



Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 07:14 am BST

PDB ID : 5H7D
Title : Crystal structure of the YgjG-protein A-Zpa963-calmodulin complex
Authors : Youn, S.J.; Kwon, N.Y.; Lee, J.H.; Kim, J.H.; Lee, H.; Lee, J.O.
Deposited on : 2016-11-17
Resolution : 2.57 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

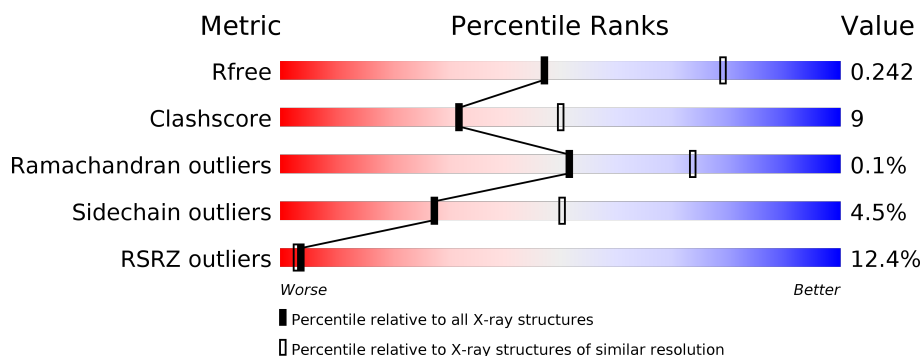
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3676 (2.60-2.56)
Clashscore	141614	4049 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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

Mol	Chain	Length	Quality of chain
1	A	499	<div> <div>5%</div> <div>81% 17% ..</div> </div>
1	B	499	<div> <div>8%</div> <div>83% 15% ..</div> </div>
1	C	499	<div> <div>6%</div> <div>80% 18% ..</div> </div>
1	D	499	<div> <div>6%</div> <div>82% 15% ..</div> </div>
1	I	499	<div> <div>5%</div> <div>82% 16% ..</div> </div>
1	J	499	<div> <div>7%</div> <div>81% 17% ..</div> </div>

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Mol	Chain	Length	Quality of chain
1	M	499	<div><div></div><div>6%</div><div>84%</div><div>14%</div><div>••</div></div>
1	N	499	<div><div></div><div>8%</div><div>83%</div><div>15%</div><div>••</div></div>
2	E	120	<div><div></div><div>25%</div><div>64%</div><div>24%</div><div>6%</div><div>6%</div></div>
2	F	120	<div><div></div><div>49%</div><div>62%</div><div>26%</div><div>5%</div><div>•</div><div>7%</div></div>
2	G	120	<div><div></div><div>18%</div><div>63%</div><div>25%</div><div>6%</div><div>6%</div></div>
2	H	120	<div><div></div><div>50%</div><div>63%</div><div>26%</div><div>•</div><div>7%</div></div>
2	K	120	<div><div></div><div>19%</div><div>62%</div><div>28%</div><div>5%</div><div>6%</div></div>
2	L	120	<div><div></div><div>48%</div><div>68%</div><div>22%</div><div>•</div><div>7%</div></div>
2	O	120	<div><div></div><div>22%</div><div>63%</div><div>25%</div><div>6%</div><div>6%</div></div>
2	P	120	<div><div></div><div>60%</div><div>63%</div><div>22%</div><div>8%</div><div>7%</div></div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 37132 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Putrescine aminotransferase,Immunoglobulin G-binding protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			3775	2396	651	706	22			
1	B	495	Total	C	N	O	S	0	0	0
			3775	2396	651	706	22			
1	C	495	Total	C	N	O	S	0	0	0
			3775	2396	651	706	22			
1	D	495	Total	C	N	O	S	0	0	0
			3775	2396	651	706	22			
1	I	495	Total	C	N	O	S	0	0	0
			3775	2396	651	706	22			
1	J	495	Total	C	N	O	S	0	0	0
			3775	2396	651	706	22			
1	M	495	Total	C	N	O	S	0	0	0
			3775	2396	651	706	22			
1	N	495	Total	C	N	O	S	0	0	0
			3775	2396	651	706	22			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLY	-	expression tag	UNP P42588
A	4	SER	-	expression tag	UNP P42588
A	5	HIS	-	expression tag	UNP P42588
A	6	MET	-	expression tag	UNP P42588
A	456	VAL	ASN	engineered mutation	UNP P38507
A	474	ALA	GLY	engineered mutation	UNP P38507
B	3	GLY	-	expression tag	UNP P42588
B	4	SER	-	expression tag	UNP P42588
B	5	HIS	-	expression tag	UNP P42588
B	6	MET	-	expression tag	UNP P42588
B	456	VAL	ASN	engineered mutation	UNP P38507
B	474	ALA	GLY	engineered mutation	UNP P38507

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Chain	Residue	Modelled	Actual	Comment	Reference
C	3	GLY	-	expression tag	UNP P42588
C	4	SER	-	expression tag	UNP P42588
C	5	HIS	-	expression tag	UNP P42588
C	6	MET	-	expression tag	UNP P42588
C	456	VAL	ASN	engineered mutation	UNP P38507
C	474	ALA	GLY	engineered mutation	UNP P38507
D	3	GLY	-	expression tag	UNP P42588
D	4	SER	-	expression tag	UNP P42588
D	5	HIS	-	expression tag	UNP P42588
D	6	MET	-	expression tag	UNP P42588
D	456	VAL	ASN	engineered mutation	UNP P38507
D	474	ALA	GLY	engineered mutation	UNP P38507
I	3	GLY	-	expression tag	UNP P42588
I	4	SER	-	expression tag	UNP P42588
I	5	HIS	-	expression tag	UNP P42588
I	6	MET	-	expression tag	UNP P42588
I	456	VAL	ASN	engineered mutation	UNP P38507
I	474	ALA	GLY	engineered mutation	UNP P38507
J	3	GLY	-	expression tag	UNP P42588
J	4	SER	-	expression tag	UNP P42588
J	5	HIS	-	expression tag	UNP P42588
J	6	MET	-	expression tag	UNP P42588
J	456	VAL	ASN	engineered mutation	UNP P38507
J	474	ALA	GLY	engineered mutation	UNP P38507
M	3	GLY	-	expression tag	UNP P42588
M	4	SER	-	expression tag	UNP P42588
M	5	HIS	-	expression tag	UNP P42588
M	6	MET	-	expression tag	UNP P42588
M	456	VAL	ASN	engineered mutation	UNP P38507
M	474	ALA	GLY	engineered mutation	UNP P38507
N	3	GLY	-	expression tag	UNP P42588
N	4	SER	-	expression tag	UNP P42588
N	5	HIS	-	expression tag	UNP P42588
N	6	MET	-	expression tag	UNP P42588
N	456	VAL	ASN	engineered mutation	UNP P38507
N	474	ALA	GLY	engineered mutation	UNP P38507

- Molecule 2 is a protein called Zpa963, Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	113	Total	C	N	O	S	0	0	0
			872	544	143	181	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	112	Total	C	N	O	S	0	0	0
			857	536	139	178	4			
2	G	113	Total	C	N	O	S	0	0	0
			872	544	143	181	4			
2	H	112	Total	C	N	O	S	0	0	0
			857	536	139	178	4			
2	K	113	Total	C	N	O	S	0	0	0
			872	544	143	181	4			
2	L	112	Total	C	N	O	S	0	0	0
			857	536	139	178	4			
2	O	113	Total	C	N	O	S	0	0	0
			872	544	143	181	4			
2	P	112	Total	C	N	O	S	0	0	0
			857	536	139	178	4			

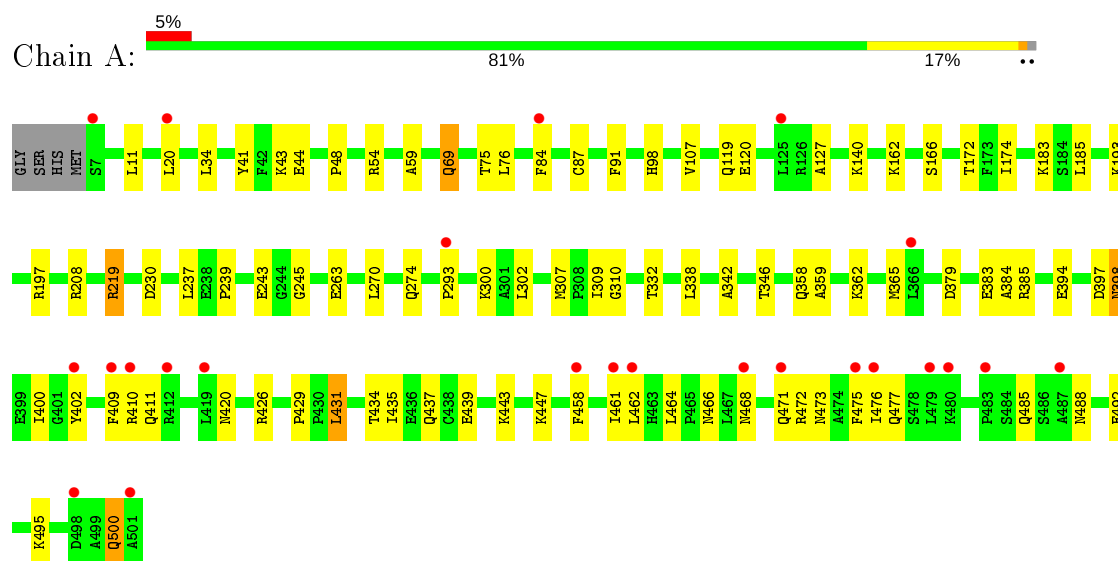
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	2	Total	Ca	0	0
			2	2		
3	G	2	Total	Ca	0	0
			2	2		
3	K	2	Total	Ca	0	0
			2	2		
3	E	2	Total	Ca	0	0
			2	2		
3	H	2	Total	Ca	0	0
			2	2		
3	O	2	Total	Ca	0	0
			2	2		
3	L	2	Total	Ca	0	0
			2	2		
3	F	2	Total	Ca	0	0
			2	2		

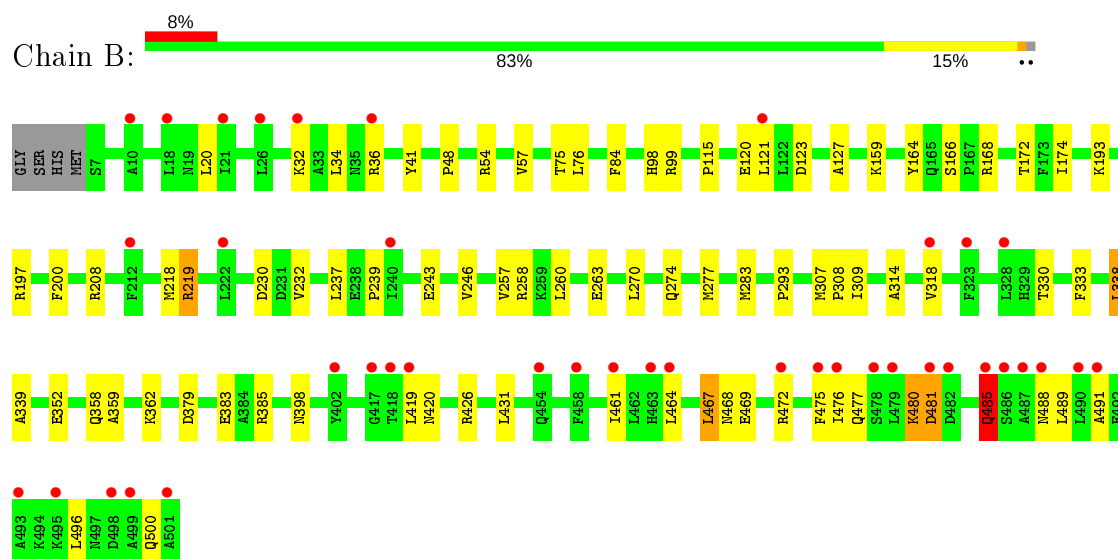
3 Residue-property plots [i](#)

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

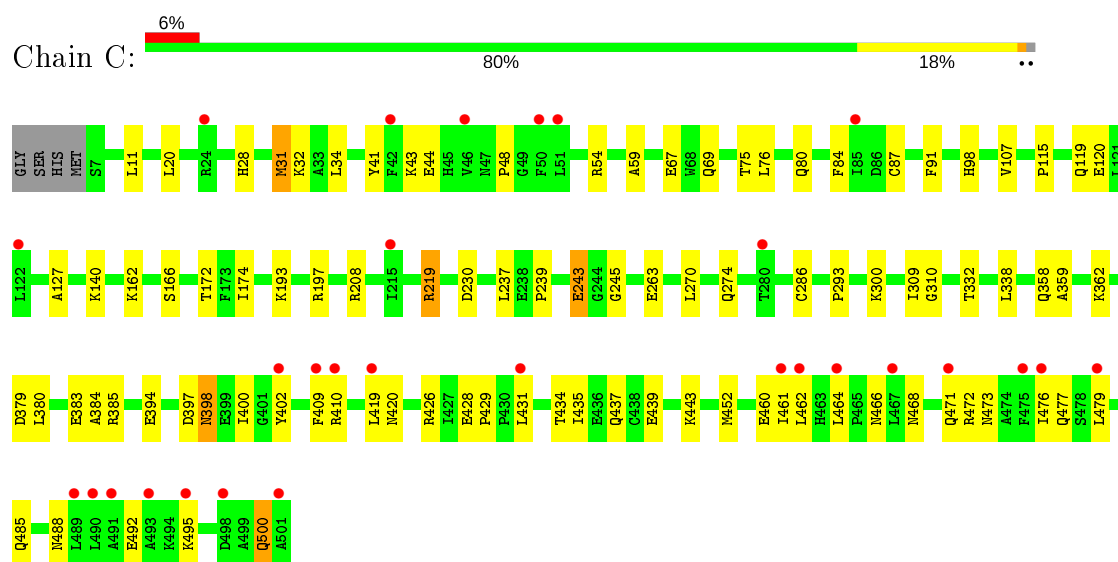
- Molecule 1: Putrescine aminotransferase,Immunoglobulin G-binding protein A



