



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:30 AM UTC

PDB ID : 1IS7 / pdb_00001is7
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 ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

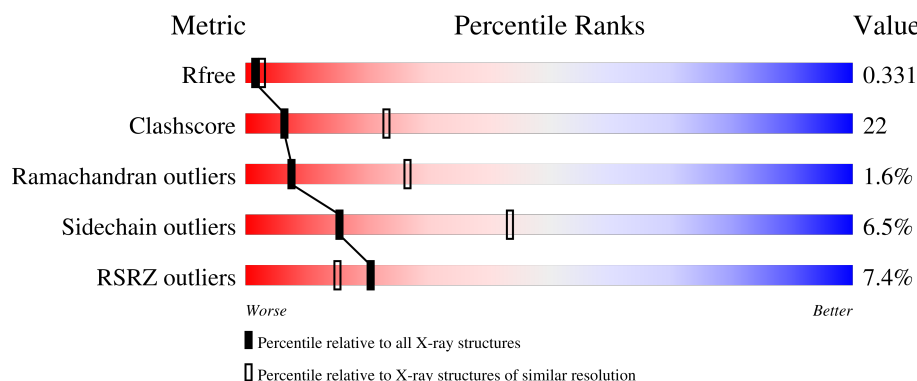
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	230	4% 51% 28% • 16%
1	B	230	7% 53% 27% • 16%
1	C	230	11% 50% 30% • 16%
1	D	230	8% 52% 26% 7% 16%
1	E	230	7% 51% 29% • 16%

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Mol	Chain	Length	Quality of chain
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	
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 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
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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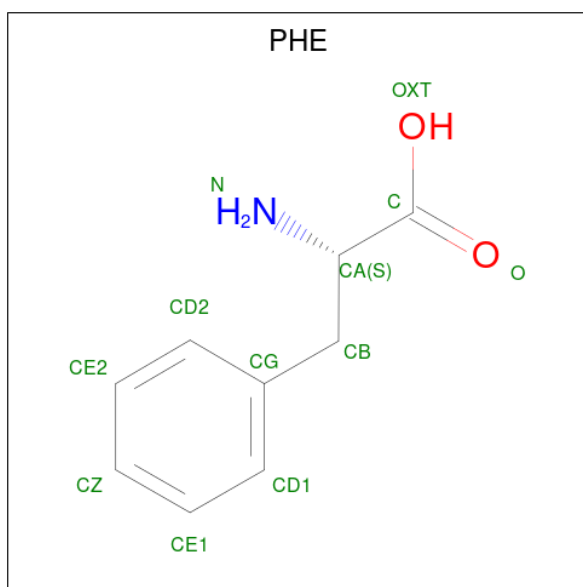
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	84	Total 676	C 428	N 117	O 124	S 7	0	0	0
2	P	84	Total 676	C 428	N 117	O 124	S 7	0	0	0
2	Q	84	Total 676	C 428	N 117	O 124	S 7	0	0	0
2	R	84	Total 676	C 428	N 117	O 124	S 7	0	0	0
2	S	84	Total 676	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 (CCD ID: K) (formula: K).

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

- Molecule 4 is PHENYLALANINE (CCD ID: PHE) (formula: C₉H₁₁NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		
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	P	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	R	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		

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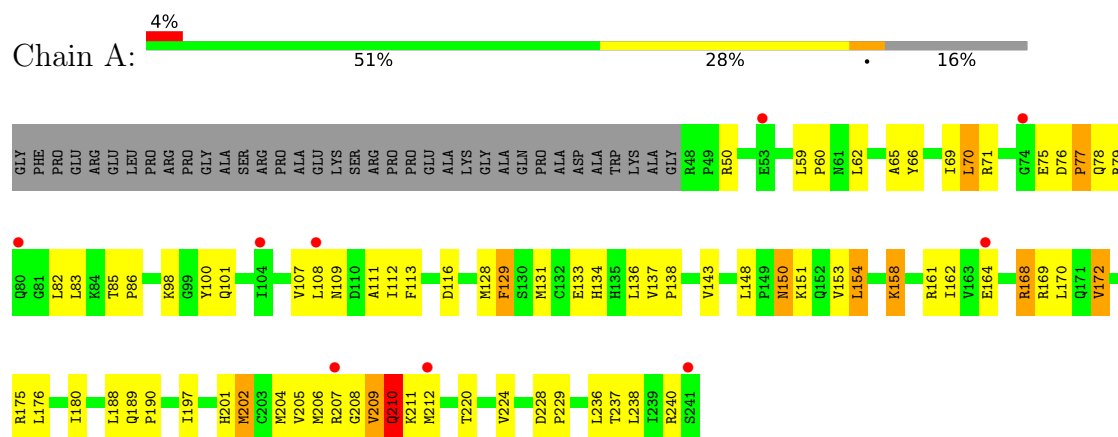
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	5	Total O 5 5	0	0
5	D	4	Total O 4 4	0	0
5	E	6	Total O 6 6	0	0
5	F	6	Total O 6 6	0	0
5	G	9	Total O 9 9	0	0
5	H	5	Total O 5 5	0	0
5	I	3	Total O 3 3	0	0
5	J	4	Total O 4 4	0	0
5	K	8	Total O 8 8	0	0
5	L	9	Total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

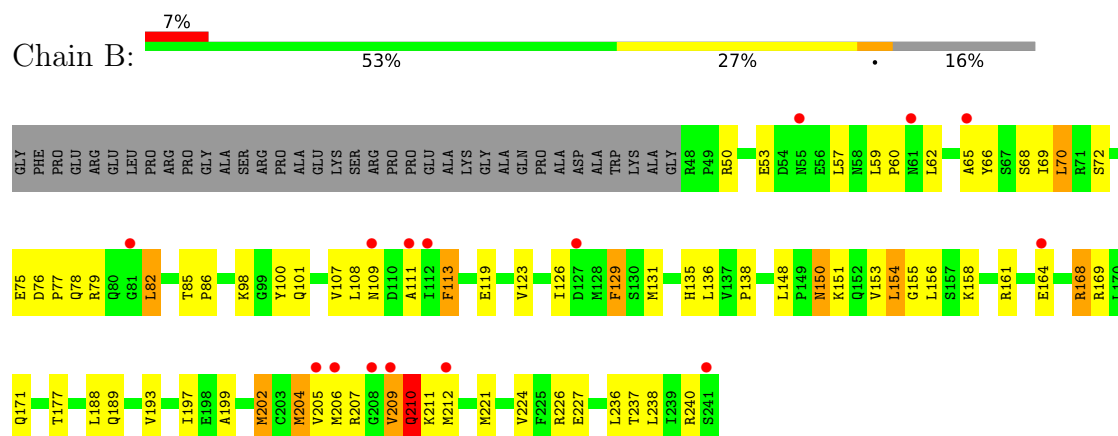
3 Residue-property plots [i](#)

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.

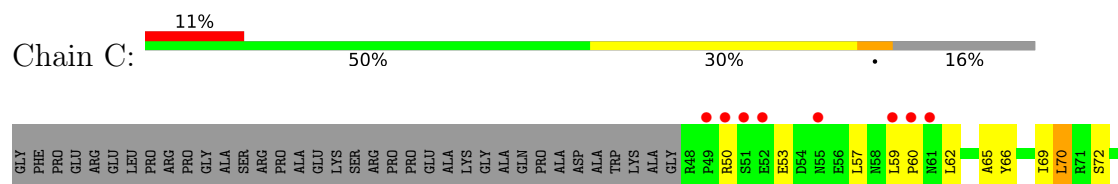
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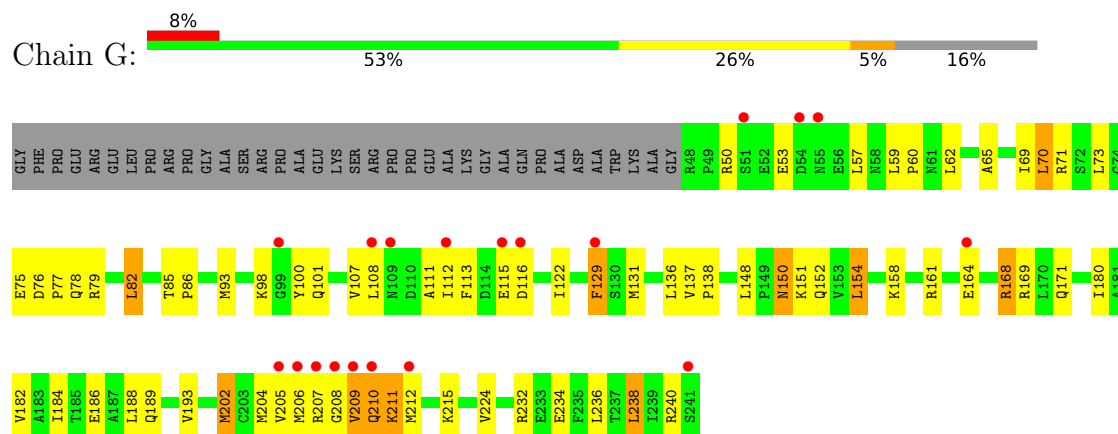
• Molecule 1: GTP Cyclohydrolase I



