



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 02:55 AM GMT

PDB ID : 1IS7
Title : Crystal structure of rat GTPCHI/GFRP stimulatory complex
Authors : Maita, N.; Okada, K.; Hatakeyama, K.; Hakoshima, T.
Deposited on : 2001-11-18
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

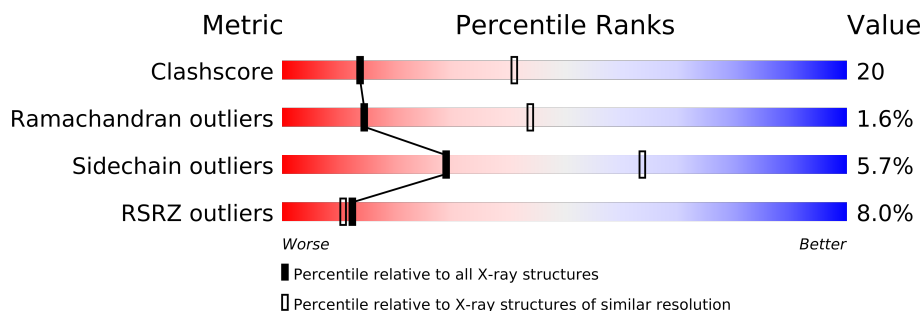
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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))
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	230	
1	B	230	
1	C	230	
1	D	230	
1	E	230	
1	F	230	
1	G	230	
1	H	230	
1	I	230	
1	J	230	
2	K	84	
2	L	84	
2	M	84	
2	N	84	
2	O	84	
2	P	84	

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Mol	Chain	Length	Quality of chain
2	Q	84	
2	R	84	
2	S	84	
2	T	84	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 22375 atoms, of which 0 are hydrogen and 0 are deuterium.

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 GTP Cyclohydrolase I.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	194	Total	C	N	O	S	0	0	0
			1536	967	271	287	11			
1	B	194	Total	C	N	O	S	0	0	0
			1536	967	271	287	11			
1	C	194	Total	C	N	O	S	0	0	0
			1536	967	271	287	11			
1	D	194	Total	C	N	O	S	0	0	0
			1536	967	271	287	11			
1	E	194	Total	C	N	O	S	0	0	0
			1536	967	271	287	11			
1	F	194	Total	C	N	O	S	0	0	0
			1536	967	271	287	11			
1	G	194	Total	C	N	O	S	0	0	0
			1536	967	271	287	11			
1	H	194	Total	C	N	O	S	0	0	0
			1536	967	271	287	11			
1	I	194	Total	C	N	O	S	0	0	0
			1536	967	271	287	11			
1	J	194	Total	C	N	O	S	0	0	0
			1536	967	271	287	11			

- Molecule 2 is a protein called GTP Cyclohydrolase I Feedback Regulatory Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	84	Total	C	N	O	S	0	0	0
			676	428	117	124	7			
2	L	84	Total	C	N	O	S	0	0	0
			676	428	117	124	7			
2	M	84	Total	C	N	O	S	0	0	0
			676	428	117	124	7			
2	N	84	Total	C	N	O	S	0	0	0
			676	428	117	124	7			

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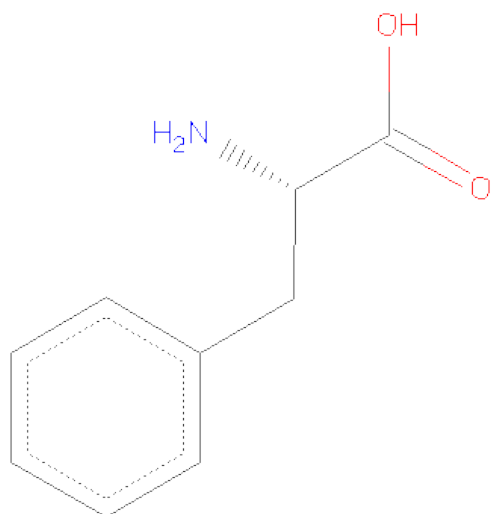
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	84	Total 676	C 428	N 117	O 124	S 7	0	0	0
2	P	84	Total 676	C 428	N 117	O 124	S 7	0	0	0
2	Q	84	Total 676	C 428	N 117	O 124	S 7	0	0	0
2	R	84	Total 676	C 428	N 117	O 124	S 7	0	0	0
2	S	84	Total 676	C 428	N 117	O 124	S 7	0	0	0
2	T	84	Total 676	C 428	N 117	O 124	S 7	0	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total 1	K 1	0	0
3	Q	1	Total 1	K 1	0	0
3	K	1	Total 1	K 1	0	0
3	T	1	Total 1	K 1	0	0
3	N	1	Total 1	K 1	0	0
3	O	1	Total 1	K 1	0	0
3	R	1	Total 1	K 1	0	0
3	L	1	Total 1	K 1	0	0
3	S	1	Total 1	K 1	0	0
3	M	1	Total 1	K 1	0	0

- Molecule 4 is PHENYLALANINE (three-letter code: PHE) (formula: C₉H₁₁NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	R	1	Total	C	N	O	0	0
			12	9	1	2		
4	R	1	Total	C	N	O	0	0
			12	9	1	2		
4	P	1	Total	C	N	O	0	0
			12	9	1	2		
4	S	1	Total	C	N	O	0	0
			12	9	1	2		
4	T	1	Total	C	N	O	0	0
			12	9	1	2		
4	M	1	Total	C	N	O	0	0
			12	9	1	2		
4	N	1	Total	C	N	O	0	0
			12	9	1	2		
4	O	1	Total	C	N	O	0	0
			12	9	1	2		
4	K	1	Total	C	N	O	0	0
			12	9	1	2		
4	L	1	Total	C	N	O	0	0
			12	9	1	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total	O	0	0
			3	3		
5	B	4	Total	O	0	0
			4	4		

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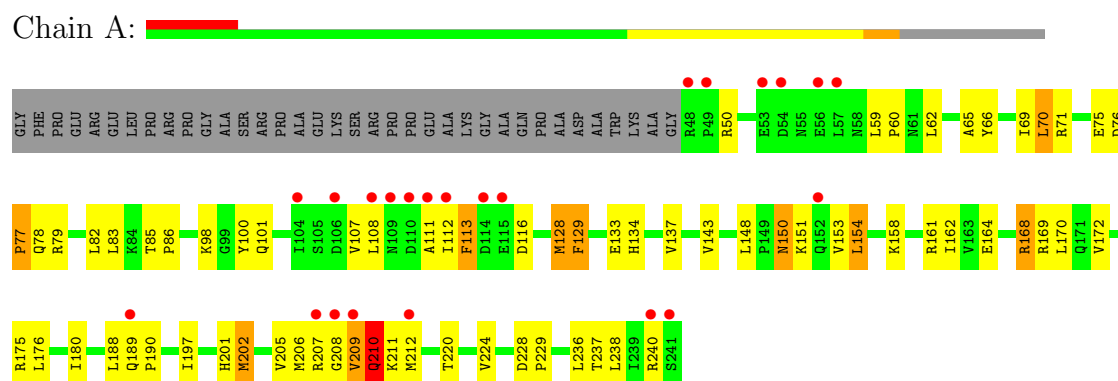
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	5	Total O 5 5	0	0
5	D	4	Total O 4 4	0	0
5	E	6	Total O 6 6	0	0
5	F	6	Total O 6 6	0	0
5	G	9	Total O 9 9	0	0
5	H	5	Total O 5 5	0	0
5	I	3	Total O 3 3	0	0
5	J	4	Total O 4 4	0	0
5	K	8	Total O 8 8	0	0
5	L	9	Total O 9 9	0	0
5	N	9	Total O 9 9	0	0
5	O	9	Total O 9 9	0	0
5	P	12	Total O 12 12	0	0
5	Q	9	Total O 9 9	0	0
5	R	6	Total O 6 6	0	0
5	S	7	Total O 7 7	0	0
5	T	7	Total O 7 7	0	0

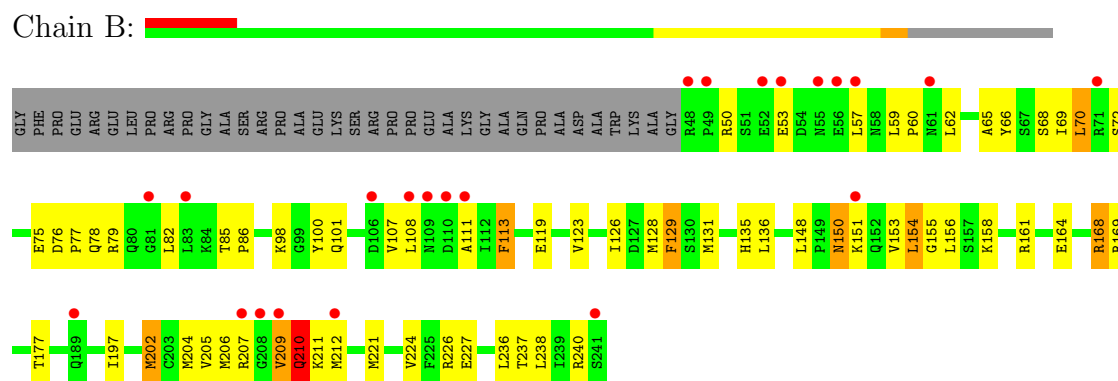
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

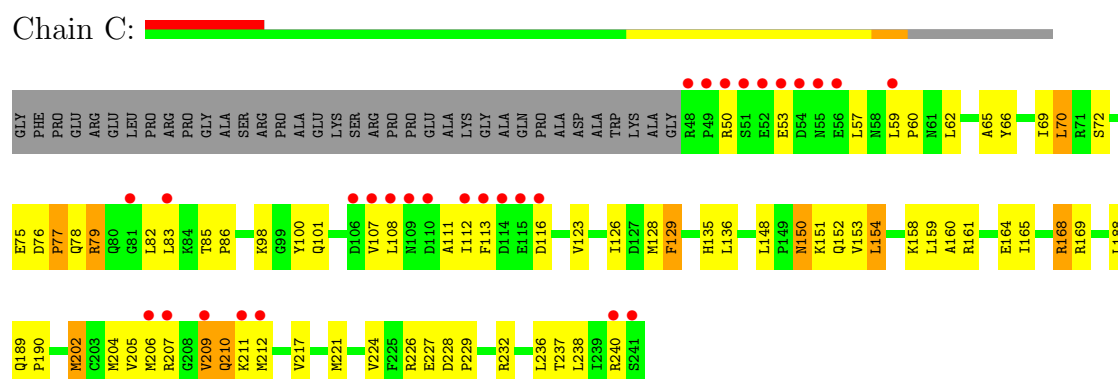
• Molecule 1: GTP Cyclohydrolase I



• Molecule 1: GTP Cyclohydrolase I

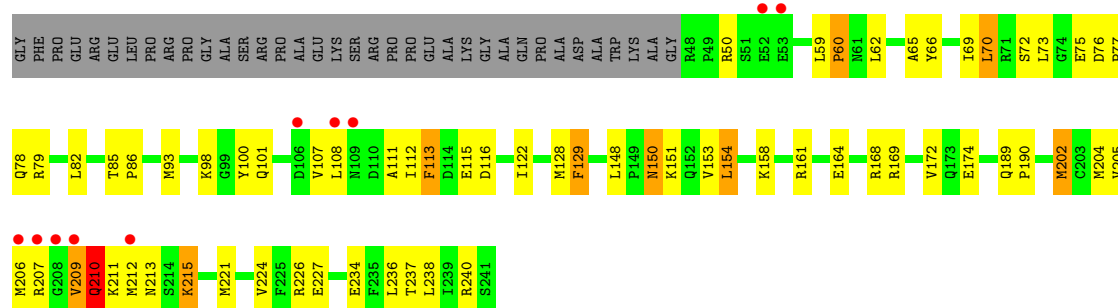


• Molecule 1: GTP Cyclohydrolase I



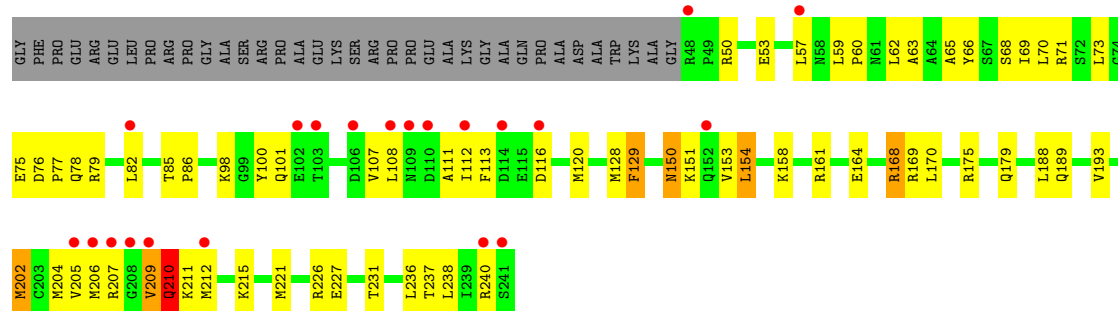
● Molecule 1: GTP Cyclohydrolase I

Chain D:



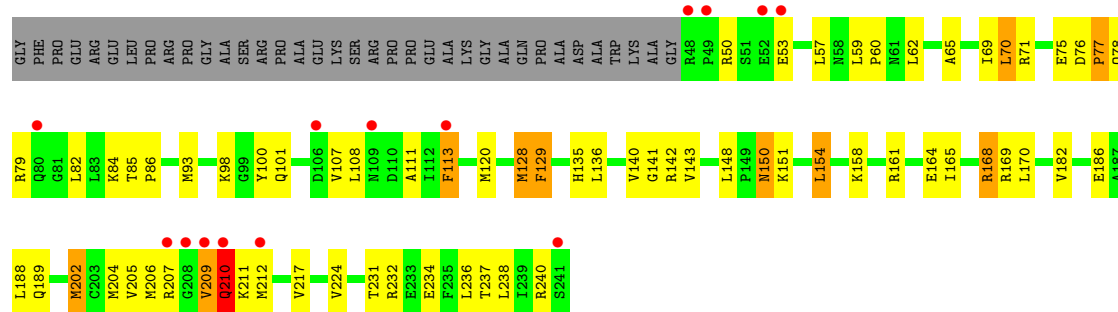
● Molecule 1: GTP Cyclohydrolase I

Chain E:



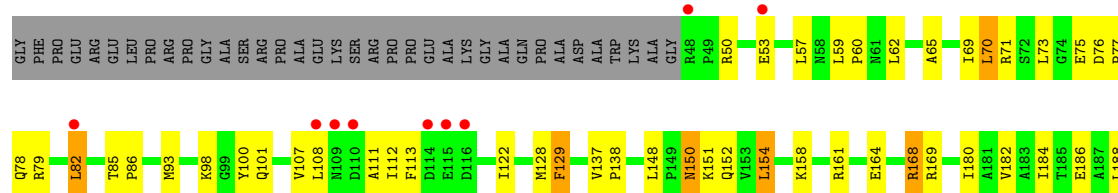
● Molecule 1: GTP Cyclohydrolase I

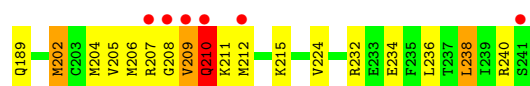
Chain F:



