



wwPDB EM Map/Model Validation Report ⓘ

Oct 17, 2016 – 02:45 PM EDT

PDB ID : 5TB0
EMDB ID: : EMD-8391
Title : Structure of rabbit RyR1 (EGTA-only dataset, all particles)
Authors : Clarke, O.B.; des Georges, A.; Zalk, R.; Marks, A.R.; Hendrickson, W.A.; Frank, J.
Deposited on : 2016-09-10
Resolution : 4.40 Å(reported)

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 : unknown
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) : rb-20027939

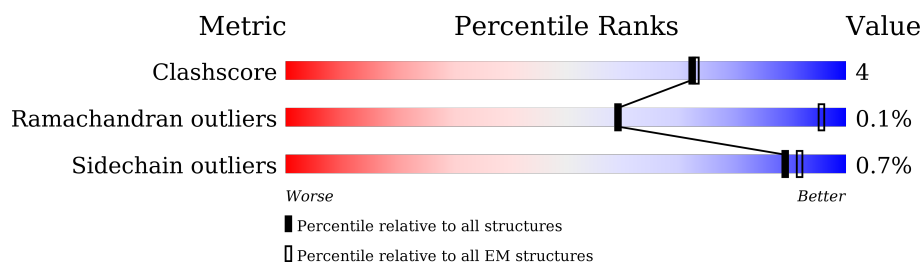
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 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	108	91% 8% .
1	F	108	90% 9% .
1	H	108	91% 8% .
1	J	108	90% 9% .
2	B	4416	85% 10% 5%
2	E	4416	85% 10% 5%
2	G	4416	85% 10% 5%
2	I	4416	85% 10% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 121272 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	F	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	A	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	H	107	Total	C	N	O	S	0	0
			818	516	144	154	4		
1	J	107	Total	C	N	O	S	0	0
			818	516	144	154	4		

- Molecule 2 is a protein called Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	G	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	E	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		
2	I	4194	Total	C	N	O	S	0	0
			29499	18686	5228	5428	157		


- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

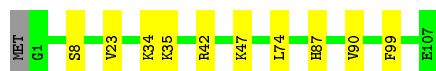
Mol	Chain	Residues	Atoms		AltConf
3	G	1	Total	Zn	0
			1	1	
3	B	1	Total	Zn	0
			1	1	
3	I	1	Total	Zn	0
			1	1	
3	E	1	Total	Zn	0
			1	1	

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.

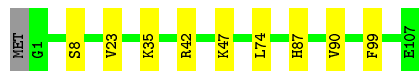
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain F: 



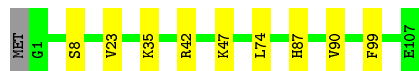
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A: 



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain H: 




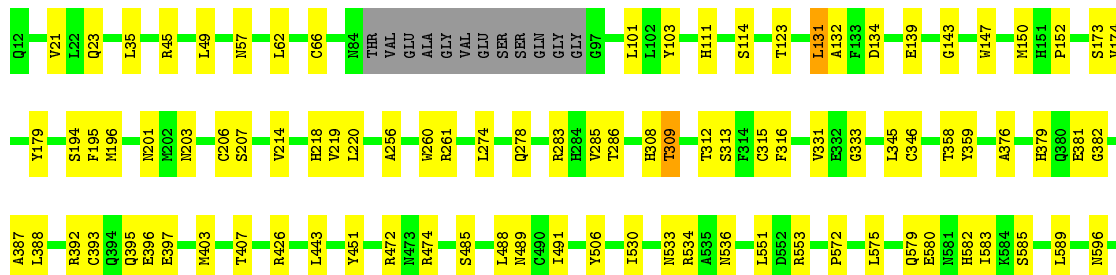
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

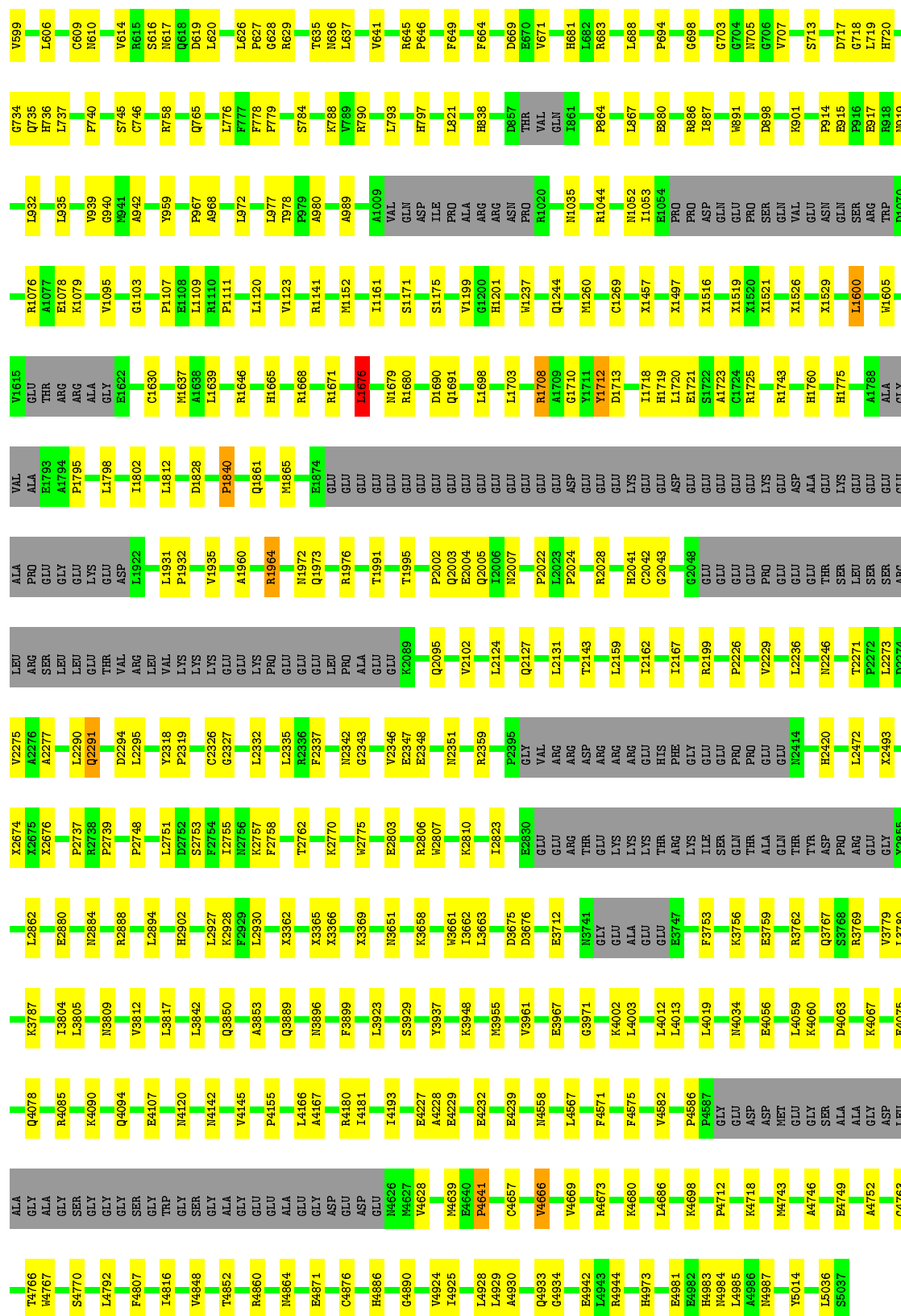
Chain J: 



- Molecule 2: Ryanodine receptor 1

Chain B: 

