Full wwPDB X-ray Structure Validation Report (i)

Dec 19, 2023 – 07:07 AM EST

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 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 (i) 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 (i)) were used in the production of this report:

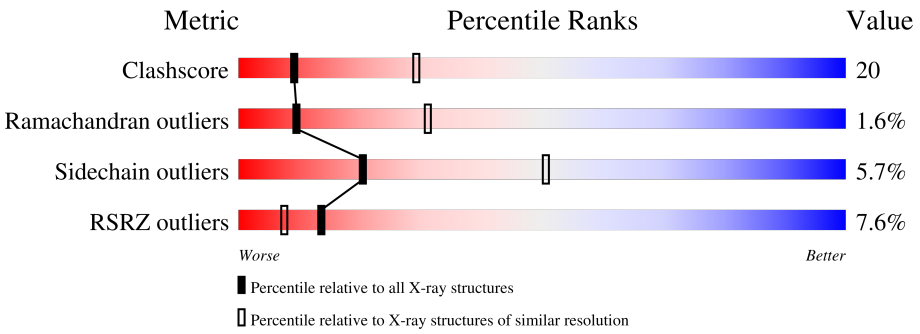
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 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 <=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	230	9% 53% 26% • 16%
1	B	230	10% 56% 25% • 16%
1	C	230	12% 53% 27% • 16%
1	D	230	4% 56% 24% • 16%
1	E	230	9% 55% 26% • 16%
1	F	230	6% 54% 25% • 16%

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Mol	Chain	Length	Quality of chain
1	G	230	6% 56% 24% • 16%
1	H	230	8% 56% 24% • 16%
1	I	230	10% 54% 25% • 16%
1	J	230	7% 56% 25% • 16%
2	K	84	5% 69% 25% 6%
2	L	84	6% 70% 23% 7%
2	M	84	% 76% 18% 6%
2	N	84	% 73% 21% 6%
2	O	84	2% 73% 21% 6%
2	P	84	2% 69% 25% 6%
2	Q	84	% 71% 24% 5%
2	R	84	4% 75% 20% 5%
2	S	84	2% 77% 17% 6%
2	T	84	2% 68% 27% 5%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 22375 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 GTP Cyclohydrolase I.

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

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

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

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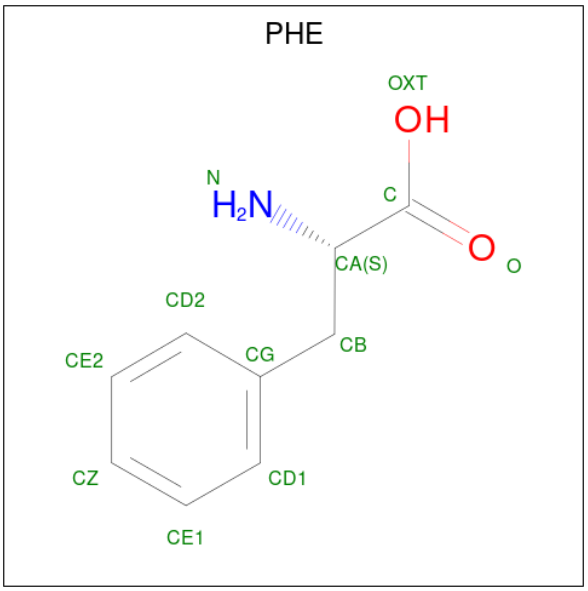
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	O	84	676	428	117	124	7	0	0	0
2	P	84	676	428	117	124	7	0	0	0
2	Q	84	676	428	117	124	7	0	0	0
2	R	84	676	428	117	124	7	0	0	0
2	S	84	676	428	117	124	7	0	0	0
2	T	84	676	428	117	124	7	0	0	0

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

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

- Molecule 4 is PHENYLALANINE (three-letter code: PHE) (formula: $C_9H_{11}NO_2$).



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

- Molecule 5 is water.

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

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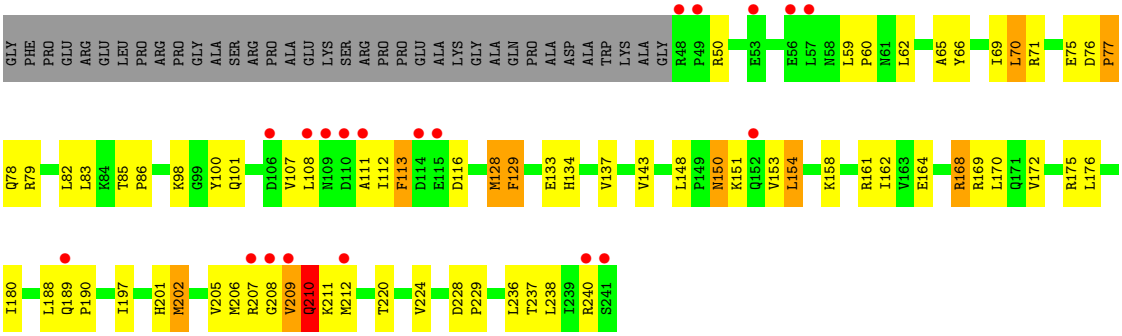
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	5	Total O 5 5	0	0
5	D	4	Total O 4 4	0	0
5	E	6	Total O 6 6	0	0
5	F	6	Total O 6 6	0	0
5	G	9	Total O 9 9	0	0
5	H	5	Total O 5 5	0	0
5	I	3	Total O 3 3	0	0
5	J	4	Total O 4 4	0	0
5	K	8	Total O 8 8	0	0
5	L	9	Total O 9 9	0	0
5	N	9	Total O 9 9	0	0
5	O	9	Total O 9 9	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 (i)

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.

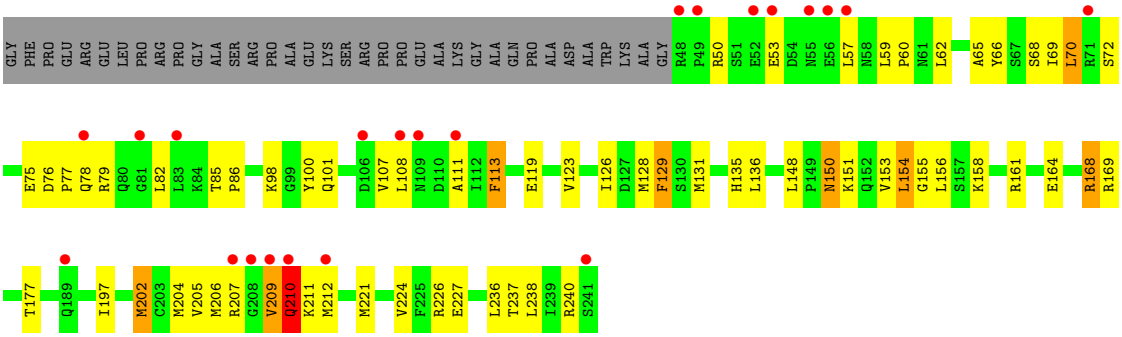
• Molecule 1: GTP Cyclohydrolase I

Chain A:



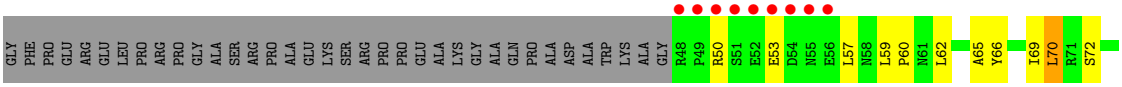
• Molecule 1: GTP Cyclohydrolase I

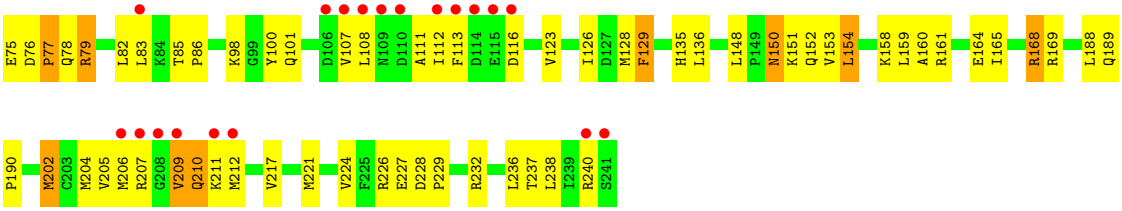
Chain B:



• Molecule 1: GTP Cyclohydrolase I

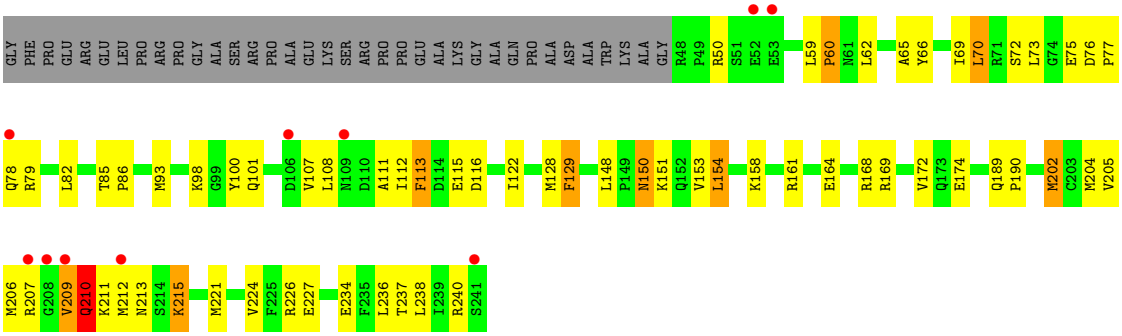
Chain C:





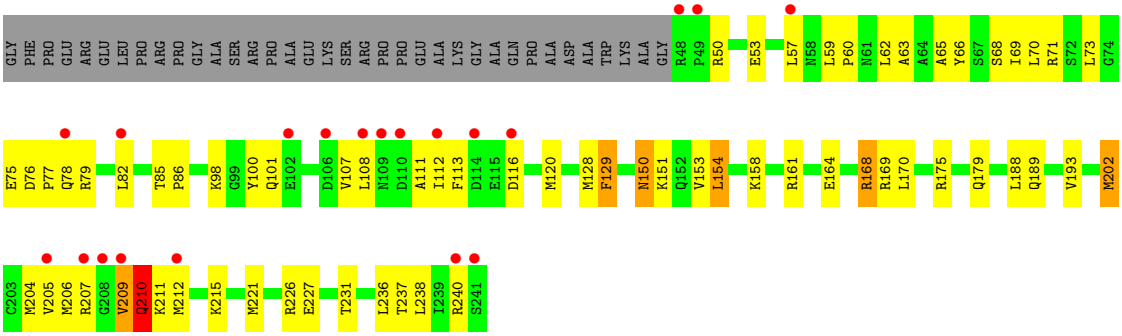
- Molecule 1: GTP Cyclohydrolase I

Chain D:



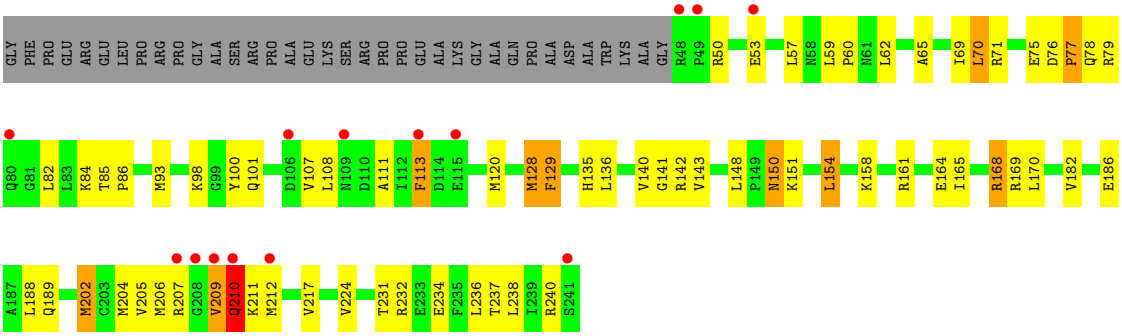
- Molecule 1: GTP Cyclohydrolase I

Chain E:



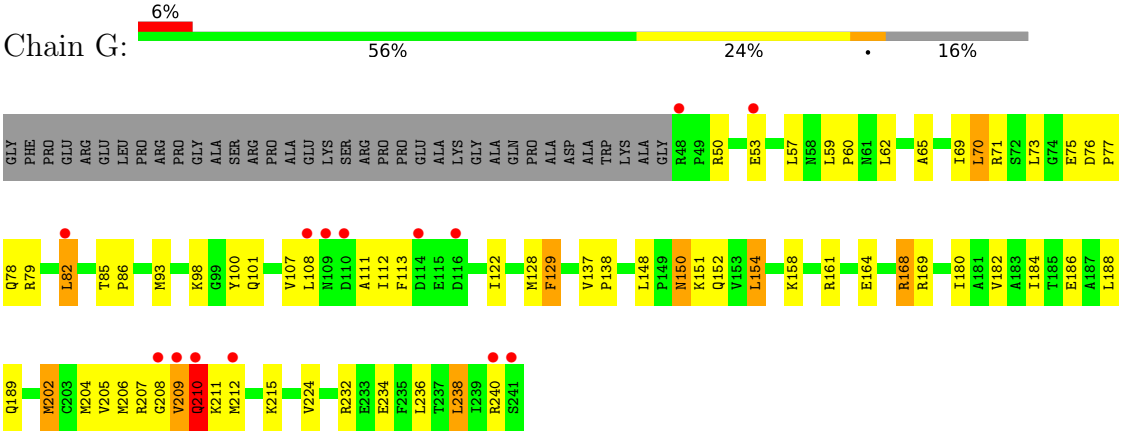
- Molecule 1: GTP Cyclohydrolase I

Chain F:



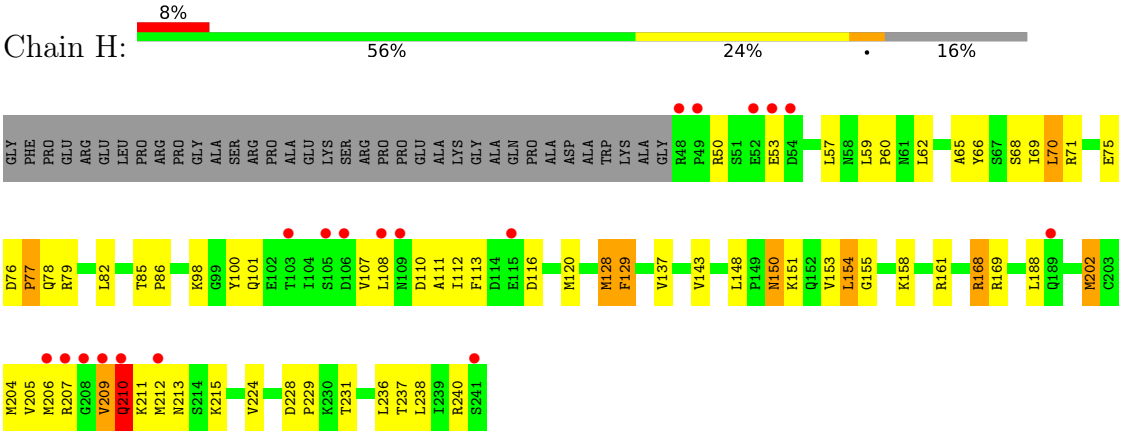
• Molecule 1: GTP Cyclohydrolase I

Chain G:



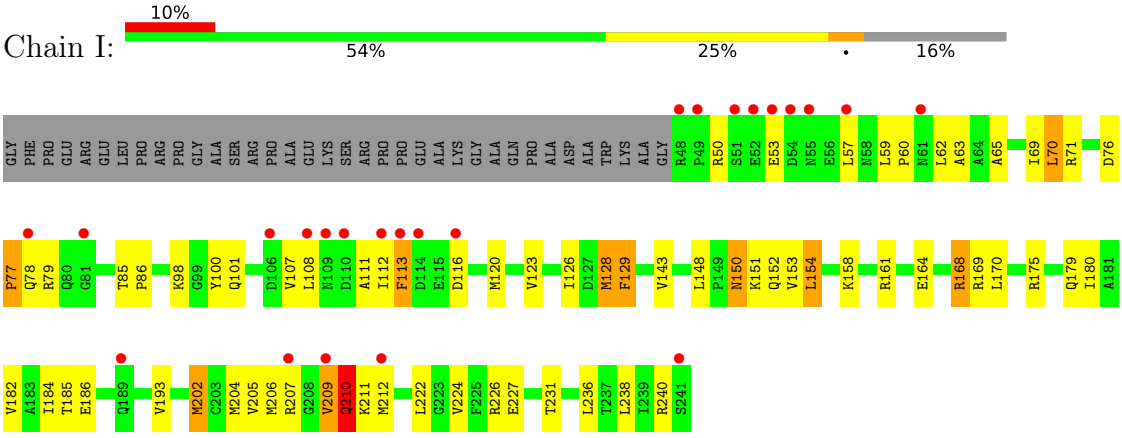
• Molecule 1: GTP Cyclohydrolase I

Chain H:



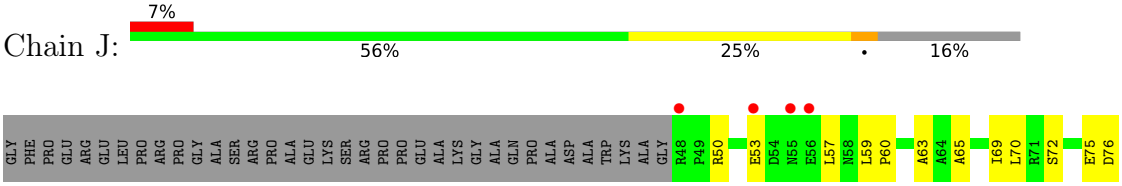
• Molecule 1: GTP Cyclohydrolase I

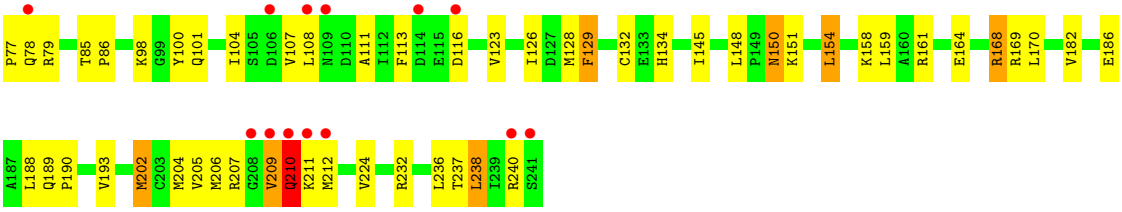
Chain I:



• Molecule 1: GTP Cyclohydrolase I

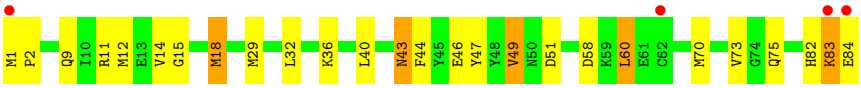
Chain J:





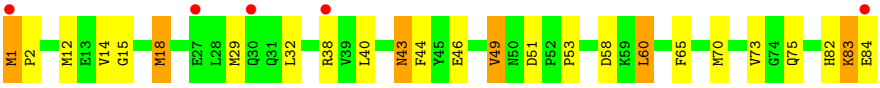
• Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain K:



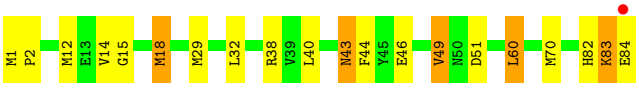
• Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain L:



• Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain M:

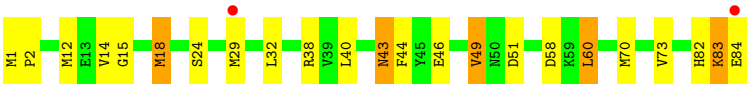


• Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain N:

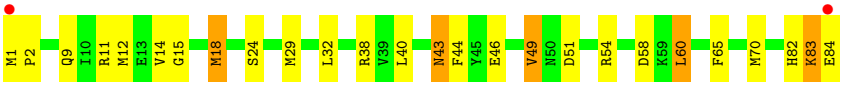
• Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain O:



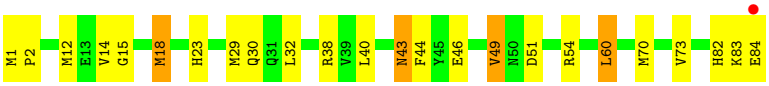
• Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain P:



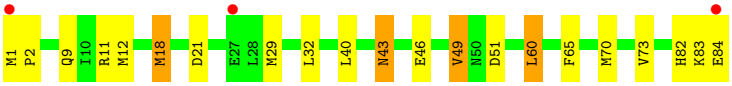
• Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

Chain Q:



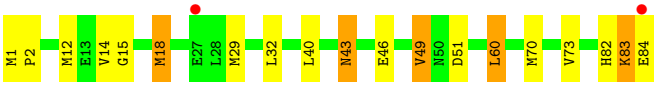
• Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

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 (i)

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
$< I/\sigma(I) >$ [1]	1.72 (at 2.51Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.228 , 0.264 0.240 , (Not available)	Depositor DCC
R_{free} test set	33257 reflections (28.50%)	wwPDB-VP
Wilson B-factor (Å^2)	52.0	Xtriage
Anisotropy	0.161	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 69.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.006 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
3	L	1	0	0	0	0
3	M	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 20.

