Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 01:20 PM JST

PDB ID : 7W7D
Title : Heme exporter HrtBA in complex with heme
Authors : Hisano, T.; Nakamura, H.; Rahman, M.M.; Tosha, T.; Shiro, Y.; Shirouzu, M.
Deposited on : 2021-12-04
Resolution : 3.40 Å(reported)

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

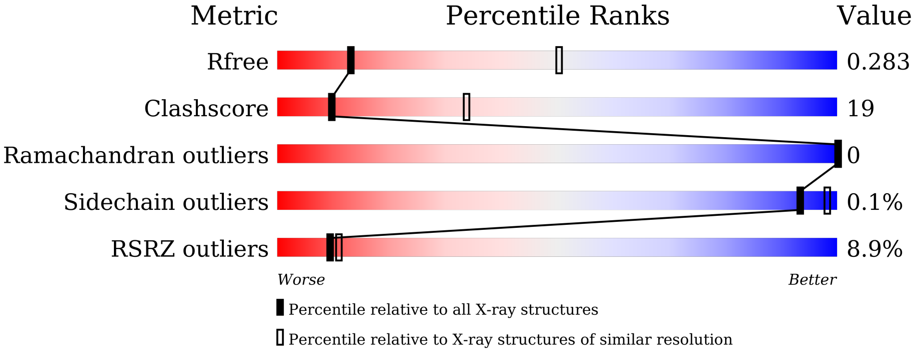
MolProbity	4.02b-467
Mogul	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	1.13
EDS	2.36
buster-report	1.1.7 (2018)
Percentile statistics	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	5.8.0158
CCP4	7.0.044 (Gargrove)
Ideal geometry (proteins)	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

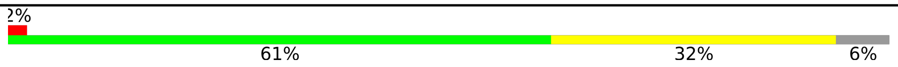
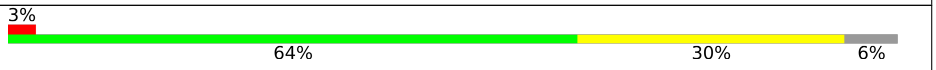
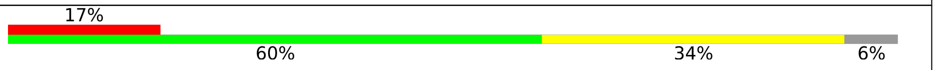
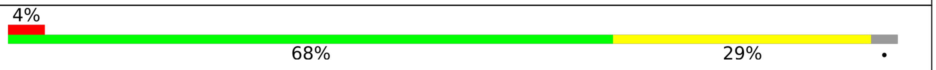
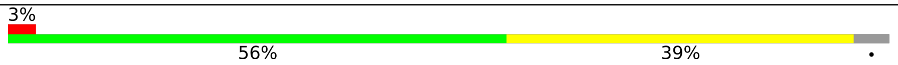
The reported resolution of this entry is 3.40 Å.

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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

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

Mol	Chain	Length	Quality of chain
1	A	231	
1	C	231	
1	E	231	
1	G	231	
1	I	231	
1	K	231	

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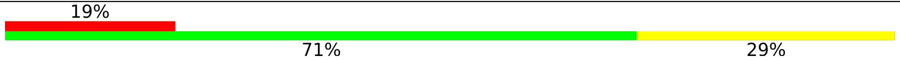
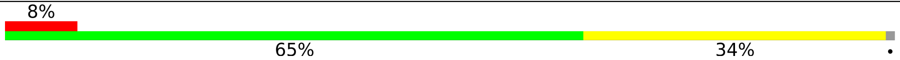
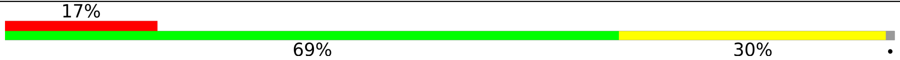
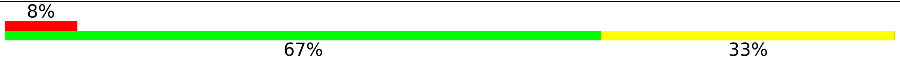
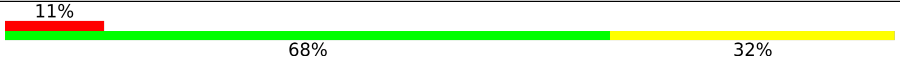
Mol	Chain	Length	Quality of chain
2	B	344	
2	D	344	
2	F	344	
2	H	344	
2	J	344	
2	L	344	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 25112 atoms, of which 60 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Putative ABC transport system, ATP-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total 1618	C 1010	N 293	O 312	S 3	0	0	0
1	C	218	Total 1634	C 1019	N 296	O 316	S 3	0	0	0
1	E	217	Total 1629	C 1016	N 295	O 315	S 3	0	0	0
1	G	225	Total 1693	C 1059	N 307	O 324	S 3	0	0	0
1	I	221	Total 1652	C 1031	N 299	O 319	S 3	0	0	0
1	K	219	Total 1639	C 1022	N 297	O 317	S 3	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	222	LYS	-	expression tag	UNP Q6NEF2
A	223	LEU	-	expression tag	UNP Q6NEF2
A	224	TRP	-	expression tag	UNP Q6NEF2
A	225	SER	-	expression tag	UNP Q6NEF2
A	226	HIS	-	expression tag	UNP Q6NEF2
A	227	PRO	-	expression tag	UNP Q6NEF2
A	228	GLN	-	expression tag	UNP Q6NEF2
A	229	PHE	-	expression tag	UNP Q6NEF2
A	230	GLU	-	expression tag	UNP Q6NEF2
A	231	LYS	-	expression tag	UNP Q6NEF2
C	222	LYS	-	expression tag	UNP Q6NEF2
C	223	LEU	-	expression tag	UNP Q6NEF2
C	224	TRP	-	expression tag	UNP Q6NEF2
C	225	SER	-	expression tag	UNP Q6NEF2
C	226	HIS	-	expression tag	UNP Q6NEF2
C	227	PRO	-	expression tag	UNP Q6NEF2
C	228	GLN	-	expression tag	UNP Q6NEF2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	229	PHE	-	expression tag	UNP Q6NEF2
C	230	GLU	-	expression tag	UNP Q6NEF2
C	231	LYS	-	expression tag	UNP Q6NEF2
E	222	LYS	-	expression tag	UNP Q6NEF2
E	223	LEU	-	expression tag	UNP Q6NEF2
E	224	TRP	-	expression tag	UNP Q6NEF2
E	225	SER	-	expression tag	UNP Q6NEF2
E	226	HIS	-	expression tag	UNP Q6NEF2
E	227	PRO	-	expression tag	UNP Q6NEF2
E	228	GLN	-	expression tag	UNP Q6NEF2
E	229	PHE	-	expression tag	UNP Q6NEF2
E	230	GLU	-	expression tag	UNP Q6NEF2
E	231	LYS	-	expression tag	UNP Q6NEF2
G	222	LYS	-	expression tag	UNP Q6NEF2
G	223	LEU	-	expression tag	UNP Q6NEF2
G	224	TRP	-	expression tag	UNP Q6NEF2
G	225	SER	-	expression tag	UNP Q6NEF2
G	226	HIS	-	expression tag	UNP Q6NEF2
G	227	PRO	-	expression tag	UNP Q6NEF2
G	228	GLN	-	expression tag	UNP Q6NEF2
G	229	PHE	-	expression tag	UNP Q6NEF2
G	230	GLU	-	expression tag	UNP Q6NEF2
G	231	LYS	-	expression tag	UNP Q6NEF2
I	222	LYS	-	expression tag	UNP Q6NEF2
I	223	LEU	-	expression tag	UNP Q6NEF2
I	224	TRP	-	expression tag	UNP Q6NEF2
I	225	SER	-	expression tag	UNP Q6NEF2
I	226	HIS	-	expression tag	UNP Q6NEF2
I	227	PRO	-	expression tag	UNP Q6NEF2
I	228	GLN	-	expression tag	UNP Q6NEF2
I	229	PHE	-	expression tag	UNP Q6NEF2
I	230	GLU	-	expression tag	UNP Q6NEF2
I	231	LYS	-	expression tag	UNP Q6NEF2
K	222	LYS	-	expression tag	UNP Q6NEF2
K	223	LEU	-	expression tag	UNP Q6NEF2
K	224	TRP	-	expression tag	UNP Q6NEF2
K	225	SER	-	expression tag	UNP Q6NEF2
K	226	HIS	-	expression tag	UNP Q6NEF2
K	227	PRO	-	expression tag	UNP Q6NEF2
K	228	GLN	-	expression tag	UNP Q6NEF2
K	229	PHE	-	expression tag	UNP Q6NEF2
K	230	GLU	-	expression tag	UNP Q6NEF2