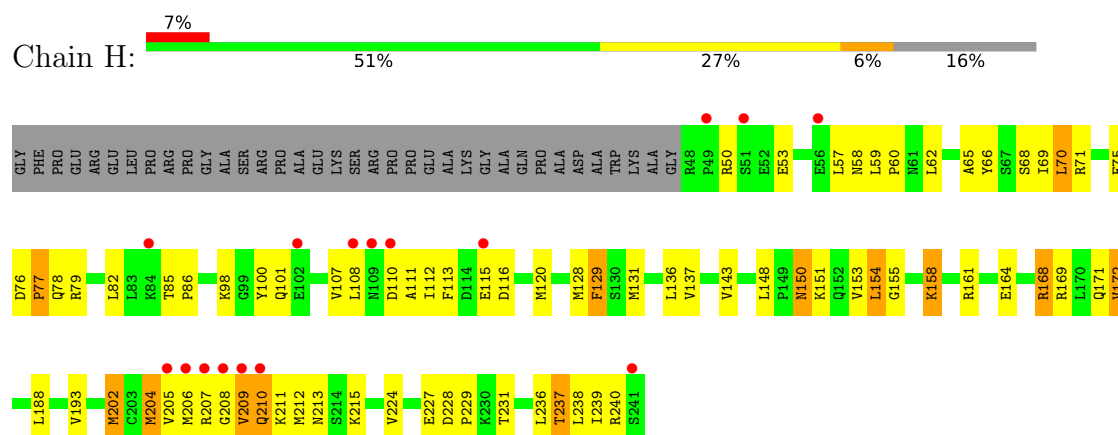
• Molecule 1: GTP Cyclohydrolase I



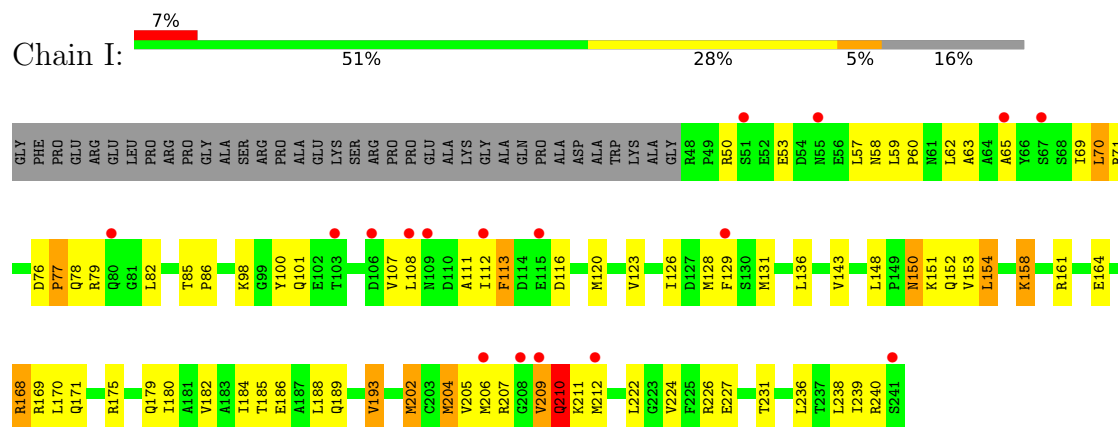
- Molecule 1: GTP Cyclohydrolase I



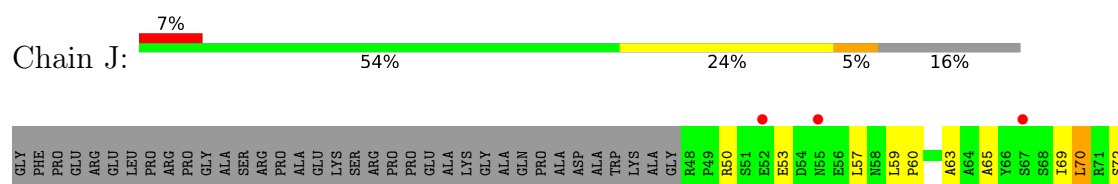
- Molecule 1: GTP Cyclohydrolase I

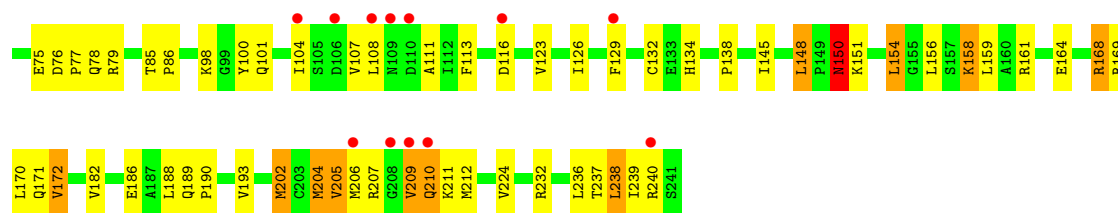


- Molecule 1: GTP Cyclohydrolase I

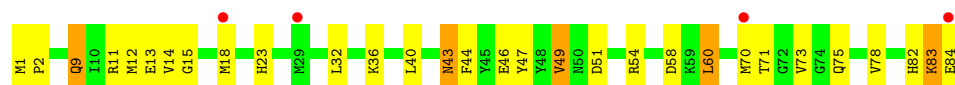


- Molecule 1: GTP Cyclohydrolase I

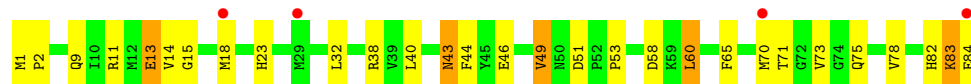




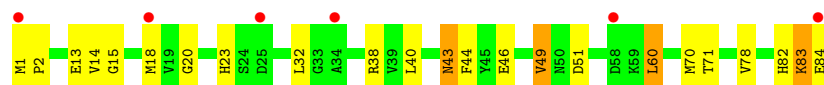
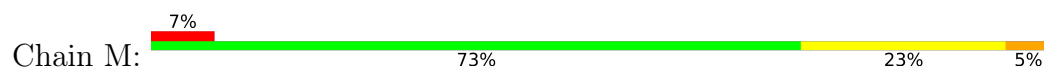
● Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein



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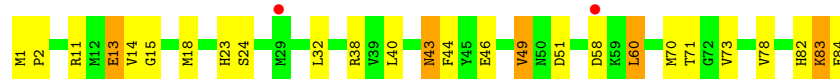
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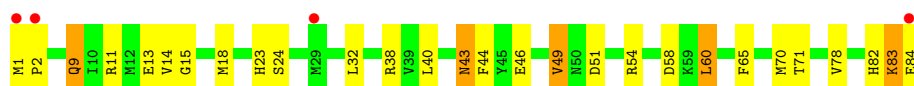


● Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

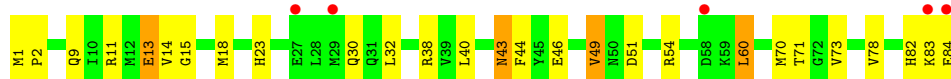


● Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein

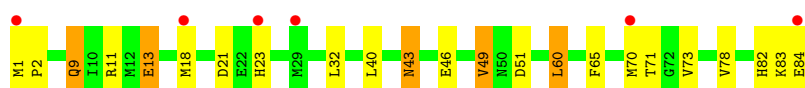
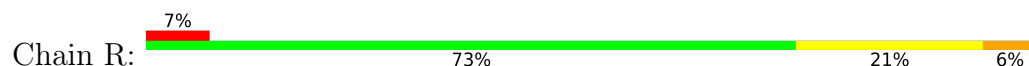




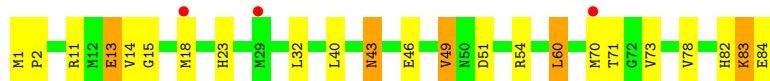
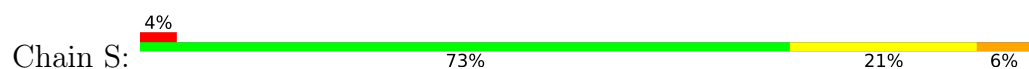
- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein



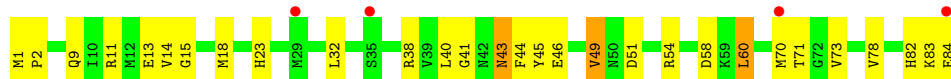
- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein



- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein



- Molecule 2: GTP Cyclohydrolase I Feedback Regulatory Protein



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 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (15.00-2.80) 99.0 (15.00-2.80)	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 0.240 , 0.331	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)	0.36 , 70.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.006 for l,-k,h	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.

