



Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 02:34 AM EST

PDB ID : 6X36
EMDB ID : EMD-22019
Title : Pig R615C RyR1 in complex with CaM, EGTA (class 3, closed)
Authors : Woll, K.W.; Haji-Ghassemi, O.; Van Petegem, F.
Deposited on : 2020-05-21
Resolution : 4.70 Å(reported)

This is a Full wwPDB EM 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/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

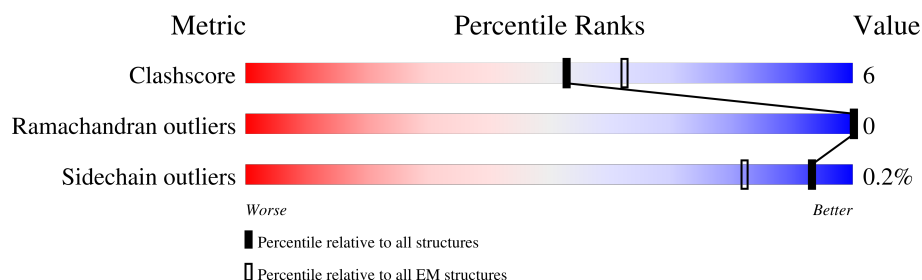
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.70 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	110	78% 17% 5%
1	D	110	78% 17% 5%
1	G	110	78% 17% 5%
1	J	110	78% 17% 5%
2	B	3531	89% 11%
2	E	3531	89% 11%
2	H	3531	89% 11%
2	K	3531	89% 11%
3	C	148	82% 8% 10%

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Mol	Chain	Length	Quality of chain
3	F	148	 82%7%10%
3	I	148	 84%5%10%
3	L	148	 82%7%10%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 100164 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	A	105	Total	C	N	O	S	0	0
			697	440	124	131	2		
1	D	105	Total	C	N	O	S	0	0
			697	440	124	131	2		
1	G	105	Total	C	N	O	S	0	0
			697	440	124	131	2		
1	J	105	Total	C	N	O	S	0	0
			697	440	124	131	2		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP P68106
A	-1	ASN	-	expression tag	UNP P68106
A	0	ALA	-	expression tag	UNP P68106
D	-2	SER	-	expression tag	UNP P68106
D	-1	ASN	-	expression tag	UNP P68106
D	0	ALA	-	expression tag	UNP P68106
G	-2	SER	-	expression tag	UNP P68106
G	-1	ASN	-	expression tag	UNP P68106
G	0	ALA	-	expression tag	UNP P68106
J	-2	SER	-	expression tag	UNP P68106
J	-1	ASN	-	expression tag	UNP P68106
J	0	ALA	-	expression tag	UNP P68106

- Molecule 2 is a protein called Ryanodine Receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	3529	Total	C	N	O	S	0	0
			23573	15059	4209	4176	129		
2	E	3529	Total	C	N	O	S	0	0
			23573	15059	4209	4176	129		
2	H	3529	Total	C	N	O	S	0	0
			23573	15059	4209	4176	129		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	K	3529	Total	C	N	O	S	0	0
			23573	15059	4209	4176	129		


- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	133	Total	C	N	O	S	0	0
			771	475	138	154	4		
3	F	133	Total	C	N	O	S	0	0
			771	475	138	154	4		
3	I	133	Total	C	N	O	S	0	0
			771	475	138	154	4		
3	L	133	Total	C	N	O	S	0	0
			771	475	138	154	4		

3 Residue-property plots [i](#)


These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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 A: 




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

Chain D: 




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

Chain G: 




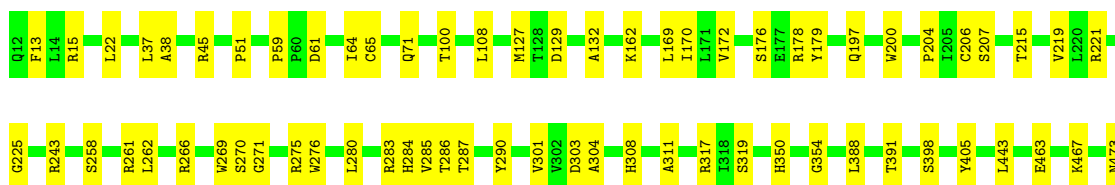
- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

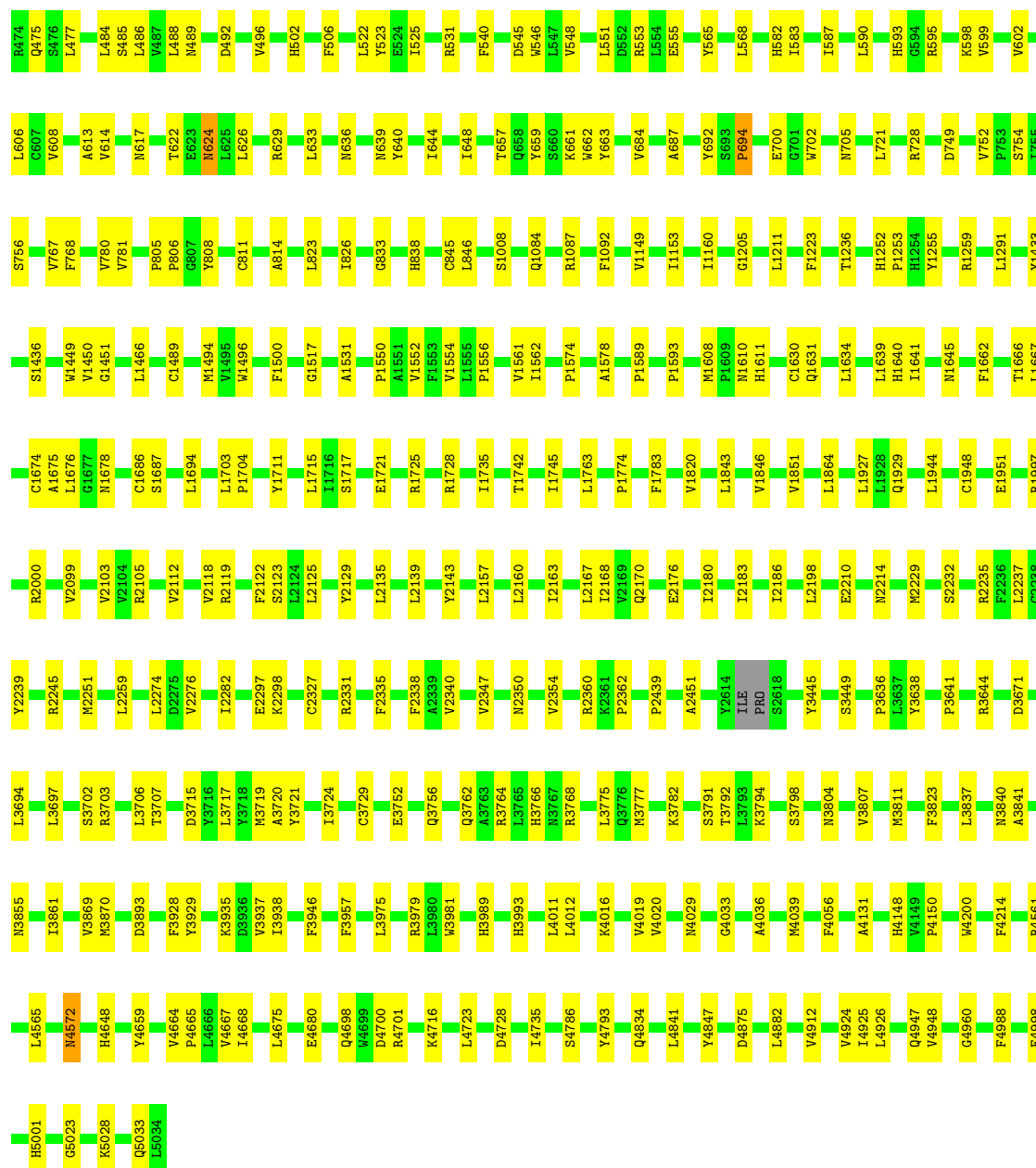
Chain J: 



- Molecule 2: Ryanodine Receptor

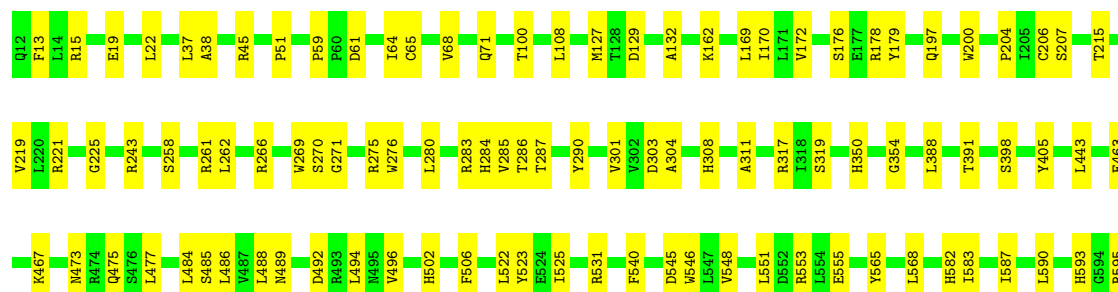
Chain B: 

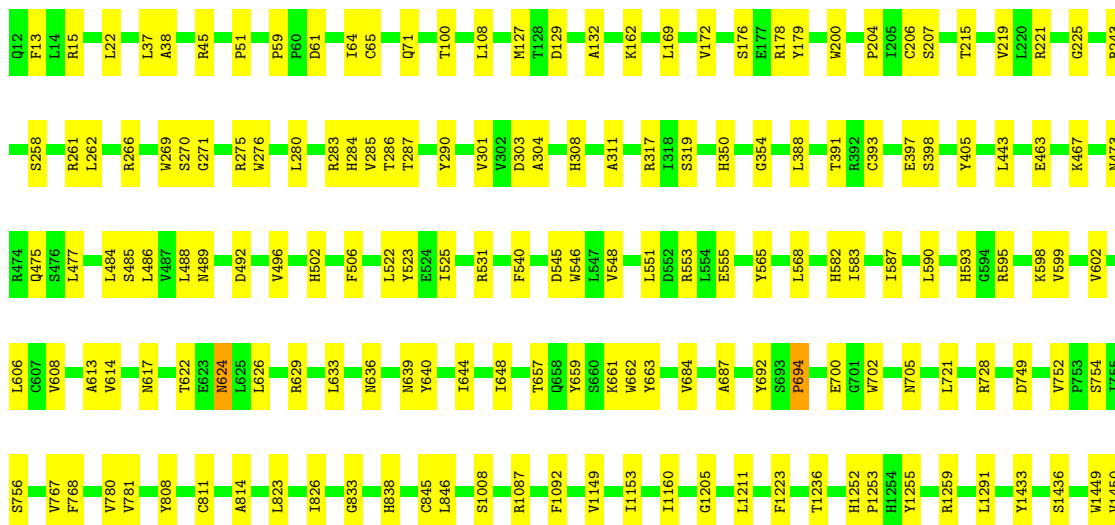




● Molecule 2: Ryanodine Receptor


Chain E: 89% 11%



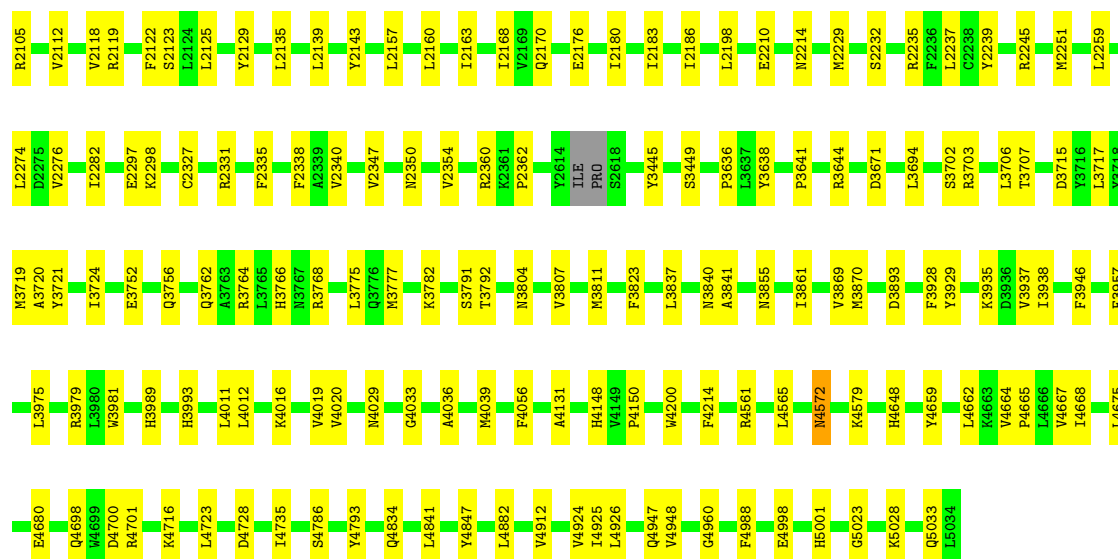


G1451	C1686	T2102	I2282	A3720	L3980	
L1466	S1687	V2103	I2297	Y3721	W3981	Y4793
C1459	L1694	R2105	K2298	I3724	H3993	Q4834
M1494	L1703	V2112	C2327	E3752	L4011	L4841
Y1496	P1704	V2118	R2331	Q3756	L4012	Y4847
F1500	Y1711	R2119	F2338	Q3762	V4020	L4882
G1517	L1715	F2122	A2339	A3763	N4029	V4912
A1531	L1716	L2124	V2340	I3765	G4033	V4924
P1550	S1717	L2125	V2347	H3766	A4036	I4925
A1551	E1721	Y2129	N2350	R3767	M4039	L4926
P1552	R1725	L2135	V2354	L3775	F4056	Q4947
F1553	R1728	L2139	R2360	Q3776	A4131	V4948
V1554	I1735	Y2143	P2361	K3777	H4148	Q4960
P1556	T1742	L2157	P2362	K3782	V4149	F4988
V1561	I1745	L2160	P2439	S3791	P4150	E4988
I1562	L1763	I2163	A2451	N3804	W4200	H5001
P1574	L1774	L2168	Y2614	V3807	F4214	G5023
A1578	P1774	V2169	PRO	K3811	R4561	K5028
P1589	F1783	Q2170	S2618	F3823	L4665	Q5033
P1592	V1820	E2176	Y3445	L3837	N4572	L5034
P1593	L1843	I2180	S3449	N3840	H4648	
M1608	V1846	I2183	P3636	A3841	V4664	
N1610	V1851	I2186	L3637	N3855	P4665	
H1611	L1864	L2198	Y3638	I3861	L4666	
C1630	L1927	E2210	P3641	V3869	I4668	
Q1631	L1928	N2214	R3644	N3870	L4675	
L1639	Q1929	M2229	D3671	D3893	E4680	
H1640	L1944	S2232	L3694	F3928	Q4698	
I1641	C1948	R2235	S3702	Y3929	V4699	
N1645	E1951	F2236	R3703	T3938	D4700	
F1662	T1666	L2237	L3706	F3946	R4701	
T1667	R1997	M2251	T3707	F3967	K4716	
C1674	R2000	Y3715	D3715	L4723	L4723	
A1675	L2098	Y3716	K3716	L3975	D4728	
G1677	V2099	L3717	Y3718	R3979	I4735	
N1678		V2276	M3719			