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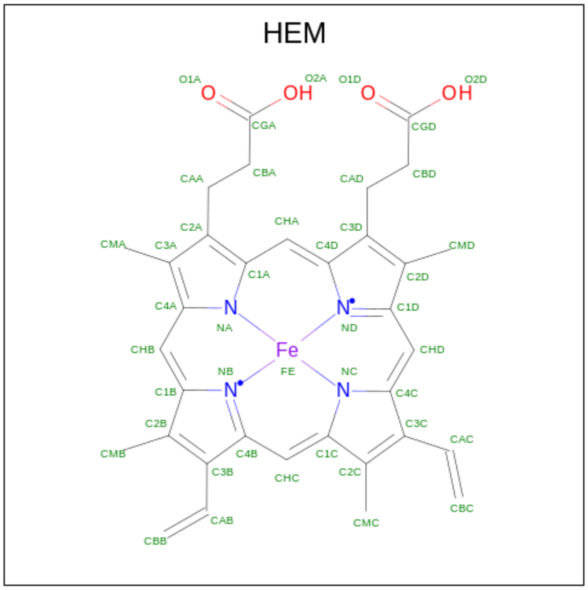
Chain	Residue	Modelled	Actual	Comment	Reference
K	231	LYS	-	expression tag	UNP Q6NEF2

- Molecule 2 is a protein called Putative ABC transport system integral membrane protein.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	B	341	Total C N O S 2510 1612 422 471 5	0	0	0
2	D	343	Total C N O S 2522 1619 424 474 5	0	0	0
2	F	342	Total C N O S 2515 1615 423 472 5	0	0	0
2	H	341	Total C N O S 2510 1612 422 471 5	0	0	0
2	J	343	Total C N O S 2522 1619 424 474 5	0	0	0
2	L	343	Total C N O S 2522 1619 424 474 5	0	0	0

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$) (labeled as "Ligand of Interest" by depositor).

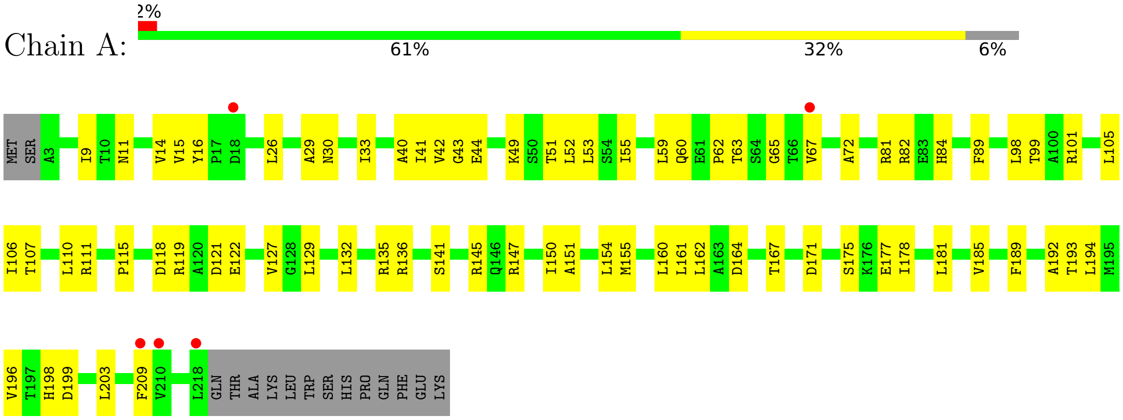


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total C Fe H N O 73 34 1 30 4 4	0	0
3	F	1	Total C Fe H N O 73 34 1 30 4 4	0	0