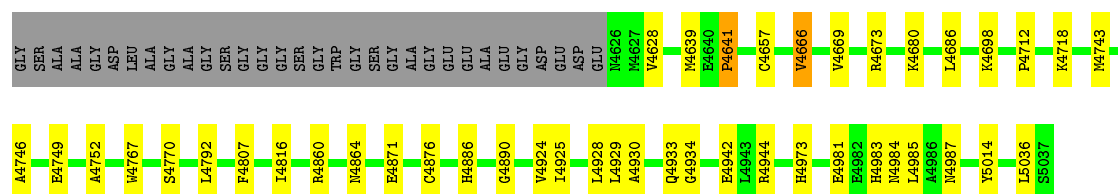




- Molecule 2: Ryanodine receptor 1

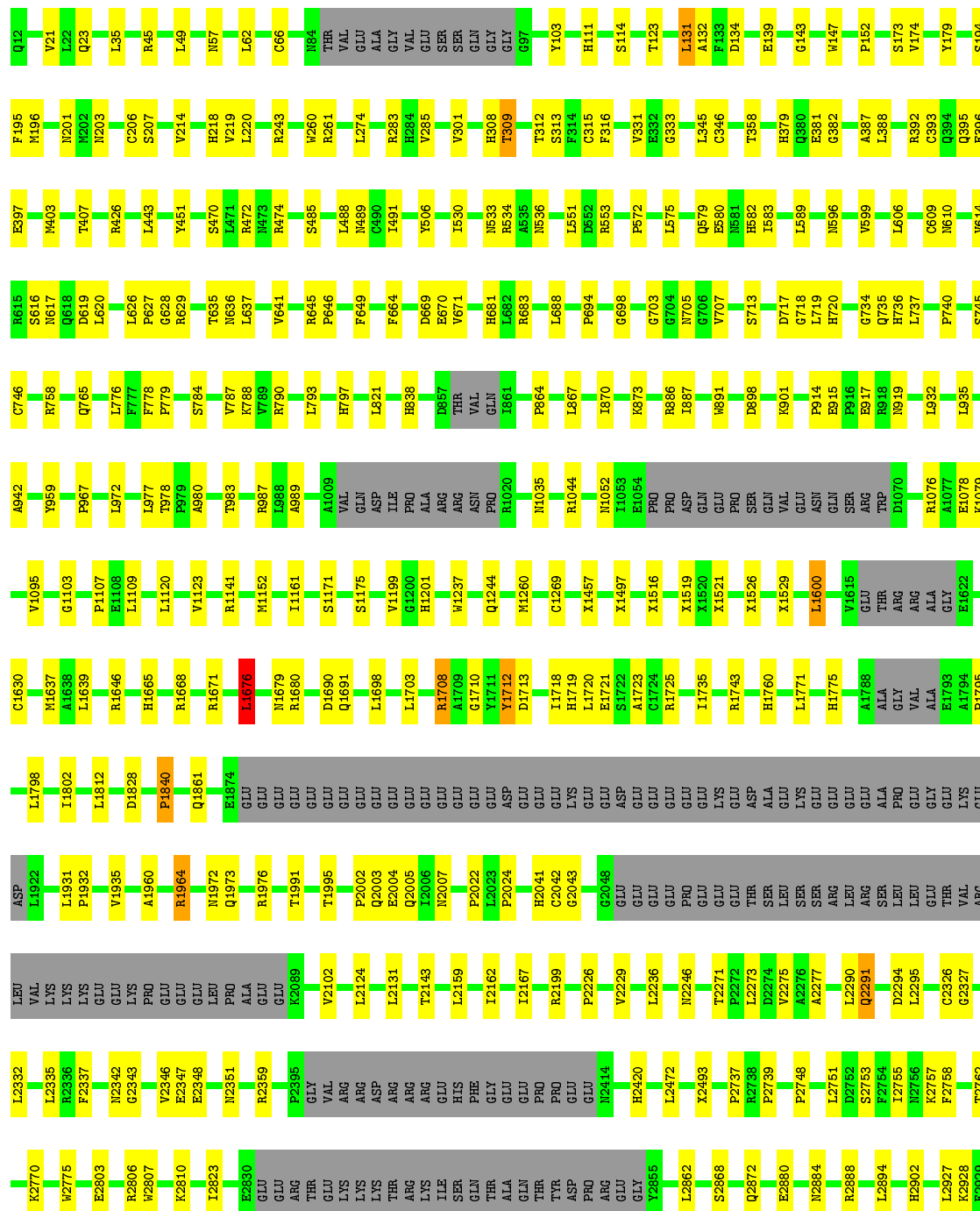
Chain G: 85% 10% 5%

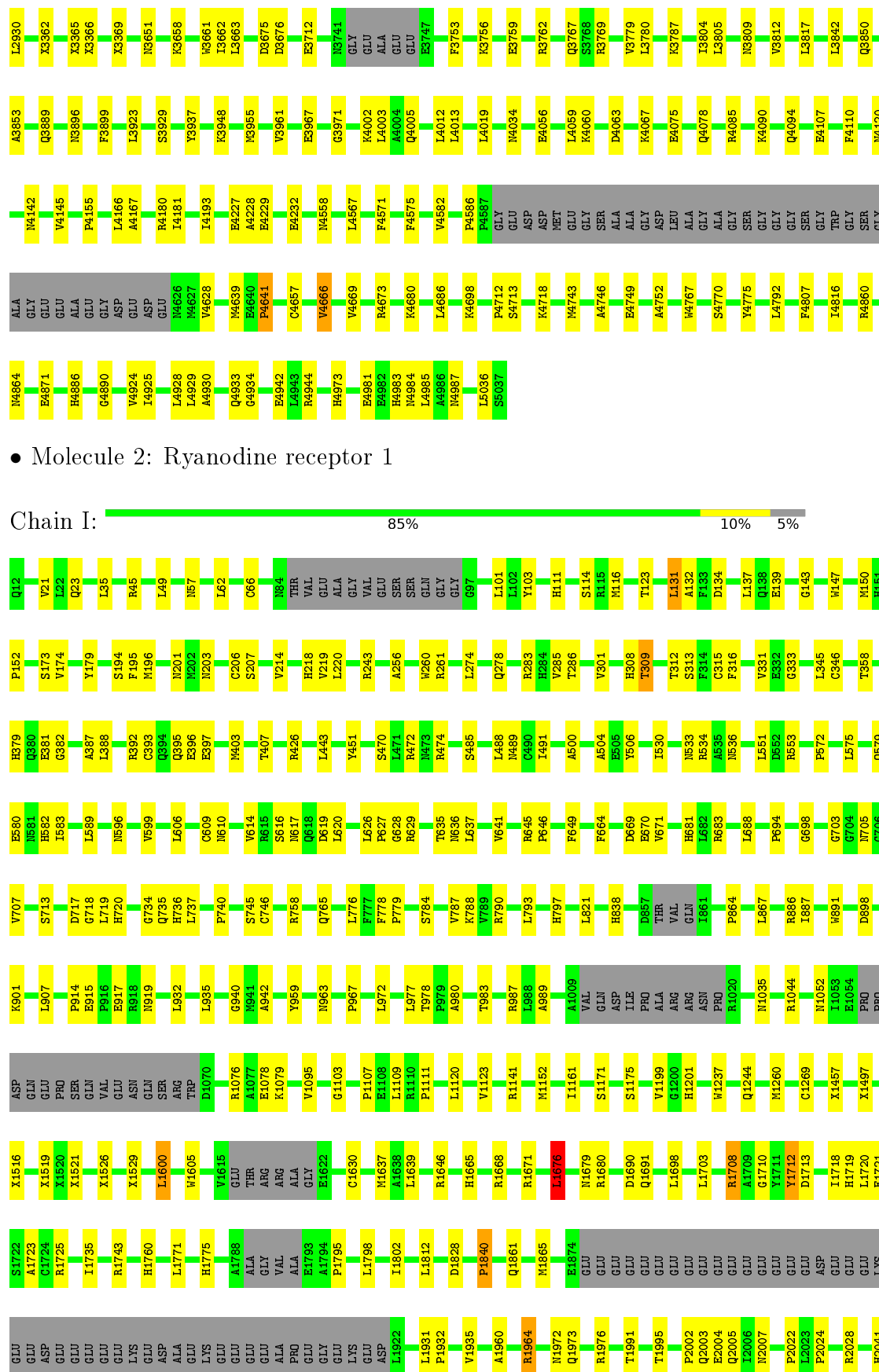


• Molecule 2: Ryanodine receptor 1

Chain E: 85% 10% 5%





N4984	P4712	GLY	F3753	SER	GLU	C2042
L4985	K4718	GLU	K3756	GLN	PRO	G2043
A4986	ASP	ASP	M4034	THR	PRO	G2048
N4987	M4743	MET	E3759	ALA	GLU	GLU
L5036	GLU	GLU	E4056	GLN	GLU	GLU
S5037	A4746	GLY	R3762	THR	N2414	GLU
	E4749	SER	Q3767	TYR	H2420	GLU
	A4752	ALA	S3768	ASP	L2236	GLU
	A4752	ALA	R3769	PRO	L2472	PRO
	G4763	ASP	D4063	ARG	N2246	GLU
	T4766	LEU	K4067	GLY	X2493	GLU
	W4767	ALA	E4075	Y2855	T2271	THR
	W4767	GLY	Q4078	S2868	P2272	SER
	S4770	SER	K3787	X2675	L2273	LEU
	L4792	GLY	S3803	Q2872	V2275	SER
	F4807	GLY	I3804	E2880	A2276	ARG
	I4816	GLY	L3805	E2884	A2277	LEU
	V4848	GLY	N3809	N2884	L2290	ARG
	T4852	SER	V3812	R2888	Q2291	SER
	R4860	TRP	L3817	L2894	D2294	LEU
	N4864	SER	E4107	H2902	L2295	GLU
	E4871	GLY	M4120	L2927	C3326	THR
	C4876	ALA	M4142	L2930	G2327	VAL
	H4886	GLY	V4145	X3362	L2332	LEU
	G4890	GLU	P4155	X3365	L2335	VAL
	V4924	ASP	L4166	X3366	R2336	LYS
	I4925	GLU	A4167	X3369	F2337	LYS
	L4928	ASP	R4180	L3923	N2342	GLU
	L4929	GLU	I4181	S3929	G2343	GLU
	A4930	GLU	I4193	Y3937	V2346	GLU
	Q4933	GLU	E4227	I3661	E2347	LEU
	G4934	GLU	A4228	L3663	E2348	PRO
	E4942	GLU	E4232	D3675	N2351	ALA
	L4943	GLU	E4232	D3676	R2359	GLU
	R4944	GLU	M4558	E3712	P2395	GLU
	H4973	GLU	L4567	C3733	GLY	Q2095
	E4981	GLU	F4571	N3741	VAL	V2102
	E4982	GLU	F4575	GLY	ARG	L2124
	H4983	GLU	V4582	GLU	ASP	Q2127
		GLU	P4586	ALA	ARG	L2131
		GLU	P4587	GLU	GLU	L2159
		GLU		GLU	HIS	L2162
		GLU		GLU	PHE	
		GLU		GLU	GLY	
		GLU		GLU	ILE	

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	55564	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.31	0/834	0.53	0/1123
1	F	0.31	0/834	0.53	0/1123
1	H	0.31	0/834	0.53	0/1123
1	J	0.31	0/834	0.53	0/1123
2	B	0.32	0/25428	0.56	9/34534 (0.0%)
2	E	0.32	0/25428	0.56	9/34534 (0.0%)
2	G	0.32	0/25428	0.56	9/34534 (0.0%)
2	I	0.32	0/25428	0.56	9/34534 (0.0%)
All	All	0.32	0/105048	0.56	36/142628 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	F	0	1
1	H	0	1
1	J	0	1
2	B	0	18
2	E	0	18
2	G	0	18
2	I	0	18
All	All	0	76

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	131	LEU	CA-CB-CG	8.74	135.39	115.30
2	B	131	LEU	CA-CB-CG	8.73	135.38	115.30
2	I	131	LEU	CA-CB-CG	8.72	135.36	115.30
2	E	131	LEU	CA-CB-CG	8.72	135.36	115.30
2	I	1676	LEU	CA-CB-CG	6.26	129.70	115.30
2	G	1676	LEU	CA-CB-CG	6.25	129.69	115.30
2	B	1676	LEU	CA-CB-CG	6.25	129.69	115.30
2	E	1676	LEU	CA-CB-CG	6.25	129.67	115.30
2	G	1600	LEU	CA-CB-CG	6.14	129.42	115.30
2	B	1600	LEU	CA-CB-CG	6.13	129.40	115.30
2	E	1600	LEU	CA-CB-CG	6.13	129.40	115.30
2	I	1600	LEU	CA-CB-CG	6.12	129.37	115.30
2	B	688	LEU	CA-CB-CG	5.92	128.92	115.30
2	I	688	LEU	CA-CB-CG	5.92	128.92	115.30
2	E	688	LEU	CA-CB-CG	5.92	128.91	115.30
2	G	688	LEU	CA-CB-CG	5.91	128.90	115.30
2	E	977	LEU	CA-CB-CG	5.91	128.90	115.30
2	I	977	LEU	CA-CB-CG	5.91	128.90	115.30
2	B	977	LEU	CA-CB-CG	5.91	128.89	115.30
2	G	977	LEU	CA-CB-CG	5.91	128.88	115.30
2	G	2290	LEU	CA-CB-CG	5.62	128.22	115.30
2	E	2290	LEU	CA-CB-CG	5.61	128.21	115.30
2	B	2290	LEU	CA-CB-CG	5.60	128.18	115.30
2	I	2290	LEU	CA-CB-CG	5.59	128.16	115.30
2	I	4985	LEU	CA-CB-CG	5.46	127.85	115.30
2	B	4985	LEU	CA-CB-CG	5.44	127.81	115.30
2	G	4985	LEU	CA-CB-CG	5.44	127.81	115.30
2	E	4985	LEU	CA-CB-CG	5.42	127.77	115.30
2	G	3663	LEU	CA-CB-CG	5.29	127.47	115.30
2	I	3663	LEU	CA-CB-CG	5.28	127.44	115.30
2	B	3663	LEU	CA-CB-CG	5.27	127.43	115.30
2	E	3663	LEU	CA-CB-CG	5.26	127.40	115.30
2	G	4639	MET	C-N-CA	5.07	134.38	121.70
2	I	4639	MET	C-N-CA	5.07	134.37	121.70
2	B	4639	MET	C-N-CA	5.06	134.34	121.70
2	E	4639	MET	C-N-CA	5.06	134.34	121.70

There are no chirality outliers.

All (76) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	8	SER	Peptide
2	B	139	GLU	Peptide

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Mol	Chain	Res	Type	Group
2	B	1676	LEU	Peptide
2	B	1690	ASP	Peptide
2	B	1712	TYR	Peptide
2	B	1720	LEU	Peptide
2	B	1795	PRO	Peptide
2	B	1828	ASP	Peptide
2	B	1840	PRO	Peptide
2	B	2291	GLN	Peptide
2	B	2343	GLY	Peptide
2	B	2472	LEU	Peptide
2	B	2807	TRP	Peptide
2	B	312	THR	Peptide
2	B	3971	GLY	Peptide
2	B	4641	PRO	Peptide
2	B	4666	VAL	Peptide
2	B	4807	PHE	Peptide
2	B	694	PRO	Peptide
2	E	139	GLU	Peptide
2	E	1676	LEU	Peptide
2	E	1690	ASP	Peptide
2	E	1712	TYR	Peptide
2	E	1720	LEU	Peptide
2	E	1795	PRO	Peptide
2	E	1828	ASP	Peptide
2	E	1840	PRO	Peptide
2	E	2291	GLN	Peptide
2	E	2343	GLY	Peptide
2	E	2472	LEU	Peptide
2	E	2807	TRP	Peptide
2	E	312	THR	Peptide
2	E	3971	GLY	Peptide
2	E	4641	PRO	Peptide
2	E	4666	VAL	Peptide
2	E	4807	PHE	Peptide
2	E	694	PRO	Peptide
1	F	8	SER	Peptide
2	G	139	GLU	Peptide
2	G	1676	LEU	Peptide
2	G	1690	ASP	Peptide
2	G	1712	TYR	Peptide
2	G	1720	LEU	Peptide
2	G	1795	PRO	Peptide

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Mol	Chain	Res	Type	Group
2	G	1828	ASP	Peptide
2	G	1840	PRO	Peptide
2	G	2291	GLN	Peptide
2	G	2343	GLY	Peptide
2	G	2472	LEU	Peptide
2	G	2807	TRP	Peptide
2	G	312	THR	Peptide
2	G	3971	GLY	Peptide
2	G	4641	PRO	Peptide
2	G	4666	VAL	Peptide
2	G	4807	PHE	Peptide
2	G	694	PRO	Peptide
1	H	8	SER	Peptide
2	I	139	GLU	Peptide
2	I	1676	LEU	Peptide
2	I	1690	ASP	Peptide
2	I	1712	TYR	Peptide
2	I	1720	LEU	Peptide
2	I	1795	PRO	Peptide
2	I	1828	ASP	Peptide
2	I	1840	PRO	Peptide
2	I	2291	GLN	Peptide
2	I	2343	GLY	Peptide
2	I	2472	LEU	Peptide
2	I	2807	TRP	Peptide
2	I	312	THR	Peptide
2	I	3971	GLY	Peptide
2	I	4641	PRO	Peptide
2	I	4666	VAL	Peptide
2	I	4807	PHE	Peptide
2	I	694	PRO	Peptide
1	J	8	SER	Peptide

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	818	0	824	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	818	0	824	6	0
1	H	818	0	824	5	0
1	J	818	0	824	6	0
2	B	29499	0	24749	236	0
2	E	29499	0	24750	227	0
2	G	29499	0	24749	236	0
2	I	29499	0	24749	237	0
3	B	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
3	I	1	0	0	0	0
All	All	121272	0	102293	929	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 4.