● Molecule 1: GTP Cyclohydrolase I

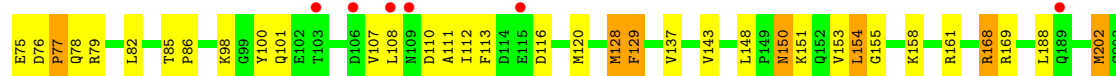
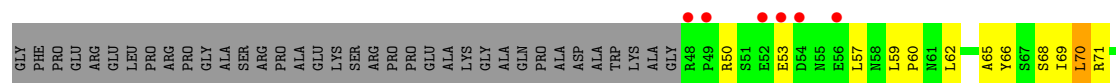
Chain G:





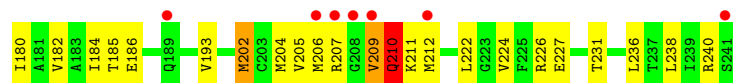
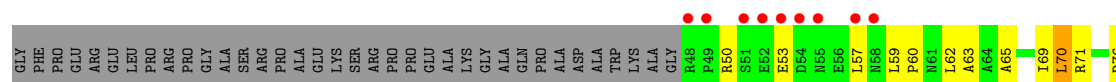
• Molecule 1: GTP Cyclohydrolase I

Chain H:



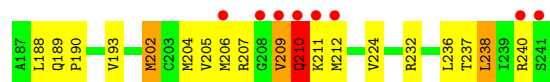
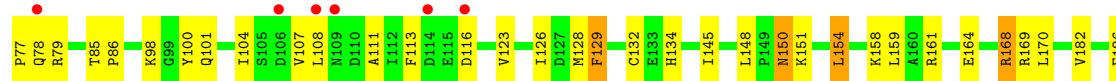
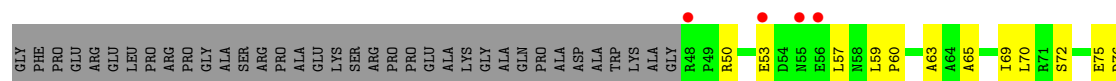
• Molecule 1: GTP Cyclohydrolase I

Chain I:



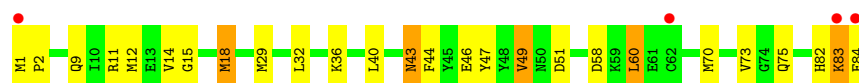
• Molecule 1: GTP Cyclohydrolase I

Chain J:



• Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain K:



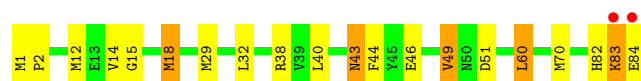
• Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain L: 



- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain M: 



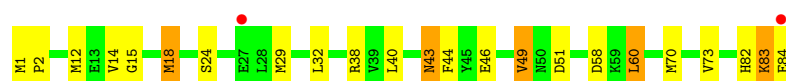
- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain N: 



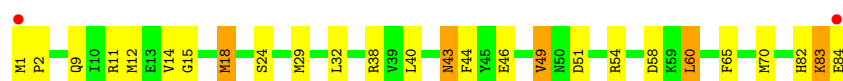
- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain O: 



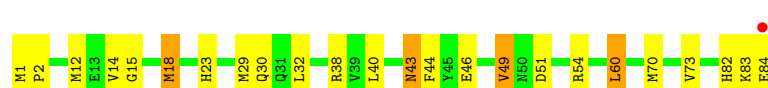
- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain P: 



- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain Q: 



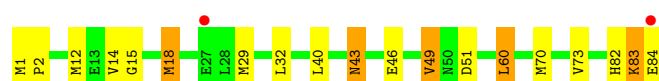
- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain R: 



- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain S: 



- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain T: 

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	124.15Å 111.72Å 126.11Å 90.00° 97.37° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80 15.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.7 (15.00-2.80) 99.2 (15.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 2.51Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.228 , 0.264 0.241 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 45.2	EDS
Estimated twinning fraction	0.006 for l,-k,h	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	5 of 116689 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	22375	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.50 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.0964e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.42	0/1561	0.64	0/2107
1	B	0.43	0/1561	0.63	0/2107
1	C	0.44	0/1561	0.64	0/2107
1	D	0.43	0/1561	0.65	0/2107
1	E	0.44	0/1561	0.65	0/2107
1	F	0.43	0/1561	0.63	0/2107
1	G	0.44	0/1561	0.64	0/2107
1	H	0.44	0/1561	0.65	0/2107
1	I	0.44	0/1561	0.63	0/2107
1	J	0.43	0/1561	0.65	0/2107
2	K	0.40	0/690	0.77	5/931 (0.5%)
2	L	0.40	0/690	0.76	5/931 (0.5%)
2	M	0.42	0/690	0.77	5/931 (0.5%)
2	N	0.47	1/690 (0.1%)	0.74	4/931 (0.4%)
2	O	0.41	0/690	0.75	5/931 (0.5%)
2	P	0.42	0/690	0.77	5/931 (0.5%)
2	Q	0.42	0/690	0.77	5/931 (0.5%)
2	R	0.41	0/690	0.76	5/931 (0.5%)
2	S	0.39	0/690	0.76	5/931 (0.5%)
2	T	0.41	0/690	0.77	5/931 (0.5%)
All	All	0.43	1/22510 (0.0%)	0.68	49/30380 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	29	MET	CG-SD	5.74	1.96	1.81

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	1	MET	CG-SD-CE	6.04	109.87	100.20
2	L	29	MET	CG-SD-CE	6.00	109.80	100.20
2	S	29	MET	CG-SD-CE	5.99	109.78	100.20
2	O	29	MET	CG-SD-CE	5.97	109.75	100.20
2	K	1	MET	CG-SD-CE	5.96	109.74	100.20
2	L	1	MET	CG-SD-CE	5.94	109.70	100.20
2	K	29	MET	CG-SD-CE	5.94	109.70	100.20
2	R	70	MET	CG-SD-CE	5.92	109.67	100.20
2	P	1	MET	CG-SD-CE	5.92	109.67	100.20
2	S	70	MET	CG-SD-CE	5.92	109.67	100.20
2	P	70	MET	CG-SD-CE	5.91	109.66	100.20
2	K	70	MET	CG-SD-CE	5.91	109.65	100.20
2	O	12	MET	CG-SD-CE	5.90	109.64	100.20
2	Q	70	MET	CG-SD-CE	5.89	109.63	100.20
2	O	70	MET	CG-SD-CE	5.89	109.63	100.20
2	Q	12	MET	CG-SD-CE	5.89	109.62	100.20
2	T	70	MET	CG-SD-CE	5.89	109.62	100.20
2	Q	1	MET	CG-SD-CE	5.88	109.61	100.20
2	Q	29	MET	CG-SD-CE	5.88	109.61	100.20
2	N	1	MET	CG-SD-CE	5.86	109.58	100.20
2	N	70	MET	CG-SD-CE	5.86	109.57	100.20
2	L	70	MET	CG-SD-CE	5.86	109.57	100.20
2	T	1	MET	CG-SD-CE	5.85	109.57	100.20
2	M	70	MET	CG-SD-CE	5.85	109.56	100.20
2	M	29	MET	CG-SD-CE	5.85	109.56	100.20
2	O	1	MET	CG-SD-CE	5.84	109.55	100.20
2	S	1	MET	CG-SD-CE	5.84	109.55	100.20
2	R	1	MET	CG-SD-CE	5.83	109.53	100.20
2	P	29	MET	CG-SD-CE	5.82	109.51	100.20
2	S	12	MET	CG-SD-CE	5.79	109.46	100.20
2	P	12	MET	CG-SD-CE	5.78	109.45	100.20
2	R	29	MET	CG-SD-CE	5.78	109.45	100.20
2	N	12	MET	CG-SD-CE	5.77	109.43	100.20
2	R	12	MET	CG-SD-CE	5.77	109.43	100.20
2	T	29	MET	CG-SD-CE	5.76	109.41	100.20
2	K	12	MET	CG-SD-CE	5.74	109.39	100.20
2	M	12	MET	CG-SD-CE	5.72	109.36	100.20
2	T	12	MET	CG-SD-CE	5.72	109.36	100.20
2	L	12	MET	CG-SD-CE	5.71	109.34	100.20
2	P	18	MET	CG-SD-CE	5.69	109.31	100.20
2	Q	18	MET	CG-SD-CE	5.69	109.30	100.20
2	M	18	MET	CG-SD-CE	5.63	109.21	100.20
2	S	18	MET	CG-SD-CE	5.62	109.19	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	18	MET	CG-SD-CE	5.62	109.18	100.20
2	T	18	MET	CG-SD-CE	5.60	109.16	100.20
2	N	18	MET	CG-SD-CE	5.59	109.14	100.20
2	O	18	MET	CG-SD-CE	5.58	109.14	100.20
2	R	18	MET	CG-SD-CE	5.55	109.08	100.20
2	L	18	MET	CG-SD-CE	5.53	109.05	100.20

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1536	0	1557	81	0
1	B	1536	0	1557	88	0
1	C	1536	0	1557	84	0
1	D	1536	0	1557	83	0
1	E	1536	0	1557	83	0
1	F	1536	0	1557	87	0
1	G	1536	0	1557	83	0
1	H	1536	0	1557	79	0
1	I	1536	0	1557	85	0
1	J	1536	0	1557	76	0
2	K	676	0	677	20	0
2	L	676	0	677	21	0
2	M	676	0	677	15	0
2	N	676	0	677	18	0
2	O	676	0	677	20	0
2	P	676	0	677	22	0
2	Q	676	0	677	18	1
2	R	676	0	677	16	0
2	S	676	0	677	15	0
2	T	676	0	677	19	1
3	K	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	1	0	0	0	0
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	1	0	0	0	0
3	T	1	0	0	0	0
4	K	12	0	8	1	0
4	L	12	0	8	1	0
4	M	12	0	8	0	0
4	N	12	0	8	0	0
4	O	12	0	8	0	0
4	P	12	0	8	0	0
4	R	24	0	16	0	0
4	S	12	0	8	0	0
4	T	12	0	8	0	0
5	A	3	0	0	0	0
5	B	4	0	0	0	0
5	C	5	0	0	1	0
5	D	4	0	0	0	0
5	E	6	0	0	0	0
5	F	6	0	0	0	0
5	G	9	0	0	1	0
5	H	5	0	0	0	0
5	I	3	0	0	0	0
5	J	4	0	0	0	0
5	K	8	0	0	1	0
5	L	9	0	0	2	0
5	N	9	0	0	0	0
5	O	9	0	0	0	0
5	P	12	0	0	0	0
5	Q	9	0	0	0	0
5	R	6	0	0	0	0
5	S	7	0	0	0	0
5	T	7	0	0	0	0
All	All	22375	0	22420	893	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 20.