● Molecule 2: Ryanodine Receptor

Chain K:  89% 11%

Q12	G225	R474	L606	V767	L1466	L1694
F13	R243	Q475	G607	F768	C1489	L1703
L14	S258	S476	V608	V780	M1489	P1704
R15	L261	L477	A613	V781	Y1495	Y1711
L22	L262	L484	V614	Y808	W1496	L1715
L37	R266	S485	N617	C811	F1500	S1717
A38	R45	L486	T622	A814	G1517	E1721
R45	W269	N489	N624	L623	A1531	R1725
P51	G271	D492	L626	I826	P1550	R1728
P59	R275	V496	R629	G833	A1551	I1735
D61	W276	H502	L633	H838	F1552	T1742
I64	L280	F506	N636	C945	V1554	I1745
C65	R283	L522	N639	L846	L1555	L1763
Q71	H284	Y523	N640	S1008	P1556	P1774
T100	V285	E524	I525	R1087	V1561	A1578
L108	T286	I525	I644	F1092	I1562	P1589
M127	T287	R531	I648	F1092	P1574	V1820
T128	Y290	F540	T657	F1092	A1578	L1843
D129	V301	D545	Q658	V1149	P1589	V1846
A132	D303	W546	Y659	T1183	P1609	V1851
K162	A304	L547	S660	I1180	P1630	L1864
L169	H308	V548	K661	G1205	Q1631	L1927
I170	A311	L551	W662	L1211	L1639	L1928
L171	R317	D552	Y663	F1223	H1640	Q1929
V172	I318	R553	V694	T1236	I1641	L1944
S176	S319	L554	Y694	H1252	N1645	C1948
E177	S319	E555	Y694	P1253	F1662	E1951
R178	H350	Y565	E700	H1254	T1666	R1997
Y179	G354	L568	G701	Y1255	L1667	R2000
Q197	L388	H582	W702	H1255	C1674	L2098
W200	T391	I583	N705	L1259	A1675	V2099
P204	S398	I587	L721	L1291	F1677	T2102
I266	Y405	L590	R728	Y1433	N1678	V2103
S207	R593	H593	D749	S1436	C1686	V2104
L443	R595	G594	A1675	W1449	S1687	
T215	E463	K598	V752	V1450		
V219	K467	V599	S754	G1451		
L221	N473	V602	S756			



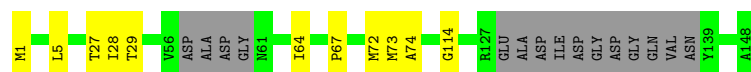
• Molecule 3: Calmodulin-1

Chain C: 82% 8% 10%



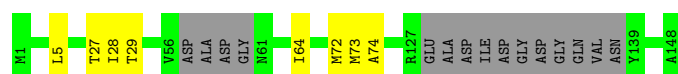
• Molecule 3: Calmodulin-1

Chain F: 82% 7% 10%



• Molecule 3: Calmodulin-1

Chain I: 84% 5% 10%



• Molecule 3: Calmodulin-1

Chain L: 82% 7% 10%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	7038	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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	0.25	0/711	0.43	0/971
1	D	0.25	0/711	0.43	0/971
1	G	0.25	0/711	0.43	0/971
1	J	0.25	0/711	0.43	0/971
2	B	0.24	0/22309	0.41	3/30536 (0.0%)
2	E	0.24	0/22309	0.41	3/30536 (0.0%)
2	H	0.24	0/22309	0.41	3/30536 (0.0%)
2	K	0.24	0/22309	0.41	3/30536 (0.0%)
3	C	0.25	0/774	0.43	0/1059
3	F	0.25	0/774	0.43	0/1059
3	I	0.25	0/774	0.43	0/1059
3	L	0.25	0/774	0.43	0/1059
All	All	0.24	0/95176	0.41	12/130264 (0.0%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	2362	PRO	CA-N-CD	-5.72	103.49	111.50
2	B	2362	PRO	CA-N-CD	-5.70	103.52	111.50
2	H	2362	PRO	CA-N-CD	-5.70	103.53	111.50
2	E	2362	PRO	CA-N-CD	-5.69	103.53	111.50
2	E	694	PRO	CA-N-CD	-5.37	103.98	111.50
2	B	694	PRO	CA-N-CD	-5.34	104.02	111.50
2	K	694	PRO	CA-N-CD	-5.31	104.06	111.50
2	H	694	PRO	CA-N-CD	-5.31	104.06	111.50
2	E	127	MET	CA-CB-CG	5.15	122.05	113.30
2	B	127	MET	CA-CB-CG	5.15	122.05	113.30
2	K	127	MET	CA-CB-CG	5.14	122.04	113.30
2	H	127	MET	CA-CB-CG	5.12	122.01	113.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	697	0	604	12	0
1	D	697	0	604	12	0
1	G	697	0	604	11	0
1	J	697	0	604	12	0
2	B	23573	0	19309	249	0
2	E	23573	0	19309	243	0
2	H	23573	0	19309	231	0
2	K	23573	0	19309	237	0
3	C	771	0	513	9	0
3	F	771	0	513	8	0
3	I	771	0	513	5	0
3	L	771	0	513	8	0
All	All	100164	0	81704	1011	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 6.