All (929) 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)
2:I:2291:GLN:HB3	2:I:2294:ASP:H	1.55	0.72
2:B:2291:GLN:HB3	2:B:2294:ASP:H	1.55	0.71
2:G:2291:GLN:HB3	2:G:2294:ASP:H	1.55	0.71
2:E:2291:GLN:HB3	2:E:2294:ASP:H	1.55	0.71
2:B:1260:MET:HB2	2:B:1269:CYS:H	1.62	0.65
2:B:331:VAL:HG12	2:B:333:GLY:H	1.61	0.65
2:E:1260:MET:HB2	2:E:1269:CYS:H	1.62	0.65
2:G:1260:MET:HB2	2:G:1269:CYS:H	1.62	0.65
2:I:331:VAL:HG12	2:I:333:GLY:H	1.61	0.64
2:G:1721:GLU:OE2	2:G:1725:ARG:NH2	2.31	0.64
2:E:331:VAL:HG12	2:E:333:GLY:H	1.61	0.64
2:E:942:ALA:HB2	2:E:1052:ASN:HB2	1.80	0.64
2:I:1260:MET:HB2	2:I:1269:CYS:H	1.62	0.64
2:I:1721:GLU:OE2	2:I:1725:ARG:NH2	2.31	0.64
2:G:942:ALA:HB2	2:G:1052:ASN:HB2	1.80	0.64
2:E:1721:GLU:OE2	2:E:1725:ARG:NH2	2.31	0.63
2:I:942:ALA:HB2	2:I:1052:ASN:HB2	1.80	0.63
2:I:379:HIS:HD2	2:I:382:GLY:H	1.47	0.63
2:B:942:ALA:HB2	2:B:1052:ASN:HB2	1.80	0.63
2:G:331:VAL:HG12	2:G:333:GLY:H	1.61	0.63
2:G:788:LYS:HG2	2:G:1630:CYS:H	1.64	0.63
2:B:1721:GLU:OE2	2:B:1725:ARG:NH2	2.31	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:788:LYS:HG2	2:I:1630:CYS:H	1.64	0.62
2:B:379:HIS:HD2	2:B:382:GLY:H	1.47	0.62
2:E:2347:GLU:O	2:E:2351:ASN:N	2.32	0.62
2:E:788:LYS:HG2	2:E:1630:CYS:H	1.64	0.61
2:B:788:LYS:HG2	2:B:1630:CYS:H	1.64	0.61
2:E:646:PRO:HD2	2:E:779:PRO:HB2	1.83	0.61
2:G:646:PRO:HD2	2:G:779:PRO:HB2	1.83	0.61
2:E:379:HIS:HD2	2:E:382:GLY:H	1.47	0.61
2:B:4973:HIS:NE2	2:I:4227:GLU:OE2	2.29	0.61
2:G:379:HIS:HD2	2:G:382:GLY:H	1.47	0.61
2:B:1519:UNK:HA	2:B:1526:UNK:HA	1.83	0.60
2:B:646:PRO:HD2	2:B:779:PRO:HB2	1.83	0.60
2:I:646:PRO:HD2	2:I:779:PRO:HB2	1.83	0.60
2:E:1519:UNK:HA	2:E:1526:UNK:HA	1.83	0.60
2:B:2347:GLU:O	2:B:2351:ASN:N	2.32	0.60
2:B:3937:TYR:O	2:B:4002:LYS:NZ	2.35	0.60
2:B:2748:PRO:HD2	2:B:2751:LEU:HD12	1.83	0.60
2:G:2748:PRO:HD2	2:G:2751:LEU:HD12	1.83	0.60
2:I:3937:TYR:O	2:I:4002:LYS:NZ	2.35	0.60
2:B:4984:ASN:OD1	2:B:4987:ASN:N	2.34	0.59
2:G:2347:GLU:O	2:G:2351:ASN:N	2.32	0.59
2:I:1519:UNK:HA	2:I:1526:UNK:HA	1.83	0.59
2:I:4180:ARG:NH1	2:I:4981:GLU:OE1	2.36	0.59
2:B:3675:ASP:OD1	2:B:3769:ARG:NH2	2.36	0.59
2:G:1519:UNK:HA	2:G:1526:UNK:HA	1.83	0.59
2:G:3937:TYR:O	2:G:4002:LYS:NZ	2.35	0.59
2:B:4227:GLU:OE2	2:E:4973:HIS:NE2	2.29	0.59
2:E:3937:TYR:O	2:E:4002:LYS:NZ	2.35	0.59
2:E:4180:ARG:NH1	2:E:4981:GLU:OE1	2.36	0.59
2:G:179:TYR:OH	2:I:2359:ARG:NH2	2.36	0.59
2:G:2359:ARG:NH2	2:E:179:TYR:OH	2.36	0.59
2:E:2748:PRO:HD2	2:E:2751:LEU:HD12	1.83	0.59
2:I:2748:PRO:HD2	2:I:2751:LEU:HD12	1.83	0.59
2:B:1079:LYS:NZ	2:B:1107:PRO:O	2.36	0.59
2:I:4984:ASN:OD1	2:I:4987:ASN:N	2.34	0.59
2:B:4180:ARG:NH1	2:B:4981:GLU:OE1	2.36	0.59
2:G:3675:ASP:OD1	2:G:3769:ARG:NH2	2.36	0.59
2:G:4180:ARG:NH1	2:G:4981:GLU:OE1	2.36	0.59
2:I:2347:GLU:O	2:I:2351:ASN:N	2.32	0.59
2:B:2291:GLN:HB2	2:B:2295:LEU:HG	1.85	0.58
2:E:580:GLU:HG2	2:E:583:ILE:HD11	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1079:LYS:NZ	2:G:1107:PRO:O	2.36	0.58
2:G:4227:GLU:OE2	2:I:4973:HIS:NE2	2.26	0.58
2:G:580:GLU:HG2	2:G:583:ILE:HD11	1.85	0.58
2:I:2291:GLN:HB2	2:I:2295:LEU:HG	1.85	0.58
1:J:74:LEU:HB2	1:J:99:PHE:HB2	1.85	0.58
2:E:1079:LYS:NZ	2:E:1107:PRO:O	2.36	0.58
2:E:3675:ASP:OD1	2:E:3769:ARG:NH2	2.36	0.58
1:H:74:LEU:HB2	1:H:99:PHE:HB2	1.85	0.58
2:I:1079:LYS:NZ	2:I:1107:PRO:O	2.36	0.58
2:G:2291:GLN:HB2	2:G:2295:LEU:HG	1.85	0.58
1:A:74:LEU:HB2	1:A:99:PHE:HB2	1.85	0.58
2:E:2291:GLN:HB2	2:E:2295:LEU:HG	1.85	0.58
2:G:1743:ARG:O	2:G:1964:ARG:NH2	2.37	0.58
2:G:4984:ASN:OD1	2:G:4987:ASN:N	2.34	0.58
2:B:35:LEU:HD13	2:B:49:LEU:HD13	1.86	0.57
1:F:74:LEU:HB2	1:F:99:PHE:HB2	1.85	0.57
2:G:4582:VAL:HG11	2:E:4860:ARG:HD2	1.86	0.57
2:I:3675:ASP:OD1	2:I:3769:ARG:NH2	2.36	0.57
1:F:42:ARG:HG2	2:E:1691:GLN:HG2	1.87	0.57
2:I:4567:LEU:HA	2:I:4816:ILE:HD12	1.87	0.57
2:B:4567:LEU:HA	2:B:4816:ILE:HD12	1.87	0.57
2:B:4860:ARG:HD2	2:E:4582:VAL:HG11	1.87	0.57
2:G:393:CYS:SG	2:G:395:GLN:NE2	2.77	0.57
2:B:664:PHE:HB2	2:B:746:CYS:HB2	1.87	0.57
2:I:1743:ARG:O	2:I:1964:ARG:NH2	2.37	0.57
2:I:664:PHE:HB2	2:I:746:CYS:HB2	1.87	0.57
2:G:4567:LEU:HA	2:G:4816:ILE:HD12	1.87	0.57
2:B:4582:VAL:HG11	2:I:4860:ARG:HD2	1.86	0.57
2:B:580:GLU:HG2	2:B:583:ILE:HD11	1.85	0.57
2:G:35:LEU:HD13	2:G:49:LEU:HD13	1.86	0.57
2:G:4942:GLU:HA	2:I:4944:ARG:HH22	1.70	0.57
2:B:2359:ARG:NH2	2:I:179:TYR:OH	2.37	0.57
2:I:2755:ILE:HD13	2:I:2810:LYS:HG2	1.87	0.57
2:I:580:GLU:HG2	2:I:583:ILE:HD11	1.85	0.57
2:I:393:CYS:SG	2:I:395:GLN:NE2	2.77	0.57
2:B:393:CYS:SG	2:B:395:GLN:NE2	2.77	0.57
2:B:745:SER:HB2	2:B:758:ARG:HB3	1.87	0.57
2:B:1743:ARG:O	2:B:1964:ARG:NH2	2.37	0.56
2:E:1152:MET:HB2	2:E:1161:ILE:HB	1.87	0.56
2:E:393:CYS:SG	2:E:395:GLN:NE2	2.77	0.56
2:E:664:PHE:HB2	2:E:746:CYS:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:4933:GLN:NE2	2:I:4933:GLN:OE1	2.38	0.56
2:I:745:SER:HB2	2:I:758:ARG:HB3	1.87	0.56
2:E:4984:ASN:OD1	2:E:4987:ASN:N	2.34	0.56
2:E:719:LEU:HD22	2:E:735:GLN:HG2	1.87	0.56
2:I:35:LEU:HD13	2:I:49:LEU:HD13	1.86	0.56
2:B:2755:ILE:HD13	2:B:2810:LYS:HG2	1.87	0.56
2:B:719:LEU:HD22	2:B:735:GLN:HG2	1.87	0.56
2:E:1743:ARG:O	2:E:1964:ARG:NH2	2.37	0.56
2:E:35:LEU:HD13	2:E:49:LEU:HD13	1.86	0.56
2:E:2755:ILE:HD13	2:E:2810:LYS:HG2	1.87	0.56
2:E:745:SER:HB2	2:E:758:ARG:HB3	1.87	0.56
2:E:4567:LEU:HA	2:E:4816:ILE:HD12	1.87	0.56
2:G:2042:CYS:SG	2:G:2043:GLY:N	2.78	0.56
2:G:641:VAL:HG21	2:G:705:ASN:HA	1.87	0.56
2:G:664:PHE:HB2	2:G:746:CYS:HB2	1.87	0.56
2:G:745:SER:HB2	2:G:758:ARG:HB3	1.87	0.56
2:I:23:GLN:OE1	2:I:203:ASN:ND2	2.34	0.56
2:B:1152:MET:HB2	2:B:1161:ILE:HB	1.87	0.56
2:E:641:VAL:HG21	2:E:705:ASN:HA	1.87	0.56
2:G:1152:MET:HB2	2:G:1161:ILE:HB	1.87	0.56
2:E:2042:CYS:SG	2:E:2043:GLY:N	2.78	0.56
2:B:23:GLN:OE1	2:B:203:ASN:ND2	2.34	0.56
2:G:2755:ILE:HD13	2:G:2810:LYS:HG2	1.87	0.56
2:E:4864:ASN:ND2	2:E:4871:GLU:OE1	2.39	0.56
2:G:2342:ASN:N	2:G:2342:ASN:OD1	2.39	0.56
2:I:719:LEU:HD22	2:I:735:GLN:HG2	1.87	0.56
2:B:179:TYR:OH	2:E:2359:ARG:NH2	2.38	0.56
2:E:2803:GLU:OE2	2:E:2806:ARG:NH1	2.39	0.56
2:G:4973:HIS:NE2	2:E:4227:GLU:OE2	2.32	0.56
2:B:2770:LYS:HB3	2:B:2775:TRP:HB2	1.88	0.55
2:G:719:LEU:HD22	2:G:735:GLN:HG2	1.87	0.55
2:I:1152:MET:HB2	2:I:1161:ILE:HB	1.87	0.55
2:I:2042:CYS:SG	2:I:2043:GLY:N	2.78	0.55
2:G:4864:ASN:ND2	2:G:4871:GLU:OE1	2.39	0.55
2:E:485:SER:O	2:E:489:ASN:N	2.38	0.55
2:G:2770:LYS:HB3	2:G:2775:TRP:HB2	1.88	0.55
2:G:626:LEU:HG	2:G:628:GLY:H	1.72	0.55
2:I:2770:LYS:HB3	2:I:2775:TRP:HB2	1.88	0.55
2:I:4864:ASN:ND2	2:I:4871:GLU:OE1	2.39	0.55
2:B:614:VAL:HG22	2:B:616:SER:H	1.72	0.55
2:E:614:VAL:HG22	2:E:616:SER:H	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2737:PRO:O	2:I:2888:ARG:NH2	2.40	0.55
2:B:2342:ASN:N	2:B:2342:ASN:OD1	2.39	0.55
2:I:626:LEU:HG	2:I:628:GLY:H	1.72	0.55
2:B:4864:ASN:ND2	2:B:4871:GLU:OE1	2.39	0.55
2:E:2770:LYS:HB3	2:E:2775:TRP:HB2	1.89	0.55
2:E:2737:PRO:O	2:E:2888:ARG:NH2	2.40	0.55
2:G:2803:GLU:OE2	2:G:2806:ARG:NH1	2.39	0.55
2:I:315:CYS:SG	2:I:316:PHE:N	2.80	0.55
2:G:614:VAL:HG22	2:G:616:SER:H	1.72	0.55
2:I:619:ASP:OD1	2:I:1680:ARG:NH1	2.38	0.55
2:E:23:GLN:OE1	2:E:203:ASN:ND2	2.34	0.55
2:I:614:VAL:HG22	2:I:616:SER:H	1.72	0.55
2:B:2803:GLU:OE2	2:B:2806:ARG:NH1	2.39	0.55
2:E:626:LEU:HG	2:E:628:GLY:H	1.72	0.55
2:G:2737:PRO:O	2:G:2888:ARG:NH2	2.40	0.55
2:G:315:CYS:SG	2:G:316:PHE:N	2.80	0.55
2:B:2737:PRO:O	2:B:2888:ARG:NH2	2.40	0.54
2:I:2803:GLU:OE2	2:I:2806:ARG:NH1	2.39	0.54
2:B:641:VAL:HG21	2:B:705:ASN:HA	1.87	0.54
2:E:3809:ASN:HB3	2:E:3812:VAL:HG22	1.89	0.54
2:G:2739:PRO:HB3	2:G:2884:ASN:HB3	1.89	0.54
2:G:3809:ASN:HB3	2:G:3812:VAL:HG22	1.89	0.54
2:G:671:VAL:HG22	2:G:740:PRO:HG3	1.89	0.54
2:B:626:LEU:HG	2:B:628:GLY:H	1.72	0.54
2:E:2739:PRO:HB3	2:E:2884:ASN:HB3	1.89	0.54
2:E:315:CYS:SG	2:E:316:PHE:N	2.80	0.54
2:G:2346:VAL:HG22	2:G:2348:GLU:H	1.73	0.54
2:I:641:VAL:HG21	2:I:705:ASN:HA	1.87	0.54
2:I:2739:PRO:HB3	2:I:2884:ASN:HB3	1.89	0.54
2:I:3809:ASN:HB3	2:I:3812:VAL:HG22	1.89	0.54
2:B:2346:VAL:HG22	2:B:2348:GLU:H	1.73	0.54
2:B:315:CYS:SG	2:B:316:PHE:N	2.80	0.54
2:E:3817:LEU:HD13	2:E:3899:PHE:HD1	1.73	0.54
2:I:2342:ASN:OD1	2:I:2342:ASN:N	2.39	0.54
2:B:3809:ASN:HB3	2:B:3812:VAL:HG22	1.89	0.54
2:E:1679:ASN:ND2	2:E:1798:LEU:O	2.41	0.54
2:B:671:VAL:HG22	2:B:740:PRO:HG3	1.89	0.54
2:E:2342:ASN:OD1	2:E:2342:ASN:N	2.39	0.54
2:I:3817:LEU:HD13	2:I:3899:PHE:HD1	1.73	0.54
2:B:1679:ASN:ND2	2:B:1798:LEU:O	2.41	0.54
2:B:3817:LEU:HD13	2:B:3899:PHE:HD1	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:358:THR:HG21	2:B:382:GLY:HA2	1.90	0.53
2:E:2003:GLN:O	2:E:2007:ASN:ND2	2.42	0.53
2:B:4930:ALA:O	2:B:4934:GLY:N	2.42	0.53
2:G:4930:ALA:O	2:G:4934:GLY:N	2.42	0.53
2:I:2346:VAL:HG22	2:I:2348:GLU:H	1.73	0.53
2:G:2003:GLN:O	2:G:2007:ASN:ND2	2.42	0.53
2:I:2003:GLN:O	2:I:2007:ASN:ND2	2.42	0.53
2:E:4090:LYS:O	2:E:4094:GLN:N	2.40	0.53
2:E:4075:GLU:HA	2:E:4078:GLN:HB2	1.91	0.53
2:I:671:VAL:HG22	2:I:740:PRO:HG3	1.89	0.53
2:E:671:VAL:HG22	2:E:740:PRO:HG3	1.89	0.53
2:I:1679:ASN:ND2	2:I:1798:LEU:O	2.41	0.53
2:I:1691:GLN:HE22	2:I:1802:ILE:HG12	1.74	0.53
2:I:4930:ALA:O	2:I:4934:GLY:N	2.42	0.53
2:B:1691:GLN:HE22	2:B:1802:ILE:HG12	1.74	0.53
2:B:2739:PRO:HB3	2:B:2884:ASN:HB3	1.89	0.53
2:E:2346:VAL:HG22	2:E:2348:GLU:H	1.73	0.53
2:E:4571:PHE:O	2:E:4575:PHE:N	2.42	0.53
2:E:4930:ALA:O	2:E:4934:GLY:N	2.41	0.53
2:G:1679:ASN:ND2	2:G:1798:LEU:O	2.41	0.53
2:G:3817:LEU:HD13	2:G:3899:PHE:HD1	1.73	0.53
2:B:2003:GLN:O	2:B:2007:ASN:ND2	2.42	0.53
2:B:4075:GLU:HA	2:B:4078:GLN:HB2	1.91	0.53
2:G:358:THR:HG21	2:G:382:GLY:HA2	1.90	0.53
2:E:358:THR:HG21	2:E:382:GLY:HA2	1.90	0.52
2:I:4571:PHE:O	2:I:4575:PHE:N	2.42	0.52
2:B:4571:PHE:O	2:B:4575:PHE:N	2.42	0.52
2:B:572:PRO:HA	2:B:575:LEU:HD13	1.92	0.52
2:G:4571:PHE:O	2:G:4575:PHE:N	2.42	0.52
2:E:619:ASP:OD1	2:E:1680:ARG:NH1	2.39	0.52
2:G:2199:ARG:NH2	2:G:2246:ASN:OD1	2.43	0.52
2:G:619:ASP:OD1	2:G:1680:ARG:NH1	2.38	0.52
2:I:2199:ARG:NH2	2:I:2246:ASN:OD1	2.43	0.52
2:I:358:THR:HG21	2:I:382:GLY:HA2	1.90	0.52
2:B:485:SER:O	2:B:489:ASN:N	2.38	0.52
2:E:1691:GLN:HE22	2:E:1802:ILE:HG12	1.74	0.52
2:I:635:THR:HB	2:I:1639:LEU:HD23	1.92	0.52
2:I:4181:ILE:HG23	2:I:4193:ILE:HB	1.92	0.52
2:B:2199:ARG:NH2	2:B:2246:ASN:OD1	2.43	0.52
2:I:4075:GLU:HA	2:I:4078:GLN:HB2	1.91	0.52
2:I:533:ASN:ND2	2:I:536:ASN:OD1	2.38	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1691:GLN:HE22	2:G:1802:ILE:HG12	1.74	0.52
2:G:669:ASP:OD2	2:G:790:ARG:NH2	2.43	0.52
2:I:173:SER:OG	2:I:174:VAL:N	2.43	0.52
2:I:572:PRO:HA	2:I:575:LEU:HD13	1.92	0.52
2:G:4181:ILE:HG23	2:G:4193:ILE:HB	1.92	0.52
2:E:4181:ILE:HG23	2:E:4193:ILE:HB	1.92	0.52
2:G:635:THR:HB	2:G:1639:LEU:HD23	1.92	0.52