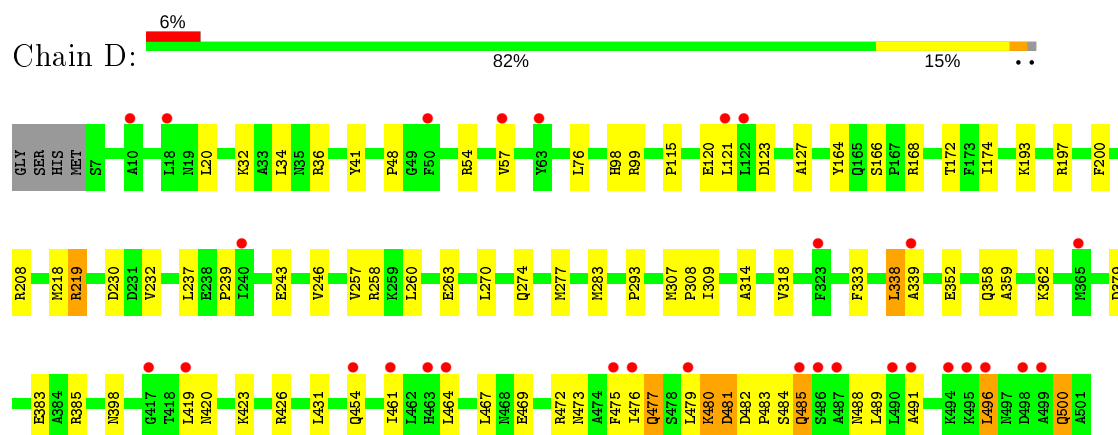
- Molecule 1: Putrescine aminotransferase,Immunoglobulin G-binding protein A



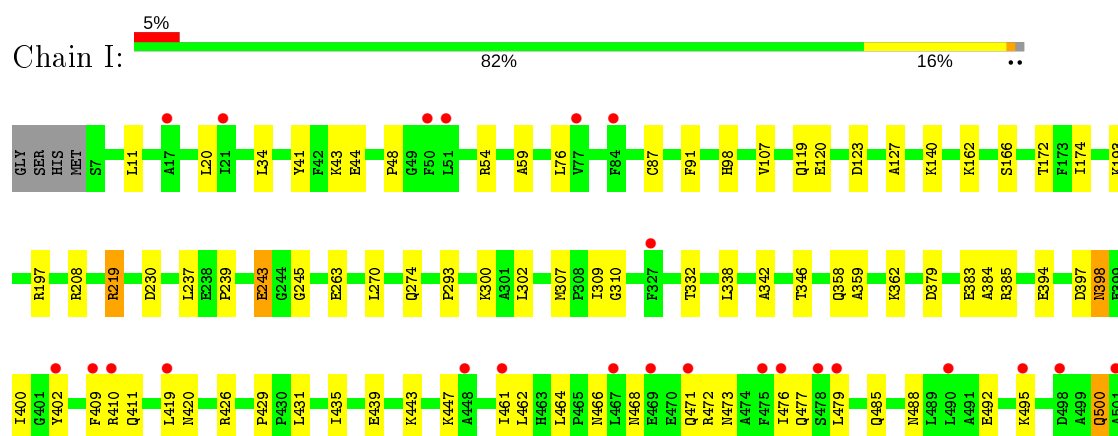
- Molecule 1: Putrescine aminotransferase,Immunoglobulin G-binding protein A



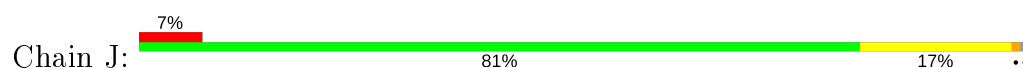
- Molecule 1: Putrescine aminotransferase,Immunoglobulin G-binding protein A

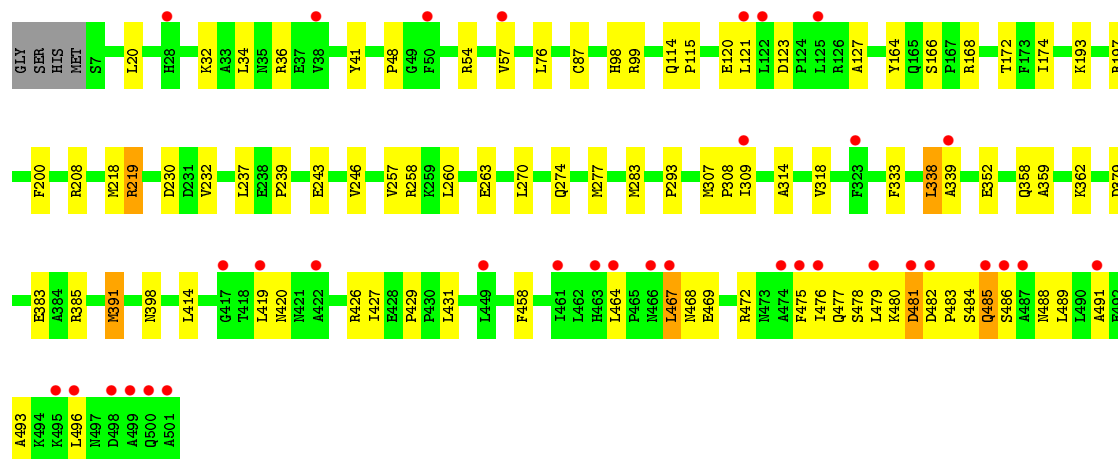


- Molecule 1: Putrescine aminotransferase,Immunoglobulin G-binding protein A

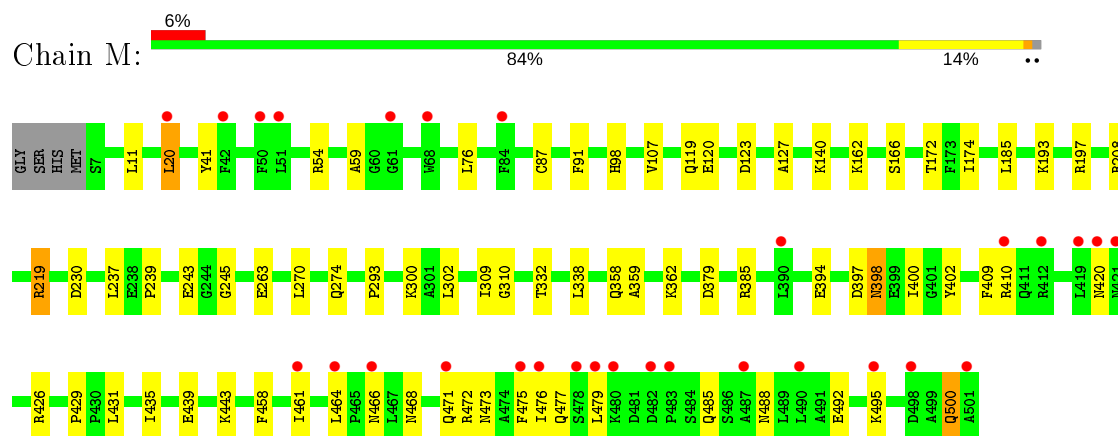


- Molecule 1: Putrescine aminotransferase,Immunoglobulin G-binding protein A

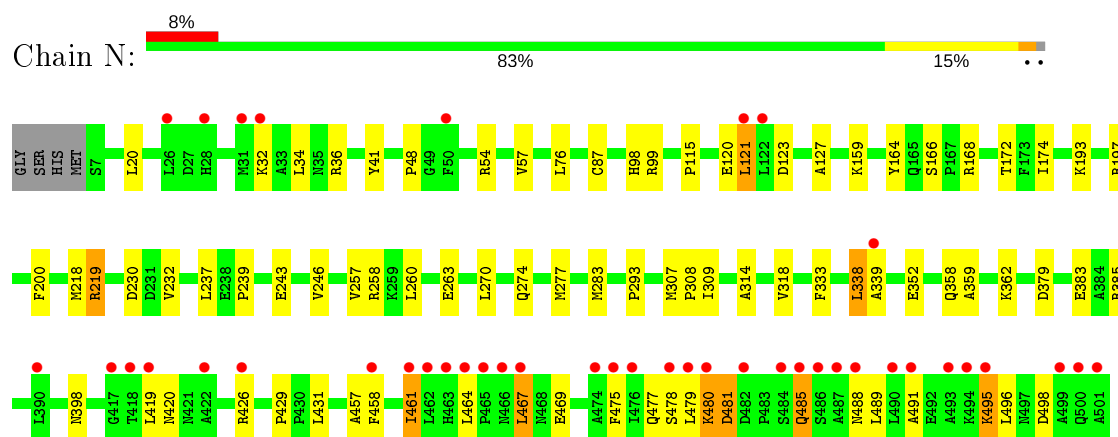




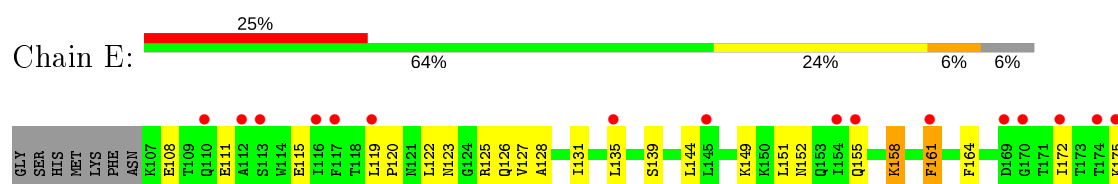
- Molecule 1: Putrescine aminotransferase,Immunoglobulin G-binding protein A

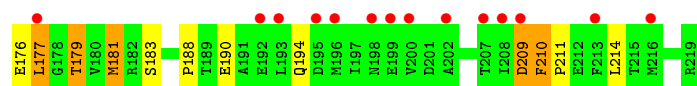


- Molecule 1: Putrescine aminotransferase,Immunoglobulin G-binding protein A

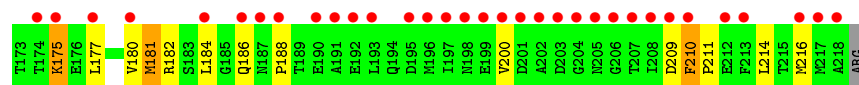
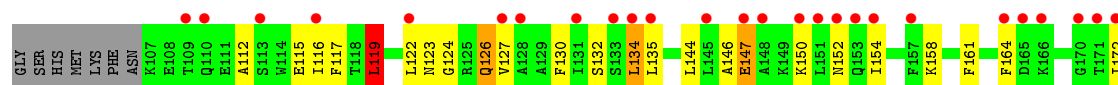


- Molecule 2: Zpa963,Calmodulin

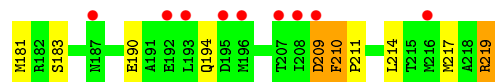
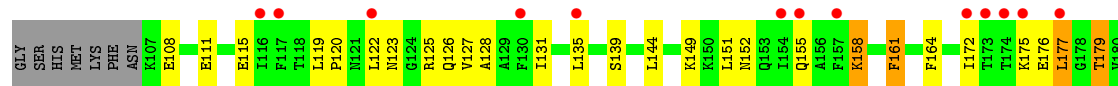




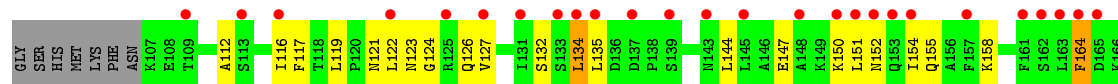
• Molecule 2: Zpa963,Calmodulin



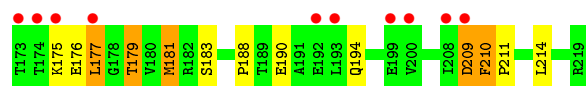
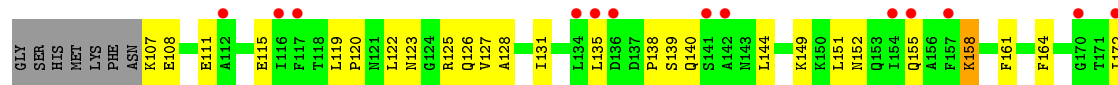
• Molecule 2: Zpa963,Calmodulin



• Molecule 2: Zpa963,Calmodulin

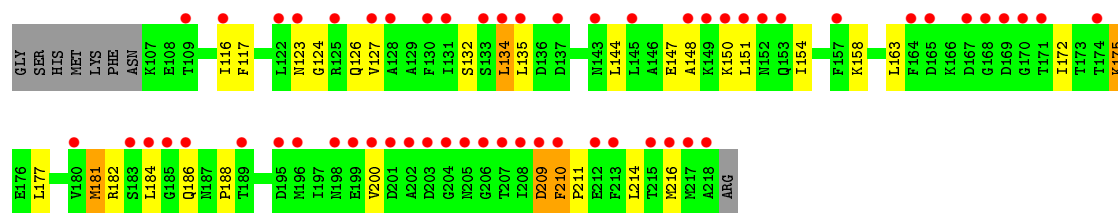


• Molecule 2: Zpa963,Calmodulin

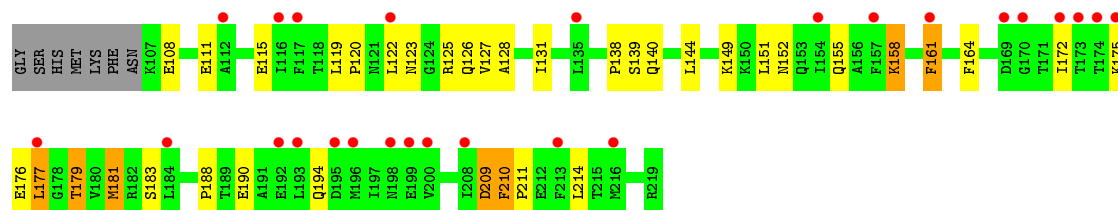


• Molecule 2: Zpa963,Calmodulin

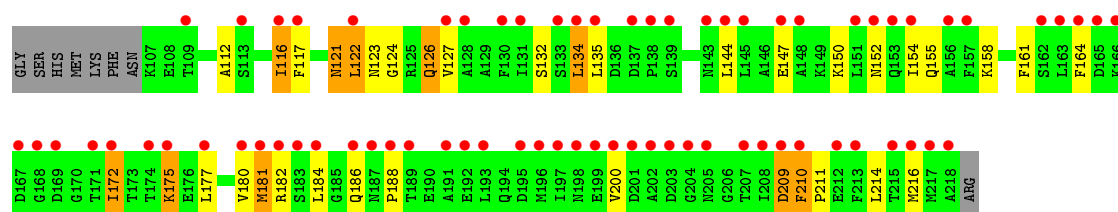




● Molecule 2: Zpa963,Calmodulin



● Molecule 2: Zpa963,Calmodulin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	79.49 Å 155.38 Å 155.49 Å 84.84° 89.68° 89.56°	Depositor
Resolution (Å)	50.00 – 2.57 47.70 – 2.57	Depositor EDS
% Data completeness (in resolution range)	89.5 (50.00-2.57) 89.4 (47.70-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.58 Å)	Xtriage
Refinement program	REFMAC 5.8.0155	Depositor
R, R_{free}	0.204 , 0.241 0.204 , 0.242	Depositor DCC
R_{free} test set	21075 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.014	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.397 for h,-k,-l 0.387 for -h,l,k 0.439 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	37132	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.43	0/3845	0.52	0/5203
1	B	0.47	0/3845	0.57	0/5203
1	C	0.45	1/3845 (0.0%)	0.54	1/5203 (0.0%)
1	D	0.47	0/3845	0.56	0/5203
1	I	0.44	0/3845	0.54	0/5203
1	J	0.46	0/3845	0.57	0/5203
1	M	0.44	0/3845	0.53	1/5203 (0.0%)
1	N	0.47	0/3845	0.56	0/5203
2	E	0.58	0/884	0.69	0/1194
2	F	0.66	0/869	0.86	3/1175 (0.3%)
2	G	0.58	0/884	0.68	0/1194
2	H	0.65	0/869	0.82	1/1175 (0.1%)
2	K	0.57	0/884	0.69	0/1194
2	L	0.63	0/869	0.84	2/1175 (0.2%)
2	O	0.57	0/884	0.70	0/1194
2	P	0.63	0/869	0.84	1/1175 (0.1%)
All	All	0.49	1/37772 (0.0%)	0.60	9/51100 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	460	GLU	CD-OE2	5.33	1.31	1.25

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	31	MET	CG-SD-CE	-7.73	87.83	100.20
2	F	119	LEU	CB-CG-CD2	5.82	120.89	111.00
2	P	184	LEU	CA-CB-CG	5.53	128.01	115.30
2	L	163	LEU	CB-CG-CD1	5.52	120.38	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	184	LEU	CA-CB-CG	5.51	127.97	115.30
2	H	184	LEU	CA-CB-CG	5.46	127.86	115.30
2	F	184	LEU	CA-CB-CG	5.38	127.68	115.30
2	F	122	LEU	CA-CB-CG	5.18	127.22	115.30
1	M	20	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3775	0	3801	61	0
1	B	3775	0	3801	60	0
1	C	3775	0	3801	65	0
1	D	3775	0	3801	63	0
1	I	3775	0	3801	58	0
1	J	3775	0	3801	61	0
1	M	3775	0	3801	54	0
1	N	3775	0	3801	56	0
2	E	872	0	846	32	0
2	F	857	0	829	35	0
2	G	872	0	846	32	0
2	H	857	0	829	31	0
2	K	872	0	846	32	0
2	L	857	0	829	23	0
2	O	872	0	846	34	0
2	P	857	0	829	34	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
3	G	2	0	0	0	0
3	H	2	0	0	0	0
3	K	2	0	0	0	0
3	L	2	0	0	0	0
3	O	2	0	0	0	0
3	P	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	37132	0	37108	660	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 9.