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

5 Model quality [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	0.51	0/1561	0.94	2/2107 (0.1%)
1	B	0.52	0/1561	0.95	4/2107 (0.2%)
1	C	0.56	0/1561	0.97	4/2107 (0.2%)
1	D	0.57	0/1561	0.97	4/2107 (0.2%)
1	E	0.55	0/1561	0.95	4/2107 (0.2%)
1	F	0.55	0/1561	0.94	3/2107 (0.1%)
1	G	0.57	0/1561	0.93	2/2107 (0.1%)
1	H	0.54	0/1561	0.96	5/2107 (0.2%)
1	I	0.53	0/1561	0.92	3/2107 (0.1%)
1	J	0.51	0/1561	0.96	6/2107 (0.3%)
2	K	0.47	0/690	0.95	2/931 (0.2%)
2	L	0.46	0/690	0.94	2/931 (0.2%)
2	M	0.50	0/690	0.96	2/931 (0.2%)
2	N	0.57	2/690 (0.3%)	0.93	2/931 (0.2%)
2	O	0.51	0/690	0.93	1/931 (0.1%)
2	P	0.49	0/690	0.92	2/931 (0.2%)
2	Q	0.53	0/690	0.94	2/931 (0.2%)
2	R	0.48	0/690	0.95	2/931 (0.2%)
2	S	0.47	0/690	0.96	1/931 (0.1%)
2	T	0.51	0/690	0.97	1/931 (0.1%)
All	All	0.53	2/22510 (0.0%)	0.95	54/30380 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	29	MET	CG-SD	6.13	1.96	1.80
2	N	29	MET	SD-CE	5.57	1.93	1.79

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	171	GLN	N-CA-C	7.07	118.83	108.86
1	C	171	GLN	N-CA-C	6.54	118.89	109.14
1	G	171	GLN	N-CA-C	6.38	118.25	109.18
2	R	78	VAL	N-CA-C	6.38	117.04	108.11
1	E	171	GLN	N-CA-C	6.30	117.75	108.86
1	J	171	GLN	N-CA-C	6.25	117.67	108.86
2	M	78	VAL	N-CA-C	6.21	116.81	108.11
2	N	78	VAL	N-CA-C	6.16	116.73	108.11
1	F	171	GLN	N-CA-C	6.10	117.46	108.86
1	I	239	ILE	N-CA-C	-6.09	106.29	113.42
2	S	78	VAL	N-CA-C	6.09	116.64	108.11
2	K	9	GLN	N-CA-C	6.01	119.00	109.50
1	A	172	VAL	N-CA-C	-5.94	99.50	108.17
1	C	204	MET	N-CA-C	-5.94	107.02	114.56
2	L	9	GLN	N-CA-C	5.92	118.70	109.52
1	I	171	GLN	N-CA-C	5.91	117.19	108.86
1	A	109	ASN	N-CA-C	5.85	119.24	111.75
1	J	204	MET	N-CA-C	-5.77	105.87	114.64
2	T	78	VAL	N-CA-C	5.76	116.17	108.11
1	B	171	GLN	N-CA-C	5.72	116.92	108.86
1	C	172	VAL	N-CA-C	-5.70	99.29	107.78
1	B	109	ASN	N-CA-C	5.66	119.00	111.75
2	O	78	VAL	N-CA-C	5.65	116.62	108.48
2	R	9	GLN	N-CA-C	5.51	118.20	109.50
2	Q	78	VAL	N-CA-C	5.47	116.36	108.48
1	H	227	GLU	N-CA-C	5.47	119.12	112.23
1	D	204	MET	N-CA-C	-5.42	106.41	114.64
1	H	172	VAL	N-CA-C	-5.39	100.36	108.12
1	J	239	ILE	N-CA-C	-5.38	107.13	113.42
2	L	78	VAL	N-CA-C	5.36	116.20	108.48
1	F	239	ILE	N-CA-C	-5.33	107.18	113.42
1	E	204	MET	N-CA-C	-5.31	106.57	114.64
1	B	199	ALA	N-CA-C	5.29	117.12	109.07
1	H	171	GLN	N-CA-C	5.28	117.01	109.14
2	P	78	VAL	N-CA-C	5.28	116.32	108.46
1	F	204	MET	N-CA-C	-5.28	106.62	114.64
1	D	172	VAL	N-CA-C	-5.27	99.92	107.78
1	B	204	MET	N-CA-C	-5.26	106.64	114.64
1	H	204	MET	N-CA-C	-5.24	106.67	114.64
1	I	204	MET	N-CA-C	-5.22	106.70	114.64
1	J	205	VAL	N-CA-C	-5.18	106.02	110.74
1	G	211	LYS	N-CA-C	5.14	116.58	109.54
2	Q	9	GLN	N-CA-C	5.13	117.47	109.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	239	ILE	N-CA-C	-5.11	107.44	113.42
1	C	109	ASN	N-CA-C	5.10	118.27	111.75
2	K	78	VAL	N-CA-C	5.10	115.82	108.48
1	E	227	GLU	N-CA-C	5.08	118.63	112.23
1	J	150	ASN	N-CA-C	-5.07	101.39	108.54
1	E	122	ILE	N-CA-C	5.05	115.39	108.12
1	J	172	VAL	N-CA-C	-5.04	100.28	107.78
2	M	20	GLY	N-CA-C	5.03	117.83	110.38
1	H	239	ILE	N-CA-C	-5.03	107.54	113.42
2	N	9	GLN	N-CA-C	5.03	117.31	109.52
2	P	9	GLN	N-CA-C	5.02	117.31	109.52

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1536	0	1557	89	0
1	B	1536	0	1557	94	0
1	C	1536	0	1557	89	0
1	D	1536	0	1557	90	0
1	E	1536	0	1557	89	0
1	F	1536	0	1557	96	0
1	G	1536	0	1557	88	0
1	H	1536	0	1557	87	0
1	I	1536	0	1557	89	0
1	J	1536	0	1557	83	0
2	K	676	0	677	25	0
2	L	676	0	677	28	0
2	M	676	0	677	20	0
2	N	676	0	677	21	0
2	O	676	0	677	24	0
2	P	676	0	677	25	0
2	Q	676	0	677	23	1
2	R	676	0	677	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S	676	0	677	20	0
2	T	676	0	677	25	1
3	K	1	0	0	0	0
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	3	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	983	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 22.