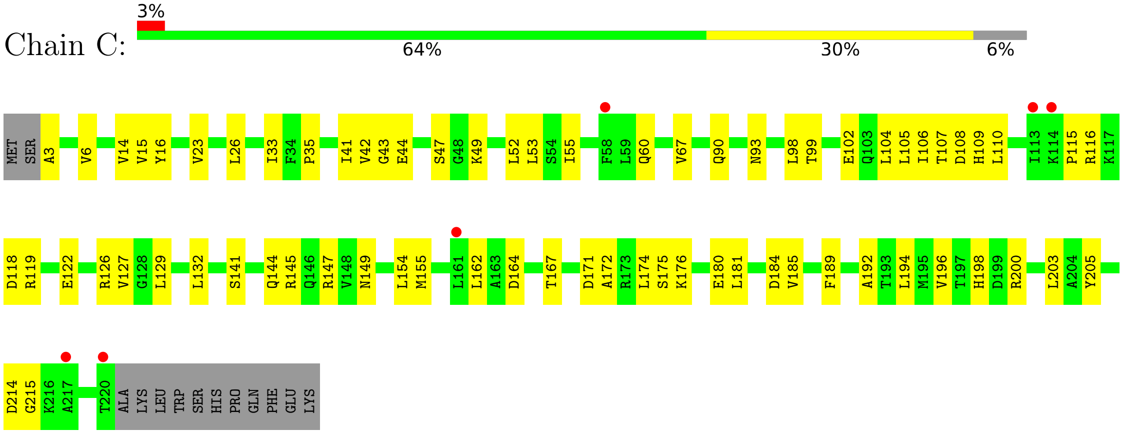
3 Residue-property plots

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

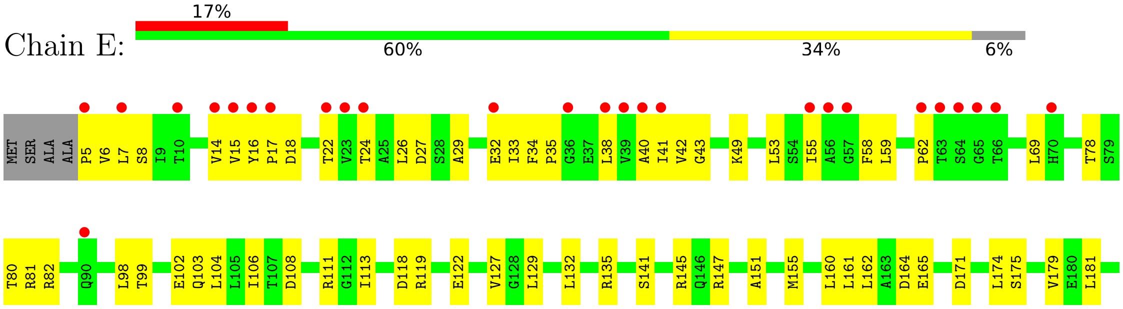
- Molecule 1: Putative ABC transport system, ATP-binding protein

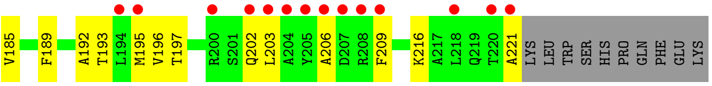


- Molecule 1: Putative ABC transport system, ATP-binding protein



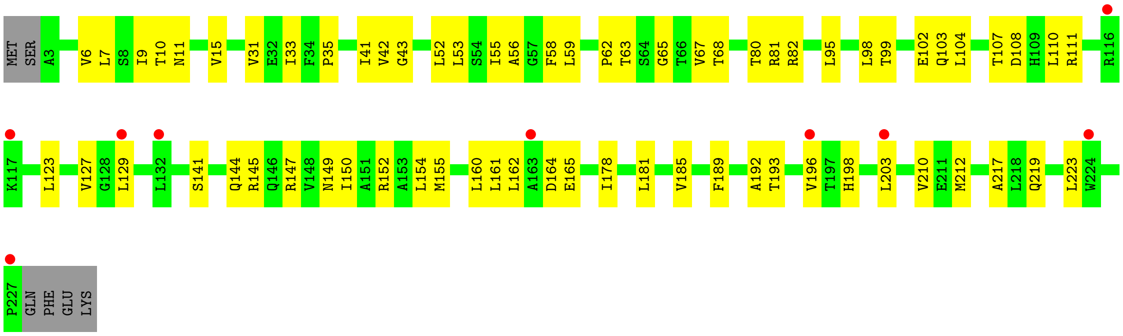
- Molecule 1: Putative ABC transport system, ATP-binding protein





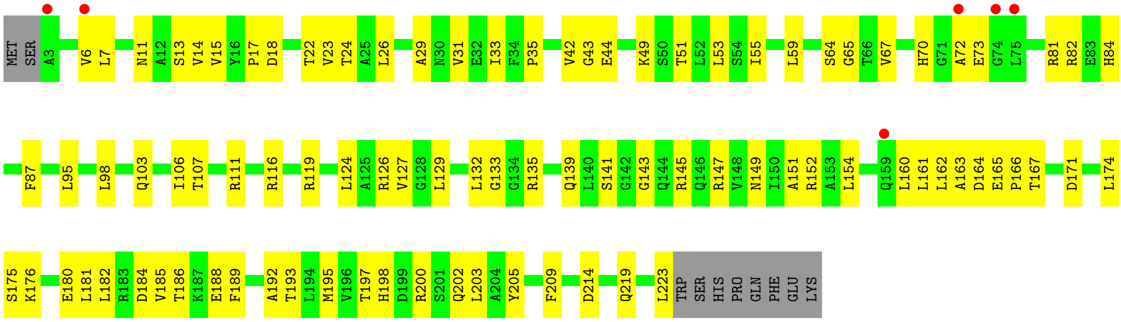
- Molecule 1: Putative ABC transport system, ATP-binding protein

Chain G:



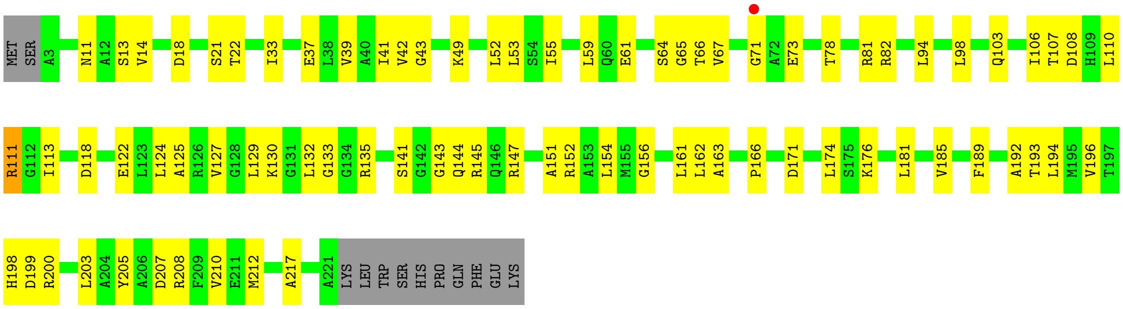
- Molecule 1: Putative ABC transport system, ATP-binding protein

Chain I:



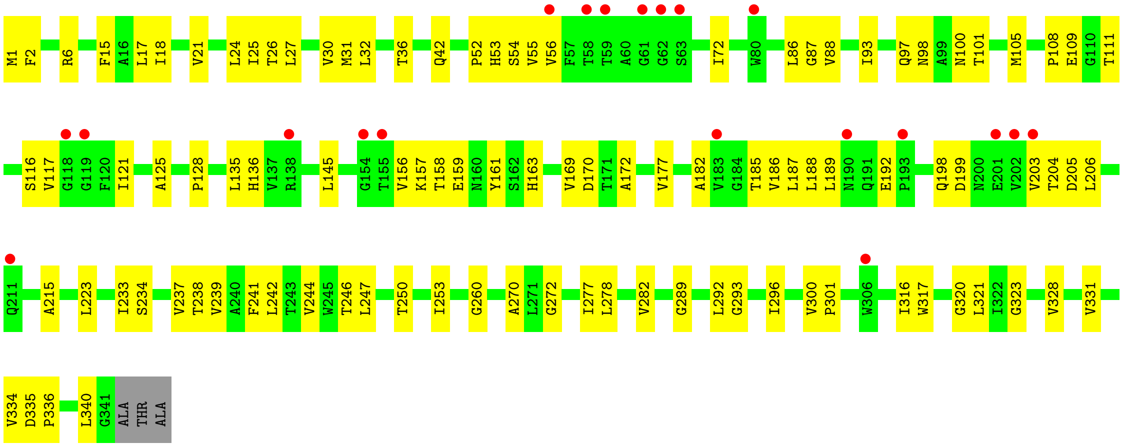
- Molecule 1: Putative ABC transport system, ATP-binding protein

Chain K:



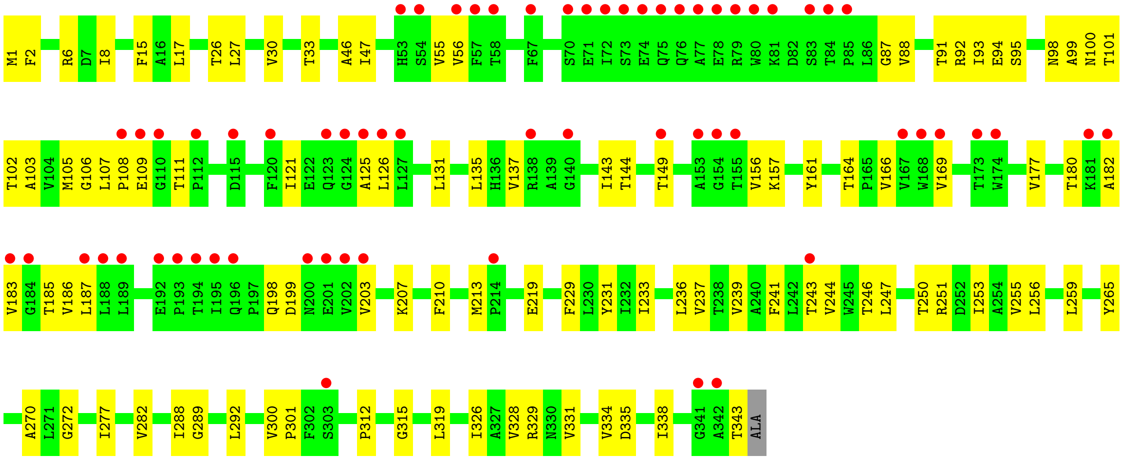
- Molecule 2: Putative ABC transport system integral membrane protein

Chain B:



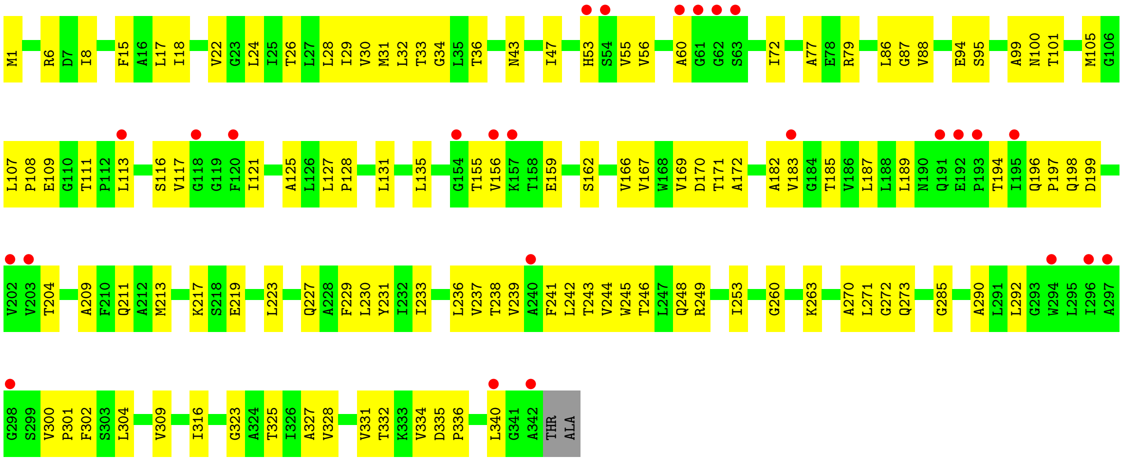
- Molecule 2: Putative ABC transport system integral membrane protein

Chain D:

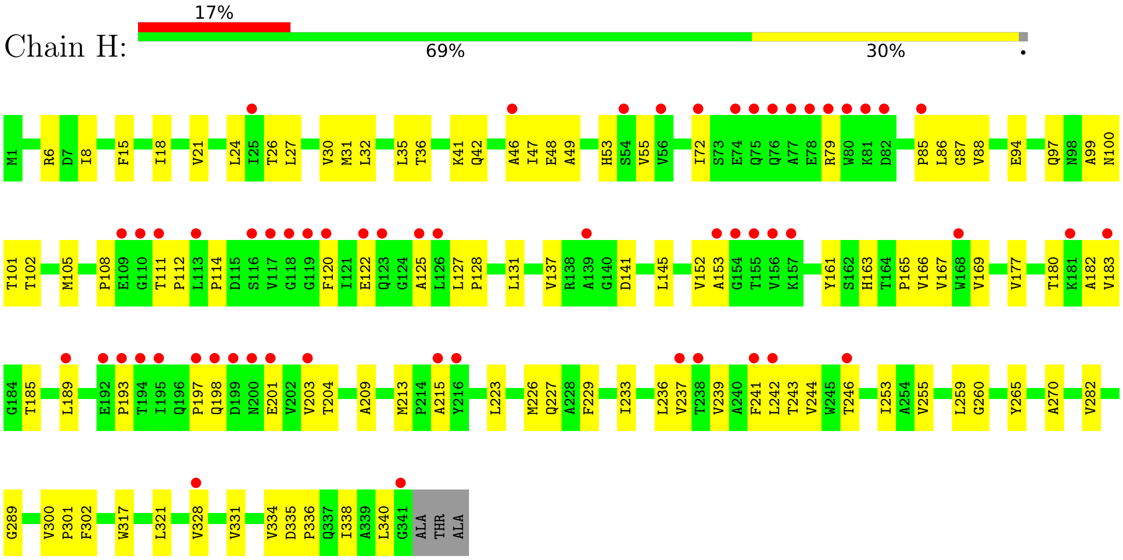


- Molecule 2: Putative ABC transport system integral membrane protein

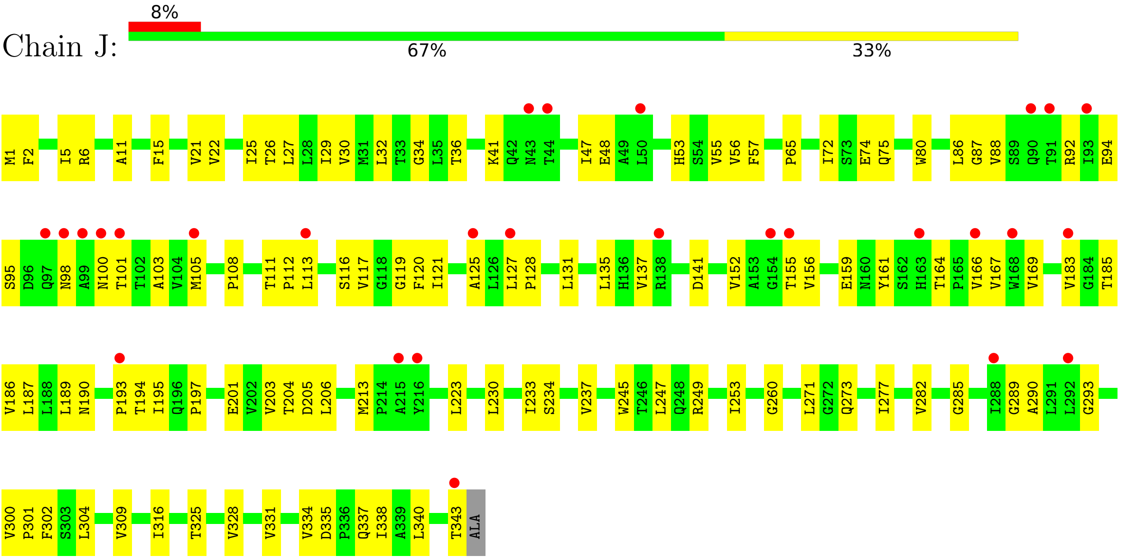
Chain F:



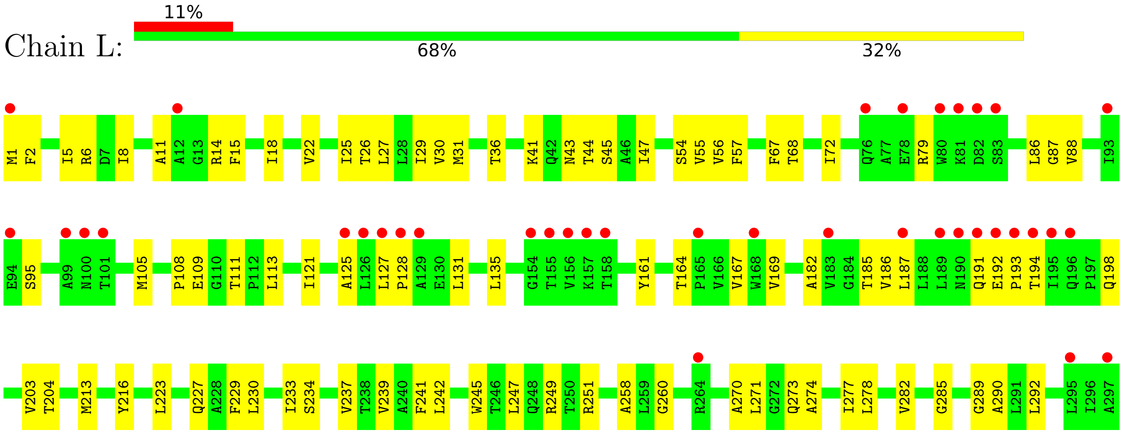
- Molecule 2: Putative ABC transport system integral membrane protein



- Molecule 2: Putative ABC transport system integral membrane protein



- Molecule 2: Putative ABC transport system integral membrane protein




V300
P301
F302
S303
L304
V309
I316
W317
G320
L321
I322
G323
A324
T325
I326
A327
V328
R329
N330
V331
V334
D335
P336
Q337
I338
A339
L340
G341
A342
T343
ALA

4 Data and refinement statistics ⓘ

Property	**Value**	**Source**
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	82.58Å 135.03Å 160.97Å 112.49° 100.41° 93.78°	Depositor
Resolution (Å)	49.29 – 3.40 49.29 – 3.27	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.29-3.40) 83.0 (49.29-3.27)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.53 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.255 , 0.285 0.255 , 0.283	Depositor DCC
R_{free} test set	2947 reflections (3.13%)	wwPDB-VP
Wilson B-factor (Å^2)	103.8	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 71.2	EDS
L-test for twinning[2]	$< \|L\| >$ = 0.48, $< L^2 >$ = 0.31	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	25112	wwPDB-VP
Average B, all atoms (Å^2)	167.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.26	0/1637	0.50	0/2216
1	C	0.27	0/1653	0.51	0/2238
1	E	0.24	0/1648	0.50	0/2230
1	G	0.26	0/1716	0.52	0/2325
1	I	0.27	0/1671	0.52	0/2263
1	K	0.27	0/1658	0.53	0/2245
2	B	0.26	0/2556	0.45	0/3495
2	D	0.24	0/2568	0.44	0/3512
2	F	0.25	0/2561	0.45	0/3502
2	H	0.24	0/2556	0.44	0/3495
2	J	0.24	0/2568	0.45	0/3512
2	L	0.24	0/2568	0.44	0/3512
All	All	0.25	0/25360	0.47	0/34545

There are no bond length outliers.

There are no bond angle outliers.

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	1618	0	1664	78	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1634	0	1679	72	0
1	E	1629	0	1675	73	0
1	G	1693	0	1737	61	0
1	I	1652	0	1697	85	0
1	K	1639	0	1684	78	0
2	B	2510	0	2588	91	0
2	D	2522	0	2600	85	0
2	F	2515	0	2593	121	0
2	H	2510	0	2588	105	0
2	J	2522	0	2600	92	0
2	L	2522	0	2600	93	0
3	D	43	30	30	7	0
3	F	43	30	30	9	0
All	All	25052	60	25765	979	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 19.

