:37:GLN:OE1	1:C:37:GLN:HA	2.20	0.42
1:C:508:VAL:HG11	1:C:539:ARG:NH2	2.34	0.42
1:F:202:LYS:C	1:F:204:PRO:HD3	2.44	0.42
1:F:550:ASN:HB2	1:F:586:PRO:HA	2.02	0.42
2:G:402:PHE:O	2:G:404:ARG:N	2.50	0.42
2:G:453:THR:HG22	2:G:454:ASP:N	2.34	0.42
2:G:500:GLN:C	2:G:514:LEU:HD21	2.45	0.42
1:A:476:PHE:HE2	1:A:482:ILE:HD13	1.85	0.42
1:C:398:VAL:HA	1:C:399:PRO:HD3	1.93	0.42
1:E:626:LEU:HG	1:F:399:PRO:HG3	1.79	0.42
1:A:192:GLN:HG3	1:A:228:ILE:O	2.20	0.41
1:B:459:ARG:HG3	1:B:526:PRO:HG3	2.00	0.41
1:C:476:PHE:HE2	1:C:482:ILE:HD13	1.85	0.41
1:D:482:ILE:HD12	1:D:497:VAL:HG11	2.02	0.41
1:E:87:PRO:HB2	1:E:109:LEU:CD1	2.51	0.41
1:E:313:ALA:HB1	1:E:335:LEU:HD11	2.01	0.41
1:F:654:TYR:HD1	1:F:656:CYS:SG	2.42	0.41
2:G:74:LYS:O	2:G:76:HIS:N	2.54	0.41
2:G:427:VAL:HG12	2:G:429:TYR:H	1.85	0.41
1:B:196:PRO:HG3	1:B:215:TYR:OH	2.19	0.41
1:B:476:PHE:HE2	1:B:482:ILE:HD13	1.85	0.41
1:C:57:ARG:HG3	1:C:58:ARG:HG3	2.02	0.41
1:D:692:GLU:CD	1:E:440:TYR:CD1	2.95	0.41
1:E:149:VAL:HG22	1:E:151:PRO:HD3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:GLN:OE1	1:B:37:GLN:HA	2.20	0.41
1:B:204:PRO:HD2	1:B:212:MET:SD	2.60	0.41
1:C:525:ASP:HA	1:C:526:PRO:HD3	1.86	0.41
1:C:541:ASP:HB3	1:F:677:TYR:CE1	2.55	0.41
1:E:203:LEU:HD23	1:E:203:LEU:HA	1.84	0.41
1:E:204:PRO:HD2	1:E:212:MET:SD	2.60	0.41
1:E:633:LEU:HD12	1:E:633:LEU:C	2.46	0.41
1:F:192:GLN:HG3	1:F:228:ILE:O	2.20	0.41
2:G:56:SER:HB3	2:G:58:HIS:CD2	2.54	0.41
2:G:244:TYR:HA	2:G:266:GLY:O	2.21	0.41
2:G:416:ILE:O	2:G:417:ASN:HB2	2.20	0.41
1:A:87:PRO:HB2	1:A:109:LEU:CD1	2.51	0.41
1:D:37:GLN:OE1	1:D:37:GLN:HA	2.20	0.41
1:D:663:LEU:CD2	1:D:698:SER:HB2	2.51	0.41
1:E:476:PHE:HE2	1:E:482:ILE:HD13	1.85	0.41
1:F:196:PRO:HG3	1:F:215:TYR:OH	2.20	0.41
2:G:223:ASP:N	2:G:224:PRO:CD	2.83	0.41
2:G:427:VAL:CG2	2:G:429:TYR:OH	2.69	0.41
1:A:482:ILE:HD12	1:A:497:VAL:HG11	2.02	0.41
1:B:149:VAL:HG22	1:B:151:PRO:HD3	2.02	0.41
1:B:633:LEU:HD12	1:B:633:LEU:C	2.46	0.41
1:B:692:GLU:CD	1:D:440:TYR:CE1	2.99	0.41
1:C:196:PRO:HG3	1:C:215:TYR:OH	2.19	0.41
1:D:204:PRO:HD2	1:D:212:MET:SD	2.60	0.41