All (660) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:ILE:HD11	1:A:475:PHE:HB3	1.28	1.14
1:M:461:ILE:HD11	1:M:475:PHE:HB3	1.30	1.12
1:D:485:GLN:HB2	1:D:489:LEU:HG	1.30	1.11
1:B:461:ILE:HD11	1:B:475:PHE:HB3	1.26	1.08
1:N:485:GLN:HB2	1:N:489:LEU:HG	1.35	1.07
2:F:175:LYS:HE2	2:F:175:LYS:H	1.22	1.04
1:C:274:GLN:HE22	1:C:426:ARG:HH21	1.05	0.95
2:O:161:PHE:HE2	2:O:210:PHE:HA	1.34	0.92
2:E:158:LYS:HG2	2:E:210:PHE:HZ	1.35	0.92
2:O:161:PHE:CE2	2:O:210:PHE:HA	2.05	0.92
2:E:161:PHE:CE2	2:E:210:PHE:HA	2.05	0.91
2:O:158:LYS:HG2	2:O:210:PHE:HZ	1.35	0.90
2:G:158:LYS:HG2	2:G:210:PHE:HZ	1.36	0.90
1:M:245:GLY:O	1:M:385:ARG:NH1	2.05	0.90
1:C:245:GLY:O	1:C:385:ARG:NH1	2.05	0.90
1:I:245:GLY:O	1:I:385:ARG:NH1	2.05	0.90
1:A:245:GLY:O	1:A:385:ARG:NH1	2.05	0.89
2:K:158:LYS:HG2	2:K:210:PHE:HZ	1.36	0.89
2:G:161:PHE:CE2	2:G:210:PHE:HA	2.12	0.84
2:E:161:PHE:HE2	2:E:210:PHE:HA	1.39	0.83
1:B:481:ASP:N	1:B:481:ASP:OD1	2.13	0.82
1:C:274:GLN:HE22	1:C:426:ARG:NH2	1.77	0.82
1:I:274:GLN:OE1	1:I:426:ARG:NH2	2.13	0.81
1:M:274:GLN:OE1	1:M:426:ARG:NH2	2.17	0.78
1:J:485:GLN:O	1:J:489:LEU:HB2	1.82	0.78
1:I:243:GLU:OE1	1:I:426:ARG:NH1	2.17	0.77
1:A:274:GLN:OE1	1:A:426:ARG:NH2	2.17	0.77
1:M:119:GLN:NE2	1:M:332:THR:O	2.17	0.77
1:I:119:GLN:NE2	1:I:332:THR:O	2.17	0.77
2:L:175:LYS:H	2:L:175:LYS:HE2	1.48	0.77
2:H:175:LYS:HE2	2:H:175:LYS:H	1.50	0.76
1:A:119:GLN:NE2	1:A:332:THR:O	2.16	0.76
1:N:481:ASP:OD1	1:N:481:ASP:N	2.18	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:175:LYS:HE2	2:F:175:LYS:N	2.00	0.75
1:C:243:GLU:OE1	1:C:426:ARG:NH1	2.16	0.74
1:C:119:GLN:NE2	1:C:332:THR:O	2.17	0.74
1:I:59:ALA:HB2	1:I:410:ARG:HH21	1.53	0.73
1:M:59:ALA:HB2	1:M:410:ARG:HH21	1.53	0.73
2:P:123:ASN:H	2:P:126:GLN:HE21	1.37	0.73
1:C:31:MET:CE	1:C:80:GLN:HG2	2.18	0.73
2:G:211:PRO:O	2:G:214:LEU:N	2.21	0.72
1:A:59:ALA:HB2	1:A:410:ARG:HH21	1.53	0.72
2:P:134:LEU:HG	2:P:144:LEU:HD23	1.70	0.72
1:C:59:ALA:HB2	1:C:410:ARG:HH21	1.53	0.72
2:O:158:LYS:HG2	2:O:210:PHE:CZ	2.24	0.71
2:K:211:PRO:O	2:K:214:LEU:N	2.23	0.71
1:J:458:PHE:HB2	1:J:479:LEU:HD21	1.70	0.71
2:L:134:LEU:HG	2:L:144:LEU:HD23	1.70	0.71
2:G:158:LYS:HG2	2:G:210:PHE:CZ	2.25	0.71
1:M:464:LEU:O	1:M:472:ARG:NH2	2.24	0.71
1:I:464:LEU:O	1:I:472:ARG:NH2	2.24	0.70
2:K:158:LYS:HG2	2:K:210:PHE:CZ	2.24	0.70
1:A:464:LEU:O	1:A:472:ARG:NH2	2.24	0.70
1:I:342:ALA:O	1:I:346:THR:HG23	1.92	0.70
1:M:492:GLU:HA	1:M:495:LYS:HE3	1.74	0.70
1:C:464:LEU:O	1:C:472:ARG:NH2	2.24	0.70
1:C:492:GLU:HA	1:C:495:LYS:HE3	1.73	0.70
1:I:492:GLU:HA	1:I:495:LYS:HE3	1.74	0.70
2:K:123:ASN:OD1	2:K:126:GLN:NE2	2.24	0.70
2:P:211:PRO:O	2:P:214:LEU:N	2.24	0.70
1:A:342:ALA:O	1:A:346:THR:HG23	1.92	0.70
2:H:211:PRO:O	2:H:214:LEU:N	2.25	0.69
2:G:123:ASN:OD1	2:G:126:GLN:NE2	2.24	0.69
1:D:461:ILE:HD11	1:D:475:PHE:CG	2.26	0.69
2:H:117:PHE:HA	2:H:127:VAL:HG21	1.73	0.69
2:O:123:ASN:OD1	2:O:126:GLN:NE2	2.24	0.69
2:O:211:PRO:O	2:O:214:LEU:N	2.25	0.69
1:C:31:MET:HE3	1:C:80:GLN:HG2	1.73	0.69
2:F:211:PRO:O	2:F:214:LEU:N	2.26	0.69
1:A:492:GLU:HA	1:A:495:LYS:HE3	1.74	0.69
2:E:123:ASN:OD1	2:E:126:GLN:NE2	2.24	0.69
2:L:211:PRO:O	2:L:214:LEU:N	2.25	0.69
2:E:211:PRO:O	2:E:214:LEU:N	2.26	0.68
1:A:59:ALA:HB3	1:A:410:ARG:HE	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:117:PHE:HA	2:L:127:VAL:HG21	1.76	0.68
1:C:59:ALA:HB3	1:C:410:ARG:HE	1.59	0.67
1:B:461:ILE:HD11	1:B:475:PHE:CB	2.16	0.67
1:J:218:MET:HE3	1:J:257:VAL:HG13	1.76	0.67
1:I:59:ALA:HB3	1:I:410:ARG:HE	1.58	0.67
1:M:59:ALA:HB3	1:M:410:ARG:HE	1.58	0.67
2:P:123:ASN:OD1	2:P:126:GLN:NE2	2.28	0.66
2:F:134:LEU:HG	2:F:144:LEU:HD23	1.77	0.66
2:P:117:PHE:HA	2:P:127:VAL:HG21	1.78	0.65
2:F:200:VAL:HG21	2:F:216:MET:HG3	1.78	0.65
2:H:164:PHE:CD2	2:H:172:ILE:HD13	2.32	0.65
1:C:385:ARG:NH2	1:C:394:GLU:OE1	2.29	0.65
2:H:200:VAL:HG21	2:H:216:MET:HG3	1.78	0.65
1:A:385:ARG:NH2	1:A:394:GLU:OE1	2.29	0.65
1:C:28:HIS:O	1:C:31:MET:HG3	1.96	0.65
2:P:200:VAL:HG21	2:P:216:MET:HG3	1.79	0.64
2:L:200:VAL:HG21	2:L:216:MET:HG3	1.78	0.64
1:D:485:GLN:HB2	1:D:489:LEU:CG	2.18	0.64
1:I:385:ARG:NH2	1:I:394:GLU:OE1	2.29	0.64
1:I:409:PHE:HE1	1:J:121:LEU:HD11	1.63	0.64
1:M:385:ARG:NH2	1:M:394:GLU:OE1	2.30	0.64
1:B:218:MET:HE3	1:B:257:VAL:HG13	1.80	0.64
1:D:218:MET:HE1	1:D:257:VAL:HG13	1.80	0.64
1:N:457:ALA:O	1:N:461:ILE:HG22	1.98	0.64
2:H:121:ASN:OD1	2:H:152:ASN:ND2	2.29	0.64
1:C:409:PHE:HE1	1:D:121:LEU:HD21	1.62	0.63
2:E:158:LYS:HG2	2:E:210:PHE:CZ	2.24	0.63
1:J:258:ARG:HH21	1:J:293:PRO:HA	1.63	0.63
1:N:115:PRO:HA	1:N:338:LEU:HD13	1.80	0.63
1:N:485:GLN:HB2	1:N:489:LEU:CG	2.20	0.63
1:A:435:ILE:H	1:A:435:ILE:HD12	1.64	0.62
1:D:258:ARG:HH21	1:D:293:PRO:HA	1.64	0.62
1:N:258:ARG:HH21	1:N:293:PRO:HA	1.64	0.62
1:B:258:ARG:HH21	1:B:293:PRO:HA	1.64	0.62
2:F:117:PHE:HA	2:F:127:VAL:HG21	1.80	0.62
2:H:122:LEU:HD21	2:H:151:LEU:HD23	1.81	0.62
1:B:481:ASP:CG	2:F:124:GLY:H	2.03	0.62
1:C:435:ILE:HD12	1:C:435:ILE:H	1.65	0.62
2:F:164:PHE:HD2	2:F:172:ILE:HD12	1.64	0.62
1:I:485:GLN:OE1	1:I:488:ASN:ND2	2.32	0.62
1:M:485:GLN:OE1	1:M:488:ASN:ND2	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:477:GLN:HA	2:F:124:GLY:HA3	1.81	0.61
1:I:435:ILE:H	1:I:435:ILE:HD12	1.66	0.61
1:M:398:ASN:OD1	1:M:398:ASN:N	2.33	0.61
2:P:175:LYS:HE2	2:P:175:LYS:H	1.65	0.61
1:C:398:ASN:OD1	1:C:398:ASN:N	2.33	0.61
1:N:218:MET:HE3	1:N:257:VAL:HG13	1.83	0.60
1:A:127:ALA:HB1	1:B:41:TYR:HB2	1.83	0.60
1:A:398:ASN:N	1:A:398:ASN:OD1	2.33	0.60
2:H:112:ALA:O	2:H:116:ILE:HG12	2.01	0.60
2:G:190:GLU:OE1	2:G:194:GLN:NE2	2.34	0.60
1:I:398:ASN:OD1	1:I:398:ASN:N	2.33	0.60
1:M:435:ILE:H	1:M:435:ILE:HD12	1.67	0.60
1:N:477:GLN:HA	2:P:124:GLY:HA3	1.84	0.60
1:C:127:ALA:HB1	1:D:41:TYR:HB2	1.83	0.60
2:E:190:GLU:OE1	2:E:194:GLN:NE2	2.34	0.60
1:B:309:ILE:HD12	1:B:339:ALA:HB1	1.84	0.60
2:H:150:LYS:O	2:H:154:ILE:HD12	2.02	0.60
2:O:190:GLU:OE1	2:O:194:GLN:NE2	2.34	0.60
1:C:485:GLN:OE1	1:C:488:ASN:ND2	2.32	0.60
1:D:309:ILE:HD12	1:D:339:ALA:HB1	1.84	0.60
1:M:54:ARG:HD3	1:N:120:GLU:O	2.02	0.59
1:I:127:ALA:HB1	1:J:41:TYR:HB2	1.82	0.59
1:B:464:LEU:O	1:B:472:ARG:NH2	2.34	0.59
2:G:161:PHE:HE2	2:G:210:PHE:HA	1.62	0.59
1:A:54:ARG:HD3	1:B:120:GLU:O	2.02	0.59
1:M:107:VAL:HG13	1:M:338:LEU:HD22	1.84	0.59
1:A:107:VAL:HG13	1:A:338:LEU:HD22	1.84	0.59
1:A:485:GLN:OE1	1:A:488:ASN:ND2	2.33	0.59
2:H:158:LYS:HG2	2:H:210:PHE:CE2	2.37	0.59
1:C:107:VAL:HG13	1:C:338:LEU:HD22	1.84	0.59
2:E:126:GLN:HE22	2:E:155:GLN:HE22	1.51	0.59
1:D:496:LEU:O	1:D:500:GLN:HG2	2.03	0.59
2:E:123:ASN:H	2:E:126:GLN:HE21	1.51	0.59
2:P:158:LYS:HG2	2:P:210:PHE:CE2	2.37	0.59
2:G:123:ASN:H	2:G:126:GLN:HE21	1.51	0.59
1:I:107:VAL:HG13	1:I:338:LEU:HD22	1.84	0.59
1:J:481:ASP:OD1	1:J:481:ASP:N	2.33	0.59
2:G:126:GLN:HE22	2:G:155:GLN:HE22	1.51	0.58
1:D:461:ILE:CD1	1:D:475:PHE:HB3	2.33	0.58
1:J:309:ILE:HD12	1:J:339:ALA:HB1	1.84	0.58
1:N:309:ILE:HD12	1:N:339:ALA:HB1	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:MET:HG3	1:C:32:LYS:N	2.18	0.58
1:C:274:GLN:NE2	1:C:428:GLU:OE2	2.37	0.58
2:F:115:GLU:O	2:F:119:LEU:HD23	2.03	0.58
1:N:458:PHE:HB2	1:N:479:LEU:HD21	1.86	0.58
1:B:485:GLN:HB2	1:B:489:LEU:HD23	1.85	0.57
2:O:126:GLN:HE22	2:O:155:GLN:HE22	1.51	0.57
1:B:32:LYS:HE2	1:B:36:ARG:HH11	1.69	0.57
1:D:32:LYS:HE2	1:D:36:ARG:HH11	1.70	0.57
2:K:126:GLN:HE22	2:K:155:GLN:HE22	1.51	0.57
1:D:464:LEU:O	1:D:472:ARG:NH2	2.38	0.57
1:C:41:TYR:HB2	1:D:127:ALA:HB1	1.87	0.57
1:N:32:LYS:HE2	1:N:36:ARG:HH11	1.69	0.57
2:O:123:ASN:H	2:O:126:GLN:HE21	1.51	0.57
2:H:134:LEU:HG	2:H:144:LEU:HD23	1.85	0.57
1:J:464:LEU:O	1:J:472:ARG:NH2	2.38	0.57
1:A:409:PHE:HE1	1:B:121:LEU:HD11	1.68	0.57
1:I:359:ALA:HB2	1:I:431:LEU:HG	1.87	0.57
1:I:54:ARG:HD3	1:J:120:GLU:O	2.04	0.57
2:K:123:ASN:H	2:K:126:GLN:HE21	1.51	0.57
1:C:466:ASN:ND2	1:C:500:GLN:O	2.38	0.56
2:E:172:ILE:HG21	2:E:177:LEU:HD13	1.87	0.56
1:I:243:GLU:HG3	1:I:419:LEU:HB2	1.87	0.56
1:J:477:GLN:HA	2:L:124:GLY:HA3	1.86	0.56
1:A:466:ASN:ND2	1:A:500:GLN:O	2.38	0.56
2:G:126:GLN:OE1	2:G:155:GLN:NE2	2.38	0.56
2:O:172:ILE:HG21	2:O:177:LEU:HD13	1.87	0.56
1:I:466:ASN:HD21	1:I:500:GLN:HB2	1.70	0.56
1:I:466:ASN:ND2	1:I:500:GLN:O	2.39	0.56
2:K:126:GLN:OE1	2:K:155:GLN:NE2	2.38	0.56
1:M:466:ASN:ND2	1:M:500:GLN:O	2.39	0.56
1:A:120:GLU:O	1:B:54:ARG:HD2	2.05	0.56
1:C:243:GLU:HG3	1:C:419:LEU:HB2	1.88	0.56
2:E:126:GLN:OE1	2:E:155:GLN:NE2	2.39	0.56
1:J:32:LYS:HE2	1:J:36:ARG:HH11	1.70	0.56
2:L:150:LYS:O	2:L:154:ILE:HD12	2.04	0.56
1:M:127:ALA:HB1	1:N:41:TYR:HB2	1.86	0.56
1:M:466:ASN:HD21	1:M:500:GLN:HB2	1.71	0.56
1:I:41:TYR:HB2	1:J:127:ALA:HB1	1.87	0.56
2:O:126:GLN:OE1	2:O:155:GLN:NE2	2.39	0.56
2:P:150:LYS:O	2:P:154:ILE:HD12	2.06	0.56
1:C:54:ARG:HD3	1:D:120:GLU:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:TYR:HB2	1:B:127:ALA:HB1	1.88	0.56
1:D:472:ARG:O	1:D:475:PHE:N	2.39	0.55
1:A:466:ASN:HD21	1:A:500:GLN:HB2	1.71	0.55
1:C:466:ASN:HD21	1:C:500:GLN:HB2	1.71	0.55
2:F:126:GLN:O	2:F:130:PHE:HD1	1.90	0.55
2:F:150:LYS:O	2:F:154:ILE:HD12	2.05	0.55
1:D:461:ILE:HD11	1:D:475:PHE:HB3	1.87	0.55
1:D:461:ILE:HD11	1:D:475:PHE:CB	2.36	0.55
1:B:274:GLN:HE22	1:B:426:ARG:NH2	2.05	0.55
1:B:208:ARG:NH1	1:C:208:ARG:HD3	2.22	0.54
2:H:172:ILE:HG21	2:H:177:LEU:HD23	1.89	0.54
1:N:274:GLN:HE22	1:N:426:ARG:NH2	2.06	0.54
2:P:116:ILE:HD12	2:P:134:LEU:HD11	1.88	0.54
1:J:208:ARG:NH1	1:M:208:ARG:HD3	2.23	0.54
1:D:274:GLN:HE22	1:D:426:ARG:NH2	2.06	0.54
1:M:120:GLU:O	1:N:54:ARG:HD2	2.08	0.54
1:M:41:TYR:HB2	1:N:127:ALA:HB1	1.88	0.54
2:P:161:PHE:CZ	2:P:172:ILE:HG13	2.42	0.54
1:B:461:ILE:CD1	1:B:475:PHE:HB3	2.19	0.54
2:G:108:GLU:N	2:G:108:GLU:OE1	2.41	0.54
2:G:161:PHE:CZ	2:G:210:PHE:HA	2.42	0.54
2:O:108:GLU:N	2:O:108:GLU:OE1	2.41	0.54
1:B:480:LYS:HE2	2:F:117:PHE:O	2.07	0.54
2:G:172:ILE:HG21	2:G:177:LEU:HD13	1.90	0.54
2:K:108:GLU:OE1	2:K:108:GLU:N	2.41	0.54
1:J:274:GLN:HE22	1:J:426:ARG:NH2	2.06	0.54
1:D:383:GLU:OE2	1:D:385:ARG:NH1	2.42	0.53
1:A:174:ILE:HD13	1:A:208:ARG:HB2	1.91	0.53
2:E:108:GLU:N	2:E:108:GLU:OE1	2.41	0.53
1:C:174:ILE:HD13	1:C:208:ARG:HB2	1.91	0.53
2:K:126:GLN:NE2	2:K:155:GLN:HE22	2.06	0.53
2:G:126:GLN:NE2	2:G:155:GLN:HE22	2.06	0.53
1:I:174:ILE:HD13	1:I:208:ARG:HB2	1.90	0.53
2:O:126:GLN:NE2	2:O:155:GLN:HE22	2.06	0.53
1:B:383:GLU:OE2	1:B:385:ARG:NH1	2.42	0.53
1:I:473:ASN:O	1:I:477:GLN:HB2	2.08	0.53
1:B:464:LEU:HB2	1:B:467:LEU:HD21	1.89	0.53
1:J:379:ASP:OD1	1:J:379:ASP:N	2.41	0.53
2:L:158:LYS:HG2	2:L:210:PHE:CZ	2.44	0.53
1:N:379:ASP:N	1:N:379:ASP:OD1	2.41	0.53
2:F:146:ALA:O	2:F:150:LYS:HG3	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:209:ASP:OD1	2:L:209:ASP:N	2.40	0.53
1:I:120:GLU:O	1:J:54:ARG:HD2	2.10	0.52
1:M:174:ILE:HD13	1:M:208:ARG:HB2	1.91	0.52
2:F:177:LEU:HB3	2:F:181:MET:HE2	1.91	0.52
1:C:120:GLU:O	1:D:54:ARG:HD2	2.08	0.52
2:E:126:GLN:NE2	2:E:155:GLN:HE22	2.06	0.52
1:C:439:GLU:O	1:C:443:LYS:HG3	2.10	0.52
1:A:208:ARG:HD3	1:D:208:ARG:NH1	2.24	0.52
1:C:473:ASN:O	1:C:477:GLN:HB2	2.09	0.52
2:E:120:PRO:HD2	2:E:152:ASN:HD21	1.75	0.52
1:J:391:MET:HG3	1:J:427:ILE:HB	1.92	0.52
2:K:172:ILE:HG21	2:K:177:LEU:HD13	1.91	0.52
1:C:31:MET:HE1	1:C:80:GLN:HG2	1.92	0.51
2:G:120:PRO:HD2	2:G:152:ASN:HD21	1.75	0.51
2:K:120:PRO:HD2	2:K:152:ASN:HD21	1.75	0.51
1:N:218:MET:HE2	1:N:260:LEU:HD23	1.91	0.51
1:C:359:ALA:HB2	1:C:431:LEU:HG	1.91	0.51
2:L:182:ARG:HA	2:L:186:GLN:O	2.11	0.51
2:L:177:LEU:HB3	2:L:181:MET:CE	2.40	0.51
2:P:182:ARG:HA	2:P:186:GLN:O	2.11	0.51
1:A:439:GLU:O	1:A:443:LYS:HG3	2.11	0.51
1:C:397:ASP:OD1	1:C:400:ILE:N	2.36	0.51
2:H:151:LEU:O	2:H:155:GLN:HG2	2.10	0.51
1:M:439:GLU:O	1:M:443:LYS:HG3	2.10	0.51
2:O:120:PRO:HD2	2:O:152:ASN:HD21	1.75	0.51
2:P:177:LEU:HB3	2:P:181:MET:CE	2.40	0.51
2:F:177:LEU:HB3	2:F:181:MET:CE	2.40	0.51
1:I:439:GLU:O	1:I:443:LYS:HG3	2.11	0.51
2:H:182:ARG:HA	2:H:186:GLN:O	2.11	0.51
1:J:277:MET:HA	1:J:283:MET:HE3	1.91	0.51
2:K:161:PHE:CE2	2:K:210:PHE:HA	2.46	0.51
1:A:359:ALA:HB2	1:A:431:LEU:HG	1.92	0.51
1:C:409:PHE:CE1	1:D:121:LEU:HD21	2.45	0.51
2:O:127:VAL:O	2:O:131:ILE:HG12	2.11	0.51
2:H:177:LEU:HB3	2:H:181:MET:CE	2.41	0.50
2:G:127:VAL:O	2:G:131:ILE:HG12	2.11	0.50
1:J:383:GLU:OE2	1:J:385:ARG:NH1	2.41	0.50
2:K:127:VAL:O	2:K:131:ILE:HG12	2.11	0.50
2:L:181:MET:HB2	2:L:188:PRO:HG3	1.94	0.50
1:C:434:THR:HG22	1:C:437:GLN:HG3	1.94	0.50
1:J:164:TYR:O	1:J:168:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:ASP:OD1	1:A:400:ILE:N	2.36	0.50
2:H:181:MET:HB2	2:H:188:PRO:HG3	1.94	0.50
1:M:473:ASN:O	1:M:477:GLN:HB2	2.11	0.50
1:N:383:GLU:OE2	1:N:385:ARG:NH1	2.42	0.50
1:A:473:ASN:O	1:A:477:GLN:HB2	2.11	0.50
1:D:172:THR:HG21	1:D:230:ASP:HB3	1.93	0.50
1:J:486:SER:O	1:J:489:LEU:HB3	2.11	0.50
1:N:164:TYR:O	1:N:168:ARG:NH1	2.45	0.50
2:P:181:MET:HB2	2:P:188:PRO:HG3	1.94	0.50
1:A:434:THR:HG22	1:A:437:GLN:HG3	1.94	0.50
1:J:464:LEU:HB2	1:J:467:LEU:HD21	1.94	0.50
1:D:218:MET:HE3	1:D:260:LEU:HD23	1.93	0.50
2:H:123:ASN:OD1	2:H:126:GLN:NE2	2.45	0.50
2:L:158:LYS:HE2	2:L:210:PHE:CZ	2.47	0.50
2:F:182:ARG:HA	2:F:186:GLN:O	2.11	0.49
2:E:122:LEU:HD23	2:E:155:GLN:OE1	2.12	0.49
2:G:122:LEU:HD23	2:G:155:GLN:OE1	2.12	0.49
2:O:158:LYS:HE3	2:O:210:PHE:CE1	2.47	0.49
2:E:127:VAL:O	2:E:131:ILE:HG12	2.11	0.49
2:F:181:MET:HB2	2:F:188:PRO:HG3	1.94	0.49
2:E:111:GLU:O	2:E:115:GLU:HG2	2.13	0.49
2:G:111:GLU:O	2:G:115:GLU:HG2	2.13	0.49
2:O:122:LEU:HD23	2:O:155:GLN:OE1	2.12	0.49
2:E:119:LEU:HD22	2:E:152:ASN:HD22	1.76	0.49
2:E:158:LYS:HE3	2:E:210:PHE:CE1	2.47	0.49
2:O:119:LEU:HD22	2:O:152:ASN:HD22	1.77	0.49
1:B:164:TYR:O	1:B:168:ARG:NH1	2.45	0.49
1:C:20:LEU:HD11	1:C:34:LEU:HD22	1.94	0.49
2:K:122:LEU:HD23	2:K:155:GLN:OE1	2.12	0.49
1:A:468:ASN:H	1:A:471:GLN:HE22	1.60	0.49
1:D:164:TYR:O	1:D:168:ARG:NH1	2.45	0.49
1:I:193:LYS:HD2	1:I:420:ASN:HA	1.95	0.49
1:I:300:LYS:HA	1:J:333:PHE:CZ	2.47	0.49
2:P:121:ASN:H	2:P:152:ASN:HD21	1.59	0.49
1:B:218:MET:HE2	1:B:260:LEU:HD23	1.93	0.49
1:M:11:LEU:HD11	1:N:352:GLU:HG3	1.95	0.49
2:L:172:ILE:CG2	2:L:177:LEU:HD23	2.43	0.49
1:M:193:LYS:HD2	1:M:420:ASN:HA	1.95	0.49
1:B:172:THR:HG21	1:B:230:ASP:HB3	1.95	0.48
2:F:164:PHE:CD1	2:F:180:VAL:HG21	2.48	0.48
2:G:119:LEU:HD22	2:G:152:ASN:HD22	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:172:THR:HG21	1:J:230:ASP:HB3	1.94	0.48
2:K:111:GLU:O	2:K:115:GLU:HG2	2.12	0.48
2:K:119:LEU:HD22	2:K:152:ASN:HD22	1.77	0.48
1:A:193:LYS:HD2	1:A:420:ASN:HA	1.96	0.48
1:D:454:GLN:HG3	1:D:479:LEU:HD21	1.95	0.48
2:F:164:PHE:HD2	2:F:172:ILE:CD1	2.26	0.48
1:N:172:THR:HG21	1:N:230:ASP:HB3	1.95	0.48
2:O:111:GLU:O	2:O:115:GLU:HG2	2.13	0.48
1:A:476:ILE:HD11	2:E:128:ALA:HA	1.95	0.48
2:H:172:ILE:CG2	2:H:177:LEU:HD23	2.43	0.48
1:I:172:THR:HG21	1:I:230:ASP:HB3	1.95	0.48
2:O:209:ASP:N	2:O:209:ASP:OD1	2.40	0.48
2:F:172:ILE:CG2	2:F:177:LEU:HD23	2.44	0.48
1:C:468:ASN:H	1:C:471:GLN:HE22	1.60	0.48
1:B:20:LEU:HD11	1:B:34:LEU:HD13	1.96	0.48
1:B:230:ASP:OD1	1:C:197:ARG:NH2	2.47	0.48
1:I:309:ILE:HG13	1:I:310:GLY:N	2.28	0.48
1:M:172:THR:HG21	1:M:230:ASP:HB3	1.95	0.48
1:M:468:ASN:H	1:M:471:GLN:HE22	1.60	0.48
