



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 01:44 PM BST

PDB ID : 1ZKU
EMDB ID: : EMD-1126
Title : Fitting of the gp9 structure in the EM density of bacteriophage T4 extended tail
Authors : Kostyuchenko, V.A.
Deposited on : 2005-05-04
Resolution : 15.00 Å(reported)
Based on PDB ID : 1S2E

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

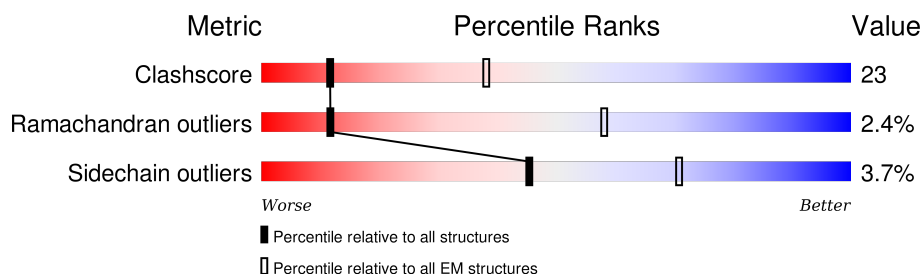
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY










The reported resolution of this entry is 15.00 Å.

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












Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	288	 70% 25% 5%
1	B	288	 70% 25% 5%
1	C	288	 72% 24% 5%
1	D	288	 70% 25% 5%
1	E	288	 70% 25% 5%
1	F	288	 71% 24% 5%
1	G	288	 71% 24% 5%
1	H	288	 70% 25% 5%
1	I	288	 70% 25% 5%

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Mol	Chain	Length	Quality of chain
1	J	288	 70%25%5%
1	K	288	 70%25%5%
1	L	288	 71%24%5%
1	M	288	 70%25%5%
1	N	288	 70%25%5%
1	O	288	 70%25%5%
1	P	288	 70%25%5%
1	Q	288	 70%25%5%
1	R	288	 71%24%5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 39420 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Baseplate structural protein Gp9.

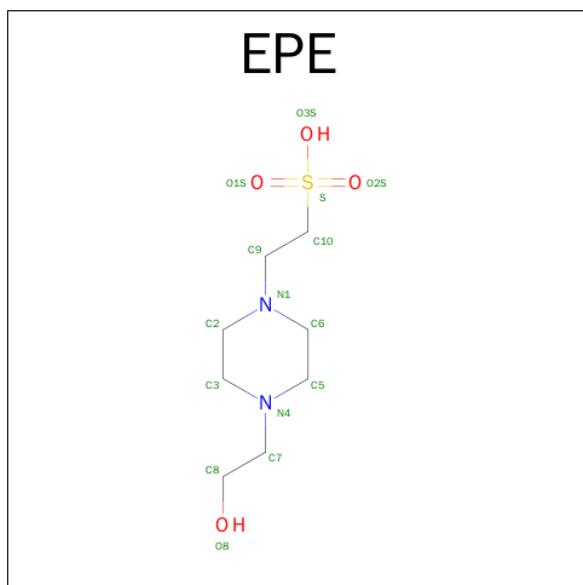
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	B	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	C	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	D	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	E	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	F	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	G	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	H	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	I	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	J	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	K	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	L	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	M	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	N	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	O	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	P	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		
1	Q	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	288	Total	C	N	O	S	0	0
			2175	1354	366	446	9		

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C₈H₁₈N₂O₄S).



Mol	Chain	Residues	Atoms					AltConf
2	A	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	B	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	C	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	D	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	E	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	F	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	G	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	H	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	I	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	J	1	Total	C	N	O	S	0
			15	8	2	4	1	

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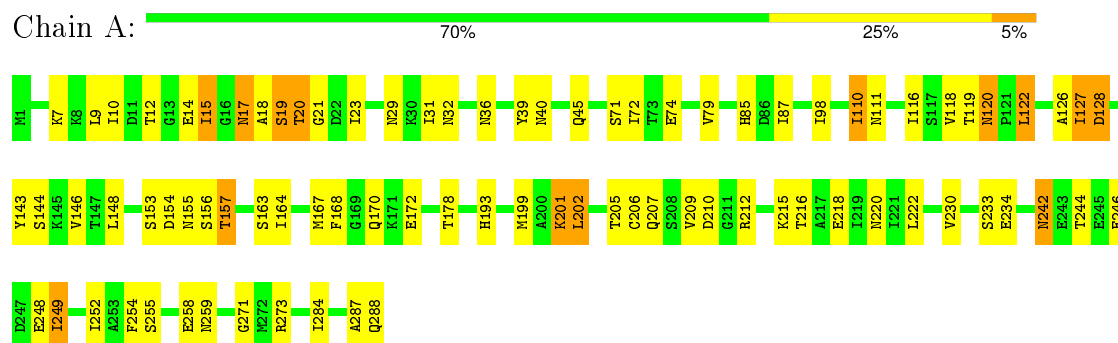
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Mol	Chain	Residues	Atoms					AltConf
2	K	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	L	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	M	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	N	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	O	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	P	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	Q	1	Total	C	N	O	S	0
			15	8	2	4	1	
2	R	1	Total	C	N	O	S	0
			15	8	2	4	1	

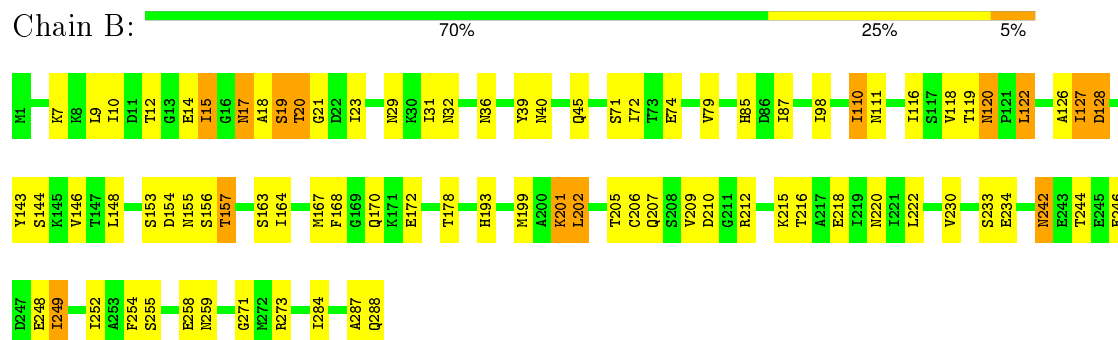
3 Residue-property plots

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

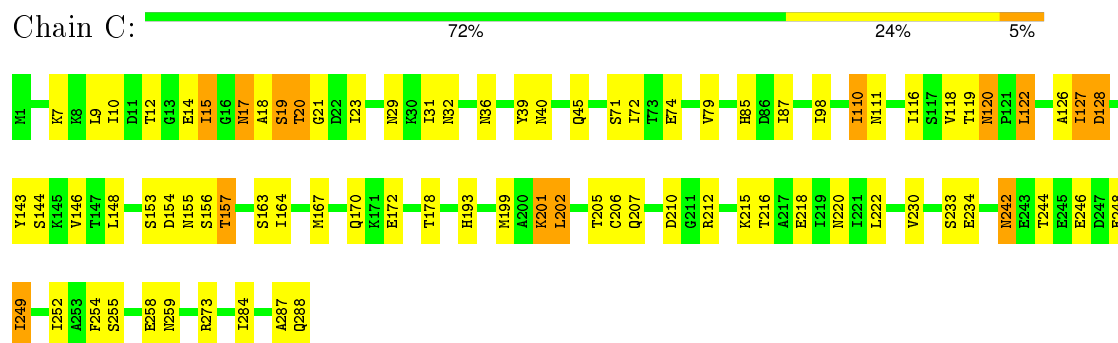
- Molecule 1: Baseplate structural protein Gp9



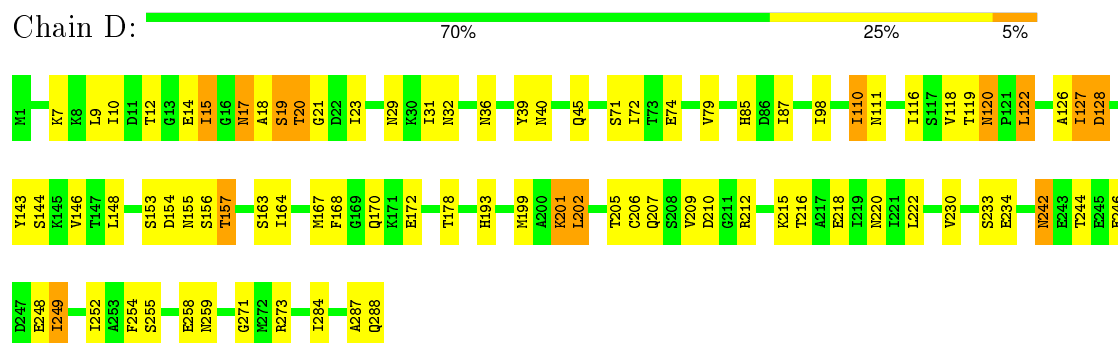
- Molecule 1: Baseplate structural protein Gp9



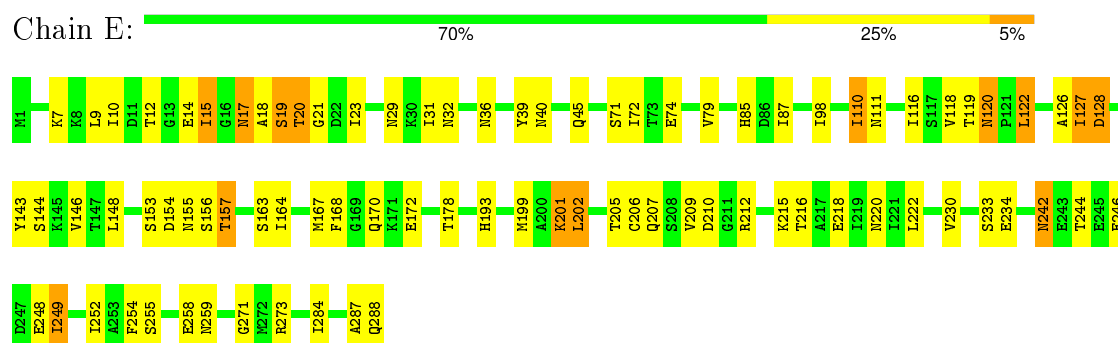
- Molecule 1: Baseplate structural protein Gp9



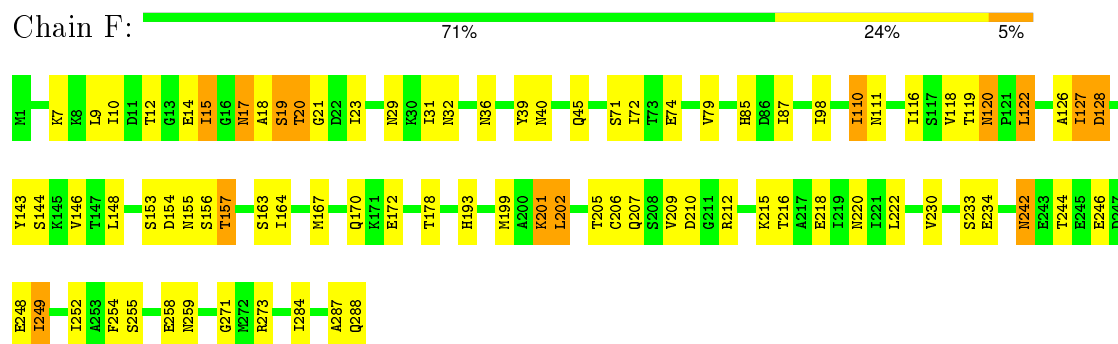
- Molecule 1: Baseplate structural protein Gp9



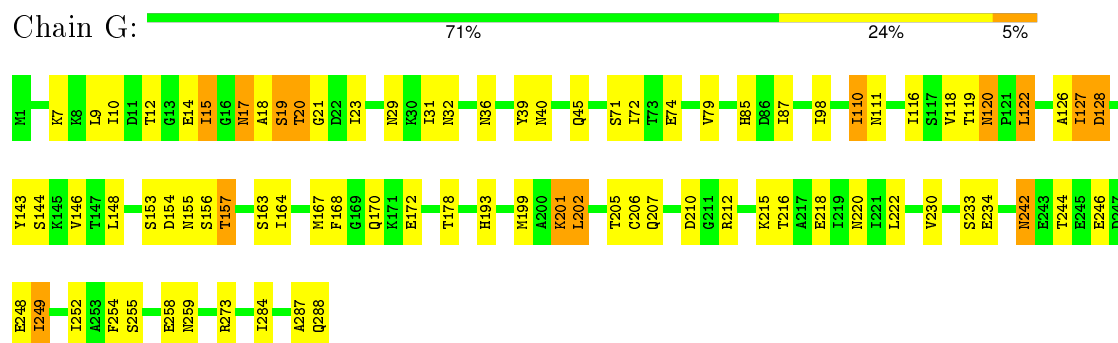
- Molecule 1: Baseplate structural protein Gp9



- Molecule 1: Baseplate structural protein Gp9

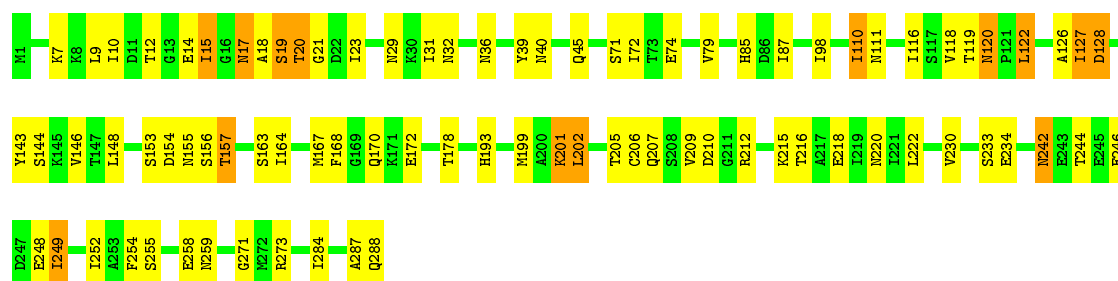


- Molecule 1: Baseplate structural protein Gp9



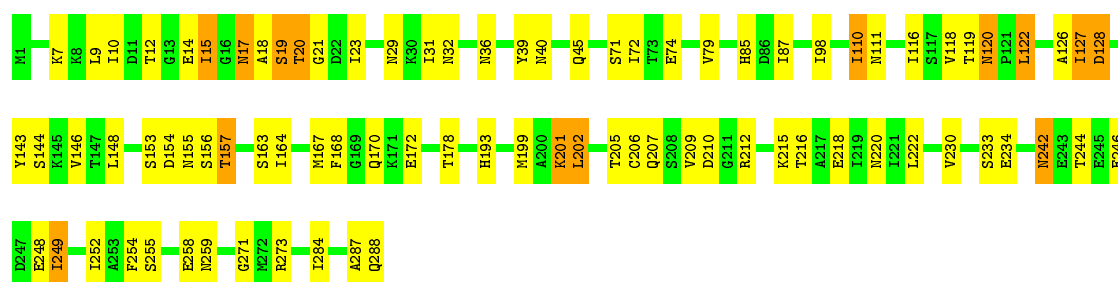
- Molecule 1: Baseplate structural protein Gp9

Chain H: 



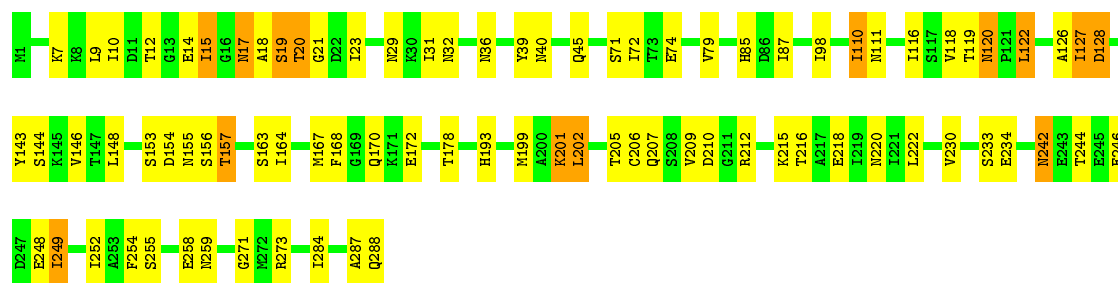
- Molecule 1: Baseplate structural protein Gp9

Chain I: 



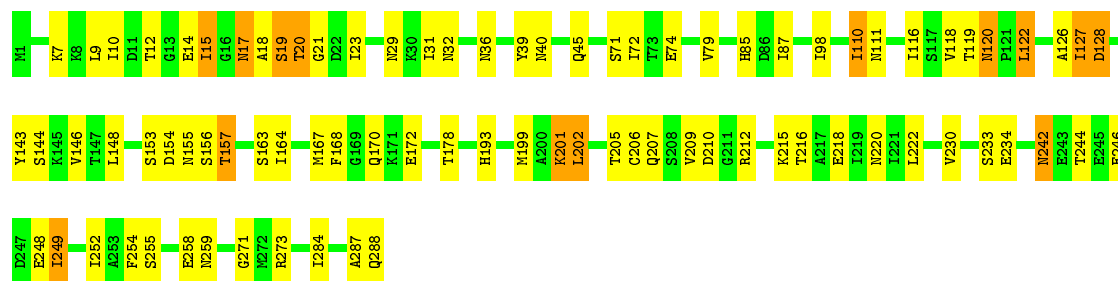
- Molecule 1: Baseplate structural protein Gp9

Chain J: 

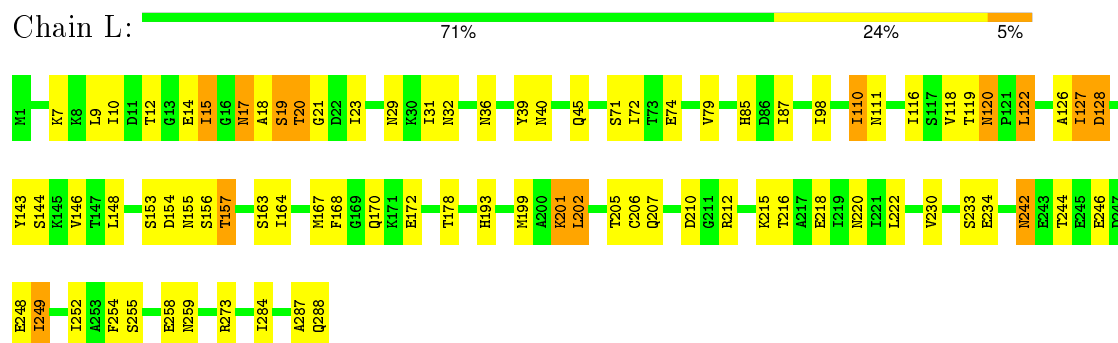


- Molecule 1: Baseplate structural protein Gp9

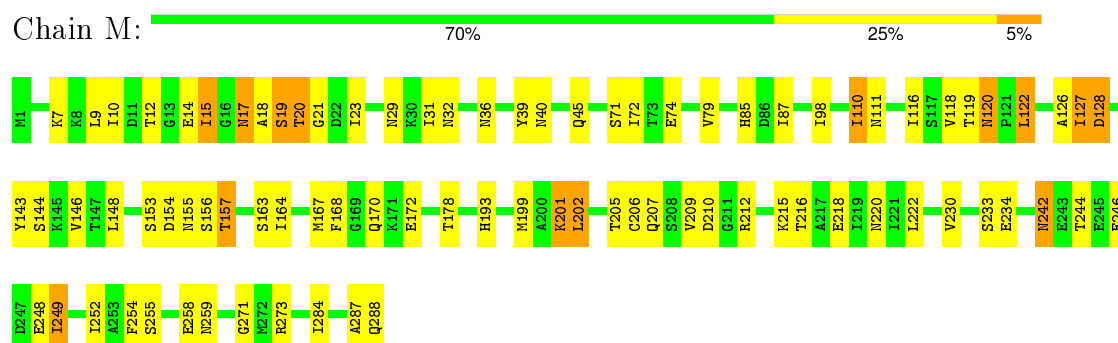
Chain K: 



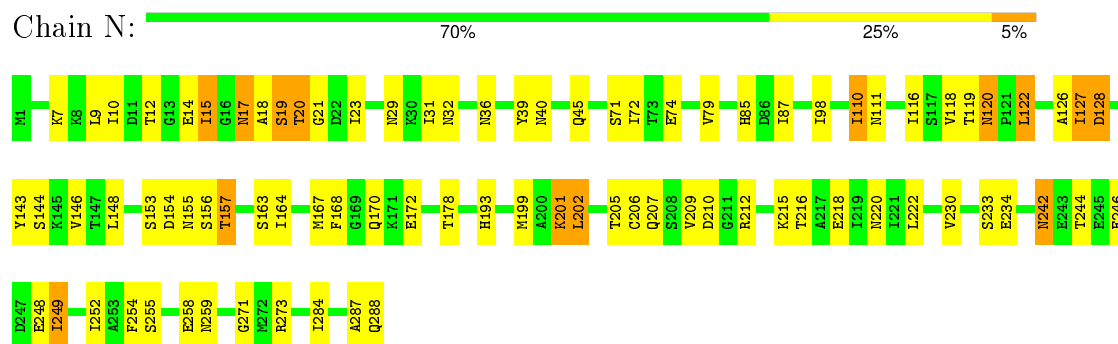
- Molecule 1: Baseplate structural protein Gp9



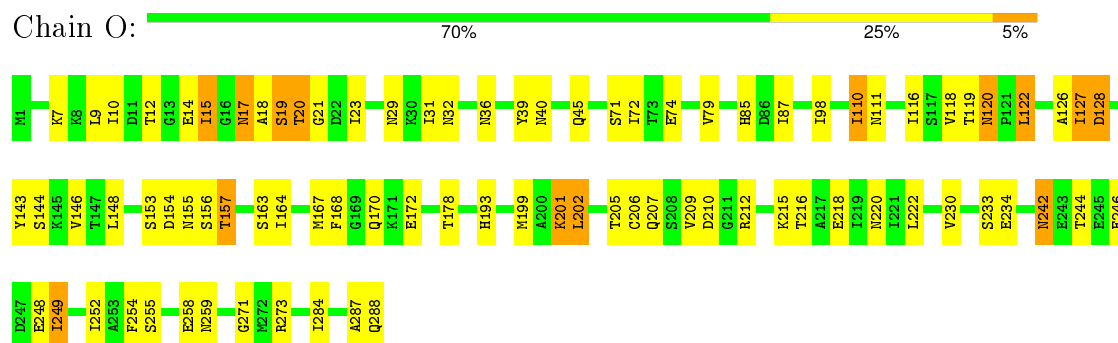
- Molecule 1: Baseplate structural protein Gp9



- Molecule 1: Baseplate structural protein Gp9

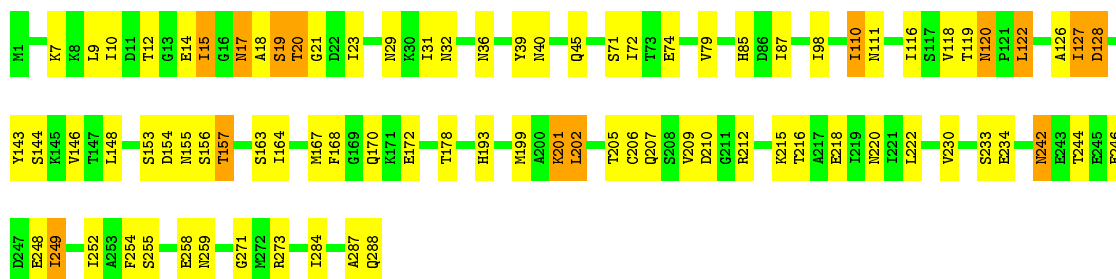


- Molecule 1: Baseplate structural protein Gp9



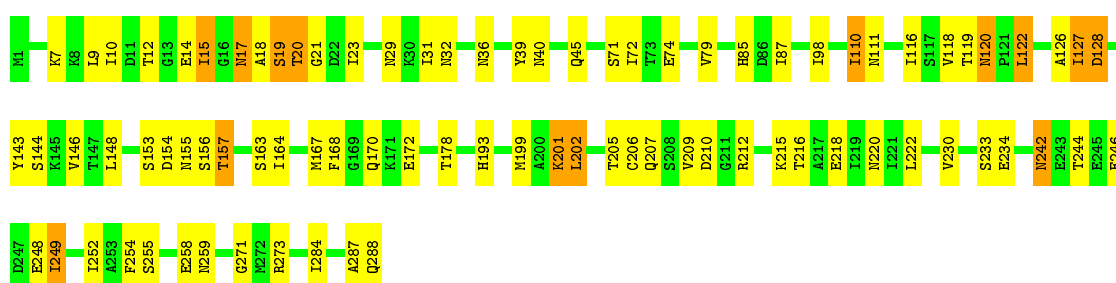
- Molecule 1: Baseplate structural protein Gp9

Chain P:  70% 25% 5%



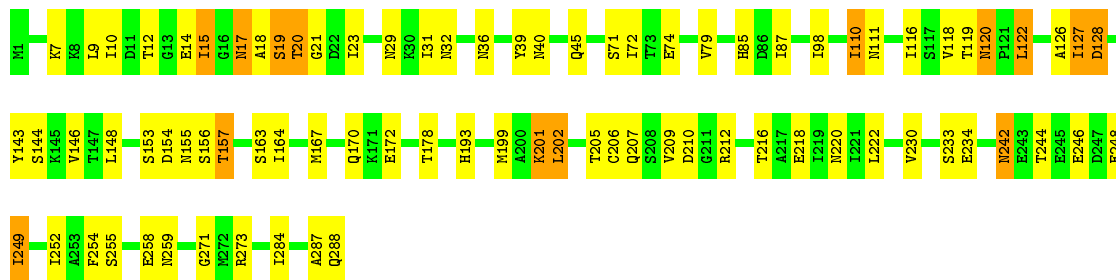
- Molecule 1: Baseplate structural protein Gp9

Chain Q:  70% 25% 5%



- Molecule 1: Baseplate structural protein Gp9

Chain R:  71% 24% 5%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH IMAGE	Depositor
Microscope	PHILIPS CM300 FEG	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	0.8	Depositor
Maximum defocus (nm)	3.2	Depositor
Magnification	45000	Depositor
Image detector	FILM	Depositor

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: EPE

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	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	0.37	0/2205	0.67	1/2988 (0.0%)
1	B	0.37	0/2205	0.67	1/2988 (0.0%)
1	C	0.37	0/2205	0.67	1/2988 (0.0%)
1	D	0.37	0/2205	0.67	1/2988 (0.0%)
1	E	0.37	0/2205	0.67	1/2988 (0.0%)
1	F	0.37	0/2205	0.67	1/2988 (0.0%)
1	G	0.37	0/2205	0.67	1/2988 (0.0%)
1	H	0.37	0/2205	0.67	1/2988 (0.0%)
1	I	0.37	0/2205	0.67	1/2988 (0.0%)
1	J	0.37	0/2205	0.67	1/2988 (0.0%)
1	K	0.37	0/2205	0.67	1/2988 (0.0%)
1	L	0.37	0/2205	0.67	1/2988 (0.0%)
1	M	0.37	0/2205	0.67	1/2988 (0.0%)
1	N	0.37	0/2205	0.67	1/2988 (0.0%)
1	O	0.37	0/2205	0.67	1/2988 (0.0%)
1	P	0.37	0/2205	0.67	1/2988 (0.0%)
1	Q	0.37	0/2205	0.67	1/2988 (0.0%)
1	R	0.37	0/2205	0.67	1/2988 (0.0%)
All	All	0.37	0/39690	0.67	18/53784 (0.0%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	19	SER	CA-C-N	-7.11	101.56	117.20
1	M	19	SER	CA-C-N	-7.11	101.56	117.20
1	A	19	SER	CA-C-N	-7.11	101.57	117.20
1	C	19	SER	CA-C-N	-7.11	101.57	117.20
1	I	19	SER	CA-C-N	-7.11	101.57	117.20
1	J	19	SER	CA-C-N	-7.11	101.57	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	19	SER	CA-C-N	-7.11	101.57	117.20
1	R	19	SER	CA-C-N	-7.11	101.57	117.20
1	F	19	SER	CA-C-N	-7.09	101.60	117.20
1	G	19	SER	CA-C-N	-7.09	101.61	117.20
1	O	19	SER	CA-C-N	-7.09	101.60	117.20
1	P	19	SER	CA-C-N	-7.09	101.61	117.20
1	B	19	SER	CA-C-N	-7.08	101.63	117.20
1	K	19	SER	CA-C-N	-7.08	101.63	117.20
1	H	19	SER	CA-C-N	-7.07	101.65	117.20
1	Q	19	SER	CA-C-N	-7.07	101.65	117.20
1	E	19	SER	CA-C-N	-7.06	101.66	117.20
1	N	19	SER	CA-C-N	-7.06	101.66	117.20

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	2175	0	2157	123	0
1	B	2175	0	2157	121	0
1	C	2175	0	2157	119	0
1	D	2175	0	2157	125	0
1	E	2175	0	2157	123	0
1	F	2175	0	2157	122	0
1	G	2175	0	2157	120	0
1	H	2175	0	2157	123	0
1	I	2175	0	2157	120	0
1	J	2175	0	2157	121	0
1	K	2175	0	2157	124	0
1	L	2175	0	2157	121	0
1	M	2175	0	2157	121	0
1	N	2175	0	2157	124	0
1	O	2175	0	2157	123	0
1	P	2175	0	2157	123	0
1	Q	2175	0	2157	122	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	R	2175	0	2157	121	0
2	A	15	0	18	3	0
2	B	15	0	18	3	0
2	C	15	0	18	3	0
2	D	15	0	18	4	0
2	E	15	0	18	3	0
2	F	15	0	18	3	0
2	G	15	0	18	3	0
2	H	15	0	18	3	0
2	I	15	0	18	3	0
2	J	15	0	18	3	0
2	K	15	0	18	3	0
2	L	15	0	18	3	0
2	M	15	0	18	3	0
2	N	15	0	18	3	0
2	O	15	0	18	3	0
2	P	15	0	18	3	0
2	Q	15	0	18	3	0
2	R	15	0	18	3	0
All	All	39420	0	39150	1808	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 23.