All (1011) 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:E:100:THR:HG21	2:E:162:LYS:HE3	1.58	0.86
2:H:100:THR:HG21	2:H:162:LYS:HE3	1.58	0.86
2:K:100:THR:HG21	2:K:162:LYS:HE3	1.58	0.85
2:B:100:THR:HG21	2:B:162:LYS:HE3	1.58	0.85
2:B:1774:PRO:HG3	2:B:2157:LEU:HB3	1.67	0.77
2:E:590:LEU:HD13	2:E:599:VAL:HG21	1.66	0.77
2:H:590:LEU:HD13	2:H:599:VAL:HG21	1.66	0.77
2:K:590:LEU:HD13	2:K:599:VAL:HG21	1.66	0.77
2:K:1774:PRO:HG3	2:K:2157:LEU:HB3	1.67	0.77
2:E:1774:PRO:HG3	2:E:2157:LEU:HB3	1.67	0.76
2:B:590:LEU:HD13	2:B:599:VAL:HG21	1.66	0.76
2:H:1774:PRO:HG3	2:H:2157:LEU:HB3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2210:GLU:OE2	2:B:2214:ASN:ND2	2.23	0.72
2:E:523:TYR:OH	2:E:553:ARG:NH1	2.23	0.71
2:H:275:ARG:HA	2:H:275:ARG:NH1	2.05	0.71
2:H:4960:GLY:H	2:H:5023:GLY:HA2	1.56	0.71
2:B:275:ARG:NH1	2:B:275:ARG:HA	2.05	0.71
2:H:3719:MET:SD	2:H:3791:SER:OG	2.48	0.71
2:K:2210:GLU:OE2	2:K:2214:ASN:ND2	2.23	0.71
2:K:3719:MET:SD	2:K:3791:SER:OG	2.48	0.71
2:K:4960:GLY:H	2:K:5023:GLY:HA2	1.55	0.71
2:E:4960:GLY:H	2:E:5023:GLY:HA2	1.55	0.71
2:B:523:TYR:OH	2:B:553:ARG:NH1	2.23	0.71
2:B:3719:MET:SD	2:B:3791:SER:OG	2.48	0.71
2:K:523:TYR:OH	2:K:553:ARG:NH1	2.23	0.71
2:H:523:TYR:OH	2:H:553:ARG:NH1	2.23	0.70
2:E:3719:MET:SD	2:E:3791:SER:OG	2.48	0.70
2:E:2210:GLU:OE2	2:E:2214:ASN:ND2	2.23	0.70
2:E:275:ARG:HA	2:E:275:ARG:NH1	2.05	0.70
2:H:2210:GLU:OE2	2:H:2214:ASN:ND2	2.23	0.70
2:K:275:ARG:NH1	2:K:275:ARG:HA	2.05	0.70
2:B:4960:GLY:H	2:B:5023:GLY:HA2	1.55	0.69
2:H:3929:TYR:HH	2:H:3993:HIS:HD1	1.38	0.69
2:H:219:VAL:HG21	2:H:398:SER:HB2	1.74	0.68
2:B:219:VAL:HG21	2:B:398:SER:HB2	1.74	0.68
2:H:2237:LEU:HG	2:H:2276:VAL:HG21	1.76	0.68
2:E:2237:LEU:HG	2:E:2276:VAL:HG21	1.76	0.68
2:K:4659:TYR:HH	2:K:4786:SER:HG	1.41	0.68
2:B:648:ILE:HG23	2:B:814:ALA:HB3	1.76	0.68
2:K:648:ILE:HG23	2:K:814:ALA:HB3	1.76	0.68
2:E:648:ILE:HG23	2:E:814:ALA:HB3	1.76	0.68
2:K:219:VAL:HG21	2:K:398:SER:HB2	1.74	0.68
2:E:1763:LEU:HD12	2:E:1864:LEU:HD11	1.76	0.68
2:E:219:VAL:HG21	2:E:398:SER:HB2	1.74	0.67
2:H:1763:LEU:HD12	2:H:1864:LEU:HD11	1.76	0.67
2:H:4723:LEU:HA	2:H:4735:ILE:HD11	1.76	0.67
2:E:176:SER:HB2	2:E:178:ARG:HH21	1.59	0.67
2:B:4723:LEU:HA	2:B:4735:ILE:HD11	1.76	0.67
2:H:548:VAL:HA	2:H:551:LEU:HD12	1.77	0.67
2:K:4723:LEU:HA	2:K:4735:ILE:HD11	1.76	0.67
2:B:176:SER:HB2	2:B:178:ARG:HH21	1.59	0.67
2:K:1763:LEU:HD12	2:K:1864:LEU:HD11	1.76	0.67
2:K:2237:LEU:HG	2:K:2276:VAL:HG21	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:548:VAL:HA	2:E:551:LEU:HD12	1.77	0.67
2:H:648:ILE:HG23	2:H:814:ALA:HB3	1.76	0.67
2:H:176:SER:HB2	2:H:178:ARG:HH21	1.59	0.66
2:B:1763:LEU:HD12	2:B:1864:LEU:HD11	1.76	0.66
2:B:2237:LEU:HG	2:B:2276:VAL:HG21	1.76	0.66
2:K:176:SER:HB2	2:K:178:ARG:HH21	1.59	0.66
2:E:4723:LEU:HA	2:E:4735:ILE:HD11	1.76	0.66
2:H:1451:GLY:HA3	2:H:1494:MET:HA	1.78	0.66
2:H:1820:VAL:HG22	2:H:1927:LEU:HD13	1.78	0.65
2:E:1820:VAL:HG22	2:E:1927:LEU:HD13	1.78	0.65
2:E:4882:LEU:HD11	2:H:4912:VAL:HG21	1.78	0.65
2:B:1820:VAL:HG22	2:B:1927:LEU:HD13	1.78	0.65
2:K:4698:GLN:OE1	2:K:4701:ARG:NH1	2.29	0.65
2:B:2143:TYR:HB3	2:B:2198:LEU:HD13	1.79	0.65
2:H:4882:LEU:HD11	2:K:4912:VAL:HG21	1.79	0.65
2:B:548:VAL:HA	2:B:551:LEU:HD12	1.77	0.65
2:H:4698:GLN:OE1	2:H:4701:ARG:NH1	2.29	0.65
2:K:1820:VAL:HG22	2:K:1927:LEU:HD13	1.78	0.65
2:B:1451:GLY:HA3	2:B:1494:MET:HA	1.78	0.65
2:E:1451:GLY:HA3	2:E:1494:MET:HA	1.78	0.65
2:K:548:VAL:HA	2:K:551:LEU:HD12	1.77	0.64
2:B:4882:LEU:HD11	2:E:4912:VAL:HG21	1.79	0.64
2:E:4698:GLN:OE1	2:E:4701:ARG:NH1	2.29	0.64
2:B:4698:GLN:OE1	2:B:4701:ARG:NH1	2.29	0.64
2:E:2143:TYR:HB3	2:E:2198:LEU:HD13	1.79	0.64
2:H:553:ARG:NH2	2:H:555:GLU:OE1	2.28	0.64
2:K:1451:GLY:HA3	2:K:1494:MET:HA	1.78	0.64
2:H:2103:VAL:HG11	2:H:2125:LEU:HD13	1.80	0.64
2:H:684:VAL:HG23	2:H:781:VAL:HG22	1.81	0.63
2:K:2103:VAL:HG11	2:K:2125:LEU:HD13	1.80	0.63
2:B:4912:VAL:HG21	2:K:4882:LEU:HD11	1.81	0.63
2:H:2143:TYR:HB3	2:H:2198:LEU:HD13	1.79	0.63
2:B:684:VAL:HG23	2:B:781:VAL:HG22	1.80	0.63
2:B:663:TYR:HB2	2:B:808:TYR:HB3	1.81	0.63
2:E:4659:TYR:HH	2:E:4786:SER:HG	1.47	0.63
2:E:2103:VAL:HG11	2:E:2125:LEU:HD13	1.80	0.62
2:E:38:ALA:HB1	2:E:64:ILE:HG12	1.81	0.62
2:B:38:ALA:HB1	2:B:64:ILE:HG12	1.81	0.62
2:H:1236:THR:OG1	2:H:1608:MET:SD	2.57	0.62
2:H:663:TYR:HB2	2:H:808:TYR:HB3	1.81	0.62
2:K:684:VAL:HG23	2:K:781:VAL:HG22	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2103:VAL:HG11	2:B:2125:LEU:HD13	1.81	0.62
2:E:684:VAL:HG23	2:E:781:VAL:HG22	1.80	0.62
2:K:663:TYR:HB2	2:K:808:TYR:HB3	1.81	0.62
2:K:2143:TYR:HB3	2:K:2198:LEU:HD13	1.79	0.62
2:E:1236:THR:OG1	2:E:1608:MET:SD	2.57	0.62
2:K:1236:THR:OG1	2:K:1608:MET:SD	2.57	0.62
2:E:4200:TRP:HB2	2:E:4988:PHE:HZ	1.65	0.62
2:H:4200:TRP:HB2	2:H:4988:PHE:HZ	1.65	0.62
2:E:1742:THR:HG23	2:E:1745:ILE:HD12	1.82	0.61
2:H:1153:ILE:HG13	2:H:1160:ILE:HG12	1.82	0.61
2:B:1717:SER:HA	2:B:1721:GLU:HB2	1.82	0.61
2:E:659:TYR:O	2:E:662:TRP:NE1	2.32	0.61
2:K:1153:ILE:HG13	2:K:1160:ILE:HG12	1.82	0.61
2:K:1742:THR:HG23	2:K:1745:ILE:HD12	1.82	0.61
2:E:1556:PRO:HA	2:E:1561:VAL:HG21	1.82	0.61
2:H:1717:SER:HA	2:H:1721:GLU:HB2	1.82	0.61
2:B:4200:TRP:HB2	2:B:4988:PHE:HZ	1.65	0.61
2:H:221:ARG:NH1	2:H:258:SER:OG	2.34	0.61
2:E:13:PHE:CG	2:E:162:LYS:HE2	2.35	0.61
2:H:13:PHE:CG	2:H:162:LYS:HE2	2.35	0.61
2:H:1742:THR:HG23	2:H:1745:ILE:HD12	1.82	0.61
2:K:13:PHE:CG	2:K:162:LYS:HE2	2.35	0.61
2:B:1742:THR:HG23	2:B:1745:ILE:HD12	1.82	0.61
2:E:1717:SER:HA	2:E:1721:GLU:HB2	1.82	0.61
2:H:1556:PRO:HA	2:H:1561:VAL:HG21	1.82	0.61
2:B:659:TYR:O	2:B:662:TRP:NE1	2.32	0.61
2:B:1236:THR:OG1	2:B:1608:MET:SD	2.57	0.61
2:H:38:ALA:HB1	2:H:64:ILE:HG12	1.81	0.61
2:K:38:ALA:HB1	2:K:64:ILE:HG12	1.81	0.61
2:E:663:TYR:HB2	2:E:808:TYR:HB3	1.81	0.61
2:K:1717:SER:HA	2:K:1721:GLU:HB2	1.82	0.60
2:B:728:ARG:NH2	2:B:1489:CYS:SG	2.74	0.60
2:B:13:PHE:CG	2:B:162:LYS:HE2	2.35	0.60
2:K:553:ARG:NH2	2:K:555:GLU:OE1	2.28	0.60
2:K:1556:PRO:HA	2:K:1561:VAL:HG21	1.82	0.60
2:K:728:ARG:NH2	2:K:1489:CYS:SG	2.74	0.60
2:B:1153:ILE:HG13	2:B:1160:ILE:HG12	1.82	0.60
2:E:221:ARG:NH1	2:E:258:SER:OG	2.34	0.60
2:H:728:ARG:NH2	2:H:1489:CYS:SG	2.74	0.60
2:B:221:ARG:NH1	2:B:258:SER:OG	2.34	0.60
2:E:728:ARG:NH2	2:E:1489:CYS:SG	2.74	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1153:ILE:HG13	2:E:1160:ILE:HG12	1.82	0.60
2:K:221:ARG:NH1	2:K:258:SER:OG	2.34	0.60
2:K:4200:TRP:HB2	2:K:4988:PHE:HZ	1.65	0.60
2:B:1556:PRO:HA	2:B:1561:VAL:HG21	1.82	0.59
2:H:1630:CYS:SG	2:H:1631:GLN:N	2.75	0.59
2:E:4998:GLU:HA	2:E:5001:HIS:HE1	1.67	0.59
2:H:4998:GLU:HA	2:H:5001:HIS:HE1	1.66	0.59
2:K:225:GLY:H	2:K:388:LEU:HA	1.67	0.59
2:H:3777:MET:SD	2:H:3792:THR:OG1	2.60	0.59
2:B:225:GLY:H	2:B:388:LEU:HA	1.67	0.59
2:B:4659:TYR:HH	2:B:4786:SER:HG	1.51	0.59
2:K:1676:LEU:HD12	2:K:2168:ILE:HG21	1.85	0.59
2:H:1676:LEU:HD12	2:H:2168:ILE:HG21	1.85	0.59
2:E:1449:TRP:HD1	2:E:1496:TRP:HA	1.68	0.59
2:E:1630:CYS:SG	2:E:1631:GLN:N	2.75	0.59
2:E:1676:LEU:HD12	2:E:2168:ILE:HG21	1.85	0.59
2:K:1630:CYS:SG	2:K:1631:GLN:N	2.76	0.59
2:K:1449:TRP:HD1	2:K:1496:TRP:HA	1.68	0.59
2:H:225:GLY:H	2:H:388:LEU:HA	1.67	0.58
2:K:1694:LEU:HD23	2:K:1715:LEU:HB2	1.85	0.58
2:B:4998:GLU:HA	2:B:5001:HIS:HE1	1.66	0.58
2:E:553:ARG:NH2	2:E:555:GLU:OE1	2.28	0.58
2:E:3777:MET:SD	2:E:3792:THR:OG1	2.60	0.58
2:E:1694:LEU:HD23	2:E:1715:LEU:HB2	1.85	0.58
2:H:1694:LEU:HD23	2:H:1715:LEU:HB2	1.85	0.58
2:B:1630:CYS:SG	2:B:1631:GLN:N	2.76	0.58
2:B:1676:LEU:HD12	2:B:2168:ILE:HG21	1.85	0.58
2:B:1694:LEU:HD23	2:B:1715:LEU:HB2	1.85	0.58
2:H:1449:TRP:HD1	2:H:1496:TRP:HA	1.68	0.58
2:K:3777:MET:SD	2:K:3792:THR:OG1	2.59	0.58
2:B:1449:TRP:HD1	2:B:1496:TRP:HA	1.68	0.58
2:B:1466:LEU:HD21	2:B:1496:TRP:CD1	2.39	0.58
2:E:225:GLY:H	2:E:388:LEU:HA	1.67	0.58
2:K:1466:LEU:HD21	2:K:1496:TRP:CD1	2.39	0.58
2:E:303:ASP:OD1	2:E:304:ALA:N	2.35	0.58
2:E:2297:GLU:OE1	2:E:2360:ARG:NH1	2.36	0.58
2:K:5028:LYS:O	2:K:5033:GLN:N	2.31	0.58
2:B:3777:MET:SD	2:B:3792:THR:OG1	2.60	0.58
2:E:1466:LEU:HD21	2:E:1496:TRP:CD1	2.39	0.58
2:K:4998:GLU:HA	2:K:5001:HIS:HE1	1.67	0.58
2:E:266:ARG:NH1	2:E:269:TRP:O	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1674:CYS:HA	2:E:1678:ASN:HB3	1.86	0.57
2:B:1674:CYS:HA	2:B:1678:ASN:HB3	1.86	0.57
2:B:4648:HIS:HE2	2:B:4793:TYR:HH	1.52	0.57
2:B:553:ARG:NH2	2:B:555:GLU:OE1	2.28	0.57
2:H:2297:GLU:OE1	2:H:2360:ARG:NH1	2.36	0.57
1:A:73:LYS:HA	1:A:100:ASP:HA	1.87	0.57
2:H:1674:CYS:HA	2:H:1678:ASN:HB3	1.86	0.57
2:H:266:ARG:NH1	2:H:269:TRP:O	2.37	0.57
2:K:266:ARG:NH1	2:K:269:TRP:O	2.37	0.57
2:K:1674:CYS:HA	2:K:1678:ASN:HB3	1.86	0.57
2:B:303:ASP:OD1	2:B:304:ALA:N	2.35	0.57
2:H:1466:LEU:HD21	2:H:1496:TRP:CD1	2.39	0.57
2:H:3869:VAL:HG22	2:H:3870:MET:HE2	1.87	0.57
1:J:73:LYS:HA	1:J:100:ASP:HA	1.87	0.57
2:K:1087:ARG:HE	2:K:1223:PHE:HE1	1.52	0.57
2:K:2297:GLU:OE1	2:K:2360:ARG:NH1	2.36	0.57
2:B:266:ARG:NH1	2:B:269:TRP:O	2.37	0.57
2:E:2122:PHE:O	2:E:3721:TYR:OH	2.23	0.57
2:E:2000:ARG:CZ	3:F:114:GLY:H	2.18	0.57
2:H:2122:PHE:O	2:H:3721:TYR:OH	2.23	0.57
2:B:266:ARG:O	2:B:270:SER:OG	2.23	0.56
2:E:5028:LYS:O	2:E:5033:GLN:N	2.31	0.56
2:K:659:TYR:O	2:K:662:TRP:NE1	2.32	0.56
2:B:284:HIS:CD2	2:B:287:THR:H	2.23	0.56
2:B:1087:ARG:HE	2:B:1223:PHE:HE1	1.52	0.56
2:H:284:HIS:CD2	2:H:287:THR:H	2.23	0.56
2:K:2000:ARG:CZ	3:L:114:GLY:H	2.18	0.56
2:E:1087:ARG:HE	2:E:1223:PHE:HE1	1.52	0.56
2:E:284:HIS:CD2	2:E:287:THR:H	2.23	0.56