All (983) 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:204:MET:HE3	1:G:211:LYS:HD3	1.49	0.92
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:B:204:MET:HE3	1:B:211:LYS:HD3	1.54	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:H:204:MET:HE3	1:H:211:LYS:HD3	1.56	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:202:MET:HG2	1:D:206:MET:HE2	1.60	0.84
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
2:L:18:MET:HE1	2:L:46:GLU:CD	2.04	0.82
1:B:205:VAL:HG22	1:B:212:MET:HA	1.61	0.81
1:J:204:MET:HE3	1:J:211:LYS:HD3	1.60	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
2:R:18:MET:HE1	2:R:46:GLU:CD	2.05	0.81
1:E:59:LEU:HB3	1:E:60:PRO:HD3	1.63	0.81
1:J:202:MET:HG2	1:J:206:MET:HE2	1.61	0.80
2:O:18:MET:HE1	2:O:46:GLU:CD	2.07	0.80
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
2:S:18:MET:HE1	2:S:46:GLU:CD	2.06	0.79
1:E:111:ALA:HB3	1:E:158:LYS:HG2	1.64	0.79
2:T:18:MET:HE1	2:T:46:GLU:CD	2.07	0.78
2:R:70:MET:HE3	2:S:71:THR:HG22	1.64	0.78
1:I:202:MET:HG2	1:I:206:MET:HE2	1.66	0.77
1:A:202:MET:HG2	1:A:206:MET:HE2	1.65	0.77
1:E:204:MET:HE3	1:E:211:LYS:HD3	1.65	0.77
1:B:59:LEU:HB3	1:B:60:PRO:HD3	1.67	0.76
2:M:18:MET:HE1	2:M:46:GLU:CD	2.10	0.76
1:C:204:MET:HE3	1:C:211:LYS:HD3	1.68	0.75
2:P:18:MET:HE1	2:P:46:GLU:CD	2.11	0.75
2:O:43:ASN:HD22	2:O:43:ASN:H	1.33	0.75
2:Q:70:MET:HE3	2:R:71:THR:HG22	1.67	0.75
2:P:71:THR:HG22	2:T:70:MET:HE3	1.69	0.75
2:K:18:MET:HE1	2:K:46:GLU:CD	2.10	0.75
1:H:70:LEU:HB3	1:H:77:PRO:HG3	1.69	0.74
2:K:70:MET:HE3	2:L:71:THR:HG22	1.68	0.74
2:Q:18:MET:HE1	2:Q:46:GLU:CD	2.13	0.74
2:T:43:ASN:HD22	2:T:43:ASN:H	1.35	0.74
1:E:202:MET:HG2	1:E:206:MET:HE2	1.70	0.74
1:A:107:VAL:HG22	1:A:161:ARG:HD3	1.69	0.74
2:N:18:MET:HE1	2:N:46:GLU:CD	2.11	0.74
1:A:148:LEU:HD12	1:A:224:VAL:HG21	1.68	0.73
1:F:204:MET:HE3	1:F:211:LYS:HD3	1.70	0.73
1:E:209:VAL:HG13	1:E:210:GLN:N	2.03	0.72
2:P:70:MET:HE3	2:Q:71:THR:HG22	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:S:70:MET:HE3	2:T:71:THR:HG22	1.71	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:F:202:MET:HG2	1:F:206:MET:HE2	1.71	0.70
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
1:D:204:MET:HE3	1:D:211:LYS:HD3	1.72	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: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: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:H:202:MET:HG2	1:H:206:MET:HE2	1.75	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
1:J:98:LYS:O	1:J:101:GLN:HG2	1.94	0.67
1:F:202:MET:HG2	1:F:206:MET:CE	2.23	0.67
2:K:43:ASN:H	2:K:43:ASN:HD22	1.41	0.67
2:S:18:MET:HE1	2:S:46:GLU:CG	2.25	0.67
1:A:59:LEU:HB3	1:A:60:PRO:HD3	1.76	0.67
1:D:202:MET:HG2	1:D:206:MET:CE	2.24	0.67
2:Q:18:MET:HE1	2:Q:46:GLU:CG	2.24	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
2:L:70:MET:HE3	2:M:71:THR:HG22	1.76	0.67
1:I:85:THR:HB	1:I:86:PRO:HD3	1.77	0.67
2:M:70:MET:HE3	2:N:71:THR:HG22	1.77	0.66
2:N:43:ASN:H	2:N:43:ASN:HD22	1.41	0.66
1:I:202:MET:HG2	1:I:206:MET:CE	2.24	0.66
2:R:18:MET:HE1	2:R:46:GLU:CG	2.24	0.66
1:G:100:TYR:CZ	1:G:169:ARG:HB2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:N:70:MET:HE3	2:O:71:THR:HG22	1.78	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
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
2:K:71:THR:HG22	2:O:70:MET:HE3	1.78	0.64
1:B:131:MET:HE1	1:B:136:LEU:O	1.97	0.64
1:I:150:ASN:O	1:I:151:LYS:HB2	1.98	0.64
2:L:18:MET:HE1	2:L:46:GLU:CG	2.27	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: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:18:MET:HE1	2:O:46:GLU:CG	2.27	0.63
2:O:43:ASN:HD22	2:O:43:ASN:N	1.94	0.63
1:A:202:MET:HG2	1:A:206:MET:CE	2.27	0.63
1:D:111:ALA:HB3	1:D:158:LYS:HG2	1.81	0.63
2:M:18:MET:HE1	2:M:46:GLU:CG	2.28	0.63
1:A:150:ASN:O	1:A:151:LYS:HB2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:MET:HE2	1:C:212:MET:HE3	1.80	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:C:76:ASP:C	1:C:78:GLN:H	2.06	0.63
1:B:202:MET:HG2	1:B:206:MET:HE2	1.80	0.62
1:G:150:ASN:O	1:G:151:LYS:HB2	1.97	0.62
1:G:207:ARG:C	1:G:209:VAL:H	2.07	0.62
1:A:164:GLU:CD	1:A:168:ARG:HD2	2.25	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:C:112:ILE:HD11	1:C:152:GLN:CD	2.25	0.61
1:H:207:ARG:C	1:H:209:VAL:H	2.09	0.61
1:A:205:VAL:HG22	1:A:212:MET:CA	2.25	0.61
1:C:59:LEU:HB3	1:C:60:PRO:HD3	1.82	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:C:207:ARG:C	1:C:209:VAL:H	2.09	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:C:209:VAL:HG13	1:C:210:GLN:N	2.06	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:C:164:GLU:CD	1:C:168:ARG:HD2	2.25	0.60
1:F:111:ALA:HB3	1:F:158:LYS:HG2	1.83	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
1:E:168:ARG:HH22	1:F:206:MET:HB3	1.66	0.60
1:B:207:ARG:C	1:B:209:VAL:H	2.09	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:J:202:MET:HG2	1:J:206:MET:CE	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:207:ARG:C	1:E:209:VAL:H	2.10	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
2:N:18:MET:HE1	2:N:46:GLU:CG	2.32	0.59
2:P:18:MET:HE1	2:P:46:GLU:CG	2.33	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:I:131:MET:HE1	1:I:136:LEU:O	2.03	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:D:207:ARG:C	1:D:209:VAL:H	2.09	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:F:207:ARG:C	1:F:209:VAL:H	2.12	0.58
1:G:111:ALA:HB3	1:G:158:LYS:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:J:207:ARG:C	1:J:209:VAL:H	2.11	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
1:D:65:ALA:O	1:D:69:ILE:HG13	2.04	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: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: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:H:76:ASP:C	1:H:78:GLN:H	2.12	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
2:T:18:MET:HE1	2:T:46:GLU:CG	2.33	0.57
1:A:207:ARG:C	1:A:209:VAL:H	2.12	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
1:I:76:ASP:C	1:I:78:GLN:H	2.12	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
1:J:164:GLU:CD	1:J:168:ARG:HD2	2.30	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: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
1:E:70:LEU:HB3	1:E:77:PRO:HG3	1.87	0.56
1:A:131:MET:HE1	1:A:136:LEU:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:62:LEU:CD2	1:G:69:ILE:HG23	2.35	0.56
1:I:207:ARG:C	1:I:209:VAL:H	2.13	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
2:Q:18:MET:HE1	2:Q:46:GLU:HB2	1.88	0.56
2:R:49:VAL:CG1	2:R:51:ASP:H	2.19	0.56
2:Q:18:MET:CE	2:Q:46:GLU:HB2	2.36	0.56
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:B:98:LYS:NZ	1:B:168:ARG:HD3	2.21	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:B:164:GLU:CD	1:B:168:ARG:HD2	2.31	0.55
1:A:148:LEU:CD1	1:A:224:VAL:HG21	2.36	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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:204:MET:HE3	1:I:211:LYS:HD3	1.87	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
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
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: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
2:K:18:MET:HE1	2:K:46:GLU:CG	2.37	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:E:164:GLU:CD	1:E:168:ARG:HD2	2.33	0.53
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
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:A:76:ASP:C	1:A:78:GLN:H	2.16	0.53
1:E:107:VAL:HG22	1:E:161:ARG:CD	2.32	0.53
1:I:164:GLU:CD	1:I:168:ARG:HD2	2.32	0.53
2:Q:18:MET:HE1	2:Q:46:GLU:CB	2.39	0.53
1:B:98:LYS:O	1:B:101:GLN:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:S:18:MET:CE	2:S:46:GLU:HB2	2.39	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: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
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:J:202:MET:CG	1:J:206:MET:HE2	2.34	0.53
1:A:210:GLN:CB	1:I:210:GLN:HB3	2.19	0.53
1:D:164:GLU:CD	1:D:168:ARG:HD2	2.34	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:A:202:MET:CG	1:A:206:MET:HE2	2.37	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:A:138:PRO:HG3	1:J:206:MET:HE1	1.91	0.52
1:H:202:MET:HG2	1:H:206:MET:CE	2.37	0.52
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:M:18:MET:HE1	2:M:46:GLU:HB2	1.93	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:202:MET:HG2	1:B:206:MET:CE	2.40	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
1:B:111:ALA:HB3	1:B:158:LYS:CG	2.40	0.51
1:F:76:ASP:C	1:F:78:GLN:H	2.19	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
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:K:14:VAL:HG22	2:K:15:GLY:N	2.26	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: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
1:E:209:VAL:HG23	1:J:209:VAL:HG23	1.93	0.51
1:G:76:ASP:C	1:G:78:GLN:H	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:O:18:MET:CE	2:O:46:GLU:HB2	2.40	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:A:204:MET:HE3	1:A:211:LYS:HD3	1.93	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: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
2:P:1:MET:HE1	2:P:23:HIS:O	2.10	0.50
1:B:210:GLN:HG2	1:I:129:PHE:CZ	2.46	0.50
1:C:188:LEU:O	1:C:189:GLN:C	2.54	0.50
1:E:113:PHE:N	1:E:113:PHE:CD1	2.80	0.50
1:G:164:GLU:CD	1:G:168:ARG:HD2	2.36	0.50
1:G:188:LEU:O	1:G:189:GLN:C	2.54	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:76:ASP:C	1:H:78:GLN:N	2.70	0.50
1:H:204:MET:O	1:H:211:LYS:HB2	2.12	0.50
2:M:18:MET:CE	2:M:46:GLU:HB2	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:A:113:PHE:CD1	1:A:113:PHE:N	2.79	0.49
1:A:206:MET:HE1	1:J:138:PRO:HG3	1.92	0.49
1:D:59:LEU:HB3	1:D:60:PRO:CD	2.31	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
2:S:18:MET:HE1	2:S:46:GLU:HB2	1.94	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:78:GLN:O	1:C:79:ARG:C	2.55	0.49
1:C:129:PHE:HZ	1:H:210:GLN:HG2	1.78	0.49
1:C:138:PRO:HG3	1:H:206:MET:HE1	1.93	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
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:F:202:MET:HE2	1:F:212:MET:HE3	1.93	0.49
1:J:150:ASN:O	1:J:151:LYS:HB2	2.13	0.49
2:R:1:MET:HE1	2:R:23:HIS:O	2.12	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: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
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:F:164:GLU:CD	1:F:168:ARG:HD2	2.38	0.48
2:S:18:MET:HE1	2:S:46:GLU:CB	2.43	0.48
1:E:76:ASP:C	1:E:78:GLN:H	2.21	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:L:18:MET:CE	2:L:46:GLU:HB2	2.42	0.48
2:M:18:MET:HE1	2:M:46:GLU:CB	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:204:MET:HE3	1:G:211:LYS:CD	2.32	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:K:12:MET:HE2	5:L:2008:HOH:O	2.13	0.48
2:T:83:LYS:HG2	2:T:84:GLU:N	2.29	0.48
1:C:107:VAL:HG12	1:C:158:LYS:HG3	1.93	0.48
1:E:112:ILE:HG23	1:E:112:ILE:O	2.12	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:C:204:MET:HE3	1:C:211:LYS:CD	2.41	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