All (1808) 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:B:18:ALA:HB3	1:B:23:ILE:HD11	1.41	1.03
1:Q:18:ALA:HB3	1:Q:23:ILE:HD11	1.41	1.02
1:E:18:ALA:HB3	1:E:23:ILE:HD11	1.41	1.02
1:I:18:ALA:HB3	1:I:23:ILE:HD11	1.41	1.02
1:F:18:ALA:HB3	1:F:23:ILE:HD11	1.41	1.02
1:H:14:GLU:CA	1:H:17:ASN:HD21	1.73	1.02
1:F:14:GLU:CA	1:F:17:ASN:HD21	1.73	1.02
1:M:18:ALA:HB3	1:M:23:ILE:HD11	1.41	1.01
1:J:14:GLU:CA	1:J:17:ASN:HD21	1.73	1.01
1:E:14:GLU:CA	1:E:17:ASN:HD21	1.73	1.01
1:I:14:GLU:CA	1:I:17:ASN:HD21	1.73	1.01
1:R:14:GLU:CA	1:R:17:ASN:HD21	1.73	1.01
1:H:18:ALA:HB3	1:H:23:ILE:HD11	1.41	1.01
1:C:14:GLU:CA	1:C:17:ASN:HD21	1.73	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:14:GLU:CA	1:G:17:ASN:HD21	1.73	1.01
1:M:14:GLU:CA	1:M:17:ASN:HD21	1.73	1.01
1:K:18:ALA:HB3	1:K:23:ILE:HD11	1.41	1.01
1:L:14:GLU:CA	1:L:17:ASN:HD21	1.73	1.01
1:K:14:GLU:C	1:K:17:ASN:HD21	1.64	1.01
1:C:242:ASN:H	1:C:242:ASN:HD22	1.01	1.01
1:C:14:GLU:C	1:C:17:ASN:HD21	1.64	1.00
1:A:14:GLU:C	1:A:17:ASN:HD21	1.64	1.00
1:P:14:GLU:CA	1:P:17:ASN:HD21	1.73	1.00
1:O:14:GLU:CA	1:O:17:ASN:HD21	1.73	1.00
1:N:14:GLU:C	1:N:17:ASN:HD21	1.64	1.00
1:Q:14:GLU:C	1:Q:17:ASN:HD21	1.64	1.00
1:O:18:ALA:HB3	1:O:23:ILE:HD11	1.41	1.00
1:R:18:ALA:HB3	1:R:23:ILE:HD11	1.41	1.00
1:D:14:GLU:CA	1:D:17:ASN:HD21	1.73	1.00
1:H:14:GLU:C	1:H:17:ASN:HD21	1.64	1.00
1:K:14:GLU:CA	1:K:17:ASN:HD21	1.73	1.00
1:A:14:GLU:CA	1:A:17:ASN:HD21	1.73	1.00
1:P:14:GLU:C	1:P:17:ASN:HD21	1.64	1.00
1:D:14:GLU:C	1:D:17:ASN:HD21	1.64	1.00
1:P:18:ALA:HB3	1:P:23:ILE:HD11	1.41	1.00
1:B:14:GLU:C	1:B:17:ASN:HD21	1.64	1.00
1:N:18:ALA:HB3	1:N:23:ILE:HD11	1.41	1.00
1:B:14:GLU:CA	1:B:17:ASN:HD21	1.73	1.00
1:R:14:GLU:C	1:R:17:ASN:HD21	1.64	1.00
1:G:18:ALA:HB3	1:G:23:ILE:HD11	1.41	1.00
1:O:14:GLU:C	1:O:17:ASN:HD21	1.64	0.99
1:L:18:ALA:HB3	1:L:23:ILE:HD11	1.41	0.99
1:J:242:ASN:HD22	1:J:242:ASN:H	1.01	0.99
1:N:14:GLU:CA	1:N:17:ASN:HD21	1.73	0.99
1:C:18:ALA:HB3	1:C:23:ILE:HD11	1.41	0.99
1:E:14:GLU:C	1:E:17:ASN:HD21	1.64	0.99
1:M:14:GLU:C	1:M:17:ASN:HD21	1.64	0.99
1:G:14:GLU:C	1:G:17:ASN:HD21	1.64	0.99
1:D:18:ALA:HB3	1:D:23:ILE:HD11	1.41	0.99
1:Q:14:GLU:CA	1:Q:17:ASN:HD21	1.73	0.99
1:A:18:ALA:HB3	1:A:23:ILE:HD11	1.41	0.99
1:M:242:ASN:HD22	1:M:242:ASN:H	1.01	0.99
1:I:14:GLU:C	1:I:17:ASN:HD21	1.64	0.98
1:L:14:GLU:C	1:L:17:ASN:HD21	1.64	0.98
1:J:18:ALA:HB3	1:J:23:ILE:HD11	1.41	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:14:GLU:C	1:J:17:ASN:HD21	1.64	0.98
1:R:242:ASN:H	1:R:242:ASN:HD22	1.01	0.98
1:F:14:GLU:C	1:F:17:ASN:HD21	1.64	0.98
1:F:242:ASN:H	1:F:242:ASN:HD22	1.01	0.97
1:P:242:ASN:H	1:P:242:ASN:HD22	1.01	0.96
1:G:242:ASN:H	1:G:242:ASN:HD22	1.01	0.96
1:O:242:ASN:H	1:O:242:ASN:HD22	1.01	0.95
1:A:242:ASN:HD22	1:A:242:ASN:H	1.01	0.94
1:I:242:ASN:HD22	1:I:242:ASN:H	1.01	0.94
1:L:242:ASN:H	1:L:242:ASN:HD22	1.01	0.93
1:D:242:ASN:H	1:D:242:ASN:HD22	1.01	0.93
1:H:242:ASN:HD22	1:H:242:ASN:H	1.01	0.93
1:K:242:ASN:H	1:K:242:ASN:HD22	1.01	0.92
1:Q:242:ASN:HD22	1:Q:242:ASN:H	1.01	0.92
1:E:242:ASN:HD22	1:E:242:ASN:H	1.01	0.91
1:N:242:ASN:H	1:N:242:ASN:ND2	1.69	0.90
1:D:242:ASN:H	1:D:242:ASN:ND2	1.69	0.90
1:B:242:ASN:ND2	1:B:242:ASN:H	1.69	0.90
1:N:242:ASN:HD22	1:N:242:ASN:H	1.01	0.90
1:I:234:GLU:H	2:I:309:EPE:H82	1.37	0.90
1:A:242:ASN:ND2	1:A:242:ASN:H	1.69	0.90
1:B:242:ASN:HD22	1:B:242:ASN:H	1.01	0.90
1:O:234:GLU:H	2:O:315:EPE:H82	1.37	0.90
1:J:234:GLU:H	2:J:310:EPE:H82	1.37	0.90
1:M:234:GLU:H	2:M:313:EPE:H82	1.37	0.90
1:G:242:ASN:H	1:G:242:ASN:ND2	1.69	0.90
1:L:234:GLU:H	2:L:312:EPE:H82	1.37	0.90
1:F:234:GLU:H	2:F:306:EPE:H82	1.37	0.90
1:P:234:GLU:H	2:P:316:EPE:H82	1.37	0.90
1:A:234:GLU:H	2:A:301:EPE:H82	1.37	0.89
1:G:234:GLU:H	2:G:307:EPE:H82	1.37	0.89
1:Q:234:GLU:H	2:Q:317:EPE:H82	1.37	0.89
1:O:242:ASN:H	1:O:242:ASN:ND2	1.69	0.89
1:I:242:ASN:ND2	1:I:242:ASN:H	1.69	0.89
1:H:242:ASN:H	1:H:242:ASN:ND2	1.69	0.89
1:F:242:ASN:ND2	1:F:242:ASN:H	1.69	0.89
1:R:234:GLU:H	2:R:318:EPE:H82	1.37	0.89
1:L:242:ASN:ND2	1:L:242:ASN:H	1.69	0.88
1:D:234:GLU:H	2:D:304:EPE:H82	1.37	0.88
1:R:242:ASN:ND2	1:R:242:ASN:H	1.69	0.88
1:P:242:ASN:H	1:P:242:ASN:ND2	1.69	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:GLU:H	2:B:302:EPE:H82	1.37	0.88
1:C:242:ASN:H	1:C:242:ASN:ND2	1.69	0.88
1:J:242:ASN:ND2	1:J:242:ASN:H	1.69	0.88
1:K:242:ASN:H	1:K:242:ASN:ND2	1.69	0.88
1:M:242:ASN:ND2	1:M:242:ASN:H	1.69	0.87
1:Q:242:ASN:ND2	1:Q:242:ASN:H	1.69	0.87
1:C:234:GLU:H	2:C:303:EPE:H82	1.37	0.87
1:N:234:GLU:H	2:N:314:EPE:H82	1.37	0.86
1:K:234:GLU:H	2:K:311:EPE:H82	1.37	0.86
1:E:234:GLU:H	2:E:305:EPE:H82	1.37	0.86
1:H:234:GLU:H	2:H:308:EPE:H82	1.37	0.86
1:E:242:ASN:ND2	1:E:242:ASN:H	1.69	0.85
1:E:119:THR:C	1:E:120:ASN:HD22	1.81	0.84
1:Q:119:THR:C	1:Q:120:ASN:HD22	1.81	0.84
1:F:119:THR:C	1:F:120:ASN:HD22	1.81	0.84
1:A:119:THR:C	1:A:120:ASN:HD22	1.81	0.84
1:P:119:THR:C	1:P:120:ASN:HD22	1.81	0.84
1:K:119:THR:C	1:K:120:ASN:HD22	1.81	0.84
1:M:119:THR:C	1:M:120:ASN:HD22	1.81	0.84
1:R:14:GLU:C	1:R:17:ASN:ND2	2.31	0.84
1:R:119:THR:C	1:R:120:ASN:HD22	1.81	0.84
1:B:119:THR:C	1:B:120:ASN:HD22	1.81	0.84
1:N:14:GLU:C	1:N:17:ASN:ND2	2.31	0.84
1:C:14:GLU:C	1:C:17:ASN:ND2	2.31	0.83
1:Q:14:GLU:C	1:Q:17:ASN:ND2	2.31	0.83
1:O:119:THR:C	1:O:120:ASN:HD22	1.81	0.83
1:G:14:GLU:C	1:G:17:ASN:ND2	2.31	0.83
1:D:14:GLU:C	1:D:17:ASN:ND2	2.31	0.83
1:C:119:THR:C	1:C:120:ASN:HD22	1.81	0.83
1:K:14:GLU:C	1:K:17:ASN:ND2	2.31	0.83
1:P:14:GLU:C	1:P:17:ASN:ND2	2.31	0.83
1:N:119:THR:C	1:N:120:ASN:HD22	1.81	0.83
1:E:14:GLU:C	1:E:17:ASN:ND2	2.31	0.83
1:A:14:GLU:C	1:A:17:ASN:ND2	2.31	0.83
1:M:14:GLU:C	1:M:17:ASN:ND2	2.31	0.83
1:O:18:ALA:O	1:O:23:ILE:HD13	1.79	0.83
1:G:119:THR:C	1:G:120:ASN:HD22	1.81	0.83
1:O:14:GLU:C	1:O:17:ASN:ND2	2.31	0.83
1:C:18:ALA:O	1:C:23:ILE:HD13	1.79	0.83
1:A:18:ALA:O	1:A:23:ILE:HD13	1.79	0.83
1:D:119:THR:C	1:D:120:ASN:HD22	1.81	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:14:GLU:C	1:F:17:ASN:ND2	2.31	0.82
1:M:18:ALA:O	1:M:23:ILE:HD13	1.79	0.82
1:K:18:ALA:O	1:K:23:ILE:HD13	1.79	0.82
1:B:14:GLU:C	1:B:17:ASN:ND2	2.31	0.82
1:H:119:THR:C	1:H:120:ASN:HD22	1.81	0.82
1:R:18:ALA:O	1:R:23:ILE:HD13	1.79	0.82
1:H:14:GLU:C	1:H:17:ASN:ND2	2.31	0.82
1:J:14:GLU:C	1:J:17:ASN:ND2	2.31	0.82
1:H:18:ALA:O	1:H:23:ILE:HD13	1.79	0.82
1:I:119:THR:C	1:I:120:ASN:HD22	1.81	0.82
1:I:201:LYS:HD3	1:I:220:ASN:OD1	1.80	0.82
1:L:201:LYS:HD3	1:L:220:ASN:OD1	1.80	0.82
1:F:201:LYS:HD3	1:F:220:ASN:OD1	1.80	0.82
1:Q:18:ALA:O	1:Q:23:ILE:HD13	1.79	0.82
1:F:18:ALA:O	1:F:23:ILE:HD13	1.79	0.82
1:L:18:ALA:O	1:L:23:ILE:HD13	1.79	0.82
1:J:201:LYS:HD3	1:J:220:ASN:OD1	1.80	0.82
1:L:119:THR:C	1:L:120:ASN:HD22	1.81	0.82
1:I:14:GLU:C	1:I:17:ASN:ND2	2.31	0.82
1:K:201:LYS:HD3	1:K:220:ASN:OD1	1.80	0.82
1:J:119:THR:C	1:J:120:ASN:HD22	1.81	0.82
1:M:201:LYS:HD3	1:M:220:ASN:OD1	1.80	0.82
1:G:18:ALA:O	1:G:23:ILE:HD13	1.79	0.82
1:A:201:LYS:HD3	1:A:220:ASN:OD1	1.80	0.82
1:B:18:ALA:O	1:B:23:ILE:HD13	1.79	0.82
1:J:18:ALA:O	1:J:23:ILE:HD13	1.79	0.82
1:D:201:LYS:HD3	1:D:220:ASN:OD1	1.80	0.82
1:O:201:LYS:HD3	1:O:220:ASN:OD1	1.80	0.82
1:P:201:LYS:HD3	1:P:220:ASN:OD1	1.80	0.82
1:L:14:GLU:C	1:L:17:ASN:ND2	2.31	0.82
1:N:18:ALA:O	1:N:23:ILE:HD13	1.79	0.82
1:G:201:LYS:HD3	1:G:220:ASN:OD1	1.80	0.82
1:Q:201:LYS:HD3	1:Q:220:ASN:OD1	1.80	0.82
1:P:18:ALA:O	1:P:23:ILE:HD13	1.79	0.81
1:E:201:LYS:HD3	1:E:220:ASN:OD1	1.80	0.81
1:C:201:LYS:HD3	1:C:220:ASN:OD1	1.80	0.81
1:R:201:LYS:HD3	1:R:220:ASN:OD1	1.80	0.81
1:E:18:ALA:O	1:E:23:ILE:HD13	1.79	0.81
1:D:18:ALA:O	1:D:23:ILE:HD13	1.79	0.81
1:H:201:LYS:HD3	1:H:220:ASN:OD1	1.80	0.81
1:N:201:LYS:HD3	1:N:220:ASN:OD1	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:18:ALA:O	1:I:23:ILE:HD13	1.79	0.80
1:B:201:LYS:HD3	1:B:220:ASN:OD1	1.80	0.80
1:D:17:ASN:H	1:D:17:ASN:HD22	1.30	0.80
1:B:17:ASN:HD22	1:B:17:ASN:H	1.31	0.79
1:F:17:ASN:H	1:F:17:ASN:HD22	1.31	0.79
1:G:17:ASN:HD22	1:G:17:ASN:H	1.31	0.79
1:A:17:ASN:HD22	1:A:17:ASN:H	1.30	0.79
1:Q:17:ASN:HD22	1:Q:17:ASN:H	1.31	0.79
1:L:17:ASN:HD22	1:L:17:ASN:H	1.31	0.79
1:I:17:ASN:HD22	1:I:17:ASN:H	1.31	0.78
1:P:17:ASN:H	1:P:17:ASN:HD22	1.31	0.78
1:J:17:ASN:HD22	1:J:17:ASN:H	1.30	0.78
1:E:17:ASN:H	1:E:17:ASN:HD22	1.31	0.78
1:C:17:ASN:H	1:C:17:ASN:HD22	1.31	0.78
1:J:15:ILE:N	1:J:17:ASN:HD21	1.82	0.78
1:R:15:ILE:N	1:R:17:ASN:HD21	1.82	0.78
1:O:234:GLU:H	2:O:315:EPE:C8	1.97	0.78
1:F:234:GLU:H	2:F:306:EPE:C8	1.97	0.78
1:G:15:ILE:N	1:G:17:ASN:HD21	1.82	0.78
1:M:15:ILE:N	1:M:17:ASN:HD21	1.82	0.78
1:M:17:ASN:H	1:M:17:ASN:HD22	1.30	0.78
1:L:234:GLU:H	2:L:312:EPE:C8	1.97	0.78
1:L:15:ILE:N	1:L:17:ASN:HD21	1.82	0.78
1:C:234:GLU:H	2:C:303:EPE:C8	1.97	0.78
1:I:234:GLU:H	2:I:309:EPE:C8	1.97	0.78
1:G:234:GLU:H	2:G:307:EPE:C8	1.97	0.78
1:N:17:ASN:H	1:N:17:ASN:HD22	1.31	0.77
1:D:15:ILE:N	1:D:17:ASN:HD21	1.82	0.77
1:Q:15:ILE:N	1:Q:17:ASN:HD21	1.82	0.77
1:F:15:ILE:N	1:F:17:ASN:HD21	1.82	0.77
1:O:17:ASN:H	1:O:17:ASN:HD22	1.31	0.77
1:H:15:ILE:N	1:H:17:ASN:HD21	1.82	0.77
1:H:17:ASN:H	1:H:17:ASN:HD22	1.31	0.77
1:M:234:GLU:H	2:M:313:EPE:C8	1.97	0.77
1:A:234:GLU:H	2:A:301:EPE:C8	1.97	0.77
1:N:234:GLU:H	2:N:314:EPE:C8	1.97	0.77
1:B:15:ILE:N	1:B:17:ASN:HD21	1.82	0.77
1:P:234:GLU:H	2:P:316:EPE:C8	1.97	0.77
1:R:17:ASN:H	1:R:17:ASN:HD22	1.31	0.77
1:O:15:ILE:N	1:O:17:ASN:HD21	1.82	0.77
1:R:234:GLU:H	2:R:318:EPE:C8	1.97	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:GLU:H	2:B:302:EPE:C8	1.97	0.77
1:N:15:ILE:N	1:N:17:ASN:HD21	1.82	0.77
1:K:234:GLU:H	2:K:311:EPE:C8	1.97	0.77
1:E:15:ILE:N	1:E:17:ASN:HD21	1.82	0.77
1:C:15:ILE:N	1:C:17:ASN:HD21	1.82	0.77
1:K:15:ILE:N	1:K:17:ASN:HD21	1.82	0.77
1:P:15:ILE:N	1:P:17:ASN:HD21	1.82	0.77
1:K:17:ASN:H	1:K:17:ASN:HD22	1.31	0.77
1:E:234:GLU:H	2:E:305:EPE:C8	1.97	0.77
1:J:234:GLU:H	2:J:310:EPE:C8	1.97	0.76
1:Q:234:GLU:H	2:Q:317:EPE:C8	1.97	0.76
1:D:234:GLU:H	2:D:304:EPE:C8	1.97	0.76
1:I:15:ILE:N	1:I:17:ASN:HD21	1.82	0.76
1:A:15:ILE:N	1:A:17:ASN:HD21	1.82	0.76
1:H:234:GLU:H	2:H:308:EPE:C8	1.97	0.75
1:D:40:ASN:HD22	1:D:45:GLN:HG2	1.52	0.75
1:K:14:GLU:CA	1:K:17:ASN:ND2	2.50	0.75
1:B:14:GLU:CA	1:B:17:ASN:ND2	2.50	0.75
1:J:40:ASN:HD22	1:J:45:GLN:HG2	1.52	0.75
1:L:40:ASN:HD22	1:L:45:GLN:HG2	1.52	0.75
1:D:127:ILE:O	1:D:128:ASP:HB2	1.87	0.75
1:Q:127:ILE:O	1:Q:128:ASP:HB2	1.87	0.75
1:N:40:ASN:HD22	1:N:45:GLN:HG2	1.52	0.75
1:F:14:GLU:CA	1:F:17:ASN:ND2	2.50	0.75
1:M:14:GLU:CA	1:M:17:ASN:ND2	2.50	0.75
1:F:40:ASN:HD22	1:F:45:GLN:HG2	1.52	0.75
1:J:127:ILE:O	1:J:128:ASP:HB2	1.87	0.75
1:L:127:ILE:O	1:L:128:ASP:HB2	1.87	0.75
1:Q:40:ASN:HD22	1:Q:45:GLN:HG2	1.52	0.75
1:M:40:ASN:HD22	1:M:45:GLN:HG2	1.52	0.75
1:G:40:ASN:HD22	1:G:45:GLN:HG2	1.52	0.75
1:E:127:ILE:O	1:E:128:ASP:HB2	1.87	0.75
1:B:40:ASN:HD22	1:B:45:GLN:HG2	1.52	0.75
1:P:40:ASN:HD22	1:P:45:GLN:HG2	1.52	0.75
1:K:40:ASN:HD22	1:K:45:GLN:HG2	1.52	0.75
1:R:40:ASN:HD22	1:R:45:GLN:HG2	1.52	0.74
1:Q:14:GLU:CA	1:Q:17:ASN:ND2	2.50	0.74
1:R:127:ILE:O	1:R:128:ASP:HB2	1.87	0.74
1:C:14:GLU:CA	1:C:17:ASN:ND2	2.50	0.74
1:E:40:ASN:HD22	1:E:45:GLN:HG2	1.52	0.74
1:K:127:ILE:O	1:K:128:ASP:HB2	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:14:GLU:CA	1:N:17:ASN:ND2	2.50	0.74
1:H:40:ASN:HD22	1:H:45:GLN:HG2	1.52	0.74
1:M:127:ILE:O	1:M:128:ASP:HB2	1.87	0.74
1:C:127:ILE:O	1:C:128:ASP:HB2	1.87	0.74
1:P:14:GLU:CA	1:P:17:ASN:ND2	2.50	0.74
1:R:144:SER:HB2	1:R:164:ILE:HD11	1.70	0.74
1:O:127:ILE:O	1:O:128:ASP:HB2	1.87	0.74
1:C:40:ASN:HD22	1:C:45:GLN:HG2	1.52	0.74
1:H:127:ILE:O	1:H:128:ASP:HB2	1.87	0.74
1:O:40:ASN:HD22	1:O:45:GLN:HG2	1.52	0.74
1:P:127:ILE:O	1:P:128:ASP:HB2	1.87	0.74
1:E:14:GLU:CA	1:E:17:ASN:ND2	2.50	0.73
1:L:144:SER:HB2	1:L:164:ILE:HD11	1.70	0.73
1:B:127:ILE:O	1:B:128:ASP:HB2	1.87	0.73
1:I:144:SER:HB2	1:I:164:ILE:HD11	1.70	0.73
1:C:144:SER:HB2	1:C:164:ILE:HD11	1.70	0.73
1:L:14:GLU:CA	1:L:17:ASN:ND2	2.50	0.73
1:H:18:ALA:HB3	1:H:23:ILE:CD1	2.19	0.73
1:A:14:GLU:CA	1:A:17:ASN:ND2	2.50	0.73
1:B:144:SER:HB2	1:B:164:ILE:HD11	1.70	0.73
1:I:40:ASN:HD22	1:I:45:GLN:HG2	1.52	0.73
1:O:14:GLU:CA	1:O:17:ASN:ND2	2.50	0.73
1:G:127:ILE:O	1:G:128:ASP:HB2	1.87	0.73
1:I:127:ILE:O	1:I:128:ASP:HB2	1.87	0.73
1:H:144:SER:HB2	1:H:164:ILE:HD11	1.70	0.73
1:A:40:ASN:HD22	1:A:45:GLN:HG2	1.52	0.73
1:D:14:GLU:CA	1:D:17:ASN:ND2	2.50	0.73
1:N:127:ILE:O	1:N:128:ASP:HB2	1.87	0.73
1:G:144:SER:HB2	1:G:164:ILE:HD11	1.70	0.73
1:A:18:ALA:HB3	1:A:23:ILE:CD1	2.19	0.73
1:G:120:ASN:N	1:G:120:ASN:HD22	1.87	0.73
1:Q:144:SER:HB2	1:Q:164:ILE:HD11	1.70	0.73
1:J:15:ILE:N	1:J:17:ASN:ND2	2.37	0.73
1:G:14:GLU:CA	1:G:17:ASN:ND2	2.50	0.73
1:Q:15:ILE:N	1:Q:17:ASN:ND2	2.37	0.73
1:J:144:SER:HB2	1:J:164:ILE:HD11	1.70	0.73
1:P:144:SER:HB2	1:P:164:ILE:HD11	1.70	0.72
1:R:15:ILE:N	1:R:17:ASN:ND2	2.37	0.72
1:O:15:ILE:N	1:O:17:ASN:ND2	2.37	0.72
1:P:18:ALA:HB3	1:P:23:ILE:CD1	2.19	0.72
1:B:15:ILE:N	1:B:17:ASN:ND2	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:120:ASN:N	1:I:120:ASN:HD22	1.87	0.72
1:N:199:MET:HG3	1:O:216:THR:HG21	1.72	0.72
1:H:199:MET:HG3	1:I:216:THR:HG21	1.72	0.72
1:O:144:SER:HB2	1:O:164:ILE:HD11	1.70	0.72
1:P:216:THR:HG21	1:R:199:MET:HG3	1.71	0.72
1:N:144:SER:HB2	1:N:164:ILE:HD11	1.70	0.72
1:A:216:THR:HG21	1:C:199:MET:HG3	1.71	0.72
1:H:15:ILE:N	1:H:17:ASN:ND2	2.37	0.72
1:D:15:ILE:N	1:D:17:ASN:ND2	2.37	0.72
1:F:120:ASN:HD22	1:F:120:ASN:N	1.87	0.72
1:A:144:SER:HB2	1:A:164:ILE:HD11	1.70	0.72
1:D:216:THR:HG21	1:F:199:MET:HG3	1.72	0.72
1:E:15:ILE:N	1:E:17:ASN:ND2	2.37	0.72
1:Q:199:MET:HG3	1:R:216:THR:HG21	1.72	0.72
1:B:18:ALA:HB3	1:B:23:ILE:CD1	2.19	0.72
1:M:18:ALA:HB3	1:M:23:ILE:CD1	2.19	0.72
1:C:15:ILE:N	1:C:17:ASN:ND2	2.37	0.72
1:N:15:ILE:N	1:N:17:ASN:ND2	2.37	0.72
1:A:120:ASN:HD22	1:A:120:ASN:N	1.87	0.72
1:C:120:ASN:N	1:C:120:ASN:HD22	1.87	0.72
1:K:15:ILE:N	1:K:17:ASN:ND2	2.37	0.72
1:R:18:ALA:HB3	1:R:23:ILE:CD1	2.19	0.72
1:G:216:THR:HG21	1:I:199:MET:HG3	1.71	0.72
1:P:199:MET:HG3	1:Q:216:THR:HG21	1.71	0.72
1:L:199:MET:HG3	1:L:216:THR:HG21	1.71	0.72
1:I:18:ALA:HB3	1:I:23:ILE:CD1	2.19	0.72
1:G:15:ILE:N	1:G:17:ASN:ND2	2.37	0.72
1:L:15:ILE:N	1:L:17:ASN:ND2	2.37	0.72
1:R:120:ASN:HD22	1:R:120:ASN:N	1.87	0.72
1:J:216:THR:HG21	1:L:199:MET:HG3	1.71	0.72
1:K:144:SER:HB2	1:K:164:ILE:HD11	1.70	0.72
1:F:127:ILE:O	1:F:128:ASP:HB2	1.87	0.72
1:D:144:SER:HB2	1:D:164:ILE:HD11	1.70	0.72
1:E:144:SER:HB2	1:E:164:ILE:HD11	1.70	0.72
1:K:18:ALA:HB3	1:K:23:ILE:CD1	2.19	0.72
1:A:15:ILE:N	1:A:17:ASN:ND2	2.37	0.72
1:L:120:ASN:HD22	1:L:120:ASN:N	1.87	0.72
1:B:199:MET:HG3	1:C:216:THR:HG21	1.71	0.72
1:E:199:MET:HG3	1:F:216:THR:HG21	1.72	0.72
1:A:127:ILE:O	1:A:128:ASP:HB2	1.87	0.72
1:F:18:ALA:HB3	1:F:23:ILE:CD1	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:15:ILE:N	1:I:17:ASN:ND2	2.37	0.72
1:I:110:ILE:HD12	1:I:167:MET:HE3	1.72	0.72
1:M:144:SER:HB2	1:M:164:ILE:HD11	1.70	0.72
1:D:120:ASN:HD22	1:D:120:ASN:N	1.87	0.71
1:D:199:MET:HG3	1:E:216:THR:HG21	1.71	0.71
1:M:120:ASN:N	1:M:120:ASN:HD22	1.87	0.71
1:M:216:THR:HG21	1:O:199:MET:HG3	1.72	0.71
1:M:15:ILE:N	1:M:17:ASN:ND2	2.37	0.71
1:G:199:MET:HG3	1:H:216:THR:HG21	1.71	0.71
1:F:144:SER:HB2	1:F:164:ILE:HD11	1.70	0.71
1:P:15:ILE:N	1:P:17:ASN:ND2	2.37	0.71
1:M:199:MET:HG3	1:N:216:THR:HG21	1.71	0.71
1:F:15:ILE:N	1:F:17:ASN:ND2	2.37	0.71
1:I:14:GLU:CA	1:I:17:ASN:ND2	2.50	0.71
1:N:120:ASN:HD22	1:N:120:ASN:N	1.87	0.71
1:Q:120:ASN:N	1:Q:120:ASN:HD22	1.87	0.71
1:O:120:ASN:HD22	1:O:120:ASN:N	1.87	0.71
1:J:14:GLU:CA	1:J:17:ASN:ND2	2.50	0.71
1:R:14:GLU:CA	1:R:17:ASN:ND2	2.50	0.71
1:B:120:ASN:HD22	1:B:120:ASN:N	1.87	0.71
1:C:242:ASN:HD22	1:C:242:ASN:N	1.85	0.70
1:C:18:ALA:HB3	1:C:23:ILE:CD1	2.19	0.70
1:P:120:ASN:HD22	1:P:120:ASN:N	1.87	0.70
1:J:120:ASN:N	1:J:120:ASN:HD22	1.87	0.70
1:H:14:GLU:CA	1:H:17:ASN:ND2	2.50	0.70
1:G:110:ILE:HD12	1:G:167:MET:HE3	1.73	0.70
1:N:18:ALA:HB3	1:N:23:ILE:CD1	2.19	0.70
1:E:120:ASN:HD22	1:E:120:ASN:N	1.87	0.70
1:J:199:MET:HG3	1:K:216:THR:HG21	1.71	0.70
1:K:120:ASN:HD22	1:K:120:ASN:N	1.87	0.70
1:A:199:MET:HG3	1:B:216:THR:HG21	1.71	0.70
1:H:120:ASN:HD22	1:H:120:ASN:N	1.87	0.70
1:C:110:ILE:HD12	1:C:167:MET:HE3	1.73	0.70
1:E:18:ALA:HB3	1:E:23:ILE:CD1	2.19	0.69
1:R:110:ILE:HD12	1:R:167:MET:HE3	1.71	0.69
1:L:18:ALA:HB3	1:L:23:ILE:CD1	2.19	0.69
1:R:242:ASN:N	1:R:242:ASN:HD22	1.85	0.69
1:H:242:ASN:HD22	1:H:242:ASN:N	1.85	0.69
1:K:242:ASN:N	1:K:242:ASN:HD22	1.85	0.69
1:J:110:ILE:HD12	1:J:167:MET:HE3	1.75	0.68
1:E:242:ASN:HD22	1:E:242:ASN:N	1.85	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:18:ALA:HB3	1:G:23:ILE:CD1	2.19	0.68
1:K:14:GLU:HA	1:K:17:ASN:OD1	1.94	0.68
1:L:14:GLU:HA	1:L:17:ASN:OD1	1.94	0.68
1:J:14:GLU:HA	1:J:17:ASN:OD1	1.94	0.68
1:O:18:ALA:HB3	1:O:23:ILE:CD1	2.19	0.68
1:D:14:GLU:HA	1:D:17:ASN:OD1	1.94	0.68
1:J:18:ALA:HB3	1:J:23:ILE:CD1	2.19	0.68
1:O:242:ASN:N	1:O:242:ASN:HD22	1.85	0.68
1:I:14:GLU:HA	1:I:17:ASN:OD1	1.94	0.68
1:N:110:ILE:HD12	1:N:167:MET:HE3	1.75	0.68
1:Q:18:ALA:HB3	1:Q:23:ILE:CD1	2.19	0.67
1:E:14:GLU:HA	1:E:17:ASN:OD1	1.94	0.67
1:A:14:GLU:HA	1:A:17:ASN:OD1	1.94	0.67
1:P:14:GLU:HA	1:P:17:ASN:OD1	1.94	0.67
1:O:14:GLU:HA	1:O:17:ASN:OD1	1.94	0.67
1:N:14:GLU:HA	1:N:17:ASN:OD1	1.94	0.67
1:N:242:ASN:HD22	1:N:242:ASN:N	1.85	0.67
1:C:14:GLU:HA	1:C:17:ASN:OD1	1.94	0.67
1:D:18:ALA:HB3	1:D:23:ILE:CD1	2.19	0.67
1:J:164:ILE:HG23	1:K:170:GLN:HA	1.77	0.67
1:H:14:GLU:HA	1:H:17:ASN:OD1	1.94	0.67
1:R:14:GLU:HA	1:R:17:ASN:OD1	1.94	0.67
1:B:242:ASN:N	1:B:242:ASN:HD22	1.85	0.67
1:P:164:ILE:HG23	1:Q:170:GLN:HA	1.77	0.67
1:M:164:ILE:HG23	1:N:170:GLN:HA	1.77	0.67
1:F:14:GLU:HA	1:F:17:ASN:OD1	1.94	0.67
1:N:164:ILE:HG23	1:O:170:GLN:HA	1.77	0.67
1:K:164:ILE:HG23	1:L:170:GLN:HA	1.77	0.67
1:D:164:ILE:HG23	1:E:170:GLN:HA	1.77	0.67
1:E:164:ILE:HG23	1:F:170:GLN:HA	1.77	0.67
1:M:14:GLU:HA	1:M:17:ASN:OD1	1.94	0.67
1:H:164:ILE:HG23	1:I:170:GLN:HA	1.77	0.67
1:G:164:ILE:HG23	1:H:170:GLN:HA	1.77	0.67
1:A:164:ILE:HG23	1:B:170:GLN:HA	1.77	0.66
1:P:170:GLN:HA	1:R:164:ILE:HG23	1.77	0.66
1:B:14:GLU:HA	1:B:17:ASN:OD1	1.94	0.66
1:Q:242:ASN:HD22	1:Q:242:ASN:N	1.85	0.66
1:B:164:ILE:HG23	1:C:170:GLN:HA	1.77	0.66
1:M:170:GLN:HA	1:O:164:ILE:HG23	1.77	0.66
1:G:14:GLU:HA	1:G:17:ASN:OD1	1.94	0.66
1:Q:14:GLU:HA	1:Q:17:ASN:OD1	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:14:GLU:CB	1:Q:17:ASN:HD21	2.09	0.66
1:I:205:THR:OG1	1:I:216:THR:HG23	1.96	0.66
1:B:14:GLU:CB	1:B:17:ASN:HD21	2.09	0.66
1:Q:205:THR:OG1	1:Q:216:THR:HG23	1.96	0.66
1:N:205:THR:OG1	1:N:216:THR:HG23	1.96	0.66
1:K:205:THR:OG1	1:K:216:THR:HG23	1.96	0.66
1:M:110:ILE:HD12	1:M:167:MET:HE3	1.78	0.66
1:N:14:GLU:CB	1:N:17:ASN:HD21	2.09	0.66
1:G:170:GLN:HA	1:I:164:ILE:HG23	1.77	0.66
1:D:205:THR:OG1	1:D:216:THR:HG23	1.96	0.66
1:E:14:GLU:CB	1:E:17:ASN:HD21	2.09	0.66
1:L:14:GLU:CB	1:L:17:ASN:HD21	2.09	0.66
1:K:14:GLU:CB	1:K:17:ASN:HD21	2.09	0.66
1:L:242:ASN:HD22	1:L:242:ASN:N	1.85	0.66
1:Q:164:ILE:HG23	1:R:170:GLN:HA	1.77	0.66
1:G:205:THR:OG1	1:G:216:THR:HG23	1.96	0.66
1:C:205:THR:OG1	1:C:216:THR:HG23	1.96	0.66
1:H:14:GLU:CB	1:H:17:ASN:HD21	2.09	0.66
1:J:170:GLN:HA	1:L:164:ILE:HG23	1.77	0.66
1:I:14:GLU:CB	1:I:17:ASN:HD21	2.09	0.65
1:D:14:GLU:CB	1:D:17:ASN:HD21	2.09	0.65
1:P:205:THR:OG1	1:P:216:THR:HG23	1.96	0.65
1:A:205:THR:OG1	1:A:216:THR:HG23	1.96	0.65
1:B:205:THR:OG1	1:B:216:THR:HG23	1.96	0.65
1:D:170:GLN:HA	1:F:164:ILE:HG23	1.77	0.65
1:L:205:THR:OG1	1:L:216:THR:HG23	1.96	0.65
1:J:205:THR:OG1	1:J:216:THR:HG23	1.96	0.65
1:F:205:THR:OG1	1:F:216:THR:HG23	1.96	0.65
1:E:205:THR:OG1	1:E:216:THR:HG23	1.96	0.65
1:H:205:THR:OG1	1:H:216:THR:HG23	1.96	0.65
1:R:205:THR:OG1	1:R:216:THR:HG23	1.96	0.65
1:G:14:GLU:CB	1:G:17:ASN:HD21	2.09	0.65
1:O:14:GLU:CB	1:O:17:ASN:HD21	2.09	0.65
1:A:170:GLN:HA	1:C:164:ILE:HG23	1.77	0.65
1:F:14:GLU:CB	1:F:17:ASN:HD21	2.09	0.65
1:R:14:GLU:CB	1:R:17:ASN:HD21	2.09	0.65
1:C:14:GLU:CB	1:C:17:ASN:HD21	2.09	0.65
1:P:14:GLU:CB	1:P:17:ASN:HD21	2.09	0.65
1:B:110:ILE:HD12	1:B:167:MET:HE3	1.78	0.64
1:M:205:THR:OG1	1:M:216:THR:HG23	1.96	0.64
1:J:14:GLU:CB	1:J:17:ASN:HD21	2.09	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:14:GLU:CB	1:M:17:ASN:HD21	2.09	0.64
1:A:14:GLU:CB	1:A:17:ASN:HD21	2.09	0.64
1:O:205:THR:OG1	1:O:216:THR:HG23	1.96	0.64
1:H:110:ILE:HD12	1:H:167:MET:HE3	1.79	0.64
1:B:164:ILE:CG2	1:C:170:GLN:HA	2.28	0.63
1:E:164:ILE:CG2	1:F:170:GLN:HA	2.28	0.63
1:P:170:GLN:HA	1:R:164:ILE:CG2	2.29	0.63
1:H:164:ILE:CG2	1:I:170:GLN:HA	2.28	0.63
1:K:164:ILE:CG2	1:L:170:GLN:HA	2.28	0.63
1:M:164:ILE:CG2	1:N:170:GLN:HA	2.29	0.63
1:J:164:ILE:CG2	1:K:170:GLN:HA	2.29	0.63
1:M:170:GLN:HA	1:O:164:ILE:CG2	2.29	0.63
1:F:230:VAL:HG12	1:F:255:SER:HA	1.81	0.63
1:O:230:VAL:HG12	1:O:255:SER:HA	1.81	0.63
1:A:170:GLN:HA	1:C:164:ILE:CG2	2.29	0.63
1:G:164:ILE:CG2	1:H:170:GLN:HA	2.29	0.63
1:N:164:ILE:CG2	1:O:170:GLN:HA	2.28	0.63
1:H:230:VAL:HG12	1:H:255:SER:HA	1.81	0.63
1:I:230:VAL:HG12	1:I:255:SER:HA	1.81	0.63
1:G:170:GLN:HA	1:I:164:ILE:CG2	2.29	0.63
1:D:170:GLN:HA	1:F:164:ILE:CG2	2.29	0.63
1:Q:230:VAL:HG12	1:Q:255:SER:HA	1.81	0.63
1:I:242:ASN:N	1:I:242:ASN:HD22	1.85	0.63
1:B:242:ASN:ND2	1:B:242:ASN:N	2.45	0.63
1:P:164:ILE:CG2	1:Q:170:GLN:HA	2.29	0.63
1:L:230:VAL:HG12	1:L:255:SER:HA	1.81	0.62
1:R:230:VAL:HG12	1:R:255:SER:HA	1.81	0.62
1:Q:164:ILE:CG2	1:R:170:GLN:HA	2.29	0.62
1:A:164:ILE:CG2	1:B:170:GLN:HA	2.29	0.62
1:E:230:VAL:HG12	1:E:255:SER:HA	1.81	0.62
1:K:230:VAL:HG12	1:K:255:SER:HA	1.81	0.62
1:H:17:ASN:N	1:H:17:ASN:HD22	1.96	0.62
1:J:170:GLN:HA	1:L:164:ILE:CG2	2.29	0.62
1:M:230:VAL:HG12	1:M:255:SER:HA	1.81	0.62
1:D:164:ILE:CG2	1:E:170:GLN:HA	2.29	0.62
1:N:230:VAL:HG12	1:N:255:SER:HA	1.81	0.62
1:J:230:VAL:HG12	1:J:255:SER:HA	1.81	0.62
1:C:230:VAL:HG12	1:C:255:SER:HA	1.81	0.62
1:M:248:GLU:O	1:M:249:ILE:HB	2.00	0.62
1:G:230:VAL:HG12	1:G:255:SER:HA	1.81	0.62
1:A:230:VAL:HG12	1:A:255:SER:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:VAL:HG12	1:D:255:SER:HA	1.81	0.62
1:I:248:GLU:O	1:I:249:ILE:HB	2.00	0.62
1:P:230:VAL:HG12	1:P:255:SER:HA	1.81	0.62
1:N:248:GLU:O	1:N:249:ILE:HB	2.00	0.61
1:B:230:VAL:HG12	1:B:255:SER:HA	1.81	0.61
1:L:248:GLU:O	1:L:249:ILE:HB	2.00	0.61
1:O:248:GLU:O	1:O:249:ILE:HB	2.00	0.61
1:L:110:ILE:HD12	1:L:167:MET:HE3	1.82	0.61
1:K:110:ILE:HD12	1:K:167:MET:HE3	1.82	0.61
1:F:248:GLU:O	1:F:249:ILE:HB	2.00	0.61
1:G:248:GLU:O	1:G:249:ILE:HB	2.00	0.61
1:A:248:GLU:O	1:A:249:ILE:HB	2.00	0.61
1:F:110:ILE:HD12	1:F:167:MET:HE3	1.82	0.61
1:J:248:GLU:O	1:J:249:ILE:HB	2.00	0.61
1:B:248:GLU:O	1:B:249:ILE:HB	2.00	0.61
1:R:248:GLU:O	1:R:249:ILE:HB	2.00	0.61
1:C:248:GLU:O	1:C:249:ILE:HB	2.00	0.61
1:P:248:GLU:O	1:P:249:ILE:HB	2.00	0.61
1:D:248:GLU:O	1:D:249:ILE:HB	2.00	0.61
1:E:110:ILE:HD12	1:E:167:MET:HE3	1.80	0.61
1:K:242:ASN:ND2	1:K:242:ASN:N	2.45	0.61
1:Q:248:GLU:O	1:Q:249:ILE:HB	2.00	0.61
1:P:110:ILE:HD12	1:P:167:MET:HE3	1.81	0.61
1:D:10:ILE:H	1:E:32:ASN:HD21	1.49	0.60
1:K:248:GLU:O	1:K:249:ILE:HB	2.00	0.60
1:D:32:ASN:HD21	1:F:10:ILE:H	1.50	0.60
1:E:248:GLU:O	1:E:249:ILE:HB	2.00	0.60
1:G:32:ASN:HD21	1:I:10:ILE:H	1.49	0.60
1:J:17:ASN:N	1:J:17:ASN:HD22	1.96	0.60
1:H:248:GLU:O	1:H:249:ILE:HB	2.00	0.60
1:A:10:ILE:H	1:B:32:ASN:HD21	1.50	0.60
1:L:17:ASN:HD22	1:L:17:ASN:N	1.96	0.60
1:G:10:ILE:H	1:H:32:ASN:HD21	1.50	0.60
1:A:32:ASN:HD21	1:C:10:ILE:H	1.50	0.60
1:P:10:ILE:H	1:Q:32:ASN:HD21	1.50	0.60
1:J:32:ASN:HD21	1:L:10:ILE:H	1.50	0.60
1:M:10:ILE:H	1:N:32:ASN:HD21	1.49	0.60
1:M:32:ASN:HD21	1:O:10:ILE:H	1.50	0.60
1:P:32:ASN:HD21	1:R:10:ILE:H	1.49	0.60
1:J:10:ILE:H	1:K:32:ASN:HD21	1.50	0.60
1:M:242:ASN:N	1:M:242:ASN:ND2	2.45	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:242:ASN:N	1:G:242:ASN:HD22	1.85	0.60
1:B:15:ILE:C	1:B:17:ASN:H	2.06	0.59
1:F:242:ASN:HD22	1:F:242:ASN:N	1.85	0.59
1:D:110:ILE:HD12	1:D:167:MET:HE3	1.84	0.59
1:F:15:ILE:C	1:F:17:ASN:H	2.06	0.59
1:C:15:ILE:C	1:C:17:ASN:H	2.06	0.59
1:D:15:ILE:C	1:D:17:ASN:H	2.06	0.59
1:Q:110:ILE:HD12	1:Q:167:MET:HE3	1.84	0.59
1:G:15:ILE:C	1:G:17:ASN:H	2.06	0.59
1:E:15:ILE:C	1:E:17:ASN:H	2.06	0.58
1:P:15:ILE:C	1:P:17:ASN:H	2.06	0.58
1:N:18:ALA:CB	1:N:23:ILE:HD11	2.27	0.58
1:I:242:ASN:ND2	1:I:242:ASN:N	2.45	0.58
1:O:110:ILE:HD12	1:O:167:MET:HE3	1.85	0.58
1:F:14:GLU:O	1:F:15:ILE:HB	2.04	0.58
1:D:242:ASN:N	1:D:242:ASN:HD22	1.85	0.58
1:I:15:ILE:C	1:I:17:ASN:H	2.06	0.58
1:O:14:GLU:O	1:O:15:ILE:HB	2.04	0.58
1:O:15:ILE:C	1:O:17:ASN:H	2.06	0.58
1:N:10:ILE:H	1:O:32:ASN:HD21	1.50	0.58
1:A:110:ILE:HD12	1:A:167:MET:HE3	1.84	0.58
1:J:15:ILE:C	1:J:17:ASN:H	2.06	0.58
1:I:17:ASN:HD22	1:I:17:ASN:N	1.96	0.58
1:P:14:GLU:O	1:P:15:ILE:HB	2.04	0.58
1:B:14:GLU:O	1:B:15:ILE:HB	2.04	0.58
1:H:242:ASN:N	1:H:242:ASN:ND2	2.45	0.58
1:Q:10:ILE:H	1:R:32:ASN:HD21	1.50	0.58
1:E:14:GLU:O	1:E:15:ILE:HB	2.04	0.58
1:M:15:ILE:C	1:M:17:ASN:H	2.06	0.58
1:R:14:GLU:O	1:R:15:ILE:HB	2.04	0.58
1:C:14:GLU:O	1:C:15:ILE:HB	2.04	0.58
1:A:14:GLU:O	1:A:15:ILE:HB	2.04	0.58
1:N:14:GLU:O	1:N:15:ILE:HB	2.04	0.58
1:K:10:ILE:H	1:L:32:ASN:HD21	1.50	0.57
1:I:14:GLU:O	1:I:15:ILE:HB	2.04	0.57
1:L:15:ILE:C	1:L:17:ASN:H	2.06	0.57
1:Q:17:ASN:HD22	1:Q:17:ASN:N	1.96	0.57
1:L:242:ASN:ND2	1:L:242:ASN:N	2.45	0.57
1:E:10:ILE:H	1:F:32:ASN:HD21	1.50	0.57
1:H:10:ILE:H	1:I:32:ASN:HD21	1.50	0.57
1:H:15:ILE:C	1:H:17:ASN:H	2.06	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:15:ILE:C	1:K:17:ASN:H	2.06	0.57
1:J:14:GLU:O	1:J:15:ILE:HB	2.04	0.57
1:L:14:GLU:O	1:L:15:ILE:HB	2.04	0.57
1:A:15:ILE:C	1:A:17:ASN:H	2.06	0.57
1:B:10:ILE:H	1:C:32:ASN:HD21	1.50	0.57
1:P:242:ASN:N	1:P:242:ASN:HD22	1.85	0.57
1:H:14:GLU:O	1:H:15:ILE:HB	2.04	0.57
1:D:14:GLU:O	1:D:15:ILE:HB	2.04	0.57
1:A:242:ASN:HD22	1:A:242:ASN:N	1.85	0.57
1:C:98:ILE:O	1:C:127:ILE:HG12	2.05	0.57
1:M:14:GLU:O	1:M:15:ILE:HB	2.04	0.57
1:Q:15:ILE:C	1:Q:17:ASN:H	2.06	0.57
1:B:17:ASN:HD22	1:B:17:ASN:N	1.96	0.57
1:D:98:ILE:O	1:D:127:ILE:HG12	2.05	0.57
1:R:98:ILE:O	1:R:127:ILE:HG12	2.05	0.57
1:B:98:ILE:O	1:B:127:ILE:HG12	2.05	0.57
1:A:98:ILE:O	1:A:127:ILE:HG12	2.05	0.57
1:Q:14:GLU:O	1:Q:15:ILE:HB	2.04	0.56
1:J:18:ALA:CB	1:J:23:ILE:HD11	2.27	0.56
1:P:98:ILE:O	1:P:127:ILE:HG12	2.05	0.56
1:N:98:ILE:O	1:N:127:ILE:HG12	2.05	0.56
1:Q:71:SER:OG	1:Q:74:GLU:HG3	2.06	0.56
1:K:14:GLU:O	1:K:15:ILE:HB	2.04	0.56
1:J:98:ILE:O	1:J:127:ILE:HG12	2.05	0.56
1:L:98:ILE:O	1:L:127:ILE:HG12	2.05	0.56
1:E:98:ILE:O	1:E:127:ILE:HG12	2.05	0.56