All (979) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:26:LEU:HD11	1:E:29:ALA:HB2	1.27	1.16
1:I:127:VAL:HG13	1:I:181:LEU:HD21	1.40	1.01
2:D:253:ILE:HD13	2:D:331:VAL:HG23	1.41	1.01
1:C:14:VAL:HG23	1:C:55:ILE:HD11	1.43	1.00
1:K:132:LEU:HD22	1:K:135:ARG:HE	1.28	0.99
2:D:108:PRO:HG2	2:D:111:THR:HG21	1.41	0.99
1:A:127:VAL:HG13	1:A:181:LEU:HD21	1.46	0.97
2:H:180:THR:HG22	2:H:182:ALA:H	1.32	0.95
1:A:53:LEU:HD11	1:A:162:LEU:HB3	1.49	0.93
1:E:14:VAL:HG22	1:E:62:PRO:HA	1.50	0.93
1:E:53:LEU:HD11	1:E:162:LEU:HB3	1.52	0.92
2:B:253:ILE:HD13	2:B:331:VAL:HG23	1.52	0.92
2:H:36:THR:HG22	2:H:223:LEU:HD13	1.53	0.90
3:D:401:HEM:HBC2	3:D:401:HEM:HMC2	1.52	0.89
2:H:125:ALA:HA	2:H:169:VAL:HG12	1.54	0.89
1:G:55:ILE:HD11	1:G:62:PRO:HG3	1.55	0.89
2:F:79:ARG:HH12	2:F:198:GLN:HB2	1.39	0.88
2:B:117:VAL:HG13	2:B:156:VAL:HG11	1.54	0.87
1:C:41:ILE:HD13	1:C:52:LEU:HD23	1.57	0.86
2:F:211:GLN:HG3	2:F:217:LYS:HD2	1.57	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:108:PRO:HG2	2:F:111:THR:HG21	1.59	0.85
3:D:401:HEM:HMB2	3:D:401:HEM:HBB2	1.59	0.84
2:H:94:GLU:HG3	2:H:99:ALA:HB2	1.61	0.82
1:I:176:LYS:NZ	1:I:205:TYR:OH	2.12	0.81
1:K:55:ILE:CG2	1:K:67:VAL:HG21	2.10	0.81
2:D:108:PRO:HG2	2:D:111:THR:CG2	2.11	0.80
3:F:401:HEM:HMB2	3:F:401:HEM:HBB2	1.63	0.80
2:F:302:PHE:HE2	2:F:304:LEU:HD12	1.46	0.80
3:F:401:HEM:HMC2	3:F:401:HEM:HBC2	1.60	0.80
1:E:15:VAL:HG22	1:E:24:THR:HG22	1.62	0.80
1:C:53:LEU:HD11	1:C:162:LEU:HB3	1.65	0.79
1:G:55:ILE:HG12	1:G:67:VAL:HG21	1.64	0.79
2:J:92:ARG:NH1	2:J:94:GLU:OE1	2.16	0.78
1:I:182:LEU:O	1:I:186:THR:HG23	1.83	0.78
1:G:53:LEU:HD11	1:G:162:LEU:HB3	1.66	0.78
1:C:104:LEU:HB3	1:C:155:MET:HG3	1.64	0.77
1:E:59:LEU:HD13	2:F:340:LEU:HD11	1.65	0.77
1:A:16:TYR:HE1	1:A:60:GLN:HE22	1.32	0.77
2:D:125:ALA:HA	2:D:169:VAL:HG12	1.65	0.77
1:K:107:THR:O	1:K:111:ARG:NE	2.18	0.77
1:I:132:LEU:HB3	1:I:135:ARG:HD3	1.67	0.77
2:B:26:THR:HG21	2:B:282:VAL:HG22	1.66	0.76
1:K:132:LEU:HD22	1:K:135:ARG:NE	2.00	0.76
1:C:14:VAL:CG2	1:C:55:ILE:HD11	2.16	0.76
2:D:185:THR:HG23	2:D:186:VAL:HG23	1.67	0.75
1:E:26:LEU:HD11	1:E:29:ALA:CB	2.14	0.75
1:I:154:LEU:HD11	1:I:185:VAL:HG11	1.67	0.75
1:G:203:LEU:HD23	1:G:223:LEU:HD11	1.67	0.74
1:C:41:ILE:CD1	1:C:194:LEU:HD11	2.17	0.74
2:D:156:VAL:HG12	2:D:157:LYS:H	1.51	0.74
2:H:42:GLN:HG3	2:H:163:HIS:HA	1.70	0.74
2:H:32:LEU:O	2:H:36:THR:HG23	1.88	0.74
1:A:147:ARG:NH2	1:A:177:GLU:OE1	2.21	0.74
2:H:137:VAL:HG13	2:H:141:ASP:HB2	1.70	0.74
1:K:14:VAL:CG2	1:K:55:ILE:HD11	2.18	0.73
1:G:108:ASP:OD1	1:G:111:ARG:NH2	2.20	0.73
3:D:401:HEM:HBC2	3:D:401:HEM:CMC	2.18	0.73
2:B:36:THR:HG22	2:B:223:LEU:HB3	1.69	0.73
2:F:244:VAL:HG12	2:H:244:VAL:HG12	1.70	0.73
1:G:59:LEU:CD1	2:H:340:LEU:HD11	2.19	0.73
2:F:125:ALA:HA	2:F:169:VAL:HG12	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:117:VAL:HG13	2:B:156:VAL:CG1	2.18	0.72
1:C:42:VAL:CG2	1:C:203:LEU:HD21	2.19	0.72
2:L:56:VAL:HG22	2:L:203:VAL:HG22	1.71	0.72
1:I:143:GLY:O	1:I:147:ARG:HG3	1.89	0.72
1:K:127:VAL:HG12	1:K:147:ARG:HB3	1.70	0.72
2:L:31:MET:HE1	2:L:292:LEU:HD23	1.70	0.72
1:K:200:ARG:HA	1:K:203:LEU:HD13	1.72	0.72
1:K:127:VAL:HG13	1:K:181:LEU:HD21	1.71	0.72
1:K:98:LEU:HD11	1:K:106:ILE:HD12	1.71	0.72
1:G:55:ILE:CD1	1:G:62:PRO:HG3	2.19	0.72
2:H:253:ILE:HG22	2:H:334:VAL:HG11	1.69	0.72
2:J:26:THR:HG22	2:J:316:ILE:HD13	1.70	0.72
1:A:154:LEU:HD11	1:A:185:VAL:HG11	1.72	0.72
1:E:17:PRO:HA	1:E:22:THR:HA	1.72	0.72
1:E:127:VAL:HG12	1:E:147:ARG:HB3	1.71	0.72
2:B:128:PRO:HB3	2:B:158:THR:HG22	1.71	0.71
1:G:59:LEU:HD12	2:H:340:LEU:HD11	1.72	0.71
2:H:137:VAL:HG11	2:H:152:VAL:HG21	1.71	0.71
1:E:102:GLU:OE2	2:F:6:ARG:NH1	2.24	0.71
2:F:108:PRO:HG2	2:F:111:THR:CG2	2.19	0.71
1:A:127:VAL:HG13	1:A:181:LEU:CD2	2.20	0.71
1:C:127:VAL:HG13	1:C:181:LEU:HD21	1.71	0.71
1:G:95:LEU:HD12	1:G:98:LEU:HD12	1.73	0.71
1:G:127:VAL:HG13	1:G:181:LEU:HD21	1.72	0.71
1:K:132:LEU:CD2	1:K:135:ARG:HE	2.04	0.71
1:C:127:VAL:O	1:C:147:ARG:HD3	1.91	0.70
2:F:211:GLN:OE1	2:F:217:LYS:NZ	2.21	0.70
2:L:108:PRO:HD2	2:L:111:THR:HG21	1.73	0.70
1:K:127:VAL:HG11	1:K:147:ARG:O	1.92	0.70
1:C:55:ILE:HG23	1:C:67:VAL:HG21	1.73	0.70