1:I:468:ASN:H	1:I:471:GLN:HE22	1.60	0.48
1:I:307:MET:CE	1:J:338:LEU:HD23	2.43	0.48
1:D:20:LEU:HD11	1:D:34:LEU:HD13	1.96	0.48
1:J:20:LEU:HD11	1:J:34:LEU:HD13	1.95	0.48
1:M:309:ILE:HG13	1:M:310:GLY:N	2.28	0.48
1:J:475:PHE:O	1:J:478:SER:OG	2.25	0.47
1:M:458:PHE:O	1:M:461:ILE:HG22	2.13	0.47
1:A:20:LEU:HD11	1:A:34:LEU:HD22	1.96	0.47
1:N:243:GLU:HG2	1:N:419:LEU:HB2	1.97	0.47
2:O:158:LYS:HE3	2:O:210:PHE:HE1	1.79	0.47
1:B:115:PRO:HA	1:B:338:LEU:HD13	1.96	0.47
1:C:193:LYS:HD2	1:C:420:ASN:HA	1.97	0.47
1:M:492:GLU:O	1:M:495:LYS:HB2	2.14	0.47
1:A:172:THR:HG21	1:A:230:ASP:HB3	1.95	0.47
1:C:309:ILE:HG13	1:C:310:GLY:N	2.28	0.47
2:H:177:LEU:HB3	2:H:181:MET:HE2	1.95	0.47
1:J:243:GLU:HG2	1:J:419:LEU:HB2	1.97	0.47
1:M:359:ALA:HB2	1:M:431:LEU:HG	1.96	0.47
1:N:20:LEU:HD11	1:N:34:LEU:HD13	1.96	0.47
1:D:473:ASN:O	1:D:477:GLN:HB3	2.15	0.47
1:D:243:GLU:HG2	1:D:419:LEU:HB2	1.97	0.47
1:C:172:THR:HG21	1:C:230:ASP:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:411:GLN:OE1	1:I:447:LYS:HE3	2.15	0.47
2:P:172:ILE:CG2	2:P:177:LEU:HD23	2.45	0.47
1:D:481:ASP:N	1:D:481:ASP:OD1	2.41	0.47
2:H:123:ASN:H	2:H:126:GLN:HE21	1.63	0.47
1:M:300:LYS:HA	1:N:333:PHE:CZ	2.49	0.47
1:N:219:ARG:NH2	1:N:263:GLU:OE2	2.47	0.47
1:A:162:LYS:HE3	1:B:200:PHE:O	2.15	0.47
1:A:309:ILE:HG13	1:A:310:GLY:N	2.29	0.47
1:C:162:LYS:HE3	1:D:200:PHE:O	2.15	0.47
1:D:479:LEU:HD22	2:H:117:PHE:CZ	2.49	0.47
1:D:473:ASN:ND2	2:H:132:SER:OG	2.42	0.47
2:K:209:ASP:OD1	2:K:209:ASP:N	2.40	0.47
1:A:492:GLU:O	1:A:495:LYS:HB2	2.16	0.46
1:C:379:ASP:N	1:C:379:ASP:OD1	2.41	0.46
1:C:492:GLU:O	1:C:495:LYS:HB2	2.16	0.46
1:N:277:MET:HA	1:N:283:MET:HE3	1.96	0.46
1:B:243:GLU:HG2	1:B:419:LEU:HB2	1.97	0.46
1:D:219:ARG:NH2	1:D:263:GLU:OE2	2.48	0.46
1:D:482:ASP:N	1:D:483:PRO:HD3	2.30	0.46
1:I:492:GLU:O	1:I:495:LYS:HB2	2.15	0.46
2:L:172:ILE:HG21	2:L:177:LEU:HD23	1.95	0.46
1:C:91:PHE:HD1	1:C:426:ARG:CZ	2.29	0.46
1:I:162:LYS:HE3	1:J:200:PHE:O	2.16	0.46
1:A:379:ASP:OD1	1:A:379:ASP:N	2.41	0.46
2:F:112:ALA:O	2:F:116:ILE:HG12	2.16	0.46
1:I:300:LYS:HA	1:J:333:PHE:HZ	1.81	0.46
1:N:461:ILE:CD1	1:N:475:PHE:HB3	2.46	0.46
1:A:358:GLN:HB3	1:A:362:LYS:HE3	1.98	0.46
1:B:488:ASN:O	1:B:491:ALA:HB3	2.15	0.46
1:M:358:GLN:HB3	1:M:362:LYS:HE3	1.98	0.46
1:N:480:LYS:HE3	2:P:117:PHE:O	2.16	0.46
1:A:270:LEU:HD12	1:A:293:PRO:HG3	1.98	0.46
1:I:397:ASP:OD1	1:I:400:ILE:N	2.36	0.46
1:A:411:GLN:OE1	1:A:447:LYS:HE3	2.16	0.46
1:C:300:LYS:HA	1:D:333:PHE:CZ	2.51	0.46
2:F:130:PHE:HE2	2:F:147:GLU:OE1	1.98	0.46
2:H:119:LEU:HB3	2:H:152:ASN:OD1	2.16	0.46
1:M:409:PHE:HE1	1:N:121:LEU:HD11	1.81	0.46
1:C:358:GLN:HB3	1:C:362:LYS:HE3	1.98	0.46
1:I:20:LEU:HD11	1:I:34:LEU:HD22	1.98	0.46
1:M:162:LYS:HE3	1:N:200:PHE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ARG:NH2	1:B:263:GLU:OE2	2.48	0.45
1:A:300:LYS:HA	1:B:333:PHE:CZ	2.51	0.45
2:E:161:PHE:CZ	2:E:210:PHE:HA	2.51	0.45
1:I:11:LEU:HD11	1:J:352:GLU:HG3	1.98	0.45
1:M:397:ASP:OD1	1:M:400:ILE:N	2.36	0.45
1:C:243:GLU:CG	1:C:419:LEU:HB2	2.46	0.45
2:G:219:ARG:HH11	2:G:219:ARG:HB3	1.81	0.45
1:I:243:GLU:CG	1:I:419:LEU:HB2	2.45	0.45
1:J:219:ARG:NH2	1:J:263:GLU:OE2	2.47	0.45
1:J:488:ASN:O	1:J:491:ALA:HB3	2.16	0.45
2:E:158:LYS:HE3	2:E:210:PHE:HE1	1.81	0.45
1:C:476:ILE:HD11	2:G:128:ALA:HA	1.99	0.45
2:H:172:ILE:HG21	2:H:177:LEU:CD2	2.46	0.45
1:A:307:MET:CE	1:B:338:LEU:HD23	2.47	0.45
1:B:461:ILE:HD13	1:B:476:ILE:HD13	1.98	0.45
1:C:270:LEU:HD12	1:C:293:PRO:HG3	1.98	0.45
2:F:116:ILE:HD13	2:F:134:LEU:HD13	1.98	0.45
1:I:358:GLN:HB3	1:I:362:LYS:HE3	1.98	0.45
2:K:123:ASN:H	2:K:126:GLN:NE2	2.15	0.45
1:A:183:LYS:HD2	1:B:330:THR:H	1.82	0.45
1:D:193:LYS:HD2	1:D:420:ASN:HA	1.98	0.45
2:G:209:ASP:OD1	2:G:209:ASP:N	2.40	0.45
1:J:193:LYS:HD2	1:J:420:ASN:HA	1.98	0.45
1:J:218:MET:HE2	1:J:260:LEU:HD23	1.98	0.45
2:O:123:ASN:H	2:O:126:GLN:NE2	2.15	0.45
2:P:126:GLN:HE22	2:P:155:GLN:HE21	1.65	0.45
1:A:11:LEU:HD11	1:B:352:GLU:HG3	1.97	0.45
2:E:190:GLU:O	2:E:194:GLN:HB2	2.17	0.45
2:F:123:ASN:ND2	2:F:126:GLN:OE1	2.50	0.45
2:F:154:ILE:O	2:F:158:LYS:HG3	2.17	0.45
2:G:190:GLU:O	2:G:194:GLN:HB2	2.17	0.45
2:G:158:LYS:HE3	2:G:210:PHE:CE1	2.52	0.45
1:J:482:ASP:N	1:J:483:PRO:HD3	2.31	0.45
1:M:219:ARG:NH2	1:M:263:GLU:OE1	2.50	0.45
2:O:211:PRO:HA	2:O:214:LEU:HG	1.99	0.45
1:B:307:MET:HE3	1:B:308:PRO:HD2	1.99	0.45
1:D:76:LEU:HD21	1:D:98:HIS:CE1	2.52	0.45
1:I:76:LEU:HD21	1:I:98:HIS:CE1	2.52	0.45
1:J:464:LEU:HD11	1:J:493:ALA:HB1	1.99	0.45
1:M:123:ASP:N	1:M:123:ASP:OD1	2.40	0.45
1:N:193:LYS:HD2	1:N:420:ASN:HA	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:76:LEU:HD21	1:N:98:HIS:CE1	2.52	0.45
1:B:477:GLN:HA	2:F:124:GLY:CA	2.46	0.44
1:I:123:ASP:N	1:I:123:ASP:OD1	2.40	0.44
1:D:489:LEU:HD23	1:D:489:LEU:HA	1.75	0.44
1:J:76:LEU:HD21	1:J:98:HIS:CE1	2.53	0.44
2:L:200:VAL:HG21	2:L:216:MET:CG	2.46	0.44
2:P:158:LYS:HE2	2:P:210:PHE:CZ	2.53	0.44
2:P:175:LYS:CE	2:P:175:LYS:H	2.29	0.44
1:B:76:LEU:HD21	1:B:98:HIS:CE1	2.52	0.44
1:C:219:ARG:NH2	1:C:263:GLU:OE1	2.49	0.44
1:I:219:ARG:NH2	1:I:263:GLU:OE1	2.49	0.44
1:B:193:LYS:HD2	1:B:420:ASN:HA	1.99	0.44
1:D:358:GLN:HB3	1:D:362:LYS:HE3	1.99	0.44
2:F:119:LEU:HD12	2:F:152:ASN:HB2	2.00	0.44
1:J:123:ASP:N	1:J:123:ASP:OD1	2.40	0.44
1:B:358:GLN:HB3	1:B:362:LYS:HE3	1.99	0.44
1:D:307:MET:HE3	1:D:308:PRO:HD2	2.00	0.44
1:I:270:LEU:HD12	1:I:293:PRO:HG3	1.98	0.44
2:K:175:LYS:O	2:K:179:THR:HG22	2.18	0.44
1:M:274:GLN:HE21	1:M:274:GLN:HB2	1.54	0.44
2:O:190:GLU:O	2:O:194:GLN:HB2	2.17	0.44
2:P:112:ALA:O	2:P:116:ILE:HG13	2.17	0.44
2:P:200:VAL:HG21	2:P:216:MET:CG	2.46	0.44
1:B:123:ASP:N	1:B:123:ASP:OD1	2.40	0.44
2:F:158:LYS:HA	2:F:210:PHE:HE2	1.81	0.44
1:M:243:GLU:OE2	1:M:274:GLN:NE2	2.50	0.44
1:M:76:LEU:HD21	1:M:98:HIS:CE1	2.53	0.44
2:O:172:ILE:HD13	2:O:172:ILE:HG21	1.67	0.44
1:J:358:GLN:HB3	1:J:362:LYS:HE3	1.99	0.44
2:K:164:PHE:O	2:K:176:GLU:HB3	2.18	0.44
1:A:219:ARG:NH2	1:A:263:GLU:OE1	2.50	0.44
1:C:461:ILE:HD12	1:C:479:LEU:HD12	1.99	0.44
1:M:270:LEU:HD12	1:M:293:PRO:HG3	1.99	0.44
1:N:123:ASP:N	1:N:123:ASP:OD1	2.41	0.44
1:N:358:GLN:HB3	1:N:362:LYS:HE3	1.99	0.44
1:J:314:ALA:HB1	1:J:318:VAL:CG2	2.48	0.44
2:O:175:LYS:O	2:O:179:THR:HG22	2.18	0.44
1:D:246:VAL:O	1:D:385:ARG:HD2	2.18	0.43
2:F:200:VAL:HG21	2:F:216:MET:CG	2.47	0.43
2:H:181:MET:O	2:H:186:GLN:HB2	2.18	0.43
1:J:115:PRO:HA	1:J:338:LEU:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:314:ALA:HB1	1:N:318:VAL:CG2	2.48	0.43
2:P:132:SER:O	2:P:135:LEU:HG	2.18	0.43
1:B:193:LYS:O	1:B:197:ARG:HG3	2.18	0.43
1:B:481:ASP:OD2	2:F:123:ASN:HB2	2.18	0.43
1:C:76:LEU:HD21	1:C:98:HIS:CE1	2.52	0.43
1:D:193:LYS:O	1:D:197:ARG:HG3	2.18	0.43
2:P:122:LEU:HD23	2:P:126:GLN:CD	2.38	0.43
2:F:119:LEU:HD12	2:F:152:ASN:CB	2.48	0.43
1:J:193:LYS:O	1:J:197:ARG:HG3	2.18	0.43
1:N:239:PRO:HG3	1:N:270:LEU:HD22	2.00	0.43
1:D:123:ASP:OD1	1:D:123:ASP:N	2.41	0.43
1:D:239:PRO:HG3	1:D:270:LEU:HD22	2.01	0.43
1:C:11:LEU:HD11	1:D:352:GLU:HG3	2.00	0.43
2:G:175:LYS:O	2:G:179:THR:HG22	2.18	0.43
1:N:193:LYS:O	1:N:197:ARG:HG3	2.18	0.43
1:A:243:GLU:OE2	1:A:274:GLN:NE2	2.50	0.43
1:A:76:LEU:HD21	1:A:98:HIS:CE1	2.53	0.43
1:D:115:PRO:HA	1:D:338:LEU:HD13	2.00	0.43
2:G:164:PHE:O	2:G:176:GLU:HB3	2.18	0.43
1:I:461:ILE:HD12	1:I:479:LEU:HD12	1.99	0.43
1:J:230:ASP:OD1	1:M:197:ARG:NH2	2.49	0.43
1:J:246:VAL:O	1:J:385:ARG:HD2	2.18	0.43
1:J:239:PRO:HG3	1:J:270:LEU:HD22	2.01	0.43
1:J:307:MET:HE3	1:J:308:PRO:HD2	2.00	0.43
1:N:174:ILE:HD11	1:N:232:VAL:HG21	2.01	0.43
1:N:464:LEU:CB	1:N:467:LEU:HD21	2.48	0.43
1:N:488:ASN:O	1:N:491:ALA:HB3	2.18	0.43
2:E:209:ASP:OD1	2:E:209:ASP:N	2.40	0.43
1:I:302:LEU:HD23	1:I:309:ILE:HG21	2.01	0.43
1:I:476:ILE:HD11	2:K:128:ALA:HA	2.01	0.43
1:M:302:LEU:HD23	1:M:309:ILE:HG21	2.00	0.43
1:N:270:LEU:HD12	1:N:293:PRO:HG3	2.01	0.43
2:O:164:PHE:O	2:O:176:GLU:HB3	2.18	0.43
1:B:314:ALA:HB1	1:B:318:VAL:CG2	2.48	0.43
1:M:458:PHE:HB2	1:M:479:LEU:HD21	1.99	0.43
1:B:54:ARG:HA	1:B:57:VAL:HG22	2.00	0.43
1:D:277:MET:HA	1:D:283:MET:HE3	1.99	0.43
1:D:54:ARG:HA	1:D:57:VAL:HG22	2.00	0.43
2:E:164:PHE:O	2:E:176:GLU:HB3	2.18	0.43
1:I:91:PHE:HD1	1:I:426:ARG:CZ	2.32	0.43
1:J:54:ARG:HA	1:J:57:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:190:GLU:O	2:K:194:GLN:HB2	2.19	0.43
2:L:177:LEU:HB3	2:L:181:MET:HE2	1.99	0.43
1:B:174:ILE:HD11	1:B:232:VAL:HG21	2.01	0.43
1:D:174:ILE:HD11	1:D:232:VAL:HG21	2.01	0.43
1:D:314:ALA:HB1	1:D:318:VAL:CG2	2.48	0.43
1:D:359:ALA:HB2	1:D:431:LEU:HD22	2.00	0.43
2:L:132:SER:O	2:L:135:LEU:HG	2.19	0.43
1:M:379:ASP:OD1	1:M:379:ASP:N	2.41	0.43
1:B:379:ASP:OD1	1:B:379:ASP:N	2.41	0.43
1:B:359:ALA:HB2	1:B:431:LEU:HD22	2.00	0.43
1:B:461:ILE:HD13	1:B:461:ILE:HG21	1.74	0.43
1:D:270:LEU:HD12	1:D:293:PRO:HG3	2.01	0.43
1:D:482:ASP:C	1:D:484:SER:H	2.22	0.43
2:F:132:SER:O	2:F:135:LEU:HG	2.19	0.43
1:I:379:ASP:OD1	1:I:379:ASP:N	2.41	0.43
1:J:270:LEU:HD12	1:J:293:PRO:HG3	2.01	0.43
2:L:181:MET:O	2:L:186:GLN:HB2	2.19	0.43
1:N:246:VAL:O	1:N:385:ARG:HD2	2.18	0.43
1:A:239:PRO:HG3	1:A:270:LEU:HD22	2.00	0.42
1:A:458:PHE:O	1:A:461:ILE:HG22	2.18	0.42
1:B:246:VAL:O	1:B:385:ARG:HD2	2.19	0.42
1:C:193:LYS:O	1:C:197:ARG:HG3	2.19	0.42
1:I:274:GLN:HB2	1:I:274:GLN:HE21	1.55	0.42
1:B:270:LEU:HD12	1:B:293:PRO:HG3	2.01	0.42
1:I:193:LYS:O	1:I:197:ARG:HG3	2.19	0.42
1:J:174:ILE:HD11	1:J:232:VAL:HG21	2.01	0.42
2:K:149:LYS:O	2:K:152:ASN:HB3	2.19	0.42
1:M:193:LYS:O	1:M:197:ARG:HG3	2.19	0.42
1:N:485:GLN:H	1:N:485:GLN:HG3	1.36	0.42
1:A:193:LYS:O	1:A:197:ARG:HG3	2.19	0.42
1:A:302:LEU:HD23	1:A:309:ILE:HG21	2.00	0.42
1:B:239:PRO:HG3	1:B:270:LEU:HD22	2.01	0.42
1:B:468:ASN:H	1:B:468:ASN:ND2	2.17	0.42
1:B:475:PHE:HD1	1:B:489:LEU:HD11	1.84	0.42
1:C:380:LEU:HD13	1:C:452:MET:HE2	2.01	0.42
2:H:164:PHE:HD2	2:H:172:ILE:HD13	1.83	0.42
1:J:414:LEU:HA	1:J:414:LEU:HD12	1.92	0.42
1:M:91:PHE:HD1	1:M:426:ARG:CZ	2.32	0.42
1:M:300:LYS:HA	1:N:333:PHE:HZ	1.84	0.42
1:A:91:PHE:HD1	1:A:426:ARG:CZ	2.33	0.42
1:C:383:GLU:HG2	1:C:384:ALA:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:464:LEU:N	1:D:472:ARG:HH22	2.18	0.42
2:F:181:MET:O	2:F:186:GLN:HB2	2.19	0.42
1:J:480:LYS:HB3	2:L:124:GLY:HA2	2.02	0.42
1:M:461:ILE:HG21	1:M:461:ILE:HD13	1.83	0.42
2:P:172:ILE:HG21	2:P:177:LEU:HD23	2.00	0.42
2:E:149:LYS:O	2:E:152:ASN:HB3	2.20	0.42
2:E:175:LYS:O	2:E:179:THR:HG22	2.18	0.42
2:G:149:LYS:O	2:G:152:ASN:HB3	2.19	0.42
1:I:462:LEU:HD11	2:K:135:LEU:HD21	2.01	0.42
1:J:464:LEU:CB	1:J:467:LEU:HD21	2.49	0.42
1:I:197:ARG:NH2	1:N:230:ASP:OD1	2.50	0.42
2:O:149:LYS:O	2:O:152:ASN:HB3	2.20	0.42
2:K:181:MET:HB2	2:K:188:PRO:HG3	2.02	0.42
1:D:379:ASP:OD1	1:D:379:ASP:N	2.41	0.42
2:F:161:PHE:CE1	2:F:172:ILE:HD12	2.54	0.42
2:H:200:VAL:HG21	2:H:216:MET:CG	2.46	0.42
1:J:114:GLN:HA	1:J:115:PRO:HD3	1.96	0.42
2:K:158:LYS:HE3	2:K:210:PHE:HE1	1.84	0.42
2:L:148:ALA:O	2:L:151:LEU:HB3	2.19	0.42
2:P:181:MET:O	2:P:186:GLN:HB2	2.19	0.42
2:H:132:SER:O	2:H:135:LEU:HG	2.20	0.42
1:C:43:LYS:HG2	1:C:44:GLU:HG2	2.02	0.42
1:A:462:LEU:HD11	2:E:135:LEU:HD21	2.02	0.42
2:L:116:ILE:HG13	2:L:117:PHE:N	2.34	0.42
1:N:54:ARG:HA	1:N:57:VAL:HG22	2.01	0.42
1:C:239:PRO:HG3	1:C:270:LEU:HD22	2.01	0.42
1:N:307:MET:HE3	1:N:308:PRO:HD2	2.01	0.42
1:A:197:ARG:NH2	1:D:230:ASP:OD1	2.49	0.41
1:J:482:ASP:C	1:J:484:SER:H	2.24	0.41
1:J:485:GLN:H	1:J:485:GLN:HG3	1.41	0.41
2:K:177:LEU:HD12	2:K:177:LEU:HA	1.84	0.41
2:K:172:ILE:CG2	2:K:177:LEU:HD13	2.50	0.41
2:G:158:LYS:HE3	2:G:210:PHE:HE1	1.83	0.41
2:P:121:ASN:N	2:P:152:ASN:HD21	2.17	0.41
1:B:477:GLN:O	1:B:481:ASP:OD1	2.38	0.41
2:E:181:MET:HB2	2:E:188:PRO:HG3	2.01	0.41
2:O:177:LEU:HD12	2:O:177:LEU:HA	1.84	0.41
2:P:164:PHE:CD2	2:P:172:ILE:HD12	2.55	0.41
2:P:177:LEU:HB3	2:P:181:MET:HE3	2.01	0.41
1:A:383:GLU:HG2	1:A:384:ALA:N	2.36	0.41
1:M:185:LEU:HD21	1:N:159:LYS:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:123:ASN:H	2:E:126:GLN:NE2	2.15	0.41
2:K:158:LYS:HE3	2:K:210:PHE:CE1	2.55	0.41
1:C:67:GLU:HG3	1:D:121:LEU:HB2	2.02	0.41
2:K:126:GLN:CD	2:K:155:GLN:HE22	2.24	0.41
1:M:239:PRO:HG3	1:M:270:LEU:HD22	2.01	0.41
1:M:476:ILE:HD11	2:O:128:ALA:HA	2.03	0.41
2:P:164:PHE:HD1	2:P:180:VAL:HG21	1.86	0.41
1:A:185:LEU:HD21	1:B:159:LYS:HG2	2.02	0.41
1:C:462:LEU:HD11	2:G:135:LEU:HD21	2.02	0.41
2:G:126:GLN:CD	2:G:155:GLN:HE22	2.24	0.41
1:N:475:PHE:O	1:N:478:SER:OG	2.30	0.41
2:O:126:GLN:CD	2:O:155:GLN:HE22	2.24	0.41
2:O:172:ILE:CG2	2:O:177:LEU:HD13	2.51	0.41
2:O:181:MET:HB2	2:O:188:PRO:HG3	2.03	0.41
2:P:209:ASP:OD1	2:P:209:ASP:N	2.40	0.41
1:J:359:ALA:HB2	1:J:431:LEU:HD22	2.01	0.41
1:J:87:CYS:HA	1:J:429:PRO:HB3	2.03	0.41
1:J:468:ASN:ND2	1:J:468:ASN:H	2.18	0.41
1:N:359:ALA:HB2	1:N:431:LEU:HD22	2.02	0.41
1:N:458:PHE:O	1:N:461:ILE:HG23	2.20	0.41
1:B:277:MET:HA	1:B:283:MET:HE3	2.02	0.41
1:D:479:LEU:HD22	2:H:117:PHE:HZ	1.84	0.41
1:A:43:LYS:HG2	1:A:44:GLU:HG2	2.03	0.41
1:I:239:PRO:HG3	1:I:270:LEU:HD22	2.01	0.41
1:D:477:GLN:O	2:H:124:GLY:HA3	2.21	0.41
1:N:495:LYS:HA	1:N:498:ASP:OD2	2.21	0.41
1:A:461:ILE:HG21	1:A:461:ILE:HD13	1.85	0.40
1:C:87:CYS:HA	1:C:429:PRO:HB3	2.03	0.40
2:G:172:ILE:CG2	2:G:177:LEU:HD13	2.50	0.40
2:K:119:LEU:HA	2:K:120:PRO:HD3	1.90	0.40
1:J:481:ASP:OD2	2:L:123:ASN:HB3	2.22	0.40
1:N:87:CYS:HA	1:N:429:PRO:HB3	2.03	0.40
1:B:75:THR:HA	1:B:84:PHE:O	2.21	0.40
1:D:423:LYS:HE3	1:D:423:LYS:HB2	2.00	0.40
1:D:488:ASN:O	1:D:491:ALA:HB3	2.21	0.40
1:I:383:GLU:HG2	1:I:384:ALA:N	2.35	0.40
2:K:138:PRO:C	2:K:140:GLN:H	2.25	0.40
2:G:123:ASN:H	2:G:126:GLN:NE2	2.15	0.40
1:D:480:LYS:HG3	2:H:127:VAL:HG11	2.03	0.40
1:I:43:LYS:HG2	1:I:44:GLU:HG2	2.02	0.40
1:I:87:CYS:HA	1:I:429:PRO:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:480:LYS:HG3	2:P:127:VAL:HG11	2.03	0.40
1:A:69:GLN:HE21	1:A:69:GLN:HB3	1.75	0.40
1:A:75:THR:HA	1:A:84:PHE:O	2.22	0.40
1:C:270:LEU:HD13	1:C:286:CYS:HB3	2.04	0.40
2:E:126:GLN:CD	2:E:155:GLN:HE22	2.25	0.40
2:O:138:PRO:C	2:O:140:GLN:H	2.25	0.40
2:P:126:GLN:HE22	2:P:155:GLN:NE2	2.20	0.40
1:A:87:CYS:HA	1:A:429:PRO:HB3	2.03	0.40
1:C:75:THR:HA	1:C:84:PHE:O	2.22	0.40
2:E:172:ILE:CG2	2:E:177:LEU:HD13	2.51	0.40
1:M:87:CYS:HA	1:M:429:PRO:HB3	2.03	0.40
1:N:461:ILE:HD12	1:N:475:PHE:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	493/499 (99%)	472 (96%)	21 (4%)	0	100	100
1	B	493/499 (99%)	470 (95%)	22 (4%)	1 (0%)	47	69
1	C	493/499 (99%)	473 (96%)	19 (4%)	1 (0%)	47	69
1	D	493/499 (99%)	470 (95%)	23 (5%)	0	100	100
1	I	493/499 (99%)	472 (96%)	21 (4%)	0	100	100
1	J	493/499 (99%)	469 (95%)	24 (5%)	0	100	100
1	M	493/499 (99%)	472 (96%)	21 (4%)	0	100	100
1	N	493/499 (99%)	470 (95%)	23 (5%)	0	100	100
2	E	111/120 (92%)	105 (95%)	5 (4%)	1 (1%)	17	34
2	F	110/120 (92%)	103 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	G	111/120 (92%)	104 (94%)	6 (5%)	1 (1%)	17	34
2	H	110/120 (92%)	102 (93%)	8 (7%)	0	100	100
2	K	111/120 (92%)	105 (95%)	5 (4%)	1 (1%)	17	34
2	L	110/120 (92%)	103 (94%)	7 (6%)	0	100	100
2	O	111/120 (92%)	104 (94%)	6 (5%)	1 (1%)	17	34
2	P	110/120 (92%)	103 (94%)	7 (6%)	0	100	100
All	All	4828/4952 (98%)	4597 (95%)	225 (5%)	6 (0%)	51	73