1:O:98:ILE:O	1:O:127:ILE:HG12	2.05	0.56
1:H:98:ILE:O	1:H:127:ILE:HG12	2.05	0.56
1:E:71:SER:OG	1:E:74:GLU:HG3	2.06	0.56
1:J:71:SER:OG	1:J:74:GLU:HG3	2.06	0.56
1:R:71:SER:OG	1:R:74:GLU:HG3	2.06	0.56
1:N:71:SER:OG	1:N:74:GLU:HG3	2.06	0.56
1:C:18:ALA:CB	1:C:23:ILE:HD11	2.27	0.56
1:K:98:ILE:O	1:K:127:ILE:HG12	2.05	0.56
1:O:71:SER:OG	1:O:74:GLU:HG3	2.06	0.56
1:P:71:SER:OG	1:P:74:GLU:HG3	2.06	0.56
1:B:71:SER:OG	1:B:74:GLU:HG3	2.06	0.56
1:O:110:ILE:HG23	1:O:167:MET:HE1	1.88	0.56
1:A:71:SER:OG	1:A:74:GLU:HG3	2.06	0.56
1:N:15:ILE:C	1:N:17:ASN:H	2.06	0.56
1:M:98:ILE:O	1:M:127:ILE:HG12	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:SER:OG	1:D:74:GLU:HG3	2.06	0.56
1:G:14:GLU:O	1:G:15:ILE:HB	2.04	0.56
1:O:18:ALA:CB	1:O:23:ILE:HD11	2.27	0.56
1:I:71:SER:OG	1:I:74:GLU:HG3	2.06	0.56
1:R:15:ILE:C	1:R:17:ASN:H	2.06	0.56
1:A:14:GLU:HA	1:A:17:ASN:ND2	2.21	0.56
1:A:242:ASN:ND2	1:A:242:ASN:N	2.45	0.56
1:M:71:SER:OG	1:M:74:GLU:HG3	2.06	0.56
1:A:79:VAL:HG11	1:A:85:HIS:HE2	1.71	0.56
1:P:233:SER:HA	2:P:316:EPE:H81	1.88	0.56
1:F:98:ILE:O	1:F:127:ILE:HG12	2.05	0.56
1:K:14:GLU:HA	1:K:17:ASN:ND2	2.21	0.56
1:D:14:GLU:HA	1:D:17:ASN:ND2	2.21	0.56
1:A:233:SER:HA	2:A:301:EPE:H81	1.88	0.56
1:I:98:ILE:O	1:I:127:ILE:HG12	2.05	0.56
1:C:71:SER:OG	1:C:74:GLU:HG3	2.06	0.56
1:D:193:HIS:CD2	1:F:118:VAL:HG21	2.41	0.56
1:F:71:SER:OG	1:F:74:GLU:HG3	2.06	0.56
1:N:118:VAL:HG21	1:O:193:HIS:CD2	2.41	0.56
1:Q:18:ALA:CB	1:Q:23:ILE:HD11	2.27	0.55
1:N:17:ASN:N	1:N:17:ASN:HD22	1.96	0.55
1:H:233:SER:HA	2:H:308:EPE:H81	1.88	0.55
1:G:193:HIS:CD2	1:I:118:VAL:HG21	2.41	0.55
1:A:193:HIS:CD2	1:C:118:VAL:HG21	2.41	0.55
1:R:79:VAL:HG11	1:R:85:HIS:HE2	1.71	0.55
1:H:71:SER:OG	1:H:74:GLU:HG3	2.06	0.55
1:P:14:GLU:HA	1:P:17:ASN:ND2	2.21	0.55
1:N:14:GLU:HA	1:N:17:ASN:ND2	2.21	0.55
1:L:201:LYS:HE2	1:L:218:GLU:OE2	2.07	0.55
1:G:98:ILE:O	1:G:127:ILE:HG12	2.05	0.55
1:I:111:ASN:HD22	1:I:143:TYR:H	1.55	0.55
1:Q:118:VAL:HG21	1:R:193:HIS:CD2	2.41	0.55
1:K:118:VAL:HG21	1:L:193:HIS:CD2	2.41	0.55
1:K:71:SER:OG	1:K:74:GLU:HG3	2.06	0.55
1:L:111:ASN:HD22	1:L:143:TYR:H	1.55	0.55
1:B:14:GLU:HA	1:B:17:ASN:ND2	2.21	0.55
1:G:233:SER:HA	2:G:307:EPE:H81	1.88	0.55
1:I:144:SER:HB2	1:I:164:ILE:CD1	2.37	0.55
1:P:79:VAL:HG11	1:P:85:HIS:HE2	1.71	0.55
1:F:111:ASN:HD22	1:F:143:TYR:H	1.55	0.55
1:H:72:ILE:H	1:H:72:ILE:HD12	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ILE:H	1:B:72:ILE:HD12	1.72	0.55
1:E:233:SER:HA	2:E:305:EPE:H81	1.88	0.55
1:Q:98:ILE:O	1:Q:127:ILE:HG12	2.05	0.55
1:F:144:SER:HB2	1:F:164:ILE:CD1	2.37	0.55
1:J:193:HIS:CD2	1:L:118:VAL:HG21	2.41	0.55
1:I:79:VAL:HG11	1:I:85:HIS:HE2	1.71	0.55
1:D:118:VAL:HG21	1:E:193:HIS:CD2	2.41	0.55
1:H:111:ASN:HD22	1:H:143:TYR:H	1.55	0.55
1:O:79:VAL:HG11	1:O:85:HIS:HE2	1.71	0.55
1:J:118:VAL:HG21	1:K:193:HIS:CD2	2.41	0.55
1:L:71:SER:OG	1:L:74:GLU:HG3	2.06	0.55
1:P:193:HIS:CD2	1:R:118:VAL:HG21	2.41	0.55
1:J:233:SER:HA	2:J:310:EPE:H81	1.88	0.55
1:P:201:LYS:HE2	1:P:218:GLU:OE2	2.07	0.55
1:Q:110:ILE:HG23	1:Q:167:MET:HE1	1.89	0.55
1:G:111:ASN:HD22	1:G:143:TYR:H	1.55	0.55
1:C:79:VAL:HG11	1:C:85:HIS:HE2	1.71	0.55
1:G:118:VAL:HG21	1:H:193:HIS:CD2	2.41	0.55
1:B:111:ASN:HD22	1:B:143:TYR:H	1.55	0.55
1:I:18:ALA:CB	1:I:23:ILE:HD11	2.27	0.55
1:O:201:LYS:HE2	1:O:218:GLU:OE2	2.07	0.55
1:A:201:LYS:HE2	1:A:218:GLU:OE2	2.07	0.55
1:Q:144:SER:HB2	1:Q:164:ILE:CD1	2.37	0.55
1:M:193:HIS:CD2	1:O:118:VAL:HG21	2.41	0.55
1:J:111:ASN:HD22	1:J:143:TYR:H	1.55	0.55
1:L:79:VAL:HG11	1:L:85:HIS:HE2	1.71	0.55
1:A:118:VAL:HG21	1:B:193:HIS:CD2	2.41	0.55
1:J:72:ILE:H	1:J:72:ILE:HD12	1.72	0.55
1:D:72:ILE:H	1:D:72:ILE:HD12	1.72	0.55
1:R:72:ILE:HD12	1:R:72:ILE:H	1.72	0.55
1:H:14:GLU:HA	1:H:17:ASN:ND2	2.21	0.55
1:G:14:GLU:HA	1:G:17:ASN:ND2	2.21	0.55
1:Q:14:GLU:HA	1:Q:17:ASN:ND2	2.21	0.55
1:E:201:LYS:HE2	1:E:218:GLU:OE2	2.07	0.55
1:R:201:LYS:HE2	1:R:218:GLU:OE2	2.07	0.55
1:B:79:VAL:HG11	1:B:85:HIS:HE2	1.71	0.55
1:P:210:ASP:OD2	1:P:212:ARG:HD3	2.07	0.55
1:E:111:ASN:HD22	1:E:143:TYR:H	1.55	0.55
1:Q:233:SER:HA	2:Q:317:EPE:H81	1.88	0.55
1:C:233:SER:HA	2:C:303:EPE:H81	1.88	0.55
1:J:201:LYS:HE2	1:J:218:GLU:OE2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:210:ASP:OD2	1:G:212:ARG:HD3	2.07	0.55
1:J:210:ASP:OD2	1:J:212:ARG:HD3	2.07	0.55
1:D:210:ASP:OD2	1:D:212:ARG:HD3	2.07	0.55
1:K:210:ASP:OD2	1:K:212:ARG:HD3	2.07	0.55
1:B:118:VAL:HG21	1:C:193:HIS:CD2	2.41	0.55
1:F:18:ALA:CB	1:F:23:ILE:HD11	2.27	0.55
1:M:14:GLU:HA	1:M:17:ASN:ND2	2.21	0.55
1:C:201:LYS:HE2	1:C:218:GLU:OE2	2.07	0.55
1:A:210:ASP:OD2	1:A:212:ARG:HD3	2.07	0.55
1:R:233:SER:HA	2:R:318:EPE:H81	1.88	0.55
1:D:233:SER:HA	2:D:304:EPE:H81	1.88	0.55
1:G:201:LYS:HE2	1:G:218:GLU:OE2	2.07	0.55
1:D:201:LYS:HE2	1:D:218:GLU:OE2	2.07	0.55
1:N:201:LYS:HE2	1:N:218:GLU:OE2	2.07	0.55
1:Q:201:LYS:HE2	1:Q:218:GLU:OE2	2.07	0.55
1:L:144:SER:HB2	1:L:164:ILE:CD1	2.37	0.55
1:M:210:ASP:OD2	1:M:212:ARG:HD3	2.07	0.55
1:D:79:VAL:HG11	1:D:85:HIS:HE2	1.71	0.55
1:Q:210:ASP:OD2	1:Q:212:ARG:HD3	2.07	0.55
1:E:210:ASP:OD2	1:E:212:ARG:HD3	2.07	0.55
1:G:71:SER:OG	1:G:74:GLU:HG3	2.06	0.55
1:G:72:ILE:H	1:G:72:ILE:HD12	1.72	0.55
1:N:210:ASP:OD2	1:N:212:ARG:HD3	2.07	0.55
1:R:14:GLU:HA	1:R:17:ASN:ND2	2.21	0.54
1:A:17:ASN:HD22	1:A:17:ASN:N	1.96	0.54
1:M:242:ASN:HD22	1:M:242:ASN:N	1.85	0.54
1:F:233:SER:HA	2:F:306:EPE:H81	1.88	0.54
1:N:233:SER:HA	2:N:314:EPE:H81	1.88	0.54
1:K:233:SER:HA	2:K:311:EPE:H81	1.88	0.54
1:C:144:SER:HB2	1:C:164:ILE:CD1	2.37	0.54
1:O:111:ASN:HD22	1:O:143:TYR:H	1.55	0.54
1:H:118:VAL:HG21	1:I:193:HIS:CD2	2.41	0.54
1:F:20:THR:O	1:F:21:GLY:C	2.46	0.54
1:P:118:VAL:HG21	1:Q:193:HIS:CD2	2.41	0.54
1:R:210:ASP:OD2	1:R:212:ARG:HD3	2.07	0.54
1:O:20:THR:O	1:O:21:GLY:C	2.46	0.54
1:P:72:ILE:H	1:P:72:ILE:HD12	1.72	0.54
1:M:72:ILE:HD12	1:M:72:ILE:H	1.72	0.54
1:J:14:GLU:HA	1:J:17:ASN:ND2	2.21	0.54
1:I:14:GLU:HA	1:I:17:ASN:ND2	2.21	0.54
1:O:242:ASN:ND2	1:O:242:ASN:N	2.45	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:233:SER:HA	2:O:315:EPE:H81	1.88	0.54
1:M:201:LYS:HE2	1:M:218:GLU:OE2	2.07	0.54
1:B:201:LYS:HE2	1:B:218:GLU:OE2	2.07	0.54
1:A:144:SER:HB2	1:A:164:ILE:CD1	2.37	0.54
1:Q:111:ASN:HD22	1:Q:143:TYR:H	1.55	0.54
1:D:111:ASN:HD22	1:D:143:TYR:H	1.55	0.54
1:Q:72:ILE:H	1:Q:72:ILE:HD12	1.72	0.54
1:P:144:SER:HB2	1:P:164:ILE:CD1	2.37	0.54
1:D:144:SER:HB2	1:D:164:ILE:CD1	2.37	0.54
1:I:210:ASP:OD2	1:I:212:ARG:HD3	2.07	0.54
1:K:111:ASN:HD22	1:K:143:TYR:H	1.55	0.54
1:M:118:VAL:HG21	1:N:193:HIS:CD2	2.41	0.54
1:A:72:ILE:HD12	1:A:72:ILE:H	1.72	0.54
1:C:72:ILE:HD12	1:C:72:ILE:H	1.72	0.54
1:R:111:ASN:HD22	1:R:143:TYR:H	1.55	0.54
1:E:17:ASN:HD22	1:E:17:ASN:N	1.96	0.54
1:L:14:GLU:HA	1:L:17:ASN:ND2	2.21	0.54
1:I:201:LYS:HE2	1:I:218:GLU:OE2	2.07	0.54
1:O:210:ASP:OD2	1:O:212:ARG:HD3	2.07	0.54
1:E:118:VAL:HG21	1:F:193:HIS:CD2	2.41	0.54
1:Q:79:VAL:HG11	1:Q:85:HIS:HE2	1.71	0.54
1:F:79:VAL:HG11	1:F:85:HIS:HE2	1.71	0.54
1:M:111:ASN:HD22	1:M:143:TYR:H	1.55	0.54
1:O:72:ILE:H	1:O:72:ILE:HD12	1.72	0.54
1:E:72:ILE:HD12	1:E:72:ILE:H	1.72	0.54
1:N:79:VAL:HG11	1:N:85:HIS:HE2	1.72	0.54
1:K:20:THR:O	1:K:21:GLY:C	2.46	0.54
1:F:17:ASN:HD22	1:F:17:ASN:N	1.96	0.54
1:C:14:GLU:HA	1:C:17:ASN:ND2	2.21	0.54
1:O:14:GLU:HA	1:O:17:ASN:ND2	2.21	0.54
1:I:233:SER:HA	2:I:309:EPE:H81	1.88	0.54
1:F:201:LYS:HE2	1:F:218:GLU:OE2	2.07	0.54
1:D:29:ASN:OD1	1:F:12:THR:HG21	2.08	0.54
1:P:29:ASN:OD1	1:R:12:THR:HG21	2.08	0.54
1:L:72:ILE:HD12	1:L:72:ILE:H	1.72	0.54
1:H:79:VAL:HG11	1:H:85:HIS:HE2	1.71	0.54
1:H:210:ASP:OD2	1:H:212:ARG:HD3	2.07	0.54
1:F:14:GLU:HA	1:F:17:ASN:ND2	2.21	0.54
1:H:201:LYS:HE2	1:H:218:GLU:OE2	2.07	0.54
1:B:144:SER:HB2	1:B:164:ILE:CD1	2.37	0.54
1:C:210:ASP:OD2	1:C:212:ARG:HD3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:79:VAL:HG11	1:J:85:HIS:HE2	1.71	0.54
1:A:29:ASN:OD1	1:C:12:THR:HG21	2.08	0.54
1:C:111:ASN:HD22	1:C:143:TYR:H	1.55	0.54
1:B:20:THR:O	1:B:21:GLY:C	2.46	0.54
1:G:144:SER:HB2	1:G:164:ILE:CD1	2.37	0.54
1:K:146:VAL:HG22	1:K:164:ILE:HD13	1.90	0.54
1:E:12:THR:HG21	1:F:29:ASN:OD1	2.08	0.54
1:H:12:THR:HG21	1:I:29:ASN:OD1	2.08	0.54
1:F:210:ASP:OD2	1:F:212:ARG:HD3	2.07	0.54
1:R:18:ALA:CB	1:R:23:ILE:HD11	2.27	0.54
1:K:201:LYS:HE2	1:K:218:GLU:OE2	2.07	0.54
1:J:144:SER:HB2	1:J:164:ILE:CD1	2.37	0.54
1:O:144:SER:HB2	1:O:164:ILE:CD1	2.37	0.54
1:M:144:SER:HB2	1:M:164:ILE:CD1	2.37	0.54
1:H:20:THR:O	1:H:21:GLY:C	2.46	0.54
1:G:79:VAL:HG11	1:G:85:HIS:HE2	1.71	0.54
1:M:29:ASN:OD1	1:O:12:THR:HG21	2.08	0.54
1:L:233:SER:HA	2:L:312:EPE:H81	1.88	0.54
1:B:233:SER:HA	2:B:302:EPE:H81	1.88	0.54
1:C:146:VAL:HG22	1:C:164:ILE:HD13	1.90	0.54
1:D:110:ILE:HG23	1:D:167:MET:HE1	1.89	0.54
1:D:20:THR:O	1:D:21:GLY:C	2.46	0.54
1:G:12:THR:HG21	1:H:29:ASN:OD1	2.08	0.54
1:I:72:ILE:H	1:I:72:ILE:HD12	1.72	0.54
1:H:146:VAL:HG22	1:H:164:ILE:HD13	1.90	0.54
1:B:210:ASP:OD2	1:B:212:ARG:HD3	2.07	0.54
1:K:72:ILE:H	1:K:72:ILE:HD12	1.72	0.54
1:G:170:GLN:HG2	1:I:164:ILE:HG21	1.90	0.53
1:B:164:ILE:HG21	1:C:170:GLN:HG2	1.91	0.53
1:G:164:ILE:HG21	1:H:170:GLN:HG2	1.91	0.53
1:J:164:ILE:HG21	1:K:170:GLN:HG2	1.91	0.53
1:E:164:ILE:HG21	1:F:170:GLN:HG2	1.91	0.53
1:A:110:ILE:HG23	1:A:167:MET:HE1	1.89	0.53
1:M:79:VAL:HG11	1:M:85:HIS:HE2	1.71	0.53
1:N:72:ILE:HD12	1:N:72:ILE:H	1.72	0.53
1:R:144:SER:HB2	1:R:164:ILE:CD1	2.37	0.53
1:B:146:VAL:HG22	1:B:164:ILE:HD13	1.90	0.53
1:Q:164:ILE:HG21	1:R:170:GLN:HG2	1.91	0.53
1:P:146:VAL:HG22	1:P:164:ILE:HD13	1.90	0.53
1:F:146:VAL:HG22	1:F:164:ILE:HD13	1.90	0.53
1:D:12:THR:HG21	1:E:29:ASN:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:VAL:HG11	1:E:85:HIS:HE2	1.72	0.53
1:A:12:THR:HG21	1:B:29:ASN:OD1	2.08	0.53
1:B:12:THR:HG21	1:C:29:ASN:OD1	2.08	0.53
1:P:12:THR:HG21	1:Q:29:ASN:OD1	2.08	0.53
1:B:18:ALA:CB	1:B:23:ILE:HD11	2.27	0.53
1:N:146:VAL:HG22	1:N:164:ILE:HD13	1.90	0.53
1:R:20:THR:O	1:R:21:GLY:C	2.46	0.53
1:K:79:VAL:HG11	1:K:85:HIS:HE2	1.71	0.53
1:G:146:VAL:HG22	1:G:164:ILE:HD13	1.90	0.53
1:P:111:ASN:HD22	1:P:143:TYR:H	1.55	0.53
1:F:72:ILE:HD12	1:F:72:ILE:H	1.72	0.53
1:E:14:GLU:HA	1:E:17:ASN:ND2	2.21	0.53
1:M:233:SER:HA	2:M:313:EPE:H81	1.88	0.53
1:K:144:SER:HB2	1:K:164:ILE:CD1	2.37	0.53
1:D:170:GLN:HG2	1:F:164:ILE:HG21	1.90	0.53
1:A:111:ASN:HD22	1:A:143:TYR:H	1.55	0.53
1:N:111:ASN:HD22	1:N:143:TYR:H	1.55	0.53
1:A:20:THR:O	1:A:21:GLY:C	2.46	0.53
1:Q:20:THR:O	1:Q:21:GLY:C	2.46	0.53
1:K:17:ASN:N	1:K:17:ASN:HD22	1.96	0.53
1:N:164:ILE:HG21	1:O:170:GLN:HG2	1.91	0.53
1:K:12:THR:HG21	1:L:29:ASN:OD1	2.08	0.53
1:L:210:ASP:OD2	1:L:212:ARG:HD3	2.07	0.53
1:J:12:THR:HG21	1:K:29:ASN:OD1	2.08	0.53
1:R:146:VAL:HG22	1:R:164:ILE:HD13	1.90	0.53
1:A:146:VAL:HG22	1:A:164:ILE:HD13	1.90	0.53
1:M:146:VAL:HG22	1:M:164:ILE:HD13	1.90	0.53
1:M:164:ILE:HG21	1:N:170:GLN:HG2	1.91	0.53
1:G:29:ASN:OD1	1:I:12:THR:HG21	2.08	0.53
1:D:39:TYR:CE2	1:F:7:LYS:HB2	2.44	0.53
1:M:12:THR:HG21	1:N:29:ASN:OD1	2.08	0.53
1:N:12:THR:HG21	1:O:29:ASN:OD1	2.08	0.53
1:E:14:GLU:HB3	1:E:17:ASN:HD21	1.74	0.53
1:J:242:ASN:HD22	1:J:242:ASN:N	1.85	0.53
1:P:170:GLN:HG2	1:R:164:ILE:HG21	1.90	0.53
1:O:146:VAL:HG22	1:O:164:ILE:HD13	1.90	0.53
1:D:164:ILE:HG21	1:E:170:GLN:HG2	1.91	0.53
1:J:29:ASN:OD1	1:L:12:THR:HG21	2.08	0.53
1:N:14:GLU:HB3	1:N:17:ASN:HD21	1.74	0.53
1:B:14:GLU:HB3	1:B:17:ASN:HD21	1.74	0.53
1:L:18:ALA:CB	1:L:23:ILE:HD11	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:GLN:HG2	1:C:164:ILE:HG21	1.91	0.53
1:K:164:ILE:HG21	1:L:170:GLN:HG2	1.91	0.53
1:C:111:ASN:HD21	1:C:116:ILE:H	1.57	0.53
1:G:7:LYS:HB2	1:H:39:TYR:CE2	2.44	0.53
1:I:20:THR:O	1:I:21:GLY:C	2.46	0.53
1:P:20:THR:O	1:P:21:GLY:C	2.46	0.53
1:D:17:ASN:ND2	1:D:17:ASN:H	2.05	0.53
1:H:144:SER:HB2	1:H:164:ILE:CD1	2.37	0.53
1:M:111:ASN:HD21	1:M:116:ILE:H	1.57	0.53
1:J:7:LYS:HB2	1:K:39:TYR:CE2	2.44	0.53
1:K:7:LYS:HB2	1:L:39:TYR:CE2	2.45	0.53
1:K:14:GLU:HB3	1:K:17:ASN:HD21	1.74	0.52
1:P:18:ALA:CB	1:P:23:ILE:HD11	2.27	0.52
1:L:146:VAL:HG22	1:L:164:ILE:HD13	1.90	0.52
1:Q:146:VAL:HG22	1:Q:164:ILE:HD13	1.90	0.52
1:J:111:ASN:HD21	1:J:116:ILE:H	1.57	0.52
1:A:7:LYS:HB2	1:B:39:TYR:CE2	2.44	0.52
1:R:17:ASN:ND2	1:R:17:ASN:H	2.05	0.52
1:H:111:ASN:HD21	1:H:116:ILE:H	1.57	0.52
1:R:111:ASN:HD21	1:R:116:ILE:H	1.57	0.52
1:N:20:THR:O	1:N:21:GLY:C	2.46	0.52
1:J:153:SER:HA	1:J:157:THR:O	2.10	0.52
1:N:7:LYS:HB2	1:O:39:TYR:CE2	2.44	0.52
1:R:153:SER:HA	1:R:157:THR:O	2.10	0.52
1:A:39:TYR:CE2	1:C:7:LYS:HB2	2.44	0.52
1:H:14:GLU:HB3	1:H:17:ASN:HD21	1.74	0.52
1:H:164:ILE:HG21	1:I:170:GLN:HG2	1.91	0.52
1:Q:111:ASN:HD21	1:Q:116:ILE:H	1.57	0.52
1:N:111:ASN:HD21	1:N:116:ILE:H	1.57	0.52
1:Q:12:THR:HG21	1:R:29:ASN:OD1	2.08	0.52
1:O:153:SER:HA	1:O:157:THR:O	2.10	0.52
1:G:39:TYR:CE2	1:I:7:LYS:HB2	2.44	0.52
1:C:14:GLU:HB3	1:C:17:ASN:HD21	1.74	0.52
1:M:14:GLU:HB3	1:M:17:ASN:HD21	1.74	0.52
1:K:17:ASN:ND2	1:K:17:ASN:H	2.05	0.52
1:I:146:VAL:HG22	1:I:164:ILE:HD13	1.90	0.52
1:D:7:LYS:HB2	1:E:39:TYR:CE2	2.44	0.52
1:N:153:SER:HA	1:N:157:THR:O	2.10	0.52
1:M:20:THR:O	1:M:21:GLY:C	2.46	0.52
1:C:20:THR:O	1:C:21:GLY:C	2.46	0.52
1:R:14:GLU:HB3	1:R:17:ASN:HD21	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:VAL:HG22	1:D:164:ILE:HD13	1.90	0.52
1:E:146:VAL:HG22	1:E:164:ILE:HD13	1.90	0.52
1:K:110:ILE:HG23	1:K:167:MET:HE1	1.91	0.52
1:E:20:THR:O	1:E:21:GLY:C	2.46	0.52
1:O:244:THR:C	1:O:246:GLU:H	2.13	0.52
1:E:18:ALA:CB	1:E:23:ILE:HD11	2.27	0.52
1:J:14:GLU:HB3	1:J:17:ASN:HD21	1.74	0.52
1:I:14:GLU:HB3	1:I:17:ASN:HD21	1.74	0.52
1:P:164:ILE:HG21	1:Q:170:GLN:HG2	1.91	0.52
1:M:170:GLN:HG2	1:O:164:ILE:HG21	1.90	0.52
1:E:144:SER:HB2	1:E:164:ILE:CD1	2.37	0.52
1:G:153:SER:HA	1:G:157:THR:O	2.10	0.52
1:H:153:SER:HA	1:H:157:THR:O	2.10	0.52
1:Q:153:SER:HA	1:Q:157:THR:O	2.10	0.52
1:H:7:LYS:HB2	1:I:39:TYR:CE2	2.44	0.52
1:H:17:ASN:ND2	1:H:17:ASN:H	2.05	0.52
1:I:17:ASN:H	1:I:17:ASN:ND2	2.05	0.52
1:G:18:ALA:CB	1:G:23:ILE:HD11	2.27	0.52
1:E:111:ASN:HD21	1:E:116:ILE:H	1.57	0.52
1:A:111:ASN:HD21	1:A:116:ILE:H	1.57	0.52
1:M:17:ASN:HD22	1:M:17:ASN:N	1.96	0.52
1:M:153:SER:HA	1:M:157:THR:O	2.10	0.52
1:G:244:THR:C	1:G:246:GLU:H	2.13	0.52
1:J:20:THR:O	1:J:21:GLY:C	2.46	0.52
1:P:14:GLU:HB3	1:P:17:ASN:HD21	1.74	0.52
1:J:146:VAL:HG22	1:J:164:ILE:HD13	1.90	0.52
1:A:164:ILE:HG21	1:B:170:GLN:HG2	1.91	0.52
1:M:7:LYS:HB2	1:N:39:TYR:CE2	2.44	0.52
1:E:153:SER:HA	1:E:157:THR:O	2.10	0.52
1:R:244:THR:C	1:R:246:GLU:H	2.13	0.52
1:G:17:ASN:N	1:G:17:ASN:HD22	1.96	0.52
1:G:17:ASN:H	1:G:17:ASN:ND2	2.05	0.52
1:N:144:SER:HB2	1:N:164:ILE:CD1	2.37	0.52
1:L:111:ASN:HD21	1:L:116:ILE:H	1.57	0.52
1:O:79:VAL:HG11	1:O:85:HIS:NE2	2.25	0.52
1:D:111:ASN:HD21	1:D:116:ILE:H	1.57	0.52
1:P:39:TYR:CE2	1:R:7:LYS:HB2	2.44	0.52
1:D:153:SER:HA	1:D:157:THR:O	2.10	0.52
1:J:170:GLN:HG2	1:L:164:ILE:HG21	1.91	0.51
1:R:79:VAL:HG11	1:R:85:HIS:NE2	2.25	0.51
1:F:111:ASN:HD21	1:F:116:ILE:H	1.57	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:VAL:HG11	1:C:85:HIS:NE2	2.25	0.51
1:O:111:ASN:HD21	1:O:116:ILE:H	1.57	0.51
1:G:79:VAL:HG11	1:G:85:HIS:NE2	2.25	0.51
1:K:79:VAL:HG11	1:K:85:HIS:NE2	2.26	0.51
1:P:7:LYS:HB2	1:Q:39:TYR:CE2	2.44	0.51
1:J:244:THR:C	1:J:246:GLU:H	2.13	0.51
1:J:39:TYR:CE2	1:L:7:LYS:HB2	2.44	0.51
1:J:17:ASN:H	1:J:17:ASN:ND2	2.05	0.51
1:A:14:GLU:HB3	1:A:17:ASN:HD21	1.74	0.51
1:O:14:GLU:HB3	1:O:17:ASN:HD21	1.74	0.51
1:P:79:VAL:HG11	1:P:85:HIS:NE2	2.25	0.51
1:L:79:VAL:HG11	1:L:85:HIS:NE2	2.25	0.51
1:N:79:VAL:HG11	1:N:85:HIS:NE2	2.26	0.51
1:I:153:SER:HA	1:I:157:THR:O	2.10	0.51
1:L:244:THR:C	1:L:246:GLU:H	2.13	0.51
1:Q:14:GLU:HB3	1:Q:17:ASN:HD21	1.74	0.51
1:N:284:ILE:HD13	1:O:207:GLN:HB3	1.93	0.51
1:I:111:ASN:HD21	1:I:116:ILE:H	1.57	0.51
1:G:111:ASN:HD21	1:G:116:ILE:H	1.57	0.51
1:K:111:ASN:HD21	1:K:116:ILE:H	1.57	0.51
1:H:79:VAL:HG11	1:H:85:HIS:NE2	2.26	0.51
1:P:111:ASN:HD21	1:P:116:ILE:H	1.57	0.51
1:Q:7:LYS:HB2	1:R:39:TYR:CE2	2.45	0.51
1:M:39:TYR:CE2	1:O:7:LYS:HB2	2.44	0.51
1:M:18:ALA:CB	1:M:23:ILE:HD11	2.27	0.51
1:D:14:GLU:HB3	1:D:17:ASN:HD21	1.74	0.51
1:H:284:ILE:HD13	1:I:207:GLN:HB3	1.93	0.51
1:A:79:VAL:HG11	1:A:85:HIS:NE2	2.25	0.51
1:Q:79:VAL:HG11	1:Q:85:HIS:NE2	2.26	0.51
1:A:244:THR:C	1:A:246:GLU:H	2.13	0.51
1:C:153:SER:HA	1:C:157:THR:O	2.10	0.51
1:K:153:SER:HA	1:K:157:THR:O	2.10	0.51
1:G:242:ASN:N	1:G:242:ASN:ND2	2.45	0.51
1:B:111:ASN:HD21	1:B:116:ILE:H	1.57	0.51
1:J:79:VAL:HG11	1:J:85:HIS:NE2	2.25	0.51
1:N:244:THR:C	1:N:246:GLU:H	2.13	0.51
1:J:178:THR:O	1:L:287:ALA:HA	2.11	0.51
1:E:244:THR:C	1:E:246:GLU:H	2.13	0.51
1:L:153:SER:HA	1:L:157:THR:O	2.10	0.51
1:F:244:THR:C	1:F:246:GLU:H	2.13	0.51
1:C:17:ASN:HD22	1:C:17:ASN:N	1.96	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:17:ASN:H	1:L:17:ASN:ND2	2.05	0.51
1:E:287:ALA:HA	1:F:178:THR:O	2.11	0.51
1:H:244:THR:C	1:H:246:GLU:H	2.13	0.51
1:P:178:THR:O	1:R:287:ALA:HA	2.11	0.51
1:A:178:THR:O	1:C:287:ALA:HA	2.11	0.51
1:A:287:ALA:HA	1:B:178:THR:O	2.11	0.51
1:P:244:THR:C	1:P:246:GLU:H	2.13	0.51
1:B:7:LYS:HB2	1:C:39:TYR:CE2	2.45	0.51
1:G:14:GLU:HB3	1:G:17:ASN:HD21	1.74	0.51
1:Q:284:ILE:HD13	1:R:207:GLN:HB3	1.93	0.51
1:M:207:GLN:HB3	1:O:284:ILE:HD13	1.93	0.51
1:F:110:ILE:HG23	1:F:167:MET:HE1	1.92	0.51
1:P:153:SER:HA	1:P:157:THR:O	2.10	0.51
1:F:153:SER:HA	1:F:157:THR:O	2.10	0.51
1:H:18:ALA:CB	1:H:23:ILE:HD11	2.27	0.51
1:L:14:GLU:HB3	1:L:17:ASN:HD21	1.74	0.51
1:K:284:ILE:HD13	1:L:207:GLN:HB3	1.93	0.51
1:O:230:VAL:HG11	1:O:254:PHE:HB3	1.93	0.51
1:E:230:VAL:HG11	1:E:254:PHE:HB3	1.93	0.51
1:E:7:LYS:HB2	1:F:39:TYR:CE2	2.44	0.51
1:B:153:SER:HA	1:B:157:THR:O	2.10	0.51
1:D:178:THR:O	1:F:287:ALA:HA	2.11	0.51
1:H:287:ALA:HA	1:I:178:THR:O	2.11	0.51
1:K:244:THR:C	1:K:246:GLU:H	2.13	0.51
1:C:17:ASN:ND2	1:C:17:ASN:H	2.05	0.51
1:M:17:ASN:ND2	1:M:17:ASN:H	2.05	0.51
1:O:17:ASN:N	1:O:17:ASN:HD22	1.96	0.51
1:N:17:ASN:H	1:N:17:ASN:ND2	2.05	0.51
1:B:284:ILE:HD13	1:C:207:GLN:HB3	1.93	0.51
1:E:284:ILE:HD13	1:F:207:GLN:HB3	1.93	0.51
1:A:284:ILE:HD13	1:B:207:GLN:HB3	1.93	0.51
1:D:79:VAL:HG11	1:D:85:HIS:NE2	2.25	0.51
1:O:72:ILE:N	1:O:72:ILE:HD12	2.26	0.51
1:B:244:THR:C	1:B:246:GLU:H	2.13	0.51
1:B:287:ALA:HA	1:C:178:THR:O	2.11	0.51
1:K:18:ALA:CB	1:K:23:ILE:HD11	2.27	0.51
1:G:20:THR:O	1:G:21:GLY:C	2.46	0.51
1:M:287:ALA:HA	1:N:178:THR:O	2.11	0.51
1:D:244:THR:C	1:D:246:GLU:H	2.13	0.51
1:F:14:GLU:HB3	1:F:17:ASN:HD21	1.74	0.50
1:A:18:ALA:CB	1:A:23:ILE:HD11	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:120:ASN:ND2	1:R:120:ASN:N	2.59	0.50
1:L:72:ILE:HD12	1:L:72:ILE:N	2.26	0.50
1:M:79:VAL:HG11	1:M:85:HIS:NE2	2.25	0.50
1:E:79:VAL:HG11	1:E:85:HIS:NE2	2.26	0.50
1:F:157:THR:OG1	1:F:157:THR:O	2.29	0.50
1:K:287:ALA:HA	1:L:178:THR:O	2.11	0.50
1:P:287:ALA:HA	1:Q:178:THR:O	2.11	0.50
1:J:207:GLN:HB3	1:L:284:ILE:HD13	1.93	0.50
1:B:230:VAL:HG11	1:B:254:PHE:HB3	1.93	0.50
1:P:120:ASN:ND2	1:P:120:ASN:N	2.59	0.50
1:L:110:ILE:HG23	1:L:167:MET:HE1	1.92	0.50
1:B:72:ILE:N	1:B:72:ILE:HD12	2.26	0.50
1:F:79:VAL:HG11	1:F:85:HIS:NE2	2.25	0.50
1:D:153:SER:O	1:D:155:ASN:N	2.45	0.50
1:K:153:SER:O	1:K:155:ASN:N	2.45	0.50
1:D:287:ALA:HA	1:E:178:THR:O	2.11	0.50
1:L:20:THR:O	1:L:21:GLY:C	2.46	0.50
1:M:244:THR:C	1:M:246:GLU:H	2.13	0.50
1:A:153:SER:O	1:A:155:ASN:N	2.45	0.50
1:A:153:SER:HA	1:A:157:THR:O	2.10	0.50
1:E:17:ASN:H	1:E:17:ASN:ND2	2.05	0.50
1:R:17:ASN:HD22	1:R:17:ASN:N	1.96	0.50
1:P:242:ASN:N	1:P:242:ASN:ND2	2.45	0.50
1:P:207:GLN:HB3	1:R:284:ILE:HD13	1.93	0.50
1:P:284:ILE:HD13	1:Q:207:GLN:HB3	1.93	0.50
1:N:230:VAL:HG11	1:N:254:PHE:HB3	1.93	0.50
1:I:79:VAL:HG11	1:I:85:HIS:NE2	2.25	0.50
1:J:153:SER:O	1:J:155:ASN:N	2.45	0.50
1:N:153:SER:O	1:N:155:ASN:N	2.45	0.50
1:K:157:THR:O	1:K:157:THR:OG1	2.29	0.50
1:G:178:THR:O	1:I:287:ALA:HA	2.11	0.50
1:R:242:ASN:N	1:R:242:ASN:ND2	2.45	0.50
1:D:242:ASN:N	1:D:242:ASN:ND2	2.45	0.50
1:E:120:ASN:N	1:E:120:ASN:ND2	2.59	0.50
1:G:284:ILE:HD13	1:H:207:GLN:HB3	1.93	0.50
1:P:230:VAL:HG11	1:P:254:PHE:HB3	1.93	0.50
1:J:72:ILE:HD12	1:J:72:ILE:N	2.26	0.50
1:B:79:VAL:HG11	1:B:85:HIS:NE2	2.26	0.50
1:E:72:ILE:HD12	1:E:72:ILE:N	2.26	0.50
1:Q:244:THR:C	1:Q:246:GLU:H	2.13	0.50
1:J:242:ASN:ND2	1:J:242:ASN:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:230:VAL:HG11	1:G:254:PHE:HB3	1.93	0.50
1:G:153:SER:O	1:G:155:ASN:N	2.45	0.50
1:L:153:SER:O	1:L:155:ASN:N	2.45	0.50
1:Q:287:ALA:HA	1:R:178:THR:O	2.11	0.50
1:J:287:ALA:HA	1:K:178:THR:O	2.11	0.50
1:J:17:ASN:N	1:J:17:ASN:ND2	2.60	0.50
1:M:17:ASN:ND2	1:M:17:ASN:N	2.60	0.50
1:P:17:ASN:N	1:P:17:ASN:ND2	2.60	0.50
1:Q:17:ASN:ND2	1:Q:17:ASN:N	2.60	0.50
1:K:72:ILE:HD12	1:K:72:ILE:N	2.26	0.50
1:D:157:THR:OG1	1:D:157:THR:O	2.29	0.50
1:G:287:ALA:HA	1:H:178:THR:O	2.11	0.50
1:M:178:THR:O	1:O:287:ALA:HA	2.11	0.50
1:G:17:ASN:N	1:G:17:ASN:ND2	2.60	0.50
1:C:230:VAL:HG11	1:C:254:PHE:HB3	1.93	0.50
1:Q:72:ILE:N	1:Q:72:ILE:HD12	2.26	0.50
1:J:157:THR:O	1:J:157:THR:OG1	2.29	0.50
1:O:157:THR:OG1	1:O:157:THR:O	2.29	0.50
1:C:153:SER:O	1:C:155:ASN:N	2.45	0.50
1:I:244:THR:C	1:I:246:GLU:H	2.13	0.50
1:C:244:THR:C	1:C:246:GLU:H	2.13	0.50
1:C:120:ASN:ND2	1:C:120:ASN:N	2.59	0.50
1:H:230:VAL:HG11	1:H:254:PHE:HB3	1.93	0.50
1:L:230:VAL:HG11	1:L:254:PHE:HB3	1.93	0.50
1:N:287:ALA:HA	1:O:178:THR:O	2.11	0.50
1:R:17:ASN:ND2	1:R:17:ASN:N	2.60	0.49
1:D:17:ASN:HD22	1:D:17:ASN:N	1.96	0.49
1:B:17:ASN:ND2	1:B:17:ASN:N	2.60	0.49
1:J:120:ASN:N	1:J:120:ASN:ND2	2.59	0.49
1:J:284:ILE:HD13	1:K:207:GLN:HB3	1.93	0.49
1:R:230:VAL:HG11	1:R:254:PHE:HB3	1.93	0.49
1:D:230:VAL:HG11	1:D:254:PHE:HB3	1.93	0.49
1:G:72:ILE:N	1:G:72:ILE:HD12	2.26	0.49
1:N:72:ILE:N	1:N:72:ILE:HD12	2.26	0.49
1:H:153:SER:O	1:H:155:ASN:N	2.45	0.49
1:Q:153:SER:O	1:Q:155:ASN:N	2.45	0.49
1:B:153:SER:O	1:B:155:ASN:N	2.45	0.49
1:O:17:ASN:N	1:O:17:ASN:ND2	2.60	0.49
1:D:284:ILE:HD13	1:E:207:GLN:HB3	1.93	0.49
1:E:110:ILE:HG23	1:E:167:MET:HE1	1.94	0.49
1:D:72:ILE:N	1:D:72:ILE:HD12	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:ILE:HD12	1:C:72:ILE:N	2.26	0.49
1:R:153:SER:O	1:R:155:ASN:N	2.45	0.49
1:P:157:THR:O	1:P:157:THR:OG1	2.29	0.49
1:Q:120:ASN:ND2	1:Q:120:ASN:N	2.59	0.49
1:L:120:ASN:N	1:L:120:ASN:ND2	2.59	0.49
1:F:230:VAL:HG11	1:F:254:PHE:HB3	1.93	0.49
1:Q:230:VAL:HG11	1:Q:254:PHE:HB3	1.93	0.49
1:K:230:VAL:HG11	1:K:254:PHE:HB3	1.93	0.49
1:H:157:THR:OG1	1:H:157:THR:O	2.29	0.49
1:M:153:SER:O	1:M:155:ASN:N	2.45	0.49
1:I:153:SER:O	1:I:155:ASN:N	2.45	0.49
1:P:153:SER:O	1:P:155:ASN:N	2.45	0.49
1:A:120:ASN:ND2	1:A:120:ASN:N	2.59	0.49
1:O:120:ASN:N	1:O:120:ASN:ND2	2.59	0.49
1:G:207:GLN:HB3	1:I:284:ILE:HD13	1.93	0.49
1:A:230:VAL:HG11	1:A:254:PHE:HB3	1.93	0.49
1:A:72:ILE:HD12	1:A:72:ILE:N	2.26	0.49
1:F:72:ILE:N	1:F:72:ILE:HD12	2.26	0.49
1:O:153:SER:O	1:O:155:ASN:N	2.45	0.49
1:E:153:SER:O	1:E:155:ASN:N	2.45	0.49
1:N:120:ASN:ND2	1:N:120:ASN:N	2.59	0.49
1:M:284:ILE:HD13	1:N:207:GLN:HB3	1.93	0.49
1:I:230:VAL:HG11	1:I:254:PHE:HB3	1.93	0.49
1:P:110:ILE:HG23	1:P:167:MET:HE1	1.93	0.49
1:Q:17:ASN:ND2	1:Q:17:ASN:H	2.05	0.49
1:K:120:ASN:ND2	1:K:120:ASN:N	2.59	0.49
1:H:120:ASN:ND2	1:H:120:ASN:N	2.59	0.49
1:A:207:GLN:HB3	1:C:284:ILE:HD13	1.93	0.49
1:P:72:ILE:N	1:P:72:ILE:HD12	2.26	0.49
1:L:157:THR:OG1	1:L:157:THR:O	2.29	0.49
1:E:7:LYS:HB2	1:F:39:TYR:CD2	2.48	0.49
1:I:14:GLU:HA	1:I:17:ASN:CG	2.33	0.49
1:A:17:ASN:ND2	1:A:17:ASN:N	2.60	0.49
1:B:120:ASN:ND2	1:B:120:ASN:N	2.59	0.49
1:M:230:VAL:HG11	1:M:254:PHE:HB3	1.93	0.49
1:M:72:ILE:HD12	1:M:72:ILE:N	2.26	0.49
1:B:7:LYS:HB2	1:C:39:TYR:CD2	2.48	0.49
1:F:153:SER:O	1:F:155:ASN:N	2.45	0.49
1:E:17:ASN:ND2	1:E:17:ASN:N	2.60	0.49
1:C:18:ALA:CB	1:C:23:ILE:CD1	2.90	0.49
1:H:72:ILE:N	1:H:72:ILE:HD12	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:7:LYS:HB2	1:H:39:TYR:CD2	2.48	0.49
1:H:7:LYS:HB2	1:I:39:TYR:CD2	2.48	0.49
1:L:14:GLU:HA	1:L:17:ASN:CG	2.33	0.49
1:B:17:ASN:ND2	1:B:17:ASN:H	2.05	0.49
1:R:72:ILE:N	1:R:72:ILE:HD12	2.26	0.49
1:I:72:ILE:N	1:I:72:ILE:HD12	2.26	0.49
1:R:157:THR:OG1	1:R:157:THR:O	2.29	0.49
1:D:7:LYS:HB2	1:E:39:TYR:CD2	2.48	0.49
1:J:31:ILE:HD11	1:K:31:ILE:HD13	1.95	0.49
1:F:17:ASN:ND2	1:F:17:ASN:N	2.60	0.49
1:D:18:ALA:CB	1:D:23:ILE:HD11	2.27	0.49
1:M:157:THR:OG1	1:M:157:THR:O	2.29	0.49
1:Q:31:ILE:HD11	1:R:31:ILE:HD13	1.95	0.49
1:F:14:GLU:HA	1:F:17:ASN:CG	2.33	0.48
1:K:17:ASN:N	1:K:17:ASN:ND2	2.60	0.48
1:D:207:GLN:HB3	1:F:284:ILE:HD13	1.93	0.48
1:A:39:TYR:CD2	1:C:7:LYS:HB2	2.48	0.48
1:Q:7:LYS:HB2	1:R:39:TYR:CD2	2.48	0.48
1:A:157:THR:O	1:A:157:THR:OG1	2.29	0.48
1:B:31:ILE:HD11	1:C:31:ILE:HD13	1.95	0.48
1:F:18:ALA:CB	1:F:23:ILE:CD1	2.90	0.48
1:G:14:GLU:HA	1:G:17:ASN:CG	2.33	0.48
1:F:120:ASN:ND2	1:F:120:ASN:N	2.59	0.48
1:J:230:VAL:HG11	1:J:254:PHE:HB3	1.93	0.48
1:P:7:LYS:HB2	1:Q:39:TYR:CD2	2.48	0.48
1:K:31:ILE:HD11	1:L:31:ILE:HD13	1.95	0.48
1:H:18:ALA:CB	1:H:23:ILE:CD1	2.90	0.48
1:A:14:GLU:HA	1:A:17:ASN:CG	2.33	0.48
1:P:14:GLU:HA	1:P:17:ASN:CG	2.33	0.48
1:H:110:ILE:HG23	1:H:167:MET:HE1	1.96	0.48
1:N:31:ILE:HD11	1:O:31:ILE:HD13	1.95	0.48
1:G:31:ILE:HD13	1:I:31:ILE:HD11	1.95	0.48
1:H:17:ASN:N	1:H:17:ASN:ND2	2.60	0.48
1:O:14:GLU:HA	1:O:17:ASN:CG	2.33	0.48
1:A:18:ALA:CB	1:A:23:ILE:CD1	2.90	0.48
1:D:39:TYR:CD2	1:F:7:LYS:HB2	2.48	0.48
1:K:7:LYS:HB2	1:L:39:TYR:CD2	2.48	0.48
1:A:7:LYS:HB2	1:B:39:TYR:CD2	2.48	0.48
1:M:39:TYR:CD2	1:O:7:LYS:HB2	2.48	0.48
1:H:14:GLU:HA	1:H:17:ASN:CG	2.33	0.48
1:E:14:GLU:HA	1:E:17:ASN:CG	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:7:LYS:HB2	1:N:39:TYR:CD2	2.48	0.48
1:J:31:ILE:HD13	1:L:31:ILE:HD11	1.95	0.48
1:M:170:GLN:HG2	1:O:164:ILE:CG2	2.44	0.48
1:P:31:ILE:HD11	1:Q:31:ILE:HD13	1.95	0.48
1:M:31:ILE:HD11	1:N:31:ILE:HD13	1.95	0.48
1:M:18:ALA:CB	1:M:23:ILE:CD1	2.90	0.48
1:R:14:GLU:HA	1:R:17:ASN:CG	2.33	0.48
1:C:14:GLU:HA	1:C:17:ASN:CG	2.33	0.48
1:P:17:ASN:H	1:P:17:ASN:ND2	2.05	0.48
1:P:18:ALA:CB	1:P:23:ILE:CD1	2.90	0.48
1:P:39:TYR:CD2	1:R:7:LYS:HB2	2.48	0.48
1:J:39:TYR:CD2	1:L:7:LYS:HB2	2.48	0.48
1:M:31:ILE:HD13	1:O:31:ILE:HD11	1.95	0.48
1:H:31:ILE:HD11	1:I:31:ILE:HD13	1.95	0.48
1:J:14:GLU:HA	1:J:17:ASN:CG	2.33	0.48
1:K:14:GLU:HA	1:K:17:ASN:CG	2.33	0.48
1:P:170:GLN:HG2	1:R:164:ILE:CG2	2.44	0.48
1:M:164:ILE:CG2	1:N:170:GLN:HG2	2.44	0.48
1:G:39:TYR:CD2	1:I:7:LYS:HB2	2.48	0.48
1:I:17:ASN:ND2	1:I:17:ASN:N	2.60	0.48
1:B:14:GLU:HA	1:B:17:ASN:CG	2.33	0.48
1:A:31:ILE:HD13	1:C:31:ILE:HD11	1.95	0.48
1:E:31:ILE:HD11	1:F:31:ILE:HD13	1.95	0.48
1:D:14:GLU:HA	1:D:17:ASN:CG	2.33	0.48
1:A:31:ILE:HD11	1:B:31:ILE:HD13	1.95	0.48