1:F:571:VAL:CG2	1:F:655:ASN:HA	2.48	0.41
1:A:552:PHE:CD2	1:C:690:PHE:CZ	2.92	0.41
1:A:633:LEU:HD12	1:A:633:LEU:C	2.45	0.41
1:A:663:LEU:CD2	1:A:698:SER:HB2	2.50	0.41
1:B:151:PRO:HG2	1:B:213:LEU:HD12	2.01	0.41
1:B:482:ILE:HD12	1:B:497:VAL:HG11	2.02	0.41
1:C:633:LEU:C	1:C:633:LEU:HD12	2.46	0.41
1:D:493:LEU:HA	1:D:539:ARG:NH2	2.35	0.41
1:D:533:LEU:HD23	1:D:533:LEU:HA	1.84	0.41
2:G:77:ILE:HD13	2:G:144:ILE:HD11	2.02	0.41
2:G:274:GLY:HA2	2:G:284:THR:CG2	2.51	0.41
2:G:316:SER:HB2	2:G:323:ILE:CD1	2.51	0.41
1:A:547:TRP:HB2	1:C:689:SER:OG	2.20	0.41
1:C:87:PRO:HB2	1:C:109:LEU:CD1	2.51	0.41
1:D:87:PRO:HB2	1:D:109:LEU:CD1	2.51	0.41
1:D:315:LEU:HD11	1:D:333:ASP:HB3	2.03	0.41
1:E:151:PRO:HG2	1:E:213:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:582:VAL:CG1	1:E:585:ALA:HB2	2.51	0.41
2:G:287:LEU:CD1	2:G:379:GLY:HA3	2.49	0.41
2:G:342:MET:HG3	2:G:421:ILE:HG12	2.02	0.41
2:G:434:ILE:CG1	2:G:435:VAL:N	2.83	0.41
1:A:37:GLN:OE1	1:A:37:GLN:HA	2.20	0.41
1:B:57:ARG:HG3	1:B:58:ARG:HG3	2.02	0.41
1:B:404:PHE:CE2	1:B:406:GLY:HA2	2.56	0.41
1:C:151:PRO:HG2	1:C:213:LEU:HD12	2.02	0.41
1:D:57:ARG:HG3	1:D:58:ARG:HG3	2.02	0.41
1:D:68:ASN:ND2	1:D:87:PRO:HG3	2.36	0.41
1:E:309:LEU:HD23	1:E:309:LEU:HA	1.89	0.41
1:E:398:VAL:HA	1:E:399:PRO:HD3	1.93	0.41
1:A:404:PHE:CE2	1:A:406:GLY:HA2	2.56	0.41
1:B:68:ASN:ND2	1:B:87:PRO:HG3	2.36	0.41
1:B:654:TYR:CG	1:B:670:PHE:CD2	3.09	0.41
1:C:149:VAL:HG22	1:C:151:PRO:HD3	2.02	0.41
1:C:556:ILE:HD11	1:D:324:GLN:OE1	2.21	0.41
1:C:663:LEU:CD2	1:C:698:SER:HB2	2.50	0.41
1:D:404:PHE:CE2	1:D:406:GLY:HA2	2.56	0.41
1:D:582:VAL:CG1	1:D:585:ALA:HB2	2.51	0.41
1:E:57:ARG:HG3	1:E:58:ARG:HG3	2.02	0.41
1:F:151:PRO:HG2	1:F:213:LEU:HD12	2.01	0.41
1:F:633:LEU:HD12	1:F:633:LEU:C	2.46	0.41
2:G:48:PHE:C	2:G:50:GLY:H	2.29	0.41
2:G:229:ALA:C	2:G:230:HIS:CD2	2.99	0.41
2:G:392:THR:O	2:G:395:LEU:HD12	2.21	0.41
2:G:427:VAL:HG21	2:G:429:TYR:CZ	2.55	0.41
1:A:68:ASN:ND2	1:A:87:PRO:HG3	2.36	0.41
1:A:493:LEU:HD22	1:A:539:ARG:CZ	2.51	0.41
1:A:564:VAL:HG23	1:A:649:THR:HG21	2.03	0.41
1:A:582:VAL:CG1	1:A:585:ALA:HB2	2.51	0.41