All (893) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:210:GLN:HB3	1:I:210:GLN:HB3	1.27	1.14
1:A:205:VAL:HG22	1:A:212:MET:HA	1.42	1.01
1:H:205:VAL:HG13	1:H:212:MET:HB2	1.41	1.01
1:J:209:VAL:HG13	1:J:210:GLN:H	1.25	1.00
1:I:205:VAL:HG13	1:I:212:MET:HB2	1.41	1.00
1:G:205:VAL:HG22	1:G:212:MET:HA	1.41	0.99
1:G:205:VAL:HG13	1:G:212:MET:HB2	1.44	0.99
1:E:205:VAL:HG13	1:E:212:MET:HB2	1.42	0.99
1:C:209:VAL:HG13	1:C:210:GLN:H	1.26	0.98
1:A:209:VAL:HG13	1:A:210:GLN:H	1.25	0.98
1:E:209:VAL:HG13	1:E:210:GLN:H	1.29	0.98
1:F:205:VAL:HG13	1:F:212:MET:HB2	1.44	0.98
1:C:205:VAL:HG13	1:C:212:MET:HB2	1.46	0.97
1:F:205:VAL:HG22	1:F:212:MET:HA	1.43	0.97
1:D:209:VAL:HG13	1:D:210:GLN:H	1.29	0.94
1:A:205:VAL:HG13	1:A:212:MET:HB2	1.47	0.94
1:D:205:VAL:HG13	1:D:212:MET:HB2	1.51	0.93
1:D:59:LEU:HB3	1:D:60:PRO:HD3	1.50	0.93
1:I:209:VAL:HG13	1:I:210:GLN:H	1.30	0.93
1:F:209:VAL:HG13	1:F:210:GLN:H	1.33	0.93
1:G:209:VAL:HG13	1:G:210:GLN:H	1.31	0.91
1:J:205:VAL:HG13	1:J:212:MET:HB2	1.51	0.91
1:H:205:VAL:HG22	1:H:212:MET:HA	1.50	0.91
1:E:107:VAL:HG22	1:E:161:ARG:HD3	1.52	0.91
1:H:209:VAL:HG13	1:H:210:GLN:H	1.35	0.90
1:H:107:VAL:HG22	1:H:161:ARG:HD3	1.54	0.90
1:I:205:VAL:HG22	1:I:212:MET:HA	1.53	0.89
1:J:205:VAL:HG22	1:J:212:MET:HA	1.53	0.88
1:E:205:VAL:HG22	1:E:212:MET:HA	1.56	0.86
1:B:209:VAL:HG13	1:B:210:GLN:H	1.36	0.86
1:D:107:VAL:HG22	1:D:161:ARG:HD3	1.57	0.86
1:J:107:VAL:HG22	1:J:161:ARG:HD3	1.55	0.86
1:C:210:GLN:HB3	1:G:210:GLN:HB3	1.56	0.85
2:Q:18:MET:HE3	2:Q:46:GLU:HB2	1.58	0.85
1:B:205:VAL:HG13	1:B:212:MET:HB2	1.57	0.85
1:D:205:VAL:HG22	1:D:212:MET:HA	1.57	0.84
2:M:18:MET:HE1	2:M:46:GLU:HB2	1.59	0.83
1:F:107:VAL:HG22	1:F:161:ARG:HD3	1.61	0.82
1:C:205:VAL:HG22	1:C:212:MET:HA	1.59	0.82
1:F:59:LEU:HB3	1:F:60:PRO:HD3	1.60	0.82
1:B:205:VAL:HG22	1:B:212:MET:HA	1.61	0.81
1:I:111:ALA:HB3	1:I:158:LYS:HG2	1.60	0.81
1:I:107:VAL:HG22	1:I:161:ARG:HD3	1.63	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:59:LEU:HB3	1:E:60:PRO:HD3	1.63	0.81
1:H:59:LEU:HB3	1:H:60:PRO:HD3	1.64	0.80
1:G:107:VAL:HG22	1:G:161:ARG:HD3	1.65	0.79
1:E:111:ALA:HB3	1:E:158:LYS:HG2	1.64	0.79
2:S:18:MET:HE1	2:S:46:GLU:HB2	1.62	0.79
2:L:18:MET:HE3	2:L:46:GLU:HB2	1.66	0.77
2:O:18:MET:HE3	2:O:46:GLU:HB2	1.67	0.77
1:B:59:LEU:HB3	1:B:60:PRO:HD3	1.67	0.76
2:O:43:ASN:HD22	2:O:43:ASN:H	1.33	0.75
1:H:204:MET:HE3	1:H:211:LYS:HD3	1.69	0.75
1:H:70:LEU:HB3	1:H:77:PRO:HG3	1.69	0.74
2:T:43:ASN:HD22	2:T:43:ASN:H	1.35	0.74
1:A:107:VAL:HG22	1:A:161:ARG:HD3	1.69	0.74
1:A:148:LEU:HD12	1:A:224:VAL:HG21	1.68	0.73
2:T:18:MET:HE1	2:T:46:GLU:HB2	1.71	0.73
1:E:209:VAL:HG13	1:E:210:GLN:N	2.03	0.72
2:Q:43:ASN:H	2:Q:43:ASN:HD22	1.37	0.72
1:A:129:PHE:HZ	1:J:210:GLN:HG2	1.53	0.72
1:C:107:VAL:HG22	1:C:161:ARG:HD3	1.72	0.72
1:G:204:MET:HE3	1:G:211:LYS:HD3	1.72	0.72
1:I:59:LEU:HB3	1:I:60:PRO:HD3	1.71	0.72
1:H:148:LEU:HD12	1:H:224:VAL:HG21	1.72	0.72
1:D:210:GLN:HB3	1:F:210:GLN:HB3	1.72	0.71
1:B:226:ARG:HD2	1:B:227:GLU:OE2	1.92	0.70
1:I:209:VAL:HG13	1:I:210:GLN:N	2.06	0.70
1:A:116:ASP:OD1	1:A:151:LYS:HE3	1.92	0.70
2:P:43:ASN:HD22	2:P:43:ASN:H	1.38	0.70
1:J:111:ALA:HB3	1:J:158:LYS:HG2	1.73	0.69
1:J:50:ARG:HB3	1:J:101:GLN:HB3	1.74	0.69
1:J:204:MET:HE3	1:J:211:LYS:HD3	1.74	0.69
1:A:111:ALA:HB3	1:A:158:LYS:HG2	1.72	0.69
1:D:209:VAL:HG13	1:D:210:GLN:N	2.06	0.69
2:N:18:MET:HE3	2:N:46:GLU:HB2	1.75	0.69
2:R:43:ASN:H	2:R:43:ASN:HD22	1.39	0.69
2:M:43:ASN:HD22	2:M:43:ASN:H	1.41	0.69
1:F:148:LEU:HD12	1:F:224:VAL:HG21	1.74	0.68
1:A:209:VAL:HG13	1:A:210:GLN:N	2.03	0.68
1:B:206:MET:HB3	1:I:168:ARG:HH22	1.59	0.68
1:G:98:LYS:O	1:G:101:GLN:HG2	1.94	0.68
2:R:18:MET:HE3	2:R:46:GLU:HB2	1.76	0.68
1:J:98:LYS:O	1:J:101:GLN:HG2	1.94	0.67
1:C:204:MET:HE3	1:C:211:LYS:HD3	1.76	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:202:MET:HG2	1:I:206:MET:CE	2.24	0.67
1:B:204:MET:HE3	1:B:211:LYS:HD3	1.75	0.67
1:D:202:MET:HG2	1:D:206:MET:CE	2.24	0.67
1:F:202:MET:HG2	1:F:206:MET:CE	2.23	0.67
2:K:43:ASN:HD22	2:K:43:ASN:H	1.41	0.67
1:A:59:LEU:HB3	1:A:60:PRO:HD3	1.76	0.67
1:B:148:LEU:HD12	1:B:224:VAL:HG21	1.75	0.67
2:L:43:ASN:H	2:L:43:ASN:HD22	1.41	0.67
1:A:70:LEU:HB3	1:A:77:PRO:HG3	1.77	0.67
1:I:85:THR:HB	1:I:86:PRO:HD3	1.77	0.67
2:N:43:ASN:HD22	2:N:43:ASN:H	1.41	0.66
1:G:100:TYR:CZ	1:G:169:ARG:HB2	2.30	0.66
1:J:209:VAL:CG1	1:J:210:GLN:H	2.06	0.66
1:J:79:ARG:HB3	1:J:79:ARG:HH11	1.60	0.66
1:E:98:LYS:O	1:E:101:GLN:HG2	1.95	0.66
1:B:79:ARG:HH11	1:B:79:ARG:HB3	1.60	0.66
1:A:143:VAL:HG22	1:A:197:ILE:HG12	1.78	0.66
1:B:209:VAL:HG13	1:B:210:GLN:N	2.11	0.66
1:F:209:VAL:HG13	1:F:210:GLN:N	2.09	0.66
1:F:205:VAL:HG22	1:F:212:MET:CA	2.23	0.65
1:G:148:LEU:HD12	1:G:224:VAL:HG21	1.78	0.65
1:A:65:ALA:O	1:A:69:ILE:HG13	1.96	0.65
1:J:209:VAL:HG13	1:J:210:GLN:N	2.06	0.65
2:P:18:MET:HE1	2:P:46:GLU:HB2	1.77	0.65
1:C:50:ARG:HB3	1:C:101:GLN:HB3	1.77	0.65
1:C:98:LYS:O	1:C:101:GLN:HG2	1.96	0.65
1:G:205:VAL:HG22	1:G:212:MET:CA	2.22	0.65
1:F:79:ARG:HH11	1:F:79:ARG:HB3	1.62	0.65
1:H:205:VAL:CG1	1:H:212:MET:HB2	2.24	0.65
1:B:111:ALA:HB3	1:B:158:LYS:HG2	1.77	0.65
1:G:59:LEU:HB3	1:G:60:PRO:HD3	1.79	0.65
1:A:100:TYR:CZ	1:A:169:ARG:HB2	2.32	0.65
2:S:43:ASN:H	2:S:43:ASN:HD22	1.44	0.65
1:A:202:MET:HG2	1:A:206:MET:CE	2.27	0.64
1:B:98:LYS:HZ3	1:B:168:ARG:HD3	1.63	0.64
1:F:202:MET:HG2	1:F:206:MET:HE2	1.78	0.64
1:I:150:ASN:O	1:I:151:LYS:HB2	1.98	0.64
1:D:209:VAL:CG1	1:D:211:LYS:HE2	2.28	0.64
1:C:65:ALA:O	1:C:69:ILE:HG13	1.97	0.64
1:E:209:VAL:CG1	1:E:210:GLN:H	2.08	0.64
1:G:209:VAL:HG13	1:G:210:GLN:N	2.09	0.64
1:D:98:LYS:O	1:D:101:GLN:HG2	1.98	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:168:ARG:HH22	1:I:206:MET:HB3	1.62	0.63
1:A:75:GLU:O	1:A:77:PRO:HD3	1.98	0.63
1:D:148:LEU:HD12	1:D:224:VAL:HG21	1.80	0.63
1:I:205:VAL:CG1	1:I:212:MET:HB2	2.25	0.63
2:O:43:ASN:N	2:O:43:ASN:HD22	1.94	0.63
1:F:65:ALA:O	1:F:69:ILE:HG13	1.98	0.63
1:D:111:ALA:HB3	1:D:158:LYS:HG2	1.81	0.63
1:A:150:ASN:O	1:A:151:LYS:HB2	1.98	0.63
1:E:205:VAL:CG1	1:E:212:MET:HB2	2.25	0.63
1:C:209:VAL:HG13	1:C:210:GLN:N	2.06	0.63
1:E:79:ARG:HB3	1:E:79:ARG:HH11	1.63	0.63
1:G:150:ASN:O	1:G:151:LYS:HB2	1.97	0.62
1:B:107:VAL:HG12	1:B:158:LYS:HG3	1.81	0.62
1:H:209:VAL:HG13	1:H:210:GLN:N	2.10	0.62
1:I:50:ARG:HB3	1:I:101:GLN:HB3	1.80	0.62
1:C:209:VAL:CG1	1:C:210:GLN:H	2.08	0.62
1:C:79:ARG:HH11	1:C:79:ARG:HB3	1.65	0.62
1:F:150:ASN:O	1:F:151:LYS:HB2	2.00	0.62
1:A:209:VAL:CG1	1:A:210:GLN:H	2.06	0.61
1:D:206:MET:HB3	1:G:168:ARG:HH22	1.64	0.61
1:A:205:VAL:HG22	1:A:212:MET:CA	2.25	0.61
1:E:204:MET:HE3	1:E:211:LYS:HD3	1.82	0.61
1:J:202:MET:HG2	1:J:206:MET:CE	2.30	0.61
2:S:18:MET:HE1	2:S:46:GLU:CB	2.30	0.61
1:C:59:LEU:HB3	1:C:60:PRO:HD3	1.82	0.61
1:E:66:TYR:CD2	1:E:69:ILE:HD12	2.35	0.61
1:A:85:THR:HB	1:A:86:PRO:HD3	1.83	0.61
1:H:111:ALA:HB3	1:H:158:LYS:HG2	1.82	0.61
2:P:43:ASN:N	2:P:43:ASN:HD22	1.97	0.61
1:B:206:MET:SD	1:I:129:PHE:HB3	2.41	0.60
1:E:210:GLN:HG2	1:F:129:PHE:HZ	1.66	0.60
1:H:205:VAL:HG22	1:H:212:MET:CA	2.26	0.60
1:J:100:TYR:CZ	1:J:169:ARG:HB2	2.36	0.60
1:F:111:ALA:HB3	1:F:158:LYS:HG2	1.83	0.60
1:D:202:MET:HG2	1:D:206:MET:HE1	1.81	0.60
1:E:168:ARG:HH22	1:F:206:MET:HB3	1.66	0.60
1:E:111:ALA:HB3	1:E:158:LYS:CG	2.30	0.60
1:E:66:TYR:HD2	1:E:69:ILE:HD12	1.66	0.60
1:E:150:ASN:O	1:E:151:LYS:HB2	2.00	0.60
1:I:164:GLU:HG3	1:I:168:ARG:HG3	1.83	0.60
1:F:204:MET:HE3	1:F:211:LYS:HD3	1.83	0.60
2:R:43:ASN:N	2:R:43:ASN:HD22	1.99	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:205:VAL:O	1:H:210:GLN:HA	2.02	0.60
1:H:98:LYS:O	1:H:101:GLN:HG2	2.01	0.60
1:C:79:ARG:O	1:C:83:LEU:HG	2.01	0.60
1:C:70:LEU:HB3	1:C:77:PRO:HG3	1.84	0.60
1:A:129:PHE:CZ	1:J:210:GLN:HG2	2.36	0.60
2:L:18:MET:HE3	2:L:46:GLU:CB	2.32	0.60
1:G:65:ALA:O	1:G:69:ILE:HG13	2.01	0.60
1:D:100:TYR:CZ	1:D:169:ARG:HB2	2.37	0.60
2:Q:43:ASN:N	2:Q:43:ASN:HD22	1.97	0.60
2:N:43:ASN:HD22	2:N:43:ASN:N	1.99	0.60
1:J:59:LEU:HB3	1:J:60:PRO:HD3	1.83	0.60
1:B:205:VAL:O	1:B:210:GLN:HA	2.02	0.59
2:O:43:ASN:H	2:O:43:ASN:ND2	1.99	0.59
1:C:116:ASP:OD1	1:C:151:LYS:HE3	2.02	0.59
2:T:43:ASN:HD22	2:T:43:ASN:N	1.96	0.59
1:I:148:LEU:HD12	1:I:224:VAL:HG21	1.84	0.59
1:F:100:TYR:CZ	1:F:169:ARG:HB2	2.37	0.59
1:I:111:ALA:HB3	1:I:158:LYS:CG	2.29	0.59
1:C:123:VAL:HG12	1:C:126:ILE:HD11	1.84	0.59
1:G:205:VAL:O	1:G:210:GLN:HA	2.03	0.59
1:G:205:VAL:CG1	1:G:212:MET:HB2	2.27	0.59
1:E:65:ALA:O	1:E:69:ILE:HG13	2.02	0.59
1:B:150:ASN:O	1:B:151:LYS:HB2	2.01	0.59
1:F:75:GLU:O	1:F:77:PRO:HD3	2.02	0.59
1:B:164:GLU:HG3	1:B:168:ARG:HG3	1.83	0.59
1:F:98:LYS:O	1:F:101:GLN:HG2	2.03	0.59
1:B:236:LEU:O	1:B:240:ARG:HB2	2.03	0.59
1:C:205:VAL:HG22	1:C:212:MET:CA	2.33	0.59
1:J:75:GLU:O	1:J:77:PRO:HD3	2.03	0.59
1:A:207:ARG:HG2	1:A:207:ARG:HH11	1.67	0.59
1:J:98:LYS:HZ3	1:J:168:ARG:HD3	1.68	0.59
1:J:207:ARG:HH11	1:J:207:ARG:HG2	1.67	0.59
2:M:43:ASN:N	2:M:43:ASN:HD22	2.00	0.59
1:H:65:ALA:O	1:H:68:SER:HB3	2.03	0.59
1:I:98:LYS:O	1:I:101:GLN:HG2	2.02	0.58
1:J:98:LYS:NZ	1:J:168:ARG:HD3	2.19	0.58
1:I:100:TYR:CZ	1:I:169:ARG:HB2	2.38	0.58
1:G:111:ALA:HB3	1:G:158:LYS:HG2	1.85	0.58
1:H:150:ASN:O	1:H:151:LYS:HB2	2.04	0.58
1:H:79:ARG:HH11	1:H:79:ARG:HB3	1.69	0.58
1:F:205:VAL:O	1:F:210:GLN:HA	2.03	0.58
2:P:43:ASN:ND2	2:P:43:ASN:H	2.02	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:116:ASP:OD1	1:H:151:LYS:HE3	2.03	0.58
1:B:129:PHE:CZ	1:I:210:GLN:HG2	2.38	0.58
1:E:206:MET:HB3	1:F:168:ARG:HH22	1.67	0.58
1:D:79:ARG:HB3	1:D:79:ARG:HH11	1.68	0.58
2:T:43:ASN:ND2	2:T:43:ASN:H	2.01	0.58
2:Q:18:MET:HE3	2:Q:46:GLU:CB	2.33	0.58
1:D:236:LEU:O	1:D:240:ARG:HB2	2.03	0.58
1:G:207:ARG:C	1:G:209:VAL:H	2.07	0.57
1:H:107:VAL:HG22	1:H:161:ARG:CD	2.30	0.57