2:B:173:SER:OG	2:B:174:VAL:N	2.43	0.51
2:E:572:PRO:HA	2:E:575:LEU:HD13	1.92	0.51
2:G:4075:GLU:HA	2:G:4078:GLN:HB2	1.91	0.51
1:A:42:ARG:HG2	2:B:1691:GLN:HG2	1.92	0.51
2:B:635:THR:HB	2:B:1639:LEU:HD23	1.92	0.51
2:I:1516:UNK:N	2:I:1529:UNK:O	2.44	0.51
2:I:4059:LEU:HD13	2:I:4167:ALA:HB2	1.92	0.51
2:I:4063:ASP:O	2:I:4067:LYS:NZ	2.36	0.51
2:B:4181:ILE:HG23	2:B:4193:ILE:HB	1.92	0.51
2:B:619:ASP:OD1	2:B:1680:ARG:NH1	2.38	0.51
2:I:4673:ARG:HH22	2:I:4698:LYS:HB2	1.75	0.51
2:E:2199:ARG:NH2	2:E:2246:ASN:OD1	2.43	0.51
2:B:4933:GLN:NE2	2:E:4933:GLN:OE1	2.43	0.51
2:G:4673:ARG:HH22	2:G:4698:LYS:HB2	1.75	0.51
2:G:572:PRO:HA	2:G:575:LEU:HD13	1.92	0.51
2:I:4003:LEU:HB2	2:I:4013:LEU:HD13	1.93	0.51
2:B:2042:CYS:SG	2:B:2043:GLY:N	2.78	0.51
2:B:4063:ASP:O	2:B:4067:LYS:NZ	2.36	0.51
2:B:533:ASN:ND2	2:B:536:ASN:OD1	2.38	0.51
2:B:596:ASN:HB3	2:B:599:VAL:HG22	1.93	0.51
2:G:173:SER:OG	2:G:174:VAL:N	2.43	0.51
2:G:4003:LEU:HB2	2:G:4013:LEU:HD13	1.93	0.51
2:G:4860:ARG:HD2	2:I:4582:VAL:HG11	1.92	0.51
2:I:4090:LYS:O	2:I:4094:GLN:N	2.40	0.51
2:B:4003:LEU:HB2	2:B:4013:LEU:HD13	1.93	0.51
2:B:717:ASP:OD1	2:B:720:HIS:ND1	2.44	0.51
2:E:1516:UNK:N	2:E:1529:UNK:O	2.44	0.51
2:G:717:ASP:OD1	2:G:720:HIS:ND1	2.44	0.51
2:I:717:ASP:OD1	2:I:720:HIS:ND1	2.44	0.51
2:B:4942:GLU:HA	2:E:4944:ARG:HH22	1.76	0.51
2:E:4673:ARG:HH22	2:E:4698:LYS:HB2	1.75	0.51
2:I:596:ASN:HB3	2:I:599:VAL:HG22	1.93	0.51
2:B:4680:LYS:HD3	2:B:4686:LEU:HD22	1.93	0.51
2:B:4944:ARG:HH22	2:I:4942:GLU:HA	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4003:LEU:HB2	2:E:4013:LEU:HD13	1.93	0.50
2:G:1718:ILE:HG13	2:G:1719:HIS:CD2	2.46	0.50
2:G:596:ASN:HB3	2:G:599:VAL:HG22	1.93	0.50
2:I:1103:GLY:HA3	2:I:1123:VAL:HA	1.94	0.50
2:I:4743:MET:HB3	2:I:4746:ALA:HB3	1.93	0.50
2:B:4059:LEU:HD13	2:B:4167:ALA:HB2	1.92	0.50
2:E:4059:LEU:HD13	2:E:4167:ALA:HB2	1.92	0.50
2:I:1718:ILE:HG13	2:I:1719:HIS:CD2	2.46	0.50
2:B:609:CYS:SG	2:B:610:ASN:N	2.85	0.50
2:G:1516:UNK:N	2:G:1529:UNK:O	2.44	0.50
2:G:4090:LYS:O	2:G:4094:GLN:N	2.40	0.50
2:G:4059:LEU:HD13	2:G:4167:ALA:HB2	1.92	0.50
2:G:609:CYS:SG	2:G:610:ASN:N	2.85	0.50
2:B:1516:UNK:N	2:B:1529:UNK:O	2.44	0.50
2:B:1718:ILE:HG13	2:B:1719:HIS:CD2	2.46	0.50
2:B:4933:GLN:OE1	2:I:4933:GLN:NE2	2.44	0.50
2:E:669:ASP:OD2	2:E:790:ARG:NH2	2.42	0.50
2:E:426:ARG:HB2	2:E:506:TYR:HA	1.94	0.50
2:E:717:ASP:OD1	2:E:720:HIS:ND1	2.44	0.50
2:G:23:GLN:OE1	2:G:203:ASN:ND2	2.34	0.50
2:G:396:GLU:OE2	2:G:451:TYR:OH	2.28	0.50
2:B:1103:GLY:HA3	2:B:1123:VAL:HA	1.94	0.50
2:B:4673:ARG:HH22	2:B:4698:LYS:HB2	1.75	0.50
2:E:1718:ILE:HG13	2:E:1719:HIS:CD2	2.46	0.50
2:G:4944:ARG:HH22	2:E:4942:GLU:HA	1.76	0.50
2:I:396:GLU:OE2	2:I:451:TYR:OH	2.28	0.50
2:I:4680:LYS:HD3	2:I:4686:LEU:HD22	1.93	0.50
2:I:609:CYS:SG	2:I:610:ASN:N	2.85	0.50
2:B:683:ARG:NH1	2:B:707:VAL:O	2.43	0.50
2:E:173:SER:OG	2:E:174:VAL:N	2.43	0.50
1:F:87:HIS:HD2	1:F:90:VAL:HB	1.77	0.50
2:G:627:PRO:O	2:G:629:ARG:NH1	2.45	0.50
2:B:111:HIS:CD2	2:B:114:SER:H	2.30	0.50
2:B:2002:PRO:HA	2:B:2005:GLN:HB3	1.94	0.50
2:B:669:ASP:OD2	2:B:790:ARG:NH2	2.43	0.50
2:I:627:PRO:O	2:I:629:ARG:NH1	2.45	0.50
2:I:864:PRO:HD2	2:I:867:LEU:HD12	1.94	0.50
2:E:111:HIS:CD2	2:E:114:SER:H	2.30	0.50
2:E:4680:LYS:HD3	2:E:4686:LEU:HD22	1.93	0.50
2:E:635:THR:HB	2:E:1639:LEU:HD23	1.92	0.50
2:G:1103:GLY:HA3	2:G:1123:VAL:HA	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1698:LEU:N	2:G:1712:TYR:OH	2.45	0.50
1:J:42:ARG:HG2	2:I:1691:GLN:HG2	1.94	0.50
2:B:627:PRO:O	2:B:629:ARG:NH1	2.45	0.49
2:E:596:ASN:HB3	2:E:599:VAL:HG22	1.93	0.49
2:E:683:ARG:NH1	2:E:707:VAL:O	2.43	0.49
2:I:637:LEU:HD23	2:I:1637:MET:HB3	1.94	0.49
2:I:214:VAL:HG12	2:I:274:LEU:HD12	1.94	0.49
2:I:989:ALA:O	2:I:1035:ASN:ND2	2.44	0.49
2:G:1244:GLN:OE1	2:G:1646:ARG:NH1	2.45	0.49
2:I:2002:PRO:HA	2:I:2005:GLN:HB3	1.94	0.49
2:I:488:LEU:HD23	2:I:491:ILE:HD12	1.94	0.49
1:J:35:LYS:HD3	2:I:636:ASN:HD21	1.77	0.49
2:B:989:ALA:O	2:B:1035:ASN:ND2	2.44	0.49
2:B:3753:PHE:HA	2:B:3756:LYS:HB3	1.93	0.49
2:B:488:LEU:HD23	2:B:491:ILE:HD12	1.94	0.49
2:E:609:CYS:SG	2:E:610:ASN:N	2.85	0.49
2:E:683:ARG:HG2	2:E:717:ASP:HB3	1.95	0.49
2:G:214:VAL:HG12	2:G:274:LEU:HD12	1.94	0.49
2:G:533:ASN:ND2	2:G:536:ASN:OD1	2.38	0.49
1:H:87:HIS:HD2	1:H:90:VAL:HB	1.77	0.49
2:I:707:VAL:HG23	2:I:713:SER:HB2	1.94	0.49
2:B:4090:LYS:O	2:B:4094:GLN:N	2.40	0.49
2:B:864:PRO:HD2	2:B:867:LEU:HD12	1.94	0.49
2:E:206:CYS:SG	2:E:207:SER:N	2.85	0.49
2:G:4743:MET:HB3	2:G:4746:ALA:HB3	1.93	0.49
2:G:707:VAL:HG23	2:G:713:SER:HB2	1.94	0.49
2:I:1244:GLN:OE1	2:I:1646:ARG:NH1	2.45	0.49
2:I:206:CYS:SG	2:I:207:SER:N	2.85	0.49
2:I:3753:PHE:HA	2:I:3756:LYS:HB3	1.93	0.49
2:I:2332:LEU:HD13	2:I:2335:LEU:HD12	1.95	0.49
2:B:1698:LEU:N	2:B:1712:TYR:OH	2.45	0.49
2:B:214:VAL:HG12	2:B:274:LEU:HD12	1.94	0.49
2:E:4924:VAL:HA	2:E:4928:LEU:HB2	1.94	0.49
2:G:2894:LEU:HD11	2:G:2902:HIS:HB2	1.94	0.49
2:G:4680:LYS:HD3	2:G:4686:LEU:HD22	1.93	0.49
2:G:637:LEU:HD23	2:G:1637:MET:HB3	1.94	0.49
2:I:3842:LEU:O	2:I:3929:SER:OG	2.31	0.49
2:I:426:ARG:HB2	2:I:506:TYR:HA	1.93	0.49
2:B:1244:GLN:OE1	2:B:1646:ARG:NH1	2.45	0.49
2:B:1703:LEU:HD12	2:B:1708:ARG:HB2	1.95	0.49
2:E:1244:GLN:OE1	2:E:1646:ARG:NH1	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:214:VAL:HG12	2:E:274:LEU:HD12	1.94	0.49
2:E:3753:PHE:HA	2:E:3756:LYS:HB3	1.93	0.49
2:E:627:PRO:O	2:E:629:ARG:NH1	2.45	0.49
2:G:111:HIS:CD2	2:G:114:SER:H	2.30	0.49
2:G:488:LEU:HD23	2:G:491:ILE:HD12	1.94	0.49
2:B:2332:LEU:HD13	2:B:2335:LEU:HD12	1.95	0.49
2:B:426:ARG:HB2	2:B:506:TYR:HA	1.93	0.49
2:E:4743:MET:HB3	2:E:4746:ALA:HB3	1.93	0.49
2:G:206:CYS:SG	2:G:207:SER:N	2.85	0.49
2:G:3842:LEU:O	2:G:3929:SER:OG	2.31	0.49
2:I:111:HIS:CD2	2:I:114:SER:H	2.30	0.49
2:I:1703:LEU:HD12	2:I:1708:ARG:HB2	1.95	0.49
1:A:87:HIS:HD2	1:A:90:VAL:HB	1.77	0.49
2:B:683:ARG:HG2	2:B:717:ASP:HB3	1.95	0.49
2:E:637:LEU:HD23	2:E:1637:MET:HB3	1.94	0.49
2:G:2002:PRO:HA	2:G:2005:GLN:HB3	1.94	0.49
2:G:4933:GLN:OE1	2:E:4933:GLN:NE2	2.46	0.49
2:G:426:ARG:HB2	2:G:506:TYR:HA	1.94	0.49
2:G:864:PRO:HD2	2:G:867:LEU:HD12	1.94	0.49
2:I:1698:LEU:N	2:I:1712:TYR:OH	2.45	0.49
2:B:2894:LEU:HD11	2:B:2902:HIS:HB2	1.94	0.49
2:E:1103:GLY:HA3	2:E:1123:VAL:HA	1.94	0.49
2:E:2002:PRO:HA	2:E:2005:GLN:HB3	1.94	0.49
2:G:3753:PHE:HA	2:G:3756:LYS:HB3	1.93	0.49
2:B:2131:LEU:HD23	2:B:3662:ILE:HB	1.95	0.48
2:E:989:ALA:O	2:E:1035:ASN:ND2	2.44	0.48
2:E:1698:LEU:N	2:E:1712:TYR:OH	2.45	0.48
2:E:838:HIS:HA	2:E:1201:HIS:HB3	1.95	0.48
2:G:4063:ASP:O	2:G:4067:LYS:NZ	2.36	0.48
2:B:707:VAL:HG23	2:B:713:SER:HB2	1.94	0.48
2:E:2420:HIS:ND1	2:E:2493:UNK:O	2.47	0.48
2:I:2131:LEU:HD23	2:I:3662:ILE:HB	1.96	0.48
2:I:3948:LYS:HG2	2:I:4012:LEU:HD22	1.95	0.48
2:I:485:SER:O	2:I:489:ASN:N	2.38	0.48
2:I:683:ARG:NH1	2:I:707:VAL:O	2.43	0.48
2:I:669:ASP:OD2	2:I:790:ARG:NH2	2.43	0.48
2:B:4743:MET:HB3	2:B:4746:ALA:HB3	1.93	0.48
2:B:838:HIS:HA	2:B:1201:HIS:HB3	1.95	0.48
2:E:2894:LEU:HD11	2:E:2902:HIS:HB2	1.94	0.48
2:G:683:ARG:HG2	2:G:717:ASP:HB3	1.95	0.48
2:I:4924:VAL:HA	2:I:4928:LEU:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1960:ALA:O	2:B:1964:ARG:NE	2.46	0.48
2:B:206:CYS:SG	2:B:207:SER:N	2.85	0.48
2:B:3842:LEU:O	2:B:3929:SER:OG	2.31	0.48
2:B:395:GLN:NE2	2:B:397:GLU:OE1	2.47	0.48
2:E:488:LEU:HD23	2:E:491:ILE:HD12	1.94	0.48
2:G:2758:PHE:O	2:G:2762:THR:N	2.47	0.48
2:I:2894:LEU:HD11	2:I:2902:HIS:HB2	1.94	0.48
2:B:3767:GLN:NE2	2:B:3804:ILE:O	2.47	0.48
2:B:637:LEU:HD23	2:B:1637:MET:HB3	1.94	0.48
2:E:864:PRO:HD2	2:E:867:LEU:HD12	1.94	0.48
2:G:1991:THR:O	2:G:1995:THR:OG1	2.32	0.48
2:G:4060:LYS:NZ	2:G:4107:GLU:OE2	2.47	0.48
2:G:4924:VAL:HA	2:G:4928:LEU:HB2	1.94	0.48
2:E:1991:THR:O	2:E:1995:THR:OG1	2.32	0.48
2:I:683:ARG:HG2	2:I:717:ASP:HB3	1.95	0.48
2:B:1991:THR:O	2:B:1995:THR:OG1	2.32	0.48
2:E:1960:ALA:O	2:E:1964:ARG:NE	2.46	0.48
2:E:395:GLN:NE2	2:E:397:GLU:OE1	2.47	0.48
2:G:3948:LYS:HG2	2:G:4012:LEU:HD22	1.96	0.48
2:G:485:SER:O	2:G:489:ASN:N	2.38	0.48
2:B:4924:VAL:HA	2:B:4928:LEU:HB2	1.94	0.48
2:E:707:VAL:HG23	2:E:713:SER:HB2	1.94	0.48
2:G:2131:LEU:HD23	2:G:3662:ILE:HB	1.96	0.48
1:H:35:LYS:HD3	2:G:636:ASN:HD21	1.79	0.48
2:E:2131:LEU:HD23	2:E:3662:ILE:HB	1.96	0.48
2:E:4060:LYS:NZ	2:E:4107:GLU:OE2	2.47	0.48
2:I:1991:THR:O	2:I:1995:THR:OG1	2.32	0.48
2:I:4666:VAL:HG23	2:I:4669:VAL:HB	1.96	0.48
2:I:681:HIS:HB3	2:I:784:SER:HB3	1.96	0.48
2:E:3767:GLN:NE2	2:E:3804:ILE:O	2.47	0.48
2:G:838:HIS:HA	2:G:1201:HIS:HB3	1.95	0.48
2:G:2332:LEU:HD13	2:G:2335:LEU:HD12	1.95	0.48
2:G:887:ILE:HG21	2:G:959:TYR:HA	1.96	0.48
2:E:1703:LEU:HD12	2:E:1708:ARG:HB2	1.95	0.47
2:E:2332:LEU:HD13	2:E:2335:LEU:HD12	1.95	0.47
2:E:4666:VAL:HG23	2:E:4669:VAL:HB	1.96	0.47
2:G:1703:LEU:HD12	2:G:1708:ARG:HB2	1.95	0.47
2:G:3767:GLN:NE2	2:G:3804:ILE:O	2.47	0.47
1:A:35:LYS:HD3	2:B:636:ASN:HD21	1.79	0.47
2:G:1671:ARG:NH2	2:G:1710:GLY:O	2.47	0.47
2:G:2420:HIS:ND1	2:G:2493:UNK:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3658:LYS:HA	2:I:3661:TRP:CD2	2.49	0.47
1:J:87:HIS:HD2	1:J:90:VAL:HB	1.77	0.47
2:B:1671:ARG:NH2	2:B:1710:GLY:O	2.47	0.47
2:E:4063:ASP:O	2:E:4067:LYS:NZ	2.36	0.47
2:G:681:HIS:HB3	2:G:784:SER:HB3	1.96	0.47
2:I:2758:PHE:O	2:I:2762:THR:N	2.47	0.47
2:I:395:GLN:NE2	2:I:397:GLU:OE1	2.47	0.47
2:B:2758:PHE:O	2:B:2762:THR:N	2.47	0.47
2:B:3658:LYS:HA	2:B:3661:TRP:CD2	2.49	0.47
2:E:887:ILE:HG21	2:E:959:TYR:HA	1.96	0.47
2:G:219:VAL:HG13	2:G:285:VAL:HG21	1.97	0.47
2:G:3658:LYS:HA	2:G:3661:TRP:CD2	2.49	0.47
2:G:683:ARG:NH1	2:G:707:VAL:O	2.43	0.47
2:I:3767:GLN:NE2	2:I:3804:ILE:O	2.47	0.47
2:E:1671:ARG:NH2	2:E:1710:GLY:O	2.47	0.47
2:E:533:ASN:ND2	2:E:536:ASN:OD1	2.38	0.47
1:H:42:ARG:HG2	2:G:1691:GLN:HG2	1.97	0.47
2:B:4155:PRO:HD2	2:B:5036:LEU:HD23	1.97	0.47
2:G:2159:LEU:HA	2:G:2162:ILE:HD12	1.97	0.47
2:G:395:GLN:NE2	2:G:397:GLU:OE1	2.47	0.47
2:I:1671:ARG:NH2	2:I:1710:GLY:O	2.47	0.47
2:I:395:GLN:HG3	2:I:397:GLU:H	1.80	0.47
2:I:4060:LYS:NZ	2:I:4107:GLU:OE2	2.47	0.47
2:I:838:HIS:HA	2:I:1201:HIS:HB3	1.95	0.47
2:B:972:LEU:O	2:B:1044:ARG:NH2	2.48	0.47
2:B:2420:HIS:ND1	2:B:2493:UNK:O	2.47	0.47
2:B:3948:LYS:HG2	2:B:4012:LEU:HD22	1.96	0.47
2:E:1171:SER:OG	2:E:1175:SER:N	2.42	0.47
2:E:3842:LEU:O	2:E:3929:SER:OG	2.31	0.47
2:E:3948:LYS:HG2	2:E:4012:LEU:HD22	1.96	0.47
2:E:4155:PRO:HD2	2:E:5036:LEU:HD23	1.97	0.47
2:I:1960:ALA:O	2:I:1964:ARG:NE	2.46	0.47
2:I:887:ILE:HG21	2:I:959:TYR:HA	1.96	0.47
2:B:1812:LEU:HD21	2:B:1861:GLN:HG2	1.97	0.47
2:B:395:GLN:HG3	2:B:397:GLU:H	1.80	0.47
2:B:396:GLU:OE2	2:B:451:TYR:OH	2.28	0.47
2:B:4060:LYS:NZ	2:B:4107:GLU:OE2	2.47	0.47
2:B:681:HIS:HB3	2:B:784:SER:HB3	1.96	0.47