1:B:582:VAL:CG1	1:B:585:ALA:HB2	2.51	0.41
1:D:633:LEU:C	1:D:633:LEU:HD12	2.46	0.41
1:E:68:ASN:ND2	1:E:87:PRO:HG3	2.36	0.41
1:E:404:PHE:CE2	1:E:406:GLY:HA2	2.56	0.41
1:F:149:VAL:HG22	1:F:151:PRO:HD3	2.03	0.41
1:B:315:LEU:HD11	1:B:333:ASP:HB3	2.03	0.40
1:C:508:VAL:N	1:C:509:GLU:N	2.67	0.40
1:C:582:VAL:CG1	1:C:585:ALA:HB2	2.51	0.40
1:D:149:VAL:HG22	1:D:151:PRO:HD3	2.02	0.40
2:G:232:ILE:HD12	2:G:345:MET:HE2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:427:VAL:CG2	2:G:429:TYR:CZ	3.04	0.40
3:H:31:ILE:HG21	3:H:138:TYR:CZ	2.56	0.40
1:A:409:ILE:HG22	2:G:194:PHE:CD2	2.53	0.40
1:B:203:LEU:HD23	1:B:203:LEU:HA	1.83	0.40
1:B:508:VAL:CG1	1:B:527:HIS:CD2	3.03	0.40
1:C:404:PHE:CE2	1:C:406:GLY:HA2	2.56	0.40
1:C:559:CYS:C	1:C:560:MET:CA	2.93	0.40
1:E:315:LEU:HD11	1:E:333:ASP:HB3	2.03	0.40
1:F:564:VAL:HG23	1:F:649:THR:HG21	2.03	0.40
2:G:337:GLY:HA2	2:G:424:LYS:O	2.22	0.40
1:D:690:PHE:CE2	1:E:540:ARG:C	2.44	0.40
2:G:135:GLY:HA3	2:G:138:HIS:O	2.21	0.40
2:G:164:ASN:HD22	2:G:166:ARG:HG3	1.86	0.40
2:G:268:ILE:HD13	2:G:283:TRP:CE2	2.56	0.40
1:A:309:LEU:HD23	1:A:309:LEU:HA	1.89	0.40
1:B:87:PRO:HB2	1:B:109:LEU:CD1	2.51	0.40
1:D:309:LEU:HA	1:D:309:LEU:HD23	1.88	0.40
1:D:508:VAL:CG1	1:D:527:HIS:CE1	3.04	0.40
1:E:349:PRO:HA	1:E:350:PRO:HD3	1.96	0.40
1:E:564:VAL:HG23	1:E:649:THR:HG21	2.03	0.40
1:F:37:GLN:OE1	1:F:37:GLN:HA	2.20	0.40
1:F:459:ARG:CD	1:F:526:PRO:HG3	2.52	0.40
1:F:525:ASP:HA	1:F:526:PRO:HD3	1.86	0.40
2:G:29:VAL:HA	2:G:30:PRO:HD3	1.86	0.40
2:G:400:ILE:O	2:G:402:PHE:O	2.38	0.40
1:B:565:HIS:HA	1:B:566:PRO:HA	1.96	0.40
1:B:612:ILE:HD11	1:C:577:LEU:HD13	2.03	0.40
1:B:692:GLU:CD	1:D:440:TYR:CD1	2.98	0.40
1:C:444:SER:HB3	1:C:460:ALA:HB3	2.04	0.40
1:C:533:LEU:HD23	1:C:533:LEU:HA	1.84	0.40
1:C:564:VAL:HG23	1:C:649:THR:HG21	2.03	0.40
1:D:654:TYR:CE2	1:D:670:PHE:CD1	3.09	0.40
1:E:626:LEU:O	1:F:399:PRO:HA	2.21	0.40
1:F:404:PHE:CE2	1:F:406:GLY:HA2	2.56	0.40
1:F:582:VAL:CG1	1:F:585:ALA:HB2	2.51	0.40
1:F:624:ILE:HA	1:F:625:PRO:HD2	1.94	0.40
2:G:209:HIS:O	2:G:210:PRO:C	2.65	0.40
2:G:482:VAL:HG12	2:G:482:VAL:O	2.21	0.40