All (893) 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: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:59:LEU:HB3	1:D:60:PRO:HD3	1.50	0.93
1:D:205:VAL:HG13	1:D:212:MET:HB2	1.51	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:107:VAL:HG22	1:I:161:ARG:HD3	1.63	0.81
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:A:116:ASP:OD1	1:A:151:LYS:HE3	1.92	0.70
1:I:209:VAL:HG13	1:I:210:GLN:N	2.06	0.70
2:P:43:ASN:H	2:P:43:ASN:HD22	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:M:43:ASN:HD22	2:M:43:ASN:H	1.41	0.69
2:R:43:ASN:HD22	2:R:43:ASN:H	1.39	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:MET:HE3	1:C:211:LYS:HD3	1.76	0.67
1:J:98:LYS:O	1:J:101:GLN:HG2	1.94	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
1:I:202:MET:HG2	1:I:206:MET:CE	2.24	0.67
2:K:43:ASN:H	2:K:43:ASN:HD22	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
1:A:70:LEU:HB3	1:A:77:PRO:HG3	1.77	0.67
2:L:43:ASN:H	2:L:43:ASN:HD22	1.41	0.67
1:I:85:THR:HB	1:I:86:PRO:HD3	1.77	0.67
2:N:43:ASN:H	2:N:43:ASN:HD22	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:HH11	1:J:79:ARG:HB3	1.60	0.66
1:A:143:VAL:HG22	1:A:197:ILE:HG12	1.78	0.66
1:B:79:ARG:HH11	1:B:79:ARG:HB3	1.60	0.66
1:E:98:LYS:O	1:E:101:GLN:HG2	1.95	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:F:79:ARG:HH11	1:F:79:ARG:HB3	1.62	0.65
1:G:205:VAL:HG22	1:G:212:MET:CA	2.22	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:H:205:VAL:CG1	1:H:212:MET:HB2	2.24	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:98:LYS:O	1:D:101:GLN:HG2	1.98	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:A:75:GLU:O	1:A:77:PRO:HD3	1.98	0.63
1:B:168:ARG:HH22	1:I:206:MET:HB3	1.62	0.63
1:D:148:LEU:HD12	1:D:224:VAL:HG21	1.80	0.63
1:F:65:ALA:O	1:F:69:ILE:HG13	1.98	0.63
1:I:205:VAL:CG1	1:I:212:MET:HB2	2.25	0.63
2:O:43:ASN:HD22	2:O:43:ASN:N	1.94	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:C:209:VAL:HG13	1:C:210:GLN:N	2.06	0.63
1:E:205:VAL:CG1	1:E:212:MET:HB2	2.25	0.63
1:E:79:ARG:HH11	1:E:79:ARG:HB3	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:79:ARG:HH11	1:C:79:ARG:HB3	1.65	0.62
1:C:209:VAL:CG1	1:C:210:GLN:H	2.08	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:C:59:LEU:HB3	1:C:60:PRO: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:A:85:THR:HB	1:A:86:PRO:HD3	1.83	0.61
1:E:66:TYR:CD2	1:E:69:ILE:HD12	2.35	0.61
1:H:111:ALA:HB3	1:H:158:LYS:HG2	1.82	0.61
2:P:43:ASN:HD22	2:P:43:ASN:N	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:66:TYR:HD2	1:E:69:ILE:HD12	1.66	0.60
1:E:111:ALA:HB3	1:E:158:LYS:CG	2.30	0.60
1:E:150:ASN:O	1:E:151:LYS:HB2	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:168:ARG:HH22	1:F:206:MET:HB3	1.66	0.60
1:F:204:MET:HE3	1:F:211:LYS:HD3	1.83	0.60
1:I:164:GLU:HG3	1:I:168:ARG:HG3	1.83	0.60
2:R:43:ASN:HD22	2:R:43:ASN:N	1.99	0.60
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:70:LEU:HB3	1:C:77:PRO:HG3	1.84	0.60
1:C:79:ARG:O	1:C:83:LEU:HG	2.01	0.60
1:A:129:PHE:CZ	1:J:210:GLN:HG2	2.36	0.60
1:D:100:TYR:CZ	1:D:169:ARG:HB2	2.37	0.60
1:G:65:ALA:O	1:G:69:ILE:HG13	2.01	0.60
2:L:18:MET:HE3	2:L:46:GLU:CB	2.32	0.60
1:J:59:LEU:HB3	1:J:60:PRO:HD3	1.83	0.60
2:N:43:ASN:HD22	2:N:43:ASN:N	1.99	0.60
2:Q:43:ASN:HD22	2:Q:43:ASN:N	1.97	0.60
1:B:205:VAL:O	1:B:210:GLN:HA	2.02	0.59
1:C:116:ASP:OD1	1:C:151:LYS:HE3	2.02	0.59
2:O:43:ASN:H	2:O:43:ASN:ND2	1.99	0.59
1:F:100:TYR:CZ	1:F:169:ARG:HB2	2.37	0.59
1:I:148:LEU:HD12	1:I:224:VAL:HG21	1.84	0.59
2:T:43:ASN:HD22	2:T:43:ASN:N	1.96	0.59
1:C:123:VAL:HG12	1:C:126:ILE:HD11	1.84	0.59
1:I:111:ALA:HB3	1:I:158:LYS:CG	2.29	0.59
1:B:150:ASN:O	1:B:151:LYS:HB2	2.01	0.59
1:E:65:ALA:O	1:E:69:ILE:HG13	2.02	0.59
1:F:75:GLU:O	1:F:77:PRO:HD3	2.02	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:B:164:GLU:HG3	1:B:168:ARG:HG3	1.83	0.59
1:B:236:LEU:O	1:B:240:ARG:HB2	2.03	0.59
1:F:98:LYS:O	1:F:101:GLN:HG2	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:H:65:ALA:O	1:H:68:SER:HB3	2.03	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:HD22	2:M:43:ASN:N	2.00	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:H:116:ASP:OD1	1:H:151:LYS:HE3	2.03	0.58
2:P:43:ASN:H	2:P:43:ASN:ND2	2.02	0.58
1:B:129:PHE:CZ	1:I:210:GLN:HG2	2.38	0.58
1:D:79:ARG:HB3	1:D:79:ARG:HH11	1.68	0.58
1:E:206:MET:HB3	1:F:168:ARG:HH22	1.67	0.58
2:T:43:ASN:H	2:T:43:ASN:ND2	2.01	0.58
1:D:236:LEU:O	1:D:240:ARG:HB2	2.03	0.58
2:Q:18:MET:HE3	2:Q:46:GLU:CB	2.33	0.58
1:D:65:ALA:O	1:D:69:ILE:HG13	2.04	0.57
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:A:164:GLU:CD	1:A:168:ARG:HD2	2.25	0.57
1:B:207:ARG:HG2	1:B:207:ARG:HH11	1.69	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:B:100:TYR:CZ	1:B:169:ARG:HB2	2.40	0.57
1:F:111:ALA:HB3	1:F:158:LYS:CD	2.35	0.57
1:B:66:TYR:CD2	1:B:69:ILE:HD12	2.40	0.57
2:L:49:VAL:CG1	2:L:51:ASP:H	2.17	0.57
1:E:129:PHE:HZ	1:F:210:GLN:HG2	1.70	0.57
2:N:43:ASN:H	2:N:43:ASN:ND2	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
1:C:112:ILE:HD11	1:C:152:GLN:CD	2.25	0.56
2:L:43:ASN:H	2:L:43:ASN:ND2	2.03	0.56
1:A:71:ARG:HG3	1:A:77:PRO:HG2	1.87	0.56
1:B:65:ALA:O	1:B:69:ILE:HG13	2.04	0.56
1:B:66:TYR:HD2	1:B:69:ILE:HD12	1.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:70:LEU:HB3	1:E:77:PRO:HG3	1.87	0.56
1:H:207:ARG:C	1:H:209:VAL:H	2.09	0.56
1:C:76:ASP:C	1:C:78:GLN:H	2.06	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:H:128:MET:HG2	1:H:143:VAL:HG23	1.86	0.56
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:C:207:ARG:C	1:C:209:VAL:H	2.09	0.56
1:D:62:LEU:CD2	1:G:69:ILE:HG23	2.35	0.56
1:I:209:VAL:CG1	1:I:210:GLN:H	2.12	0.56
2:L:43:ASN:HD22	2:L:43:ASN:N	1.99	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:A:79:ARG:HH11	1:A:79:ARG:HB3	1.71	0.56
1:D:205:VAL:O	1:D:210:GLN:HA	2.06	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:O:32:LEU:HD11	2:O:60:LEU:HD11	1.89	0.55
2:S:49:VAL:CG1	2:S:51:ASP:H	2.19	0.55
1:E:202:MET:HG2	1:E:206:MET:CE	2.37	0.55
1:H:209:VAL:CG1	1:H:211:LYS:HE2	2.37	0.55
2:M:43:ASN:H	2:M:43:ASN:ND2	2.05	0.55
1:A:148:LEU:CD1	1:A:224:VAL:HG21	2.36	0.55
1:B:98:LYS:NZ	1:B:168:ARG:HD3	2.21	0.55
1:C:206:MET:HG2	1:H:129:PHE:CG	2.41	0.55
1:E:205:VAL:O	1:E:210:GLN:HA	2.05	0.55
1:I:79:ARG:HB3	1:I:79:ARG:HH11	1.71	0.55
2:K:18:MET:HE3	2:K:46:GLU:HB2	1.88	0.55
1:C:53:GLU:O	1:C:57:LEU:HG	2.07	0.55
1:E:111:ALA:HB3	1:E:158:LYS:CD	2.36	0.55
1:E:207:ARG:C	1:E:209:VAL:H	2.10	0.55
1:J:145:ILE:HD13	1:J:159:LEU:HD11	1.89	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:D:70:LEU:HB3	1:D:77:PRO:HG3	1.89	0.55
2:O:83:LYS:HG2	2:O:84:GLU:N	2.22	0.55
1:B:107:VAL:HG22	1:B:161:ARG:HD3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:LEU:HD12	1:J:75:GLU:HG3	1.89	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
1:H:209:VAL:CG1	1:H:210:GLN:H	2.15	0.54
2:P:32:LEU:HD11	2:P:60:LEU:HD11	1.90	0.54
1:C:76:ASP:OD2	1:C:78:GLN:HG2	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:I:205:VAL:O	1:I:210:GLN:HA	2.08	0.54