2:B:350:HIS:HB3	2:B:354:GLY:H	1.71	0.56
2:E:266:ARG:O	2:E:270:SER:OG	2.23	0.56
2:H:833:GLY:HA3	2:H:838:HIS:CD2	2.41	0.56
2:K:266:ARG:O	2:K:270:SER:OG	2.23	0.56
2:K:833:GLY:HA3	2:K:838:HIS:CD2	2.41	0.56
2:B:2297:GLU:OE1	2:B:2360:ARG:NH1	2.36	0.56
2:B:833:GLY:HA3	2:B:838:HIS:CD2	2.41	0.56
2:K:284:HIS:CD2	2:K:287:THR:H	2.24	0.56
2:B:2122:PHE:O	2:B:3721:TYR:OH	2.23	0.56
2:K:350:HIS:HB3	2:K:354:GLY:H	1.71	0.56
2:K:2122:PHE:O	2:K:3721:TYR:OH	2.23	0.56
1:D:73:LYS:HA	1:D:100:ASP:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:639:ASN:OD1	2:E:640:TYR:N	2.39	0.56
2:K:303:ASP:OD1	2:K:304:ALA:N	2.35	0.56
2:H:1087:ARG:HE	2:H:1223:PHE:HE1	1.52	0.55
2:K:3869:VAL:HG22	2:K:3870:MET:HE2	1.87	0.55
2:B:3837:LEU:HD22	2:B:3928:PHE:HB2	1.89	0.55
2:E:833:GLY:HA3	2:E:838:HIS:CD2	2.41	0.55
1:G:73:LYS:HA	1:G:100:ASP:HA	1.87	0.55
2:H:5028:LYS:O	2:H:5033:GLN:N	2.31	0.55
2:B:3869:VAL:HG22	2:B:3870:MET:HE2	1.87	0.55
2:K:59:PRO:HD2	2:K:304:ALA:HB1	1.89	0.55
2:K:639:ASN:OD1	2:K:640:TYR:N	2.39	0.55
2:B:59:PRO:HD2	2:B:304:ALA:HB1	1.89	0.55
2:H:266:ARG:O	2:H:270:SER:OG	2.23	0.55
2:K:2180:ILE:HD11	2:K:2229:MET:HA	1.88	0.55
2:K:4648:HIS:HE2	2:K:4793:TYR:HH	1.55	0.55
2:E:3869:VAL:HG22	2:E:3870:MET:HE2	1.87	0.55
2:H:659:TYR:O	2:H:662:TRP:NE1	2.32	0.55
2:H:4648:HIS:HE2	2:H:4793:TYR:HH	1.54	0.55
2:K:2119:ARG:NH2	2:K:3715:ASP:OD1	2.39	0.55
2:K:3837:LEU:HD22	2:K:3928:PHE:HB2	1.89	0.55
2:H:3837:LEU:HD22	2:H:3928:PHE:HB2	1.89	0.55
2:K:2176:GLU:O	2:K:2180:ILE:HG12	2.07	0.55
2:B:3929:TYR:HH	2:B:3993:HIS:CE1	2.25	0.55
2:E:2180:ILE:HD11	2:E:2229:MET:HA	1.88	0.55
1:A:24:VAL:HG12	1:A:26:TYR:H	1.72	0.55
2:B:2180:ILE:HD11	2:B:2229:MET:HA	1.88	0.55
2:E:2245:ARG:HH22	3:F:1:MET:HG2	1.72	0.55
2:H:2119:ARG:NH2	2:H:3715:ASP:OD1	2.39	0.55
2:H:2135:LEU:O	2:H:2139:LEU:HG	2.07	0.55
2:H:2180:ILE:HD11	2:H:2229:MET:HA	1.88	0.55
2:B:1944:LEU:HD13	2:B:2099:VAL:HG23	1.89	0.55
2:E:22:LEU:HB2	2:E:37:LEU:HD13	1.89	0.55
2:E:2282:ILE:HD11	2:E:2338:PHE:HB3	1.89	0.55
2:H:71:GLN:HB3	2:H:108:LEU:HD12	1.89	0.55
2:H:2176:GLU:O	2:H:2180:ILE:HG12	2.07	0.55
2:K:2135:LEU:O	2:K:2139:LEU:HG	2.07	0.55
2:E:59:PRO:HD2	2:E:304:ALA:HB1	1.89	0.54
2:E:2176:GLU:O	2:E:2180:ILE:HG12	2.07	0.54
2:E:3837:LEU:HD22	2:E:3928:PHE:HB2	1.89	0.54
2:B:639:ASN:OD1	2:B:640:TYR:N	2.39	0.54
2:E:350:HIS:HB3	2:E:354:GLY:H	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2123:SER:HA	2:E:3717:LEU:HD11	1.90	0.54
2:H:59:PRO:HD2	2:H:304:ALA:HB1	1.89	0.54
2:H:2123:SER:HA	2:H:3717:LEU:HD11	1.90	0.54
2:B:2282:ILE:HD11	2:B:2338:PHE:HB3	1.89	0.54
2:B:3671:ASP:OD1	2:B:3764:ARG:NH2	2.24	0.54
1:D:24:VAL:HG12	1:D:26:TYR:H	1.73	0.54
2:E:71:GLN:HB3	2:E:108:LEU:HD12	1.89	0.54
2:E:1944:LEU:HD13	2:E:2099:VAL:HG23	1.89	0.54
2:H:1944:LEU:HD13	2:H:2099:VAL:HG23	1.89	0.54
2:K:1944:LEU:HD13	2:K:2099:VAL:HG23	1.89	0.54
2:K:3929:TYR:HH	2:K:3993:HIS:CE1	2.25	0.54
2:B:71:GLN:HB3	2:B:108:LEU:HD12	1.89	0.54
2:B:2123:SER:HA	2:B:3717:LEU:HD11	1.89	0.54
2:B:2176:GLU:O	2:B:2180:ILE:HG12	2.07	0.54
2:E:2135:LEU:O	2:E:2139:LEU:HG	2.07	0.54
2:H:639:ASN:OD1	2:H:640:TYR:N	2.39	0.54
2:B:22:LEU:HB2	2:B:37:LEU:HD13	1.89	0.54
2:B:4036:ALA:HA	2:B:4039:MET:HB2	1.90	0.54
2:H:350:HIS:HB3	2:H:354:GLY:H	1.71	0.54
2:K:1662:PHE:O	2:K:1666:THR:HG23	2.08	0.54
1:G:24:VAL:HG12	1:G:26:TYR:H	1.72	0.54
2:H:303:ASP:OD1	2:H:304:ALA:N	2.35	0.54
2:H:3807:VAL:O	2:H:3811:MET:HG2	2.08	0.54
2:B:1084:GLN:NE2	2:B:1084:GLN:HA	2.22	0.54
2:K:2123:SER:HA	2:K:3717:LEU:HD11	1.90	0.54
2:K:2282:ILE:HD11	2:K:2338:PHE:HB3	1.89	0.54
2:B:1662:PHE:O	2:B:1666:THR:HG23	2.08	0.54
2:E:4648:HIS:HE2	2:E:4793:TYR:HH	1.55	0.54
2:H:1662:PHE:O	2:H:1666:THR:HG23	2.08	0.54
2:H:3929:TYR:HH	2:H:3993:HIS:CE1	2.25	0.54
2:K:2112:VAL:HG21	2:K:2118:VAL:HB	1.89	0.54
2:K:3807:VAL:O	2:K:3811:MET:HG2	2.08	0.54
2:B:5028:LYS:O	2:B:5033:GLN:N	2.31	0.54
2:E:2112:VAL:HG21	2:E:2118:VAL:HB	1.90	0.54
2:E:3807:VAL:O	2:E:3811:MET:HG2	2.08	0.54
2:E:3929:TYR:HH	2:E:3993:HIS:CE1	2.26	0.54
2:H:4036:ALA:HA	2:H:4039:MET:HB2	1.90	0.54
2:K:2245:ARG:HH22	3:L:1:MET:HG2	1.72	0.54
2:E:2327:CYS:O	2:E:2331:ARG:HG2	2.08	0.54
2:E:4036:ALA:HA	2:E:4039:MET:HB2	1.90	0.54
2:H:262:LEU:HB3	2:H:280:LEU:HD23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:24:VAL:HG12	1:J:26:TYR:H	1.73	0.54
2:K:71:GLN:HB3	2:K:108:LEU:HD12	1.89	0.54
2:B:3807:VAL:O	2:B:3811:MET:HG2	2.08	0.53
2:E:3671:ASP:OD1	2:E:3764:ARG:NH2	2.24	0.53
2:H:22:LEU:HB2	2:H:37:LEU:HD13	1.89	0.53
2:B:2135:LEU:O	2:B:2139:LEU:HG	2.07	0.53
2:E:1662:PHE:O	2:E:1666:THR:HG23	2.08	0.53
2:B:2112:VAL:HG21	2:B:2118:VAL:HB	1.90	0.53
2:H:2112:VAL:HG21	2:H:2118:VAL:HB	1.89	0.53
2:H:2282:ILE:HD11	2:H:2338:PHE:HB3	1.89	0.53
2:H:3671:ASP:OD1	2:H:3764:ARG:NH2	2.24	0.53
2:K:4036:ALA:HA	2:K:4039:MET:HB2	1.90	0.53
2:E:262:LEU:HB3	2:E:280:LEU:HD23	1.90	0.53
2:B:2327:CYS:O	2:B:2331:ARG:HG2	2.09	0.53
2:E:1500:PHE:HD1	2:E:1531:ALA:HB1	1.74	0.53
2:B:593:HIS:HD2	2:B:1593:PRO:HG2	1.74	0.53
2:E:593:HIS:HD2	2:E:1593:PRO:HG2	1.74	0.53
2:H:3720:ALA:O	2:H:3724:ILE:HG12	2.09	0.53
2:K:593:HIS:HD2	2:K:1593:PRO:HG2	1.74	0.53
2:K:756:SER:HB2	2:K:767:VAL:HG23	1.90	0.53
2:K:1092:PHE:N	2:K:1149:VAL:O	2.38	0.53
2:H:206:CYS:HB2	2:H:271:GLY:HA3	1.91	0.53
2:H:593:HIS:HD2	2:H:1593:PRO:HG2	1.74	0.53
2:H:756:SER:HB2	2:H:767:VAL:HG23	1.90	0.53
2:K:22:LEU:HB2	2:K:37:LEU:HD13	1.90	0.53
2:B:1500:PHE:HD1	2:B:1531:ALA:HB1	1.74	0.53
2:B:3729:CYS:HG	2:B:3798:SER:HG	1.47	0.53
2:K:2327:CYS:O	2:K:2331:ARG:HG2	2.08	0.53
2:K:3840:ASN:OD1	2:K:3841:ALA:N	2.42	0.53
2:B:284:HIS:NE2	2:B:286:THR:OG1	2.40	0.52
2:E:1092:PHE:N	2:E:1149:VAL:O	2.38	0.52
2:H:2327:CYS:O	2:H:2331:ARG:HG2	2.08	0.52
2:B:2119:ARG:NH2	2:B:3715:ASP:OD1	2.39	0.52
2:K:206:CYS:HB2	2:K:271:GLY:HA3	1.91	0.52
2:B:262:LEU:HB3	2:B:280:LEU:HD23	1.90	0.52
2:E:283:ARG:NH1	2:E:290:TYR:OH	2.43	0.52
2:E:2119:ARG:NH2	2:E:3715:ASP:OD1	2.39	0.52
2:H:1500:PHE:HD1	2:H:1531:ALA:HB1	1.74	0.52
2:B:283:ARG:NH1	2:B:290:TYR:OH	2.43	0.52
2:E:3720:ALA:O	2:E:3724:ILE:HG12	2.09	0.52
2:H:283:ARG:NH1	2:H:290:TYR:OH	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:262:LEU:HB3	2:K:280:LEU:HD23	1.90	0.52
2:K:1500:PHE:HD1	2:K:1531:ALA:HB1	1.74	0.52
2:K:3720:ALA:O	2:K:3724:ILE:HG12	2.09	0.52
2:B:3840:ASN:OD1	2:B:3841:ALA:N	2.42	0.52
2:E:284:HIS:HE2	2:E:286:THR:HG1	1.56	0.52
2:B:756:SER:HB2	2:B:767:VAL:HG23	1.90	0.52
2:B:1092:PHE:N	2:B:1149:VAL:O	2.38	0.52
2:K:1687:SER:HB2	2:K:1783:PHE:CE1	2.45	0.52
2:H:1687:SER:HB2	2:H:1783:PHE:CE1	2.45	0.52
2:K:61:ASP:OD1	2:K:283:ARG:NH1	2.43	0.52
2:K:243:ARG:NH1	2:K:301:VAL:O	2.43	0.52
2:K:283:ARG:NH1	2:K:290:TYR:OH	2.43	0.52
2:K:624:ASN:O	2:K:624:ASN:ND2	2.42	0.52
2:K:1929:GLN:HE22	2:K:2105:ARG:HH22	1.58	0.52
2:K:4680:GLU:OE2	2:K:4716:LYS:NZ	2.31	0.52
2:B:243:ARG:NH1	2:B:301:VAL:O	2.43	0.52
2:B:1929:GLN:HE22	2:B:2105:ARG:HH22	1.57	0.52
2:E:1687:SER:HB2	2:E:1783:PHE:CE1	2.45	0.52
2:B:284:HIS:HE2	2:B:286:THR:HG1	1.56	0.52
2:B:1687:SER:HB2	2:B:1783:PHE:CE1	2.45	0.52
2:H:614:VAL:HG22	2:H:2170:GLN:HG3	1.92	0.52
2:K:1436:SER:HA	2:K:1517:GLY:HA2	1.92	0.52
2:B:624:ASN:O	2:B:624:ASN:ND2	2.42	0.51
2:B:1997:ARG:HA	2:B:2000:ARG:HG2	1.92	0.51
2:B:3720:ALA:O	2:B:3724:ILE:HG12	2.09	0.51
2:E:206:CYS:HB2	2:E:271:GLY:HA3	1.91	0.51
2:K:614:VAL:HG22	2:K:2170:GLN:HG3	1.92	0.51
2:H:752:VAL:HG12	2:H:754:SER:H	1.75	0.51
2:H:3840:ASN:OD1	2:H:3841:ALA:N	2.42	0.51
2:K:752:VAL:HG12	2:K:754:SER:H	1.75	0.51
2:E:4029:ASN:OD1	2:E:4033:GLY:N	2.44	0.51
2:B:1436:SER:HA	2:B:1517:GLY:HA2	1.92	0.51
2:E:61:ASP:OD1	2:E:283:ARG:NH1	2.43	0.51
2:E:3840:ASN:OD1	2:E:3841:ALA:N	2.42	0.51
2:H:3445:TYR:O	2:H:3449:SER:N	2.44	0.51
2:B:206:CYS:HB2	2:B:271:GLY:HA3	1.91	0.51
2:H:61:ASP:OD1	2:H:283:ARG:NH1	2.43	0.51
2:H:657:THR:O	2:H:1008:SER:OG	2.25	0.51
2:B:614:VAL:HG22	2:B:2170:GLN:HG3	1.92	0.51
2:B:752:VAL:HG12	2:B:754:SER:H	1.75	0.51
2:E:756:SER:HB2	2:E:767:VAL:HG23	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1997:ARG:HA	2:H:2000:ARG:HG2	1.92	0.51
2:K:284:HIS:NE2	2:K:286:THR:OG1	2.40	0.51
2:B:61:ASP:OD1	2:B:283:ARG:NH1	2.43	0.51
2:B:475:GLN:NE2	2:B:531:ARG:O	2.43	0.51
2:E:614:VAL:HG22	2:E:2170:GLN:HG3	1.92	0.51
2:E:1436:SER:HA	2:E:1517:GLY:HA2	1.92	0.51
2:H:284:HIS:NE2	2:H:286:THR:OG1	2.40	0.51
2:H:4841:LEU:HD22	2:H:4926:LEU:HD11	1.93	0.51
2:K:1997:ARG:HA	2:K:2000:ARG:HG2	1.92	0.51
2:K:4029:ASN:OD1	2:K:4033:GLY:N	2.44	0.51
2:E:657:THR:O	2:E:1008:SER:OG	2.25	0.51
2:H:276:TRP:HE3	2:H:317:ARG:HA	1.76	0.51
2:H:1436:SER:HA	2:H:1517:GLY:HA2	1.92	0.51
2:H:1929:GLN:HE22	2:H:2105:ARG:HH22	1.58	0.51
2:H:3702:SER:O	2:H:3706:LEU:HG	2.11	0.51
2:K:276:TRP:HE3	2:K:317:ARG:HA	1.76	0.51
2:B:129:ASP:HB3	2:B:132:ALA:HB2	1.93	0.51
2:B:3445:TYR:O	2:B:3449:SER:N	2.44	0.51
2:H:475:GLN:NE2	2:H:531:ARG:O	2.44	0.51
2:K:3702:SER:O	2:K:3706:LEU:HG	2.11	0.51
2:B:172:VAL:HG22	2:B:179:TYR:CE1	2.46	0.51
2:B:4561:ARG:O	2:B:4565:LEU:HG	2.11	0.51
2:E:284:HIS:NE2	2:E:286:THR:OG1	2.40	0.51
2:B:2160:LEU:HA	2:B:2163:ILE:HG22	1.94	0.50
2:E:475:GLN:NE2	2:E:531:ARG:O	2.43	0.50
2:E:624:ASN:ND2	2:E:624:ASN:O	2.42	0.50
2:E:2125:LEU:HD11	2:E:2129:TYR:CZ	2.46	0.50
1:G:1:GLY:O	1:G:77:THR:OG1	2.30	0.50
2:K:284:HIS:HE2	2:K:286:THR:HG1	1.56	0.50
2:K:636:ASN:HB3	2:K:702:TRP:HH2	1.77	0.50
1:D:1:GLY:O	1:D:77:THR:OG1	2.29	0.50
2:E:172:VAL:HG22	2:E:179:TYR:CE1	2.46	0.50
2:E:243:ARG:NH1	2:E:301:VAL:O	2.43	0.50