All (63) 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:A:690:PHE:CE1	1:F:540:ARG:NE[3_455]	0.68	1.52
1:A:690:PHE:CE2	1:F:540:ARG:CG[3_455]	0.78	1.42
1:B:541:ASP:N	1:E:690:PHE:CE2[3_455]	0.79	1.41
1:A:577:LEU:CD1	1:E:610:GLN:OE1[3_455]	0.87	1.33
1:B:540:ARG:C	1:E:690:PHE:CZ[3_455]	0.87	1.33
1:B:540:ARG:CB	1:E:690:PHE:CE1[3_455]	0.88	1.32
2:G:386:PHE:CZ	3:H:72:ASN:ND2[2_554]	0.89	1.31
1:A:690:PHE:CE1	1:F:540:ARG:CZ[3_455]	0.94	1.26
1:A:577:LEU:CG	1:E:610:GLN:OE1[3_455]	1.00	1.20
1:A:690:PHE:CE2	1:F:540:ARG:CD[3_455]	1.06	1.14
1:B:541:ASP:N	1:E:690:PHE:CZ[3_455]	1.06	1.14
2:G:365:GLN:NE2	2:G:365:GLN:NE2[2_554]	1.13	1.07
1:A:690:PHE:CD1	1:F:540:ARG:NE[3_455]	1.20	1.00
1:A:690:PHE:CD2	1:F:540:ARG:CD[3_455]	1.21	0.99
2:G:386:PHE:CE1	3:H:72:ASN:ND2[2_554]	1.21	0.99
1:A:690:PHE:CZ	1:F:540:ARG:NE[3_455]	1.22	0.98
1:A:610:GLN:OE1	1:E:577:LEU:CD1[3_455]	1.30	0.90
1:A:692:GLU:OE2	1:F:441:ASN:N[3_455]	1.30	0.90
1:A:577:LEU:CD1	1:E:610:GLN:CD[3_455]	1.31	0.89
1:B:541:ASP:CA	1:E:690:PHE:CE2[3_455]	1.35	0.85
1:A:610:GLN:OE1	1:E:577:LEU:CG[3_455]	1.39	0.81
2:G:385:THR:CG2	3:H:137:ARG:NH1[2_554]	1.43	0.77
1:B:540:ARG:CA	1:E:690:PHE:CE1[3_455]	1.45	0.75
1:A:690:PHE:CE2	1:F:540:ARG:CB[3_455]	1.47	0.73
2:G:386:PHE:CZ	3:H:72:ASN:CG[2_554]	1.49	0.71
1:B:441:ASN:N	1:E:691:GLN:OE1[3_455]	1.50	0.70
1:B:540:ARG:CA	1:E:690:PHE:CZ[3_455]	1.51	0.69
2:G:259:LYS:CE	2:G:299:ASN:O[2_554]	1.58	0.62
1:A:690:PHE:CZ	1:F:540:ARG:CD[3_455]	1.62	0.58
1:A:690:PHE:CE1	1:F:540:ARG:NH2[3_455]	1.66	0.54
2:G:365:GLN:CA	2:G:365:GLN:OE1[2_554]	1.70	0.50
1:B:540:ARG:CD	1:E:689:SER:O[3_455]	1.71	0.49
1:A:690:PHE:CZ	1:F:540:ARG:CG[3_455]	1.72	0.48
1:A:690:PHE:CZ	1:F:540:ARG:CZ[3_455]	1.81	0.39
1:B:540:ARG:CB	1:E:690:PHE:CD1[3_455]	1.81	0.39
1:A:690:PHE:CG	1:F:540:ARG:CD[3_455]	1.82	0.38
1:B:540:ARG:C	1:E:690:PHE:CE2[3_455]	1.85	0.35
1:A:610:GLN:OE1	1:E:577:LEU:CB[3_455]	1.87	0.33
1:A:690:PHE:CE2	1:F:540:ARG:NE[3_455]	1.87	0.33
1:A:690:PHE:CG	1:F:540:ARG:NE[3_455]	1.87	0.33
1:A:692:GLU:OE2	1:F:441:ASN:CA[3_455]	1.90	0.30
2:G:365:GLN:CD	2:G:365:GLN:NE2[2_554]	1.92	0.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:259:LYS:CD	2:G:300:GLY:CA[2_554]	1.93	0.27
1:A:690:PHE:CD1	1:F:540:ARG:CZ[3_455]	1.94	0.26
1:A:690:PHE:CD2	1:F:540:ARG:CG[3_455]	1.98	0.22
1:A:577:LEU:CB	1:E:610:GLN:NE2[3_455]	2.00	0.20
1:A:577:LEU:CG	1:E:610:GLN:CD[3_455]	2.01	0.19
1:B:540:ARG:O	1:E:690:PHE:CZ[3_455]	2.02	0.18
2:G:259:LYS:CD	2:G:300:GLY:C[2_554]	2.03	0.17
1:A:610:GLN:CD	1:E:577:LEU:CD1[3_455]	2.04	0.16
1:B:540:ARG:CB	1:E:690:PHE:CZ[3_455]	2.05	0.15
1:B:540:ARG:C	1:E:690:PHE:CE1[3_455]	2.05	0.15
1:B:541:ASP:CB	1:E:690:PHE:CE2[3_455]	2.06	0.14
1:B:541:ASP:CB	1:E:690:PHE:CD2[3_455]	2.07	0.13
1:A:577:LEU:CB	1:E:610:GLN:OE1[3_455]	2.08	0.12
1:B:540:ARG:CG	1:E:690:PHE:CE1[3_455]	2.08	0.12
1:B:541:ASP:N	1:E:690:PHE:CD2[3_455]	2.09	0.11
1:A:690:PHE:CE1	1:F:540:ARG:CD[3_455]	2.10	0.10
1:A:690:PHE:CD2	1:F:540:ARG:NE[3_455]	2.11	0.09
1:A:690:PHE:CE1	1:F:540:ARG:NH1[3_455]	2.17	0.03
1:A:690:PHE:CD1	1:F:540:ARG:CD[3_455]	2.18	0.02
1:A:577:LEU:CD1	1:E:610:GLN:CG[3_455]	2.19	0.01
2:G:386:PHE:CZ	3:H:72:ASN:CB[2_554]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	648/681 (95%)	628 (97%)	18 (3%)	2 (0%)	36	72
1	B	648/681 (95%)	629 (97%)	16 (2%)	3 (0%)	24	63
1	C	648/681 (95%)	627 (97%)	17 (3%)	4 (1%)	21	59
1	D	650/681 (95%)	630 (97%)	16 (2%)	4 (1%)	21	59
1	E	650/681 (95%)	632 (97%)	15 (2%)	3 (0%)	24	63