1:I:236:LEU:O	1:I:240:ARG:HB2	2.07	0.54
1:C:153:VAL:HG12	1:C:154:LEU:N	2.22	0.54
1:C:205:VAL:CG1	1:C:212:MET:HB2	2.30	0.54
1:C:209:VAL:CG1	1:C:211:LYS:HE2	2.37	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:107:VAL:CG1	1:C:158:LYS:HG3	2.37	0.54
1:J:111:ALA:HB3	1:J:158:LYS:CD	2.37	0.54
2:P:2:PRO:HB2	2:P:82:HIS:CE1	2.43	0.54
1:C:236:LEU:O	1:C:240:ARG:HB2	2.07	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
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:G:148:LEU:CD1	1:G:224:VAL:HG21	2.37	0.54
1:I:111:ALA:HB3	1:I:158:LYS:CD	2.38	0.54
1:B:111:ALA:HB3	1:B:158:LYS:CD	2.38	0.54
1:C:111:ALA:HB3	1:C:158:LYS:HG2	1.90	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:G:70:LEU:HB3	1:G:77:PRO:HG3	1.90	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:F:236:LEU:O	1:F:240:ARG:HB2	2.08	0.53
1:H:107:VAL:HG12	1:H:158:LYS:HG3	1.90	0.53
2:K:49:VAL:CG1	2:K:51:ASP:H	2.22	0.53
2:S:43:ASN:HD22	2:S:43:ASN:N	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:107:VAL:HG22	1:E:161:ARG:CD	2.32	0.53
1:J:207:ARG:C	1:J:209:VAL:H	2.11	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:N:58:ASP:OD1	2:O:2:PRO:HD2	2.08	0.53
2:T:49:VAL:CG1	2:T:51:ASP:H	2.22	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:G:232:ARG:NE	5:G:248:HOH:O	2.40	0.53
1:H:76:ASP:C	1:H:78:GLN:H	2.12	0.53
1:J:79:ARG:HB3	1:J:79:ARG:NH1	2.24	0.53
1:B:85:THR:HB	1:B:86:PRO:HD3	1.90	0.53
1:G:207:ARG:HG2	1:G:207:ARG:HH11	1.73	0.53
2:R:18:MET:HE3	2:R:46:GLU:CB	2.39	0.53
1:E:221:MET:O	1:E:226:ARG:HB2	2.08	0.53
1:G:111:ALA:HB3	1:G:158:LYS:CD	2.38	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:B:113:PHE:CD1	1:B:113:PHE:N	2.76	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:I:205:VAL:HG22	1:I:212:MET:CA	2.32	0.52
1:C:210:GLN:NE2	1:G:210:GLN:NE2	2.58	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
2:M:18:MET:HE1	2:M:46:GLU:CB	2.35	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:C:85:THR:HB	1:C:86:PRO:HD3	1.90	0.52
1:C:206:MET:HG2	1:H:129:PHE:CB	2.39	0.52
1:G:209:VAL:CG1	1:G:211:LYS:HE2	2.39	0.52
1:H:129:PHE:HB2	1:H:168:ARG:NH2	2.24	0.52
1:D:221:MET:O	1:D:226:ARG:HB2	2.09	0.52
1:A:220:THR:HA	1:B:119:GLU:OE1	2.09	0.52
1:D:113:PHE:N	1:D:113:PHE:CD1	2.77	0.52
1:F:207:ARG:C	1:F:209:VAL:H	2.12	0.52
1:J:164:GLU:CD	1:J:168:ARG:HD2	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:M:49:VAL:CG1	2:M:51:ASP:H	2.23	0.52
2:S:2:PRO:HB2	2:S:82:HIS:CE1	2.44	0.52
2:S:43:ASN:H	2:S:43:ASN:ND2	2.06	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
1:A:137:VAL:CG1	1:A:202:MET:HB3	2.41	0.51
1:C:72:SER:HB2	1:H:62:LEU:CD2	2.41	0.51
1:C:148:LEU:HD12	1:C:224:VAL:HG21	1.92	0.51
1:G:209:VAL:CG1	1:G:210:GLN:H	2.12	0.51
1:H:113:PHE:CD1	1:H:113:PHE:N	2.78	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:A:98:LYS:O	1:A:101:GLN:HG2	2.10	0.51
1:I:207:ARG:C	1:I:209:VAL:H	2.13	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
1:F:84:LYS:NZ	1:F:84:LYS:HB3	2.25	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: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
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
2:Q:18:MET:CE	2:Q:46:GLU:HB2	2.36	0.51
1:B:111:ALA:HB3	1:B:158:LYS:CG	2.40	0.51
1:I:113:PHE:CD1	1:I:113:PHE:N	2.78	0.51
1:J:123:VAL:HG12	1:J:126:ILE:HD11	1.92	0.51
1:J:85:THR:HB	1:J:86:PRO:HD3	1.91	0.51
1:J:209:VAL:CG1	1:J:211:LYS:HE2	2.40	0.51
2:K:2:PRO:HB2	2:K:82:HIS:CE1	2.46	0.51
2:K:14:VAL:HG22	2:K:15:GLY:N	2.26	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
1:E:206:MET:HB3	1:F:168:ARG:NH2	2.24	0.51
2:M:14:VAL:HG22	2:M:15:GLY:N	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:83:LYS:HG2	2:Q:84:GLU:N	2.25	0.51
1:C:202:MET:HG2	1:C:206:MET:CE	2.41	0.51
1:C:204:MET:CE	1:C:211:LYS:HD3	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:E:170:LEU:HD12	1:F:75:GLU:HG3	1.92	0.50
1:F:209:VAL:HG11	1:F:211:LYS:HE2	1.93	0.50
2:K:83:LYS:HG2	2:K:84:GLU:N	2.26	0.50
2:L:2:PRO:HB2	2:L:82:HIS:CE1	2.46	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: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
1:G:75:GLU:O	1:G:77:PRO:HD3	2.12	0.50
2:M:83:LYS:HG2	2:M:84:GLU:N	2.26	0.50
2:O:2:PRO:HB2	2:O:82:HIS:CE1	2.46	0.50
1:D:204:MET:HE3	1:D:211:LYS:HD3	1.93	0.50
1:D:206:MET:HB3	1:G:168:ARG:NH2	2.27	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:E:113:PHE:N	1:E:113:PHE:CD1	2.80	0.50
1:J:236:LEU:O	1:J:240:ARG:HB2	2.12	0.50
2:Q:2:PRO:HB2	2:Q:82:HIS:CE1	2.47	0.50
1:A:237:THR:HA	1:A:240:ARG:CZ	2.41	0.50
1:D:207:ARG:HG2	1:D:207:ARG:HH11	1.77	0.50
1:H:204:MET:O	1:H:211:LYS:HB2	2.12	0.50
2:P:14:VAL:HG22	2:P:15:GLY:N	2.27	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:A:113:PHE:CD1	1:A:113:PHE:N	2.79	0.49
1:D:59:LEU:HB3	1:D:60:PRO:CD	2.31	0.49
1:E:112:ILE:HG23	1:E:112:ILE:O	2.12	0.49
1:F:205:VAL:CG1	1:F:212:MET:HB2	2.28	0.49
1:J:107:VAL:HG22	1:J:161:ARG:CD	2.35	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:83:LYS:HG2	2:S:84:GLU:N	2.27	0.49
1:C:100:TYR:CZ	1:C:169:ARG:HB2	2.48	0.49
1:D:205:VAL:HG22	1:D:212:MET:CA	2.37	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:E:237:THR:HA	1:E:240:ARG:CZ	2.42	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: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
2:S:73:VAL:O	2:S:73:VAL:HG13	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
1:J:150:ASN:O	1:J:151:LYS:HB2	2.13	0.49
2:T:14:VAL:HG22	2:T:15:GLY:N	2.27	0.49
1:D:226:ARG:HD2	1:D:227:GLU:OE2	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:A:76:ASP:C	1:A:78:GLN:H	2.16	0.49
1:E:164:GLU:CD	1:E:168:ARG:HD2	2.33	0.49
1:J:154:LEU:HB2	1:J:188:LEU:HD11	1.94	0.49
1:A:201:HIS:CD2	1:B:156:LEU:HD11	2.48	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
1:I:164:GLU:CD	1:I:168:ARG:HD2	2.32	0.49
2:O:49:VAL:CG1	2:O:51:ASP:H	2.26	0.49
2:S:49:VAL:HG12	2:S:51:ASP:H	1.78	0.49
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:C:168:ARG:HH22	1:H:206:MET:HB3	1.78	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:C:113:PHE:N	1:C:113:PHE:CD1	2.80	0.48
1:F:232:ARG:HD3	1:G:234:GLU:OE2	2.12	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
2:T:83:LYS:HG2	2:T:84:GLU:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:VAL:HG12	1:C:158:LYS:HG3	1.93	0.48
1:H:204:MET:CE	1:H:211:LYS:HD3	2.40	0.48
1:I:180:ILE:O	1:I:184:ILE:HG13	2.14	0.48
2:L:83:LYS:HG2	2:L:84:GLU:N	2.28	0.48
2:R:49:VAL:HG12	2:R:51:ASP:H	1.78	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:D:69:ILE:HG23	1:G:62:LEU:HD22	1.94	0.48
1:F:148:LEU:CD1	1:F:224:VAL:HG21	2.42	0.48
1:I:53:GLU:O	1:I:57:LEU:HG	2.13	0.48
1:D:69:ILE:HG23	1:G:62:LEU:CD2	2.44	0.48
1:F:50:ARG:HB3	1:F:101:GLN:HB3	1.94	0.48
1:G:53:GLU:O	1:G:57:LEU:HG	2.14	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
2:T:18:MET:HE1	2:T:46:GLU:CB	2.42	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:C:62:LEU:CD2	1:H:69:ILE:HG23	2.44	0.48
1:D:209:VAL:CG1	1:D:210:GLN:H	2.10	0.48
2:Q:14:VAL:HG22	2:Q:15:GLY:N	2.29	0.48