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:J:202:MET:HE2	1:J:212:MET:HE3	1.95	0.48
1:C:62:LEU:CD2	1:H:69:ILE:HG23	2.44	0.48
1:C:131:MET:HE1	1:C:136:LEU:O	2.13	0.48
1:D:209:VAL:CG1	1:D:210:GLN:H	2.10	0.48
2:P:14:VAL:HG22	2:P:15:GLY:N	2.27	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
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:E:188:LEU:O	1:E:189:GLN:C	2.56	0.48
1:I:207:ARG:HG2	1:I:207:ARG:HH11	1.78	0.48
1:B:76:ASP:C	1:B:78:GLN:H	2.21	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:1:MET:HE1	2:T:23:HIS:O	2.14	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:B:207:ARG:C	1:B:209:VAL:N	2.72	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
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:F:131:MET:HE1	1:F:136:LEU:O	2.13	0.47
1:I:112:ILE:HD11	1:I:152:GLN:CD	2.39	0.47
1:I:123:VAL:HG12	1:I:126:ILE:HD11	1.97	0.47
1:A:188:LEU:O	1:A:189:GLN:C	2.58	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:B:204:MET:HE3	1:B:211:LYS:CD	2.36	0.47
1:C:206:MET:HG2	1:H:129:PHE:HB3	1.96	0.47
1:D:202:MET:CG	1:D:206:MET:HE2	2.37	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:G:207:ARG:C	1:G:209:VAL:N	2.73	0.47
2:Q:73:VAL:HG13	2:Q:73:VAL:O	2.15	0.47
2:R:18:MET:CE	2:R:46:GLU:HB2	2.44	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
2:K:1:MET:HE1	2:K:23:HIS:O	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:N:1:MET:HE1	2:N:23:HIS:O	2.14	0.47
1:A:154:LEU:HB2	1:A:188:LEU:HD11	1.97	0.47
1:D:76:ASP:C	1:D:78:GLN:H	2.23	0.47
2:O:73:VAL:HG13	2:O:73:VAL:O	2.15	0.47
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:D:131:MET:HE1	1:D:136:LEU:O	2.14	0.46
1:G:85:THR:HB	1:G:86:PRO:HD3	1.96	0.46
2:P:54:ARG:HH22	2:Q:23:HIS:C	2.22	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:J:76:ASP:C	1:J:78:GLN:H	2.23	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
1:J:209:VAL:HG11	1:J:211:LYS:HE2	1.98	0.46
1:A:133:GLU:CD	1:A:175:ARG:HH22	2.23	0.46
1:G:113:PHE:CD1	1:G:113:PHE:N	2.84	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:G:131:MET:HE1	1:G:136:LEU:O	2.16	0.46
1:H:204:MET:HE3	1:H:211:LYS:CD	2.37	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:HB3	1.98	0.46
1:B:206:MET:HG2	1:I:129:PHE:CD2	2.50	0.46
1:E:207:ARG:C	1:E:209:VAL:N	2.74	0.46
1:E:209:VAL:HG12	1:E:211:LYS:HE2	1.97	0.46
1:G:112:ILE:HD11	1:G:152:GLN:CD	2.41	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
2:T:18:MET:CE	2:T:46:GLU:HB2	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:18:MET:HE1	2:L:46:GLU:HB2	1.98	0.46
2:P:58:ASP:OD1	2:Q:2:PRO:HD2	2.16	0.46
1:D:115:GLU:O	1:D:116:ASP:C	2.57	0.46
2:O:1:MET:HE1	2:O:23:HIS:O	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:E:153:VAL:HG12	1:E:154:LEU:N	2.30	0.45
1:H:128:MET:HG2	1:H:143:VAL:CG2	2.47	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:205:VAL:HG22	1:B:212:MET:CA	2.40	0.45
1:C:204:MET:CE	1:C:211:LYS:HD3	2.41	0.45
1:F:188:LEU:O	1:F:189:GLN:C	2.59	0.45
2:L:18:MET:HE1	2:L:46:GLU:CB	2.46	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
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
1:D:70:LEU:HD21	1:D:82:LEU:HG	1.97	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
1:D:204:MET:CE	1:D:211:LYS:HD3	2.45	0.45
1:A:76:ASP:C	1:A:78:GLN:N	2.75	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
1:I:76:ASP:C	1:I:78:GLN:N	2.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N:73:VAL:O	2:N:73:VAL:HG13	2.16	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:H:131:MET:HE1	1:H:136:LEU:O	2.17	0.45
1:I:79:ARG:HB3	1:I:79:ARG:NH1	2.32	0.45
2:O:18:MET:HE1	2:O:46:GLU:HB2	1.99	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: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
1:B:76:ASP:C	1:B:78:GLN:N	2.75	0.44
2:M:1:MET:HE1	2:M:23:HIS:O	2.18	0.44
2:R:11:ARG:HH11	2:R:13:GLU:CD	2.25	0.44
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:11:ARG:HH11	2:S:13:GLU:CD	2.25	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:O:14:VAL:HG22	2:O:15:GLY:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:54:ARG:HH22	2:T:23:HIS:C	2.25	0.44
1:C:210:GLN:HG2	1:H:129:PHE:HZ	1.82	0.44
1:D:58:ASN:O	1:D:59:LEU:C	2.60	0.44
1:D:85:THR:HB	1:D:86:PRO:HD3	1.99	0.44
1:D:207:ARG:C	1:D:209:VAL:N	2.75	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:H:207:ARG:C	1:H:209:VAL:N	2.76	0.44
1:J:207:ARG:C	1:J:209:VAL:N	2.76	0.44
1:E:138:PRO:HG3	1:F:206:MET:HE1	1.98	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
1:B:129:PHE:CG	1:I:206:MET:HG2	2.53	0.44
1:C:202:MET:HG2	1:C:206:MET:HE2	1.98	0.44
1:C:207:ARG:O	1:C:209:VAL:N	2.41	0.44
1:E:85:THR:HB	1:E:86:PRO:HD3	2.00	0.44
1:J:148:LEU:CD1	1:J:224:VAL:HG21	2.48	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
1:G:76:ASP:C	1:G:78:GLN:N	2.76	0.44
2:O:18:MET:HE1	2:O:46:GLU:CB	2.48	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:1:MET:HE1	2:S:23:HIS:O	2.18	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
1:H:58:ASN:O	1:H:59:LEU:C	2.60	0.43
2:Q:11:ARG:HH11	2:Q:13:GLU:CD	2.26	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
1:E:115:GLU:O	1:E:116:ASP:C	2.60	0.43
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:115:GLU:O	1:H:116:ASP:C	2.60	0.43
1:I:58:ASN:O	1:I:59:LEU:C	2.61	0.43
1:J:98:LYS:HZ1	1:J:168:ARG:HD3	1.84	0.43
1:B:150:ASN:HD22	1:B:150:ASN:HA	1.60	0.43
1:G:115:GLU:O	1:G:116:ASP:C	2.60	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:P:23:HIS:C	2:T:54:ARG:HH22	2.26	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: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:J:98:LYS:HZ3	1:J:168:ARG:HD3	1.82	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: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:E:206:MET:HE1	1:F:138:PRO:HG3	2.00	0.43
2:K:54:ARG:HH22	2:L:23:HIS:C	2.27	0.43
2:N:14:VAL:HG22	2:N:15:GLY:N	2.33	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:B:188:LEU:O	1:B:189:GLN:C	2.60	0.42
1:B:206:MET:HG2	1:I:129:PHE:CB	2.49	0.42
1:F:207:ARG:C	1:F:209:VAL:N	2.78	0.42
1:F:217:VAL:HG11	1:G:238:LEU:HG	2.01	0.42
1:H:65:ALA:O	1:H:69:ILE:HG13	2.19	0.42
2:L:1:MET:HE1	2:L:23:HIS:O	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:E:129:PHE:CG	1:F:206:MET:HG2	2.54	0.42
1:E:133:GLU:CD	1:E:175:ARG:HH22	2.27	0.42
2:L:73:VAL:O	2:L:73:VAL:HG13	2.19	0.42
1:D:112:ILE:HD11	1:D:152:GLN:CD	2.44	0.42
1:E:150:ASN:HD22	1:E:150:ASN:HA	1.62	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:A:207:ARG:C	1:A:209:VAL:N	2.77	0.42
1:B:138:PRO:HG3	1:I:206:MET:HE1	2.00	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:I:207:ARG:C	1:I:209:VAL:N	2.78	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:F:115:GLU:O	1:F:116:ASP:C	2.61	0.42
1:H:202:MET:HE2	1:H:212:MET:HE3	2.02	0.42
2:N:11:ARG:HH11	2:N:13:GLU:CD	2.27	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: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:98:LYS:HZ3	1:B:168:ARG:HD3	1.84	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:F:76:ASP:C	1:F:78:GLN:N	2.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N:18:MET:CE	2:N:46:GLU:HB2	2.50	0.42
2:O:83:LYS:HG2	2:O:84:GLU:H	1.85	0.42
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:B:202:MET:HE2	1:B:212:MET:HE3	2.02	0.42
1:C:76:ASP:C	1:C:78:GLN:N	2.72	0.42
1:C:207:ARG:C	1:C:209:VAL:N	2.73	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
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: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:E:112:ILE:HD11	1:E:152:GLN:CD	2.44	0.41
1:H:204:MET:HG2	1:H:211:LYS:HB2	2.01	0.41
1:J:188:LEU:O	1:J:189:GLN:C	2.62	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:164:GLU:HG3	1:J:168:ARG:HG3	2.02	0.41
1:F:208:GLY:C	1:F:209:VAL:HG12	2.45	0.41
1:I:128:MET:HG2	1:I:143:VAL:HG23	2.02	0.41
2:L:11:ARG:HH11	2:L:13:GLU:CD	2.26	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: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
2:Q:1:MET:HE1	2:Q:23:HIS:O	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:P:18:MET:CE	2:P:46:GLU:HB2	2.50	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
2:T:18:MET:HE1	2:T:46:GLU:HB2	2.03	0.41
1:B:237:THR:HA	1:B:240:ARG:CZ	2.51	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:188:LEU:O	1:D:189:GLN:C	2.64	0.41
1:D:189:GLN:N	1:D:190:PRO:CD	2.84	0.41
1:F:128:MET:HG2	1:F:143:VAL:CG2	2.51	0.41
1:G:112:ILE:HG23	1:G:112:ILE:O	2.21	0.41
1:G:208:GLY:C	1:G:209:VAL:HG12	2.46	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:A:220:THR:HA	1:B:119:GLU:CD	2.46	0.41
1:D:206:MET:HG2	1:G:129:PHE:CB	2.50	0.41
1:E:76:ASP:C	1:E:78:GLN:N	2.79	0.41
1:H:208:GLY:C	1:H:209:VAL:HG12	2.46	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:123:VAL:HG21	1:C:159:LEU:CD2	2.51	0.40
1:F:140:VAL:HG12	1:F:141:GLY:N	2.36	0.40
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:H:164:GLU:CD	1:H:168:ARG:HD2	2.46	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:D:76:ASP:C	1:D:78:GLN:N	2.78	0.40
1:E:58:ASN:O	1:E:59:LEU:C	2.62	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:O:11:ARG:HH11	2:O:13:GLU:CD	2.28	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:62:LEU:O	1:F:63:ALA:C	2.65	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: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:188:LEU:O	1:I:189:GLN:C	2.64	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:B:204:MET:CE	1:B:211:LYS:HD3	2.38	0.40
1:D:138:PRO:HG3	1:G:206:MET:HE1	2.04	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:131:MET:HE1	1:E:136:LEU:O	2.22	0.40
1:E:209:VAL:CG2	1:J:209:VAL:HG23	2.51	0.40
1:F:112:ILE:HD11	1:F:152:GLN:CD	2.47	0.40
1:I:71:ARG:HG3	1:I:77:PRO:HG3	2.02	0.40
1:I:153:VAL:HG12	1:I:154:LEU:N	2.37	0.40
1:I:222:LEU:HB3	2:T:41:GLY:HA3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:182:VAL:O	1:J:186:GLU:HG3	2.21	0.40
2:L:13:GLU:CD	2:L:13:GLU:H	2.29	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%)	5	20
1	B	192/230 (84%)	168 (88%)	21 (11%)	3 (2%)	7	27
1	C	192/230 (84%)	169 (88%)	19 (10%)	4 (2%)	5	20
1	D	192/230 (84%)	171 (89%)	18 (9%)	3 (2%)	7	27
1	E	192/230 (84%)	169 (88%)	20 (10%)	3 (2%)	7	27
1	F	192/230 (84%)	169 (88%)	19 (10%)	4 (2%)	5	20
1	G	192/230 (84%)	168 (88%)	21 (11%)	3 (2%)	7	27
1	H	192/230 (84%)	172 (90%)	15 (8%)	5 (3%)	4	15
1	I	192/230 (84%)	169 (88%)	19 (10%)	4 (2%)	5	20
1	J	192/230 (84%)	169 (88%)	20 (10%)	3 (2%)	7	27
2	K	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	10	34
2	L	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	10	34
2	M	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	10	34
2	N	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	10	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	O	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	10	34
2	P	82/84 (98%)	78 (95%)	3 (4%)	1 (1%)	10	34
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%)	10	34
2	T	82/84 (98%)	78 (95%)	4 (5%)	0	100	100
All	All	2740/3140 (87%)	2475 (90%)	222 (8%)	43 (2%)	7	27