1:D:31:ILE:HD11	1:E:31:ILE:HD13	1.95	0.48
1:Q:242:ASN:ND2	1:Q:242:ASN:N	2.45	0.47
1:I:120:ASN:N	1:I:120:ASN:ND2	2.59	0.47
1:H:164:ILE:CG2	1:I:170:GLN:HG2	2.44	0.47
1:Q:164:ILE:CG2	1:R:170:GLN:HG2	2.44	0.47
1:D:164:ILE:CG2	1:E:170:GLN:HG2	2.44	0.47
1:J:7:LYS:HB2	1:K:39:TYR:CD2	2.48	0.47
1:N:14:GLU:HA	1:N:17:ASN:CG	2.33	0.47
1:R:18:ALA:CB	1:R:23:ILE:CD1	2.90	0.47
1:J:164:ILE:CG2	1:K:170:GLN:HG2	2.44	0.47
1:K:164:ILE:CG2	1:L:170:GLN:HG2	2.44	0.47
1:K:110:ILE:HD13	1:K:110:ILE:HA	1.79	0.47
1:B:18:ALA:CB	1:B:23:ILE:CD1	2.90	0.47
1:P:164:ILE:CG2	1:Q:170:GLN:HG2	2.44	0.47
1:N:164:ILE:CG2	1:O:170:GLN:HG2	2.44	0.47
1:M:14:GLU:HA	1:M:17:ASN:CG	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:17:ASN:N	1:P:17:ASN:HD22	1.96	0.47
1:J:170:GLN:HG2	1:L:164:ILE:CG2	2.44	0.47
1:Q:110:ILE:HA	1:Q:110:ILE:HD13	1.79	0.47
1:N:7:LYS:HB2	1:O:39:TYR:CD2	2.48	0.47
1:G:31:ILE:HD11	1:H:31:ILE:HD13	1.95	0.47
1:I:18:ALA:CB	1:I:23:ILE:CD1	2.90	0.47
1:A:170:GLN:HG2	1:C:164:ILE:CG2	2.44	0.47
1:A:164:ILE:CG2	1:B:170:GLN:HG2	2.44	0.47
1:D:17:ASN:ND2	1:D:17:ASN:N	2.60	0.47
1:B:157:THR:OG1	1:B:157:THR:O	2.29	0.47
1:D:31:ILE:HD13	1:F:31:ILE:HD11	1.95	0.47
1:N:17:ASN:ND2	1:N:17:ASN:N	2.60	0.47
1:Q:14:GLU:HA	1:Q:17:ASN:CG	2.33	0.47
1:B:164:ILE:CG2	1:C:170:GLN:HG2	2.44	0.47
1:E:164:ILE:CG2	1:F:170:GLN:HG2	2.44	0.47
1:G:110:ILE:HA	1:G:110:ILE:HD13	1.79	0.47
1:I:157:THR:O	1:I:157:THR:OG1	2.29	0.47
1:G:170:GLN:HG2	1:I:164:ILE:CG2	2.44	0.47
1:G:164:ILE:CG2	1:H:170:GLN:HG2	2.44	0.47
1:M:287:ALA:O	1:M:288:GLN:HB2	2.15	0.47
1:N:18:ALA:CB	1:N:23:ILE:CD1	2.90	0.47
1:H:287:ALA:O	1:H:288:GLN:HB2	2.15	0.47
1:D:120:ASN:ND2	1:D:120:ASN:N	2.59	0.47
1:E:287:ALA:O	1:E:288:GLN:HB2	2.15	0.47
1:F:287:ALA:O	1:F:288:GLN:HB2	2.15	0.47
1:K:287:ALA:O	1:K:288:GLN:HB2	2.15	0.47
1:I:287:ALA:O	1:I:288:GLN:HB2	2.15	0.47
1:K:18:ALA:CB	1:K:23:ILE:CD1	2.90	0.46
1:C:242:ASN:N	1:C:242:ASN:ND2	2.45	0.46
1:P:31:ILE:HD13	1:R:31:ILE:HD11	1.95	0.46
1:C:157:THR:O	1:C:157:THR:OG1	2.29	0.46
1:P:287:ALA:O	1:P:288:GLN:HB2	2.15	0.46
1:Q:157:THR:OG1	1:Q:157:THR:O	2.29	0.46
1:L:287:ALA:O	1:L:288:GLN:HB2	2.15	0.46
1:R:287:ALA:O	1:R:288:GLN:HB2	2.15	0.46
1:D:287:ALA:O	1:D:288:GLN:HB2	2.15	0.46
1:C:287:ALA:O	1:C:288:GLN:HB2	2.15	0.46
1:A:287:ALA:O	1:A:288:GLN:HB2	2.15	0.46
1:G:287:ALA:O	1:G:288:GLN:HB2	2.15	0.46
1:D:18:ALA:CB	1:D:23:ILE:CD1	2.90	0.46
1:M:127:ILE:HD13	1:M:127:ILE:HA	1.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:18:ALA:CB	1:O:23:ILE:CD1	2.90	0.46
1:D:170:GLN:HG2	1:F:164:ILE:CG2	2.44	0.46
1:O:287:ALA:O	1:O:288:GLN:HB2	2.15	0.46
1:O:17:ASN:ND2	1:O:17:ASN:H	2.05	0.46
1:N:287:ALA:O	1:N:288:GLN:HB2	2.15	0.46
1:B:110:ILE:HG23	1:B:167:MET:HE1	1.98	0.45
1:L:18:ALA:CB	1:L:23:ILE:CD1	2.90	0.45
1:J:287:ALA:O	1:J:288:GLN:HB2	2.15	0.45
1:J:18:ALA:CB	1:J:23:ILE:CD1	2.90	0.45
1:E:157:THR:O	1:E:157:THR:OG1	2.29	0.45
1:B:287:ALA:O	1:B:288:GLN:HB2	2.15	0.45
1:F:17:ASN:H	1:F:17:ASN:ND2	2.05	0.45
1:F:242:ASN:ND2	1:F:242:ASN:N	2.45	0.45
1:Q:287:ALA:O	1:Q:288:GLN:HB2	2.15	0.45
1:N:242:ASN:ND2	1:N:242:ASN:N	2.45	0.45
1:P:110:ILE:HD13	1:P:110:ILE:HA	1.79	0.45
1:M:110:ILE:HA	1:M:110:ILE:HD13	1.79	0.45
1:F:230:VAL:HG13	1:F:230:VAL:O	2.17	0.45
1:R:230:VAL:HG13	1:R:230:VAL:O	2.17	0.45
1:K:230:VAL:O	1:K:230:VAL:HG13	2.17	0.45
1:N:230:VAL:O	1:N:230:VAL:HG13	2.17	0.45
1:C:230:VAL:O	1:C:230:VAL:HG13	2.17	0.45
1:A:202:LEU:HD23	1:A:202:LEU:N	2.32	0.45
1:F:110:ILE:HA	1:F:110:ILE:HD13	1.79	0.45
1:J:230:VAL:O	1:J:230:VAL:HG13	2.17	0.45
1:P:202:LEU:HD23	1:P:202:LEU:N	2.32	0.45
1:C:17:ASN:ND2	1:C:17:ASN:N	2.60	0.45
1:J:222:LEU:HD13	1:K:216:THR:OG1	2.17	0.45
1:H:110:ILE:HD12	1:H:167:MET:CE	2.47	0.45
1:Q:230:VAL:HG13	1:Q:230:VAL:O	2.17	0.45
1:K:202:LEU:HD23	1:K:202:LEU:N	2.32	0.45
1:N:202:LEU:HD23	1:N:202:LEU:N	2.32	0.45
1:D:202:LEU:N	1:D:202:LEU:HD23	2.32	0.45
1:B:202:LEU:HD23	1:B:202:LEU:N	2.32	0.45
1:C:126:ALA:O	1:C:127:ILE:C	2.56	0.45
1:M:222:LEU:HD13	1:N:216:THR:OG1	2.17	0.45
1:Q:202:LEU:N	1:Q:202:LEU:HD23	2.32	0.45
1:L:202:LEU:HD23	1:L:202:LEU:N	2.32	0.45
1:L:230:VAL:HG13	1:L:230:VAL:O	2.17	0.45
1:P:230:VAL:O	1:P:230:VAL:HG13	2.17	0.45
1:P:110:ILE:HD12	1:P:167:MET:CE	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:126:ALA:O	1:F:127:ILE:C	2.56	0.44
1:B:222:LEU:HD13	1:C:216:THR:OG1	2.17	0.44
1:G:284:ILE:HD11	1:H:205:THR:HG22	2.00	0.44
1:O:230:VAL:HG13	1:O:230:VAL:O	2.17	0.44
1:H:230:VAL:O	1:H:230:VAL:HG13	2.17	0.44
1:I:202:LEU:HD23	1:I:202:LEU:N	2.32	0.44
1:G:230:VAL:O	1:G:230:VAL:HG13	2.17	0.44
1:A:230:VAL:HG13	1:A:230:VAL:O	2.17	0.44
1:E:126:ALA:O	1:E:127:ILE:C	2.56	0.44
1:R:126:ALA:O	1:R:127:ILE:C	2.56	0.44
1:M:126:ALA:O	1:M:127:ILE:C	2.56	0.44
1:H:126:ALA:O	1:H:127:ILE:C	2.56	0.44
1:B:284:ILE:HD11	1:C:205:THR:HG22	2.00	0.44
1:A:110:ILE:HD12	1:A:167:MET:CE	2.47	0.44
1:N:157:THR:O	1:N:157:THR:OG1	2.29	0.44
1:I:126:ALA:O	1:I:127:ILE:C	2.56	0.44
1:Q:284:ILE:HD11	1:R:205:THR:HG22	2.00	0.44
1:E:230:VAL:HG13	1:E:230:VAL:O	2.17	0.44
1:K:110:ILE:HD12	1:K:167:MET:CE	2.47	0.44
1:Q:206:CYS:HA	1:Q:273:ARG:O	2.18	0.44
1:R:127:ILE:HD13	1:R:127:ILE:HA	1.82	0.44
1:B:126:ALA:O	1:B:127:ILE:C	2.56	0.44
1:P:205:THR:HG22	1:R:284:ILE:HD11	2.00	0.44
1:Q:222:LEU:HD13	1:R:216:THR:OG1	2.17	0.44
1:I:230:VAL:O	1:I:230:VAL:HG13	2.17	0.44
1:E:202:LEU:HD23	1:E:202:LEU:N	2.32	0.44
1:E:110:ILE:HD12	1:E:167:MET:CE	2.47	0.44
1:L:206:CYS:HA	1:L:273:ARG:O	2.18	0.44
1:O:206:CYS:HA	1:O:273:ARG:O	2.18	0.44
1:B:206:CYS:HA	1:B:273:ARG:O	2.18	0.44
1:L:126:ALA:O	1:L:127:ILE:C	2.56	0.44
1:P:126:ALA:O	1:P:127:ILE:C	2.56	0.44
1:A:205:THR:HG22	1:C:284:ILE:HD11	2.00	0.44
1:A:216:THR:OG1	1:C:222:LEU:HD13	2.17	0.44
1:D:205:THR:HG22	1:F:284:ILE:HD11	2.00	0.44
1:G:205:THR:HG22	1:I:284:ILE:HD11	2.00	0.44
1:J:205:THR:HG22	1:L:284:ILE:HD11	2.00	0.44
1:E:222:LEU:HD13	1:F:216:THR:OG1	2.17	0.44
1:M:205:THR:HG22	1:O:284:ILE:HD11	2.00	0.44
1:G:222:LEU:HD13	1:H:216:THR:OG1	2.17	0.44
1:M:110:ILE:HG23	1:M:167:MET:HE1	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:202:LEU:N	1:H:202:LEU:HD23	2.32	0.44
1:R:202:LEU:N	1:R:202:LEU:HD23	2.32	0.44
1:M:202:LEU:HD23	1:M:202:LEU:N	2.32	0.44
1:B:230:VAL:HG13	1:B:230:VAL:O	2.17	0.44
1:E:18:ALA:CB	1:E:23:ILE:CD1	2.90	0.44
1:K:126:ALA:O	1:K:127:ILE:C	2.56	0.44
1:N:222:LEU:HD13	1:O:216:THR:OG1	2.17	0.44
1:J:284:ILE:HD11	1:K:205:THR:HG22	2.00	0.44
1:R:110:ILE:HA	1:R:110:ILE:HD13	1.79	0.44
1:C:202:LEU:HD23	1:C:202:LEU:N	2.32	0.44
1:D:110:ILE:HD12	1:D:167:MET:CE	2.47	0.44
1:Q:110:ILE:HD12	1:Q:167:MET:CE	2.47	0.44
1:E:206:CYS:HA	1:E:273:ARG:O	2.18	0.44
1:A:206:CYS:HA	1:A:273:ARG:O	2.18	0.44
1:L:252:ILE:N	1:L:252:ILE:HD12	2.33	0.44
1:Q:18:ALA:CB	1:Q:23:ILE:CD1	2.90	0.44
1:A:17:ASN:ND2	1:A:17:ASN:H	2.05	0.44
1:P:216:THR:OG1	1:R:222:LEU:HD13	2.17	0.44
1:A:126:ALA:O	1:A:127:ILE:C	2.56	0.44
1:F:202:LEU:N	1:F:202:LEU:HD23	2.32	0.44
1:O:202:LEU:HD23	1:O:202:LEU:N	2.32	0.44
1:D:230:VAL:HG13	1:D:230:VAL:O	2.17	0.44
1:R:206:CYS:HA	1:R:273:ARG:O	2.18	0.44
1:N:206:CYS:HA	1:N:273:ARG:O	2.18	0.44
1:F:206:CYS:HA	1:F:273:ARG:O	2.18	0.44
1:I:206:CYS:HA	1:I:273:ARG:O	2.18	0.44
1:G:18:ALA:CB	1:G:23:ILE:CD1	2.90	0.44
1:O:110:ILE:HA	1:O:110:ILE:HD13	1.79	0.44
1:K:206:CYS:HA	1:K:273:ARG:O	2.18	0.44
1:E:252:ILE:N	1:E:252:ILE:HD12	2.33	0.44
1:O:252:ILE:N	1:O:252:ILE:HD12	2.33	0.44
1:C:252:ILE:HD12	1:C:252:ILE:N	2.33	0.44
1:P:252:ILE:N	1:P:252:ILE:HD12	2.33	0.44
1:J:252:ILE:HD12	1:J:252:ILE:N	2.33	0.44
1:G:120:ASN:ND2	1:G:120:ASN:N	2.59	0.44
1:Q:126:ALA:O	1:Q:127:ILE:C	2.56	0.44
1:P:222:LEU:HD13	1:Q:216:THR:OG1	2.17	0.44
1:D:284:ILE:HD11	1:E:205:THR:HG22	2.00	0.44
1:B:110:ILE:HD12	1:B:167:MET:CE	2.47	0.44
1:M:230:VAL:HG13	1:M:230:VAL:O	2.17	0.44
1:G:202:LEU:HD23	1:G:202:LEU:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:110:ILE:HD12	1:F:167:MET:CE	2.47	0.44
1:G:258:GLU:O	1:G:259:ASN:HB2	2.18	0.44
1:I:87:ILE:HG21	1:I:122:LEU:HG	2.00	0.44
1:M:206:CYS:HA	1:M:273:ARG:O	2.18	0.44
1:A:252:ILE:HD12	1:A:252:ILE:N	2.33	0.44
1:I:252:ILE:HD12	1:I:252:ILE:N	2.33	0.44
1:G:201:LYS:HG2	1:G:201:LYS:HZ3	1.70	0.43
1:J:126:ALA:O	1:J:127:ILE:C	2.56	0.43
1:K:222:LEU:HD13	1:L:216:THR:OG1	2.17	0.43
1:E:284:ILE:HD11	1:F:205:THR:HG22	2.00	0.43
1:I:110:ILE:HD13	1:I:110:ILE:HA	1.79	0.43
1:R:252:ILE:N	1:R:252:ILE:HD12	2.33	0.43
1:N:252:ILE:N	1:N:252:ILE:HD12	2.33	0.43
1:H:252:ILE:HD12	1:H:252:ILE:N	2.33	0.43
1:M:216:THR:OG1	1:O:222:LEU:HD13	2.17	0.43
1:C:87:ILE:HG21	1:C:122:LEU:HG	2.00	0.43
1:P:258:GLU:O	1:P:259:ASN:HB2	2.19	0.43
1:J:206:CYS:HA	1:J:273:ARG:O	2.18	0.43
1:G:252:ILE:N	1:G:252:ILE:HD12	2.33	0.43
1:B:252:ILE:HD12	1:B:252:ILE:N	2.33	0.43
1:D:126:ALA:O	1:D:127:ILE:C	2.56	0.43
1:G:126:ALA:O	1:G:127:ILE:C	2.56	0.43
1:N:126:ALA:O	1:N:127:ILE:C	2.56	0.43
1:M:258:GLU:O	1:M:259:ASN:HB2	2.19	0.43
1:A:258:GLU:O	1:A:259:ASN:HB2	2.19	0.43
1:P:87:ILE:HG21	1:P:122:LEU:HG	2.00	0.43
1:F:87:ILE:HG21	1:F:122:LEU:HG	2.00	0.43
1:N:40:ASN:ND2	1:N:45:GLN:HG2	2.28	0.43
1:H:222:LEU:HD13	1:I:216:THR:OG1	2.17	0.43
1:G:216:THR:OG1	1:I:222:LEU:HD13	2.17	0.43
1:A:222:LEU:HD13	1:B:216:THR:OG1	2.17	0.43
1:F:258:GLU:O	1:F:259:ASN:HB2	2.19	0.43
1:J:258:GLU:O	1:J:259:ASN:HB2	2.19	0.43
1:D:258:GLU:O	1:D:259:ASN:HB2	2.18	0.43
1:G:110:ILE:HD12	1:G:167:MET:CE	2.47	0.43
1:N:110:ILE:HD12	1:N:167:MET:CE	2.47	0.43
1:B:87:ILE:HG21	1:B:122:LEU:HG	2.00	0.43
1:R:87:ILE:HG21	1:R:122:LEU:HG	2.00	0.43
1:Q:252:ILE:HD12	1:Q:252:ILE:N	2.33	0.43
1:M:252:ILE:HD12	1:M:252:ILE:N	2.33	0.43
1:P:127:ILE:HA	1:P:127:ILE:HD13	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:216:THR:OG1	1:F:222:LEU:HD13	2.17	0.43
1:K:284:ILE:HD11	1:L:205:THR:HG22	2.00	0.43
1:J:216:THR:OG1	1:L:222:LEU:HD13	2.17	0.43
1:O:110:ILE:HD12	1:O:167:MET:CE	2.47	0.43
1:A:210:ASP:OD2	1:A:212:ARG:HB3	2.19	0.43
1:H:206:CYS:HA	1:H:273:ARG:O	2.18	0.43
1:M:87:ILE:HG21	1:M:122:LEU:HG	2.00	0.43
1:F:252:ILE:HD12	1:F:252:ILE:N	2.33	0.43
1:D:252:ILE:HD12	1:D:252:ILE:N	2.33	0.43
1:H:284:ILE:HD11	1:I:205:THR:HG22	2.00	0.43
1:P:284:ILE:HD11	1:Q:205:THR:HG22	2.00	0.43
1:O:210:ASP:OD2	1:O:212:ARG:HB3	2.19	0.43
1:L:210:ASP:OD2	1:L:212:ARG:HB3	2.19	0.43
1:C:206:CYS:HA	1:C:273:ARG:O	2.18	0.43
1:A:87:ILE:HG21	1:A:122:LEU:HG	2.00	0.43
1:C:258:GLU:O	1:C:259:ASN:HB2	2.19	0.43
1:J:202:LEU:HD23	1:J:202:LEU:N	2.32	0.43
1:L:110:ILE:HD12	1:L:167:MET:CE	2.47	0.43
1:M:210:ASP:OD2	1:M:212:ARG:HB3	2.19	0.43
1:R:258:GLU:O	1:R:259:ASN:HB2	2.19	0.43
1:G:206:CYS:HA	1:G:273:ARG:O	2.18	0.43
1:Q:87:ILE:HG21	1:Q:122:LEU:HG	2.00	0.43
1:K:258:GLU:O	1:K:259:ASN:HB2	2.19	0.43
1:L:87:ILE:HG21	1:L:122:LEU:HG	2.00	0.43
1:D:210:ASP:OD2	1:D:212:ARG:HB3	2.19	0.43
1:I:210:ASP:OD2	1:I:212:ARG:HB3	2.19	0.43
1:P:206:CYS:HA	1:P:273:ARG:O	2.18	0.43
1:H:258:GLU:O	1:H:259:ASN:HB2	2.19	0.43
1:K:252:ILE:N	1:K:252:ILE:HD12	2.33	0.43
1:D:206:CYS:HA	1:D:273:ARG:O	2.18	0.43
1:Q:40:ASN:ND2	1:Q:45:GLN:HG2	2.28	0.43
1:J:164:ILE:HG13	1:K:172:GLU:HB3	2.01	0.43
1:I:110:ILE:HG23	1:I:167:MET:CE	2.49	0.43
1:M:164:ILE:HG13	1:N:172:GLU:HB3	2.01	0.43
1:D:222:LEU:HD13	1:E:216:THR:OG1	2.17	0.43
1:N:110:ILE:HA	1:N:110:ILE:HD13	1.79	0.43
1:D:110:ILE:HG23	1:D:167:MET:CE	2.49	0.43
1:G:210:ASP:OD2	1:G:212:ARG:HB3	2.19	0.43
1:J:210:ASP:OD2	1:J:212:ARG:HB3	2.19	0.43
1:N:210:ASP:OD2	1:N:212:ARG:HB3	2.19	0.43
1:F:210:ASP:OD2	1:F:212:ARG:HB3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:210:ASP:OD2	1:B:212:ARG:HB3	2.19	0.43
1:G:157:THR:O	1:G:157:THR:OG1	2.29	0.43
1:P:9:LEU:HD11	1:Q:36:ASN:HD21	1.84	0.43
1:B:258:GLU:O	1:B:259:ASN:HB2	2.19	0.43
1:D:36:ASN:HD21	1:F:9:LEU:HD11	1.84	0.43
1:K:87:ILE:HG21	1:K:122:LEU:HG	2.00	0.43
1:M:9:LEU:HD11	1:N:36:ASN:HD21	1.84	0.43
1:A:9:LEU:HD11	1:B:36:ASN:HD21	1.84	0.43
1:K:15:ILE:C	1:K:17:ASN:N	2.73	0.42
1:D:40:ASN:ND2	1:D:45:GLN:HG2	2.28	0.42
1:B:164:ILE:HG13	1:C:172:GLU:HB3	2.01	0.42
1:L:215:LYS:HG2	1:L:216:THR:N	2.35	0.42
1:N:215:LYS:HG2	1:N:216:THR:N	2.34	0.42
1:B:110:ILE:HG23	1:B:167:MET:CE	2.49	0.42
1:L:110:ILE:HG23	1:L:167:MET:CE	2.49	0.42
1:Q:110:ILE:HG23	1:Q:167:MET:CE	2.49	0.42
1:O:110:ILE:HG23	1:O:167:MET:CE	2.49	0.42
1:D:9:LEU:HD11	1:E:36:ASN:HD21	1.84	0.42
1:E:9:LEU:HD11	1:F:36:ASN:HD21	1.84	0.42
1:Q:258:GLU:O	1:Q:259:ASN:HB2	2.19	0.42
1:L:17:ASN:ND2	1:L:17:ASN:N	2.60	0.42
1:D:201:LYS:HG2	1:D:201:LYS:HZ3	1.72	0.42
1:L:127:ILE:HD13	1:L:127:ILE:HA	1.82	0.42
1:G:164:ILE:HG13	1:H:172:GLU:HB3	2.01	0.42
1:N:284:ILE:HD11	1:O:205:THR:HG22	2.00	0.42
1:I:215:LYS:HG2	1:I:216:THR:N	2.35	0.42
1:D:215:LYS:HG2	1:D:216:THR:N	2.34	0.42
1:G:215:LYS:HG2	1:G:216:THR:N	2.34	0.42
1:D:164:ILE:HG13	1:E:172:GLU:HB3	2.01	0.42
1:F:215:LYS:HG2	1:F:216:THR:N	2.35	0.42
1:E:202:LEU:HD11	1:E:254:PHE:CE2	2.55	0.42
1:N:202:LEU:HD11	1:N:254:PHE:CE2	2.55	0.42
1:F:110:ILE:HG23	1:F:167:MET:CE	2.49	0.42
1:O:19:SER:O	1:O:21:GLY:N	2.52	0.42
1:K:19:SER:O	1:K:21:GLY:N	2.53	0.42
1:D:19:SER:O	1:D:21:GLY:N	2.52	0.42
1:N:19:SER:O	1:N:21:GLY:N	2.53	0.42
1:C:19:SER:O	1:C:21:GLY:N	2.52	0.42
1:N:9:LEU:HD11	1:O:36:ASN:HD21	1.84	0.42
1:H:9:LEU:HD11	1:I:36:ASN:HD21	1.84	0.42
1:G:36:ASN:HD21	1:I:9:LEU:HD11	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:126:ALA:O	1:O:127:ILE:C	2.56	0.42
1:G:172:GLU:HB3	1:I:164:ILE:HG13	2.01	0.42
1:H:164:ILE:HG13	1:I:172:GLU:HB3	2.01	0.42
1:Q:215:LYS:HG2	1:Q:216:THR:N	2.34	0.42
1:J:215:LYS:HG2	1:J:216:THR:N	2.34	0.42
1:M:284:ILE:HD11	1:N:205:THR:HG22	2.00	0.42
1:K:215:LYS:HG2	1:K:216:THR:N	2.35	0.42
1:A:284:ILE:HD11	1:B:205:THR:HG22	2.00	0.42
1:K:202:LEU:HD11	1:K:254:PHE:CE2	2.55	0.42
1:A:110:ILE:HG23	1:A:167:MET:CE	2.49	0.42
1:K:210:ASP:OD2	1:K:212:ARG:HB3	2.19	0.42
1:F:19:SER:O	1:F:21:GLY:N	2.52	0.42
1:M:19:SER:O	1:M:21:GLY:N	2.52	0.42
1:J:19:SER:O	1:J:21:GLY:N	2.52	0.42
1:G:19:SER:O	1:G:21:GLY:N	2.53	0.42
1:O:87:ILE:HG21	1:O:122:LEU:HG	2.00	0.42
1:J:15:ILE:C	1:J:17:ASN:N	2.73	0.42
1:G:15:ILE:C	1:G:17:ASN:N	2.73	0.42
1:E:164:ILE:HG13	1:F:172:GLU:HB3	2.01	0.42
1:D:172:GLU:HB3	1:F:164:ILE:HG13	2.01	0.42
1:G:110:ILE:HG23	1:G:167:MET:CE	2.49	0.42
1:M:110:ILE:HG23	1:M:167:MET:CE	2.49	0.42
1:H:110:ILE:HG23	1:H:167:MET:CE	2.49	0.42
1:L:202:LEU:HD11	1:L:254:PHE:CE2	2.55	0.42
1:R:202:LEU:HD11	1:R:254:PHE:CE2	2.55	0.42
1:C:202:LEU:HD11	1:C:254:PHE:CE2	2.55	0.42
1:P:202:LEU:HD11	1:P:254:PHE:CE2	2.55	0.42
1:L:110:ILE:HA	1:L:110:ILE:HD13	1.79	0.42
1:D:110:ILE:HA	1:D:110:ILE:HD13	1.79	0.42
1:P:210:ASP:OD2	1:P:212:ARG:HB3	2.19	0.42
1:L:19:SER:O	1:L:21:GLY:N	2.52	0.42
1:E:87:ILE:HG21	1:E:122:LEU:HG	2.00	0.42
1:A:164:ILE:HG13	1:B:172:GLU:HB3	2.01	0.42
1:J:110:ILE:HG23	1:J:167:MET:CE	2.49	0.42
1:R:19:SER:O	1:R:21:GLY:N	2.52	0.42
1:Q:19:SER:O	1:Q:21:GLY:N	2.53	0.42
1:G:87:ILE:HG21	1:G:122:LEU:HG	2.00	0.42
1:J:87:ILE:HG21	1:J:122:LEU:HG	2.00	0.42
1:F:40:ASN:ND2	1:F:45:GLN:HG2	2.28	0.42
1:J:172:GLU:HB3	1:L:164:ILE:HG13	2.01	0.42
1:O:202:LEU:HD11	1:O:254:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:110:ILE:HG23	1:K:167:MET:CE	2.49	0.42
1:E:210:ASP:OD2	1:E:212:ARG:HB3	2.19	0.42
1:R:210:ASP:OD2	1:R:212:ARG:HB3	2.19	0.42
1:B:9:LEU:HD11	1:C:36:ASN:HD21	1.84	0.42
1:P:14:GLU:HB3	1:P:17:ASN:ND2	2.35	0.42
1:E:242:ASN:ND2	1:E:242:ASN:N	2.45	0.42
1:P:172:GLU:OE1	1:R:164:ILE:HG23	2.20	0.42
1:M:215:LYS:HG2	1:M:216:THR:N	2.34	0.42
1:N:110:ILE:HG23	1:N:167:MET:CE	2.49	0.42
1:Q:210:ASP:OD2	1:Q:212:ARG:HB3	2.19	0.42
1:P:19:SER:O	1:P:21:GLY:N	2.53	0.42
1:N:87:ILE:HG21	1:N:122:LEU:HG	2.00	0.42
1:H:87:ILE:HG21	1:H:122:LEU:HG	2.00	0.42
1:A:36:ASN:HD21	1:C:9:LEU:HD11	1.84	0.42
1:G:9:LEU:HD11	1:H:36:ASN:HD21	1.84	0.42
1:L:14:GLU:HB3	1:L:17:ASN:ND2	2.35	0.42
1:D:218:GLU:OE1	1:F:201:LYS:HE3	2.20	0.42
1:P:218:GLU:OE1	1:R:201:LYS:HE3	2.20	0.42
1:A:172:GLU:OE1	1:C:164:ILE:HG23	2.20	0.42
1:P:164:ILE:HG13	1:Q:172:GLU:HB3	2.01	0.42
1:H:202:LEU:HD11	1:H:254:PHE:CE2	2.55	0.42
1:I:202:LEU:HD11	1:I:254:PHE:CE2	2.55	0.42
1:D:202:LEU:HD11	1:D:254:PHE:CE2	2.55	0.42
1:B:202:LEU:HD11	1:B:254:PHE:CE2	2.55	0.42
1:J:9:LEU:HD11	1:K:36:ASN:HD21	1.84	0.42
1:N:258:GLU:O	1:N:259:ASN:HB2	2.19	0.42
1:K:119:THR:OG1	1:K:120:ASN:ND2	2.53	0.42
1:K:201:LYS:HE3	1:L:218:GLU:OE1	2.20	0.42
1:D:201:LYS:HE3	1:E:218:GLU:OE1	2.20	0.42
1:E:201:LYS:HE3	1:F:218:GLU:OE1	2.20	0.42
1:N:201:LYS:HE3	1:O:218:GLU:OE1	2.20	0.42
1:Q:164:ILE:HG13	1:R:172:GLU:HB3	2.01	0.42
1:Q:164:ILE:HG23	1:R:172:GLU:OE1	2.20	0.42
1:R:110:ILE:HG23	1:R:167:MET:CE	2.49	0.42
1:J:110:ILE:HD12	1:J:167:MET:CE	2.47	0.42
1:C:210:ASP:OD2	1:C:212:ARG:HB3	2.19	0.42
1:A:19:SER:O	1:A:21:GLY:N	2.52	0.42
1:K:9:LEU:HD11	1:L:36:ASN:HD21	1.84	0.42
1:J:36:ASN:HD21	1:L:9:LEU:HD11	1.84	0.42
1:A:14:GLU:HB3	1:A:17:ASN:ND2	2.35	0.42
1:P:119:THR:OG1	1:P:120:ASN:ND2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:119:THR:OG1	1:N:120:ASN:ND2	2.53	0.42
1:H:201:LYS:HE3	1:I:218:GLU:OE1	2.20	0.42
1:M:201:LYS:HZ3	1:M:201:LYS:HG2	1.69	0.42
1:O:215:LYS:HG2	1:O:216:THR:N	2.35	0.42
1:A:164:ILE:HG23	1:B:172:GLU:OE1	2.20	0.42
1:C:215:LYS:HG2	1:C:216:THR:N	2.35	0.42
1:I:110:ILE:HD12	1:I:167:MET:CE	2.47	0.42
1:M:202:LEU:HD11	1:M:254:PHE:CE2	2.55	0.42
1:L:258:GLU:O	1:L:259:ASN:HB2	2.19	0.42
1:A:119:THR:OG1	1:A:120:ASN:ND2	2.53	0.41
1:A:201:LYS:HE3	1:B:218:GLU:OE1	2.20	0.41
1:Q:201:LYS:HE3	1:R:218:GLU:OE1	2.20	0.41
1:A:172:GLU:HB3	1:C:164:ILE:HG13	2.01	0.41
1:B:164:ILE:HG23	1:C:172:GLU:OE1	2.20	0.41
1:M:172:GLU:OE1	1:O:164:ILE:HG23	2.20	0.41
1:N:164:ILE:HG13	1:O:172:GLU:HB3	2.01	0.41
1:H:215:LYS:HG2	1:H:216:THR:N	2.34	0.41
1:C:110:ILE:HG23	1:C:167:MET:CE	2.49	0.41
1:F:202:LEU:HD11	1:F:254:PHE:CE2	2.55	0.41
1:Q:202:LEU:HD11	1:Q:254:PHE:CE2	2.55	0.41
1:P:110:ILE:HG23	1:P:167:MET:CE	2.49	0.41
1:H:210:ASP:OD2	1:H:212:ARG:HB3	2.19	0.41
1:B:19:SER:O	1:B:21:GLY:N	2.53	0.41
1:H:19:SER:O	1:H:21:GLY:N	2.53	0.41
1:I:19:SER:O	1:I:21:GLY:N	2.52	0.41
1:G:31:ILE:HD13	1:I:31:ILE:CD1	2.51	0.41
1:D:31:ILE:HD13	1:F:31:ILE:CD1	2.51	0.41
1:D:87:ILE:HG21	1:D:122:LEU:HG	2.00	0.41
1:O:258:GLU:O	1:O:259:ASN:HB2	2.19	0.41
1:B:15:ILE:C	1:B:17:ASN:N	2.73	0.41
1:M:119:THR:OG1	1:M:120:ASN:ND2	2.53	0.41
1:M:172:GLU:HB3	1:O:164:ILE:HG13	2.01	0.41
1:N:164:ILE:HG23	1:O:172:GLU:OE1	2.20	0.41
1:A:215:LYS:HG2	1:A:216:THR:N	2.34	0.41
1:D:172:GLU:OE1	1:F:164:ILE:HG23	2.20	0.41
1:A:202:LEU:HD11	1:A:254:PHE:CE2	2.55	0.41
1:E:19:SER:O	1:E:21:GLY:N	2.53	0.41
1:B:31:ILE:CD1	1:C:31:ILE:HD13	2.51	0.41
1:Q:9:LEU:HD11	1:R:36:ASN:HD21	1.84	0.41
1:I:258:GLU:O	1:I:259:ASN:HB2	2.19	0.41
1:M:120:ASN:N	1:M:120:ASN:ND2	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:THR:OG1	1:D:120:ASN:ND2	2.53	0.41
1:H:119:THR:OG1	1:H:120:ASN:ND2	2.53	0.41
1:J:119:THR:OG1	1:J:120:ASN:ND2	2.53	0.41
1:A:218:GLU:OE1	1:C:201:LYS:HE3	2.20	0.41
1:P:164:ILE:HG23	1:Q:172:GLU:OE1	2.20	0.41
1:E:164:ILE:HG23	1:F:172:GLU:OE1	2.20	0.41
1:E:110:ILE:HG23	1:E:167:MET:CE	2.49	0.41
1:J:31:ILE:HD13	1:L:31:ILE:CD1	2.51	0.41
1:Q:31:ILE:CD1	1:R:31:ILE:HD13	2.51	0.41
1:P:36:ASN:HD21	1:R:9:LEU:HD11	1.84	0.41
1:D:14:GLU:HB3	1:D:17:ASN:ND2	2.35	0.41
1:Q:119:THR:OG1	1:Q:120:ASN:ND2	2.53	0.41
1:G:119:THR:OG1	1:G:120:ASN:ND2	2.53	0.41
1:J:218:GLU:OE1	1:L:201:LYS:HE3	2.20	0.41
1:D:164:ILE:HG23	1:E:172:GLU:OE1	2.20	0.41
1:G:230:VAL:HG11	1:G:255:SER:N	2.36	0.41
1:D:230:VAL:HG11	1:D:255:SER:N	2.36	0.41
1:P:168:PHE:HA	1:R:163:SER:HB3	2.03	0.41
1:A:31:ILE:HD13	1:C:31:ILE:CD1	2.51	0.41
1:M:36:ASN:HD21	1:O:9:LEU:HD11	1.84	0.41
1:R:119:THR:OG1	1:R:120:ASN:ND2	2.53	0.41
1:I:119:THR:OG1	1:I:120:ASN:ND2	2.53	0.41
1:H:40:ASN:ND2	1:H:45:GLN:HG2	2.28	0.41
1:K:164:ILE:HG13	1:L:172:GLU:HB3	2.01	0.41
1:B:215:LYS:HG2	1:B:216:THR:N	2.35	0.41
1:D:163:SER:HB3	1:E:168:PHE:HA	2.03	0.41
1:E:15:ILE:C	1:E:17:ASN:N	2.73	0.41
1:G:14:GLU:HB3	1:G:17:ASN:ND2	2.35	0.41
1:C:119:THR:OG1	1:C:120:ASN:ND2	2.53	0.41
1:L:119:THR:OG1	1:L:120:ASN:ND2	2.53	0.41
1:M:218:GLU:OE1	1:O:201:LYS:HE3	2.20	0.41
1:J:172:GLU:OE1	1:L:164:ILE:HG23	2.20	0.41
1:E:215:LYS:HG2	1:E:216:THR:N	2.34	0.41
1:H:230:VAL:HG11	1:H:255:SER:N	2.36	0.41
1:I:230:VAL:HG11	1:I:255:SER:N	2.36	0.41
1:J:202:LEU:HD11	1:J:254:PHE:CE2	2.55	0.41
1:P:31:ILE:CD1	1:Q:31:ILE:HD13	2.51	0.41
1:M:31:ILE:HD13	1:O:31:ILE:CD1	2.51	0.41
1:J:168:PHE:HA	1:L:163:SER:HB3	2.03	0.41
1:M:163:SER:HB3	1:N:168:PHE:HA	2.03	0.41
1:E:258:GLU:O	1:E:259:ASN:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:14:GLU:HB3	1:I:17:ASN:ND2	2.35	0.41
1:G:218:GLU:OE1	1:I:201:LYS:HE3	2.20	0.41
1:P:201:LYS:HE3	1:Q:218:GLU:OE1	2.20	0.41
1:J:230:VAL:HG11	1:J:255:SER:N	2.36	0.41
1:J:163:SER:HB3	1:K:167:MET:O	2.21	0.41
1:R:72:ILE:H	1:R:72:ILE:CD1	2.34	0.41
1:O:72:ILE:H	1:O:72:ILE:CD1	2.34	0.41
1:M:31:ILE:CD1	1:N:31:ILE:HD13	2.51	0.41
1:E:31:ILE:CD1	1:F:31:ILE:HD13	2.51	0.41
1:Q:209:VAL:HG13	1:Q:271:GLY:O	2.21	0.41
1:G:168:PHE:HA	1:I:163:SER:HB3	2.03	0.41
1:B:209:VAL:HG13	1:B:271:GLY:O	2.21	0.41
1:B:201:LYS:HE3	1:C:218:GLU:OE1	2.20	0.41
1:G:172:GLU:OE1	1:I:164:ILE:HG23	2.20	0.41
1:A:163:SER:HB3	1:B:167:MET:O	2.21	0.41
1:L:230:VAL:HG11	1:L:255:SER:N	2.36	0.41
1:E:230:VAL:HG11	1:E:255:SER:N	2.36	0.41
1:P:167:MET:O	1:R:163:SER:HB3	2.21	0.41
1:P:163:SER:HB3	1:Q:167:MET:O	2.21	0.41
1:N:163:SER:HB3	1:O:167:MET:O	2.21	0.41
1:C:72:ILE:CD1	1:C:72:ILE:H	2.34	0.41
1:F:72:ILE:H	1:F:72:ILE:CD1	2.34	0.41
1:P:31:ILE:HD13	1:R:31:ILE:CD1	2.51	0.41
1:E:209:VAL:HG13	1:E:271:GLY:O	2.21	0.41
1:N:209:VAL:HG13	1:N:271:GLY:O	2.21	0.41
1:H:15:ILE:C	1:H:17:ASN:N	2.73	0.41
1:F:14:GLU:HB3	1:F:17:ASN:ND2	2.35	0.41
1:E:14:GLU:HB3	1:E:17:ASN:ND2	2.35	0.41
1:R:14:GLU:HB3	1:R:17:ASN:ND2	2.35	0.41
1:C:14:GLU:HB3	1:C:17:ASN:ND2	2.35	0.41
1:K:14:GLU:HB3	1:K:17:ASN:ND2	2.35	0.41
1:E:119:THR:OG1	1:E:120:ASN:ND2	2.53	0.41
1:B:119:THR:OG1	1:B:120:ASN:ND2	2.53	0.41
1:C:127:ILE:HD13	1:C:127:ILE:HA	1.82	0.41
1:H:164:ILE:HG23	1:I:172:GLU:OE1	2.20	0.41
1:G:164:ILE:HG23	1:H:172:GLU:OE1	2.20	0.41
1:J:164:ILE:HG23	1:K:172:GLU:OE1	2.20	0.41
1:M:164:ILE:HG23	1:N:172:GLU:OE1	2.20	0.41
1:H:163:SER:HB3	1:I:167:MET:O	2.21	0.41
1:H:163:SER:HB3	1:I:168:PHE:HA	2.03	0.41
1:Q:163:SER:HB3	1:R:167:MET:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:110:ILE:HG23	1:N:167:MET:HE1	2.03	0.41
1:M:168:PHE:HA	1:O:163:SER:HB3	2.03	0.41
1:M:230:VAL:HG11	1:M:255:SER:N	2.36	0.41
1:N:230:VAL:HG11	1:N:255:SER:N	2.36	0.41
1:P:230:VAL:HG11	1:P:255:SER:N	2.36	0.41
1:K:163:SER:HB3	1:L:167:MET:O	2.21	0.41
1:O:248:GLU:O	1:O:249:ILE:CB	2.69	0.41
1:D:163:SER:HB3	1:E:167:MET:O	2.21	0.41
1:A:110:ILE:HD13	1:A:110:ILE:HA	1.79	0.41
1:A:168:PHE:HA	1:C:163:SER:HB3	2.03	0.41
1:A:167:MET:O	1:C:163:SER:HB3	2.21	0.41
1:J:31:ILE:CD1	1:K:31:ILE:HD13	2.51	0.41
1:A:31:ILE:CD1	1:B:31:ILE:HD13	2.51	0.41
1:N:31:ILE:CD1	1:O:31:ILE:HD13	2.51	0.41
1:J:209:VAL:HG13	1:J:271:GLY:O	2.21	0.41
1:I:209:VAL:HG13	1:I:271:GLY:O	2.21	0.41
1:D:209:VAL:HG13	1:D:271:GLY:O	2.21	0.41
1:N:14:GLU:HB3	1:N:17:ASN:ND2	2.35	0.41
1:J:201:LYS:HE3	1:K:218:GLU:OE1	2.20	0.41
1:K:164:ILE:HG23	1:L:172:GLU:OE1	2.20	0.41
1:B:163:SER:HB3	1:C:167:MET:O	2.21	0.41
1:A:163:SER:HB3	1:B:168:PHE:HA	2.03	0.41
1:H:110:ILE:HA	1:H:110:ILE:HD13	1.79	0.41
1:G:163:SER:HB3	1:H:167:MET:O	2.21	0.41
1:G:202:LEU:HD11	1:G:254:PHE:CE2	2.55	0.41
1:A:230:VAL:HG11	1:A:255:SER:N	2.36	0.41
1:K:163:SER:HB3	1:L:168:PHE:HA	2.03	0.41
1:E:110:ILE:HA	1:E:110:ILE:HD13	1.79	0.41
1:R:209:VAL:HG13	1:R:271:GLY:O	2.21	0.41
1:M:209:VAL:HG13	1:M:271:GLY:O	2.21	0.41
1:H:14:GLU:O	1:H:15:ILE:CB	2.70	0.40
1:R:14:GLU:O	1:R:15:ILE:CB	2.69	0.40
1:A:14:GLU:O	1:A:15:ILE:CB	2.69	0.40
1:O:119:THR:OG1	1:O:120:ASN:ND2	2.53	0.40
1:G:201:LYS:HE3	1:H:218:GLU:OE1	2.20	0.40
1:E:127:ILE:HA	1:E:127:ILE:HD13	1.82	0.40
1:K:230:VAL:HG11	1:K:255:SER:N	2.36	0.40
1:E:163:SER:HB3	1:F:167:MET:O	2.21	0.40
1:D:72:ILE:CD1	1:D:72:ILE:H	2.34	0.40
1:P:209:VAL:HG13	1:P:271:GLY:O	2.21	0.40
1:A:209:VAL:HG13	1:A:271:GLY:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:14:GLU:HB3	1:J:17:ASN:ND2	2.35	0.40
1:D:234:GLU:H	2:D:304:EPE:H81	1.84	0.40
1:F:119:THR:OG1	1:F:120:ASN:ND2	2.53	0.40
1:M:201:LYS:HE3	1:N:218:GLU:OE1	2.20	0.40
1:C:110:ILE:HA	1:C:110:ILE:HD13	1.79	0.40
1:N:230:VAL:HG12	1:N:255:SER:CA	2.51	0.40
1:H:31:ILE:CD1	1:I:31:ILE:HD13	2.51	0.40
1:O:209:VAL:HG13	1:O:271:GLY:O	2.21	0.40
1:F:209:VAL:HG13	1:F:271:GLY:O	2.21	0.40
1:R:40:ASN:ND2	1:R:45:GLN:HG2	2.28	0.40
1:P:172:GLU:HB3	1:R:164:ILE:HG13	2.01	0.40
1:G:163:SER:HB3	1:H:168:PHE:HA	2.03	0.40
1:F:230:VAL:HG11	1:F:255:SER:N	2.36	0.40
1:O:230:VAL:HG11	1:O:255:SER:N	2.36	0.40
1:N:163:SER:HB3	1:O:168:PHE:HA	2.03	0.40
1:K:31:ILE:CD1	1:L:31:ILE:HD13	2.51	0.40
1:K:14:GLU:CB	1:K:17:ASN:ND2	2.83	0.40
1:N:14:GLU:O	1:N:15:ILE:CB	2.70	0.40
1:B:14:GLU:HB3	1:B:17:ASN:ND2	2.35	0.40
1:P:215:LYS:HG2	1:P:216:THR:N	2.34	0.40
1:M:167:MET:O	1:O:163:SER:HB3	2.21	0.40
1:Q:230:VAL:HG11	1:Q:255:SER:N	2.36	0.40
1:D:168:PHE:HA	1:F:163:SER:HB3	2.03	0.40
1:H:209:VAL:HG13	1:H:271:GLY:O	2.21	0.40
1:J:14:GLU:O	1:J:15:ILE:CB	2.69	0.40
1:B:14:GLU:O	1:B:15:ILE:CB	2.70	0.40
1:J:163:SER:HB3	1:K:168:PHE:HA	2.03	0.40
1:Q:248:GLU:O	1:Q:249:ILE:CB	2.69	0.40
1:P:163:SER:HB3	1:Q:168:PHE:HA	2.03	0.40
1:D:31:ILE:CD1	1:E:31:ILE:HD13	2.51	0.40
1:K:209:VAL:HG13	1:K:271:GLY:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	7	47
1	B	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	7	47
1	C	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	7	47
1	D	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	7	47
1	E	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	7	47
1	F	286/288 (99%)	264 (92%)	15 (5%)	7 (2%)	7	47
1	G	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	7	47
1	H	286/288 (99%)	264 (92%)	15 (5%)	7 (2%)	7	47
1	I	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	7	47
1	J	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	7	47
1	K	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	7	47
1	L	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	7	47
1	M	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	7	47
1	N	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	7	47
1	O	286/288 (99%)	264 (92%)	15 (5%)	7 (2%)	7	47
1	P	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	7	47
1	Q	286/288 (99%)	264 (92%)	15 (5%)	7 (2%)	7	47
1	R	286/288 (99%)	265 (93%)	14 (5%)	7 (2%)	7	47
All	All	5148/5184 (99%)	4766 (93%)	256 (5%)	126 (2%)	12	47