2:G:395:GLN:HG3	2:G:397:GLU:H	1.80	0.47
2:B:2751:LEU:HD11	2:B:2823:ILE:HG21	1.97	0.47
2:E:134:ASP:N	2:E:134:ASP:OD1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2927:LEU:HD23	2:E:2930:LEU:HD12	1.96	0.47
2:E:3779:VAL:HG23	2:E:3780:LEU:HD12	1.97	0.47
2:E:681:HIS:HB3	2:E:784:SER:HB3	1.96	0.47
2:G:4666:VAL:HG23	2:G:4669:VAL:HB	1.96	0.47
2:I:4155:PRO:HD2	2:I:5036:LEU:HD23	1.97	0.47
2:B:4239:GLU:OE2	2:B:5014:TYR:OH	2.27	0.47
2:E:2159:LEU:HA	2:E:2162:ILE:HD12	1.97	0.47
2:E:395:GLN:HG3	2:E:397:GLU:H	1.80	0.47
2:G:4155:PRO:HD2	2:G:5036:LEU:HD23	1.97	0.47
2:G:989:ALA:O	2:G:1035:ASN:ND2	2.44	0.47
2:I:219:VAL:HG13	2:I:285:VAL:HG21	1.97	0.47
2:I:2420:HIS:ND1	2:I:2493:UNK:O	2.47	0.47
2:I:4767:TRP:HE3	2:I:4770:SER:HB2	1.80	0.47
2:B:3779:VAL:HG23	2:B:3780:LEU:HD12	1.97	0.47
2:B:887:ILE:HG21	2:B:959:TYR:HA	1.96	0.46
2:E:1812:LEU:HD21	2:E:1861:GLN:HG2	1.97	0.46
2:I:2751:LEU:HD11	2:I:2823:ILE:HG21	1.97	0.46
1:A:23:VAL:HG22	1:A:47:LYS:HG2	1.97	0.46
2:B:2159:LEU:HA	2:B:2162:ILE:HD12	1.96	0.46
2:B:2277:ALA:HB1	2:B:2337:PHE:HD2	1.81	0.46
2:B:2927:LEU:HD23	2:B:2930:LEU:HD12	1.96	0.46
2:B:4666:VAL:HG23	2:B:4669:VAL:HB	1.96	0.46
2:B:4767:TRP:HE3	2:B:4770:SER:HB2	1.80	0.46
2:E:2236:LEU:HD23	2:E:2275:VAL:HG21	1.98	0.46
2:E:2758:PHE:O	2:E:2762:THR:N	2.47	0.46
2:E:972:LEU:O	2:E:1044:ARG:NH2	2.48	0.46
2:G:132:ALA:HA	2:G:194:SER:HB2	1.98	0.46
2:I:2159:LEU:HA	2:I:2162:ILE:HD12	1.97	0.46
2:B:1095:VAL:HB	2:B:1199:VAL:HG23	1.97	0.46
2:B:219:VAL:HG13	2:B:285:VAL:HG21	1.97	0.46
2:E:2277:ALA:HB1	2:E:2337:PHE:HD2	1.81	0.46
2:G:972:LEU:O	2:G:1044:ARG:NH2	2.48	0.46
2:G:2236:LEU:HD23	2:G:2275:VAL:HG21	1.98	0.46
2:G:3779:VAL:HG23	2:G:3780:LEU:HD12	1.97	0.46
1:H:23:VAL:HG22	1:H:47:LYS:HG2	1.97	0.46
2:I:972:LEU:O	2:I:1044:ARG:NH2	2.48	0.46
2:E:3658:LYS:HA	2:E:3661:TRP:CD2	2.49	0.46
2:E:3923:LEU:HD13	2:E:3961:VAL:HG11	1.98	0.46
2:E:396:GLU:OE2	2:E:451:TYR:OH	2.28	0.46
2:G:1812:LEU:HD21	2:G:1861:GLN:HG2	1.97	0.46
2:I:2927:LEU:HD23	2:I:2930:LEU:HD12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:3779:VAL:HG23	2:I:3780:LEU:HD12	1.97	0.46
2:B:1078:GLU:HG3	2:B:1237:TRP:HE1	1.81	0.46
2:B:2143:THR:O	2:B:3651:ASN:ND2	2.44	0.46
2:G:2751:LEU:HD11	2:G:2823:ILE:HG21	1.97	0.46
2:G:4749:GLU:HA	2:G:4752:ALA:HB3	1.97	0.46
2:B:134:ASP:OD1	2:B:134:ASP:N	2.48	0.46
2:G:765:GLN:NE2	2:G:1521:UNK:O	2.49	0.46
2:G:3923:LEU:HD13	2:G:3961:VAL:HG11	1.98	0.46
2:I:2326:CYS:SG	2:I:2327:GLY:N	2.89	0.46
2:I:645:ARG:HH11	2:I:778:PHE:HE1	1.64	0.46
2:B:2236:LEU:HD23	2:B:2275:VAL:HG21	1.98	0.46
2:E:219:VAL:HG13	2:E:285:VAL:HG21	1.97	0.46
2:I:132:ALA:HA	2:I:194:SER:HB2	1.98	0.46
2:G:1960:ALA:O	2:G:1964:ARG:NE	2.46	0.46
2:G:2326:CYS:SG	2:G:2327:GLY:N	2.89	0.46
2:G:2927:LEU:HD23	2:G:2930:LEU:HD12	1.96	0.46
2:G:698:GLY:HA2	2:G:703:GLY:HA2	1.98	0.46
2:I:4749:GLU:HA	2:I:4752:ALA:HB3	1.97	0.46
2:E:765:GLN:NE2	2:E:1521:UNK:O	2.49	0.46
2:G:1171:SER:OG	2:G:1175:SER:N	2.42	0.46
2:G:2277:ALA:HB1	2:G:2337:PHE:HD2	1.81	0.46
2:G:3365:UNK:O	2:G:3369:UNK:N	2.49	0.46
2:I:134:ASP:OD1	2:I:134:ASP:N	2.48	0.46
2:I:3923:LEU:HD13	2:I:3961:VAL:HG11	1.98	0.46
2:I:698:GLY:HA2	2:I:703:GLY:HA2	1.98	0.46
2:E:2326:CYS:SG	2:E:2327:GLY:N	2.89	0.45
2:G:1095:VAL:HB	2:G:1199:VAL:HG23	1.97	0.45
2:G:134:ASP:OD1	2:G:134:ASP:N	2.48	0.45
2:I:2236:LEU:HD23	2:I:2275:VAL:HG21	1.98	0.45
2:B:4749:GLU:HA	2:B:4752:ALA:HB3	1.97	0.45
2:E:1078:GLU:HG3	2:E:1237:TRP:HE1	1.81	0.45
2:I:2277:ALA:HB1	2:I:2337:PHE:HD2	1.81	0.45
2:I:765:GLN:NE2	2:I:1521:UNK:O	2.49	0.45
2:E:4749:GLU:HA	2:E:4752:ALA:HB3	1.97	0.45
2:E:4767:TRP:HE3	2:E:4770:SER:HB2	1.80	0.45
2:B:2326:CYS:SG	2:B:2327:GLY:N	2.89	0.45
2:B:3923:LEU:HD13	2:B:3961:VAL:HG11	1.98	0.45
2:I:2004:GLU:HA	2:I:2007:ASN:HD22	1.82	0.45
1:J:23:VAL:HG22	1:J:47:LYS:HG2	1.97	0.45
2:B:765:GLN:NE2	2:B:1521:UNK:O	2.49	0.45
2:B:403:MET:O	2:B:407:THR:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1095:VAL:HB	2:E:1199:VAL:HG23	1.97	0.45
2:E:4713:SER:HG	2:E:4775:TYR:HH	1.64	0.45
2:E:551:LEU:HD21	2:E:589:LEU:HD13	1.98	0.45
2:G:4767:TRP:HE3	2:G:4770:SER:HB2	1.80	0.45
2:I:4657:CYS:HB3	2:I:4792:LEU:HD11	1.99	0.45
2:B:2004:GLU:HA	2:B:2007:ASN:HD22	1.82	0.45
2:B:551:LEU:HD21	2:B:589:LEU:HD13	1.98	0.45
2:B:645:ARG:HH11	2:B:778:PHE:HE1	1.64	0.45
2:E:2753:SER:O	2:E:2757:LYS:N	2.48	0.45
2:E:2751:LEU:HD11	2:E:2823:ILE:HG21	1.97	0.45
2:E:3365:UNK:O	2:E:3369:UNK:N	2.49	0.45
2:G:2004:GLU:HA	2:G:2007:ASN:HD22	1.82	0.45
2:G:645:ARG:HH11	2:G:778:PHE:HE1	1.64	0.45
2:I:1078:GLU:HG3	2:I:1237:TRP:HE1	1.81	0.45
2:B:132:ALA:HA	2:B:194:SER:HB2	1.98	0.45
2:B:698:GLY:HA2	2:B:703:GLY:HA2	1.98	0.45
1:F:23:VAL:HG22	1:F:47:LYS:HG2	1.97	0.45
2:G:1078:GLU:HG3	2:G:1237:TRP:HE1	1.81	0.45
2:G:1457:UNK:N	2:G:1497:UNK:O	2.50	0.45
2:G:551:LEU:HD21	2:G:589:LEU:HD13	1.98	0.45
2:I:1095:VAL:HB	2:I:1199:VAL:HG23	1.98	0.45
2:B:4657:CYS:HB3	2:B:4792:LEU:HD11	1.99	0.45
2:E:132:ALA:HA	2:E:194:SER:HB2	1.98	0.45
2:I:1812:LEU:HD21	2:I:1861:GLN:HG2	1.97	0.45
2:I:4925:ILE:HA	2:I:4929:LEU:HD23	1.99	0.45
2:B:3365:UNK:O	2:B:3369:UNK:N	2.49	0.45
2:E:4558:ASN:N	2:E:4558:ASN:OD1	2.50	0.45
2:G:3756:LYS:HA	2:G:3759:GLU:HG2	1.99	0.45
2:G:3992:PHE:O	2:G:3996:PHE:N	2.41	0.45
2:I:3365:UNK:O	2:I:3369:UNK:N	2.49	0.45
2:B:379:HIS:CD2	2:B:381:GLU:H	2.35	0.45
2:E:4142:ASN:HA	2:E:4145:VAL:HG12	1.99	0.45
1:F:35:LYS:HD3	2:E:636:ASN:HD21	1.82	0.45
2:B:2753:SER:O	2:B:2757:LYS:N	2.48	0.44
2:B:886:ARG:HB3	2:B:891:TRP:HB2	2.00	0.44
2:E:2004:GLU:HA	2:E:2007:ASN:HD22	1.82	0.44
2:E:4925:ILE:HA	2:E:4929:LEU:HD23	1.99	0.44
2:I:1171:SER:OG	2:I:1175:SER:N	2.42	0.44
2:I:4142:ASN:HA	2:I:4145:VAL:HG12	1.99	0.44
2:I:45:ARG:HG2	2:I:443:LEU:HD21	1.99	0.44
2:B:4142:ASN:HA	2:B:4145:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:346:CYS:N	2:E:388:LEU:O	2.50	0.44
2:E:4229:GLU:HA	2:E:4232:GLU:HB3	2.00	0.44
2:G:4142:ASN:HA	2:G:4145:VAL:HG12	1.99	0.44
2:G:978:THR:HB	2:G:980:ALA:H	1.82	0.44
2:I:143:GLY:HA3	2:I:147:TRP:HE1	1.82	0.44
2:B:346:CYS:N	2:B:388:LEU:O	2.50	0.44
2:E:1457:UNK:N	2:E:1497:UNK:O	2.50	0.44
2:E:379:HIS:CD2	2:E:381:GLU:H	2.35	0.44
2:E:698:GLY:HA2	2:E:703:GLY:HA2	1.98	0.44
2:E:886:ARG:HB3	2:E:891:TRP:HB2	2.00	0.44
2:G:2880:GLU:O	2:G:2884:ASN:N	2.46	0.44
2:I:1457:UNK:N	2:I:1497:UNK:O	2.50	0.44
2:I:3676:ASP:OD1	2:I:3676:ASP:N	2.50	0.44
2:B:1973:GLN:HA	2:B:1976:ARG:HB3	2.00	0.44
2:B:4227:GLU:HG3	2:B:4228:ALA:H	1.82	0.44
2:E:978:THR:HB	2:E:980:ALA:H	1.82	0.44
2:G:4657:CYS:HB3	2:G:4792:LEU:HD11	1.99	0.44
2:I:403:MET:O	2:I:407:THR:N	2.50	0.44
2:I:579:GLN:H	2:I:582:HIS:HD2	1.66	0.44
2:B:1457:UNK:N	2:B:1497:UNK:O	2.50	0.44
2:B:3676:ASP:OD1	2:B:3676:ASP:N	2.50	0.44
2:B:4229:GLU:HA	2:B:4232:GLU:HB3	2.00	0.44
2:E:220:LEU:O	2:E:260:TRP:N	2.50	0.44
2:E:645:ARG:HH11	2:E:778:PHE:HE1	1.64	0.44
2:I:218:HIS:HB3	2:I:392:ARG:HD3	2.00	0.44
2:I:2226:PRO:HA	2:I:2229:VAL:HG12	2.00	0.44
2:I:379:HIS:CD2	2:I:381:GLU:H	2.35	0.44
2:I:4227:GLU:HG3	2:I:4228:ALA:H	1.82	0.44
2:I:470:SER:O	2:I:474:ARG:NE	2.43	0.44
2:B:1972:ASN:O	2:B:1976:ARG:N	2.49	0.44
2:B:4925:ILE:HA	2:B:4929:LEU:HD23	1.99	0.44
2:I:2880:GLU:O	2:I:2884:ASN:N	2.47	0.44
2:I:4886:HIS:O	2:I:4890:GLY:N	2.46	0.44
2:I:551:LEU:HD21	2:I:589:LEU:HD13	1.98	0.44
2:B:978:THR:HB	2:B:980:ALA:H	1.82	0.44
2:G:143:GLY:HA3	2:G:147:TRP:HE1	1.82	0.44
2:G:2226:PRO:HA	2:G:2229:VAL:HG12	2.00	0.44
2:G:3676:ASP:OD1	2:G:3676:ASP:N	2.50	0.44
2:G:4925:ILE:HA	2:G:4929:LEU:HD23	1.99	0.44
2:I:1760:HIS:CE1	2:I:2041:HIS:HA	2.53	0.44
2:I:3756:LYS:HA	2:I:3759:GLU:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:606:LEU:HG	2:I:617:ASN:HD22	1.82	0.44
2:B:143:GLY:HA3	2:B:147:TRP:HE1	1.82	0.44
2:G:379:HIS:CD2	2:G:381:GLU:H	2.35	0.44
2:G:886:ARG:HB3	2:G:891:TRP:HB2	2.00	0.44
2:B:3850:GLN:HA	2:B:3853:ALA:HB3	2.00	0.44
2:B:4558:ASN:N	2:B:4558:ASN:OD1	2.50	0.44
2:B:4886:HIS:O	2:B:4890:GLY:N	2.46	0.44
2:E:143:GLY:HA3	2:E:147:TRP:HE1	1.82	0.44
2:G:346:CYS:N	2:G:388:LEU:O	2.50	0.44
2:G:4227:GLU:HG3	2:G:4228:ALA:H	1.82	0.44
2:G:606:LEU:HG	2:G:617:ASN:HD22	1.82	0.44
2:I:1973:GLN:HA	2:I:1976:ARG:HB3	2.00	0.44
2:I:4229:GLU:HA	2:I:4232:GLU:HB3	2.00	0.44
2:E:243:ARG:NH1	2:E:301:VAL:O	2.46	0.43
2:E:3756:LYS:HA	2:E:3759:GLU:HG2	1.99	0.43
2:E:403:MET:O	2:E:407:THR:N	2.50	0.43
2:G:218:HIS:HB3	2:G:392:ARG:HD3	2.00	0.43
2:G:220:LEU:O	2:G:260:TRP:N	2.50	0.43
2:I:886:ARG:HB3	2:I:891:TRP:HB2	2.00	0.43
2:B:1760:HIS:CE1	2:B:2041:HIS:HA	2.53	0.43
2:B:278:GLN:N	2:B:315:CYS:SG	2.91	0.43
2:E:4227:GLU:HG3	2:E:4228:ALA:H	1.82	0.43
2:E:4657:CYS:HB3	2:E:4792:LEU:HD11	1.99	0.43
2:E:606:LEU:HG	2:E:617:ASN:HD22	1.82	0.43
2:G:451:TYR:O	2:G:474:ARG:NH1	2.45	0.43
2:G:579:GLN:H	2:G:582:HIS:HD2	1.66	0.43
2:G:718:GLY:HA3	2:G:737:LEU:HA	2.01	0.43
2:I:101:LEU:HB3	2:I:150:MET:HE1	1.99	0.43
2:I:346:CYS:N	2:I:388:LEU:O	2.50	0.43
2:B:218:HIS:HB3	2:B:392:ARG:HD3	2.00	0.43
2:B:3756:LYS:HA	2:B:3759:GLU:HG2	1.99	0.43
2:B:718:GLY:HA3	2:B:737:LEU:HA	2.01	0.43
2:E:3362:UNK:O	2:E:3366:UNK:N	2.52	0.43
2:E:530:ILE:HD13	2:E:536:ASN:HB3	2.01	0.43
2:G:243:ARG:NH1	2:G:301:VAL:O	2.46	0.43
2:G:3362:UNK:O	2:G:3366:UNK:N	2.52	0.43
2:G:4229:GLU:HA	2:G:4232:GLU:HB3	2.00	0.43
2:G:915:GLU:O	2:G:919:ASN:ND2	2.51	0.43
2:B:4586:PRO:HB3	2:B:4628:VAL:HG21	2.01	0.43
2:E:959:TYR:HB3	2:E:967:PRO:HD2	2.01	0.43
2:G:1972:ASN:O	2:G:1976:ARG:N	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:907:LEU:O	2:I:963:ASN:ND2	2.39	0.43
2:E:3850:GLN:HA	2:E:3853:ALA:HB3	2.00	0.43
2:G:530:ILE:HD13	2:G:536:ASN:HB3	2.01	0.43
2:I:2095:GLN:NE2	2:I:2127:GLN:O	2.50	0.43
2:I:4586:PRO:HB3	2:I:4628:VAL:HG21	2.01	0.43
2:B:579:GLN:H	2:B:582:HIS:HD2	1.66	0.43
2:E:345:LEU:HD22	2:E:387:ALA:HB1	2.01	0.43
2:E:3955:MET:HG3	2:E:4019:LEU:HD22	2.01	0.43
2:E:4886:HIS:O	2:E:4890:GLY:N	2.46	0.43
2:E:915:GLU:O	2:E:919:ASN:ND2	2.51	0.43
2:G:101:LEU:HB3	2:G:150:MET:HE1	2.00	0.43
2:G:1973:GLN:HA	2:G:1976:ARG:HB3	2.00	0.43
2:G:4586:PRO:HB3	2:G:4628:VAL:HG21	2.01	0.43
2:I:978:THR:HB	2:I:980:ALA:H	1.82	0.43
2:B:2226:PRO:HA	2:B:2229:VAL:HG12	2.00	0.43
2:B:309:THR:O	2:B:313:SER:OG	2.37	0.43
2:B:4712:PRO:HG2	2:B:4718:LYS:HG2	2.01	0.43
2:E:1760:HIS:CE1	2:E:2041:HIS:HA	2.53	0.43
2:E:718:GLY:HA3	2:E:737:LEU:HA	2.01	0.43
2:G:3850:GLN:HA	2:G:3853:ALA:HB3	2.00	0.43
2:I:2271:THR:HG22	2:I:2273:LEU:H	1.83	0.43
2:I:3362:UNK:O	2:I:3366:UNK:N	2.52	0.43
2:I:580:GLU:HG3	2:I:620:LEU:HD22	2.01	0.43
2:B:45:ARG:HG2	2:B:443:LEU:HD21	1.99	0.43
2:B:915:GLU:O	2:B:919:ASN:ND2	2.51	0.43
2:E:218:HIS:HB3	2:E:392:ARG:HD3	2.00	0.43
2:E:2271:THR:HG22	2:E:2273:LEU:H	1.83	0.43
2:E:45:ARG:HG2	2:E:443:LEU:HD21	2.00	0.43