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	650/681 (95%)	631 (97%)	17 (3%)	2 (0%)	36	72
2	G	480/538 (89%)	408 (85%)	55 (12%)	17 (4%)	3	20
3	H	115/577 (20%)	106 (92%)	7 (6%)	2 (2%)	7	36
All	All	4489/5201 (86%)	4291 (96%)	161 (4%)	37 (1%)	16	54

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	655	ASN
2	G	161	HIS
2	G	207	HIS
2	G	257	SER
3	H	81	ASP
3	H	129	THR
1	B	508	VAL
1	C	655	ASN
1	E	655	ASN
2	G	42	SER
2	G	75	ASP
2	G	95	VAL
2	G	147	GLY
2	G	158	GLN
2	G	159	ASP
2	G	206	GLY
2	G	278	SER
2	G	456	GLY
1	A	160	SER
1	A	175	SER
1	B	160	SER
1	B	175	SER
1	C	160	SER
1	C	175	SER
1	C	508	VAL
1	D	160	SER
1	D	175	SER
1	E	160	SER
1	E	175	SER
1	F	160	SER
1	F	175	SER
2	G	55	SER
2	G	49	ASN

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Mol	Chain	Res	Type
2	G	299	ASN
2	G	298	PRO
1	D	508	VAL
2	G	146	VAL

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	578/597 (97%)	566 (98%)	12 (2%)	47	65
1	B	578/597 (97%)	566 (98%)	12 (2%)	47	65
1	C	578/597 (97%)	566 (98%)	12 (2%)	47	65
1	D	578/597 (97%)	566 (98%)	12 (2%)	47	65
1	E	578/597 (97%)	566 (98%)	12 (2%)	47	65
1	F	578/597 (97%)	566 (98%)	12 (2%)	47	65
2	G	428/472 (91%)	400 (94%)	28 (6%)	15	37
3	H	102/506 (20%)	98 (96%)	4 (4%)	28	49
All	All	3998/4560 (88%)	3894 (97%)	104 (3%)	40	62

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	106	VAL
1	A	237	SER
1	A	238	HIS
1	A	274	LEU
1	A	298	PHE
1	A	301	THR
1	A	508	VAL
1	A	509	GLU
1	A	512	GLU
1	A	542	LYS
1	A	580	LEU

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Mol	Chain	Res	Type
1	A	626	LEU
1	B	106	VAL
1	B	237	SER
1	B	238	HIS
1	B	274	LEU
1	B	298	PHE
1	B	301	THR
1	B	508	VAL
1	B	509	GLU
1	B	512	GLU
1	B	542	LYS
1	B	580	LEU
1	B	626	LEU
1	C	106	VAL
1	C	237	SER
1	C	238	HIS
1	C	274	LEU
1	C	298	PHE
1	C	301	THR
1	C	508	VAL
1	C	509	GLU
1	C	512	GLU
1	C	542	LYS
1	C	580	LEU
1	C	626	LEU
1	D	106	VAL
1	D	237	SER
1	D	238	HIS
1	D	274	LEU
1	D	298	PHE
1	D	301	THR
1	D	508	VAL
1	D	509	GLU
1	D	512	GLU
1	D	542	LYS
1	D	580	LEU
1	D	626	LEU
1	E	106	VAL
1	E	237	SER
1	E	238	HIS
1	E	274	LEU
1	E	298	PHE

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Mol	Chain	Res	Type
1	E	301	THR
1	E	508	VAL
1	E	509	GLU
1	E	512	GLU
1	E	542	LYS
1	E	580	LEU
1	E	626	LEU
1	F	106	VAL
1	F	237	SER
1	F	238	HIS
1	F	274	LEU
1	F	298	PHE
1	F	301	THR
1	F	508	VAL
1	F	509	GLU
1	F	512	GLU
1	F	542	LYS
1	F	580	LEU
1	F	626	LEU
2	G	27	ASN
2	G	40	LEU
2	G	61	LEU
2	G	69	LEU
2	G	94	PRO
2	G	101	ASP
2	G	140	ILE
2	G	159	ASP
2	G	161	HIS
2	G	180	LEU
2	G	190	THR
2	G	218	SER
2	G	224	PRO
2	G	231	LEU
2	G	268	ILE
2	G	308	LEU
2	G	314	MET
2	G	384	LYS
2	G	389	PHE
2	G	390	ASP
2	G	413	VAL
2	G	427	VAL
2	G	436	VAL