1:H:111:ALA:HB3	1:H:158:LYS:CD	2.34	0.57
1:D:65:ALA:O	1:D:69:ILE:HG13	2.04	0.57
1:B:207:ARG:HH11	1:B:207:ARG:HG2	1.69	0.57
1:A:164:GLU:CD	1:A:168:ARG:HD2	2.25	0.57
1:C:72:SER:HB2	1:H:62:LEU:HD21	1.87	0.57
1:G:79:ARG:HH11	1:G:79:ARG:HB3	1.70	0.57
1:A:202:MET:HG2	1:A:206:MET:HE2	1.86	0.57
1:A:210:GLN:HG2	1:J:129:PHE:CZ	2.39	0.57
1:B:129:PHE:HZ	1:I:210:GLN:HG2	1.68	0.57
1:F:209:VAL:CG1	1:F:210:GLN:H	2.13	0.57
1:I:202:MET:HG2	1:I:206:MET:HE2	1.85	0.57
2:R:18:MET:HE3	2:R:46:GLU:CG	2.34	0.57
1:F:154:LEU:HB2	1:F:188:LEU:HD11	1.87	0.57
2:P:49:VAL:CG1	2:P:51:ASP:H	2.18	0.57
1:F:111:ALA:HB3	1:F:158:LYS:CD	2.35	0.57
1:B:100:TYR:CZ	1:B:169:ARG:HB2	2.40	0.57
2:L:49:VAL:CG1	2:L:51:ASP:H	2.17	0.57
1:B:66:TYR:CD2	1:B:69:ILE:HD12	2.40	0.57
1:E:129:PHE:HZ	1:F:210:GLN:HG2	1.70	0.57
2:N:43:ASN:ND2	2:N:43:ASN:H	2.03	0.57
1:A:50:ARG:HB3	1:A:101:GLN:HB3	1.87	0.57
2:K:43:ASN:HD22	2:K:43:ASN:N	1.99	0.57
2:L:43:ASN:H	2:L:43:ASN:ND2	2.03	0.56
1:C:112:ILE:HD11	1:C:152:GLN:CD	2.25	0.56
1:H:207:ARG:C	1:H:209:VAL:H	2.09	0.56
1:A:71:ARG:HG3	1:A:77:PRO:HG2	1.87	0.56
1:B:66:TYR:HD2	1:B:69:ILE:HD12	1.68	0.56
1:B:65:ALA:O	1:B:69:ILE:HG13	2.04	0.56
1:E:70:LEU:HB3	1:E:77:PRO:HG3	1.87	0.56
1:C:207:ARG:HG2	1:C:207:ARG:HH11	1.70	0.56
1:F:207:ARG:HG2	1:F:207:ARG:HH11	1.68	0.56
1:C:76:ASP:C	1:C:78:GLN:H	2.06	0.56
1:H:128:MET:HG2	1:H:143:VAL:HG23	1.86	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:209:VAL:CG1	1:F:211:LYS:HE2	2.35	0.56
1:A:205:VAL:O	1:A:210:GLN:HA	2.05	0.56
1:I:209:VAL:CG1	1:I:210:GLN:H	2.12	0.56
1:C:207:ARG:C	1:C:209:VAL:H	2.09	0.56
2:L:43:ASN:N	2:L:43:ASN:HD22	1.99	0.56
1:D:62:LEU:CD2	1:G:69:ILE:HG23	2.35	0.56
1:I:226:ARG:HD2	1:I:227:GLU:OE2	2.05	0.56
1:E:210:GLN:HG2	1:F:129:PHE:CZ	2.41	0.56
1:D:205:VAL:O	1:D:210:GLN:HA	2.06	0.56
1:A:79:ARG:HB3	1:A:79:ARG:HH11	1.71	0.56
1:C:164:GLU:CD	1:C:168:ARG:HD2	2.25	0.56
2:R:49:VAL:CG1	2:R:51:ASP:H	2.19	0.56
1:B:207:ARG:C	1:B:209:VAL:H	2.09	0.55
2:Q:43:ASN:H	2:Q:43:ASN:ND2	2.03	0.55
2:R:43:ASN:H	2:R:43:ASN:ND2	2.04	0.55
2:S:49:VAL:CG1	2:S:51:ASP:H	2.19	0.55
2:O:32:LEU:HD11	2:O:60:LEU:HD11	1.89	0.55
1:H:209:VAL:CG1	1:H:211:LYS:HE2	2.37	0.55
1:E:202:MET:HG2	1:E:206:MET:CE	2.37	0.55
2:M:43:ASN:ND2	2:M:43:ASN:H	2.05	0.55
1:B:98:LYS:NZ	1:B:168:ARG:HD3	2.21	0.55
1:E:205:VAL:O	1:E:210:GLN:HA	2.05	0.55
1:C:206:MET:HG2	1:H:129:PHE:CG	2.41	0.55
1:A:148:LEU:CD1	1:A:224:VAL:HG21	2.36	0.55
2:K:18:MET:HE3	2:K:46:GLU:HB2	1.88	0.55
1:I:79:ARG:HB3	1:I:79:ARG:HH11	1.71	0.55
1:C:53:GLU:O	1:C:57:LEU:HG	2.07	0.55
1:E:207:ARG:C	1:E:209:VAL:H	2.10	0.55
1:E:111:ALA:HB3	1:E:158:LYS:CD	2.36	0.55
2:K:43:ASN:H	2:K:43:ASN:ND2	2.05	0.55
2:L:32:LEU:HD11	2:L:60:LEU:HD11	1.89	0.55
1:J:145:ILE:HD13	1:J:159:LEU:HD11	1.89	0.55
2:O:83:LYS:HG2	2:O:84:GLU:N	2.22	0.55
1:D:70:LEU:HB3	1:D:77:PRO:HG3	1.89	0.55
1:B:107:VAL:HG22	1:B:161:ARG:HD3	1.88	0.55
1:A:170:LEU:HD12	1:J:75:GLU:HG3	1.89	0.54
1:H:209:VAL:CG1	1:H:210:GLN:H	2.15	0.54
1:E:209:VAL:CG1	1:E:211:LYS:HE2	2.36	0.54
1:H:100:TYR:CZ	1:H:169:ARG:HB2	2.42	0.54
2:P:32:LEU:HD11	2:P:60:LEU:HD11	1.90	0.54
1:I:205:VAL:O	1:I:210:GLN:HA	2.08	0.54
1:C:76:ASP:OD2	1:C:78:GLN:HG2	2.07	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:236:LEU:O	1:I:240:ARG:HB2	2.07	0.54
1:D:150:ASN:O	1:D:151:LYS:HB2	2.06	0.54
1:I:65:ALA:O	1:I:69:ILE:HG13	2.08	0.54
1:C:209:VAL:CG1	1:C:211:LYS:HE2	2.37	0.54
1:C:205:VAL:CG1	1:C:212:MET:HB2	2.30	0.54
1:D:209:VAL:HG11	1:D:211:LYS:HE2	1.90	0.54
1:J:111:ALA:HB3	1:J:158:LYS:CG	2.37	0.54
2:L:18:MET:HE3	2:L:46:GLU:CG	2.38	0.54
1:C:153:VAL:HG12	1:C:154:LEU:N	2.22	0.54
1:J:111:ALA:HB3	1:J:158:LYS:CD	2.37	0.54
1:C:107:VAL:CG1	1:C:158:LYS:HG3	2.37	0.54
2:P:2:PRO:HB2	2:P:82:HIS:CE1	2.43	0.54
1:H:202:MET:HG2	1:H:206:MET:CE	2.37	0.54
1:J:202:MET:HG2	1:J:206:MET:HE1	1.88	0.54
1:C:236:LEU:O	1:C:240:ARG:HB2	2.07	0.54
2:L:53:PRO:HG2	5:L:2012:HOH:O	2.08	0.54
1:F:85:THR:HB	1:F:86:PRO:HD3	1.90	0.54
1:D:207:ARG:C	1:D:209:VAL:H	2.09	0.54
1:I:111:ALA:HB3	1:I:158:LYS:CD	2.38	0.54
1:G:148:LEU:CD1	1:G:224:VAL:HG21	2.37	0.54
1:G:204:MET:CE	1:G:211:LYS:HD3	2.36	0.54
2:S:18:MET:HE1	2:S:46:GLU:CG	2.38	0.54
1:C:111:ALA:HB3	1:C:158:LYS:HG2	1.90	0.54
1:B:111:ALA:HB3	1:B:158:LYS:CD	2.38	0.54
1:G:107:VAL:HG12	1:G:158:LYS:HG3	1.90	0.54
2:N:49:VAL:CG1	2:N:51:ASP:H	2.21	0.54
1:G:70:LEU:HB3	1:G:77:PRO:HG3	1.90	0.54
1:H:107:VAL:HG12	1:H:158:LYS:HG3	1.90	0.53
2:S:43:ASN:N	2:S:43:ASN:HD22	2.01	0.53
2:K:49:VAL:CG1	2:K:51:ASP:H	2.22	0.53
1:F:236:LEU:O	1:F:240:ARG:HB2	2.08	0.53
1:E:129:PHE:CZ	1:F:210:GLN:HG2	2.43	0.53
1:J:70:LEU:HB3	1:J:77:PRO:HG3	1.90	0.53
1:B:206:MET:HB3	1:I:168:ARG:NH2	2.21	0.53
1:C:111:ALA:HB3	1:C:158:LYS:CD	2.39	0.53
1:C:123:VAL:CG1	1:C:126:ILE:HD11	2.38	0.53
1:B:204:MET:CE	1:B:211:LYS:HD3	2.38	0.53
1:J:207:ARG:C	1:J:209:VAL:H	2.11	0.53
1:E:107:VAL:HG22	1:E:161:ARG:CD	2.32	0.53
1:B:98:LYS:O	1:B:101:GLN:HG2	2.09	0.53
1:E:100:TYR:CZ	1:E:169:ARG:HB2	2.42	0.53
2:T:49:VAL:CG1	2:T:51:ASP:H	2.22	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:N:58:ASP:OD1	2:O:2:PRO:HD2	2.08	0.53
1:B:209:VAL:CG1	1:B:211:LYS:HE2	2.39	0.53
1:D:111:ALA:HB3	1:D:158:LYS:CD	2.39	0.53
1:J:79:ARG:HB3	1:J:79:ARG:NH1	2.24	0.53
1:H:76:ASP:C	1:H:78:GLN:H	2.12	0.53
1:G:232:ARG:NE	5:G:248:HOH:O	2.40	0.53
1:G:207:ARG:HH11	1:G:207:ARG:HG2	1.73	0.53
2:R:18:MET:HE3	2:R:46:GLU:CB	2.39	0.53
1:B:85:THR:HB	1:B:86:PRO:HD3	1.90	0.53
1:G:111:ALA:HB3	1:G:158:LYS:CD	2.38	0.53
1:E:221:MET:O	1:E:226:ARG:HB2	2.08	0.53
1:A:210:GLN:CB	1:I:210:GLN:HB3	2.19	0.53
1:J:204:MET:CE	1:J:211:LYS:HD3	2.37	0.53
1:I:205:VAL:HG22	1:I:212:MET:CA	2.32	0.52
1:D:107:VAL:HG22	1:D:161:ARG:CD	2.36	0.52
1:E:116:ASP:OD1	1:E:151:LYS:HE3	2.09	0.52
1:B:113:PHE:N	1:B:113:PHE:CD1	2.76	0.52
1:C:210:GLN:NE2	1:G:210:GLN:NE2	2.58	0.52
2:M:18:MET:HE1	2:M:46:GLU:CB	2.35	0.52
1:F:70:LEU:HB3	1:F:77:PRO:HG3	1.90	0.52
1:H:237:THR:HA	1:H:240:ARG:CZ	2.39	0.52
1:I:76:ASP:C	1:I:78:GLN:H	2.12	0.52
1:A:207:ARG:C	1:A:209:VAL:H	2.12	0.52
1:B:210:GLN:HG2	1:I:129:PHE:HZ	1.75	0.52
1:G:209:VAL:CG1	1:G:211:LYS:HE2	2.39	0.52
1:C:206:MET:HG2	1:H:129:PHE:CB	2.39	0.52
1:H:129:PHE:HB2	1:H:168:ARG:NH2	2.24	0.52
1:C:85:THR:HB	1:C:86:PRO:HD3	1.90	0.52
1:D:221:MET:O	1:D:226:ARG:HB2	2.09	0.52
1:F:207:ARG:C	1:F:209:VAL:H	2.12	0.52
1:D:113:PHE:CD1	1:D:113:PHE:N	2.77	0.52
1:A:220:THR:HA	1:B:119:GLU:OE1	2.09	0.52
1:J:164:GLU:CD	1:J:168:ARG:HD2	2.30	0.52
2:S:43:ASN:H	2:S:43:ASN:ND2	2.06	0.52
2:S:2:PRO:HB2	2:S:82:HIS:CE1	2.44	0.52
2:M:49:VAL:CG1	2:M:51:ASP:H	2.23	0.52
1:E:210:GLN:HB3	1:J:210:GLN:HB3	1.91	0.52
1:B:202:MET:HG2	1:B:206:MET:CE	2.40	0.52
1:H:50:ARG:HB3	1:H:101:GLN:HB3	1.92	0.52
1:A:111:ALA:HB3	1:A:158:LYS:CG	2.39	0.52
1:C:205:VAL:O	1:C:210:GLN:HA	2.10	0.52
1:F:113:PHE:CD1	1:F:113:PHE:N	2.78	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:137:VAL:CG1	1:A:202:MET:HB3	2.41	0.51
1:G:209:VAL:CG1	1:G:210:GLN:H	2.12	0.51
1:C:72:SER:HB2	1:H:62:LEU:CD2	2.41	0.51
2:L:49:VAL:HG12	2:L:51:ASP:H	1.75	0.51
2:P:83:LYS:HG2	2:P:84:GLU:N	2.24	0.51
1:C:148:LEU:HD12	1:C:224:VAL:HG21	1.92	0.51
1:H:113:PHE:N	1:H:113:PHE:CD1	2.78	0.51
1:I:207:ARG:C	1:I:209:VAL:H	2.13	0.51
1:A:98:LYS:O	1:A:101:GLN:HG2	2.10	0.51
1:J:107:VAL:HG12	1:J:158:LYS:HG3	1.91	0.51
1:C:129:PHE:HB3	1:H:206:MET:SD	2.50	0.51
2:K:75:GLN:OE1	4:K:1009:PHE:N	2.43	0.51
2:O:38:ARG:HG3	2:O:44:PHE:O	2.11	0.51
1:F:84:LYS:NZ	1:F:84:LYS:HB3	2.25	0.51
1:A:210:GLN:HG2	1:J:129:PHE:HZ	1.74	0.51
1:B:206:MET:HG2	1:I:129:PHE:CG	2.45	0.51
1:C:129:PHE:CZ	1:H:210:GLN:HG2	2.46	0.51
2:M:2:PRO:HB2	2:M:82:HIS:CE1	2.45	0.51
2:Q:18:MET:CE	2:Q:46:GLU:HB2	2.36	0.51
1:C:150:ASN:O	1:C:151:LYS:HB2	2.10	0.51
2:N:2:PRO:HB2	2:N:82:HIS:CE1	2.45	0.51
1:B:111:ALA:HB3	1:B:158:LYS:CG	2.40	0.51
1:J:123:VAL:HG12	1:J:126:ILE:HD11	1.92	0.51
1:I:113:PHE:N	1:I:113:PHE:CD1	2.78	0.51
1:J:209:VAL:CG1	1:J:211:LYS:HE2	2.40	0.51
1:J:85:THR:HB	1:J:86:PRO:HD3	1.91	0.51
2:K:14:VAL:HG22	2:K:15:GLY:N	2.26	0.51
2:K:2:PRO:HB2	2:K:82:HIS:CE1	2.46	0.51
1:E:206:MET:HB3	1:F:168:ARG:NH2	2.24	0.51
1:A:148:LEU:HD12	1:A:224:VAL:CG2	2.40	0.51
1:B:65:ALA:O	1:B:68:SER:HB3	2.11	0.51
2:M:14:VAL:HG22	2:M:15:GLY:N	2.24	0.51
2:Q:83:LYS:HG2	2:Q:84:GLU:N	2.25	0.51
1:C:204:MET:CE	1:C:211:LYS:HD3	2.41	0.51
1:C:202:MET:HG2	1:C:206:MET:CE	2.41	0.51
1:F:107:VAL:HG12	1:F:158:LYS:HG3	1.93	0.51
2:O:18:MET:HE3	2:O:46:GLU:CB	2.38	0.51
1:E:209:VAL:HG23	1:J:209:VAL:HG23	1.93	0.51
1:J:65:ALA:O	1:J:69:ILE:HG13	2.10	0.51
1:D:210:GLN:HG2	1:G:129:PHE:CZ	2.47	0.50
1:F:209:VAL:HG11	1:F:211:LYS:HE2	1.93	0.50
1:E:170:LEU:HD12	1:F:75:GLU:HG3	1.92	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:L:2:PRO:HB2	2:L:82:HIS:CE1	2.46	0.50
2:K:83:LYS:HG2	2:K:84:GLU:N	2.26	0.50
1:B:164:GLU:CD	1:B:168:ARG:HD2	2.31	0.50
1:E:62:LEU:HD22	1:F:69:ILE:HG23	1.92	0.50
2:N:32:LEU:HD11	2:N:60:LEU:HD11	1.92	0.50
1:D:148:LEU:CD1	1:D:224:VAL:HG21	2.41	0.50
1:G:75:GLU:O	1:G:77:PRO:HD3	2.12	0.50
2:O:2:PRO:HB2	2:O:82:HIS:CE1	2.46	0.50
1:D:213:ASN:O	1:D:215:LYS:HE2	2.11	0.50
1:F:53:GLU:O	1:F:57:LEU:HG	2.11	0.50
2:M:83:LYS:HG2	2:M:84:GLU:N	2.26	0.50
1:D:206:MET:HB3	1:G:168:ARG:NH2	2.27	0.50
1:D:204:MET:HE3	1:D:211:LYS:HD3	1.93	0.50
1:D:237:THR:HA	1:D:240:ARG:CZ	2.41	0.50
1:J:113:PHE:CD1	1:J:113:PHE:N	2.78	0.50
1:B:210:GLN:HG2	1:I:129:PHE:CZ	2.46	0.50
1:J:236:LEU:O	1:J:240:ARG:HB2	2.12	0.50
1:E:113:PHE:N	1:E:113:PHE:CD1	2.80	0.50
2:Q:2:PRO:HB2	2:Q:82:HIS:CE1	2.47	0.50
1:H:204:MET:O	1:H:211:LYS:HB2	2.12	0.50
1:D:207:ARG:HH11	1:D:207:ARG:HG2	1.77	0.50
2:P:14:VAL:HG22	2:P:15:GLY:N	2.27	0.50
1:A:237:THR:HA	1:A:240:ARG:CZ	2.41	0.50
2:R:83:LYS:HG2	2:R:84:GLU:N	2.27	0.50