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	485	GLN
2	E	139	SER
2	G	139	SER
2	K	139	SER
2	O	139	SER
1	C	115	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	396/399 (99%)	385 (97%)	11 (3%)	43	67
1	B	396/399 (99%)	382 (96%)	14 (4%)	36	59
1	C	396/399 (99%)	386 (98%)	10 (2%)	47	70
1	D	396/399 (99%)	380 (96%)	16 (4%)	31	55
1	I	396/399 (99%)	387 (98%)	9 (2%)	50	73
1	J	396/399 (99%)	382 (96%)	14 (4%)	36	59
1	M	396/399 (99%)	388 (98%)	8 (2%)	55	76
1	N	396/399 (99%)	380 (96%)	16 (4%)	31	55
2	E	95/101 (94%)	84 (88%)	11 (12%)	5	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	93/101 (92%)	85 (91%)	8 (9%)	10	19
2	G	95/101 (94%)	82 (86%)	13 (14%)	3	6
2	H	93/101 (92%)	86 (92%)	7 (8%)	13	26
2	K	95/101 (94%)	84 (88%)	11 (12%)	5	9
2	L	93/101 (92%)	86 (92%)	7 (8%)	13	26
2	O	95/101 (94%)	84 (88%)	11 (12%)	5	9
2	P	93/101 (92%)	82 (88%)	11 (12%)	5	9
All	All	3920/4000 (98%)	3743 (96%)	177 (4%)	27	50