All (126) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	20	THR
1	A	128	ASP
1	B	20	THR
1	B	128	ASP
1	C	20	THR
1	C	128	ASP
1	D	20	THR
1	D	128	ASP
1	E	20	THR
1	E	128	ASP
1	F	20	THR

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Mol	Chain	Res	Type
1	F	128	ASP
1	G	20	THR
1	G	128	ASP
1	H	20	THR
1	H	128	ASP
1	I	20	THR
1	I	128	ASP
1	J	20	THR
1	J	128	ASP
1	K	20	THR
1	K	128	ASP
1	L	20	THR
1	L	128	ASP
1	M	20	THR
1	M	128	ASP
1	N	20	THR
1	N	128	ASP
1	O	20	THR
1	O	128	ASP
1	P	20	THR
1	P	128	ASP
1	Q	20	THR
1	Q	128	ASP
1	R	20	THR
1	R	128	ASP
1	A	154	ASP
1	A	156	SER
1	B	154	ASP
1	B	156	SER
1	C	154	ASP
1	C	156	SER
1	D	154	ASP
1	D	156	SER
1	E	154	ASP
1	E	156	SER
1	F	154	ASP
1	F	156	SER
1	G	154	ASP
1	G	156	SER
1	H	154	ASP
1	H	156	SER
1	I	154	ASP