2:H:4029:ASN:OD1	2:H:4033:GLY:N	2.44	0.50
2:H:4561:ARG:O	2:H:4565:LEU:HG	2.11	0.50
2:K:1703:LEU:HD12	2:K:1704:PRO:HD2	1.94	0.50
1:A:1:GLY:O	1:A:77:THR:OG1	2.29	0.50
2:B:636:ASN:HB3	2:B:702:TRP:HH2	1.77	0.50
2:B:4029:ASN:OD1	2:B:4033:GLY:N	2.44	0.50
2:E:129:ASP:HB3	2:E:132:ALA:HB2	1.93	0.50
2:H:284:HIS:HE2	2:H:286:THR:HG1	1.58	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:624:ASN:O	2:H:624:ASN:ND2	2.42	0.50
2:B:2125:LEU:HD11	2:B:2129:TYR:CZ	2.47	0.50
2:E:752:VAL:HG12	2:E:754:SER:H	1.75	0.50
2:H:243:ARG:NH1	2:H:301:VAL:O	2.43	0.50
2:K:4561:ARG:O	2:K:4565:LEU:HG	2.12	0.50
2:E:1466:LEU:HD21	2:E:1496:TRP:HD1	1.77	0.50
2:E:1640:HIS:NE2	2:E:1645:ASN:OD1	2.30	0.50
2:E:1929:GLN:HE22	2:E:2105:ARG:HH22	1.58	0.50
2:E:3445:TYR:O	2:E:3449:SER:N	2.44	0.50
2:E:4561:ARG:O	2:E:4565:LEU:HG	2.12	0.50
2:K:2125:LEU:HD11	2:K:2129:TYR:CZ	2.46	0.50
2:B:4841:LEU:HD22	2:B:4926:LEU:HD11	1.93	0.50
2:E:692:TYR:CE2	2:E:780:VAL:HG11	2.47	0.50
2:E:3636:PRO:HD2	2:E:3638:TYR:HE1	1.77	0.50
2:E:3702:SER:O	2:E:3706:LEU:HG	2.11	0.50
2:E:4841:LEU:HD22	2:E:4926:LEU:HD11	1.93	0.50
2:H:636:ASN:HB3	2:H:702:TRP:HH2	1.77	0.50
2:H:2125:LEU:HD11	2:H:2129:TYR:CZ	2.46	0.50
2:K:502:HIS:NE2	2:K:506:PHE:HE2	2.10	0.50
2:K:845:CYS:SG	2:K:846:LEU:N	2.85	0.50
2:B:276:TRP:HE3	2:B:317:ARG:HA	1.76	0.50
2:B:4572:ASN:HD21	2:E:4847:TYR:HE2	1.59	0.50
2:E:502:HIS:NE2	2:E:506:PHE:HE2	2.10	0.50
2:H:172:VAL:HG22	2:H:179:TYR:CE1	2.46	0.50
2:H:1703:LEU:HD12	2:H:1704:PRO:HD2	1.94	0.50
2:K:3445:TYR:O	2:K:3449:SER:N	2.44	0.50
2:K:3636:PRO:HD2	2:K:3638:TYR:HE1	1.77	0.50
2:H:845:CYS:SG	2:H:846:LEU:N	2.85	0.50
2:H:1092:PHE:N	2:H:1149:VAL:O	2.38	0.50
2:H:2160:LEU:HA	2:H:2163:ILE:HG22	1.94	0.50
1:J:1:GLY:O	1:J:77:THR:OG1	2.29	0.50
2:B:275:ARG:HA	2:B:275:ARG:HH11	1.77	0.50
2:E:636:ASN:HB3	2:E:702:TRP:HH2	1.77	0.50
2:E:2160:LEU:HA	2:E:2163:ILE:HG22	1.94	0.50
2:H:692:TYR:CE2	2:H:780:VAL:HG11	2.47	0.50
2:K:692:TYR:CE2	2:K:780:VAL:HG11	2.47	0.50
2:B:1703:LEU:HD12	2:B:1704:PRO:HD2	1.93	0.49
2:B:3636:PRO:HD2	2:B:3638:TYR:HE1	1.77	0.49
2:H:1466:LEU:HD21	2:H:1496:TRP:HD1	1.77	0.49
2:H:3636:PRO:HD2	2:H:3638:TYR:HE1	1.77	0.49
2:K:172:VAL:HG22	2:K:179:TYR:CE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:502:HIS:NE2	2:B:506:PHE:HE2	2.10	0.49
2:B:3702:SER:O	2:B:3706:LEU:HG	2.11	0.49
2:E:276:TRP:HE3	2:E:317:ARG:HA	1.76	0.49
2:E:486:LEU:HA	2:E:489:ASN:HD21	1.77	0.49
2:H:129:ASP:HB3	2:H:132:ALA:HB2	1.93	0.49
2:H:486:LEU:HA	2:H:489:ASN:HD21	1.77	0.49
2:H:502:HIS:CD2	2:H:506:PHE:HE2	2.30	0.49
2:H:2347:VAL:HG23	2:H:2350:ASN:H	1.77	0.49
2:B:692:TYR:CE2	2:B:780:VAL:HG11	2.47	0.49
2:E:51:PRO:HG2	2:E:65:CYS:SG	2.53	0.49
2:H:502:HIS:NE2	2:H:506:PHE:HE2	2.10	0.49
2:K:502:HIS:CD2	2:K:506:PHE:HE2	2.30	0.49
2:E:2347:VAL:HG23	2:E:2350:ASN:H	1.77	0.49
2:K:2340:VAL:HA	2:K:2354:VAL:HG21	1.94	0.49
3:L:28:ILE:HG22	3:L:29:THR:N	2.28	0.49
2:B:845:CYS:SG	2:B:846:LEU:N	2.85	0.49
2:B:1948:CYS:HA	2:B:1951:GLU:HG2	1.94	0.49
2:E:502:HIS:CD2	2:E:506:PHE:HE2	2.31	0.49
2:E:1997:ARG:HA	2:E:2000:ARG:HG2	1.92	0.49
2:K:614:VAL:HG12	2:K:617:ASN:H	1.77	0.49
2:B:502:HIS:CD2	2:B:506:PHE:HE2	2.31	0.49
2:B:545:ASP:OD1	2:B:546:TRP:N	2.46	0.49
2:E:845:CYS:SG	2:E:846:LEU:N	2.85	0.49
2:E:1948:CYS:HA	2:E:1951:GLU:HG2	1.94	0.49
2:K:275:ARG:HA	2:K:275:ARG:HH11	1.77	0.49
2:K:657:THR:O	2:K:1008:SER:OG	2.25	0.49
2:K:4841:LEU:HD22	2:K:4926:LEU:HD11	1.93	0.49
2:B:486:LEU:HA	2:B:489:ASN:HD21	1.77	0.49
2:B:4680:GLU:OE2	2:B:4716:LYS:NZ	2.31	0.49
2:E:545:ASP:OD1	2:E:546:TRP:N	2.45	0.49
2:E:614:VAL:HG12	2:E:617:ASN:H	1.78	0.49
2:E:1703:LEU:HD12	2:E:1704:PRO:HD2	1.94	0.49
2:H:614:VAL:HG12	2:H:617:ASN:H	1.78	0.49
2:K:2347:VAL:HG23	2:K:2350:ASN:H	1.77	0.49
3:C:28:ILE:HG22	3:C:29:THR:N	2.28	0.49
2:K:545:ASP:OD1	2:K:546:TRP:N	2.45	0.49
2:H:2340:VAL:HA	2:H:2354:VAL:HG21	1.95	0.49
2:K:2160:LEU:HA	2:K:2163:ILE:HG22	1.94	0.49
2:H:545:ASP:OD1	2:H:546:TRP:N	2.45	0.49
2:K:486:LEU:HA	2:K:489:ASN:HD21	1.77	0.49
2:K:1554:VAL:HG21	2:K:1562:ILE:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:SER:HA	1:A:42:ARG:HE	1.78	0.48
2:K:475:GLN:NE2	2:K:531:ARG:O	2.43	0.48
2:B:51:PRO:HG2	2:B:65:CYS:SG	2.53	0.48
2:B:1291:LEU:HD13	2:B:1550:PRO:HG2	1.95	0.48
2:B:1554:VAL:HG21	2:B:1562:ILE:HD13	1.94	0.48
2:E:275:ARG:HA	2:E:275:ARG:HH11	1.78	0.48
2:E:1291:LEU:HD13	2:E:1550:PRO:HG2	1.95	0.48
2:H:51:PRO:HG2	2:H:65:CYS:SG	2.53	0.48
2:B:614:VAL:HG12	2:B:617:ASN:H	1.78	0.48
2:B:3935:LYS:NZ	2:B:3937:VAL:O	2.34	0.48
2:E:206:CYS:SG	2:E:207:SER:N	2.87	0.48
3:I:28:ILE:HG22	3:I:29:THR:N	2.28	0.48
2:K:662:TRP:HE3	2:K:811:CYS:HA	1.78	0.48
2:B:206:CYS:SG	2:B:207:SER:N	2.87	0.48
2:K:172:VAL:HG22	2:K:179:TYR:HE1	1.79	0.48
2:B:2340:VAL:HA	2:B:2354:VAL:HG21	1.95	0.48
2:B:4847:TYR:HE2	2:K:4572:ASN:HD21	1.56	0.48
2:E:548:VAL:HG21	2:E:582:HIS:CG	2.49	0.48
2:E:1554:VAL:HG21	2:E:1562:ILE:HD13	1.94	0.48
2:H:662:TRP:HE3	2:H:811:CYS:HA	1.79	0.48
2:H:1554:VAL:HG21	2:H:1562:ILE:HD13	1.94	0.48
2:K:51:PRO:HG2	2:K:65:CYS:SG	2.53	0.48
2:B:172:VAL:HG22	2:B:179:TYR:HE1	1.78	0.48
1:D:39:SER:HA	1:D:42:ARG:HE	1.78	0.48
3:F:28:ILE:HG22	3:F:29:THR:N	2.28	0.48
2:H:275:ARG:HA	2:H:275:ARG:HH11	1.78	0.48
2:B:548:VAL:HG21	2:B:582:HIS:CG	2.49	0.48
2:E:4648:HIS:NE2	2:E:4793:TYR:OH	2.42	0.48
2:H:172:VAL:HG22	2:H:179:TYR:HE1	1.79	0.48
2:K:129:ASP:HB3	2:K:132:ALA:HB2	1.93	0.48
2:E:172:VAL:HG22	2:E:179:TYR:HE1	1.79	0.48
2:B:1728:ARG:HE	2:B:1851:VAL:HG11	1.78	0.48
2:E:2340:VAL:HA	2:E:2354:VAL:HG21	1.95	0.48
1:G:39:SER:HA	1:G:42:ARG:HE	1.78	0.48
2:H:1291:LEU:HD13	2:H:1550:PRO:HG2	1.95	0.48
2:K:206:CYS:SG	2:K:207:SER:N	2.87	0.48
2:K:565:TYR:HB2	2:K:602:VAL:HG22	1.96	0.48
2:B:565:TYR:HB2	2:B:602:VAL:HG22	1.96	0.48
2:B:2000:ARG:CZ	3:C:114:GLY:H	2.26	0.48
2:B:2347:VAL:HG23	2:B:2350:ASN:H	1.77	0.48
2:H:206:CYS:SG	2:H:207:SER:N	2.87	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1466:LEU:HD21	2:K:1496:TRP:HD1	1.77	0.48
2:B:317:ARG:HG2	2:B:319:SER:H	1.79	0.47
2:B:662:TRP:HE3	2:B:811:CYS:HA	1.79	0.47
2:K:1948:CYS:HA	2:K:1951:GLU:HG2	1.94	0.47
3:C:5:LEU:HD21	3:C:74:ALA:HA	1.96	0.47
2:H:548:VAL:HG21	2:H:582:HIS:CG	2.49	0.47
2:H:565:TYR:HB2	2:H:602:VAL:HG22	1.96	0.47
2:H:833:GLY:HA3	2:H:838:HIS:HD2	1.79	0.47
2:H:4680:GLU:OE2	2:H:4716:LYS:NZ	2.31	0.47
2:K:1728:ARG:HE	2:K:1851:VAL:HG11	1.78	0.47
2:E:833:GLY:HA3	2:E:838:HIS:HD2	1.79	0.47
2:E:1728:ARG:HE	2:E:1851:VAL:HG11	1.78	0.47
2:H:1948:CYS:HA	2:H:1951:GLU:HG2	1.94	0.47
2:K:276:TRP:CE3	2:K:317:ARG:HA	2.50	0.47
2:B:833:GLY:HA3	2:B:838:HIS:HD2	1.79	0.47
2:E:317:ARG:HG2	2:E:319:SER:H	1.79	0.47
1:G:52:LYS:HG2	1:G:54:GLU:H	1.80	0.47
2:K:1291:LEU:HD13	2:K:1550:PRO:HG2	1.95	0.47
2:E:565:TYR:HB2	2:E:602:VAL:HG22	1.96	0.47
2:H:176:SER:HB2	2:H:178:ARG:NH2	2.28	0.47
2:K:833:GLY:HA3	2:K:838:HIS:HD2	1.79	0.47
2:B:1466:LEU:HD21	2:B:1496:TRP:HD1	1.77	0.47
3:F:5:LEU:HD21	3:F:74:ALA:HA	1.96	0.47
2:H:1728:ARG:HE	2:H:1851:VAL:HG11	1.78	0.47
2:B:276:TRP:CE3	2:B:317:ARG:HA	2.50	0.47
1:D:52:LYS:HG2	1:D:54:GLU:H	1.80	0.47
2:H:276:TRP:CE3	2:H:317:ARG:HA	2.50	0.47
1:J:39:SER:HA	1:J:42:ARG:HE	1.78	0.47
2:K:4214:PHE:CE1	2:K:4948:VAL:HG11	2.50	0.47
3:L:5:LEU:HD21	3:L:74:ALA:HA	1.96	0.47
3:L:28:ILE:HG22	3:L:29:THR:H	1.80	0.47
2:B:2245:ARG:HH22	3:C:1:MET:HG2	1.79	0.47
2:E:694:PRO:HG2	2:E:826:ILE:HB	1.97	0.47
1:J:52:LYS:HG2	1:J:54:GLU:H	1.80	0.47
2:B:4214:PHE:CE1	2:B:4948:VAL:HG11	2.50	0.47
3:C:28:ILE:HG22	3:C:29:THR:H	1.80	0.47
2:E:662:TRP:HE3	2:E:811:CYS:HA	1.78	0.47
2:E:4680:GLU:OE2	2:E:4716:LYS:NZ	2.31	0.47
2:H:694:PRO:HG2	2:H:826:ILE:HB	1.97	0.47
2:H:4214:PHE:CE1	2:H:4948:VAL:HG11	2.49	0.47
2:K:176:SER:HB2	2:K:178:ARG:NH2	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:276:TRP:CE3	2:E:317:ARG:HA	2.50	0.47
3:I:28:ILE:HG22	3:I:29:THR:H	1.80	0.47
2:K:548:VAL:HG21	2:K:582:HIS:CG	2.49	0.47
2:K:694:PRO:HG2	2:K:826:ILE:HB	1.97	0.47
2:K:1450:VAL:HA	2:K:1552:VAL:HG23	1.97	0.47
1:D:77:THR:HB	1:D:80:VAL:HG22	1.98	0.46
2:E:2259:LEU:HB3	2:E:2298:LYS:HZ1	1.79	0.46
2:E:4214:PHE:CE1	2:E:4948:VAL:HG11	2.50	0.46
2:B:2239:TYR:CE2	3:C:67:PRO:HG3	2.50	0.46
2:B:3938:ILE:HG21	2:B:3946:PHE:CD1	2.51	0.46
2:H:1728:ARG:HH21	2:H:1851:VAL:HG11	1.81	0.46
3:I:5:LEU:HD21	3:I:74:ALA:HA	1.96	0.46
2:K:1433:TYR:CE1	2:K:1578:ALA:HB2	2.50	0.46
1:G:74:LEU:N	1:G:99:PHE:O	2.48	0.46
2:H:3938:ILE:HG21	2:H:3946:PHE:CD1	2.51	0.46
2:K:317:ARG:HG2	2:K:319:SER:H	1.79	0.46
2:K:3938:ILE:HG21	2:K:3946:PHE:CD1	2.50	0.46
1:A:52:LYS:HG2	1:A:54:GLU:H	1.80	0.46
2:B:694:PRO:HG2	2:B:826:ILE:HB	1.97	0.46
2:E:1087:ARG:NE	2:E:1223:PHE:HE1	2.13	0.46
2:E:3641:PRO:HG2	2:E:3644:ARG:HH21	1.81	0.46
2:E:3938:ILE:HG21	2:E:3946:PHE:CD1	2.51	0.46
2:H:1433:TYR:CE1	2:H:1578:ALA:HB2	2.50	0.46
2:K:1728:ARG:HH21	2:K:1851:VAL:HG11	1.80	0.46
1:G:77:THR:HB	1:G:80:VAL:HG22	1.98	0.46
2:H:1450:VAL:HA	2:H:1552:VAL:HG23	1.97	0.46
1:J:77:THR:HB	1:J:80:VAL:HG22	1.98	0.46
2:B:215:THR:OG1	2:B:271:GLY:O	2.33	0.46
2:B:221:ARG:N	2:B:391:THR:O	2.42	0.46
2:B:1087:ARG:NE	2:B:1223:PHE:HE1	2.13	0.46
2:B:2259:LEU:HD13	2:B:2298:LYS:HZ1	1.81	0.46
2:B:4728:ASP:N	2:B:4728:ASP:OD1	2.49	0.46
2:E:4947:GLN:OE1	2:E:4947:GLN:N	2.49	0.46
2:H:317:ARG:HG2	2:H:319:SER:H	1.79	0.46
2:H:3703:ARG:O	2:H:3707:THR:HG23	2.16	0.46
2:K:3641:PRO:HG2	2:K:3644:ARG:HH21	1.81	0.46
2:B:4947:GLN:OE1	2:B:4947:GLN:N	2.49	0.46
2:K:700:GLU:H	2:K:705:ASN:HD21	1.64	0.46
2:E:1433:TYR:CE1	2:E:1578:ALA:HB2	2.50	0.46