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
1	I	210	GLN
1	A	210	GLN
1	D	210	GLN
1	G	210	GLN

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Mol	Chain	Res	Type
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%)	161 (95%)	9 (5%)	20	52
1	B	170/196 (87%)	159 (94%)	11 (6%)	15	43
1	C	170/196 (87%)	160 (94%)	10 (6%)	18	48
1	D	170/196 (87%)	157 (92%)	13 (8%)	12	36
1	E	170/196 (87%)	158 (93%)	12 (7%)	13	39
1	F	170/196 (87%)	159 (94%)	11 (6%)	15	43
1	G	170/196 (87%)	161 (95%)	9 (5%)	20	52
1	H	170/196 (87%)	157 (92%)	13 (8%)	12	36
1	I	170/196 (87%)	159 (94%)	11 (6%)	15	43
1	J	170/196 (87%)	159 (94%)	11 (6%)	15	43
2	K	76/76 (100%)	71 (93%)	5 (7%)	15	43
2	L	76/76 (100%)	71 (93%)	5 (7%)	15	43
2	M	76/76 (100%)	71 (93%)	5 (7%)	15	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	N	76/76 (100%)	71 (93%)	5 (7%)	15	43
2	O	76/76 (100%)	71 (93%)	5 (7%)	15	43
2	P	76/76 (100%)	71 (93%)	5 (7%)	15	43
2	Q	76/76 (100%)	71 (93%)	5 (7%)	15	43
2	R	76/76 (100%)	71 (93%)	5 (7%)	15	43
2	S	76/76 (100%)	71 (93%)	5 (7%)	15	43
2	T	76/76 (100%)	71 (93%)	5 (7%)	15	43
All	All	2460/2720 (90%)	2300 (94%)	160 (6%)	15	43