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Mol	Chain	Res	Type
2	G	457	THR
2	G	476	LEU
2	G	485	GLU
2	G	487	THR
2	G	501	LEU
3	H	26	LYS
3	H	30	THR
3	H	55	GLU
3	H	125	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	GLN
1	A	392	GLN
1	A	403	ASN
1	A	465	HIS
1	B	403	ASN
1	B	465	HIS
1	B	534	HIS
1	B	660	GLN
1	B	696	ASN
1	C	83	HIS
1	C	403	ASN
1	C	465	HIS
1	C	565	HIS
1	D	83	HIS
1	D	392	GLN
1	D	403	ASN
1	E	153	HIS
1	E	324	GLN
1	E	392	GLN
1	E	403	ASN
1	E	465	HIS
1	F	324	GLN
1	F	403	ASN
1	F	465	HIS
1	F	696	ASN
2	G	27	ASN
2	G	28	ASN
2	G	76	HIS
2	G	89	GLN

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Mol	Chain	Res	Type
2	G	158	GLN
2	G	164	ASN
2	G	215	GLN
2	G	216	HIS
2	G	256	HIS
2	G	262	HIS
2	G	370	GLN
2	G	406	HIS
2	G	411	ASN
2	G	417	ASN
2	G	430	GLN
2	G	433	GLN
2	G	511	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	3
1	A	2
1	C	2
1	B	1
1	F	1
1	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	559:CYS	C	560:MET	N	2.86
1	B	559:CYS	C	560:MET	N	2.56
1	C	559:CYS	C	560:MET	N	2.24
1	A	508:VAL	C	509:GLU	N	1.91
1	D	559:CYS	C	560:MET	N	1.79
1	F	508:VAL	C	509:GLU	N	1.63
1	E	559:CYS	C	560:MET	N	1.19
1	D	508:VAL	C	509:GLU	N	1.10
1	D	654:TYR	C	655:ASN	N	1.05
1	C	508:VAL	C	509:GLU	N	0.85

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	656/681 (96%)	0.62	51 (7%)	19	25	287, 291, 313, 313	0
1	B	656/681 (96%)	0.50	39 (5%)	28	32	290, 308, 308, 308	0
1	C	656/681 (96%)	0.55	49 (7%)	20	26	278, 322, 327, 327	0
1	D	656/681 (96%)	0.28	29 (4%)	39	39	294, 342, 342, 342	0
1	E	656/681 (96%)	0.50	45 (6%)	23	28	304, 341, 351, 351	0
1	F	656/681 (96%)	0.56	57 (8%)	16	23	305, 348, 370, 370	0
2	G	484/538 (89%)	0.44	25 (5%)	33	35	340, 340, 340, 340	0
3	H	117/577 (20%)	0.33	8 (6%)	23	29	370, 370, 370, 370	0
All	All	4537/5201 (87%)	0.49	303 (6%)	24	29	278, 322, 348, 370	0

All (303) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	107	ILE	7.4
1	F	165	THR	6.9
1	E	320	GLU	6.1
1	D	303	ALA	6.0
1	E	244	ILE	5.6
1	A	248	ALA	4.9
1	B	172	ILE	4.9
1	A	221	PHE	4.8
1	C	385	TRP	4.8
1	F	491	ASN	4.8
1	B	171	VAL	4.8
1	B	255	PHE	4.8
1	E	432	LEU	4.7
1	F	293	TYR	4.7
1	D	256	LEU	4.6
1	E	298	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	387	LEU	4.6
1	F	183	PHE	4.6
1	A	93	ALA	4.5
1	F	471	GLU	4.4
1	C	432	LEU	4.4
1	C	346	TYR	4.3
1	E	280	ILE	4.3
1	E	256	LEU	4.3
1	A	238	HIS	4.3
1	C	515	THR	4.3
1	F	234	ALA	4.3
1	F	472	MET	4.2
2	G	479	GLU	4.2
1	E	129	CYS	4.0
1	A	220	ASP	4.0
1	A	137	CYS	4.0
1	E	445	VAL	4.0
1	A	239	PHE	3.9
1	A	500	GLU	3.9
1	F	53	LEU	3.9
1	D	331	ASP	3.9
1	B	629	ASP	3.8
1	F	303	ALA	3.8
1	A	164	LYS	3.8
2	G	333	ASN	3.8
1	A	448	VAL	3.7
1	A	286	ASP	3.7
1	B	170	GLY	3.7
1	D	500	GLU	3.7
1	F	163	ASN	3.7
1	D	137	CYS	3.7
1	B	163	ASN	3.6
1	C	443	TYR	3.6
1	C	332	GLU	3.6
1	F	447	PHE	3.5
3	H	110	SER	3.5
1	E	336	PHE	3.5
1	E	443	TYR	3.5
3	H	51	SER	3.5
1	E	609	SER	3.5
1	C	325	ALA	3.5
1	C	622	PRO	3.5