1:D:72:SER:HB2	1:G:62:LEU:HD21	1.95	0.48
1:D:164:GLU:CD	1:D:168:ARG:HD2	2.34	0.48
2:L:38:ARG:HG3	2:L:44:PHE:O	2.13	0.48
1:D:153:VAL:HG12	1:D:154:LEU:N	2.28	0.48
1:I:207:ARG:HG2	1:I:207:ARG:HH11	1.78	0.48
1:C:79:ARG:HB3	1:C:79:ARG:NH1	2.29	0.47
1:D:50:ARG:HB3	1:D:101:GLN:HB3	1.96	0.47
1:E:73:LEU:HD11	1:F:93:MET:HG3	1.96	0.47
1:H:154:LEU:HD23	1:H:155:GLY:H	1.78	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: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:I:107:VAL:HG12	1:I:158:LYS:HG3	1.96	0.47
1:A:206:MET:HB3	1:J:168:ARG:HH22	1.79	0.47
1:D:66:TYR:CD2	1:D:69:ILE:HD12	2.49	0.47
1:E:62:LEU:CD2	1:F:69:ILE:HG23	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:135:HIS:O	1:F:136:LEU:HB2	2.14	0.47
1:G:207:ARG:O	1:G:209:VAL:N	2.42	0.47
1:B:107:VAL:CG1	1:B:158:LYS:HG3	2.44	0.47
1:C:161:ARG:O	1:C:165:ILE:HG13	2.14	0.47
1:E:204:MET:O	1:E:211:LYS:HB2	2.13	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:A:133:GLU:HG3	1:A:134:HIS:CD2	2.50	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
2:Q:73:VAL:HG13	2:Q:73:VAL:O	2.15	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:H:209:VAL:HG11	1:H:211:LYS:HE2	1.97	0.47
1:I:76:ASP:O	1:I:78:GLN:N	2.48	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
1:C:209:VAL:HG11	1:C:211:LYS:HE2	1.97	0.47
1:E:206:MET:SD	1:F:129:PHE:HB3	2.54	0.47
1:G:111:ALA:CB	1:G:158:LYS:HE3	2.45	0.47
1:J:207:ARG:O	1:J:209:VAL:N	2.42	0.47
1:A:154:LEU:HB2	1:A:188:LEU:HD11	1.97	0.47
2:L:18:MET:CE	2:L:46:GLU:HB2	2.42	0.47
2:O:73:VAL:HG13	2:O:73:VAL:O	2.15	0.47
1:G:76:ASP:C	1:G:78:GLN:H	2.18	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:J:204:MET:O	1:J:211:LYS:HB2	2.15	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: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:C:129:PHE:HB2	1:C:168:ARG:NH2	2.29	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:A:76:ASP:O	1:A:78:GLN:N	2.49	0.46
1:F:150:ASN:HD22	1:F:150:ASN:HA	1.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:209:VAL:HG11	1:J:211:LYS:HE2	1.98	0.46
1:E:153:VAL:HG12	1:E:154:LEU:N	2.30	0.46
1:G:113:PHE:CD1	1:G:113:PHE:N	2.84	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: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
2:S:18:MET:CE	2:S:46:GLU:HB2	2.39	0.46
1:B:206:MET:HG2	1:I:129:PHE:HB3	1.98	0.46
1:B:206:MET:HG2	1:I:129:PHE:CD2	2.50	0.46
1:E:209:VAL:HG12	1:E:211:LYS:HE2	1.97	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
2:M:38:ARG:HG3	2:M:44:PHE:O	2.15	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:D:107:VAL:CG1	1:D:158:LYS:HG3	2.46	0.46
1:G:209:VAL:HG11	1:G:211:LYS:HE2	1.98	0.46
2:L:14:VAL:HG22	2:L:15:GLY:N	2.31	0.46
2:N:73:VAL:O	2:N:73:VAL:HG13	2.16	0.46
2:P:58:ASP:OD1	2:Q:2:PRO:HD2	2.16	0.46
1:A:133:GLU:HG2	1:A:172:VAL:HG23	1.98	0.45
1:D:164:GLU:HG3	1:D:168:ARG:HG3	1.97	0.45
1:B:129:PHE:HB3	1:I:206:MET:HG2	1.98	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
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:I:175:ARG:O	1:I:179:GLN:HG3	2.17	0.45
2:T:49:VAL:HG13	2:T:51:ASP:H	1.81	0.45
1:B:131:MET:HE1	1:B:136:LEU:O	2.16	0.45
1:B:205:VAL:HG22	1:B:212:MET:CA	2.40	0.45
1:C:188:LEU:O	1:C:189:GLN:C	2.54	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:O:49:VAL:HG13	2:O:51:ASP:H	1.81	0.45
2:P:49:VAL:HG13	2:P:51:ASP:H	1.81	0.45
2:T:18:MET:CE	2:T:46:GLU:HB2	2.45	0.45
1:A:205:VAL:CG1	1:A:212:MET:HB2	2.31	0.45
1:B:148:LEU:CD1	1:B:224:VAL:HG21	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:J:205:VAL:O	1:J:210:GLN:HA	2.16	0.45
1:D:79:ARG:HB3	1:D:79:ARG:NH1	2.31	0.45
1:F:111:ALA:HB3	1:F:158:LYS:HD3	1.99	0.45
1:I:209:VAL:CG1	1:I:211:LYS:HE2	2.45	0.45
1:J:148:LEU:HD12	1:J:224:VAL:HG21	1.97	0.45
2:K:9:GLN:O	2:K:11:ARG:N	2.46	0.45
1:D:72:SER:HB2	1:G:62:LEU:CD2	2.47	0.45
2:M:18:MET:HE2	2:M:46:GLU:CD	2.37	0.45
1:B:53:GLU:O	1:B:57:LEU:HG	2.17	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:9:GLN:O	2:T:11:ARG:N	2.47	0.45
2:T:32:LEU:HD11	2:T:60:LEU:HD11	1.98	0.45
1:A:168:ARG:HH22	1:J:206:MET:HB3	1.81	0.45
1:B:69:ILE:HG23	1:I:62:LEU:HD22	1.99	0.45
1:C:168:ARG:NH2	1:H:206:MET:HB3	2.32	0.45
1:F:234:GLU:OE2	1:J:232:ARG:HD3	2.15	0.45
2:M:32:LEU:HD11	2:M:60:LEU:HD11	1.98	0.45
2:P:49:VAL:HG12	2:P:51:ASP:H	1.81	0.45
2:Q:54:ARG:NH1	2:R:21:ASP:OD1	2.50	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
1:H:137:VAL:CG1	1:H:202:MET:HB3	2.47	0.45
2:R:32:LEU:HD11	2:R:60:LEU:HD11	1.98	0.45
1:C:153:VAL:CG1	1:C:154:LEU:N	2.80	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
1:I:79:ARG:HB3	1:I:79:ARG:NH1	2.32	0.45
2:P:43:ASN:N	2:P:43:ASN:ND2	2.64	0.45
2:P:65:PHE:CE2	2:P:83:LYS:HB2	2.51	0.45
2:T:43:ASN:N	2:T:43:ASN:ND2	2.63	0.45
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
1:H:71:ARG:HG3	1:H:77:PRO:HG2	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:VAL:HG12	1:A:154:LEU:N	2.32	0.44
1:H:112:ILE:O	1:H:112:ILE:HG23	2.17	0.44
2:P:43:ASN:ND2	2:P:44:PHE:HD2	2.15	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:C:111:ALA:HB3	1:C:158:LYS:HD3	2.00	0.44
1:E:75:GLU:O	1:E:77:PRO:HD3	2.17	0.44
1:F:59:LEU:HB3	1:F:60:PRO:CD	2.40	0.44
1:F:79:ARG:HB3	1:F:79:ARG:NH1	2.29	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:H:79:ARG:HB3	1:H:79:ARG:NH1	2.30	0.44
2:N:43:ASN:N	2:N:43:ASN:ND2	2.64	0.44
2:O:14:VAL:HG22	2:O:15:GLY:N	2.32	0.44
2:R:18:MET:CE	2:R:46:GLU:HB2	2.44	0.44
1:C:210:GLN:HG2	1:H:129:PHE:HZ	1.82	0.44
1:D:85:THR:HB	1:D:86:PRO:HD3	1.99	0.44
1:F:237:THR:HA	1:F:240:ARG:CZ	2.47	0.44
1:H:111:ALA:HB3	1:H:158:LYS:HD3	2.00	0.44
1:E:168:ARG:NH2	1:F:206:MET:HB3	2.31	0.44
1:G:236:LEU:O	1:G:240:ARG:HB2	2.18	0.44
2:P:18:MET:HE1	2:P:46:GLU:CG	2.48	0.44
1:B:129:PHE:CG	1:I:206:MET:HG2	2.53	0.44
1:C:207:ARG:O	1:C:209:VAL:N	2.41	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:F:164:GLU:CD	1:F:168:ARG:HD2	2.38	0.44
1:J:148:LEU:CD1	1:J:224:VAL:HG21	2.48	0.44
2:O:18:MET:HE3	2:O:46:GLU:CG	2.48	0.44
1:B:76:ASP:C	1:B:78:GLN:H	2.21	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:F:217:VAL:HB	1:G:122:ILE:HB	2.00	0.44
1:G:50:ARG:HB3	1:G:101:GLN:HB3	1.99	0.44
2:N:43:ASN:ND2	2:N:44:PHE:HD2	2.16	0.43
2:Q:32:LEU:HD11	2:Q:60:LEU:HD11	2.00	0.43
2:S:14:VAL:HG22	2:S:15:GLY:N	2.33	0.43
1:E:50:ARG:HB3	1:E:101:GLN:HB3	2.00	0.43
1:G:209:VAL:HG13	1:G:211:LYS:HG3	2.01	0.43
2:Q:49:VAL:HG13	2:Q:51:ASP:H	1.83	0.43
1:C:76:ASP:O	1:C:78:GLN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:236:LEU:O	1:E:240:ARG:HB2	2.17	0.43
1:G:70:LEU:HD21	1:G:82:LEU:HG	2.00	0.43
2:N:38:ARG:HG3	2:N:44:PHE:O	2.19	0.43
1:B:154:LEU:HD23	1:B:155:GLY:H	1.82	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: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:B:150:ASN:HD22	1:B:150:ASN:HA	1.60	0.43
1:H:53:GLU:O	1:H:57:LEU:HG	2.19	0.43
1:H:75:GLU:O	1:H:77:PRO:HD3	2.18	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:A:112:ILE:HG23	1:A:112:ILE:O	2.18	0.43
1:E:129:PHE:HB3	1:F:206:MET:HG2	2.00	0.43
1:E:188:LEU:O	1:E:189:GLN:C	2.56	0.43
1:F:107:VAL:CG1	1:F:158:LYS:HG3	2.49	0.43