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	LEU
1	A	129	PHE
1	A	150	ASN
1	A	154	LEU
1	A	158	LYS
1	A	168	ARG
1	A	202	MET
1	A	210	GLN
1	A	238	LEU
1	B	70	LEU
1	B	82	LEU
1	B	113	PHE
1	B	129	PHE
1	B	150	ASN
1	B	154	LEU
1	B	168	ARG
1	B	193	VAL
1	B	202	MET
1	B	210	GLN
1	B	238	LEU
1	C	70	LEU
1	C	82	LEU
1	C	150	ASN
1	C	154	LEU
1	C	168	ARG
1	C	172	VAL
1	C	190	PRO
1	C	193	VAL

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Mol	Chain	Res	Type
1	C	202	MET
1	C	238	LEU
1	D	60	PRO
1	D	70	LEU
1	D	82	LEU
1	D	113	PHE
1	D	129	PHE
1	D	150	ASN
1	D	154	LEU
1	D	158	LYS
1	D	168	ARG
1	D	193	VAL
1	D	202	MET
1	D	215	LYS
1	D	238	LEU
1	E	72	SER
1	E	82	LEU
1	E	129	PHE
1	E	150	ASN
1	E	154	LEU
1	E	158	LYS
1	E	168	ARG
1	E	193	VAL
1	E	200	THR
1	E	202	MET
1	E	210	GLN
1	E	238	LEU
1	F	70	LEU
1	F	82	LEU
1	F	129	PHE
1	F	150	ASN
1	F	154	LEU
1	F	158	LYS
1	F	168	ARG
1	F	193	VAL
1	F	202	MET
1	F	210	GLN
1	F	238	LEU
1	G	70	LEU
1	G	82	LEU
1	G	129	PHE
1	G	150	ASN

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Mol	Chain	Res	Type
1	G	154	LEU
1	G	168	ARG
1	G	193	VAL
1	G	202	MET
1	G	238	LEU
1	H	70	LEU
1	H	82	LEU
1	H	129	PHE
1	H	150	ASN
1	H	154	LEU
1	H	158	LYS
1	H	168	ARG
1	H	172	VAL
1	H	193	VAL
1	H	202	MET
1	H	213	ASN
1	H	237	THR
1	H	238	LEU
1	I	70	LEU
1	I	82	LEU
1	I	113	PHE
1	I	150	ASN
1	I	154	LEU
1	I	158	LYS
1	I	168	ARG
1	I	193	VAL
1	I	202	MET
1	I	210	GLN
1	I	238	LEU
1	J	70	LEU
1	J	148	LEU
1	J	150	ASN
1	J	154	LEU
1	J	156	LEU
1	J	158	LYS
1	J	168	ARG
1	J	172	VAL
1	J	193	VAL
1	J	202	MET
1	J	238	LEU
2	K	13	GLU
2	K	40	LEU

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Mol	Chain	Res	Type
2	K	43	ASN
2	K	49	VAL
2	K	60	LEU
2	L	13	GLU
2	L	40	LEU
2	L	43	ASN
2	L	49	VAL
2	L	60	LEU
2	M	13	GLU
2	M	40	LEU
2	M	43	ASN
2	M	49	VAL
2	M	60	LEU
2	N	13	GLU
2	N	40	LEU
2	N	43	ASN
2	N	49	VAL
2	N	60	LEU
2	O	13	GLU
2	O	40	LEU
2	O	43	ASN
2	O	49	VAL
2	O	60	LEU
2	P	13	GLU
2	P	40	LEU
2	P	43	ASN
2	P	49	VAL
2	P	60	LEU
2	Q	13	GLU
2	Q	40	LEU
2	Q	43	ASN
2	Q	49	VAL
2	Q	60	LEU
2	R	13	GLU
2	R	40	LEU
2	R	43	ASN
2	R	49	VAL
2	R	60	LEU
2	S	13	GLU
2	S	40	LEU
2	S	43	ASN
2	S	49	VAL

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Mol	Chain	Res	Type
2	S	60	LEU
2	T	13	GLU
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 (90) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	94	GLN
1	A	134	HIS
1	A	150	ASN
1	A	210	GLN
1	A	213	ASN
1	B	94	GLN
1	B	117	HIS
1	B	134	HIS
1	B	150	ASN
1	B	210	GLN
1	B	213	ASN
1	C	94	GLN
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	210	GLN
1	D	213	ASN
1	E	150	ASN
1	E	210	GLN
1	E	213	ASN
1	F	150	ASN
1	F	152	GLN
1	F	213	ASN
1	G	55	ASN
1	G	94	GLN
1	G	150	ASN
1	G	189	GLN
1	G	210	GLN

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Mol	Chain	Res	Type
1	G	213	ASN
1	H	55	ASN
1	H	94	GLN
1	H	134	HIS
1	H	150	ASN
1	H	210	GLN
1	H	213	ASN
1	I	55	ASN
1	I	94	GLN
1	I	101	GLN
1	I	134	HIS
1	I	150	ASN
1	I	152	GLN
1	I	210	GLN
1	I	213	ASN
1	J	94	GLN
1	J	150	ASN
1	J	210	GLN
1	J	213	ASN
2	K	9	GLN
2	K	42	ASN
2	K	43	ASN
2	K	75	GLN
2	K	82	HIS
2	L	9	GLN
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	N	82	HIS
2	O	42	ASN
2	O	43	ASN
2	O	82	HIS
2	P	42	ASN
2	P	43	ASN

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Mol	Chain	Res	Type
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	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 oligosaccharides 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	0.68	0	11,15,15	0.33	0
4	PHE	N	1007	-	11,12,12	0.75	0	11,15,15	0.29	0
4	PHE	M	1006	-	11,12,12	0.63	0	11,15,15	0.26	0
4	PHE	S	1004	-	11,12,12	0.65	0	11,15,15	0.24	0
4	PHE	L	1010	-	11,12,12	0.70	0	11,15,15	0.24	0
4	PHE	P	1003	-	11,12,12	0.79	0	11,15,15	0.24	0
4	PHE	R	1002	-	11,12,12	0.61	0	11,15,15	0.33	0
4	PHE	O	1008	-	11,12,12	0.70	0	11,15,15	0.29	0
4	PHE	R	1001	-	11,12,12	0.71	0	11,15,15	0.29	0
4	PHE	K	1009	-	11,12,12	0.70	0	11,15,15	0.21	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	N	1007	-	-	0/8/8/8	0/1/1/1
4	PHE	M	1006	-	-	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	P	1003	-	-	0/8/8/8	0/1/1/1
4	PHE	R	1002	-	-	6/8/8/8	0/1/1/1
4	PHE	O	1008	-	-	0/8/8/8	0/1/1/1
4	PHE	R	1001	-	-	1/8/8/8	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	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-CD1
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 ⓘ