2:E:4664:VAL:HA	2:E:4667:VAL:HG12	1.98	0.46
2:K:3935:LYS:NZ	2:K:3937:VAL:O	2.34	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:4728:ASP:OD1	2:K:4728:ASP:N	2.49	0.46
1:A:77:THR:HB	1:A:80:VAL:HG22	1.98	0.46
2:B:284:HIS:HD2	2:B:287:THR:HB	1.81	0.46
2:B:700:GLU:H	2:B:705:ASN:HD21	1.64	0.46
2:B:1433:TYR:CE1	2:B:1578:ALA:HB2	2.50	0.46
2:H:2259:LEU:HD13	2:H:2298:LYS:HZ1	1.80	0.46
2:B:4664:VAL:HA	2:B:4667:VAL:HG12	1.98	0.46
2:E:3703:ARG:O	2:E:3707:THR:HG23	2.16	0.46
2:H:215:THR:OG1	2:H:271:GLY:O	2.33	0.46
2:K:3703:ARG:O	2:K:3707:THR:HG23	2.16	0.46
2:B:661:LYS:HA	2:B:749:ASP:HA	1.99	0.45
2:B:1450:VAL:HA	2:B:1552:VAL:HG23	1.97	0.45
2:B:4200:TRP:HB2	2:B:4988:PHE:CZ	2.50	0.45
2:E:473:ASN:O	2:E:477:LEU:HD23	2.16	0.45
2:H:3641:PRO:HG2	2:H:3644:ARG:HH21	1.81	0.45
2:B:622:THR:HA	2:B:626:LEU:HD23	1.98	0.45
2:B:1252:HIS:CE1	2:B:1255:TYR:CD2	3.05	0.45
2:E:1252:HIS:CE1	2:E:1255:TYR:CD2	3.05	0.45
2:H:473:ASN:O	2:H:477:LEU:HD23	2.16	0.45
2:H:1087:ARG:NE	2:H:1223:PHE:HE1	2.13	0.45
2:K:661:LYS:HA	2:K:749:ASP:HA	1.99	0.45
2:K:1087:ARG:NE	2:K:1223:PHE:HE1	2.13	0.45
2:H:4947:GLN:N	2:H:4947:GLN:OE1	2.49	0.45
2:K:2259:LEU:HD13	2:K:2298:LYS:HZ1	1.80	0.45
2:E:176:SER:HB2	2:E:178:ARG:NH2	2.28	0.45
2:E:4728:ASP:OD1	2:E:4728:ASP:N	2.49	0.45
2:H:3893:ASP:N	2:H:3893:ASP:OD1	2.49	0.45
2:H:4572:ASN:HD21	2:K:4847:TYR:HE2	1.58	0.45
2:H:4665:PRO:HA	2:H:4668:ILE:HG12	1.99	0.45
2:K:215:THR:OG1	2:K:271:GLY:O	2.34	0.45
2:E:215:THR:OG1	2:E:271:GLY:O	2.33	0.45
2:E:1728:ARG:HH21	2:E:1851:VAL:HG11	1.81	0.45
2:E:3893:ASP:OD1	2:E:3893:ASP:N	2.49	0.45
3:F:28:ILE:HG22	3:F:29:THR:H	1.80	0.45
2:H:204:PRO:HG2	2:H:269:TRP:HE1	1.81	0.45
2:K:4665:PRO:HA	2:K:4668:ILE:HG12	1.99	0.45
2:B:204:PRO:HG2	2:B:269:TRP:HE1	1.81	0.45
2:B:3641:PRO:HG2	2:B:3644:ARG:HH21	1.81	0.45
2:E:284:HIS:HD2	2:E:287:THR:HB	1.81	0.45
2:E:661:LYS:HA	2:E:749:ASP:HA	1.99	0.45
2:E:662:TRP:CE3	2:E:811:CYS:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4011:LEU:HD12	2:E:4012:LEU:HD12	1.99	0.45
2:H:1252:HIS:CE1	2:H:1255:TYR:CD2	3.05	0.45
2:H:4728:ASP:OD1	2:H:4728:ASP:N	2.49	0.45
2:K:1252:HIS:CE1	2:K:1255:TYR:CD2	3.04	0.45
2:K:1640:HIS:NE2	2:K:1645:ASN:OD1	2.30	0.45
2:K:4664:VAL:HA	2:K:4667:VAL:HG12	1.98	0.45
2:B:662:TRP:CE3	2:B:811:CYS:HA	2.52	0.45
2:B:4924:VAL:HB	2:B:4925:ILE:HD12	1.99	0.45
2:E:522:LEU:HA	2:E:525:ILE:HG22	1.99	0.45
2:E:700:GLU:H	2:E:705:ASN:HD21	1.64	0.45
2:K:622:THR:HA	2:K:626:LEU:HD23	1.98	0.45
2:B:4648:HIS:NE2	2:B:4793:TYR:OH	2.42	0.45
2:E:1450:VAL:HA	2:E:1552:VAL:HG23	1.98	0.45
1:A:78:PRO:HB3	1:A:96:THR:HA	1.99	0.45
2:B:473:ASN:O	2:B:477:LEU:HD23	2.16	0.45
2:B:3703:ARG:O	2:B:3707:THR:HG23	2.16	0.45
2:E:3656:ALA:O	2:E:3660:THR:OG1	2.27	0.45
2:E:4665:PRO:HA	2:E:4668:ILE:HG12	1.99	0.45
2:H:284:HIS:HD2	2:H:287:THR:HB	1.81	0.45
2:H:700:GLU:H	2:H:705:ASN:HD21	1.64	0.45
2:K:662:TRP:CE3	2:K:811:CYS:HA	2.52	0.45
2:K:4947:GLN:N	2:K:4947:GLN:OE1	2.49	0.45
2:B:485:SER:O	2:B:489:ASN:ND2	2.50	0.45
2:H:661:LYS:HA	2:H:749:ASP:HA	1.99	0.45
1:J:78:PRO:HB3	1:J:96:THR:HA	1.99	0.45
2:K:221:ARG:N	2:K:391:THR:O	2.42	0.45
2:K:4011:LEU:HD12	2:K:4012:LEU:HD12	1.99	0.45
2:H:221:ARG:N	2:H:391:THR:O	2.42	0.44
2:K:284:HIS:HD2	2:K:287:THR:HB	1.81	0.44
2:K:598:LYS:O	2:K:602:VAL:HG23	2.18	0.44
2:B:492:ASP:O	2:B:496:VAL:HG13	2.18	0.44
2:B:522:LEU:HA	2:B:525:ILE:HG22	1.99	0.44
1:D:78:PRO:HB3	1:D:96:THR:HA	1.99	0.44
2:E:485:SER:O	2:E:489:ASN:ND2	2.50	0.44
2:H:644:ILE:HG21	2:H:823:LEU:HD13	2.00	0.44
2:H:662:TRP:CE3	2:H:811:CYS:HA	2.52	0.44
2:H:4664:VAL:HA	2:H:4667:VAL:HG12	1.98	0.44
2:K:3893:ASP:OD1	2:K:3893:ASP:N	2.49	0.44
2:B:1728:ARG:HH21	2:B:1851:VAL:HG11	1.80	0.44
2:E:463:GLU:O	2:E:467:LYS:HG2	2.18	0.44
2:E:644:ILE:HG21	2:E:823:LEU:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:34:LYS:HD2	2:H:629:ARG:HE	1.82	0.44
2:B:657:THR:O	2:B:1008:SER:OG	2.25	0.44
2:B:4665:PRO:HA	2:B:4668:ILE:HG12	1.99	0.44
2:E:622:THR:HA	2:E:626:LEU:HD23	1.98	0.44
2:E:3636:PRO:HB2	2:E:3638:TYR:HD1	1.83	0.44
2:K:4056:PHE:HE2	2:K:4131:ALA:HB3	1.83	0.44
2:B:176:SER:HB2	2:B:178:ARG:NH2	2.28	0.44
2:B:463:GLU:O	2:B:467:LYS:HG2	2.18	0.44
2:E:204:PRO:HG2	2:E:269:TRP:HE1	1.81	0.44
2:E:492:ASP:O	2:E:496:VAL:HG13	2.18	0.44
2:E:4056:PHE:HE2	2:E:4131:ALA:HB3	1.83	0.44
1:G:78:PRO:HB3	1:G:96:THR:HA	1.99	0.44
2:H:492:ASP:O	2:H:496:VAL:HG13	2.18	0.44
2:H:622:THR:HA	2:H:626:LEU:HD23	1.98	0.44
2:H:3762:GLN:HB3	2:H:3766:HIS:CE1	2.53	0.44
2:B:598:LYS:O	2:B:602:VAL:HG23	2.18	0.44
2:E:3975:LEU:HD21	2:E:3979:ARG:HH21	1.83	0.44
2:H:598:LYS:O	2:H:602:VAL:HG23	2.18	0.44
2:K:204:PRO:HG2	2:K:269:TRP:HE1	1.81	0.44
2:K:463:GLU:O	2:K:467:LYS:HG2	2.18	0.44
2:K:473:ASN:O	2:K:477:LEU:HD23	2.16	0.44
2:K:485:SER:O	2:K:489:ASN:ND2	2.50	0.44
2:K:3671:ASP:OD1	2:K:3764:ARG:NH2	2.24	0.44
2:B:644:ILE:HG21	2:B:823:LEU:HD13	2.00	0.44
2:B:3975:LEU:HD21	2:B:3979:ARG:HH21	1.83	0.44
2:B:4056:PHE:HE2	2:B:4131:ALA:HB3	1.83	0.44
2:B:4664:VAL:CG2	2:B:4665:PRO:HD3	2.48	0.44
2:E:1735:ILE:HG22	2:E:2198:LEU:HD11	2.00	0.44
2:K:308:HIS:HB2	2:K:311:ALA:HB3	2.00	0.44
2:K:644:ILE:HG21	2:K:823:LEU:HD13	2.00	0.44
2:K:1735:ILE:HG22	2:K:2198:LEU:HD11	2.00	0.44
2:B:3636:PRO:HB2	2:B:3638:TYR:HD1	1.83	0.44
2:E:598:LYS:O	2:E:602:VAL:HG23	2.18	0.44
1:G:30:LEU:HD11	1:G:36:PHE:HB3	2.00	0.44
2:H:4011:LEU:HD12	2:H:4012:LEU:HD12	1.99	0.44
2:K:3762:GLN:HB3	2:K:3766:HIS:CE1	2.53	0.44
2:K:4200:TRP:HB2	2:K:4988:PHE:CZ	2.50	0.44
2:B:1610:ASN:OD1	2:B:1611:HIS:N	2.51	0.44
1:D:74:LEU:N	1:D:99:PHE:O	2.48	0.44
2:H:4056:PHE:HE2	2:H:4131:ALA:HB3	1.83	0.44
1:J:30:LEU:HD11	1:J:36:PHE:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:4664:VAL:CG2	2:K:4665:PRO:HD3	2.48	0.44
2:H:308:HIS:HB2	2:H:311:ALA:HB3	2.00	0.43
2:H:4924:VAL:HB	2:H:4925:ILE:HD12	1.99	0.43
2:H:1735:ILE:HG22	2:H:2198:LEU:HD11	2.00	0.43
2:H:3636:PRO:HB2	2:H:3638:TYR:HD1	1.83	0.43
2:B:1640:HIS:NE2	2:B:1645:ASN:OD1	2.30	0.43
2:B:3975:LEU:HD21	2:B:3979:ARG:NH2	2.34	0.43
2:E:662:TRP:CH2	2:E:814:ALA:HB2	2.54	0.43
2:E:1092:PHE:O	2:E:1149:VAL:N	2.48	0.43
2:K:492:ASP:O	2:K:496:VAL:HG13	2.18	0.43
2:B:3893:ASP:OD1	2:B:3893:ASP:N	2.49	0.43
2:E:2239:TYR:CE2	3:F:67:PRO:HG3	2.54	0.43
2:E:4664:VAL:CG2	2:E:4665:PRO:HD3	2.48	0.43
2:H:485:SER:O	2:H:489:ASN:ND2	2.50	0.43
2:H:522:LEU:HA	2:H:525:ILE:HG22	1.99	0.43
1:J:34:LYS:HD2	2:K:629:ARG:HE	1.82	0.43
2:B:488:LEU:HD11	2:B:540:PHE:HE1	1.84	0.43
2:E:583:ILE:O	2:E:587:ILE:HG12	2.19	0.43
2:E:3975:LEU:HD21	2:E:3979:ARG:NH2	2.34	0.43
2:E:4924:VAL:HB	2:E:4925:ILE:HD12	1.99	0.43
2:H:4664:VAL:CG2	2:H:4665:PRO:HD3	2.48	0.43
2:K:4148:HIS:CE1	2:K:4150:PRO:HD2	2.54	0.43
2:B:662:TRP:CH2	2:B:814:ALA:HB2	2.54	0.43
2:B:1084:GLN:HA	2:B:1084:GLN:HE21	1.83	0.43
1:D:34:LYS:HD2	2:E:629:ARG:HE	1.82	0.43
2:E:4148:HIS:CE1	2:E:4150:PRO:HD2	2.54	0.43
3:I:27:THR:HA	3:I:64:ILE:H	1.84	0.43
2:K:522:LEU:HA	2:K:525:ILE:HG22	1.99	0.43
2:K:2239:TYR:CE2	3:L:67:PRO:HG3	2.54	0.43
2:K:3975:LEU:HD21	2:K:3979:ARG:NH2	2.34	0.43
2:B:1735:ILE:HG22	2:B:2198:LEU:HD11	2.00	0.43
2:B:4011:LEU:HD12	2:B:4012:LEU:HD12	1.99	0.43
2:E:488:LEU:HD11	2:E:540:PHE:HE1	1.84	0.43
2:E:3762:GLN:HB3	2:E:3766:HIS:CE1	2.53	0.43
2:E:4200:TRP:HB2	2:E:4988:PHE:CZ	2.50	0.43
2:K:3636:PRO:HB2	2:K:3638:TYR:HD1	1.83	0.43
2:E:308:HIS:HB2	2:E:311:ALA:HB3	2.00	0.43
2:E:3929:TYR:OH	2:E:3993:HIS:ND1	2.38	0.43
2:E:3957:PHE:CD1	2:E:4020:VAL:HG11	2.54	0.43
3:F:27:THR:HA	3:F:64:ILE:H	1.84	0.43
2:H:1205:GLY:HA2	2:H:1211:LEU:HD21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1610:ASN:OD1	2:H:1611:HIS:N	2.51	0.43
2:H:3804:ASN:OD1	2:H:3807:VAL:HG23	2.19	0.43
2:H:4200:TRP:HB2	2:H:4988:PHE:CZ	2.50	0.43
2:K:488:LEU:HD11	2:K:540:PHE:HE1	1.84	0.43
2:K:583:ILE:O	2:K:587:ILE:HG12	2.19	0.43
2:K:662:TRP:CH2	2:K:814:ALA:HB2	2.54	0.43
2:E:3855:ASN:HB2	2:E:3861:ILE:HB	2.01	0.43
2:E:4214:PHE:HE1	2:E:4948:VAL:HG11	1.84	0.43
2:E:4572:ASN:HD21	2:H:4847:TYR:HE2	1.59	0.43
2:H:463:GLU:O	2:H:467:LYS:HG2	2.18	0.43
2:H:4148:HIS:CE1	2:H:4150:PRO:HD2	2.54	0.43
2:K:2160:LEU:HA	2:K:2160:LEU:HD23	1.83	0.43
2:K:2183:ILE:HA	2:K:2186:ILE:HG22	2.01	0.43
2:K:3957:PHE:CD1	2:K:4020:VAL:HG11	2.54	0.43
2:K:4924:VAL:HB	2:K:4925:ILE:HD12	1.99	0.43
1:A:34:LYS:HD2	2:B:629:ARG:HE	1.83	0.43
2:B:583:ILE:O	2:B:587:ILE:HG12	2.19	0.43
2:B:1259:ARG:HH22	2:B:1593:PRO:HA	1.84	0.43
2:H:285:VAL:O	2:H:405:TYR:HB2	2.19	0.43
2:H:1259:ARG:HH22	2:H:1593:PRO:HA	1.84	0.43
2:H:2183:ILE:HA	2:H:2186:ILE:HG22	2.01	0.43
2:H:3957:PHE:CD1	2:H:4020:VAL:HG11	2.54	0.43
2:H:3975:LEU:HD21	2:H:3979:ARG:HH21	1.82	0.43
2:H:3975:LEU:HD21	2:H:3979:ARG:NH2	2.34	0.43
2:H:4214:PHE:HE1	2:H:4948:VAL:HG11	1.84	0.43
2:K:1259:ARG:HH22	2:K:1593:PRO:HA	1.84	0.43
2:K:3975:LEU:HD21	2:K:3979:ARG:HH21	1.82	0.43
3:L:27:THR:HA	3:L:64:ILE:H	1.84	0.43
2:B:2183:ILE:HA	2:B:2186:ILE:HG22	2.01	0.42
2:B:3762:GLN:HB3	2:B:3766:HIS:CE1	2.53	0.42
2:B:3804:ASN:OD1	2:B:3807:VAL:HG23	2.19	0.42
2:B:3855:ASN:HB2	2:B:3861:ILE:HB	2.01	0.42
1:D:30:LEU:HD11	1:D:36:PHE:HB3	2.00	0.42
2:H:1703:LEU:HD21	2:H:1711:TYR:HD2	1.84	0.42
2:B:308:HIS:HB2	2:B:311:ALA:HB3	2.00	0.42
2:B:1703:LEU:HD21	2:B:1711:TYR:HD2	1.85	0.42
2:E:2183:ILE:HA	2:E:2186:ILE:HG22	2.01	0.42
2:E:3697:LEU:HD12	2:E:3697:LEU:HA	1.89	0.42
2:H:488:LEU:HD11	2:H:540:PHE:HE1	1.84	0.42
2:K:261:ARG:HH21	2:K:283:ARG:HE	1.67	0.42
1:A:30:LEU:HD11	1:A:36:PHE:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3957:PHE:CD1	2:B:4020:VAL:HG11	2.54	0.42