1:F:207:ARG:HG2	1:F:207:ARG:NH1	2.34	0.43
1:A:107:VAL:HG12	1:A:158:LYS:HG3	2.01	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: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
1:I:112:ILE:HD11	1:I:152:GLN:CD	2.39	0.43
2:P:24:SER:OG	2:T:54:ARG:NH1	2.49	0.43
1:A:209:VAL:HG22	1:I:210:GLN:HB2	2.01	0.42
1:B:207:ARG:HG2	1:B:207:ARG:NH1	2.34	0.42
1:C:237:THR:HA	1:C:240:ARG:CZ	2.49	0.42
1:I:129:PHE:HB2	1:I:168:ARG:NH2	2.34	0.42
1:I:204:MET:O	1:I:211:LYS:HB2	2.18	0.42
1:J:209:VAL:HG13	1:J:211:LYS:HG3	2.00	0.42
1:A:75:GLU:HG3	1:J:170:LEU:HD12	2.00	0.42
1:A:188:LEU:O	1:A:189:GLN:C	2.58	0.42
1:B:206:MET:HG2	1:I:129:PHE:CB	2.49	0.42
1:F:217:VAL:HG11	1:G:238:LEU:HG	2.01	0.42
1:G:207:ARG:C	1:G:209:VAL:N	2.73	0.42
1:H:65:ALA:O	1:H:69:ILE:HG13	2.19	0.42
1:B:72:SER:HB2	1:I:62:LEU:HD21	2.01	0.42
1:C:62:LEU:HD22	1:H:69:ILE:HG23	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:LEU:HB2	1:C:188:LEU:HD11	2.02	0.42
1:D:111:ALA:CB	1:D:158:LYS:HE3	2.49	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:E:204:MET:CE	1:E:211:LYS:HD3	2.46	0.42
2:K:18:MET:HE3	2:K:46:GLU:CG	2.50	0.42
2:L:73:VAL:O	2:L:73:VAL:HG13	2.19	0.42
2:N:18:MET:HE3	2:N:46:GLU:CB	2.46	0.42
1:E:150:ASN:HD22	1:E:150:ASN:HA	1.62	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
2:T:73:VAL:O	2:T:73:VAL:HG13	2.18	0.42
1:A:107:VAL:HG22	1:A:161:ARG:CD	2.44	0.42
1:A:129:PHE:CG	1:J:206:MET:HG2	2.55	0.42
1:B:211:LYS:HE3	1:C:160:ALA:HB1	2.02	0.42
1:D:112:ILE:HG23	1:D:112:ILE:O	2.20	0.42
1:H:66:TYR:CD2	1:H:69:ILE:HD12	2.54	0.42
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:E:63:ALA:O	1:E:86:PRO:HB3	2.19	0.42
1:F:82:LEU:HA	1:F:82:LEU:HD12	1.84	0.42
1:G:137:VAL:CG1	1:G:202:MET:HB2	2.50	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:C:111:ALA:HB3	1:C:158:LYS:CG	2.49	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:B:82:LEU:HD12	1:B:82:LEU:HA	1.86	0.42
1:D:76:ASP:C	1:D:78:GLN:H	2.23	0.42
1:D:172:VAL:CG1	1:D:174:GLU:OE1	2.68	0.42
1:G:79:ARG:HB3	1:G:79:ARG:NH1	2.35	0.42
2:L:1:MET:N	5:L:2009:HOH:O	2.49	0.42
2:M:49:VAL:HG13	2:M:51:ASP:H	1.85	0.42
1:B:135:HIS:O	1:B:136:LEU:HB2	2.20	0.42
1:B:154:LEU:HD21	1:B:158:LYS:HB3	2.02	0.42
1:D:168:ARG:NH2	1:G:206:MET:HB3	2.35	0.42
1:G:180:ILE:O	1:G:184:ILE:HG13	2.20	0.42
1:G:215:LYS:HE2	1:G:215:LYS:HB2	1.78	0.42
1:H:120:MET:CE	1:H:231:THR:HG23	2.50	0.42
2:O:83:LYS:HG2	2:O:84:GLU:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:GLY:O	1:A:209:VAL:HB	2.20	0.42
1:B:148:LEU:HD23	1:B:148:LEU:HA	1.92	0.42
1:C:98:LYS:HZ3	1:C:168:ARG:HD3	1.85	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:A:176:LEU:O	1:A:180:ILE:HG13	2.21	0.41
1:D:129:PHE:CZ	1:G:210:GLN:HG2	2.55	0.41
1:E:120:MET:CE	1:E:231:THR:HG23	2.50	0.41
1:E:202:MET:HG2	1:E:206:MET:HE2	2.02	0.41
1:G:164:GLU:HG3	1:G:168:ARG:HG3	2.01	0.41
1:H:207:ARG:O	1:H:209:VAL:N	2.49	0.41
1:I:107:VAL:CG1	1:I:158:LYS:HG3	2.50	0.41
1:A:228:ASP:HA	1:A:229:PRO:HD2	1.92	0.41
1:D:129:PHE:CB	1:G:206:MET:HG2	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
2:O:18:MET:HE1	2:O:46:GLU:CD	2.40	0.41
2:Q:18:MET:HE3	2:Q:46:GLU:CG	2.50	0.41
1:A:133:GLU:CD	1:A:175:ARG:HH22	2.23	0.41
1:B:153:VAL:CG1	1:B:154:LEU:N	2.82	0.41
1:C:226:ARG:HD2	1:C:227:GLU:OE2	2.20	0.41
1:D:189:GLN:N	1:D:190:PRO:HD3	2.36	0.41
1:E:79:ARG:NH2	1:E:82:LEU:HD13	2.35	0.41
1:F:111:ALA:CB	1:F:158:LYS:HE3	2.50	0.41
1:F:142:ARG:HG2	1:F:142:ARG:HH11	1.84	0.41
1:J:76:ASP:C	1:J:78:GLN:H	2.23	0.41
1:J:164:GLU:HG3	1:J:168:ARG:HG3	2.02	0.41
1:I:128:MET:HG2	1:I:143:VAL:HG23	2.02	0.41
2:P:18:MET:HE1	2:P:46:GLU:CB	2.45	0.41
1:B:177:THR:OG1	1:B:197:ILE:HD12	2.21	0.41
1:C:135:HIS:O	1:C:136:LEU:HB2	2.20	0.41
1:G:112:ILE:HD11	1:G:152:GLN:CD	2.41	0.41
1:H:111:ALA:CB	1:H:158:LYS:HE3	2.50	0.41
1:J:104:ILE:O	1:J:104:ILE:HG12	2.21	0.41
1:A:128:MET:HG2	1:A:143:VAL:HG23	2.02	0.41
1:E:129:PHE:HB3	1:F:206:MET:SD	2.61	0.41
1:E:236:LEU:HD23	1:E:236:LEU:HA	1.89	0.41
1:H:154:LEU:HD21	1:H:158:LYS:HB3	2.02	0.41
1:J:79:ARG:NH1	1:J:79:ARG:CB	2.83	0.41
2:N:18:MET:HE1	2:N:46:GLU:CD	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:PHE:CB	1:J:206:MET:HG2	2.50	0.41
1:C:66:TYR:CD2	1:C:69:ILE:HD12	2.56	0.41
1:F:107:VAL:HG22	1:F:161:ARG:CD	2.40	0.41
1:H:154:LEU:HD23	1:H:155:GLY:N	2.36	0.41
1:H:154:LEU:HB2	1:H:188:LEU:HD11	2.01	0.41
2:K:36:LYS:HD2	2:K:47:TYR:CZ	2.56	0.41
2:K:58:ASP:OD1	2:L:2:PRO:HD2	2.21	0.41
2:K:60:LEU:HD12	2:K:60:LEU:HA	1.90	0.41
2:N:54:ARG:NH1	2:O:24:SER:OG	2.53	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
2:P:2:PRO:HD2	2:T:58:ASP:OD1	2.20	0.41
1:B:237:THR:HA	1:B:240:ARG:CZ	2.51	0.41
1:C:207:ARG:C	1:C:209:VAL:N	2.73	0.41
1:C:232:ARG:HD3	1:D:234:GLU:OE2	2.21	0.41
1:D:66:TYR:HD2	1:D:69:ILE:HD12	1.86	0.41
1:D:82:LEU:HD12	1:D:82:LEU:HA	1.89	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:E:207:ARG:C	1:E:209:VAL:N	2.74	0.41
1:F:128:MET:HG2	1:F:143:VAL:CG2	2.51	0.41
1:F:140:VAL:HG12	1:F:141:GLY:N	2.36	0.41
1:F:204:MET:CE	1:F:211:LYS:HD3	2.48	0.41
1:G:112:ILE:HG23	1:G:112:ILE:O	2.21	0.41
1:H:85:THR:HB	1:H:86:PRO:HD3	2.03	0.41
1:H:215:LYS:HE2	1:H:215:LYS:HB2	1.87	0.41
1:I:63:ALA:O	1:I:86:PRO:HB3	2.21	0.41
1:I:185:THR:OG1	1:I:193:VAL:HG11	2.21	0.41
1:J:189:GLN:N	1:J:190:PRO:CD	2.84	0.41
2:K:43:ASN:ND2	2:K:44:PHE:HD2	2.19	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: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
1:F:188:LEU:O	1:F:189:GLN:C	2.59	0.41
2:S:43:ASN:N	2:S:43:ASN:ND2	2.67	0.41
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:C:123:VAL:HG21	1:C:159:LEU:CD2	2.51	0.40
1:F:209:VAL:HG13	1:F:211:LYS:HG3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:148:LEU:CD1	1:H:224:VAL:HG21	2.47	0.40
1:A:62:LEU:HD21	1:J:72:SER:HB2	2.04	0.40
1:A:236:LEU:O	1:A:240:ARG:HB2	2.21	0.40
1:E:71:ARG:HG3	1:E:77:PRO:HG2	2.02	0.40
1:E:215:LYS:HB2	1:E:215:LYS:HE2	1.90	0.40
1:J:63:ALA:O	1:J:86:PRO:HB3	2.21	0.40
1:J:132:CYS:SG	1:J:134:HIS:HB2	2.61	0.40
1:J:164:GLU:O	1:J:168:ARG:HG3	2.21	0.40
2:R:65:PHE:CE2	2:R:83:LYS:HB2	2.56	0.40
1:E:164:GLU:HG3	1:E:168:ARG:HG3	2.04	0.40
1:F:182:VAL:O	1:F:186:GLU:HG3	2.21	0.40
1:G:208:GLY:O	1:G:209:VAL:HB	2.21	0.40
1:I:112:ILE:HD11	1:I:152:GLN:NE2	2.35	0.40
1:J:123:VAL:CG1	1:J:126:ILE:HD11	2.52	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:C:78:GLN:NE2	5:C:246:HOH:O	2.54	0.40
1:C:217:VAL:HB	1:D:122:ILE:HB	2.02	0.40
1:E:107:VAL:CG1	1:E:158:LYS:HG3	2.52	0.40
1:I:76:ASP:C	1:I:78:GLN:N	2.74	0.40
1:I:153:VAL:HG12	1:I:154:LEU:N	2.37	0.40
1:J:238:LEU:HD12	1:J:238:LEU:HA	1.90	0.40
2:L:75:GLN:OE1	4:L:1010:PHE:N	2.53	0.40
2:M:14:VAL:CG2	2:M:15:GLY:N	2.84	0.40
1:A:189:GLN:N	1:A:190:PRO:CD	2.85	0.40
1:D:148:LEU:HD12	1:D:224:VAL:CG2	2.50	0.40
1:D:206:MET:SD	1:G:129:PHE:HB3	2.61	0.40
1:E:209:VAL:CG2	1:J:209:VAL:HG23	2.51	0.40
1:I:71:ARG:HG3	1:I:77:PRO:HG3	2.02	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	Interatomic distance (Å)	Clash overlap (Å)
2:Q:30:GLN:NE2	2:T:45:TYR:OH[2_556]	2.01	0.19