2:E:470:SER:O	2:E:474:ARG:NE	2.43	0.43
2:E:62:LEU:O	2:E:261:ARG:NH2	2.52	0.43
2:G:45:ARG:HG2	2:G:443:LEU:HD21	1.99	0.43
2:I:1109:LEU:HA	2:I:1120:LEU:HD21	2.01	0.43
2:I:111:HIS:HD2	2:I:114:SER:H	1.66	0.43
2:I:195:PHE:HB3	2:I:196:MET:HG2	2.01	0.43
2:I:530:ILE:HD13	2:I:536:ASN:HB3	2.01	0.43
2:I:718:GLY:HA3	2:I:737:LEU:HA	2.01	0.43
2:B:2102:VAL:HB	2:B:2124:LEU:HD12	2.00	0.43
2:B:21:VAL:HG12	2:B:66:CYS:HA	2.00	0.43
2:B:2271:THR:HG22	2:B:2273:LEU:H	1.83	0.43
2:B:2880:GLU:O	2:B:2884:ASN:N	2.46	0.43
2:B:345:LEU:HD22	2:B:387:ALA:HB1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:530:ILE:HD13	2:B:536:ASN:HB3	2.01	0.43
2:B:898:ASP:HB3	2:B:901:LYS:HB2	2.01	0.43
2:E:195:PHE:HB3	2:E:196:MET:HG2	2.01	0.43
2:E:2226:PRO:HA	2:E:2229:VAL:HG12	2.00	0.43
2:G:1760:HIS:CE1	2:G:2041:HIS:HA	2.53	0.43
2:G:2095:GLN:NE2	2:G:2127:GLN:O	2.50	0.43
2:G:309:THR:O	2:G:313:SER:OG	2.37	0.43
2:G:403:MET:O	2:G:407:THR:N	2.50	0.43
2:I:1972:ASN:O	2:I:1976:ARG:N	2.49	0.43
2:G:345:LEU:HD22	2:G:387:ALA:HB1	2.01	0.43
2:I:4712:PRO:HG2	2:I:4718:LYS:HG2	2.01	0.43
2:I:932:LEU:HA	2:I:935:LEU:HD12	2.01	0.43
2:B:101:LEU:HB3	2:B:150:MET:HE1	2.01	0.42
2:B:111:HIS:HD2	2:B:114:SER:H	1.66	0.42
2:B:3955:MET:HG3	2:B:4019:LEU:HD22	2.01	0.42
2:B:4763:GLY:O	2:B:4766:THR:OG1	2.34	0.42
2:B:734:GLY:O	2:B:736:HIS:ND1	2.52	0.42
2:E:309:THR:O	2:E:313:SER:OG	2.37	0.42
2:E:579:GLN:H	2:E:582:HIS:HD2	1.66	0.42
2:G:4712:PRO:HG2	2:G:4718:LYS:HG2	2.01	0.42
2:I:793:LEU:HD22	2:I:821:LEU:HD13	2.01	0.42
2:I:915:GLU:O	2:I:919:ASN:ND2	2.51	0.42
2:E:111:HIS:HD2	2:E:114:SER:H	1.66	0.42
2:E:103:TYR:HB3	2:E:152:PRO:HD3	2.01	0.42
2:E:1931:LEU:HB3	2:E:1935:VAL:HB	2.02	0.42
2:E:2143:THR:O	2:E:3651:ASN:ND2	2.44	0.42
2:E:4586:PRO:HB3	2:E:4628:VAL:HG21	2.01	0.42
2:G:1109:LEU:HA	2:G:1120:LEU:HD21	2.01	0.42
2:G:195:PHE:HB3	2:G:196:MET:HG2	2.01	0.42
2:G:959:TYR:HB3	2:G:967:PRO:HD2	2.01	0.42
2:I:3850:GLN:HA	2:I:3853:ALA:HB3	2.00	0.42
2:B:1109:LEU:HA	2:B:1120:LEU:HD21	2.01	0.42
2:E:580:GLU:HG3	2:E:620:LEU:HD22	2.01	0.42
2:G:1931:LEU:HB3	2:G:1935:VAL:HB	2.02	0.42
2:G:940:GLY:O	2:G:1052:ASN:N	2.50	0.42
2:I:309:THR:O	2:I:313:SER:OG	2.37	0.42
2:I:898:ASP:HB3	2:I:901:LYS:HB2	2.01	0.42
2:B:959:TYR:HB3	2:B:967:PRO:HD2	2.01	0.42
2:E:793:LEU:HD12	2:E:797:HIS:HB2	2.02	0.42
2:G:2102:VAL:HB	2:G:2124:LEU:HD12	2.00	0.42
2:G:62:LEU:O	2:G:261:ARG:NH2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1171:SER:OG	2:B:1175:SER:N	2.42	0.42
2:B:220:LEU:O	2:B:260:TRP:N	2.50	0.42
2:B:606:LEU:HG	2:B:617:ASN:HD22	1.82	0.42
2:B:580:GLU:HG3	2:B:620:LEU:HD22	2.01	0.42
2:B:62:LEU:O	2:B:261:ARG:NH2	2.52	0.42
2:E:21:VAL:HG12	2:E:66:CYS:HA	2.00	0.42
2:E:4712:PRO:HG2	2:E:4718:LYS:HG2	2.01	0.42
2:E:932:LEU:HA	2:E:935:LEU:HD12	2.01	0.42
2:I:123:THR:OG1	2:I:134:ASP:OD1	2.38	0.42
2:I:21:VAL:HG12	2:I:66:CYS:HA	2.00	0.42
2:I:3992:PHE:O	2:I:3996:PHE:N	2.41	0.42
2:E:451:TYR:O	2:E:474:ARG:NH1	2.45	0.42
2:G:3955:MET:HG3	2:G:4019:LEU:HD22	2.01	0.42
2:G:4558:ASN:OD1	2:G:4558:ASN:N	2.50	0.42
2:I:3955:MET:HG3	2:I:4019:LEU:HD22	2.01	0.42
2:B:195:PHE:HB3	2:B:196:MET:HG2	2.01	0.42
2:B:3362:UNK:O	2:B:3366:UNK:N	2.52	0.42
2:B:793:LEU:HD22	2:B:821:LEU:HD13	2.01	0.42
2:E:1973:GLN:HA	2:E:1976:ARG:HB3	2.00	0.42
1:F:34:LYS:HD3	2:E:629:ARG:HD2	2.01	0.42
2:G:103:TYR:HB3	2:G:152:PRO:HD3	2.01	0.42
2:I:2102:VAL:HB	2:I:2124:LEU:HD12	2.00	0.42
2:I:261:ARG:HB3	2:I:283:ARG:HB3	2.02	0.42
2:B:932:LEU:HA	2:B:935:LEU:HD12	2.01	0.42
2:E:3676:ASP:N	2:E:3676:ASP:OD1	2.50	0.42
2:E:898:ASP:HB3	2:E:901:LYS:HB2	2.01	0.42
2:G:2753:SER:O	2:G:2757:LYS:N	2.48	0.42
2:G:4101:LYS:HA	2:G:4101:LYS:HD3	1.86	0.42
2:I:2753:SER:O	2:I:2757:LYS:N	2.48	0.42
2:B:1665:HIS:HA	2:B:1668:ARG:HG2	2.02	0.42
2:B:649:PHE:HB3	2:B:776:LEU:HB3	2.02	0.42
2:E:123:THR:OG1	2:E:134:ASP:OD1	2.38	0.42
2:E:793:LEU:HD22	2:E:821:LEU:HD13	2.01	0.42
2:G:580:GLU:HG3	2:G:620:LEU:HD22	2.01	0.42
2:G:870:ILE:HD12	2:G:870:ILE:HA	1.95	0.42
2:I:220:LEU:O	2:I:260:TRP:N	2.50	0.42
2:I:62:LEU:O	2:I:261:ARG:NH2	2.52	0.42
2:I:940:GLY:O	2:I:1052:ASN:N	2.50	0.42
2:B:1723:ALA:HB1	2:B:1775:HIS:HD2	1.85	0.42
2:B:23:GLN:HB3	2:B:201:ASN:HB2	2.02	0.42
2:E:23:GLN:HB3	2:E:201:ASN:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:21:VAL:HG12	2:G:66:CYS:HA	2.00	0.42
2:G:2271:THR:HG22	2:G:2273:LEU:H	1.83	0.42
2:G:472:ARG:NH2	2:G:3712:GLU:OE2	2.53	0.42
2:I:1665:HIS:HA	2:I:1668:ARG:HG2	2.02	0.42
2:I:345:LEU:HD22	2:I:387:ALA:HB1	2.01	0.42
2:I:4056:GLU:HG2	2:I:4166:LEU:HD23	2.02	0.42
2:I:4558:ASN:OD1	2:I:4558:ASN:N	2.50	0.42
2:B:4056:GLU:HG2	2:B:4166:LEU:HD23	2.02	0.41
2:B:583:ILE:HG13	2:B:583:ILE:H	1.70	0.41
2:B:880:GLU:OE1	2:B:968:ALA:N	2.43	0.41
2:E:2102:VAL:HB	2:E:2124:LEU:HD12	2.00	0.41
2:G:470:SER:O	2:G:474:ARG:NE	2.43	0.41
2:I:670:GLU:HG3	2:I:787:VAL:HG13	2.03	0.41
2:B:793:LEU:HD12	2:B:797:HIS:HB2	2.01	0.41
2:B:914:PRO:HD2	2:B:917:GLU:HB2	2.02	0.41
2:B:940:GLY:O	2:B:1052:ASN:N	2.50	0.41
2:E:1109:LEU:HA	2:E:1120:LEU:HD21	2.01	0.41
2:E:1723:ALA:HB1	2:E:1775:HIS:HD2	1.85	0.41
2:E:472:ARG:NH2	2:E:3712:GLU:OE2	2.53	0.41
2:E:914:PRO:HD2	2:E:917:GLU:HB2	2.02	0.41
2:G:123:THR:OG1	2:G:134:ASP:OD1	2.38	0.41
2:G:23:GLN:HB3	2:G:201:ASN:HB2	2.02	0.41
2:I:243:ARG:NH1	2:I:301:VAL:O	2.46	0.41
2:I:959:TYR:HB3	2:I:967:PRO:HD2	2.01	0.41
2:E:649:PHE:HB3	2:E:776:LEU:HB3	2.02	0.41
2:E:983:THR:O	2:E:987:ARG:N	2.52	0.41
2:G:4239:GLU:OE2	2:G:5014:TYR:OH	2.27	0.41
2:G:793:LEU:HD12	2:G:797:HIS:HB2	2.01	0.41
2:G:898:ASP:HB3	2:G:901:LYS:HB2	2.01	0.41
2:I:1931:LEU:HB3	2:I:1935:VAL:HB	2.02	0.41
2:I:793:LEU:HD12	2:I:797:HIS:HB2	2.01	0.41
2:B:103:TYR:HB3	2:B:152:PRO:HD3	2.01	0.41
2:B:1931:LEU:HB3	2:B:1935:VAL:HB	2.02	0.41
2:E:2868:SER:O	2:E:2872:GLN:N	2.39	0.41
2:G:793:LEU:HD22	2:G:821:LEU:HD13	2.01	0.41
2:I:1735:ILE:HG23	2:I:1771:LEU:HB2	2.02	0.41
2:I:1676:LEU:HD23	2:I:2167:ILE:HG23	2.03	0.41
2:B:1676:LEU:HD23	2:B:2167:ILE:HG23	2.03	0.41
2:B:261:ARG:HB3	2:B:283:ARG:HB3	2.02	0.41
2:E:1665:HIS:HA	2:E:1668:ARG:HG2	2.02	0.41
2:E:1972:ASN:O	2:E:1976:ARG:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4056:GLU:HG2	2:E:4166:LEU:HD23	2.02	0.41
2:G:1665:HIS:HA	2:G:1668:ARG:HG2	2.02	0.41
2:G:1723:ALA:HB1	2:G:1775:HIS:HD2	1.85	0.41
2:G:2874:MET:O	2:G:2878:LEU:N	2.43	0.41
2:G:4056:GLU:HG2	2:G:4166:LEU:HD23	2.02	0.41
2:G:111:HIS:HD2	2:G:114:SER:H	1.66	0.41
2:I:1723:ALA:HB1	2:I:1775:HIS:HD2	1.85	0.41
2:I:472:ARG:NH2	2:I:3712:GLU:OE2	2.53	0.41
2:I:4763:GLY:O	2:I:4766:THR:OG1	2.34	0.41
1:J:87:HIS:HA	1:J:88:PRO:HD3	1.90	0.41
2:B:2862:LEU:HB3	2:B:2928:LYS:HB3	2.03	0.41
2:E:734:GLY:O	2:E:736:HIS:ND1	2.52	0.41
2:G:261:ARG:HB3	2:G:283:ARG:HB3	2.02	0.41
2:G:670:GLU:HG3	2:G:787:VAL:HG13	2.03	0.41
2:E:1676:LEU:HD23	2:E:2167:ILE:HG23	2.03	0.41
2:E:1735:ILE:HG23	2:E:1771:LEU:HB2	2.02	0.41
2:G:1735:ILE:HG23	2:G:1771:LEU:HB2	2.02	0.41
2:G:1865:MET:N	2:G:1865:MET:SD	2.94	0.41
2:G:2022:PRO:HB2	2:G:2024:PRO:HD2	2.03	0.41
2:G:4860:ARG:HG3	2:G:4876:CYS:HB3	2.03	0.41
2:G:932:LEU:HA	2:G:935:LEU:HD12	2.01	0.41
2:I:103:TYR:HB3	2:I:152:PRO:HD3	2.01	0.41
2:I:451:TYR:O	2:I:474:ARG:NH1	2.45	0.41
2:I:914:PRO:HD2	2:I:917:GLU:HB2	2.02	0.41
2:B:2095:GLN:NE2	2:B:2127:GLN:O	2.50	0.41
2:B:472:ARG:NH2	2:B:3712:GLU:OE2	2.53	0.41
2:B:582:HIS:O	2:B:585:SER:OG	2.30	0.41
2:I:2674:UNK:O	2:I:2676:UNK:N	2.54	0.41
2:I:2868:SER:O	2:I:2872:GLN:N	2.39	0.41
2:E:2862:LEU:HB3	2:E:2928:LYS:HB3	2.03	0.41
2:E:3889:GLN:HG3	2:E:3967:GLU:HG3	2.03	0.41
2:E:4005:GLN:HE21	2:E:4110:PHE:HE1	1.69	0.41
2:G:2674:UNK:O	2:G:2676:UNK:N	2.54	0.41
2:G:939:VAL:HG22	2:G:1053:ILE:HG12	2.03	0.41
2:I:734:GLY:O	2:I:736:HIS:ND1	2.52	0.41
2:B:123:THR:OG1	2:B:134:ASP:OD1	2.38	0.41
2:E:2022:PRO:HB2	2:E:2024:PRO:HD2	2.03	0.41
2:G:256:ALA:HB1	2:G:286:THR:HG21	2.03	0.41
2:G:2868:SER:O	2:G:2872:GLN:N	2.39	0.41
2:G:3733:CYS:HB2	2:G:3803:SER:HB3	2.03	0.41
2:I:1865:MET:SD	2:I:1865:MET:N	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:2022:PRO:HB2	2:I:2024:PRO:HD2	2.03	0.41
2:I:278:GLN:N	2:I:315:CYS:SG	2.91	0.41
2:I:4848:VAL:O	2:I:4852:THR:OG1	2.32	0.41
2:I:4860:ARG:HG3	2:I:4876:CYS:HB3	2.03	0.41
2:B:2022:PRO:HB2	2:B:2024:PRO:HD2	2.03	0.40
2:B:4860:ARG:HG3	2:B:4876:CYS:HB3	2.03	0.40
2:G:2143:THR:O	2:G:3651:ASN:ND2	2.44	0.40
2:G:649:PHE:HB3	2:G:776:LEU:HB3	2.02	0.40
2:G:914:PRO:HD2	2:G:917:GLU:HB2	2.02	0.40
2:I:23:GLN:HB3	2:I:201:ASN:HB2	2.02	0.40
2:I:500:ALA:HB1	2:I:504:ALA:HB2	2.03	0.40
2:B:1865:MET:SD	2:B:1865:MET:N	2.94	0.40
2:B:2674:UNK:O	2:B:2676:UNK:N	2.54	0.40
2:B:57:ASN:HD22	2:B:308:HIS:HB2	1.87	0.40
2:B:359:TYR:HA	2:B:376:ALA:HA	2.03	0.40
2:B:3889:GLN:HG3	2:B:3967:GLU:HG3	2.03	0.40
2:E:1671:ARG:NH2	2:E:1713:ASP:HB3	2.36	0.40
2:E:2880:GLU:O	2:E:2884:ASN:N	2.47	0.40
2:E:57:ASN:HD22	2:E:308:HIS:HB2	1.87	0.40
2:E:670:GLU:HG3	2:E:787:VAL:HG13	2.03	0.40
2:G:1671:ARG:NH2	2:G:1713:ASP:HB3	2.36	0.40
2:G:1676:LEU:HD23	2:G:2167:ILE:HG23	2.03	0.40
2:G:4886:HIS:O	2:G:4890:GLY:N	2.46	0.40
2:I:1671:ARG:NH2	2:I:1713:ASP:HB3	2.36	0.40
2:I:2022:PRO:O	2:I:2028:ARG:NH2	2.54	0.40
2:B:1111:PRO:HD3	2:B:1605:TRP:HE1	1.86	0.40
2:B:1671:ARG:NH2	2:B:1713:ASP:HB3	2.36	0.40
2:B:4848:VAL:O	2:B:4852:THR:OG1	2.32	0.40
2:G:57:ASN:HD22	2:G:308:HIS:HB2	1.87	0.40
2:I:1111:PRO:HD3	2:I:1605:TRP:HE1	1.86	0.40
2:I:256:ALA:HB1	2:I:286:THR:HG21	2.03	0.40
2:I:983:THR:O	2:I:987:ARG:N	2.52	0.40
2:B:256:ALA:HB1	2:B:286:THR:HG21	2.03	0.40
2:E:870:ILE:HD12	2:E:873:LYS:HB2	2.04	0.40
2:G:1641:ILE:HA	2:G:1642:PRO:HD3	1.90	0.40
2:G:4929:LEU:HA	2:G:4929:LEU:HD13	1.95	0.40
2:B:2022:PRO:O	2:B:2028:ARG:NH2	2.54	0.40
2:B:2318:TYR:HA	2:B:2319:PRO:HD3	1.94	0.40
2:B:451:TYR:O	2:B:474:ARG:NH1	2.45	0.40
2:B:939:VAL:HG22	2:B:1053:ILE:HG12	2.03	0.40
2:E:261:ARG:HB3	2:E:283:ARG:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:734:GLY:O	2:G:736:HIS:ND1	2.52	0.40
2:I:116:MET:HB2	2:I:137:LEU:HD12	2.04	0.40
2:I:57:ASN:HD22	2:I:308:HIS:HB2	1.87	0.40
2:I:3733:CYS:HB2	2:I:3803:SER:HB3	2.03	0.40
2:I:649:PHE:HB3	2:I:776:LEU:HB3	2.02	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 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	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	F	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	H	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
1	J	105/108 (97%)	95 (90%)	10 (10%)	0	100	100
2	B	3235/4416 (73%)	2874 (89%)	357 (11%)	4 (0%)	56	90
2	E	3235/4416 (73%)	2873 (89%)	358 (11%)	4 (0%)	56	90
2	G	3235/4416 (73%)	2875 (89%)	356 (11%)	4 (0%)	56	90
2	I	3235/4416 (73%)	2873 (89%)	358 (11%)	4 (0%)	56	90
All	All	13360/18096 (74%)	11875 (89%)	1469 (11%)	16 (0%)	59	90