1:A:111:ALA:HB3	1:A:158:LYS:CD	2.42	0.49
1:E:226:ARG:HD2	1:E:227:GLU:OE2	2.11	0.49
1:F:205:VAL:CG1	1:F:212:MET:HB2	2.28	0.49
1:D:59:LEU:HB3	1:D:60:PRO:CD	2.31	0.49
1:J:107:VAL:HG22	1:J:161:ARG:CD	2.35	0.49
1:E:112:ILE:HG23	1:E:112:ILE:O	2.12	0.49
1:A:113:PHE:N	1:A:113:PHE:CD1	2.79	0.49
2:S:83:LYS:HG2	2:S:84:GLU:N	2.27	0.49
1:D:205:VAL:HG22	1:D:212:MET:CA	2.37	0.49
1:C:100:TYR:CZ	1:C:169:ARG:HB2	2.48	0.49
1:J:53:GLU:O	1:J:57:LEU:HG	2.13	0.49
1:C:129:PHE:HZ	1:H:210:GLN:HG2	1.78	0.49
1:H:153:VAL:HG12	1:H:154:LEU:N	2.27	0.49
2:O:18:MET:CE	2:O:46:GLU:HB2	2.40	0.49
1:E:237:THR:HA	1:E:240:ARG:CZ	2.42	0.49
1:B:50:ARG:HB3	1:B:101:GLN:HB3	1.93	0.49
1:D:210:GLN:HG2	1:G:129:PHE:HZ	1.77	0.49
2:R:2:PRO:HB2	2:R:82:HIS:CE1	2.47	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:S:73:VAL:HG13	2:S:73:VAL:O	2.12	0.49
1:A:66:TYR:CD2	1:A:69:ILE:HD12	2.48	0.49
1:B:153:VAL:HG12	1:B:154:LEU:N	2.28	0.49
2:T:14:VAL:HG22	2:T:15:GLY:N	2.27	0.49
1:J:150:ASN:O	1:J:151:LYS:HB2	2.13	0.49
1:E:75:GLU:HG3	1:F:170:LEU:HD12	1.95	0.49
2:N:49:VAL:HG12	2:N:51:ASP:H	1.76	0.49
1:D:226:ARG:HD2	1:D:227:GLU:OE2	2.13	0.49
1:E:164:GLU:CD	1:E:168:ARG:HD2	2.33	0.49
1:A:76:ASP:C	1:A:78:GLN:H	2.16	0.49
1:J:154:LEU:HB2	1:J:188:LEU:HD11	1.94	0.49
1:I:164:GLU:CD	1:I:168:ARG:HD2	2.32	0.49
1:B:221:MET:O	1:B:226:ARG:HB2	2.13	0.49
1:C:69:ILE:HG23	1:H:62:LEU:HD22	1.95	0.49
2:S:49:VAL:HG12	2:S:51:ASP:H	1.78	0.49
1:A:201:HIS:CD2	1:B:156:LEU:HD11	2.48	0.49
2:O:49:VAL:CG1	2:O:51:ASP:H	2.26	0.49
1:C:168:ARG:HH22	1:H:206:MET:HB3	1.78	0.48
1:A:98:LYS:HZ3	1:A:168:ARG:HD3	1.77	0.48
1:A:98:LYS:NZ	1:A:168:ARG:HD3	2.28	0.48
1:H:111:ALA:HB3	1:H:158:LYS:CG	2.43	0.48
1:I:116:ASP:OD1	1:I:151:LYS:HE3	2.13	0.48
1:J:237:THR:HA	1:J:240:ARG:CZ	2.44	0.48
2:T:2:PRO:HB2	2:T:82:HIS:CE1	2.48	0.48
1:B:168:ARG:NH2	1:I:206:MET:HB3	2.27	0.48
1:G:204:MET:O	1:G:211:LYS:HB2	2.13	0.48
1:J:116:ASP:OD1	1:J:151:LYS:HE3	2.13	0.48
1:F:232:ARG:HD3	1:G:234:GLU:OE2	2.12	0.48
1:C:113:PHE:N	1:C:113:PHE:CD1	2.80	0.48
2:T:83:LYS:HG2	2:T:84:GLU:N	2.29	0.48
1:H:204:MET:CE	1:H:211:LYS:HD3	2.40	0.48
1:C:107:VAL:HG12	1:C:158:LYS:HG3	1.93	0.48
2:R:49:VAL:HG12	2:R:51:ASP:H	1.78	0.48
2:L:83:LYS:HG2	2:L:84:GLU:N	2.28	0.48
1:I:180:ILE:O	1:I:184:ILE:HG13	2.14	0.48
1:A:209:VAL:CG1	1:A:211:LYS:HE2	2.44	0.48
1:B:129:PHE:CB	1:I:206:MET:HG2	2.44	0.48
1:F:148:LEU:CD1	1:F:224:VAL:HG21	2.42	0.48
1:D:69:ILE:HG23	1:G:62:LEU:HD22	1.94	0.48
1:I:53:GLU:O	1:I:57:LEU:HG	2.13	0.48
1:F:50:ARG:HB3	1:F:101:GLN:HB3	1.94	0.48
2:T:18:MET:HE1	2:T:46:GLU:CB	2.42	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:69:ILE:HG23	1:G:62:LEU:CD2	2.44	0.48
1:G:71:ARG:HG3	1:G:77:PRO:HG2	1.94	0.48
1:H:236:LEU:O	1:H:240:ARG:HB2	2.13	0.48
2:Q:49:VAL:CG1	2:Q:51:ASP:H	2.27	0.48
1:G:53:GLU:O	1:G:57:LEU:HG	2.14	0.48
1:D:107:VAL:HG12	1:D:158:LYS:HG3	1.96	0.48
1:F:111:ALA:HB3	1:F:158:LYS:CG	2.44	0.48
1:I:70:LEU:HD23	1:I:77:PRO:HB3	1.96	0.48
1:D:209:VAL:CG1	1:D:210:GLN:H	2.10	0.48
1:C:62:LEU:CD2	1:H:69:ILE:HG23	2.44	0.48
2:Q:14:VAL:HG22	2:Q:15:GLY:N	2.29	0.48
1:D:164:GLU:CD	1:D:168:ARG:HD2	2.34	0.48
1:D:72:SER:HB2	1:G:62:LEU:HD21	1.95	0.48
2:L:38:ARG:HG3	2:L:44:PHE:O	2.13	0.48
1:I:207:ARG:HG2	1:I:207:ARG:HH11	1.78	0.48
1:D:153:VAL:HG12	1:D:154:LEU:N	2.28	0.48
1:H:154:LEU:HD23	1:H:155:GLY:H	1.78	0.47
1:D:50:ARG:HB3	1:D:101:GLN:HB3	1.96	0.47
1:C:79:ARG:HB3	1:C:79:ARG:NH1	2.29	0.47
1:E:73:LEU:HD11	1:F:93:MET:HG3	1.96	0.47
1:B:209:VAL:CG1	1:B:210:GLN:H	2.16	0.47
1:B:209:VAL:HG23	1:H:209:VAL:HG23	1.96	0.47
1:D:111:ALA:HB3	1:D:158:LYS:CG	2.44	0.47
1:I:107:VAL:HG12	1:I:158:LYS:HG3	1.96	0.47
1:G:107:VAL:CG1	1:G:158:LYS:HG3	2.44	0.47
1:H:76:ASP:O	1:H:78:GLN:N	2.47	0.47
1:A:206:MET:HB3	1:J:168:ARG:HH22	1.79	0.47
1:G:207:ARG:O	1:G:209:VAL:N	2.42	0.47
1:E:62:LEU:CD2	1:F:69:ILE:HG23	2.44	0.47
1:D:66:TYR:CD2	1:D:69:ILE:HD12	2.49	0.47
1:F:135:HIS:O	1:F:136:LEU:HB2	2.14	0.47
1:E:204:MET:O	1:E:211:LYS:HB2	2.13	0.47
1:C:161:ARG:O	1:C:165:ILE:HG13	2.14	0.47
1:B:107:VAL:CG1	1:B:158:LYS:HG3	2.44	0.47
1:I:123:VAL:HG12	1:I:126:ILE:HD11	1.97	0.47
1:B:70:LEU:HB3	1:B:77:PRO:HG3	1.96	0.47
1:B:123:VAL:HG12	1:B:126:ILE:HD11	1.97	0.47
1:A:129:PHE:HB3	1:J:206:MET:HG2	1.96	0.47
1:C:206:MET:HG2	1:H:129:PHE:HB3	1.96	0.47
1:D:207:ARG:O	1:D:209:VAL:N	2.43	0.47
1:E:107:VAL:HG12	1:E:158:LYS:HG3	1.95	0.47
1:A:133:GLU:HG3	1:A:134:HIS:CD2	2.50	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:Q:73:VAL:HG13	2:Q:73:VAL:O	2.15	0.47
1:H:209:VAL:HG11	1:H:211:LYS:HE2	1.97	0.47
1:E:69:ILE:HG23	1:F:62:LEU:CD2	2.45	0.47
1:F:71:ARG:HG3	1:F:77:PRO:HG2	1.96	0.47
1:I:76:ASP:O	1:I:78:GLN:N	2.48	0.47
1:E:206:MET:SD	1:F:129:PHE:HB3	2.54	0.47
1:J:207:ARG:O	1:J:209:VAL:N	2.42	0.47
1:C:209:VAL:HG11	1:C:211:LYS:HE2	1.97	0.47
1:G:111:ALA:CB	1:G:158:LYS:HE3	2.45	0.47
1:B:62:LEU:HD22	1:I:69:ILE:HG23	1.96	0.47
1:B:75:GLU:O	1:B:77:PRO:HD3	2.15	0.47
2:L:18:MET:CE	2:L:46:GLU:HB2	2.42	0.47
1:A:154:LEU:HB2	1:A:188:LEU:HD11	1.97	0.47
2:O:73:VAL:HG13	2:O:73:VAL:O	2.15	0.47
1:J:204:MET:O	1:J:211:LYS:HB2	2.15	0.46
1:I:107:VAL:HG22	1:I:161:ARG:CD	2.40	0.46
1:I:123:VAL:CG1	1:I:126:ILE:HD11	2.45	0.46
1:G:76:ASP:C	1:G:78:GLN:H	2.18	0.46
1:A:206:MET:SD	1:J:129:PHE:HB3	2.56	0.46
1:D:73:LEU:HD11	1:G:93:MET:HG3	1.96	0.46
1:G:85:THR:HB	1:G:86:PRO:HD3	1.96	0.46
1:C:129:PHE:HB2	1:C:168:ARG:NH2	2.29	0.46
1:B:79:ARG:HB3	1:B:79:ARG:NH1	2.26	0.46
1:C:75:GLU:O	1:C:77:PRO:HD3	2.15	0.46
1:F:76:ASP:C	1:F:78:GLN:H	2.19	0.46
2:P:9:GLN:O	2:P:11:ARG:N	2.44	0.46
1:J:209:VAL:HG11	1:J:211:LYS:HE2	1.98	0.46
1:F:150:ASN:HA	1:F:150:ASN:HD22	1.56	0.46
1:A:76:ASP:O	1:A:78:GLN:N	2.49	0.46
1:I:202:MET:HG2	1:I:206:MET:HE1	1.97	0.46
2:L:58:ASP:OD1	2:M:2:PRO:HD2	2.15	0.46
1:E:153:VAL:HG12	1:E:154:LEU:N	2.30	0.46
1:G:113:PHE:N	1:G:113:PHE:CD1	2.84	0.46
2:S:18:MET:CE	2:S:46:GLU:HB2	2.39	0.46
1:E:65:ALA:O	1:E:68:SER:HB3	2.16	0.46
1:I:120:MET:CE	1:I:231:THR:HG23	2.46	0.46
1:B:206:MET:HG2	1:I:129:PHE:CD2	2.50	0.46
1:B:206:MET:HG2	1:I:129:PHE:HB3	1.98	0.46
1:E:209:VAL:HG12	1:E:211:LYS:HE2	1.97	0.46
2:M:38:ARG:HG3	2:M:44:PHE:O	2.15	0.46
1:G:138:PRO:O	1:G:202:MET:HG3	2.15	0.46
2:K:32:LEU:HD11	2:K:60:LEU:HD11	1.98	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:107:VAL:CG1	1:D:158:LYS:HG3	2.46	0.46
1:D:75:GLU:O	1:D:77:PRO:HD3	2.16	0.46
1:D:93:MET:HG3	1:G:73:LEU:HD11	1.97	0.46
1:G:209:VAL:HG11	1:G:211:LYS:HE2	1.98	0.46
2:P:58:ASP:OD1	2:Q:2:PRO:HD2	2.16	0.46
2:N:73:VAL:HG13	2:N:73:VAL:O	2.16	0.46
2:L:14:VAL:HG22	2:L:15:GLY:N	2.31	0.46
1:D:164:GLU:HG3	1:D:168:ARG:HG3	1.97	0.45
1:A:133:GLU:HG2	1:A:172:VAL:HG23	1.98	0.45
1:B:129:PHE:HB3	1:I:206:MET:HG2	1.98	0.45
1:H:202:MET:HG2	1:H:206:MET:HE3	1.98	0.45
1:H:207:ARG:HG2	1:H:207:ARG:HH11	1.81	0.45
1:D:168:ARG:HH22	1:G:206:MET:HB3	1.79	0.45
1:D:204:MET:CE	1:D:211:LYS:HD3	2.45	0.45
1:H:128:MET:HG2	1:H:143:VAL:CG2	2.47	0.45
2:T:49:VAL:HG13	2:T:51:ASP:H	1.81	0.45
1:I:175:ARG:O	1:I:179:GLN:HG3	2.17	0.45
1:B:205:VAL:HG22	1:B:212:MET:CA	2.40	0.45
1:G:164:GLU:CD	1:G:168:ARG:HD2	2.36	0.45
1:G:188:LEU:O	1:G:189:GLN:C	2.54	0.45
2:T:18:MET:CE	2:T:46:GLU:HB2	2.45	0.45
2:P:49:VAL:HG13	2:P:51:ASP:H	1.81	0.45
1:C:188:LEU:O	1:C:189:GLN:C	2.54	0.45
2:O:49:VAL:HG13	2:O:51:ASP:H	1.81	0.45
1:B:131:MET:HE1	1:B:136:LEU:O	2.16	0.45
1:A:205:VAL:CG1	1:A:212:MET:HB2	2.31	0.45
1:J:205:VAL:O	1:J:210:GLN:HA	2.16	0.45
1:B:148:LEU:CD1	1:B:224:VAL:HG21	2.43	0.45
1:D:70:LEU:HD21	1:D:82:LEU:HG	1.97	0.45
1:H:76:ASP:C	1:H:78:GLN:N	2.70	0.45
1:I:209:VAL:CG1	1:I:211:LYS:HE2	2.45	0.45
1:F:111:ALA:HB3	1:F:158:LYS:HD3	1.99	0.45
1:D:79:ARG:HB3	1:D:79:ARG:NH1	2.31	0.45
2:K:9:GLN:O	2:K:11:ARG:N	2.46	0.45
1:J:148:LEU:HD12	1:J:224:VAL:HG21	1.97	0.45
2:M:18:MET:HE2	2:M:46:GLU:CD	2.37	0.45
1:D:72:SER:HB2	1:G:62:LEU:CD2	2.47	0.45
1:G:154:LEU:HB2	1:G:188:LEU:HD11	1.97	0.45
2:P:38:ARG:HG3	2:P:44:PHE:O	2.17	0.45
2:T:32:LEU:HD11	2:T:60:LEU:HD11	1.98	0.45
2:T:9:GLN:O	2:T:11:ARG:N	2.47	0.45
1:B:53:GLU:O	1:B:57:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:168:ARG:NH2	1:H:206:MET:HB3	2.32	0.45
1:A:168:ARG:HH22	1:J:206:MET:HB3	1.81	0.45
2:P:49:VAL:HG12	2:P:51:ASP:H	1.81	0.45
1:B:69:ILE:HG23	1:I:62:LEU:HD22	1.99	0.45
2:M:32:LEU:HD11	2:M:60:LEU:HD11	1.98	0.45
1:F:234:GLU:OE2	1:J:232:ARG:HD3	2.15	0.45
2:Q:54:ARG:NH1	2:R:21:ASP:OD1	2.50	0.45
1:H:137:VAL:CG1	1:H:202:MET:HB3	2.47	0.45
1:C:209:VAL:HG23	1:G:209:VAL:HG23	1.98	0.45
1:D:129:PHE:HZ	1:G:210:GLN:HG2	1.82	0.45
1:D:209:VAL:HG12	1:D:211:LYS:HE2	1.97	0.45
1:E:69:ILE:HG23	1:F:62:LEU:HD22	1.98	0.45
2:R:32:LEU:HD11	2:R:60:LEU:HD11	1.98	0.45
1:E:207:ARG:O	1:E:209:VAL:N	2.44	0.45
1:F:204:MET:O	1:F:211:LYS:HB2	2.17	0.45
2:T:43:ASN:ND2	2:T:43:ASN:N	2.63	0.45
2:P:43:ASN:N	2:P:43:ASN:ND2	2.64	0.45
1:I:79:ARG:HB3	1:I:79:ARG:NH1	2.32	0.45
1:C:153:VAL:CG1	1:C:154:LEU:N	2.80	0.45
2:P:65:PHE:CE2	2:P:83:LYS:HB2	2.51	0.45
1:H:71:ARG:HG3	1:H:77:PRO:HG2	1.99	0.44
1:A:70:LEU:HD21	1:A:82:LEU:HG	1.99	0.44
1:C:78:GLN:O	1:C:79:ARG:C	2.55	0.44
2:K:2:PRO:HD2	2:O:58:ASP:OD1	2.16	0.44
2:N:83:LYS:HG2	2:N:84:GLU:N	2.31	0.44
2:N:14:VAL:HG22	2:N:15:GLY:N	2.33	0.44
2:P:43:ASN:ND2	2:P:44:PHE:HD2	2.15	0.44
1:A:153:VAL:HG12	1:A:154:LEU:N	2.32	0.44
2:R:9:GLN:O	2:R:11:ARG:N	2.47	0.44
2:S:32:LEU:HD11	2:S:60:LEU:HD11	1.99	0.44
1:H:112:ILE:O	1:H:112:ILE:HG23	2.17	0.44
1:F:59:LEU:HB3	1:F:60:PRO:CD	2.40	0.44
1:G:111:ALA:HB3	1:G:158:LYS:CG	2.46	0.44
1:G:154:LEU:HD21	1:G:158:LYS:HB3	1.99	0.44
1:C:111:ALA:HB3	1:C:158:LYS:HD3	2.00	0.44
2:R:18:MET:CE	2:R:46:GLU:HB2	2.44	0.44
2:N:43:ASN:ND2	2:N:43:ASN:N	2.64	0.44
1:F:79:ARG:NH1	1:F:79:ARG:HB3	2.29	0.44
1:H:79:ARG:HB3	1:H:79:ARG:NH1	2.30	0.44