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%)	0.34	9 (4%) 37 29	21, 53, 102, 110	0
1	B	194/230 (84%)	0.39	15 (7%) 19 14	22, 55, 101, 110	0
1	C	194/230 (84%)	0.56	26 (13%) 7 5	20, 52, 102, 111	0
1	D	194/230 (84%)	0.42	19 (9%) 13 9	17, 50, 101, 110	0
1	E	194/230 (84%)	0.39	16 (8%) 17 13	17, 54, 101, 110	0
1	F	194/230 (84%)	0.34	13 (6%) 24 17	17, 53, 102, 111	0
1	G	194/230 (84%)	0.44	19 (9%) 13 9	17, 50, 101, 110	0
1	H	194/230 (84%)	0.37	16 (8%) 17 13	17, 53, 102, 110	0
1	I	194/230 (84%)	0.41	17 (8%) 15 11	21, 56, 101, 110	0
1	J	194/230 (84%)	0.33	15 (7%) 19 14	20, 53, 102, 110	0
2	K	84/84 (100%)	0.30	4 (4%) 35 28	24, 51, 71, 90	0
2	L	84/84 (100%)	0.27	4 (4%) 35 28	24, 53, 72, 91	0
2	M	84/84 (100%)	0.25	6 (7%) 22 16	24, 52, 71, 91	0
2	N	84/84 (100%)	0.17	4 (4%) 35 28	25, 52, 70, 90	0
2	O	84/84 (100%)	0.20	2 (2%) 59 49	23, 51, 70, 90	0
2	P	84/84 (100%)	0.23	4 (4%) 35 28	23, 50, 70, 89	0
2	Q	84/84 (100%)	0.33	5 (5%) 27 21	22, 50, 68, 89	0
2	R	84/84 (100%)	0.21	6 (7%) 22 16	24, 50, 71, 90	0
2	S	84/84 (100%)	0.13	3 (3%) 46 37	21, 52, 70, 89	0
2	T	84/84 (100%)	0.44	4 (4%) 35 28	23, 50, 71, 90	0
All	All	2780/3140 (88%)	0.35	207 (7%) 20 15	17, 52, 100, 111	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	55	ASN	5.4
1	E	109	ASN	5.3
1	G	109	ASN	5.3
1	C	106	ASP	4.5
1	I	109	ASN	4.3
1	C	51	SER	4.3
1	C	209	VAL	3.9
1	D	109	ASN	3.9
1	G	209	VAL	3.9
1	F	241	SER	3.9
1	D	208	GLY	3.8
1	F	212	MET	3.8
1	G	210	GLN	3.7
1	J	108	LEU	3.7
1	I	241	SER	3.7
1	C	59	LEU	3.6
1	A	80	GLN	3.6
1	H	241	SER	3.6
1	G	207	ARG	3.5
1	G	115	GLU	3.5
1	E	108	LEU	3.5
2	O	29	MET	3.5
1	G	205	VAL	3.5
1	E	205	VAL	3.5
1	H	209	VAL	3.5
1	B	241	SER	3.5
1	H	49	PRO	3.5
2	P	2	PRO	3.4
1	G	206	MET	3.3
1	C	208	GLY	3.3
1	G	241	SER	3.3
1	I	67	SER	3.3
1	C	116	ASP	3.3
2	Q	58	ASP	3.3
1	B	109	ASN	3.3
1	G	55	ASN	3.3
2	P	84	GLU	3.3
2	T	84	GLU	3.3
1	G	212	MET	3.3
1	C	109	ASN	3.2
1	J	55	ASN	3.2
1	J	206	MET	3.2
1	B	208	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	209	VAL	3.2
1	C	206	MET	3.2
1	C	212	MET	3.2
1	E	115	GLU	3.2
1	G	108	LEU	3.1
1	J	110	ASP	3.1
1	J	109	ASN	3.1
1	B	209	VAL	3.1
1	B	164	GLU	3.1
2	K	84	GLU	3.1
1	H	206	MET	3.1
1	F	207	ARG	3.1
1	G	129	PHE	3.1
1	J	209	VAL	3.1
1	C	50	ARG	3.1
2	Q	29	MET	3.0
1	H	109	ASN	3.0
1	J	106	ASP	3.0
2	P	1	MET	3.0
1	D	207	ARG	3.0
1	D	240	ARG	3.0
1	I	80	GLN	3.0
1	H	56	GLU	2.9
2	T	35	SER	2.9
2	T	29	MET	2.9
1	J	208	GLY	2.9
1	H	115	GLU	2.9
1	I	112	ILE	2.9
1	E	55	ASN	2.9
1	I	108	LEU	2.9
1	I	212	MET	2.8
2	K	29	MET	2.8
1	E	241	SER	2.8
1	E	208	GLY	2.8
1	A	108	LEU	2.8
1	D	106	ASP	2.8
1	C	108	LEU	2.8
1	I	208	GLY	2.8
1	D	103	THR	2.7
2	O	58	ASP	2.7
1	B	212	MET	2.7
1	C	49	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	J	240	ARG	2.7
2	L	70	MET	2.7
1	E	240	ARG	2.7
1	G	116	ASP	2.7
1	D	205	VAL	2.7
1	B	206	MET	2.7
2	K	70	MET	2.7
2	R	23	HIS	2.7
1	D	55	ASN	2.7
1	B	65	ALA	2.6
2	L	18	MET	2.6
1	C	77	PRO	2.6
1	F	109	ASN	2.6
1	I	55	ASN	2.6
1	C	52	GLU	2.6
1	J	129	PHE	2.6
1	D	87	TRP	2.6
1	F	52	GLU	2.6
1	I	209	VAL	2.6
2	M	25	ASP	2.6
1	D	54	ASP	2.6
1	C	205	VAL	2.6
1	H	205	VAL	2.6
2	T	70	MET	2.6
2	R	84	GLU	2.6
1	F	240	ARG	2.5
2	R	18	MET	2.5
1	C	114	ASP	2.5
1	D	157	SER	2.5
1	I	51	SER	2.5
1	J	67	SER	2.5
1	E	209	VAL	2.5
1	H	102	GLU	2.5
2	L	29	MET	2.5
2	N	29	MET	2.5
2	S	29	MET	2.5
1	F	209	VAL	2.5
2	M	84	GLU	2.5
1	B	127	ASP	2.5
1	E	112	ILE	2.5
1	G	208	GLY	2.5
1	B	111	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	212	MET	2.4
1	E	206	MET	2.4
2	P	29	MET	2.4
1	B	112	ILE	2.4
2	Q	84	GLU	2.4
1	C	80	GLN	2.4
1	F	106	ASP	2.4
1	G	164	GLU	2.4
1	F	80	GLN	2.4
1	E	103	THR	2.4
1	B	81	GLY	2.4
1	C	79	ARG	2.4
1	J	210	GLN	2.4
1	A	212	MET	2.4
1	H	108	LEU	2.4
1	H	207	ARG	2.3
1	D	241	SER	2.3
1	B	61	ASN	2.3
1	D	84	LYS	2.3
2	M	34	ALA	2.3
2	R	29	MET	2.3
2	S	70	MET	2.3
1	A	104	ILE	2.3
1	C	104	ILE	2.3
1	G	51	SER	2.3
1	C	60	PRO	2.3
1	C	113	PHE	2.2
1	E	164	GLU	2.2
2	Q	83	LYS	2.2
1	G	112	ILE	2.2
1	C	103	THR	2.2
1	F	206	MET	2.2
2	M	18	MET	2.2
1	A	164	GLU	2.2
1	D	164	GLU	2.2
1	J	104	ILE	2.2
1	E	129	PHE	2.2
1	C	210	GLN	2.2
2	M	58	ASP	2.2
1	I	206	MET	2.2
2	K	18	MET	2.2
1	C	83	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	115	GLU	2.2
1	I	65	ALA	2.2
2	N	84	GLU	2.2
1	E	207	ARG	2.1
1	B	55	ASN	2.1
1	C	61	ASN	2.1
1	B	205	VAL	2.1
1	F	205	VAL	2.1
1	H	110	ASP	2.1
1	H	51	SER	2.1
2	Q	27	GLU	2.1
1	D	206	MET	2.1
2	M	1	MET	2.1
1	G	54	ASP	2.1
1	G	99	GLY	2.1
2	R	70	MET	2.1
1	I	103	THR	2.1
1	A	207	ARG	2.1
1	F	48	ARG	2.1
1	A	241	SER	2.1
1	H	84	LYS	2.1
1	D	112	ILE	2.1
2	L	84	GLU	2.1
1	E	212	MET	2.0
2	N	2	PRO	2.0
1	A	74	GLY	2.0
1	D	129	PHE	2.0
1	H	208	GLY	2.0
1	I	129	PHE	2.0
1	I	106	ASP	2.0
1	J	116	ASP	2.0
1	A	53	GLU	2.0
1	I	115	GLU	2.0
1	J	52	GLU	2.0
2	N	70	MET	2.0
2	S	18	MET	2.0
1	H	210	GLN	2.0
2	R	1	MET	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 oligosaccharides 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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	K	R	2001	1/1	0.91	0.07	56,56,56,56	0
4	PHE	K	1009	12/12	0.91	0.11	37,40,43,43	0
3	K	S	2002	1/1	0.92	0.08	53,53,53,53	0
3	K	T	2003	1/1	0.93	0.07	38,38,38,38	0
3	K	K	2006	1/1	0.94	0.04	48,48,48,48	0
3	K	O	2010	1/1	0.94	0.06	52,52,52,52	0
4	PHE	O	1008	12/12	0.94	0.08	28,33,34,34	0
4	PHE	R	1002	12/12	0.94	0.08	25,29,33,34	0
3	K	M	2008	1/1	0.95	0.04	43,43,43,43	0
4	PHE	N	1007	12/12	0.95	0.07	20,24,26,28	0
4	PHE	L	1010	12/12	0.96	0.07	28,30,31,35	0
3	K	L	2007	1/1	0.96	0.05	48,48,48,48	0
3	K	Q	2005	1/1	0.96	0.09	39,39,39,39	0
4	PHE	R	1001	12/12	0.96	0.06	17,21,23,25	0
3	K	N	2009	1/1	0.96	0.06	42,42,42,42	0
4	PHE	S	1004	12/12	0.96	0.06	17,22,26,28	0
4	PHE	T	1005	12/12	0.96	0.06	24,28,32,33	0
4	PHE	M	1006	12/12	0.97	0.05	23,27,30,32	0
4	PHE	P	1003	12/12	0.97	0.07	26,27,29,30	0
3	K	P	2004	1/1	0.97	0.04	43,43,43,43	0

6.5 Other polymers ⓘ

There are no such residues in this entry.