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Mol	Chain	Res	Type
1	I	156	SER
1	J	154	ASP
1	J	156	SER
1	K	154	ASP
1	K	156	SER
1	L	154	ASP
1	L	156	SER
1	M	154	ASP
1	M	156	SER
1	N	154	ASP
1	N	156	SER
1	O	154	ASP
1	O	156	SER
1	P	154	ASP
1	P	156	SER
1	Q	154	ASP
1	Q	156	SER
1	R	154	ASP
1	R	156	SER
1	A	127	ILE
1	B	127	ILE
1	C	127	ILE
1	D	127	ILE
1	E	127	ILE
1	F	127	ILE
1	G	127	ILE
1	H	127	ILE
1	I	127	ILE
1	J	127	ILE
1	K	127	ILE
1	L	127	ILE
1	M	127	ILE
1	N	127	ILE
1	O	127	ILE
1	P	127	ILE
1	Q	127	ILE
1	R	127	ILE
1	B	15	ILE
1	E	15	ILE
1	H	15	ILE
1	K	15	ILE
1	N	15	ILE

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Mol	Chain	Res	Type
1	Q	15	ILE
1	A	15	ILE
1	C	15	ILE
1	D	15	ILE
1	F	15	ILE
1	G	15	ILE
1	I	15	ILE
1	J	15	ILE
1	L	15	ILE
1	M	15	ILE
1	O	15	ILE
1	P	15	ILE
1	R	15	ILE
1	A	249	ILE
1	B	249	ILE
1	C	249	ILE
1	D	249	ILE
1	E	249	ILE
1	F	249	ILE
1	G	249	ILE
1	H	249	ILE
1	I	249	ILE
1	J	249	ILE
1	K	249	ILE
1	L	249	ILE
1	M	249	ILE
1	N	249	ILE
1	O	249	ILE
1	P	249	ILE
1	Q	249	ILE
1	R	249	ILE