2:E:1205:GLY:HA2	2:E:1211:LEU:HD21	2.00	0.42
2:E:1259:ARG:HH22	2:E:1593:PRO:HA	1.84	0.42
2:E:3804:ASN:OD1	2:E:3807:VAL:HG23	2.19	0.42
2:E:1703:LEU:HD21	2:E:1711:TYR:HD2	1.84	0.42
2:E:3694:LEU:HD23	2:E:3768:ARG:HG3	2.02	0.42
2:H:662:TRP:CH2	2:H:814:ALA:HB2	2.54	0.42
2:K:285:VAL:O	2:K:405:TYR:HB2	2.19	0.42
2:B:568:LEU:HD13	2:B:606:LEU:HD21	2.02	0.42
2:B:4148:HIS:CE1	2:B:4150:PRO:HD2	2.54	0.42
3:C:72:MET:SD	3:C:73:MET:N	2.93	0.42
2:H:3855:ASN:HB2	2:H:3861:ILE:HB	2.01	0.42
2:K:1610:ASN:OD1	2:K:1611:HIS:N	2.51	0.42
2:K:1686:CYS:HB3	2:K:1783:PHE:HZ	1.85	0.42
2:K:3855:ASN:HB2	2:K:3861:ILE:HB	2.01	0.42
2:B:484:LEU:O	2:B:488:LEU:HD23	2.20	0.42
2:B:2160:LEU:HA	2:B:2160:LEU:HD23	1.83	0.42
2:B:3694:LEU:HD23	2:B:3768:ARG:HG3	2.02	0.42
3:C:27:THR:HA	3:C:64:ILE:H	1.84	0.42
2:E:285:VAL:O	2:E:405:TYR:HB2	2.19	0.42
2:E:1610:ASN:OD1	2:E:1611:HIS:N	2.51	0.42
2:E:3794:LYS:HD3	2:E:3794:LYS:HA	1.86	0.42
2:E:3979:ARG:HH11	2:E:3981:TRP:HB3	1.85	0.42
2:H:1843:LEU:HA	2:H:1846:VAL:HG12	2.02	0.42
2:H:4675:LEU:HD21	2:H:4700:ASP:HB3	2.02	0.42
3:I:72:MET:SD	3:I:73:MET:N	2.93	0.42
2:K:45:ARG:HG2	2:K:443:LEU:HD21	2.01	0.42
2:K:568:LEU:HD13	2:K:606:LEU:HD21	2.02	0.42
2:K:1843:LEU:HA	2:K:1846:VAL:HG12	2.02	0.42
2:K:4214:PHE:HE1	2:K:4948:VAL:HG11	1.84	0.42
2:K:4675:LEU:HD21	2:K:4700:ASP:HB3	2.02	0.42
2:B:1843:LEU:HA	2:B:1846:VAL:HG12	2.02	0.42
2:E:2160:LEU:HA	2:E:2160:LEU:HD23	1.83	0.42
2:E:2232:SER:O	2:E:2235:ARG:HG2	2.20	0.42
2:H:2232:SER:O	2:H:2235:ARG:HG2	2.20	0.42
2:B:1634:LEU:HD23	2:B:1634:LEU:HA	1.90	0.42
2:B:2245:ARG:HA	2:B:2245:ARG:HD3	1.97	0.42
2:E:692:TYR:HE2	2:E:780:VAL:HG11	1.85	0.42
2:H:583:ILE:O	2:H:587:ILE:HG12	2.19	0.42
2:K:3804:ASN:OD1	2:K:3807:VAL:HG23	2.19	0.42
2:B:1205:GLY:HA2	2:B:1211:LEU:HD21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:45:ARG:HG2	2:E:443:LEU:HD21	2.02	0.42
2:E:169:LEU:O	2:E:200:TRP:HB2	2.20	0.42
2:E:1843:LEU:HA	2:E:1846:VAL:HG12	2.02	0.42
2:E:4675:LEU:HD21	2:E:4700:ASP:HB3	2.02	0.42
2:H:1686:CYS:HB3	2:H:1783:PHE:HZ	1.85	0.42
2:K:1205:GLY:HA2	2:K:1211:LEU:HD21	2.01	0.42
2:K:1675:ALA:O	2:K:1725:ARG:NH1	2.49	0.42
1:A:74:LEU:N	1:A:99:PHE:O	2.48	0.42
2:B:285:VAL:O	2:B:405:TYR:HB2	2.19	0.42
1:D:24:VAL:HG13	1:D:102:GLU:H	1.84	0.42
3:F:72:MET:SD	3:F:73:MET:N	2.93	0.42
2:H:608:VAL:HG12	2:H:613:ALA:HB2	2.02	0.42
2:K:1703:LEU:HD21	2:K:1711:TYR:HD2	1.84	0.42
2:K:3979:ARG:HH11	2:K:3981:TRP:HB3	1.85	0.42
2:B:2232:SER:O	2:B:2235:ARG:HG2	2.20	0.41
2:B:2235:ARG:NH2	3:C:65:ASP:OD2	2.52	0.41
2:B:3775:LEU:HD22	2:B:3823:PHE:CE1	2.55	0.41
2:E:1686:CYS:HB3	2:E:1783:PHE:HZ	1.85	0.41
2:H:45:ARG:HG2	2:H:443:LEU:HD21	2.01	0.41
2:B:4675:LEU:HD21	2:B:4700:ASP:HB3	2.02	0.41
2:E:221:ARG:N	2:E:391:THR:O	2.42	0.41
2:E:484:LEU:O	2:E:488:LEU:HD23	2.20	0.41
2:H:3979:ARG:HH11	2:H:3981:TRP:HB3	1.85	0.41
2:K:285:VAL:HG23	2:K:286:THR:HG23	2.02	0.41
2:K:484:LEU:O	2:K:488:LEU:HD23	2.20	0.41
2:K:608:VAL:HG12	2:K:613:ALA:HB2	2.02	0.41
1:A:24:VAL:HG13	1:A:102:GLU:H	1.84	0.41
2:B:45:ARG:HG2	2:B:443:LEU:HD21	2.01	0.41
2:B:633:LEU:HD23	2:B:1639:LEU:HD22	2.03	0.41
2:B:1686:CYS:HB3	2:B:1783:PHE:HZ	1.85	0.41
2:E:2237:LEU:HD11	2:E:2251:MET:SD	2.61	0.41
2:H:692:TYR:HE2	2:H:780:VAL:HG11	1.85	0.41
2:H:3694:LEU:HD23	2:H:3768:ARG:HG3	2.01	0.41
2:K:633:LEU:HD23	2:K:1639:LEU:HD22	2.02	0.41
2:K:721:LEU:HD12	2:K:768:PHE:CE1	2.56	0.41
2:B:692:TYR:HE2	2:B:780:VAL:HG11	1.85	0.41
2:B:2237:LEU:HD11	2:B:2251:MET:SD	2.61	0.41
2:E:633:LEU:HD23	2:E:1639:LEU:HD22	2.02	0.41
2:E:4701:ARG:HB3	2:E:4701:ARG:CZ	2.50	0.41
2:H:261:ARG:HH21	2:H:283:ARG:HE	1.67	0.41
2:H:568:LEU:HD13	2:H:606:LEU:HD21	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:633:LEU:HD23	2:H:1639:LEU:HD22	2.02	0.41
2:H:1640:HIS:NE2	2:H:1645:ASN:OD1	2.30	0.41
2:K:169:LEU:O	2:K:200:TRP:HB2	2.20	0.41
2:K:1574:PRO:HG3	2:K:1589:PRO:HA	2.02	0.41
2:B:486:LEU:HA	2:B:489:ASN:ND2	2.36	0.41
2:E:486:LEU:HA	2:E:489:ASN:ND2	2.36	0.41
2:H:484:LEU:O	2:H:488:LEU:HD23	2.20	0.41
2:H:595:ARG:HH12	2:H:1641:ILE:HD11	1.86	0.41
2:H:3752:GLU:O	2:H:3756:GLN:HG2	2.21	0.41
2:H:3782:LYS:N	2:H:3782:LYS:HD2	2.36	0.41
2:H:4701:ARG:CZ	2:H:4701:ARG:HB3	2.51	0.41
1:J:24:VAL:HG13	1:J:102:GLU:H	1.84	0.41
1:J:74:LEU:N	1:J:99:PHE:O	2.48	0.41
2:K:3775:LEU:HD22	2:K:3823:PHE:CE1	2.56	0.41
3:L:72:MET:SD	3:L:73:MET:N	2.93	0.41
2:B:261:ARG:HH21	2:B:283:ARG:HE	1.68	0.41
2:B:3979:ARG:HH11	2:B:3981:TRP:HB3	1.85	0.41
2:E:1592:PRO:HA	2:E:1593:PRO:HD3	1.95	0.41
2:E:595:ARG:HH12	2:E:1641:ILE:HD11	1.86	0.41
2:E:1252:HIS:CD2	2:E:1253:PRO:HD2	2.56	0.41
2:H:486:LEU:HA	2:H:489:ASN:ND2	2.36	0.41
2:H:1574:PRO:HG3	2:H:1589:PRO:HA	2.03	0.41
2:K:2232:SER:O	2:K:2235:ARG:HG2	2.20	0.41
2:K:3694:LEU:HD23	2:K:3768:ARG:HG3	2.02	0.41
2:K:3782:LYS:HD2	2:K:3782:LYS:N	2.36	0.41
2:B:169:LEU:O	2:B:200:TRP:HB2	2.20	0.41
2:E:721:LEU:HD12	2:E:768:PHE:CE1	2.56	0.41
2:E:1634:LEU:HD23	2:E:1634:LEU:HA	1.90	0.41
2:E:3775:LEU:HD22	2:E:3823:PHE:CE1	2.55	0.41
2:H:285:VAL:HG23	2:H:286:THR:HG23	2.02	0.41
2:H:1252:HIS:CD2	2:H:1253:PRO:HD2	2.56	0.41
2:H:2439:PRO:HB2	2:H:2451:ALA:HB1	2.03	0.41
2:K:1092:PHE:O	2:K:1149:VAL:N	2.48	0.41
2:K:1667:LEU:HD21	2:K:1711:TYR:CD1	2.56	0.41
1:A:34:LYS:HB3	2:B:629:ARG:HH21	1.86	0.41
2:B:1574:PRO:HG3	2:B:1589:PRO:HA	2.03	0.41
2:B:1675:ALA:O	2:B:1725:ARG:NH1	2.49	0.41
2:B:3752:GLU:O	2:B:3756:GLN:HG2	2.20	0.41
2:B:4214:PHE:HE1	2:B:4948:VAL:HG11	1.84	0.41
2:E:568:LEU:HD13	2:E:606:LEU:HD21	2.02	0.41
2:E:687:ALA:HB3	2:E:780:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2439:PRO:HB2	2:E:2451:ALA:HB1	2.03	0.41
2:E:3782:LYS:HD2	2:E:3782:LYS:N	2.36	0.41
2:E:3935:LYS:NZ	2:E:3937:VAL:O	2.34	0.41
1:G:24:VAL:HG13	1:G:102:GLU:H	1.84	0.41
2:H:1092:PHE:O	2:H:1149:VAL:N	2.48	0.41
2:H:2237:LEU:HD11	2:H:2251:MET:SD	2.61	0.41
2:K:595:ARG:HH12	2:K:1641:ILE:HD11	1.86	0.41
2:K:3752:GLU:O	2:K:3756:GLN:HG2	2.20	0.41
2:K:4701:ARG:HB3	2:K:4701:ARG:CZ	2.50	0.41
2:B:721:LEU:HD12	2:B:768:PHE:CE1	2.55	0.41
2:B:1667:LEU:HD21	2:B:1711:TYR:CD1	2.56	0.41
2:E:4016:LYS:HA	2:E:4019:VAL:HG22	2.03	0.41
2:H:169:LEU:O	2:H:200:TRP:HB2	2.20	0.41
2:H:3775:LEU:HD22	2:H:3823:PHE:CE1	2.55	0.41
2:B:595:ARG:HH12	2:B:1641:ILE:HD11	1.86	0.40
2:B:805:PRO:HA	2:B:806:PRO:HD3	1.96	0.40
2:B:2274:LEU:HD11	2:B:2335:PHE:CG	2.56	0.40
2:B:3782:LYS:HD2	2:B:3782:LYS:N	2.36	0.40
1:D:34:LYS:HB3	2:E:629:ARG:HH21	1.86	0.40
2:E:285:VAL:HG23	2:E:286:THR:HG23	2.02	0.40
2:E:1675:ALA:O	2:E:1725:ARG:NH1	2.49	0.40
2:H:1675:ALA:O	2:H:1725:ARG:NH1	2.49	0.40
1:J:34:LYS:HB3	2:K:629:ARG:HH21	1.86	0.40
2:B:1252:HIS:CD2	2:B:1253:PRO:HD2	2.56	0.40
2:B:2439:PRO:HB2	2:B:2451:ALA:HB1	2.03	0.40
2:B:3794:LYS:HD3	2:B:3794:LYS:HA	1.86	0.40
2:B:4701:ARG:CZ	2:B:4701:ARG:HB3	2.50	0.40
2:E:19:GLU:HA	2:E:68:VAL:HA	2.03	0.40
2:H:721:LEU:HD12	2:H:768:PHE:CE1	2.56	0.40
2:K:170:ILE:HD13	2:K:197:GLN:HG2	2.02	0.40
2:K:1252:HIS:CD2	2:K:1253:PRO:HD2	2.56	0.40
2:K:2274:LEU:HD11	2:K:2335:PHE:CG	2.56	0.40
2:B:170:ILE:HD13	2:B:197:GLN:HG2	2.02	0.40
2:B:4875:ASP:O	2:K:4579:LYS:HA	2.21	0.40
2:E:261:ARG:HH21	2:E:283:ARG:HE	1.67	0.40
2:E:3929:TYR:OH	2:E:3989:HIS:HB3	2.21	0.40
2:H:1592:PRO:HA	2:H:1593:PRO:HD3	1.95	0.40
2:H:1667:LEU:HD21	2:H:1711:TYR:CD1	2.56	0.40
2:K:2237:LEU:HD11	2:K:2251:MET:SD	2.61	0.40
2:B:285:VAL:HG23	2:B:286:THR:HG23	2.02	0.40
2:B:3929:TYR:OH	2:B:3989:HIS:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:494:LEU:HD23	2:E:494:LEU:HA	1.93	0.40
2:E:3762:GLN:O	2:E:3766:HIS:CG	2.75	0.40
2:K:3929:TYR:OH	2:K:3989:HIS:HB3	2.21	0.40
2:K:4016:LYS:HA	2:K:4019:VAL:HG22	2.03	0.40
2:B:608:VAL:HG12	2:B:613:ALA:HB2	2.02	0.40
2:B:687:ALA:HB3	2:B:780:VAL:HG21	2.02	0.40
2:B:2167:LEU:HD13	2:B:2210:GLU:OE1	2.22	0.40
2:B:3697:LEU:HD12	2:B:3697:LEU:HA	1.89	0.40
2:B:4016:LYS:HA	2:B:4019:VAL:HG22	2.03	0.40
2:E:170:ILE:HD13	2:E:197:GLN:HG2	2.02	0.40
2:H:393:CYS:HB2	2:H:397:GLU:OE1	2.22	0.40
2:H:687:ALA:HB3	2:H:780:VAL:HG21	2.03	0.40
2:H:2098:LEU:O	2:H:2102:THR:HG23	2.22	0.40
2:K:2098:LEU:O	2:K:2102:THR:HG23	2.22	0.40
2:K:4662:LEU:O	2:K:4665:PRO:HD2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	101/110 (92%)	99 (98%)	2 (2%)	0	100	100
1	D	101/110 (92%)	99 (98%)	2 (2%)	0	100	100
1	G	101/110 (92%)	99 (98%)	2 (2%)	0	100	100
1	J	101/110 (92%)	99 (98%)	2 (2%)	0	100	100
2	B	3103/3531 (88%)	3035 (98%)	68 (2%)	0	100	100
2	E	3103/3531 (88%)	3036 (98%)	67 (2%)	0	100	100
2	H	3103/3531 (88%)	3035 (98%)	68 (2%)	0	100	100
2	K	3103/3531 (88%)	3035 (98%)	68 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	127/148 (86%)	122 (96%)	5 (4%)	0	100	100
3	F	127/148 (86%)	122 (96%)	5 (4%)	0	100	100
3	I	127/148 (86%)	122 (96%)	5 (4%)	0	100	100
3	L	127/148 (86%)	122 (96%)	5 (4%)	0	100	100
All	All	13324/15156 (88%)	13025 (98%)	299 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	58/90 (64%)	58 (100%)	0	100	100
1	D	58/90 (64%)	58 (100%)	0	100	100
1	G	58/90 (64%)	58 (100%)	0	100	100
1	J	58/90 (64%)	58 (100%)	0	100	100
2	B	1784/2792 (64%)	1780 (100%)	4 (0%)	93	96
2	E	1784/2792 (64%)	1780 (100%)	4 (0%)	93	96
2	H	1784/2792 (64%)	1780 (100%)	4 (0%)	93	96
2	K	1784/2792 (64%)	1780 (100%)	4 (0%)	93	96
3	C	34/126 (27%)	34 (100%)	0	100	100
3	F	34/126 (27%)	34 (100%)	0	100	100
3	I	34/126 (27%)	34 (100%)	0	100	100
3	L	34/126 (27%)	34 (100%)	0	100	100
All	All	7504/12032 (62%)	7488 (100%)	16 (0%)	93	96