All (177) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	PRO
1	A	69	GLN
1	A	140	LYS
1	A	166	SER
1	A	219	ARG
1	A	237	LEU
1	A	365	MET
1	A	398	ASN
1	A	402	TYR
1	A	431	LEU
1	A	500	GLN
1	B	48	PRO
1	B	99	ARG
1	B	166	SER
1	B	219	ARG
1	B	237	LEU
1	B	338	LEU
1	B	398	ASN
1	B	467	LEU
1	B	469	GLU
1	B	480	LYS
1	B	481	ASP
1	B	485	GLN
1	B	496	LEU
1	B	500	GLN
2	E	125	ARG
2	E	144	LEU
2	E	151	LEU

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Mol	Chain	Res	Type
2	E	158	LYS
2	E	161	PHE
2	E	177	LEU
2	E	179	THR
2	E	181	MET
2	E	183	SER
2	E	209	ASP
2	E	210	PHE
2	F	119	LEU
2	F	126	GLN
2	F	134	LEU
2	F	147	GLU
2	F	175	LYS
2	F	181	MET
2	F	209	ASP
2	F	210	PHE
1	C	48	PRO
1	C	69	GLN
1	C	140	LYS
1	C	166	SER
1	C	219	ARG
1	C	237	LEU
1	C	243	GLU
1	C	398	ASN
1	C	402	TYR
1	C	500	GLN
1	D	48	PRO
1	D	99	ARG
1	D	166	SER
1	D	219	ARG
1	D	237	LEU
1	D	338	LEU
1	D	398	ASN
1	D	467	LEU
1	D	469	GLU
1	D	476	ILE
1	D	477	GLN
1	D	480	LYS
1	D	481	ASP
1	D	485	GLN
1	D	496	LEU
1	D	500	GLN