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 PDB entries followed by that with respect to all EM entries.

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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	244/244 (100%)	235 (96%)	9 (4%)	41	73
1	B	244/244 (100%)	235 (96%)	9 (4%)	41	73
1	C	244/244 (100%)	235 (96%)	9 (4%)	41	73
1	D	244/244 (100%)	235 (96%)	9 (4%)	41	73
1	E	244/244 (100%)	235 (96%)	9 (4%)	41	73
1	F	244/244 (100%)	235 (96%)	9 (4%)	41	73
1	G	244/244 (100%)	235 (96%)	9 (4%)	41	73
1	H	244/244 (100%)	235 (96%)	9 (4%)	41	73
1	I	244/244 (100%)	235 (96%)	9 (4%)	41	73
1	J	244/244 (100%)	235 (96%)	9 (4%)	41	73
1	K	244/244 (100%)	235 (96%)	9 (4%)	41	73
1	L	244/244 (100%)	235 (96%)	9 (4%)	41	73
1	M	244/244 (100%)	235 (96%)	9 (4%)	41	73
1	N	244/244 (100%)	235 (96%)	9 (4%)	41	73
1	O	244/244 (100%)	235 (96%)	9 (4%)	41	73
1	P	244/244 (100%)	235 (96%)	9 (4%)	41	73
1	Q	244/244 (100%)	235 (96%)	9 (4%)	41	73
1	R	244/244 (100%)	235 (96%)	9 (4%)	41	73
All	All	4392/4392 (100%)	4230 (96%)	162 (4%)	45	73

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	110	ILE
1	A	120	ASN
1	A	122	LEU
1	A	148	LEU
1	A	157	THR
1	A	201	LYS
1	A	202	LEU
1	A	242	ASN
1	B	17	ASN
1	B	110	ILE

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Mol	Chain	Res	Type
1	B	120	ASN
1	B	122	LEU
1	B	148	LEU
1	B	157	THR
1	B	201	LYS
1	B	202	LEU
1	B	242	ASN
1	C	17	ASN
1	C	110	ILE
1	C	120	ASN
1	C	122	LEU
1	C	148	LEU
1	C	157	THR
1	C	201	LYS
1	C	202	LEU
1	C	242	ASN
1	D	17	ASN
1	D	110	ILE
1	D	120	ASN
1	D	122	LEU
1	D	148	LEU
1	D	157	THR
1	D	201	LYS
1	D	202	LEU
1	D	242	ASN
1	E	17	ASN
1	E	110	ILE
1	E	120	ASN
1	E	122	LEU
1	E	148	LEU
1	E	157	THR
1	E	201	LYS
1	E	202	LEU
1	E	242	ASN
1	F	17	ASN
1	F	110	ILE
1	F	120	ASN
1	F	122	LEU
1	F	148	LEU
1	F	157	THR
1	F	201	LYS
1	F	202	LEU

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Mol	Chain	Res	Type
1	F	242	ASN
1	G	17	ASN
1	G	110	ILE
1	G	120	ASN
1	G	122	LEU
1	G	148	LEU
1	G	157	THR
1	G	201	LYS
1	G	202	LEU
1	G	242	ASN
1	H	17	ASN
1	H	110	ILE
1	H	120	ASN
1	H	122	LEU
1	H	148	LEU
1	H	157	THR
1	H	201	LYS
1	H	202	LEU
1	H	242	ASN
1	I	17	ASN
1	I	110	ILE
1	I	120	ASN
1	I	122	LEU
1	I	148	LEU
1	I	157	THR
1	I	201	LYS
1	I	202	LEU
1	I	242	ASN
1	J	17	ASN
1	J	110	ILE
1	J	120	ASN
1	J	122	LEU
1	J	148	LEU
1	J	157	THR
1	J	201	LYS
1	J	202	LEU
1	J	242	ASN
1	K	17	ASN
1	K	110	ILE
1	K	120	ASN
1	K	122	LEU
1	K	148	LEU

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Mol	Chain	Res	Type
1	K	157	THR
1	K	201	LYS
1	K	202	LEU
1	K	242	ASN
1	L	17	ASN
1	L	110	ILE
1	L	120	ASN
1	L	122	LEU
1	L	148	LEU
1	L	157	THR
1	L	201	LYS
1	L	202	LEU
1	L	242	ASN
1	M	17	ASN
1	M	110	ILE
1	M	120	ASN
1	M	122	LEU
1	M	148	LEU
1	M	157	THR
1	M	201	LYS
1	M	202	LEU
1	M	242	ASN
1	N	17	ASN
1	N	110	ILE
1	N	120	ASN
1	N	122	LEU
1	N	148	LEU
1	N	157	THR
1	N	201	LYS
1	N	202	LEU
1	N	242	ASN
1	O	17	ASN
1	O	110	ILE
1	O	120	ASN
1	O	122	LEU
1	O	148	LEU
1	O	157	THR
1	O	201	LYS
1	O	202	LEU
1	O	242	ASN
1	P	17	ASN
1	P	110	ILE

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Mol	Chain	Res	Type
1	P	120	ASN
1	P	122	LEU
1	P	148	LEU
1	P	157	THR
1	P	201	LYS
1	P	202	LEU
1	P	242	ASN
1	Q	17	ASN
1	Q	110	ILE
1	Q	120	ASN
1	Q	122	LEU
1	Q	148	LEU
1	Q	157	THR
1	Q	201	LYS
1	Q	202	LEU
1	Q	242	ASN
1	R	17	ASN
1	R	110	ILE
1	R	120	ASN
1	R	122	LEU
1	R	148	LEU
1	R	157	THR
1	R	201	LYS
1	R	202	LEU
1	R	242	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (198) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	32	ASN
1	A	36	ASN
1	A	40	ASN
1	A	59	GLN
1	A	111	ASN
1	A	120	ASN
1	A	125	GLN
1	A	155	ASN
1	A	227	ASN
1	A	242	ASN
1	B	17	ASN
1	B	32	ASN