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	192/230 (84%)	171 (89%)	17 (9%)	4 (2%)	7	23
1	B	192/230 (84%)	168 (88%)	21 (11%)	3 (2%)	9	31
1	C	192/230 (84%)	169 (88%)	19 (10%)	4 (2%)	7	23
1	D	192/230 (84%)	171 (89%)	18 (9%)	3 (2%)	9	31
1	E	192/230 (84%)	169 (88%)	20 (10%)	3 (2%)	9	31
1	F	192/230 (84%)	169 (88%)	19 (10%)	4 (2%)	7	23
1	G	192/230 (84%)	168 (88%)	21 (11%)	3 (2%)	9	31
1	H	192/230 (84%)	172 (90%)	15 (8%)	5 (3%)	5	18
1	I	192/230 (84%)	169 (88%)	19 (10%)	4 (2%)	7	23
1	J	192/230 (84%)	169 (88%)	20 (10%)	3 (2%)	9	31
2	K	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	13	39
2	L	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	13	39
2	M	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	13	39
2	N	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	13	39
2	O	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	13	39
2	P	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	13	39
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%)	13	39
2	T	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
All	All	2740/3140 (87%)	2475 (90%)	222 (8%)	43 (2%)	9	31

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	108	LEU

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Mol	Chain	Res	Type
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
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	170/196 (87%)	160 (94%)	10 (6%)	19	49
1	B	170/196 (87%)	160 (94%)	10 (6%)	19	49
1	C	170/196 (87%)	159 (94%)	11 (6%)	17	44
1	D	170/196 (87%)	159 (94%)	11 (6%)	17	44
1	E	170/196 (87%)	161 (95%)	9 (5%)	22	54
1	F	170/196 (87%)	160 (94%)	10 (6%)	19	49
1	G	170/196 (87%)	160 (94%)	10 (6%)	19	49
1	H	170/196 (87%)	159 (94%)	11 (6%)	17	44
1	I	170/196 (87%)	160 (94%)	10 (6%)	19	49
1	J	170/196 (87%)	161 (95%)	9 (5%)	22	54
2	K	76/76 (100%)	72 (95%)	4 (5%)	22	54
2	L	76/76 (100%)	72 (95%)	4 (5%)	22	54
2	M	76/76 (100%)	72 (95%)	4 (5%)	22	54
2	N	76/76 (100%)	72 (95%)	4 (5%)	22	54
2	O	76/76 (100%)	72 (95%)	4 (5%)	22	54
2	P	76/76 (100%)	72 (95%)	4 (5%)	22	54
2	Q	76/76 (100%)	72 (95%)	4 (5%)	22	54
2	R	76/76 (100%)	72 (95%)	4 (5%)	22	54
2	S	76/76 (100%)	72 (95%)	4 (5%)	22	54
2	T	76/76 (100%)	72 (95%)	4 (5%)	22	54
All	All	2460/2720 (90%)	2319 (94%)	141 (6%)	20	50

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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

Sometimes 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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	T	1005	-	11,12,12	0.65	0	14,15,15	0.65	0
4	PHE	R	1002	-	11,12,12	0.59	0	14,15,15	0.65	0
4	PHE	R	1001	-	11,12,12	0.68	0	14,15,15	0.51	0
4	PHE	P	1003	-	11,12,12	0.75	0	14,15,15	0.53	0
4	PHE	O	1008	-	11,12,12	0.66	0	14,15,15	0.55	0
4	PHE	M	1006	-	11,12,12	0.60	0	14,15,15	0.60	0
4	PHE	N	1007	-	11,12,12	0.71	0	14,15,15	0.63	0
4	PHE	S	1004	-	11,12,12	0.63	0	14,15,15	0.50	0
4	PHE	L	1010	-	11,12,12	0.66	0	14,15,15	0.53	0
4	PHE	K	1009	-	11,12,12	0.66	0	14,15,15	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	T	1005	-	-	0/8/8/8	0/1/1/1
4	PHE	R	1002	-	-	6/8/8/8	0/1/1/1
4	PHE	R	1001	-	-	1/8/8/8	0/1/1/1
4	PHE	P	1003	-	-	0/8/8/8	0/1/1/1
4	PHE	O	1008	-	-	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	S	1004	-	-	2/8/8/8	0/1/1/1
4	PHE	L	1010	-	-	0/8/8/8	0/1/1/1
4	PHE	K	1009	-	-	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.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	R	1002	PHE	OXT-C-CA-N
4	R	1002	PHE	CA-CB-CG-CD1
4	R	1002	PHE	N-CA-CB-CG
4	R	1002	PHE	C-CA-CB-CG
4	S	1004	PHE	N-CA-CB-CG
4	R	1002	PHE	CA-CB-CG-CD2

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Mol	Chain	Res	Type	Atoms
4	R	1002	PHE	O-C-CA-N
4	S	1004	PHE	C-CA-CB-CG
4	R	1001	PHE	OXT-C-CA-N