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Mol	Chain	Res	Type
2	G	125	ARG
2	G	144	LEU
2	G	151	LEU
2	G	158	LYS
2	G	161	PHE
2	G	177	LEU
2	G	179	THR
2	G	181	MET
2	G	183	SER
2	G	209	ASP
2	G	210	PHE
2	G	217	MET
2	G	219	ARG
2	H	134	LEU
2	H	147	GLU
2	H	164	PHE
2	H	175	LYS
2	H	181	MET
2	H	209	ASP
2	H	210	PHE
1	I	48	PRO
1	I	140	LYS
1	I	166	SER
1	I	219	ARG
1	I	237	LEU
1	I	243	GLU
1	I	398	ASN
1	I	402	TYR
1	I	500	GLN
1	J	48	PRO
1	J	99	ARG
1	J	166	SER
1	J	219	ARG
1	J	237	LEU
1	J	338	LEU
1	J	391	MET
1	J	398	ASN
1	J	467	LEU
1	J	469	GLU
1	J	476	ILE
1	J	481	ASP
1	J	485	GLN

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Mol	Chain	Res	Type
1	J	496	LEU
2	K	107	LYS
2	K	125	ARG
2	K	144	LEU
2	K	151	LEU
2	K	158	LYS
2	K	177	LEU
2	K	179	THR
2	K	181	MET
2	K	183	SER
2	K	209	ASP
2	K	210	PHE
2	L	126	GLN
2	L	134	LEU
2	L	147	GLU
2	L	175	LYS
2	L	181	MET
2	L	209	ASP
2	L	210	PHE
1	M	20	LEU
1	M	140	LYS
1	M	166	SER
1	M	219	ARG
1	M	237	LEU
1	M	398	ASN
1	M	402	TYR
1	M	500	GLN
1	N	48	PRO
1	N	99	ARG
1	N	121	LEU
1	N	166	SER
1	N	219	ARG
1	N	237	LEU
1	N	338	LEU
1	N	398	ASN
1	N	461	ILE
1	N	467	LEU
1	N	469	GLU
1	N	480	LYS
1	N	481	ASP
1	N	485	GLN
1	N	495	LYS

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Mol	Chain	Res	Type
1	N	496	LEU
2	O	125	ARG
2	O	144	LEU
2	O	151	LEU
2	O	158	LYS
2	O	161	PHE
2	O	177	LEU
2	O	179	THR
2	O	181	MET
2	O	183	SER
2	O	209	ASP
2	O	210	PHE
2	P	116	ILE
2	P	121	ASN
2	P	122	LEU
2	P	126	GLN
2	P	134	LEU
2	P	147	GLU
2	P	172	ILE
2	P	175	LYS
2	P	181	MET
2	P	209	ASP
2	P	210	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	B	274	GLN
1	B	468	ASN
1	B	471	GLN
1	B	500	GLN
2	E	126	GLN
2	E	152	ASN
2	E	155	GLN
1	C	69	GLN
1	C	274	GLN
1	D	274	GLN
1	D	454	GLN
1	D	468	ASN
1	D	471	GLN
1	D	477	GLN

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Mol	Chain	Res	Type
2	G	110	GLN
2	G	126	GLN
2	G	152	ASN
2	G	155	GLN
2	H	126	GLN
1	I	69	GLN
1	J	274	GLN
1	J	454	GLN
1	J	468	ASN
2	K	110	GLN
2	K	126	GLN
2	K	152	ASN
2	K	155	GLN
1	N	274	GLN
2	O	126	GLN
2	O	152	ASN
2	O	155	GLN
2	P	126	GLN
2	P	152	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	495/499 (99%)	0.61	24 (4%) 30 26	45, 69, 137, 163	0
1	B	495/499 (99%)	0.77	40 (8%) 12 9	43, 62, 126, 159	0
1	C	495/499 (99%)	0.61	29 (5%) 22 19	42, 65, 86, 98	0
1	D	495/499 (99%)	0.75	30 (6%) 21 17	44, 62, 129, 162	0
1	I	495/499 (99%)	0.51	24 (4%) 30 26	44, 68, 130, 155	0
1	J	495/499 (99%)	0.62	35 (7%) 16 13	44, 61, 128, 162	0
1	M	495/499 (99%)	0.57	29 (5%) 22 19	46, 69, 137, 164	0
1	N	495/499 (99%)	0.74	42 (8%) 10 8	44, 63, 128, 160	0
2	E	113/120 (94%)	1.39	30 (26%) 0 0	103, 125, 147, 155	0
2	F	112/120 (93%)	3.49	59 (52%) 0 0	163, 203, 250, 261	0
2	G	113/120 (94%)	1.04	22 (19%) 1 0	97, 119, 151, 160	0
2	H	112/120 (93%)	2.63	60 (53%) 0 0	147, 183, 233, 246	0
2	K	113/120 (94%)	1.18	23 (20%) 1 0	97, 117, 142, 153	0
2	L	112/120 (93%)	2.96	57 (50%) 0 0	166, 201, 241, 251	0
2	O	113/120 (94%)	1.21	26 (23%) 0 0	103, 127, 156, 162	0
2	P	112/120 (93%)	3.03	72 (64%) 0 0	170, 192, 227, 237	0
All	All	4860/4952 (98%)	0.92	602 (12%) 4 3	42, 70, 188, 261	0

All (602) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	208	ILE	21.6
2	F	200	VAL	20.5
2	F	208	ILE	16.9
2	P	208	ILE	16.2
2	F	205	ASN	14.1

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Mol	Chain	Res	Type	RSRZ
2	L	209	ASP	13.6
2	H	205	ASN	12.2
2	L	131	ILE	12.1
2	F	203	ASP	12.0
2	H	208	ILE	11.9
2	K	172	ILE	11.5
2	F	218	ALA	11.1
2	F	131	ILE	11.1
2	F	204	GLY	11.0
2	P	200	VAL	10.7
2	G	172	ILE	10.3
2	L	134	LEU	10.0
2	H	209	ASP	9.9
2	H	131	ILE	9.9
2	P	205	ASN	9.8
2	F	210	PHE	9.5
1	N	464	LEU	9.4
2	H	134	LEU	9.3
2	L	203	ASP	9.1
2	F	134	LEU	9.0
2	H	157	PHE	8.9
2	E	172	ILE	8.7
2	F	122	LEU	8.7
2	P	134	LEU	8.7
2	P	131	ILE	8.6
2	H	207	THR	8.5
2	F	199	GLU	8.5
2	F	193	LEU	8.4
2	O	172	ILE	8.4
1	N	501	ALA	8.4
2	F	171	THR	8.3
2	F	209	ASP	8.3
1	N	486	SER	8.3
1	N	485	GLN	8.1
1	B	487	ALA	8.0
2	L	207	THR	8.0
2	L	212	GLU	7.9
2	P	209	ASP	7.9
1	D	495	LYS	7.8
2	F	198	ASN	7.8
2	P	157	PHE	7.8
2	E	193	LEU	7.7

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Mol	Chain	Res	Type	RSRZ
2	F	196	MET	7.7
1	D	464	LEU	7.6
1	N	463	HIS	7.3
1	B	463	HIS	7.2
1	M	501	ALA	7.1
2	P	213	PHE	7.1
1	B	485	GLN	7.1
2	F	135	LEU	7.0
1	I	475	PHE	6.9
1	B	417	GLY	6.9
2	F	191	ALA	6.8
1	N	487	ALA	6.8
1	N	461	ILE	6.8
2	H	171	THR	6.7
2	L	201	ASP	6.7
2	L	135	LEU	6.7
2	F	186	GLN	6.7
2	F	212	GLU	6.6
2	H	169	ASP	6.6
2	P	174	THR	6.6
2	P	122	LEU	6.6
2	O	174	THR	6.6
2	L	127	VAL	6.6
1	J	495	LYS	6.5
2	H	170	GLY	6.5
2	L	205	ASN	6.5
2	F	157	PHE	6.5
2	E	117	PHE	6.4
2	H	174	THR	6.4
2	P	196	MET	6.4
2	L	122	LEU	6.4
2	G	193	LEU	6.3
2	L	169	ASP	6.3
2	L	200	VAL	6.3
1	B	464	LEU	6.3
2	L	171	THR	6.3
2	L	202	ALA	6.2
2	P	199	GLU	6.1
1	I	495	LYS	6.1
1	B	486	SER	6.1
2	L	218	ALA	6.0
1	J	485	GLN	6.0

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Mol	Chain	Res	Type	RSRZ
1	J	464	LEU	6.0
1	C	490	LEU	6.0
2	L	198	ASN	6.0
2	L	213	PHE	5.9
1	C	495	LYS	5.9
2	H	206	GLY	5.9
2	P	135	LEU	5.8
2	O	117	PHE	5.7
2	K	173	THR	5.7
2	P	164	PHE	5.7
2	F	150	LYS	5.7
2	O	200	VAL	5.7
2	P	218	ALA	5.7
2	H	164	PHE	5.7
2	P	167	ASP	5.7
2	H	203	ASP	5.6
1	A	410	ARG	5.6
2	P	210	PHE	5.6
2	F	164	PHE	5.6
2	P	171	THR	5.5
1	C	501	ALA	5.5
1	M	475	PHE	5.5
1	B	476	ILE	5.5
1	N	476	ILE	5.5
2	G	208	ILE	5.4
2	E	195	ASP	5.4
2	H	201	ASP	5.4
1	N	491	ALA	5.3
1	B	501	ALA	5.3
2	P	183	SER	5.3
1	M	490	LEU	5.3
1	B	495	LYS	5.2
2	L	157	PHE	5.2
2	P	127	VAL	5.2
2	L	217	MET	5.2
2	H	200	VAL	5.2
2	H	184	LEU	5.2
2	H	217	MET	5.2
2	P	166	LYS	5.1
2	F	165	ASP	5.1
1	N	28	HIS	5.1
2	F	207	THR	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	475	PHE	5.1
1	D	476	ILE	5.1
1	B	491	ALA	5.1
2	F	152	ASN	5.1
2	P	175	LYS	5.0
2	H	202	ALA	5.0
2	L	184	LEU	5.0
2	P	186	GLN	5.0
2	F	127	VAL	5.0
1	D	461	ILE	5.0
2	P	165	ASP	5.0
2	O	199	GLU	5.0
2	E	198	ASN	4.9
2	L	164	PHE	4.9
2	F	187	ASN	4.9
2	O	195	ASP	4.9
2	H	191	ALA	4.9
1	A	479	LEU	4.9
2	E	112	ALA	4.9
1	N	495	LYS	4.9
2	F	172	ILE	4.9
2	O	112	ALA	4.9
2	H	135	LEU	4.8
1	N	484	SER	4.8
2	P	151	LEU	4.8
2	F	180	VAL	4.8
2	E	116	ILE	4.8
2	H	127	VAL	4.8
1	J	475	PHE	4.8
1	N	479	LEU	4.8
1	D	486	SER	4.7
1	N	488	ASN	4.7
1	J	461	ILE	4.7
1	M	479	LEU	4.7
2	L	128	ALA	4.7
2	H	186	GLN	4.7
2	L	145	LEU	4.7
1	C	475	PHE	4.7
1	I	501	ALA	4.6
2	F	116	ILE	4.6
2	L	206	GLY	4.6
2	E	196	MET	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	471	GLN	4.6
2	H	162	SER	4.6
2	L	153	GLN	4.5
2	P	169	ASP	4.5
1	J	419	LEU	4.5
2	E	200	VAL	4.5
2	O	193	LEU	4.5
2	H	175	LYS	4.5
2	P	201	ASP	4.5
1	D	485	GLN	4.5
2	E	175	LYS	4.5
1	D	417	GLY	4.5
2	H	204	GLY	4.4
1	J	501	ALA	4.4
2	L	150	LYS	4.4
2	O	122	LEU	4.4
2	H	172	ILE	4.4
2	P	198	ASN	4.4
2	O	177	LEU	4.4
1	J	486	SER	4.4
2	H	125	ARG	4.3
2	P	203	ASP	4.3
2	H	218	ALA	4.3
1	J	487	ALA	4.3
2	F	184	LEU	4.3
1	N	458	PHE	4.3
1	I	479	LEU	4.3
1	D	499	ALA	4.3
2	F	128	ALA	4.3
2	P	212	GLU	4.3
2	K	193	LEU	4.2
1	A	461	ILE	4.2
2	P	153	GLN	4.2
2	P	207	THR	4.2
2	P	191	ALA	4.2
2	E	199	GLU	4.2
2	F	170	GLY	4.2
2	F	174	THR	4.1
2	G	174	THR	4.1
2	L	151	LEU	4.1
2	K	174	THR	4.1
1	J	463	HIS	4.1