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Mol	Chain	Res	Type	RSRZ
1	E	208	GLU	3.4
2	G	218	SER	3.4
2	G	378	PRO	3.4
1	E	447	PHE	3.4
1	A	163	ASN	3.4
1	C	517	CYS	3.4
1	E	436	ALA	3.3
1	B	650	GLU	3.3
2	G	286	PHE	3.3
1	F	138	LYS	3.3
1	F	235	LEU	3.3
1	D	255	PHE	3.3
1	C	165	THR	3.3
1	C	554	ALA	3.2
1	C	231	ASP	3.2
1	F	445	VAL	3.2
1	C	456	LYS	3.2
1	A	223	SER	3.2
1	B	616	PRO	3.2
1	A	303	ALA	3.2
1	F	385	TRP	3.2
1	D	293	TYR	3.2
1	A	346	TYR	3.1
1	D	164	LYS	3.1
1	C	454	LYS	3.1
1	F	664	SER	3.1
1	E	317	LYS	3.1
3	H	70	ASN	3.1
1	D	588	LEU	3.1
2	G	257	SER	3.1
1	E	532	ALA	3.1
1	D	532	ALA	3.0
1	E	137	CYS	3.0
2	G	215	GLN	3.0
1	B	189	ASP	3.0
1	C	615	SER	3.0
1	D	189	ASP	3.0
1	F	512	GLU	3.0
1	C	349	PRO	3.0
1	D	488	PHE	3.0
1	B	106	VAL	3.0
1	C	361	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
3	H	108	ALA	3.0
1	D	171	VAL	3.0
1	E	435	VAL	3.0
1	B	280	ILE	2.9
1	B	556	ILE	2.9
1	F	310	LEU	2.9
1	C	293	TYR	2.9
1	A	596	PHE	2.9
1	C	163	ASN	2.9
1	E	47	ASP	2.9
1	A	170	GLY	2.9
1	D	198	LEU	2.9
2	G	32	LEU	2.9
1	B	702	PRO	2.9
1	C	613	CYS	2.9
1	F	486	MET	2.9
1	C	403	ASN	2.9
1	E	448	VAL	2.9
1	B	281	VAL	2.8
1	F	244	ILE	2.8
1	C	242	PHE	2.8
1	C	430	ASP	2.8
2	G	324	VAL	2.8
1	A	129	CYS	2.8
1	C	102	PRO	2.8
1	E	456	LYS	2.8
3	H	106	LYS	2.8
1	F	182	LEU	2.8
1	A	208	GLU	2.8
1	A	655	ASN	2.8
1	C	577	LEU	2.8
1	B	686	THR	2.8
1	E	296	LEU	2.8
1	A	116	LEU	2.8
2	G	176	LEU	2.8
1	C	629	ASP	2.8
1	A	70	VAL	2.7
1	F	130	GLY	2.7
1	B	522	SER	2.7
1	C	555	SER	2.7
1	F	164	LYS	2.7
1	E	582	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	608	GLY	2.7
1	F	463	PRO	2.7
1	E	599	LEU	2.7
1	F	457	LYS	2.7
2	G	246	PHE	2.7
1	C	655	ASN	2.7
1	E	355	LEU	2.7
1	D	226	ILE	2.6
2	G	101	ASP	2.6
1	B	447	PHE	2.6
1	F	430	ASP	2.6
2	G	111	LEU	2.6
1	F	412	PRO	2.6
1	E	439	VAL	2.6
1	C	549	ALA	2.6
1	F	248	ALA	2.6
1	E	254	TYR	2.6
1	C	616	PRO	2.6
1	B	563	GLU	2.6
1	F	236	VAL	2.6
1	D	273	ASP	2.5
1	A	493	LEU	2.5
1	A	522	SER	2.5
1	F	256	LEU	2.5
1	B	127	LEU	2.5
1	C	700	ASP	2.5
1	C	76	ASN	2.5
1	F	137	CYS	2.5
1	B	626	LEU	2.5
1	D	554	ALA	2.5
1	F	129	CYS	2.5
2	G	100	ARG	2.5
1	C	330	SER	2.5
1	E	608	GLY	2.5
1	E	203	LEU	2.4
1	F	578	LEU	2.4
1	F	686	THR	2.4
2	G	311	VAL	2.4
1	A	388	GLY	2.4
1	A	492	GLN	2.4
1	A	422	LEU	2.4