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1708	ARG
2	G	1708	ARG
2	E	1708	ARG
2	I	1708	ARG
2	B	1932	PRO

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Mol	Chain	Res	Type
2	G	1932	PRO
2	E	1932	PRO
2	I	1932	PRO
2	B	1840	PRO
2	B	4641	PRO
2	G	1840	PRO
2	G	4641	PRO
2	E	1840	PRO
2	E	4641	PRO
2	I	1840	PRO
2	I	4641	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 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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	88/89 (99%)	88 (100%)	0	100	100
1	F	88/89 (99%)	88 (100%)	0	100	100
1	H	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2493/3022 (82%)	2476 (99%)	17 (1%)	88	94
2	E	2493/3022 (82%)	2476 (99%)	17 (1%)	88	94
2	G	2493/3022 (82%)	2476 (99%)	17 (1%)	88	94
2	I	2493/3022 (82%)	2476 (99%)	17 (1%)	88	94
All	All	10324/12444 (83%)	10256 (99%)	68 (1%)	89	94

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	131	LEU
2	B	309	THR
2	B	534	ARG
2	B	553	ARG

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Mol	Chain	Res	Type
2	B	1076	ARG
2	B	1141	ARG
2	B	1600	LEU
2	B	1676	LEU
2	B	1964	ARG
2	B	3762	ARG
2	B	3787	LYS
2	B	3805	LEU
2	B	3896	ASN
2	B	4034	ASN
2	B	4085	ARG
2	B	4120	ASN
2	B	4983	HIS
2	G	131	LEU
2	G	309	THR
2	G	534	ARG
2	G	553	ARG
2	G	1076	ARG
2	G	1141	ARG
2	G	1600	LEU
2	G	1676	LEU
2	G	1964	ARG
2	G	3762	ARG
2	G	3787	LYS
2	G	3805	LEU
2	G	3896	ASN
2	G	4034	ASN
2	G	4085	ARG
2	G	4120	ASN
2	G	4983	HIS
2	E	131	LEU
2	E	309	THR
2	E	534	ARG
2	E	553	ARG
2	E	1076	ARG
2	E	1141	ARG
2	E	1600	LEU
2	E	1676	LEU
2	E	1964	ARG
2	E	3762	ARG
2	E	3787	LYS
2	E	3805	LEU