2:H:193:PRO:HG3	2:H:203:VAL:HG11	1.73	0.70
2:F:302:PHE:CE2	2:F:304:LEU:HD12	2.27	0.70
1:E:6:VAL:O	1:E:69:LEU:HD12	1.92	0.70
1:A:127:VAL:O	1:A:147:ARG:HD3	1.92	0.70
1:I:167:THR:HB	1:I:175:SER:HB3	1.73	0.70
2:D:1:MET:CE	2:D:272:GLY:HA3	2.22	0.69
1:I:127:VAL:HG21	1:I:151:ALA:HB2	1.74	0.69
2:B:156:VAL:HG12	2:B:157:LYS:N	2.06	0.69
2:H:128:PRO:HG2	2:H:131:LEU:HB3	1.72	0.69
2:D:94:GLU:HG3	2:D:99:ALA:HB2	1.74	0.69
3:F:401:HEM:HBC2	3:F:401:HEM:CMC	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:117:VAL:HG13	2:J:156:VAL:HB	1.74	0.69
1:K:111:ARG:HH12	1:K:156:GLY:HA3	1.57	0.69
1:A:42:VAL:CG2	1:A:203:LEU:HD21	2.23	0.69
2:F:32:LEU:O	2:F:36:THR:HG23	1.92	0.69
2:H:41:LYS:NZ	2:H:48:GLU:OE1	2.25	0.69
2:J:116:SER:OG	2:J:159:GLU:OE2	2.10	0.69
2:B:17:LEU:HD21	2:D:239:VAL:HG12	1.75	0.68
2:B:270:ALA:HB3	2:B:328:VAL:HG11	1.75	0.68
1:E:127:VAL:O	1:E:147:ARG:HD3	1.94	0.68
2:F:304:LEU:HD21	2:F:309:VAL:CG2	2.23	0.68
2:F:271:LEU:HD21	2:F:325:THR:HG22	1.75	0.68
1:I:55:ILE:CG2	1:I:67:VAL:HG21	2.23	0.68
2:B:317:TRP:CH2	2:B:321:LEU:HD11	2.29	0.68
1:C:55:ILE:CG2	1:C:67:VAL:HG21	2.24	0.67
1:A:119:ARG:NH1	1:A:155:MET:O	2.27	0.67
2:D:326:ILE:O	2:D:329:ARG:NH1	2.26	0.67
1:E:129:LEU:HD22	1:E:132:LEU:HD12	1.76	0.67
1:G:127:VAL:HG13	1:G:181:LEU:CD2	2.23	0.67
3:D:401:HEM:HBB2	3:D:401:HEM:CMB	2.24	0.67
1:E:15:VAL:HG22	1:E:24:THR:CG2	2.24	0.67
2:D:56:VAL:HG22	2:D:203:VAL:HG22	1.76	0.67
2:F:246:THR:HG21	2:F:328:VAL:HG22	1.76	0.67
2:L:31:MET:CE	2:L:292:LEU:HD23	2.25	0.67
2:D:98:ASN:HB3	2:D:135:LEU:HD23	1.75	0.67
1:A:127:VAL:HG12	1:A:147:ARG:HB3	1.76	0.67
3:F:401:HEM:HBB2	3:F:401:HEM:CMB	2.24	0.67
1:I:59:LEU:CD1	2:J:340:LEU:HD11	2.25	0.67
2:F:304:LEU:HD21	2:F:309:VAL:HG23	1.76	0.67
2:D:315:GLY:O	2:D:319:LEU:HD23	1.96	0.66
1:E:127:VAL:HG11	1:E:147:ARG:O	1.95	0.66
1:G:7:LEU:HB3	1:G:33:ILE:HG22	1.76	0.66
1:C:127:VAL:HG12	1:C:147:ARG:HB3	1.78	0.66
2:B:36:THR:CG2	2:B:223:LEU:HB3	2.26	0.66
1:C:3:ALA:HB3	1:K:61:GLU:HG2	1.76	0.66
1:E:119:ARG:NH1	1:E:155:MET:O	2.28	0.66
2:L:26:THR:HG22	2:L:316:ILE:HD13	1.77	0.66
1:K:143:GLY:O	1:K:147:ARG:HG3	1.96	0.66
2:F:117:VAL:HG13	2:F:156:VAL:HB	1.77	0.66
2:H:88:VAL:HG22	2:H:105:MET:HG2	1.78	0.66
1:K:13:SER:HB2	1:K:64:SER:OG	1.96	0.66
2:B:1:MET:CE	2:B:272:GLY:HA3	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:14:VAL:HG21	1:I:55:ILE:HD11	1.76	0.65
2:D:47:ILE:HD12	2:D:213:MET:CE	2.25	0.65
2:H:128:PRO:HG2	2:H:131:LEU:CB	2.26	0.65
2:B:244:VAL:HG11	2:D:244:VAL:HG13	1.79	0.65
2:F:24:LEU:HD12	2:H:236:LEU:HD12	1.79	0.65
2:F:29:ILE:HG21	2:F:231:TYR:HE1	1.60	0.65
2:L:29:ILE:HD11	2:L:230:LEU:HB2	1.78	0.65
1:I:160:LEU:HD12	1:I:192:ALA:O	1.96	0.65
3:F:401:HEM:HMC3	2:H:35:LEU:HD21	1.78	0.64
1:I:127:VAL:HG12	1:I:147:ARG:HB3	1.78	0.64
2:J:26:THR:O	2:J:30:VAL:HG23	1.96	0.64
1:A:167:THR:HB	1:A:175:SER:HB3	1.79	0.64
2:J:125:ALA:HA	2:J:169:VAL:HG12	1.80	0.64
1:C:41:ILE:CD1	1:C:52:LEU:HD23	2.27	0.64
1:K:200:ARG:HA	1:K:203:LEU:CD1	2.26	0.64
1:K:82:ARG:HB2	2:L:260:GLY:HA3	1.79	0.64
2:B:156:VAL:HG12	2:B:157:LYS:H	1.60	0.64
2:F:113:LEU:HD21	2:F:121:ILE:HD11	1.77	0.64
1:A:171:ASP:HB2	1:C:214:ASP:OD1	1.98	0.64
2:L:87:GLY:O	2:L:105:MET:HA	1.97	0.64
1:C:141:SER:OG	1:C:144:GLN:HG3	1.98	0.63
1:I:44:GLU:HA	1:I:44:GLU:OE1	1.97	0.63
2:L:328:VAL:HG13	2:L:331:VAL:HG21	1.80	0.63
2:H:328:VAL:HG13	2:H:331:VAL:HG21	1.79	0.63
2:L:302:PHE:CE2	2:L:304:LEU:HD13	2.33	0.63
1:C:108:ASP:OD2	1:C:116:ARG:HG2	1.97	0.63
2:L:79:ARG:HH12	2:L:198:GLN:HB2	1.63	0.63
1:A:9:ILE:HG23	1:A:67:VAL:HG22	1.80	0.63
2:J:32:LEU:O	2:J:36:THR:HG23	1.98	0.63
2:H:223:LEU:O	2:H:227:GLN:HG3	1.99	0.63
1:E:127:VAL:HG13	1:E:181:LEU:HD21	1.80	0.63
1:C:49:LYS:HB3	1:C:196:VAL:HG13	1.81	0.62
2:H:127:LEU:HD23	2:H:167:VAL:HG13	1.81	0.62
2:L:125:ALA:HA	2:L:169:VAL:HG12	1.81	0.62
2:H:125:ALA:CA	2:H:169:VAL:HG12	2.28	0.62
1:E:27:ASP:OD2	1:E:216:LYS:HE2	2.00	0.62
1:E:209:PHE:CE1	1:E:221:ALA:HB3	2.34	0.62
1:G:104:LEU:CD2	1:G:152:ARG:HA	2.30	0.62
2:J:193:PRO:HG3	2:J:203:VAL:HG11	1.81	0.62
2:J:328:VAL:HG13	2:J:331:VAL:HG21	1.81	0.62