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	1010	PHE	1	0
4	K	1009	PHE	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.06	20 (10%)	6	3	21, 53, 102, 110	0
1	B	194/230 (84%)	0.16	22 (11%)	5	3	22, 55, 101, 110	0
1	C	194/230 (84%)	0.32	28 (14%)	2	1	20, 52, 102, 111	0
1	D	194/230 (84%)	-0.06	10 (5%)	27	18	17, 50, 101, 110	0
1	E	194/230 (84%)	0.06	20 (10%)	6	3	17, 54, 101, 110	0
1	F	194/230 (84%)	0.01	14 (7%)	15	8	17, 53, 102, 111	0
1	G	194/230 (84%)	0.03	14 (7%)	15	8	17, 50, 101, 110	0
1	H	194/230 (84%)	0.11	19 (9%)	7	4	17, 53, 102, 110	0
1	I	194/230 (84%)	0.23	24 (12%)	4	2	21, 56, 101, 110	0
1	J	194/230 (84%)	0.05	17 (8%)	10	5	20, 53, 102, 110	0
2	K	84/84 (100%)	-0.10	4 (4%)	30	21	24, 51, 71, 90	0
2	L	84/84 (100%)	-0.10	5 (5%)	21	14	24, 53, 72, 91	0
2	M	84/84 (100%)	-0.12	1 (1%)	79	73	24, 52, 71, 91	0
2	N	84/84 (100%)	-0.29	1 (1%)	79	73	25, 52, 70, 90	0
2	O	84/84 (100%)	-0.27	2 (2%)	59	49	23, 51, 70, 90	0
2	P	84/84 (100%)	-0.17	2 (2%)	59	49	23, 50, 70, 89	0
2	Q	84/84 (100%)	-0.20	1 (1%)	79	73	22, 50, 68, 89	0
2	R	84/84 (100%)	-0.17	3 (3%)	42	32	24, 50, 71, 90	0
2	S	84/84 (100%)	-0.22	2 (2%)	59	49	21, 52, 70, 89	0
2	T	84/84 (100%)	-0.10	2 (2%)	59	49	23, 50, 71, 90	0
All	All	2780/3140 (88%)	0.02	211 (7%)	13	7	17, 52, 100, 111	0

All (211) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	109	ASN	12.6
1	B	109	ASN	8.1
1	H	109	ASN	7.6
1	G	108	LEU	7.0
1	E	109	ASN	6.8
1	I	109	ASN	6.8
1	D	109	ASN	6.6
1	J	109	ASN	6.6
1	G	109	ASN	6.5
1	F	109	ASN	6.4
1	H	209	VAL	5.9
1	C	49	PRO	5.9
2	M	84	GLU	5.5
1	I	209	VAL	5.4
2	S	84	GLU	5.4
1	C	116	ASP	5.1
1	C	110	ASP	5.1
1	I	48	ARG	5.0
1	H	48	ARG	4.8
1	F	209	VAL	4.7
2	R	84	GLU	4.7
1	J	208	GLY	4.7
1	J	209	VAL	4.7
1	A	110	ASP	4.6
1	H	49	PRO	4.5
1	C	108	LEU	4.5
1	I	241	SER	4.3
1	A	106	ASP	4.3
2	K	84	GLU	4.2
1	B	241	SER	4.2
1	H	241	SER	4.2
1	G	53	GLU	4.2
2	L	84	GLU	4.2
1	C	114	ASP	4.1
1	D	207	ARG	4.1
1	C	51	SER	4.1
1	C	48	ARG	4.1
1	D	106	ASP	4.1
1	E	207	ARG	4.0
1	A	241	SER	4.0
1	A	109	ASN	4.0
1	I	212	MET	4.0
1	B	83	LEU	4.0

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Mol	Chain	Res	Type	RSRZ
2	T	84	GLU	4.0
1	B	108	LEU	3.9
1	B	55	ASN	3.9
1	I	49	PRO	3.9
1	J	108	LEU	3.8
1	B	208	GLY	3.8
1	B	209	VAL	3.8
1	E	108	LEU	3.8
1	F	241	SER	3.8
1	G	210	GLN	3.8
1	F	208	GLY	3.7
1	J	55	ASN	3.7
1	C	56	GLU	3.7
1	C	212	MET	3.7
1	C	83	LEU	3.7
1	G	241	SER	3.7
1	J	116	ASP	3.7
1	G	48	ARG	3.6
1	G	209	VAL	3.6
1	J	210	GLN	3.6
1	F	113	PHE	3.6
1	A	111	ALA	3.6
1	C	209	VAL	3.6
1	C	52	GLU	3.6
1	I	110	ASP	3.6
1	H	210	GLN	3.6
1	B	48	ARG	3.6
1	F	207	ARG	3.6
2	N	84	GLU	3.6
1	B	57	LEU	3.5
1	B	111	ALA	3.5
2	P	1	MET	3.5
1	A	49	PRO	3.4
1	H	52	GLU	3.4
1	I	51	SER	3.4
1	I	52	GLU	3.4
1	E	106	ASP	3.4
1	I	55	ASN	3.4
1	E	205	VAL	3.4
1	C	112	ILE	3.3
1	E	209	VAL	3.3
1	A	56	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	53	GLU	3.3
1	H	208	GLY	3.3
1	F	212	MET	3.3
1	I	78	GLN	3.3
1	A	209	VAL	3.2
1	D	209	VAL	3.2
1	B	212	MET	3.2
1	A	207	ARG	3.2
1	J	106	ASP	3.2
1	H	54	ASP	3.2
1	B	56	GLU	3.2
1	B	207	ARG	3.1
1	C	115	GLU	3.1
1	G	116	ASP	3.1
1	A	108	LEU	3.1
1	C	50	ARG	3.1
1	E	57	LEU	3.1
2	L	30	GLN	3.1
1	I	53	GLU	3.1
1	J	114	ASP	3.1
1	C	55	ASN	3.1
1	D	208	GLY	3.1
1	H	115	GLU	3.0
1	E	241	SER	3.0
1	E	116	ASP	3.0
1	A	208	GLY	3.0
1	I	112	ILE	3.0
1	B	53	GLU	3.0
1	C	206	MET	3.0
1	C	211	LYS	2.9
1	H	108	LEU	2.9
1	H	207	ARG	2.9
1	A	53	GLU	2.9
1	C	106	ASP	2.9
1	G	208	GLY	2.9
1	H	53	GLU	2.9
1	J	48	ARG	2.9
1	B	189	GLN	2.9
2	Q	84	GLU	2.9
1	I	114	ASP	2.8
1	A	57	LEU	2.8
1	B	106	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	210	GLN	2.8
1	E	49	PRO	2.8
1	C	113	PHE	2.8
1	E	208	GLY	2.8
1	J	78	GLN	2.7
1	J	211	LYS	2.7
1	J	56	GLU	2.7
1	C	207	ARG	2.7
1	I	207	ARG	2.7
1	I	57	LEU	2.7
1	F	48	ARG	2.7
1	A	152	GLN	2.7
1	B	49	PRO	2.7
1	D	212	MET	2.6
2	K	83	LYS	2.6
2	O	84	GLU	2.6
1	G	212	MET	2.6
2	L	27	GLU	2.6
1	C	241	SER	2.6
2	P	84	GLU	2.6
1	E	82	LEU	2.6
1	A	114	ASP	2.5
1	I	189	GLN	2.5
1	E	48	ARG	2.5
1	E	212	MET	2.5
1	H	106	ASP	2.5
1	J	241	SER	2.5
1	I	108	LEU	2.5
1	F	106	ASP	2.5
2	K	62	CYS	2.5
1	F	49	PRO	2.4
1	J	212	MET	2.4
1	J	240	ARG	2.4
1	A	48	ARG	2.4
1	E	114	ASP	2.4
1	I	113	PHE	2.4
1	F	53	GLU	2.4
1	A	189	GLN	2.4
1	G	114	ASP	2.4
1	I	54	ASP	2.4
2	R	1	MET	2.4
1	D	52	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	115	GLU	2.3
1	E	240	ARG	2.3
2	S	27	GLU	2.3
1	C	208	GLY	2.3
1	D	241	SER	2.3
1	G	240	ARG	2.3
1	E	102	GLU	2.3
1	B	210	GLN	2.3
1	E	110	ASP	2.3
1	I	116	ASP	2.3
2	K	1	MET	2.3
1	A	212	MET	2.3
1	G	82	LEU	2.3
2	R	27	GLU	2.3
2	L	38	ARG	2.2
1	F	115	GLU	2.2
1	H	189	GLN	2.2
2	L	1	MET	2.2
2	T	1	MET	2.2
1	B	52	GLU	2.2
1	A	240	ARG	2.2
1	I	106	ASP	2.2
1	E	112	ILE	2.2
1	C	54	ASP	2.2
1	D	78	GLN	2.2
1	I	81	GLY	2.1
1	E	78	GLN	2.1
1	I	61	ASN	2.1
2	O	29	MET	2.1
1	B	81	GLY	2.1
1	B	71	ARG	2.1
1	F	80	GLN	2.1
1	H	212	MET	2.1
1	H	103	THR	2.1
1	D	53	GLU	2.1
1	H	105	SER	2.1
1	J	53	GLU	2.1
1	B	78	GLN	2.1
1	C	107	VAL	2.0
1	C	240	ARG	2.0
1	G	110	ASP	2.0
1	H	206	MET	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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(Å^2)	Q<0.9
3	K	R	2001	1/1	0.91	0.10	56,56,56,56	0
3	K	S	2002	1/1	0.92	0.09	53,53,53,53	0
3	K	O	2010	1/1	0.93	0.09	52,52,52,52	0
4	PHE	K	1009	12/12	0.94	0.15	37,40,43,43	0
3	K	L	2007	1/1	0.95	0.07	48,48,48,48	0
4	PHE	O	1008	12/12	0.95	0.14	28,33,34,34	0
3	K	M	2008	1/1	0.96	0.07	43,43,43,43	0
4	PHE	N	1007	12/12	0.96	0.13	20,24,26,28	0
3	K	Q	2005	1/1	0.96	0.05	39,39,39,39	0
4	PHE	R	1001	12/12	0.96	0.13	17,21,23,25	0
4	PHE	R	1002	12/12	0.96	0.13	25,29,33,34	0
4	PHE	M	1006	12/12	0.97	0.10	23,27,30,32	0
3	K	K	2006	1/1	0.97	0.05	48,48,48,48	0
3	K	P	2004	1/1	0.97	0.07	43,43,43,43	0
4	PHE	P	1003	12/12	0.97	0.13	26,27,29,30	0
3	K	N	2009	1/1	0.97	0.06	42,42,42,42	0
4	PHE	L	1010	12/12	0.97	0.13	28,30,31,35	0
4	PHE	S	1004	12/12	0.97	0.12	17,22,26,28	0
4	PHE	T	1005	12/12	0.97	0.12	24,28,32,33	0
3	K	T	2003	1/1	0.98	0.06	38,38,38,38	0

6.5 Other polymers (i)

There are no such residues in this entry.