1:E:75:GLU:O	1:E:77:PRO:HD3	2.17	0.44
2:O:14:VAL:HG22	2:O:15:GLY:N	2.32	0.44
1:C:210:GLN:HG2	1:H:129:PHE:HZ	1.82	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:111:ALA:HB3	1:H:158:LYS:HD3	2.00	0.44
1:F:237:THR:HA	1:F:240:ARG:CZ	2.47	0.44
1:D:85:THR:HB	1:D:86:PRO:HD3	1.99	0.44
1:E:168:ARG:NH2	1:F:206:MET:HB3	2.31	0.44
2:P:18:MET:HE1	2:P:46:GLU:CG	2.48	0.44
1:G:236:LEU:O	1:G:240:ARG:HB2	2.18	0.44
1:B:129:PHE:CG	1:I:206:MET:HG2	2.53	0.44
1:F:164:GLU:CD	1:F:168:ARG:HD2	2.38	0.44
1:C:207:ARG:O	1:C:209:VAL:N	2.41	0.44
2:O:18:MET:HE3	2:O:46:GLU:CG	2.48	0.44
1:J:148:LEU:CD1	1:J:224:VAL:HG21	2.48	0.44
1:E:76:ASP:C	1:E:78:GLN:H	2.21	0.44
1:E:85:THR:HB	1:E:86:PRO:HD3	2.00	0.44
1:B:129:PHE:HB3	1:I:206:MET:SD	2.58	0.44
1:E:207:ARG:HH11	1:E:207:ARG:HG2	1.83	0.44
1:G:50:ARG:HB3	1:G:101:GLN:HB3	1.99	0.44
1:F:217:VAL:HB	1:G:122:ILE:HB	2.00	0.44
1:B:76:ASP:C	1:B:78:GLN:H	2.21	0.44
2:N:43:ASN:ND2	2:N:44:PHE:HD2	2.16	0.43
2:S:14:VAL:HG22	2:S:15:GLY:N	2.33	0.43
2:Q:32:LEU:HD11	2:Q:60:LEU:HD11	2.00	0.43
1:G:209:VAL:HG13	1:G:211:LYS:HG3	2.01	0.43
1:E:50:ARG:HB3	1:E:101:GLN:HB3	2.00	0.43
2:Q:49:VAL:HG13	2:Q:51:ASP:H	1.83	0.43
2:N:38:ARG:HG3	2:N:44:PHE:O	2.19	0.43
1:C:76:ASP:O	1:C:78:GLN:N	2.51	0.43
1:G:70:LEU:HD21	1:G:82:LEU:HG	2.00	0.43
1:E:236:LEU:O	1:E:240:ARG:HB2	2.17	0.43
1:B:207:ARG:O	1:B:209:VAL:N	2.40	0.43
1:F:161:ARG:O	1:F:165:ILE:HG13	2.18	0.43
1:B:154:LEU:HD23	1:B:155:GLY:H	1.82	0.43
1:I:182:VAL:O	1:I:186:GLU:HG3	2.18	0.43
2:Q:38:ARG:HG3	2:Q:44:PHE:O	2.18	0.43
1:D:206:MET:HG2	1:G:129:PHE:CG	2.53	0.43
1:G:182:VAL:O	1:G:186:GLU:HG3	2.18	0.43
1:H:75:GLU:O	1:H:77:PRO:HD3	2.18	0.43
1:B:150:ASN:HD22	1:B:150:ASN:HA	1.60	0.43
2:K:18:MET:HG3	5:K:2011:HOH:O	2.18	0.43
2:T:38:ARG:HG3	2:T:44:PHE:O	2.19	0.43
1:H:53:GLU:O	1:H:57:LEU:HG	2.19	0.43
1:E:129:PHE:HB3	1:F:206:MET:HG2	2.00	0.43
1:F:207:ARG:HG2	1:F:207:ARG:NH1	2.34	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:107:VAL:CG1	1:F:158:LYS:HG3	2.49	0.43
1:A:112:ILE:O	1:A:112:ILE:HG23	2.18	0.43
1:E:188:LEU:O	1:E:189:GLN:C	2.56	0.43
1:A:210:GLN:HB3	1:I:210:GLN:CB	2.20	0.43
1:B:207:ARG:C	1:B:209:VAL:N	2.72	0.43
1:A:107:VAL:HG12	1:A:158:LYS:HG3	2.01	0.43
1:C:221:MET:O	1:C:226:ARG:HB2	2.19	0.43
1:E:129:PHE:CB	1:F:206:MET:HG2	2.49	0.43
2:P:24:SER:OG	2:T:54:ARG:NH1	2.49	0.43
1:I:112:ILE:HD11	1:I:152:GLN:CD	2.39	0.43
1:A:209:VAL:HG22	1:I:210:GLN:HB2	2.01	0.42
1:I:204:MET:O	1:I:211:LYS:HB2	2.18	0.42
1:B:207:ARG:HG2	1:B:207:ARG:NH1	2.34	0.42
1:I:129:PHE:HB2	1:I:168:ARG:NH2	2.34	0.42
1:J:209:VAL:HG13	1:J:211:LYS:HG3	2.00	0.42
1:C:237:THR:HA	1:C:240:ARG:CZ	2.49	0.42
1:B:206:MET:HG2	1:I:129:PHE:CB	2.49	0.42
1:G:207:ARG:C	1:G:209:VAL:N	2.73	0.42
1:A:75:GLU:HG3	1:J:170:LEU:HD12	2.00	0.42
1:H:65:ALA:O	1:H:69:ILE:HG13	2.19	0.42
1:A:188:LEU:O	1:A:189:GLN:C	2.58	0.42
1:F:217:VAL:HG11	1:G:238:LEU:HG	2.01	0.42
1:E:204:MET:CE	1:E:211:LYS:HD3	2.46	0.42
1:D:202:MET:HG2	1:D:206:MET:HE2	2.01	0.42
1:E:129:PHE:CG	1:F:206:MET:HG2	2.54	0.42
1:D:111:ALA:CB	1:D:158:LYS:HE3	2.49	0.42
2:N:18:MET:HE3	2:N:46:GLU:CB	2.46	0.42
1:C:62:LEU:HD22	1:H:69:ILE:HG23	1.99	0.42
1:B:72:SER:HB2	1:I:62:LEU:HD21	2.01	0.42
2:K:18:MET:HE3	2:K:46:GLU:CG	2.50	0.42
1:C:154:LEU:HB2	1:C:188:LEU:HD11	2.02	0.42
2:L:73:VAL:O	2:L:73:VAL:HG13	2.19	0.42
1:E:202:MET:HG2	1:E:206:MET:HE3	2.00	0.42
1:F:98:LYS:NZ	1:F:168:ARG:HD3	2.35	0.42
1:J:107:VAL:CG1	1:J:158:LYS:HG3	2.50	0.42
1:E:150:ASN:HA	1:E:150:ASN:HD22	1.62	0.42
2:T:73:VAL:O	2:T:73:VAL:HG13	2.18	0.42
1:B:211:LYS:HE3	1:C:160:ALA:HB1	2.02	0.42
1:A:129:PHE:CG	1:J:206:MET:HG2	2.55	0.42
1:A:107:VAL:HG22	1:A:161:ARG:CD	2.44	0.42
1:H:66:TYR:CD2	1:H:69:ILE:HD12	2.54	0.42
1:D:112:ILE:HG23	1:D:112:ILE:O	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:K:73:VAL:O	2:K:73:VAL:HG13	2.20	0.42
1:B:69:ILE:HG23	1:I:62:LEU:CD2	2.49	0.42
1:G:137:VAL:CG1	1:G:202:MET:HB2	2.50	0.42
1:E:63:ALA:O	1:E:86:PRO:HB3	2.19	0.42
1:F:82:LEU:HD12	1:F:82:LEU:HA	1.84	0.42
1:C:111:ALA:HB3	1:C:158:LYS:CG	2.49	0.42
1:A:79:ARG:HB3	1:A:79:ARG:NH1	2.34	0.42
1:B:82:LEU:O	1:B:85:THR:HB	2.20	0.42
1:E:53:GLU:O	1:E:57:LEU:HG	2.19	0.42
1:A:158:LYS:O	1:A:162:ILE:HG13	2.20	0.42
1:G:79:ARG:HB3	1:G:79:ARG:NH1	2.35	0.42
1:B:82:LEU:HD12	1:B:82:LEU:HA	1.86	0.42
2:M:49:VAL:HG13	2:M:51:ASP:H	1.85	0.42
1:D:76:ASP:C	1:D:78:GLN:H	2.23	0.42
2:L:1:MET:N	5:L:2009:HOH:O	2.49	0.42
1:D:172:VAL:CG1	1:D:174:GLU:OE1	2.68	0.42
1:D:168:ARG:NH2	1:G:206:MET:HB3	2.35	0.42
1:B:154:LEU:HD21	1:B:158:LYS:HB3	2.02	0.42
2:O:83:LYS:HG2	2:O:84:GLU:H	1.85	0.42
1:B:135:HIS:O	1:B:136:LEU:HB2	2.20	0.42
1:G:180:ILE:O	1:G:184:ILE:HG13	2.20	0.42
1:G:215:LYS:HB2	1:G:215:LYS:HE2	1.78	0.42
1:H:120:MET:CE	1:H:231:THR:HG23	2.50	0.42
1:A:208:GLY:O	1:A:209:VAL:HB	2.20	0.42
1:C:98:LYS:HZ3	1:C:168:ARG:HD3	1.85	0.42
1:B:148:LEU:HD23	1:B:148:LEU:HA	1.92	0.42
1:C:228:ASP:HA	1:C:229:PRO:HD2	1.96	0.42
1:F:120:MET:CE	1:F:231:THR:HG23	2.49	0.42
2:P:54:ARG:HH22	2:Q:23:HIS:C	2.22	0.42
1:H:207:ARG:O	1:H:209:VAL:N	2.49	0.41
1:E:202:MET:HG2	1:E:206:MET:HE2	2.02	0.41
1:D:129:PHE:CZ	1:G:210:GLN:HG2	2.55	0.41
1:G:164:GLU:HG3	1:G:168:ARG:HG3	2.01	0.41
1:I:107:VAL:CG1	1:I:158:LYS:HG3	2.50	0.41
1:A:176:LEU:O	1:A:180:ILE:HG13	2.21	0.41
1:E:120:MET:CE	1:E:231:THR:HG23	2.50	0.41
1:H:204:MET:HG2	1:H:211:LYS:HB2	2.01	0.41
1:I:98:LYS:HZ3	1:I:168:ARG:HD3	1.85	0.41
1:D:129:PHE:CB	1:G:206:MET:HG2	2.50	0.41
2:Q:18:MET:HE3	2:Q:46:GLU:CG	2.50	0.41
2:O:18:MET:HE1	2:O:46:GLU:CD	2.40	0.41
1:A:228:ASP:HA	1:A:229:PRO:HD2	1.92	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:164:GLU:HG3	1:J:168:ARG:HG3	2.02	0.41
1:F:111:ALA:CB	1:F:158:LYS:HE3	2.50	0.41
1:B:153:VAL:CG1	1:B:154:LEU:N	2.82	0.41
1:E:79:ARG:NH2	1:E:82:LEU:HD13	2.35	0.41
1:A:133:GLU:CD	1:A:175:ARG:HH22	2.23	0.41
1:C:226:ARG:HD2	1:C:227:GLU:OE2	2.20	0.41
1:J:76:ASP:C	1:J:78:GLN:H	2.23	0.41
1:F:142:ARG:HG2	1:F:142:ARG:HH11	1.84	0.41
1:D:189:GLN:N	1:D:190:PRO:HD3	2.36	0.41
2:P:18:MET:HE1	2:P:46:GLU:CB	2.45	0.41
1:I:128:MET:HG2	1:I:143:VAL:HG23	2.02	0.41
1:H:111:ALA:CB	1:H:158:LYS:HE3	2.50	0.41
1:C:135:HIS:O	1:C:136:LEU:HB2	2.20	0.41
1:B:177:THR:OG1	1:B:197:ILE:HD12	2.21	0.41
1:J:104:ILE:HG12	1:J:104:ILE:O	2.21	0.41
1:G:112:ILE:HD11	1:G:152:GLN:CD	2.41	0.41
1:E:129:PHE:HB3	1:F:206:MET:SD	2.61	0.41
1:H:154:LEU:HD21	1:H:158:LYS:HB3	2.02	0.41
2:N:18:MET:HE1	2:N:46:GLU:CD	2.40	0.41
1:J:79:ARG:CB	1:J:79:ARG:NH1	2.83	0.41
1:A:128:MET:HG2	1:A:143:VAL:HG23	2.02	0.41
1:E:236:LEU:HA	1:E:236:LEU:HD23	1.89	0.41
1:A:129:PHE:CB	1:J:206:MET:HG2	2.50	0.41
1:H:154:LEU:HB2	1:H:188:LEU:HD11	2.01	0.41
1:H:154:LEU:HD23	1:H:155:GLY:N	2.36	0.41
1:F:107:VAL:HG22	1:F:161:ARG:CD	2.40	0.41
1:C:66:TYR:CD2	1:C:69:ILE:HD12	2.56	0.41
2:K:58:ASP:OD1	2:L:2:PRO:HD2	2.21	0.41
2:K:60:LEU:HA	2:K:60:LEU:HD12	1.90	0.41
2:K:36:LYS:HD2	2:K:47:TYR:CZ	2.56	0.41
2:N:54:ARG:NH1	2:O:24:SER:OG	2.53	0.41
2:P:2:PRO:HD2	2:T:58:ASP:OD1	2.20	0.41
1:D:115:GLU:O	1:D:116:ASP:C	2.57	0.41
1:E:175:ARG:O	1:E:179:GLN:HG3	2.20	0.41
1:H:228:ASP:HA	1:H:229:PRO:HD2	1.90	0.41
1:E:207:ARG:C	1:E:209:VAL:N	2.74	0.41
1:C:207:ARG:C	1:C:209:VAL:N	2.73	0.41
1:F:204:MET:CE	1:F:211:LYS:HD3	2.48	0.41
2:K:43:ASN:ND2	2:K:44:PHE:HD2	2.19	0.41
1:I:63:ALA:O	1:I:86:PRO:HB3	2.21	0.41
1:B:237:THR:HA	1:B:240:ARG:CZ	2.51	0.41
1:D:66:TYR:HD2	1:D:69:ILE:HD12	1.86	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:82:LEU:HA	1:D:82:LEU:HD12	1.89	0.41
2:K:49:VAL:HG13	2:K:51:ASP:H	1.84	0.41
2:L:65:PHE:CE2	2:L:83:LYS:HB2	2.56	0.41
1:D:153:VAL:CG1	1:D:154:LEU:N	2.84	0.41
1:D:189:GLN:N	1:D:190:PRO:CD	2.84	0.41
1:G:112:ILE:O	1:G:112:ILE:HG23	2.21	0.41
1:F:128:MET:HG2	1:F:143:VAL:CG2	2.51	0.41
1:J:189:GLN:N	1:J:190:PRO:CD	2.84	0.41
1:F:140:VAL:HG12	1:F:141:GLY:N	2.36	0.41
1:C:232:ARG:HD3	1:D:234:GLU:OE2	2.21	0.41
1:H:215:LYS:HB2	1:H:215:LYS:HE2	1.87	0.41
1:H:85:THR:HB	1:H:86:PRO:HD3	2.03	0.41
1:I:185:THR:OG1	1:I:193:VAL:HG11	2.21	0.41
1:A:209:VAL:HG11	1:A:211:LYS:HE2	2.03	0.41
1:D:206:MET:HG2	1:G:129:PHE:CB	2.50	0.41
2:S:43:ASN:ND2	2:S:43:ASN:N	2.67	0.41
1:F:188:LEU:O	1:F:189:GLN:C	2.59	0.41
1:F:209:VAL:HG13	1:F:211:LYS:HG3	2.02	0.40
1:H:148:LEU:CD1	1:H:224:VAL:HG21	2.47	0.40
1:C:123:VAL:HG21	1:C:159:LEU:CD2	2.51	0.40
1:A:79:ARG:O	1:A:83:LEU:HG	2.21	0.40
1:B:75:GLU:HG3	1:I:170:LEU:HD12	2.02	0.40
1:J:164:GLU:O	1:J:168:ARG:HG3	2.21	0.40
1:E:71:ARG:HG3	1:E:77:PRO:HG2	2.02	0.40
1:J:63:ALA:O	1:J:86:PRO:HB3	2.21	0.40
1:A:236:LEU:O	1:A:240:ARG:HB2	2.21	0.40
2:R:65:PHE:CE2	2:R:83:LYS:HB2	2.56	0.40
1:A:62:LEU:HD21	1:J:72:SER:HB2	2.04	0.40
1:J:132:CYS:SG	1:J:134:HIS:HB2	2.61	0.40
1:E:215:LYS:HB2	1:E:215:LYS:HE2	1.90	0.40
1:G:208:GLY:O	1:G:209:VAL:HB	2.21	0.40
1:E:164:GLU:HG3	1:E:168:ARG:HG3	2.04	0.40
1:J:123:VAL:CG1	1:J:126:ILE:HD11	2.52	0.40
1:I:112:ILE:HD11	1:I:152:GLN:NE2	2.35	0.40
1:F:182:VAL:O	1:F:186:GLU:HG3	2.21	0.40
2:R:73:VAL:O	2:R:73:VAL:HG13	2.22	0.40
1:B:202:MET:HG2	1:B:206:MET:HE3	2.01	0.40
1:E:107:VAL:CG1	1:E:158:LYS:HG3	2.52	0.40
1:C:78:GLN:NE2	5:C:246:HOH:O	2.54	0.40
1:I:76:ASP:C	1:I:78:GLN:N	2.74	0.40
2:M:14:VAL:CG2	2:M:15:GLY:N	2.84	0.40
1:C:217:VAL:HB	1:D:122:ILE:HB	2.02	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:153:VAL:HG12	1:I:154:LEU:N	2.37	0.40
2:L:75:GLN:OE1	4:L:1010:PHE:N	2.53	0.40
1:J:238:LEU:HD12	1:J:238:LEU:HA	1.90	0.40
1:E:209:VAL:CG2	1:J:209:VAL:HG23	2.51	0.40
1:D:206:MET:SD	1:G:129:PHE:HB3	2.61	0.40
1:D:148:LEU:HD12	1:D:224:VAL:CG2	2.50	0.40
1:I:71:ARG:HG3	1:I:77:PRO:HG3	2.02	0.40
1:A:189:GLN:N	1:A:190:PRO:CD	2.85	0.40
1:I:222:LEU:HB3	2:T:41:GLY:HA3	2.04	0.40
1:J:182:VAL:O	1:J:186:GLU:HG3	2.21	0.40