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Mol	Chain	Res	Type	RSRZ
1	J	323	PHE	4.1
2	H	212	GLU	4.1
2	K	208	ILE	4.1
2	P	184	LEU	4.0
1	J	121	LEU	4.0
2	E	154	ILE	4.0
2	L	149	LYS	4.0
2	L	123	ASN	4.0
2	P	172	ILE	4.0
2	K	200	VAL	4.0
1	I	410	ARG	3.9
1	A	476	ILE	3.9
1	J	476	ILE	3.9
2	H	198	ASN	3.9
2	E	169	ASP	3.9
2	H	122	LEU	3.9
2	L	210	PHE	3.9
1	C	491	ALA	3.9
2	K	116	ILE	3.9
1	J	474	ALA	3.9
2	P	138	PRO	3.9
1	C	498	ASP	3.8
2	F	201	ASP	3.8
2	P	217	MET	3.8
2	F	175	LYS	3.8
2	F	188	PRO	3.8
1	B	479	LEU	3.8
1	I	51	LEU	3.8
1	N	419	LEU	3.8
2	H	210	PHE	3.8
1	M	476	ILE	3.8
2	K	170	GLY	3.8
2	O	175	LYS	3.8
1	C	479	LEU	3.8
1	N	482	ASP	3.8
2	P	215	THR	3.8
2	H	161	PHE	3.7
2	P	204	GLY	3.7
2	O	135	LEU	3.7
2	H	195	ASP	3.7
1	A	458	PHE	3.7
2	G	175	LYS	3.7

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Mol	Chain	Res	Type	RSRZ
2	L	170	GLY	3.7
1	N	490	LEU	3.7
2	H	152	ASN	3.6
2	L	125	ARG	3.6
1	C	410	ARG	3.6
2	F	147	GLU	3.6
1	B	419	LEU	3.6
1	C	467	LEU	3.6
2	P	144	LEU	3.6
2	L	174	THR	3.6
1	I	476	ILE	3.6
2	G	116	ILE	3.6
1	M	51	LEU	3.5
2	O	192	GLU	3.5
2	E	135	LEU	3.5
1	M	420	ASN	3.5
2	G	187	ASN	3.5
1	M	464	LEU	3.4
1	D	487	ALA	3.4
1	M	495	LYS	3.4
1	M	50	PHE	3.4
1	D	491	ALA	3.4
1	N	499	ALA	3.4
2	E	216	MET	3.4
2	P	147	GLU	3.4
2	E	170	GLY	3.4
1	D	463	HIS	3.4
2	P	162	SER	3.4
1	N	465	PRO	3.4
1	C	489	LEU	3.4
2	E	208	ILE	3.3
2	G	177	LEU	3.3
2	G	155	GLN	3.3
1	N	478	SER	3.3
1	J	499	ALA	3.3
1	N	500	GLN	3.3
2	L	204	GLY	3.3
2	L	183	SER	3.3
1	C	476	ILE	3.3
2	O	116	ILE	3.3
2	O	154	ILE	3.3
1	M	410	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	498	ASP	3.3
1	M	419	LEU	3.3
2	L	199	GLU	3.3
1	I	478	SER	3.3
1	B	499	ALA	3.3
1	M	487	ALA	3.3
2	P	189	THR	3.3
1	C	50	PHE	3.3
2	P	133	SER	3.3
2	P	181	MET	3.2
2	L	196	MET	3.2
1	D	490	LEU	3.2
2	O	213	PHE	3.2
2	L	186	GLN	3.2
1	M	480	LYS	3.2
2	E	202	ALA	3.2
2	L	148	ALA	3.2
1	I	409	PHE	3.2
2	F	145	LEU	3.2
2	P	177	LEU	3.2
2	K	175	LYS	3.2
2	K	117	PHE	3.1
2	O	157	PHE	3.1
2	H	196	MET	3.1
1	N	467	LEU	3.1
1	B	482	ASP	3.1
2	H	145	LEU	3.1
2	L	137	ASP	3.1
2	F	153	GLN	3.1
1	C	461	ILE	3.1
2	E	145	LEU	3.1
2	F	151	LEU	3.1
1	M	61	GLY	3.1
2	K	141	SER	3.1
2	F	195	ASP	3.1
1	A	462	LEU	3.1
1	C	42	PHE	3.1
1	D	475	PHE	3.1
2	F	197	ILE	3.1
2	P	152	ASN	3.1
1	D	122	LEU	3.1
2	H	116	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
2	L	152	ASN	3.0
1	A	501	ALA	3.0
1	I	490	LEU	3.0
2	E	207	THR	3.0
1	D	494	LYS	3.0
1	C	409	PHE	3.0
2	H	213	PHE	3.0
2	P	195	ASP	3.0
2	H	151	LEU	3.0
1	M	20	LEU	3.0
2	F	148	ALA	3.0
2	L	165	ASP	3.0
2	F	109	THR	2.9
2	P	188	PRO	2.9
2	P	216	MET	2.9
2	H	148	ALA	2.9
2	P	187	ASN	2.9
2	F	154	ILE	2.9
2	H	143	ASN	2.9
2	E	174	THR	2.9
1	B	493	ALA	2.9
1	N	418	THR	2.9
1	B	481	ASP	2.9
1	I	50	PHE	2.9
2	K	142	ALA	2.9
2	H	168	GLY	2.9
1	B	458	PHE	2.9
2	P	109	THR	2.9
1	N	480	LYS	2.8
1	B	475	PHE	2.8
2	L	130	PHE	2.8
2	P	163	LEU	2.8
2	G	122	LEU	2.8
2	K	136	ASP	2.8
2	F	216	MET	2.8
1	A	84	PHE	2.8
1	I	327	PHE	2.8
2	G	117	PHE	2.8
1	B	10	ALA	2.8
2	P	192	GLU	2.8
2	P	182	ARG	2.8
2	K	157	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
2	F	217	MET	2.8
2	G	216	MET	2.8
2	L	216	MET	2.8
1	M	421	ASN	2.8
2	O	198	ASN	2.8
2	K	134	LEU	2.8
2	O	216	MET	2.8
2	P	168	GLY	2.7
2	G	173	THR	2.7
2	H	109	THR	2.7
2	P	193	LEU	2.7
2	L	133	SER	2.7
2	G	195	ASP	2.7
2	P	180	VAL	2.7
1	I	448	ALA	2.7
1	M	478	SER	2.7
2	O	196	MET	2.7
1	A	412	ARG	2.7
1	A	487	ALA	2.7
2	H	163	LEU	2.7
2	O	161	PHE	2.7
2	H	153	GLN	2.7
1	B	461	ILE	2.7
2	K	154	ILE	2.7
2	L	215	THR	2.7
1	J	467	LEU	2.7
1	N	121	LEU	2.7
1	C	51	LEU	2.7
1	A	402	TYR	2.7
1	I	402	TYR	2.7
1	I	498	ASP	2.7
2	O	169	ASP	2.7
1	C	419	LEU	2.6
2	H	216	MET	2.6
1	N	466	ASN	2.6
1	I	84	PHE	2.6
2	O	170	GLY	2.6
1	D	121	LEU	2.6
2	E	177	LEU	2.6
2	K	177	LEU	2.6
1	M	498	ASP	2.6
2	K	209	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	192	GLU	2.6
1	M	68	TRP	2.6
2	F	113	SER	2.6
2	P	139	SER	2.6
1	B	498	ASP	2.6
1	J	479	LEU	2.6
1	J	496	LEU	2.6
2	F	192	GLU	2.6
1	D	57	VAL	2.6
2	G	154	ILE	2.6
2	O	208	ILE	2.6
1	A	480	LYS	2.6
1	A	471	GLN	2.6
1	N	417	GLY	2.6
1	I	77	VAL	2.5
1	I	471	GLN	2.5
1	I	419	LEU	2.5
1	J	122	LEU	2.5
2	F	177	LEU	2.5
1	B	488	ASN	2.5
1	J	481	ASP	2.5
1	N	31	MET	2.5
2	P	156	ALA	2.5
1	A	419	LEU	2.5
2	F	206	GLY	2.5
2	P	197	ILE	2.5
1	N	426	ARG	2.5
2	G	207	THR	2.5
1	M	461	ILE	2.5
1	D	339	ALA	2.5
1	M	466	ASN	2.5
2	K	135	LEU	2.5
1	I	21	ILE	2.5
1	C	493	ALA	2.5
1	N	422	ALA	2.5
1	C	280	THR	2.5
2	L	189	THR	2.5
1	D	18	LEU	2.4
1	C	402	TYR	2.4
1	J	417	GLY	2.4
1	N	493	ALA	2.4
1	B	32	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	418	THR	2.4
1	B	240	ILE	2.4
1	I	461	ILE	2.4
2	H	167	ASP	2.4
1	M	84	PHE	2.4
1	N	475	PHE	2.4
1	I	17	ALA	2.4
1	J	500	GLN	2.4
2	L	143	ASN	2.4
2	L	109	THR	2.4
1	A	7	SER	2.4
1	B	328	LEU	2.4
2	O	184	LEU	2.4
2	P	117	PHE	2.4
1	B	478	SER	2.4
2	O	173	THR	2.4
1	A	20	LEU	2.4
2	E	119	LEU	2.4
1	J	498	ASP	2.3
2	P	128	ALA	2.3
1	J	57	VAL	2.3
2	H	180	VAL	2.3
1	M	482	ASP	2.3
2	H	154	ILE	2.3
1	D	323	PHE	2.3
2	F	213	PHE	2.3
2	L	168	GLY	2.3
1	A	125	LEU	2.3
1	A	498	ASP	2.3
2	H	165	ASP	2.3
2	F	166	LYS	2.3
2	E	213	PHE	2.3
1	N	339	ALA	2.3
2	H	133	SER	2.3
2	P	148	ALA	2.3
1	B	490	LEU	2.3
2	P	137	ASP	2.3
1	B	318	VAL	2.3
2	G	192	GLU	2.3
1	J	491	ALA	2.3
2	G	157	PHE	2.3
2	G	209	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	366	LEU	2.3
1	D	365	MET	2.3
1	C	85	ILE	2.3
2	H	113	SER	2.3
1	D	10	ALA	2.3
1	M	471	GLN	2.2
2	E	155	GLN	2.2
2	E	209	ASP	2.2
1	J	449	LEU	2.2
1	M	390	LEU	2.2
1	N	494	LYS	2.2
2	K	155	GLN	2.2
1	C	215	ILE	2.2
2	P	116	ILE	2.2
1	M	412	ARG	2.2
1	D	63	TYR	2.2
2	F	133	SER	2.2
1	J	422	ALA	2.2
1	N	474	ALA	2.2
2	L	116	ILE	2.2
2	P	202	ALA	2.2
1	A	483	PRO	2.2
1	B	26	LEU	2.2
1	N	32	LYS	2.2
1	D	454	GLN	2.2
1	J	50	PHE	2.2
2	K	112	ALA	2.2
1	J	466	ASN	2.2
1	J	482	ASP	2.2
1	C	464	LEU	2.2
1	I	467	LEU	2.2
1	M	483	PRO	2.2
2	G	135	LEU	2.2
2	F	202	ALA	2.2
1	B	323	PHE	2.2
2	L	185	GLY	2.2
1	D	240	ILE	2.1
2	E	161	PHE	2.1
1	B	18	LEU	2.1
1	C	462	LEU	2.1
1	D	496	LEU	2.1
2	H	137	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	472	ARG	2.1
2	H	185	GLY	2.1
2	K	199	GLU	2.1
2	G	130	PHE	2.1
2	P	113	SER	2.1
2	L	195	ASP	2.1
2	P	154	ILE	2.1
1	D	419	LEU	2.1
2	K	192	GLU	2.1
1	B	21	ILE	2.1
1	B	222	LEU	2.1
1	D	479	LEU	2.1
1	J	125	LEU	2.1
1	N	122	LEU	2.1
1	N	462	LEU	2.1
2	H	183	SER	2.1
2	G	196	MET	2.1
1	B	402	TYR	2.1
2	F	190	GLU	2.1
1	J	309	ILE	2.1
1	N	50	PHE	2.1
1	N	390	LEU	2.1
1	B	454	GLN	2.1
1	A	293	PRO	2.1
1	C	46	VAL	2.1
1	J	38	VAL	2.1
1	C	431	LEU	2.1
1	M	42	PHE	2.1
2	P	145	LEU	2.1
2	E	110	GLN	2.1
1	I	469	GLU	2.1
2	E	113	SER	2.0
2	H	139	SER	2.0
1	B	121	LEU	2.0
1	C	122	LEU	2.0
2	P	130	PHE	2.0
2	P	143	ASN	2.0
2	H	150	LYS	2.0
1	A	468	ASN	2.0
2	H	177	LEU	2.0
1	A	409	PHE	2.0
1	D	50	PHE	2.0

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Mol	Chain	Res	Type	RSRZ
1	J	339	ALA	2.0
1	J	28	HIS	2.0
2	F	110	GLN	2.0
2	L	180	VAL	2.0
1	B	36	ARG	2.0
1	C	24	ARG	2.0
1	N	26	LEU	2.0
1	B	212	PHE	2.0
2	L	167	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	CA	O	502	1/1	0.56	0.12	88,88,88,88	0
3	CA	E	502	1/1	0.77	0.13	86,86,86,86	0
3	CA	P	502	1/1	0.83	0.41	84,84,84,84	0
3	CA	O	501	1/1	0.83	0.10	79,79,79,79	0
3	CA	H	502	1/1	0.83	0.54	83,83,83,83	0
3	CA	G	502	1/1	0.83	0.18	84,84,84,84	0
3	CA	G	501	1/1	0.83	0.10	82,82,82,82	0
3	CA	P	501	1/1	0.85	0.24	89,89,89,89	0
3	CA	K	501	1/1	0.85	0.09	80,80,80,80	0
3	CA	L	501	1/1	0.87	0.22	88,88,88,88	0
3	CA	K	502	1/1	0.89	0.20	86,86,86,86	0
3	CA	H	501	1/1	0.90	0.22	90,90,90,90	0
3	CA	F	501	1/1	0.91	0.19	91,91,91,91	0
3	CA	E	501	1/1	0.91	0.12	82,82,82,82	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	CA	L	502	1/1	0.94	0.52	82,82,82,82	0
3	CA	F	502	1/1	0.94	0.53	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.