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	15	ARG

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Mol	Chain	Res	Type
2	B	624	ASN
2	B	4572	ASN
2	B	4834	GLN
2	E	15	ARG
2	E	624	ASN
2	E	4572	ASN
2	E	4834	GLN
2	H	15	ARG
2	H	624	ASN
2	H	4572	ASN
2	H	4834	GLN
2	K	15	ARG
2	K	624	ASN
2	K	4572	ASN
2	K	4834	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	138	GLN
2	B	3766	HIS
2	B	4931	GLN
2	E	138	GLN
2	E	1084	GLN
2	E	3766	HIS
2	E	4931	GLN
2	H	138	GLN
2	H	1084	GLN
2	H	3766	HIS
2	H	4931	GLN
2	K	138	GLN
2	K	1084	GLN
2	K	3766	HIS
2	K	4931	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	B	62
2	E	62
2	H	62
2	K	62

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	4331:UNK	C	4543:GLU	N	49.49
1	E	4331:UNK	C	4543:GLU	N	49.49
1	H	4331:UNK	C	4543:GLU	N	49.49
1	K	4331:UNK	C	4543:GLU	N	49.49
1	B	1050:GLY	C	1071:ARG	N	48.46
1	E	1050:GLY	C	1071:ARG	N	48.46
1	H	1050:GLY	C	1071:ARG	N	48.46
1	K	1050:GLY	C	1071:ARG	N	48.46
1	B	3603:UNK	C	3625:ARG	N	43.04
1	E	3603:UNK	C	3625:ARG	N	43.04
1	H	3603:UNK	C	3625:ARG	N	43.04
1	K	3603:UNK	C	3625:ARG	N	43.04
1	B	4241:GLN	C	4315:UNK	N	30.79

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	4241:GLN	C	4315:UNK	N	30.79
1	H	4241:GLN	C	4315:UNK	N	30.79
1	K	4241:GLN	C	4315:UNK	N	30.79
1	B	2509:ARG	C	2548:ALA	N	28.16
1	E	2509:ARG	C	2548:ALA	N	28.16
1	H	2509:ARG	C	2548:ALA	N	28.16
1	K	2509:ARG	C	2548:ALA	N	28.16
1	B	4737:GLU	C	4763:LEU	N	23.89
1	E	4737:GLU	C	4763:LEU	N	23.89
1	H	4737:GLU	C	4763:LEU	N	23.89
1	K	4737:GLU	C	4763:LEU	N	23.89
1	B	3555:UNK	C	3565:UNK	N	23.31
1	E	3555:UNK	C	3565:UNK	N	23.31
1	H	3555:UNK	C	3565:UNK	N	23.31
1	K	3555:UNK	C	3565:UNK	N	23.31
1	B	84:ASN	C	97:GLY	N	21.92
1	E	84:ASN	C	97:GLY	N	21.92
1	H	84:ASN	C	97:GLY	N	21.92
1	K	84:ASN	C	97:GLY	N	21.92
1	B	855:PRO	C	870:ILE	N	21.90
1	E	855:PRO	C	870:ILE	N	21.90
1	H	855:PRO	C	870:ILE	N	21.90
1	K	855:PRO	C	870:ILE	N	21.90
1	B	1299:GLN	C	1428:LEU	N	21.35
1	E	1299:GLN	C	1428:LEU	N	21.35
1	H	1299:GLN	C	1428:LEU	N	21.35
1	K	1299:GLN	C	1428:LEU	N	21.35
1	B	3574:UNK	C	3586:UNK	N	21.12
1	E	3574:UNK	C	3586:UNK	N	21.12
1	H	3574:UNK	C	3586:UNK	N	21.12
1	K	3574:UNK	C	3586:UNK	N	21.12
1	B	3166:UNK	C	3180:UNK	N	19.79
1	E	3166:UNK	C	3180:UNK	N	19.79
1	H	3166:UNK	C	3180:UNK	N	19.79
1	K	3166:UNK	C	3180:UNK	N	19.79
1	B	2046:GLN	C	2092:LEU	N	18.33
1	E	2046:GLN	C	2092:LEU	N	18.33
1	H	2046:GLN	C	2092:LEU	N	18.33
1	K	2046:GLN	C	2092:LEU	N	18.33
1	B	3193:UNK	C	3202:UNK	N	17.99
1	E	3193:UNK	C	3202:UNK	N	17.99
1	H	3193:UNK	C	3202:UNK	N	17.99

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	3193:UNK	C	3202:UNK	N	17.99
1	B	2653:UNK	C	2664:UNK	N	16.60
1	E	2653:UNK	C	2664:UNK	N	16.60
1	H	2653:UNK	C	2664:UNK	N	16.60
1	K	2653:UNK	C	2664:UNK	N	16.60
1	B	3238:UNK	C	3278:UNK	N	16.59
1	E	3238:UNK	C	3278:UNK	N	16.59
1	H	3238:UNK	C	3278:UNK	N	16.59
1	K	3238:UNK	C	3278:UNK	N	16.59
1	B	2978:UNK	C	2999:UNK	N	15.94
1	E	2978:UNK	C	2999:UNK	N	15.94
1	H	2978:UNK	C	2999:UNK	N	15.94
1	K	2978:UNK	C	2999:UNK	N	15.94
1	B	3733:GLU	C	3747:SER	N	15.87
1	E	3733:GLU	C	3747:SER	N	15.87
1	H	3733:GLU	C	3747:SER	N	15.87
1	K	3733:GLU	C	3747:SER	N	15.87
1	B	3384:UNK	C	3398:GLU	N	15.24
1	E	3384:UNK	C	3398:GLU	N	15.24
1	H	3384:UNK	C	3398:GLU	N	15.24
1	K	3384:UNK	C	3398:GLU	N	15.24
1	B	2479:THR	C	2497:PRO	N	15.21
1	E	2479:THR	C	2497:PRO	N	15.21
1	H	2479:THR	C	2497:PRO	N	15.21
1	K	2479:THR	C	2497:PRO	N	15.21
1	B	1501:VAL	C	1510:SER	N	15.09
1	E	1501:VAL	C	1510:SER	N	15.09
1	H	1501:VAL	C	1510:SER	N	15.09
1	K	1501:VAL	C	1510:SER	N	15.09
1	B	3335:UNK	C	3346:UNK	N	15.02
1	E	3335:UNK	C	3346:UNK	N	15.02
1	H	3335:UNK	C	3346:UNK	N	15.02
1	K	3335:UNK	C	3346:UNK	N	15.02
1	K	1871:VAL	C	1924:GLU	N	14.95
1	B	1871:VAL	C	1924:GLU	N	14.94
1	E	1871:VAL	C	1924:GLU	N	14.94
1	H	1871:VAL	C	1924:GLU	N	14.94
1	B	3018:UNK	C	3032:UNK	N	14.86
1	E	3018:UNK	C	3032:UNK	N	14.86
1	H	3018:UNK	C	3032:UNK	N	14.86
1	K	3018:UNK	C	3032:UNK	N	14.86
1	B	3062:UNK	C	3146:UNK	N	14.65

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	3062:UNK	C	3146:UNK	N	14.65
1	H	3062:UNK	C	3146:UNK	N	14.65
1	K	3062:UNK	C	3146:UNK	N	14.65
1	B	2569:LEU	C	2579:MET	N	14.52
1	E	2569:LEU	C	2579:MET	N	14.52
1	H	2569:LEU	C	2579:MET	N	14.52
1	K	2569:LEU	C	2579:MET	N	14.52
1	B	3358:UNK	C	3365:UNK	N	14.29
1	E	3358:UNK	C	3365:UNK	N	14.29
1	H	3358:UNK	C	3365:UNK	N	14.29
1	K	3358:UNK	C	3365:UNK	N	14.29
1	B	3288:UNK	C	3292:UNK	N	13.92
1	E	3288:UNK	C	3292:UNK	N	13.92
1	H	3288:UNK	C	3292:UNK	N	13.92
1	K	3288:UNK	C	3292:UNK	N	13.92
1	B	2629:PHE	C	2641:UNK	N	13.31
1	E	2629:PHE	C	2641:UNK	N	13.30
1	H	2629:PHE	C	2641:UNK	N	13.30
1	K	2629:PHE	C	2641:UNK	N	13.30
1	K	4585:PRO	C	4626:VAL	N	12.69
1	B	4585:PRO	C	4626:VAL	N	12.68
1	E	4585:PRO	C	4626:VAL	N	12.68
1	H	4585:PRO	C	4626:VAL	N	12.68
1	B	323:LEU	C	328:LYS	N	12.67
1	E	323:LEU	C	328:LYS	N	12.66
1	H	323:LEU	C	328:LYS	N	12.66
1	K	323:LEU	C	328:LYS	N	12.66
1	B	3526:UNK	C	3534:UNK	N	12.43
1	H	3526:UNK	C	3534:UNK	N	12.43
1	K	3526:UNK	C	3534:UNK	N	12.43
1	E	3526:UNK	C	3534:UNK	N	12.42
1	B	3999:ALA	C	4008:LEU	N	12.40
1	E	3999:ALA	C	4008:LEU	N	12.40
1	H	3999:ALA	C	4008:LEU	N	12.40
1	K	3999:ALA	C	4008:LEU	N	12.40
1	B	2700:UNK	C	2956:UNK	N	11.73
1	E	2700:UNK	C	2956:UNK	N	11.73
1	H	2700:UNK	C	2956:UNK	N	11.73
1	K	2700:UNK	C	2956:UNK	N	11.73
1	B	3046:UNK	C	3051:UNK	N	11.48
1	E	3046:UNK	C	3051:UNK	N	11.48
1	H	3046:UNK	C	3051:UNK	N	11.48

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	3046:UNK	C	3051:UNK	N	11.48
1	B	4090:LYS	C	4109:UNK	N	11.46
1	E	4090:LYS	C	4109:UNK	N	11.46
1	H	4090:LYS	C	4109:UNK	N	11.46
1	K	4090:LYS	C	4109:UNK	N	11.46
1	B	3461:VAL	C	3509:UNK	N	11.36
1	E	3461:VAL	C	3509:UNK	N	11.36
1	H	3461:VAL	C	3509:UNK	N	11.36
1	K	3461:VAL	C	3509:UNK	N	11.36
1	B	3425:LEU	C	3430:PRO	N	11.31
1	E	3425:LEU	C	3430:PRO	N	11.31
1	H	3425:LEU	C	3430:PRO	N	11.31
1	K	3425:LEU	C	3430:PRO	N	11.31
1	B	236:ALA	C	240:ASP	N	10.94
1	E	236:ALA	C	240:ASP	N	10.94
1	H	236:ALA	C	240:ASP	N	10.94
1	K	236:ALA	C	240:ASP	N	10.94
1	B	4218:ASN	C	4221:GLY	N	10.79
1	E	4218:ASN	C	4221:GLY	N	10.79
1	H	4218:ASN	C	4221:GLY	N	10.79
1	K	4218:ASN	C	4221:GLY	N	10.79
1	B	2014:LYS	C	2021:ASP	N	10.73
1	E	2014:LYS	C	2021:ASP	N	10.73
1	H	2014:LYS	C	2021:ASP	N	10.73
1	K	2014:LYS	C	2021:ASP	N	10.73
1	E	3308:UNK	C	3320:UNK	N	10.43
1	H	3308:UNK	C	3320:UNK	N	10.43
1	K	3308:UNK	C	3320:UNK	N	10.43
1	B	3308:UNK	C	3320:UNK	N	10.42
1	K	361:ALA	C	372:LEU	N	10.35
1	B	361:ALA	C	372:LEU	N	10.34
1	E	361:ALA	C	372:LEU	N	10.34
1	H	361:ALA	C	372:LEU	N	10.34
1	B	1750:PRO	C	1760:ARG	N	10.26
1	E	1750:PRO	C	1760:ARG	N	10.26
1	H	1750:PRO	C	1760:ARG	N	10.26
1	K	1750:PRO	C	1760:ARG	N	10.26
1	B	3216:UNK	C	3225:UNK	N	10.24
1	E	3216:UNK	C	3225:UNK	N	10.24
1	H	3216:UNK	C	3225:UNK	N	10.24
1	K	3216:UNK	C	3225:UNK	N	10.23
1	B	3544:UNK	C	3548:UNK	N	10.18

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	3544:UNK	C	3548:UNK	N	10.18
1	H	3544:UNK	C	3548:UNK	N	10.18
1	K	3544:UNK	C	3548:UNK	N	10.18
1	B	2384:ALA	C	2424:MET	N	9.57
1	E	2384:ALA	C	2424:MET	N	9.57
1	H	2384:ALA	C	2424:MET	N	9.57
1	K	2384:ALA	C	2424:MET	N	9.57
1	B	3678:GLU	C	3689:LYS	N	9.39
1	E	3678:GLU	C	3689:LYS	N	9.39
1	H	3678:GLU	C	3689:LYS	N	9.39
1	K	3678:GLU	C	3689:LYS	N	9.39
1	B	4114:UNK	C	4122:GLU	N	9.37
1	E	4114:UNK	C	4122:GLU	N	9.37
1	H	4114:UNK	C	4122:GLU	N	9.37
1	K	4114:UNK	C	4122:GLU	N	9.37
1	B	2217:GLY	C	2225:ARG	N	9.15
1	E	2217:GLY	C	2225:ARG	N	9.15
1	H	2217:GLY	C	2225:ARG	N	9.15
1	K	2217:GLY	C	2225:ARG	N	9.15
1	B	2263:GLY	C	2267:GLY	N	8.98
1	E	2263:GLY	C	2267:GLY	N	8.98
1	H	2263:GLY	C	2267:GLY	N	8.98
1	K	2263:GLY	C	2267:GLY	N	8.98
1	B	2682:UNK	C	2688:UNK	N	8.43
1	E	2682:UNK	C	2688:UNK	N	8.43
1	H	2682:UNK	C	2688:UNK	N	8.43
1	K	2682:UNK	C	2688:UNK	N	8.43
1	B	1567:GLY	C	1570:LYS	N	8.18
1	E	1567:GLY	C	1570:LYS	N	8.18
1	H	1567:GLY	C	1570:LYS	N	8.18
1	K	1567:GLY	C	1570:LYS	N	8.18
1	B	1788:PRO	C	1794:GLU	N	7.21
1	E	1788:PRO	C	1794:GLU	N	7.21
1	H	1788:PRO	C	1794:GLU	N	7.21
1	K	1788:PRO	C	1794:GLU	N	7.21
1	B	2439:PRO	C	2444:ILE	N	7.07
1	E	2439:PRO	C	2444:ILE	N	7.07
1	H	2439:PRO	C	2444:ILE	N	7.07
1	K	2439:PRO	C	2444:ILE	N	7.07
1	B	897:ARG	C	904:HIS	N	6.52
1	E	897:ARG	C	904:HIS	N	6.52
1	H	897:ARG	C	904:HIS	N	6.52

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	897:ARG	C	904:HIS	N	6.52
1	B	2367:PRO	C	2377:LEU	N	5.69
1	E	2367:PRO	C	2377:LEU	N	5.69
1	H	2367:PRO	C	2377:LEU	N	5.69
1	K	2367:PRO	C	2377:LEU	N	5.69
1	B	1275:ARG	C	1280:GLN	N	5.11
1	E	1275:ARG	C	1280:GLN	N	5.11
1	H	1275:ARG	C	1280:GLN	N	5.11
1	K	1275:ARG	C	1280:GLN	N	5.11
1	B	4864:SER	C	4873:LYS	N	4.76
1	E	4864:SER	C	4873:LYS	N	4.76
1	H	4864:SER	C	4873:LYS	N	4.76
1	K	4864:SER	C	4873:LYS	N	4.76
1	B	426:ARG	C	431:PRO	N	4.61
1	E	426:ARG	C	431:PRO	N	4.61
1	H	426:ARG	C	431:PRO	N	4.61
1	K	426:ARG	C	431:PRO	N	4.61
1	B	1478:ASP	C	1482:ASN	N	4.34
1	E	1478:ASP	C	1482:ASN	N	4.34
1	H	1478:ASP	C	1482:ASN	N	4.34
1	K	1478:ASP	C	1482:ASN	N	4.34
1	B	835:ARG	C	837:PRO	N	4.24
1	E	835:ARG	C	837:PRO	N	4.24
1	H	835:ARG	C	837:PRO	N	4.24
1	K	835:ARG	C	837:PRO	N	4.24

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-22019. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal surface views

This section was not generated.

6.5 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.