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

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:Q:30:GLN:NE2	2:T:45:TYR:OH[2_556]	2.01	0.19

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	192/230 (84%)	171 (89%)	17 (9%)	4 (2%)	11	33
1	B	192/230 (84%)	168 (88%)	21 (11%)	3 (2%)	14	44
1	C	192/230 (84%)	169 (88%)	19 (10%)	4 (2%)	11	33
1	D	192/230 (84%)	171 (89%)	18 (9%)	3 (2%)	14	44
1	E	192/230 (84%)	169 (88%)	20 (10%)	3 (2%)	14	44
1	F	192/230 (84%)	169 (88%)	19 (10%)	4 (2%)	11	33
1	G	192/230 (84%)	168 (88%)	21 (11%)	3 (2%)	14	44
1	H	192/230 (84%)	172 (90%)	15 (8%)	5 (3%)	8	26
1	I	192/230 (84%)	169 (88%)	19 (10%)	4 (2%)	11	33
1	J	192/230 (84%)	169 (88%)	20 (10%)	3 (2%)	14	44
2	K	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	19	54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	19	54
2	M	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	19	54
2	N	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	19	54
2	O	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	19	54
2	P	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	19	54
2	Q	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
2	R	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
2	S	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	19	54
2	T	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
All	All	2740/3140 (87%)	2475 (90%)	222 (8%)	43 (2%)	14	44

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	LEU
1	A	209	VAL
1	B	108	LEU
1	B	209	VAL
1	C	108	LEU
1	C	209	VAL
1	D	108	LEU
1	D	209	VAL
1	E	108	LEU
1	E	209	VAL
1	F	108	LEU
1	F	209	VAL
1	G	108	LEU
1	G	209	VAL
1	H	108	LEU
1	H	209	VAL
1	I	108	LEU
1	I	209	VAL
1	J	108	LEU
1	J	209	VAL
1	B	210	GLN
1	C	79	ARG
1	E	210	GLN
1	F	210	GLN
1	H	210	GLN

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Mol	Chain	Res	Type
1	I	210	GLN
1	A	210	GLN
1	D	210	GLN
1	G	210	GLN
1	I	77	PRO
2	O	83	LYS
1	C	77	PRO
2	L	83	LYS
2	N	83	LYS
2	P	83	LYS
1	A	77	PRO
1	H	110	ASP
1	J	210	GLN
2	K	83	LYS
2	M	83	LYS
2	S	83	LYS
1	H	77	PRO
1	F	77	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	170/196 (87%)	160 (94%)	10 (6%)	28	62
1	B	170/196 (87%)	160 (94%)	10 (6%)	28	62
1	C	170/196 (87%)	159 (94%)	11 (6%)	24	57
1	D	170/196 (87%)	159 (94%)	11 (6%)	24	57
1	E	170/196 (87%)	161 (95%)	9 (5%)	32	67
1	F	170/196 (87%)	160 (94%)	10 (6%)	28	62
1	G	170/196 (87%)	160 (94%)	10 (6%)	28	62
1	H	170/196 (87%)	159 (94%)	11 (6%)	24	57
1	I	170/196 (87%)	160 (94%)	10 (6%)	28	62
1	J	170/196 (87%)	161 (95%)	9 (5%)	32	67
2	K	76/76 (100%)	72 (95%)	4 (5%)	32	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	76/76 (100%)	72 (95%)	4 (5%)	32	67
2	M	76/76 (100%)	72 (95%)	4 (5%)	32	67
2	N	76/76 (100%)	72 (95%)	4 (5%)	32	67
2	O	76/76 (100%)	72 (95%)	4 (5%)	32	67
2	P	76/76 (100%)	72 (95%)	4 (5%)	32	67
2	Q	76/76 (100%)	72 (95%)	4 (5%)	32	67
2	R	76/76 (100%)	72 (95%)	4 (5%)	32	67
2	S	76/76 (100%)	72 (95%)	4 (5%)	32	67
2	T	76/76 (100%)	72 (95%)	4 (5%)	32	67
All	All	2460/2720 (90%)	2319 (94%)	141 (6%)	29	64

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LEU
1	A	113	PHE
1	A	128	MET
1	A	129	PHE
1	A	150	ASN
1	A	154	LEU
1	A	168	ARG
1	A	202	MET
1	A	210	GLN
1	A	238	LEU
1	B	70	LEU
1	B	113	PHE
1	B	128	MET
1	B	129	PHE
1	B	150	ASN
1	B	154	LEU
1	B	168	ARG
1	B	202	MET
1	B	210	GLN
1	B	238	LEU
1	C	70	LEU
1	C	82	LEU
1	C	128	MET
1	C	129	PHE
1	C	150	ASN

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Mol	Chain	Res	Type
1	C	154	LEU
1	C	168	ARG
1	C	190	PRO
1	C	202	MET
1	C	210	GLN
1	C	238	LEU
1	D	60	PRO
1	D	70	LEU
1	D	113	PHE
1	D	128	MET
1	D	129	PHE
1	D	150	ASN
1	D	154	LEU
1	D	202	MET
1	D	210	GLN
1	D	215	LYS
1	D	238	LEU
1	E	128	MET
1	E	129	PHE
1	E	150	ASN
1	E	154	LEU
1	E	168	ARG
1	E	193	VAL
1	E	202	MET
1	E	210	GLN
1	E	238	LEU
1	F	70	LEU
1	F	113	PHE
1	F	128	MET
1	F	129	PHE
1	F	150	ASN
1	F	154	LEU
1	F	168	ARG
1	F	202	MET
1	F	210	GLN
1	F	238	LEU
1	G	70	LEU
1	G	82	LEU
1	G	128	MET
1	G	129	PHE
1	G	150	ASN
1	G	154	LEU

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Mol	Chain	Res	Type
1	G	168	ARG
1	G	202	MET
1	G	210	GLN
1	G	238	LEU
1	H	70	LEU
1	H	82	LEU
1	H	128	MET
1	H	129	PHE
1	H	150	ASN
1	H	154	LEU
1	H	168	ARG
1	H	202	MET
1	H	210	GLN
1	H	213	ASN
1	H	238	LEU
1	I	70	LEU
1	I	113	PHE
1	I	128	MET
1	I	129	PHE
1	I	150	ASN
1	I	154	LEU
1	I	168	ARG
1	I	202	MET
1	I	210	GLN
1	I	238	LEU
1	J	128	MET
1	J	129	PHE
1	J	150	ASN
1	J	154	LEU
1	J	168	ARG
1	J	193	VAL
1	J	202	MET
1	J	210	GLN
1	J	238	LEU
2	K	40	LEU
2	K	43	ASN
2	K	49	VAL
2	K	60	LEU
2	L	40	LEU
2	L	43	ASN
2	L	49	VAL
2	L	60	LEU