1	B	198	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	667	ASN	2.4
1	B	622	PRO	2.4
1	C	678	ARG	2.4
1	D	611	VAL	2.4
2	G	405	SER	2.4
1	B	554	ALA	2.4
1	D	305	VAL	2.4
1	F	122	SER	2.4
2	G	494	LEU	2.4
1	D	629	ASP	2.4
1	E	425	TYR	2.4
2	G	345	MET	2.4
1	B	343	GLN	2.4
1	B	331	ASP	2.4
2	G	219	ARG	2.4
1	B	512	GLU	2.4
1	B	215	TYR	2.4
3	H	73	PRO	2.3
1	F	161	SER	2.3
1	C	227	LYS	2.3
2	G	230	HIS	2.3
1	E	464	PRO	2.3
1	F	124	ASN	2.3
1	C	614	ILE	2.3
1	C	239	PHE	2.3
1	A	111	ASN	2.3
1	B	575	SER	2.3
1	D	347	HIS	2.3
1	F	376	HIS	2.3
1	A	159	LEU	2.3
1	A	579	SER	2.3
1	A	648	SER	2.3
1	B	183	PHE	2.3
1	F	596	PHE	2.3
1	D	39	SER	2.3
1	E	255	PHE	2.3
1	B	118	ILE	2.3
1	C	467	GLY	2.3
1	A	432	LEU	2.3
1	A	475	VAL	2.3
1	F	386	LEU	2.3
1	A	262	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	301	THR	2.3
2	G	325	TYR	2.3
1	A	443	TYR	2.2
1	E	247	PHE	2.2
1	F	274	LEU	2.2
1	D	150	GLU	2.2
3	H	62	GLU	2.2
1	A	327	ASN	2.2
1	C	228	ILE	2.2
1	D	183	PHE	2.2
1	F	172	ILE	2.2
2	G	102	GLU	2.2
1	C	114	ASN	2.2
1	C	468	VAL	2.2
1	E	517	CYS	2.2
1	E	575	SER	2.2
1	B	226	ILE	2.2
1	A	325	ALA	2.2
1	F	52	HIS	2.2
1	F	657	SER	2.2
1	C	54	THR	2.2
1	C	148	LEU	2.2
1	E	310	LEU	2.2
1	E	438	TYR	2.2
1	E	660	GLN	2.2
1	A	529	GLY	2.2
1	A	260	PRO	2.2
2	G	411	ASN	2.2
1	B	599	LEU	2.1
1	F	184	ILE	2.1
1	D	683	HIS	2.1
1	A	222	VAL	2.1
1	E	249	SER	2.1
1	F	346	TYR	2.1
1	F	304	GLY	2.1
1	C	111	ASN	2.1
1	C	347	HIS	2.1
1	B	615	SER	2.1
1	A	332	GLU	2.1
1	A	517	CYS	2.1
1	C	254	TYR	2.1
1	F	205	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	609	SER	2.1
1	E	227	LYS	2.1
2	G	162	PHE	2.1
1	A	485	ASP	2.1
1	D	129	CYS	2.1
1	A	657	SER	2.1
1	D	492	GLN	2.1
1	E	437	SER	2.1
1	F	128	ALA	2.1
1	B	385	TRP	2.1
1	B	205	ARG	2.1
1	B	256	LEU	2.1
1	C	384	ASN	2.1
1	C	422	LEU	2.1
1	E	206	ASP	2.1
1	F	485	ASP	2.1
1	A	455	LEU	2.1
1	D	228	ILE	2.1
1	F	51	ASN	2.1
1	F	239	PHE	2.1
1	F	277	THR	2.1
1	E	318	PRO	2.1
1	E	406	GLY	2.0
1	F	255	PHE	2.0
1	E	229	PRO	2.0
2	G	93	TRP	2.0
1	B	521	LEU	2.0
1	F	336	PHE	2.0
1	C	263	PRO	2.0
1	A	506	VAL	2.0
1	F	678	ARG	2.0
1	A	609	SER	2.0
1	A	247	PHE	2.0
1	A	438	TYR	2.0
1	D	657	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	H	601	1/1	0.91	0.16	369,369,369,369	0

6.5 Other polymers [i](#)

There are no such residues in this entry.