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Mol	Chain	Res	Type
2	E	3896	ASN
2	E	4034	ASN
2	E	4085	ARG
2	E	4120	ASN
2	E	4983	HIS
2	I	131	LEU
2	I	309	THR
2	I	534	ARG
2	I	553	ARG
2	I	1076	ARG
2	I	1141	ARG
2	I	1600	LEU
2	I	1676	LEU
2	I	1964	ARG
2	I	3762	ARG
2	I	3787	LYS
2	I	3805	LEU
2	I	3896	ASN
2	I	4034	ASN
2	I	4085	ARG
2	I	4120	ASN
2	I	4983	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	87	HIS
1	A	87	HIS
1	H	87	HIS
1	J	87	HIS
2	B	57	ASN
2	B	111	HIS
2	B	113	HIS
2	B	273	HIS
2	B	379	HIS
2	B	479	GLN
2	B	582	HIS
2	B	1158	ASN
2	B	1598	GLN
2	B	1679	ASN
2	B	1688	HIS
2	B	1691	GLN

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Mol	Chain	Res	Type
2	B	1719	HIS
2	B	1775	HIS
2	B	2005	GLN
2	B	3767	GLN
2	B	3809	ASN
2	B	3896	ASN
2	B	3960	GLN
2	B	3976	ASN
2	B	4034	ASN
2	B	4120	ASN
2	B	4553	ASN
2	B	4806	ASN
2	G	57	ASN
2	G	111	HIS
2	G	113	HIS
2	G	273	HIS
2	G	379	HIS
2	G	479	GLN
2	G	582	HIS
2	G	1158	ASN
2	G	1598	GLN
2	G	1679	ASN
2	G	1688	HIS
2	G	1691	GLN
2	G	1719	HIS
2	G	1775	HIS
2	G	2005	GLN
2	G	3767	GLN
2	G	3809	ASN
2	G	3896	ASN
2	G	3960	GLN
2	G	4034	ASN
2	G	4120	ASN
2	G	4553	ASN
2	G	4806	ASN
2	E	57	ASN
2	E	111	HIS
2	E	113	HIS
2	E	273	HIS
2	E	379	HIS
2	E	479	GLN
2	E	582	HIS

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Mol	Chain	Res	Type
2	E	1158	ASN
2	E	1598	GLN
2	E	1679	ASN
2	E	1688	HIS
2	E	1691	GLN
2	E	1719	HIS
2	E	1775	HIS
2	E	2005	GLN
2	E	3767	GLN
2	E	3809	ASN
2	E	3896	ASN
2	E	3960	GLN
2	E	4034	ASN
2	E	4120	ASN
2	E	4553	ASN
2	E	4806	ASN
2	I	57	ASN
2	I	111	HIS
2	I	113	HIS
2	I	273	HIS
2	I	379	HIS
2	I	479	GLN
2	I	582	HIS
2	I	1158	ASN
2	I	1598	GLN
2	I	1679	ASN
2	I	1688	HIS
2	I	1691	GLN
2	I	1719	HIS
2	I	1775	HIS
2	I	2005	GLN
2	I	3767	GLN
2	I	3809	ASN
2	I	3896	ASN
2	I	3960	GLN
2	I	4034	ASN
2	I	4120	ASN
2	I	4553	ASN
2	I	4806	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](#)

Of 4 ligands modelled in this entry, 4 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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	G	14
2	B	14
2	I	14
2	E	14

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4345:UNK	C	4540:PHE	N	73.03
1	G	4345:UNK	C	4540:PHE	N	73.03
1	E	4345:UNK	C	4540:PHE	N	73.03
1	I	4345:UNK	C	4540:PHE	N	73.03
1	B	3613:UNK	C	3639:THR	N	46.34
1	G	3613:UNK	C	3639:THR	N	46.34
1	E	3613:UNK	C	3639:THR	N	46.34
1	I	3613:UNK	C	3639:THR	N	46.34
1	B	4253:GLU	C	4320:UNK	N	27.01
1	G	4253:GLU	C	4320:UNK	N	27.01
1	E	4253:GLU	C	4320:UNK	N	27.01
1	I	4253:GLU	C	4320:UNK	N	27.01
1	B	3163:UNK	C	3170:UNK	N	16.37
1	G	3163:UNK	C	3170:UNK	N	16.37
1	E	3163:UNK	C	3170:UNK	N	16.37
1	I	3163:UNK	C	3170:UNK	N	16.37
1	B	3063:UNK	C	3134:UNK	N	15.02
1	E	3063:UNK	C	3134:UNK	N	15.02
1	G	3063:UNK	C	3134:UNK	N	15.01
1	I	3063:UNK	C	3134:UNK	N	15.01
1	B	3468:UNK	C	3511:UNK	N	14.70
1	G	3468:UNK	C	3511:UNK	N	14.70
1	E	3468:UNK	C	3511:UNK	N	14.70
1	I	3468:UNK	C	3511:UNK	N	14.70
1	B	2703:UNK	C	2734:ASN	N	14.05
1	G	2703:UNK	C	2734:ASN	N	14.05
1	E	2703:UNK	C	2734:ASN	N	14.05
1	I	2703:UNK	C	2734:ASN	N	14.05
1	B	3236:UNK	C	3241:UNK	N	13.51
1	G	3236:UNK	C	3241:UNK	N	13.51
1	E	3236:UNK	C	3241:UNK	N	13.51
1	I	3236:UNK	C	3241:UNK	N	13.50
1	B	2976:UNK	C	2995:UNK	N	12.41
1	G	2976:UNK	C	2995:UNK	N	12.41
1	E	2976:UNK	C	2995:UNK	N	12.41
1	I	2976:UNK	C	2995:UNK	N	12.41
1	B	1564:UNK	C	1573:MET	N	12.19
1	G	1564:UNK	C	1573:MET	N	12.19
1	E	1564:UNK	C	1573:MET	N	12.19
1	I	1564:UNK	C	1573:MET	N	12.19
1	B	3254:UNK	C	3261:UNK	N	8.04
1	G	3254:UNK	C	3261:UNK	N	8.04
1	E	3254:UNK	C	3261:UNK	N	8.04

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	3254:UNK	C	3261:UNK	N	8.04
1	B	1297:UNK	C	1430:UNK	N	5.71
1	G	1297:UNK	C	1430:UNK	N	5.71
1	E	1297:UNK	C	1430:UNK	N	5.71
1	I	1297:UNK	C	1430:UNK	N	5.71
1	B	2479:LEU	C	2487:UNK	N	3.30
1	G	2479:LEU	C	2487:UNK	N	3.30
1	E	2479:LEU	C	2487:UNK	N	3.30
1	I	2479:LEU	C	2487:UNK	N	3.30
1	B	2939:ARG	C	2942:UNK	N	3.28
1	G	2939:ARG	C	2942:UNK	N	3.28
1	E	2939:ARG	C	2942:UNK	N	3.28
1	I	2939:ARG	C	2942:UNK	N	3.28