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Mol	Chain	Res	Type
2	M	40	LEU
2	M	43	ASN
2	M	49	VAL
2	M	60	LEU
2	N	40	LEU
2	N	43	ASN
2	N	49	VAL
2	N	60	LEU
2	O	40	LEU
2	O	43	ASN
2	O	49	VAL
2	O	60	LEU
2	P	40	LEU
2	P	43	ASN
2	P	49	VAL
2	P	60	LEU
2	Q	40	LEU
2	Q	43	ASN
2	Q	49	VAL
2	Q	60	LEU
2	R	40	LEU
2	R	43	ASN
2	R	49	VAL
2	R	60	LEU
2	S	40	LEU
2	S	43	ASN
2	S	49	VAL
2	S	60	LEU
2	T	40	LEU
2	T	43	ASN
2	T	49	VAL
2	T	60	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	134	HIS
1	A	150	ASN
1	A	213	ASN
1	B	55	ASN
1	B	94	GLN

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Mol	Chain	Res	Type
1	B	134	HIS
1	B	150	ASN
1	B	210	GLN
1	B	213	ASN
1	C	94	GLN
1	C	134	HIS
1	C	150	ASN
1	C	210	GLN
1	C	213	ASN
1	D	94	GLN
1	D	150	ASN
1	D	152	GLN
1	D	213	ASN
1	E	134	HIS
1	E	150	ASN
1	E	213	ASN
1	F	134	HIS
1	F	150	ASN
1	F	213	ASN
1	G	94	GLN
1	G	134	HIS
1	G	150	ASN
1	G	210	GLN
1	G	213	ASN
1	H	55	ASN
1	H	94	GLN
1	H	134	HIS
1	H	150	ASN
1	H	213	ASN
1	I	94	GLN
1	I	134	HIS
1	I	150	ASN
1	I	152	GLN
1	I	213	ASN
1	J	55	ASN
1	J	94	GLN
1	J	134	HIS
1	J	150	ASN
1	J	210	GLN
1	J	213	ASN
2	K	42	ASN
2	K	43	ASN

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Mol	Chain	Res	Type
2	K	75	GLN
2	K	82	HIS
2	L	42	ASN
2	L	43	ASN
2	L	75	GLN
2	L	82	HIS
2	M	42	ASN
2	M	43	ASN
2	M	75	GLN
2	M	82	HIS
2	N	42	ASN
2	N	43	ASN
2	N	75	GLN
2	O	42	ASN
2	O	43	ASN
2	O	75	GLN
2	O	82	HIS
2	P	42	ASN
2	P	43	ASN
2	P	75	GLN
2	P	82	HIS
2	Q	42	ASN
2	Q	43	ASN
2	Q	75	GLN
2	Q	82	HIS
2	R	42	ASN
2	R	43	ASN
2	R	82	HIS
2	S	42	ASN
2	S	43	ASN
2	S	75	GLN
2	S	82	HIS
2	T	42	ASN
2	T	43	ASN
2	T	75	GLN
2	T	82	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PHE	K	1009	-	12,12,12	0.56	0	15,15,15	0.35	0
4	PHE	L	1010	-	12,12,12	0.56	0	15,15,15	0.47	0
4	PHE	M	1006	-	12,12,12	0.51	0	15,15,15	0.39	0
4	PHE	N	1007	-	12,12,12	0.63	0	15,15,15	0.38	0
4	PHE	O	1008	-	12,12,12	0.57	0	15,15,15	0.48	0
4	PHE	P	1003	-	12,12,12	0.64	0	15,15,15	0.46	0
4	PHE	R	1001	-	12,12,12	0.57	0	15,15,15	0.40	0
4	PHE	R	1002	-	12,12,12	0.51	0	15,15,15	0.62	0
4	PHE	S	1004	-	12,12,12	0.54	0	15,15,15	0.34	0
4	PHE	T	1005	-	12,12,12	0.56	0	15,15,15	0.54	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PHE	K	1009	-	-	0/8/8/8	0/1/1/1
4	PHE	L	1010	-	-	0/8/8/8	0/1/1/1
4	PHE	M	1006	-	-	0/8/8/8	0/1/1/1
4	PHE	N	1007	-	-	0/8/8/8	0/1/1/1
4	PHE	O	1008	-	-	0/8/8/8	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PHE	P	1003	-	-	0/8/8/8	0/1/1/1
4	PHE	R	1001	-	-	0/8/8/8	0/1/1/1
4	PHE	R	1002	-	-	0/8/8/8	0/1/1/1
4	PHE	S	1004	-	-	0/8/8/8	0/1/1/1
4	PHE	T	1005	-	-	0/8/8/8	0/1/1/1

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.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	194/230 (84%)	0.05	23 (11%) 5 4	21, 53, 102, 110	0
1	B	194/230 (84%)	0.11	23 (11%) 5 4	22, 55, 101, 110	0
1	C	194/230 (84%)	0.32	29 (14%) 3 2	20, 52, 102, 111	0
1	D	194/230 (84%)	-0.08	10 (5%) 26 26	17, 50, 101, 110	0
1	E	194/230 (84%)	0.05	21 (10%) 6 5	17, 54, 101, 110	0
1	F	194/230 (84%)	0.01	14 (7%) 15 14	17, 53, 102, 111	0
1	G	194/230 (84%)	0.04	15 (7%) 13 12	17, 50, 101, 110	0
1	H	194/230 (84%)	0.13	19 (9%) 8 6	17, 53, 102, 110	0
1	I	194/230 (84%)	0.23	27 (13%) 4 3	21, 56, 101, 110	0
1	J	194/230 (84%)	0.05	18 (9%) 9 7	20, 53, 102, 111	0
2	K	84/84 (100%)	-0.15	4 (4%) 29 30	24, 51, 71, 90	0
2	L	84/84 (100%)	-0.15	5 (5%) 21 21	24, 53, 72, 91	0
2	M	84/84 (100%)	-0.16	2 (2%) 56 57	24, 52, 71, 91	0
2	N	84/84 (100%)	-0.26	1 (1%) 75 76	25, 52, 70, 90	0
2	O	84/84 (100%)	-0.26	2 (2%) 56 57	23, 51, 70, 90	0
2	P	84/84 (100%)	-0.21	2 (2%) 56 57	23, 50, 70, 89	0
2	Q	84/84 (100%)	-0.19	1 (1%) 75 76	22, 50, 68, 89	0
2	R	84/84 (100%)	-0.17	5 (5%) 21 21	24, 50, 71, 90	0
2	S	84/84 (100%)	-0.24	2 (2%) 56 57	21, 52, 70, 89	0
2	T	84/84 (100%)	-0.10	2 (2%) 56 57	23, 50, 71, 90	0
All	All	2780/3140 (88%)	0.01	225 (8%) 12 10	17, 52, 100, 111	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	109	ASN	11.2
1	B	109	ASN	8.1
1	H	109	ASN	7.9
1	E	109	ASN	7.7
1	G	109	ASN	7.4
1	I	109	ASN	7.2
1	J	109	ASN	6.8
1	D	109	ASN	6.7
1	H	209	VAL	6.6
1	F	109	ASN	6.6
1	G	108	LEU	6.4
1	C	116	ASP	5.8
1	I	209	VAL	5.8
2	M	84	GLU	5.7
1	I	48	ARG	5.5
1	J	209	VAL	5.5
2	R	84	GLU	5.2
1	C	51	SER	5.1
1	J	208	GLY	5.1
1	F	209	VAL	5.1
2	S	84	GLU	5.0
2	K	84	GLU	4.9
1	H	49	PRO	4.9
1	C	49	PRO	4.9
2	L	84	GLU	4.8
1	H	208	GLY	4.7
1	H	48	ARG	4.7
1	I	212	MET	4.6
1	I	241	SER	4.6
1	D	207	ARG	4.6
1	D	106	ASP	4.5
1	C	48	ARG	4.5
1	C	110	ASP	4.4
2	T	84	GLU	4.4
1	H	241	SER	4.3
1	C	212	MET	4.3
1	B	83	LEU	4.2
1	C	114	ASP	4.2
1	A	241	SER	4.1
1	I	207	ARG	4.1
1	J	106	ASP	4.1
1	A	109	ASN	4.1
1	E	108	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
2	N	84	GLU	4.1
1	G	241	SER	4.1
1	G	209	VAL	4.0
2	L	30	GLN	4.0
1	E	57	LEU	4.0
1	C	52	GLU	4.0
1	D	209	VAL	3.9
1	C	106	ASP	3.9
1	B	48	ARG	3.9
1	E	207	ARG	3.9
1	J	108	LEU	3.9
1	C	56	GLU	3.9
1	C	83	LEU	3.8
1	B	212	MET	3.8
1	F	208	GLY	3.8
1	I	52	GLU	3.8
1	A	106	ASP	3.8
1	E	106	ASP	3.8
2	P	1	MET	3.8
1	H	207	ARG	3.8
1	E	209	VAL	3.7
1	A	208	GLY	3.7
1	J	55	ASN	3.7
1	G	210	GLN	3.7
1	B	209	VAL	3.7
1	F	207	ARG	3.7
1	I	78	GLN	3.7
1	H	52	GLU	3.7
1	I	57	LEU	3.6
1	B	241	SER	3.6
1	C	113	PHE	3.5
1	F	212	MET	3.5
1	A	110	ASP	3.5
1	A	207	ARG	3.5
1	A	49	PRO	3.5
1	F	241	SER	3.5
1	H	108	LEU	3.5
1	G	48	ARG	3.5
1	C	108	LEU	3.5
2	Q	84	GLU	3.5
1	J	116	ASP	3.5
1	E	205	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	209	VAL	3.4
1	B	108	LEU	3.4
1	G	53	GLU	3.4
1	H	53	GLU	3.4
1	C	209	VAL	3.4
1	I	112	ILE	3.4
1	J	210	GLN	3.4
1	C	53	GLU	3.3
1	F	106	ASP	3.3
1	E	241	SER	3.3
1	C	55	ASN	3.3
1	D	208	GLY	3.3
1	I	110	ASP	3.3
2	P	84	GLU	3.3
1	G	212	MET	3.2
2	O	84	GLU	3.2
1	F	48	ARG	3.2
1	A	111	ALA	3.2
1	A	53	GLU	3.2
1	I	51	SER	3.2
1	F	113	PHE	3.2
1	J	48	ARG	3.2
1	B	111	ALA	3.2
1	H	210	GLN	3.1
1	A	56	GLU	3.1
1	B	207	ARG	3.1
1	A	108	LEU	3.1
1	C	50	ARG	3.1
1	G	208	GLY	3.1
1	B	56	GLU	3.1
1	A	152	GLN	3.1
1	B	208	GLY	3.1
1	C	207	ARG	3.1
1	C	115	GLU	3.1
1	C	206	MET	3.1
1	H	115	GLU	3.0
1	B	55	ASN	3.0
1	I	53	GLU	3.0
1	I	55	ASN	3.0
1	A	57	LEU	3.0
1	A	212	MET	3.0
1	J	240	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	J	212	MET	3.0
1	F	53	GLU	2.9
1	B	57	LEU	2.9
1	C	241	SER	2.9
1	E	212	MET	2.8
1	J	211	LYS	2.8
1	I	108	LEU	2.8
1	B	106	ASP	2.8
1	H	106	ASP	2.8
2	K	83	LYS	2.8
1	A	48	ARG	2.8
1	J	114	ASP	2.8
1	J	241	SER	2.7
1	H	54	ASP	2.7
1	E	116	ASP	2.7
1	C	112	ILE	2.7
1	C	211	LYS	2.7
2	K	62	CYS	2.7
1	D	212	MET	2.7
1	G	82	LEU	2.7
1	G	116	ASP	2.7
1	E	208	GLY	2.6
1	I	49	PRO	2.6
1	A	114	ASP	2.6
1	G	114	ASP	2.6
1	H	206	MET	2.6
1	B	53	GLU	2.6
1	G	115	GLU	2.6
1	I	114	ASP	2.6
1	H	56	GLU	2.6
1	H	212	MET	2.6
1	A	112	ILE	2.5
1	F	49	PRO	2.5
1	J	53	GLU	2.5
1	E	110	ASP	2.5
2	R	27	GLU	2.5
2	M	83	LYS	2.5
1	D	52	GLU	2.5
1	B	189	GLN	2.5
1	E	82	LEU	2.5
1	A	54	ASP	2.4
1	A	189	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	78	GLN	2.4
1	E	114	ASP	2.4
1	A	115	GLU	2.4
1	G	207	ARG	2.3
1	D	53	GLU	2.3
1	B	71	ARG	2.3
1	B	52	GLU	2.3
1	F	52	GLU	2.3
2	L	27	GLU	2.3
1	I	208	GLY	2.3
1	E	48	ARG	2.3
1	I	189	GLN	2.3
1	D	206	MET	2.3
1	H	189	GLN	2.3
1	C	240	ARG	2.2
1	H	103	THR	2.2
1	E	240	ARG	2.2
2	S	27	GLU	2.2
2	R	30	GLN	2.2
1	A	104	ILE	2.2
1	B	110	ASP	2.2
1	C	107	VAL	2.2
1	G	110	ASP	2.2
1	J	56	GLU	2.2
1	B	81	GLY	2.2
1	I	103	THR	2.2
1	C	54	ASP	2.1
1	E	112	ILE	2.1
1	J	206	MET	2.1
1	I	81	GLY	2.1
1	A	240	ARG	2.1
2	R	1	MET	2.1
1	E	102	GLU	2.1
1	C	81	GLY	2.1
1	I	58	ASN	2.1
1	C	59	LEU	2.1
1	E	206	MET	2.1
1	I	206	MET	2.1
1	I	106	ASP	2.1
2	O	27	GLU	2.1
2	T	1	MET	2.1
1	I	111	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	80	GLN	2.1
2	K	1	MET	2.0
1	I	113	PHE	2.0
1	B	49	PRO	2.0
1	B	151	LYS	2.0
1	F	210	GLN	2.0
1	B	61	ASN	2.0
1	I	54	ASP	2.0
1	E	152	GLN	2.0
1	E	103	THR	2.0
1	D	108	LEU	2.0
2	L	1	MET	2.0
2	L	38	ARG	2.0
2	R	83	LYS	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	PHE	K	1009	12/12	0.14	0.47	37,40,43,43	0
4	PHE	O	1008	12/12	0.13	0.04	28,33,34,34	0
4	PHE	L	1010	12/12	0.11	-0.27	28,30,31,35	0
4	PHE	N	1007	12/12	0.11	-0.28	20,24,26,28	0
4	PHE	R	1002	12/12	0.11	-0.32	25,29,33,34	0
4	PHE	P	1003	12/12	0.11	-0.64	26,27,29,30	0
4	PHE	R	1001	12/12	0.10	-0.65	17,21,23,25	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	PHE	S	1004	12/12	0.10	-0.68	17,22,26,28	0
4	PHE	T	1005	12/12	0.10	-1.18	24,28,32,33	0
4	PHE	M	1006	12/12	0.08	-1.21	23,27,30,32	0
3	K	R	2001	1/1	0.08	-1.41	56,56,56,56	0
3	K	Q	2005	1/1	0.06	-1.70	39,39,39,39	0
3	K	N	2009	1/1	0.06	-1.70	42,42,42,42	0
3	K	O	2010	1/1	0.07	-1.71	52,52,52,52	0
3	K	S	2002	1/1	0.07	-1.90	53,53,53,53	0
3	K	P	2004	1/1	0.06	-2.15	43,43,43,43	0
3	K	L	2007	1/1	0.06	-2.77	48,48,48,48	0
3	K	K	2006	1/1	0.04	-3.95	48,48,48,48	0
3	K	M	2008	1/1	0.06	-4.55	43,43,43,43	0
3	K	T	2003	1/1	0.07	-5.01	38,38,38,38	0

6.5 Other polymers ⓘ

There are no such residues in this entry.