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Mol	Chain	Res	Type
1	B	36	ASN
1	B	40	ASN
1	B	59	GLN
1	B	111	ASN
1	B	120	ASN
1	B	125	GLN
1	B	155	ASN
1	B	227	ASN
1	B	242	ASN
1	C	17	ASN
1	C	32	ASN
1	C	36	ASN
1	C	40	ASN
1	C	59	GLN
1	C	111	ASN
1	C	120	ASN
1	C	125	GLN
1	C	155	ASN
1	C	227	ASN
1	C	242	ASN
1	D	17	ASN
1	D	32	ASN
1	D	36	ASN
1	D	40	ASN
1	D	59	GLN
1	D	111	ASN
1	D	120	ASN
1	D	125	GLN
1	D	155	ASN
1	D	227	ASN
1	D	242	ASN
1	E	17	ASN
1	E	32	ASN
1	E	36	ASN
1	E	40	ASN
1	E	59	GLN
1	E	111	ASN
1	E	120	ASN
1	E	125	GLN
1	E	155	ASN
1	E	227	ASN
1	E	242	ASN

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Mol	Chain	Res	Type
1	F	17	ASN
1	F	32	ASN
1	F	36	ASN
1	F	40	ASN
1	F	59	GLN
1	F	111	ASN
1	F	120	ASN
1	F	125	GLN
1	F	155	ASN
1	F	227	ASN
1	F	242	ASN
1	G	17	ASN
1	G	32	ASN
1	G	36	ASN
1	G	40	ASN
1	G	59	GLN
1	G	111	ASN
1	G	120	ASN
1	G	125	GLN
1	G	155	ASN
1	G	227	ASN
1	G	242	ASN
1	H	17	ASN
1	H	32	ASN
1	H	36	ASN
1	H	40	ASN
1	H	59	GLN
1	H	111	ASN
1	H	120	ASN
1	H	125	GLN
1	H	155	ASN
1	H	227	ASN
1	H	242	ASN
1	I	17	ASN
1	I	32	ASN
1	I	36	ASN
1	I	40	ASN
1	I	59	GLN
1	I	111	ASN
1	I	120	ASN
1	I	125	GLN
1	I	155	ASN

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Mol	Chain	Res	Type
1	I	227	ASN
1	I	242	ASN
1	J	17	ASN
1	J	32	ASN
1	J	36	ASN
1	J	40	ASN
1	J	59	GLN
1	J	111	ASN
1	J	120	ASN
1	J	125	GLN
1	J	155	ASN
1	J	227	ASN
1	J	242	ASN
1	K	17	ASN
1	K	32	ASN
1	K	36	ASN
1	K	40	ASN
1	K	59	GLN
1	K	111	ASN
1	K	120	ASN
1	K	125	GLN
1	K	155	ASN
1	K	227	ASN
1	K	242	ASN
1	L	17	ASN
1	L	32	ASN
1	L	36	ASN
1	L	40	ASN
1	L	59	GLN
1	L	111	ASN
1	L	120	ASN
1	L	125	GLN
1	L	155	ASN
1	L	227	ASN
1	L	242	ASN
1	M	17	ASN
1	M	32	ASN
1	M	36	ASN
1	M	40	ASN
1	M	59	GLN
1	M	111	ASN
1	M	120	ASN

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Mol	Chain	Res	Type
1	M	125	GLN
1	M	155	ASN
1	M	227	ASN
1	M	242	ASN
1	N	17	ASN
1	N	32	ASN
1	N	36	ASN
1	N	40	ASN
1	N	59	GLN
1	N	111	ASN
1	N	120	ASN
1	N	125	GLN
1	N	155	ASN
1	N	227	ASN
1	N	242	ASN
1	O	17	ASN
1	O	32	ASN
1	O	36	ASN
1	O	40	ASN
1	O	59	GLN
1	O	111	ASN
1	O	120	ASN
1	O	125	GLN
1	O	155	ASN
1	O	227	ASN
1	O	242	ASN
1	P	17	ASN
1	P	32	ASN
1	P	36	ASN
1	P	40	ASN
1	P	59	GLN
1	P	111	ASN
1	P	120	ASN
1	P	125	GLN
1	P	155	ASN
1	P	227	ASN
1	P	242	ASN
1	Q	17	ASN
1	Q	32	ASN
1	Q	36	ASN
1	Q	40	ASN
1	Q	59	GLN

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Mol	Chain	Res	Type
1	Q	111	ASN
1	Q	120	ASN
1	Q	125	GLN
1	Q	155	ASN
1	Q	227	ASN
1	Q	242	ASN
1	R	17	ASN
1	R	32	ASN
1	R	36	ASN
1	R	40	ASN
1	R	59	GLN
1	R	111	ASN
1	R	120	ASN
1	R	125	GLN
1	R	155	ASN
1	R	227	ASN
1	R	242	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

18 ligands are modelled in this entry.

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
2	EPE	A	301	-	15,15,15	1.80	2 (13%)	19,20,20	4.35	12 (63%)
2	EPE	B	302	-	15,15,15	1.81	2 (13%)	19,20,20	4.36	12 (63%)
2	EPE	C	303	-	15,15,15	1.80	2 (13%)	19,20,20	4.35	12 (63%)
2	EPE	D	304	-	15,15,15	1.80	2 (13%)	19,20,20	4.35	12 (63%)
2	EPE	E	305	-	15,15,15	1.80	2 (13%)	19,20,20	4.36	12 (63%)
2	EPE	F	306	-	15,15,15	1.79	2 (13%)	19,20,20	4.35	12 (63%)
2	EPE	G	307	-	15,15,15	1.80	2 (13%)	19,20,20	4.34	12 (63%)
2	EPE	H	308	-	15,15,15	1.81	2 (13%)	19,20,20	4.36	12 (63%)
2	EPE	I	309	-	15,15,15	1.80	2 (13%)	19,20,20	4.35	12 (63%)
2	EPE	J	310	-	15,15,15	1.80	2 (13%)	19,20,20	4.35	12 (63%)
2	EPE	K	311	-	15,15,15	1.81	2 (13%)	19,20,20	4.36	12 (63%)
2	EPE	L	312	-	15,15,15	1.80	2 (13%)	19,20,20	4.35	12 (63%)
2	EPE	M	313	-	15,15,15	1.80	2 (13%)	19,20,20	4.35	12 (63%)
2	EPE	N	314	-	15,15,15	1.80	2 (13%)	19,20,20	4.36	12 (63%)
2	EPE	O	315	-	15,15,15	1.79	2 (13%)	19,20,20	4.36	12 (63%)
2	EPE	P	316	-	15,15,15	1.80	2 (13%)	19,20,20	4.34	12 (63%)
2	EPE	Q	317	-	15,15,15	1.80	2 (13%)	19,20,20	4.36	12 (63%)
2	EPE	R	318	-	15,15,15	1.80	2 (13%)	19,20,20	4.35	12 (63%)

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
2	EPE	A	301	-	-	0/9/19/19	0/1/1/1
2	EPE	B	302	-	-	0/9/19/19	0/1/1/1
2	EPE	C	303	-	-	0/9/19/19	0/1/1/1
2	EPE	D	304	-	-	0/9/19/19	0/1/1/1
2	EPE	E	305	-	-	0/9/19/19	0/1/1/1
2	EPE	F	306	-	-	0/9/19/19	0/1/1/1
2	EPE	G	307	-	-	0/9/19/19	0/1/1/1
2	EPE	H	308	-	-	0/9/19/19	0/1/1/1
2	EPE	I	309	-	-	0/9/19/19	0/1/1/1
2	EPE	J	310	-	-	0/9/19/19	0/1/1/1
2	EPE	K	311	-	-	0/9/19/19	0/1/1/1
2	EPE	L	312	-	-	0/9/19/19	0/1/1/1
2	EPE	M	313	-	-	0/9/19/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EPE	N	314	-	-	0/9/19/19	0/1/1/1
2	EPE	O	315	-	-	0/9/19/19	0/1/1/1
2	EPE	P	316	-	-	0/9/19/19	0/1/1/1
2	EPE	Q	317	-	-	0/9/19/19	0/1/1/1
2	EPE	R	318	-	-	0/9/19/19	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	315	EPE	C10-S	3.83	1.83	1.77
2	F	306	EPE	C10-S	3.83	1.83	1.77
2	L	312	EPE	C10-S	3.88	1.83	1.77
2	C	303	EPE	C10-S	3.88	1.83	1.77
2	R	318	EPE	C10-S	3.89	1.83	1.77
2	I	309	EPE	C10-S	3.89	1.83	1.77
2	H	308	EPE	C10-S	3.90	1.83	1.77
2	Q	317	EPE	C10-S	3.90	1.83	1.77
2	E	305	EPE	C10-S	3.90	1.83	1.77
2	N	314	EPE	C10-S	3.90	1.83	1.77
2	G	307	EPE	C10-S	3.91	1.83	1.77
2	P	316	EPE	C10-S	3.91	1.83	1.77
2	M	313	EPE	C10-S	3.91	1.83	1.77
2	D	304	EPE	C10-S	3.91	1.83	1.77
2	J	310	EPE	C10-S	3.92	1.83	1.77
2	A	301	EPE	C10-S	3.92	1.83	1.77
2	B	302	EPE	C10-S	3.92	1.83	1.77
2	K	311	EPE	C10-S	3.92	1.83	1.77
2	G	307	EPE	O3S-S	5.05	1.64	1.47
2	P	316	EPE	O3S-S	5.05	1.64	1.47
2	J	310	EPE	O3S-S	5.05	1.64	1.47
2	A	301	EPE	O3S-S	5.05	1.64	1.47
2	L	312	EPE	O3S-S	5.06	1.64	1.47
2	C	303	EPE	O3S-S	5.06	1.64	1.47
2	R	318	EPE	O3S-S	5.06	1.64	1.47
2	I	309	EPE	O3S-S	5.06	1.64	1.47
2	O	315	EPE	O3S-S	5.06	1.64	1.47
2	F	306	EPE	O3S-S	5.06	1.64	1.47
2	M	313	EPE	O3S-S	5.06	1.64	1.47
2	D	304	EPE	O3S-S	5.06	1.64	1.47
2	E	305	EPE	O3S-S	5.08	1.64	1.47
2	N	314	EPE	O3S-S	5.08	1.64	1.47
2	H	308	EPE	O3S-S	5.08	1.64	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	317	EPE	O3S-S	5.08	1.64	1.47
2	B	302	EPE	O3S-S	5.09	1.64	1.47
2	K	311	EPE	O3S-S	5.09	1.64	1.47

All (216) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	305	EPE	O3S-S-O1S	-4.88	100.45	111.26
2	B	302	EPE	O3S-S-O1S	-4.88	100.45	111.26
2	N	314	EPE	O3S-S-O1S	-4.88	100.45	111.26
2	K	311	EPE	O3S-S-O1S	-4.88	100.45	111.26
2	H	308	EPE	O3S-S-O1S	-4.88	100.46	111.26
2	Q	317	EPE	O3S-S-O1S	-4.88	100.46	111.26
2	L	312	EPE	O3S-S-O1S	-4.88	100.47	111.26
2	C	303	EPE	O3S-S-O1S	-4.88	100.47	111.26
2	R	318	EPE	O3S-S-O1S	-4.87	100.48	111.26
2	I	309	EPE	O3S-S-O1S	-4.87	100.48	111.26
2	J	310	EPE	O3S-S-O1S	-4.87	100.48	111.26
2	A	301	EPE	O3S-S-O1S	-4.87	100.48	111.26
2	O	315	EPE	O3S-S-O1S	-4.87	100.49	111.26
2	F	306	EPE	O3S-S-O1S	-4.87	100.49	111.26
2	M	313	EPE	O3S-S-O1S	-4.87	100.49	111.26
2	D	304	EPE	O3S-S-O1S	-4.87	100.49	111.26
2	G	307	EPE	O3S-S-O1S	-4.85	100.52	111.26
2	P	316	EPE	O3S-S-O1S	-4.85	100.52	111.26
2	H	308	EPE	C5-N4-C3	2.07	113.50	108.87
2	Q	317	EPE	C5-N4-C3	2.07	113.50	108.87
2	E	305	EPE	C5-N4-C3	2.07	113.51	108.87
2	N	314	EPE	C5-N4-C3	2.07	113.51	108.87
2	B	302	EPE	C5-N4-C3	2.08	113.52	108.87
2	K	311	EPE	C5-N4-C3	2.08	113.52	108.87
2	O	315	EPE	C5-N4-C3	2.08	113.52	108.87
2	R	318	EPE	C5-N4-C3	2.09	113.55	108.87
2	L	312	EPE	C5-N4-C3	2.09	113.55	108.87
2	C	303	EPE	C5-N4-C3	2.09	113.55	108.87
2	I	309	EPE	C5-N4-C3	2.09	113.56	108.87
2	F	306	EPE	C5-N4-C3	2.09	113.56	108.87
2	G	307	EPE	C5-N4-C3	2.10	113.58	108.87
2	P	316	EPE	C5-N4-C3	2.10	113.58	108.87
2	M	313	EPE	C5-N4-C3	2.10	113.58	108.87
2	D	304	EPE	C5-N4-C3	2.10	113.58	108.87
2	J	310	EPE	C5-N4-C3	2.11	113.59	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	EPE	C5-N4-C3	2.11	113.59	108.87
2	E	305	EPE	C6-N1-C2	2.82	115.19	108.87
2	N	314	EPE	C6-N1-C2	2.82	115.19	108.87
2	H	308	EPE	C6-N1-C2	2.83	115.20	108.87
2	Q	317	EPE	C6-N1-C2	2.83	115.20	108.87
2	B	302	EPE	C6-N1-C2	2.84	115.22	108.87
2	K	311	EPE	C6-N1-C2	2.84	115.22	108.87
2	M	313	EPE	C6-N1-C2	2.85	115.25	108.87
2	D	304	EPE	C6-N1-C2	2.85	115.25	108.87
2	G	307	EPE	C6-N1-C2	2.85	115.25	108.87
2	P	316	EPE	C6-N1-C2	2.85	115.25	108.87
2	J	310	EPE	C6-N1-C2	2.85	115.26	108.87
2	A	301	EPE	C6-N1-C2	2.85	115.26	108.87
2	L	312	EPE	C6-N1-C2	2.87	115.30	108.87
2	C	303	EPE	C6-N1-C2	2.87	115.30	108.87
2	I	309	EPE	C6-N1-C2	2.88	115.31	108.87
2	R	318	EPE	C6-N1-C2	2.88	115.31	108.87
2	O	315	EPE	C6-N1-C2	2.89	115.34	108.87
2	F	306	EPE	C6-N1-C2	2.89	115.34	108.87
2	G	307	EPE	C9-N1-C2	3.59	119.06	111.25
2	P	316	EPE	C9-N1-C2	3.59	119.06	111.25
2	M	313	EPE	C9-N1-C2	3.59	119.06	111.25
2	D	304	EPE	C9-N1-C2	3.59	119.06	111.25
2	J	310	EPE	C9-N1-C2	3.59	119.06	111.25
2	A	301	EPE	C9-N1-C2	3.59	119.06	111.25
2	O	315	EPE	C9-N1-C2	3.59	119.06	111.25
2	F	306	EPE	C9-N1-C2	3.59	119.06	111.25
2	I	309	EPE	C9-N1-C2	3.59	119.07	111.25
2	H	308	EPE	C9-N1-C2	3.59	119.07	111.25
2	Q	317	EPE	C9-N1-C2	3.59	119.07	111.25
2	L	312	EPE	C9-N1-C2	3.60	119.08	111.25
2	C	303	EPE	C9-N1-C2	3.60	119.08	111.25
2	B	302	EPE	C9-N1-C2	3.60	119.09	111.25
2	K	311	EPE	C9-N1-C2	3.60	119.09	111.25
2	E	305	EPE	C9-N1-C2	3.60	119.09	111.25
2	N	314	EPE	C9-N1-C2	3.60	119.09	111.25
2	R	318	EPE	C9-N1-C2	3.61	119.10	111.25
2	G	307	EPE	C6-C5-N4	3.78	118.04	110.65
2	P	316	EPE	C6-C5-N4	3.78	118.04	110.65
2	M	313	EPE	C6-C5-N4	3.79	118.05	110.65
2	D	304	EPE	C6-C5-N4	3.79	118.05	110.65
2	J	310	EPE	C6-C5-N4	3.79	118.05	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	EPE	C6-C5-N4	3.79	118.05	110.65
2	R	318	EPE	C6-C5-N4	3.81	118.08	110.65
2	F	306	EPE	C6-C5-N4	3.81	118.09	110.65
2	H	308	EPE	C6-C5-N4	3.82	118.10	110.65
2	Q	317	EPE	C6-C5-N4	3.82	118.10	110.65
2	I	309	EPE	C6-C5-N4	3.82	118.10	110.65
2	L	312	EPE	C6-C5-N4	3.82	118.10	110.65
2	C	303	EPE	C6-C5-N4	3.82	118.10	110.65
2	B	302	EPE	C6-C5-N4	3.82	118.11	110.65
2	K	311	EPE	C6-C5-N4	3.82	118.11	110.65
2	O	315	EPE	C6-C5-N4	3.82	118.11	110.65
2	E	305	EPE	C6-C5-N4	3.83	118.12	110.65
2	N	314	EPE	C6-C5-N4	3.83	118.12	110.65
2	R	318	EPE	C9-N1-C6	3.90	119.74	111.25
2	O	315	EPE	C9-N1-C6	3.91	119.75	111.25
2	F	306	EPE	C9-N1-C6	3.91	119.75	111.25
2	L	312	EPE	C9-N1-C6	3.92	119.79	111.25
2	C	303	EPE	C9-N1-C6	3.92	119.79	111.25
2	I	309	EPE	C9-N1-C6	3.93	119.81	111.25
2	B	302	EPE	C9-N1-C6	3.94	119.83	111.25
2	K	311	EPE	C9-N1-C6	3.94	119.83	111.25
2	J	310	EPE	C9-N1-C6	3.94	119.83	111.25
2	A	301	EPE	C9-N1-C6	3.94	119.83	111.25
2	G	307	EPE	C9-N1-C6	3.95	119.84	111.25
2	P	316	EPE	C9-N1-C6	3.95	119.84	111.25
2	M	313	EPE	C9-N1-C6	3.95	119.84	111.25
2	D	304	EPE	C9-N1-C6	3.95	119.84	111.25
2	E	305	EPE	C9-N1-C6	3.95	119.85	111.25
2	N	314	EPE	C9-N1-C6	3.95	119.85	111.25
2	H	308	EPE	C9-N1-C6	3.96	119.86	111.25
2	Q	317	EPE	C9-N1-C6	3.96	119.86	111.25
2	F	306	EPE	C2-C3-N4	4.05	118.56	110.65
2	J	310	EPE	C2-C3-N4	4.06	118.57	110.65
2	A	301	EPE	C2-C3-N4	4.06	118.57	110.65
2	I	309	EPE	C2-C3-N4	4.06	118.57	110.65
2	L	312	EPE	C2-C3-N4	4.06	118.57	110.65
2	C	303	EPE	C2-C3-N4	4.06	118.57	110.65
2	M	313	EPE	C2-C3-N4	4.06	118.58	110.65
2	D	304	EPE	C2-C3-N4	4.06	118.58	110.65
2	E	305	EPE	C2-C3-N4	4.06	118.58	110.65
2	N	314	EPE	C2-C3-N4	4.06	118.58	110.65
2	G	307	EPE	C2-C3-N4	4.06	118.58	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	P	316	EPE	C2-C3-N4	4.06	118.58	110.65
2	H	308	EPE	C2-C3-N4	4.07	118.59	110.65
2	Q	317	EPE	C2-C3-N4	4.07	118.59	110.65
2	O	315	EPE	O8-C8-C7	4.07	129.97	111.27
2	F	306	EPE	O8-C8-C7	4.07	129.97	111.27
2	B	302	EPE	C2-C3-N4	4.07	118.59	110.65
2	R	318	EPE	C2-C3-N4	4.07	118.59	110.65
2	K	311	EPE	C2-C3-N4	4.07	118.59	110.65
2	L	312	EPE	O8-C8-C7	4.07	129.97	111.27
2	C	303	EPE	O8-C8-C7	4.07	129.97	111.27
2	O	315	EPE	C2-C3-N4	4.07	118.60	110.65
2	R	318	EPE	O8-C8-C7	4.08	130.00	111.27
2	I	309	EPE	O8-C8-C7	4.08	130.00	111.27
2	G	307	EPE	O8-C8-C7	4.08	130.03	111.27
2	P	316	EPE	O8-C8-C7	4.08	130.03	111.27
2	D	304	EPE	O8-C8-C7	4.09	130.04	111.27
2	J	310	EPE	O8-C8-C7	4.09	130.05	111.27
2	A	301	EPE	O8-C8-C7	4.09	130.05	111.27
2	M	313	EPE	O8-C8-C7	4.10	130.09	111.27
2	N	314	EPE	O8-C8-C7	4.10	130.09	111.27
2	Q	317	EPE	O8-C8-C7	4.10	130.12	111.27
2	B	302	EPE	O8-C8-C7	4.10	130.12	111.27
2	K	311	EPE	O8-C8-C7	4.10	130.12	111.27
2	E	305	EPE	O8-C8-C7	4.11	130.13	111.27
2	H	308	EPE	O8-C8-C7	4.11	130.15	111.27
2	R	318	EPE	C7-N4-C5	4.40	120.84	111.25
2	O	315	EPE	C7-N4-C5	4.41	120.86	111.25
2	L	312	EPE	C7-N4-C5	4.42	120.86	111.25
2	C	303	EPE	C7-N4-C5	4.42	120.86	111.25
2	B	302	EPE	C7-N4-C5	4.42	120.87	111.25
2	K	311	EPE	C7-N4-C5	4.42	120.87	111.25
2	F	306	EPE	C7-N4-C5	4.42	120.87	111.25
2	G	307	EPE	C7-N4-C5	4.42	120.88	111.25
2	P	316	EPE	C7-N4-C5	4.42	120.88	111.25
2	J	310	EPE	C7-N4-C5	4.42	120.88	111.25
2	A	301	EPE	C7-N4-C5	4.42	120.88	111.25
2	Q	317	EPE	C7-N4-C5	4.43	120.89	111.25
2	N	314	EPE	C7-N4-C5	4.43	120.89	111.25
2	I	309	EPE	C7-N4-C5	4.43	120.89	111.25
2	H	308	EPE	C7-N4-C5	4.44	120.91	111.25
2	M	313	EPE	C7-N4-C5	4.44	120.91	111.25
2	D	304	EPE	C7-N4-C5	4.44	120.91	111.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	305	EPE	C7-N4-C5	4.44	120.92	111.25
2	R	318	EPE	C5-C6-N1	5.81	121.98	110.65
2	O	315	EPE	C5-C6-N1	5.81	121.98	110.65
2	F	306	EPE	C5-C6-N1	5.81	121.99	110.65
2	I	309	EPE	C5-C6-N1	5.81	122.00	110.65
2	L	312	EPE	C5-C6-N1	5.82	122.00	110.65
2	C	303	EPE	C5-C6-N1	5.82	122.00	110.65
2	J	310	EPE	C5-C6-N1	5.85	122.07	110.65
2	A	301	EPE	C5-C6-N1	5.85	122.07	110.65
2	B	302	EPE	C5-C6-N1	5.85	122.07	110.65
2	K	311	EPE	C5-C6-N1	5.85	122.07	110.65
2	M	313	EPE	C5-C6-N1	5.86	122.09	110.65
2	D	304	EPE	C5-C6-N1	5.86	122.09	110.65
2	G	307	EPE	C5-C6-N1	5.86	122.09	110.65
2	P	316	EPE	C5-C6-N1	5.86	122.09	110.65
2	E	305	EPE	C5-C6-N1	5.86	122.09	110.65
2	N	314	EPE	C5-C6-N1	5.86	122.09	110.65
2	H	308	EPE	C5-C6-N1	5.87	122.11	110.65
2	Q	317	EPE	C5-C6-N1	5.87	122.11	110.65
2	M	313	EPE	C7-N4-C3	6.54	125.49	111.25
2	D	304	EPE	C7-N4-C3	6.54	125.49	111.25
2	J	310	EPE	C7-N4-C3	6.55	125.51	111.25
2	A	301	EPE	C7-N4-C3	6.55	125.51	111.25
2	G	307	EPE	C7-N4-C3	6.56	125.53	111.25
2	P	316	EPE	C7-N4-C3	6.56	125.53	111.25
2	I	309	EPE	C7-N4-C3	6.56	125.53	111.25
2	F	306	EPE	C7-N4-C3	6.57	125.55	111.25
2	E	305	EPE	C7-N4-C3	6.57	125.55	111.25
2	L	312	EPE	C7-N4-C3	6.58	125.56	111.25
2	C	303	EPE	C7-N4-C3	6.58	125.56	111.25
2	H	308	EPE	C7-N4-C3	6.58	125.57	111.25
2	N	314	EPE	C7-N4-C3	6.59	125.59	111.25
2	B	302	EPE	C7-N4-C3	6.59	125.59	111.25
2	K	311	EPE	C7-N4-C3	6.59	125.59	111.25
2	Q	317	EPE	C7-N4-C3	6.59	125.59	111.25
2	R	318	EPE	C7-N4-C3	6.59	125.59	111.25
2	O	315	EPE	C7-N4-C3	6.59	125.60	111.25
2	G	307	EPE	O2S-S-C10	11.95	115.31	106.87
2	P	316	EPE	O2S-S-C10	11.95	115.31	106.87
2	M	313	EPE	O2S-S-C10	11.95	115.31	106.87
2	D	304	EPE	O2S-S-C10	11.95	115.31	106.87
2	J	310	EPE	O2S-S-C10	11.97	115.33	106.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	EPE	O2S-S-C10	11.97	115.33	106.87
2	B	302	EPE	O2S-S-C10	11.98	115.33	106.87
2	K	311	EPE	O2S-S-C10	11.98	115.33	106.87
2	H	308	EPE	O2S-S-C10	11.98	115.34	106.87
2	Q	317	EPE	O2S-S-C10	11.98	115.34	106.87
2	R	318	EPE	O2S-S-C10	11.99	115.34	106.87
2	I	309	EPE	O2S-S-C10	11.99	115.34	106.87
2	E	305	EPE	O2S-S-C10	12.00	115.35	106.87
2	N	314	EPE	O2S-S-C10	12.00	115.35	106.87
2	L	312	EPE	O2S-S-C10	12.02	115.36	106.87
2	C	303	EPE	O2S-S-C10	12.02	115.36	106.87
2	O	315	EPE	O2S-S-C10	12.03	115.37	106.87
2	F	306	EPE	O2S-S-C10	12.03	115.37	106.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

18 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	EPE	3	0
2	B	302	EPE	3	0
2	C	303	EPE	3	0
2	D	304	EPE	4	0
2	E	305	EPE	3	0
2	F	306	EPE	3	0
2	G	307	EPE	3	0
2	H	308	EPE	3	0
2	I	309	EPE	3	0
2	J	310	EPE	3	0
2	K	311	EPE	3	0
2	L	312	EPE	3	0
2	M	313	EPE	3	0
2	N	314	EPE	3	0
2	O	315	EPE	3	0
2	P	316	EPE	3	0
2	Q	317	EPE	3	0
2	R	318	EPE	3	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.