2:B:215:ALA:HB2	3:D:401:HEM:HBA2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:239:VAL:HG22	2:F:323:GLY:O	2.00	0.62
2:H:26:THR:O	2:H:30:VAL:HG23	2.00	0.62
2:H:86:LEU:O	2:H:185:THR:HG22	2.00	0.62
2:J:26:THR:OG1	2:J:285:GLY:HA3	1.99	0.62
1:E:33:ILE:HG22	1:E:192:ALA:HB1	1.81	0.62
1:G:203:LEU:CD2	1:G:223:LEU:HD11	2.29	0.62
2:H:270:ALA:HB3	2:H:328:VAL:HG11	1.81	0.62
2:F:26:THR:OG1	2:F:285:GLY:HA3	1.99	0.62
2:H:137:VAL:CG1	2:H:152:VAL:HG21	2.30	0.62
1:A:33:ILE:CD1	1:A:194:LEU:HG	2.30	0.61
2:B:300:VAL:HG13	3:D:401:HEM:HBB1	1.82	0.61
2:D:26:THR:O	2:D:30:VAL:HG23	1.99	0.61
2:D:180:THR:HG22	2:D:182:ALA:H	1.65	0.61
2:B:145:LEU:HG	2:B:177:VAL:HG11	1.82	0.61
2:L:26:THR:HG21	2:L:282:VAL:HG22	1.82	0.61
2:L:113:LEU:HD21	2:L:121:ILE:HD11	1.82	0.61
2:F:36:THR:HG22	2:F:223:LEU:HB3	1.81	0.61
1:I:198:HIS:HB3	1:K:198:HIS:CE1	2.35	0.61
2:J:87:GLY:O	2:J:105:MET:HA	2.01	0.61
1:I:59:LEU:HD12	2:J:340:LEU:HD11	1.81	0.61
1:I:200:ARG:HA	1:I:203:LEU:HG	1.83	0.61
1:C:104:LEU:HB3	1:C:155:MET:CG	2.31	0.61
2:F:29:ILE:HD13	2:F:231:TYR:CD1	2.36	0.61
1:G:52:LEU:O	1:G:55:ILE:HG22	1.98	0.61
1:I:81:ARG:HG2	1:I:87:PHE:HZ	1.66	0.61
1:I:132:LEU:HD22	1:I:135:ARG:HD2	1.83	0.61
1:K:33:ILE:CD1	1:K:194:LEU:HG	2.31	0.61
1:G:99:THR:O	1:G:103:GLN:HG2	2.01	0.61
1:K:154:LEU:HD21	1:K:185:VAL:HG11	1.82	0.60
2:B:36:THR:HG22	2:B:223:LEU:HD13	1.83	0.60
2:H:55:VAL:HG11	2:H:209:ALA:HB2	1.83	0.60
2:H:87:GLY:O	2:H:105:MET:HA	2.01	0.60
2:J:186:VAL:HG12	2:J:187:LEU:N	2.16	0.60
1:K:55:ILE:HG23	1:K:67:VAL:HG21	1.84	0.60
1:C:41:ILE:HD11	1:C:194:LEU:HD11	1.83	0.60
1:E:14:VAL:CG2	1:E:55:ILE:HD11	2.32	0.60
1:I:126:ARG:NH2	1:I:188:GLU:OE1	2.35	0.60
1:E:195:MET:O	1:E:197:THR:HG23	2.00	0.60
2:H:47:ILE:HD12	2:H:213:MET:CE	2.31	0.60
1:I:186:THR:HG22	1:I:193:THR:OG1	2.02	0.60
2:H:335:ASP:OD1	2:H:336:PRO:HD2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:TYR:O	1:C:23:VAL:HG12	2.02	0.59
1:I:53:LEU:HD11	1:I:162:LEU:HB3	1.83	0.59
1:K:33:ILE:HD13	1:K:194:LEU:HG	1.83	0.59
2:L:47:ILE:HG13	2:L:213:MET:CE	2.31	0.59
2:B:56:VAL:HB	2:B:187:LEU:HB2	1.84	0.59
2:F:211:GLN:CG	2:F:217:LYS:HD2	2.31	0.59
2:H:180:THR:HG22	2:H:182:ALA:N	2.12	0.59
2:L:302:PHE:HE2	2:L:304:LEU:HD13	1.67	0.59
2:H:108:PRO:HD2	2:H:111:THR:HG21	1.83	0.59
2:F:86:LEU:O	2:F:185:THR:HG22	2.01	0.59
1:I:15:VAL:HG22	1:I:24:THR:HA	1.83	0.59
1:C:42:VAL:HG21	1:C:203:LEU:HD21	1.84	0.59
2:H:36:THR:CG2	2:H:223:LEU:HB3	2.33	0.59
2:L:8:ILE:HD11	2:L:273:GLN:HG3	1.83	0.59
2:H:26:THR:HG21	2:H:282:VAL:HG22	1.84	0.59
1:I:18:ASP:CB	1:I:23:VAL:HG23	2.32	0.59
1:I:31:VAL:HA	1:I:219:GLN:OE1	2.02	0.59
2:B:26:THR:HG22	2:B:316:ILE:HG21	1.85	0.59
2:H:253:ILE:CG2	2:H:334:VAL:HG11	2.32	0.59
2:F:302:PHE:CE2	2:F:304:LEU:HB2	2.37	0.59
2:J:26:THR:HG22	2:J:316:ILE:CD1	2.33	0.59
2:J:293:GLY:HA3	2:J:302:PHE:CE2	2.38	0.59
2:J:300:VAL:CG1	2:J:301:PRO:HD2	2.33	0.59
1:A:33:ILE:CG2	1:A:192:ALA:HB1	2.33	0.59
2:F:335:ASP:OD1	2:F:336:PRO:HD2	2.03	0.59
2:D:338:ILE:HG23	2:D:343:THR:HG21	1.85	0.58
2:F:196:GLN:NE2	2:F:197:PRO:HD2	2.18	0.58
1:E:127:VAL:HG21	1:E:151:ALA:HB2	1.85	0.58
2:F:229:PHE:HE2	2:H:27:LEU:HD23	1.67	0.58
2:L:300:VAL:CG1	2:L:301:PRO:HD2	2.33	0.58
1:G:82:ARG:HB2	2:H:260:GLY:HA3	1.85	0.58
2:L:86:LEU:O	2:L:185:THR:HG22	2.03	0.58
1:C:47:SER:O	1:C:215:GLY:N	2.30	0.58
1:I:165:GLU:OE2	1:I:198:HIS:ND1	2.36	0.58
1:A:59:LEU:CD1	2:B:340:LEU:HD11	2.34	0.58
1:A:127:VAL:CG1	1:A:147:ARG:HB3	2.34	0.58
2:B:117:VAL:CG1	2:B:156:VAL:HG11	2.29	0.58
1:K:127:VAL:HG21	1:K:151:ALA:HB2	1.85	0.58
1:C:119:ARG:NH1	1:C:155:MET:O	2.35	0.58
1:E:8:SER:HA	1:E:32:GLU:HG2	1.85	0.58
1:E:38:LEU:HD22	1:E:206:ALA:HA	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:11:ASN:O	1:I:65:GLY:HA3	2.03	0.58
2:D:253:ILE:HD13	2:D:331:VAL:CG2	2.26	0.58
2:B:293:GLY:HA2	2:B:296:ILE:HG22	1.85	0.58
2:L:278:LEU:HD13	2:L:320:GLY:HA3	1.85	0.58
2:D:270:ALA:HB3	2:D:328:VAL:HG11	1.85	0.58
2:D:26:THR:HG21	2:D:282:VAL:HG22	1.86	0.58
1:C:98:LEU:HD11	1:C:106:ILE:HD12	1.85	0.57
1:G:185:VAL:HG13	1:G:189:PHE:CD2	2.40	0.57
1:I:13:SER:HB2	1:I:64:SER:OG	2.03	0.57
2:H:233:ILE:O	2:H:237:VAL:HG23	2.04	0.57
2:J:25:ILE:HG21	2:J:234:SER:HB3	1.86	0.57
1:A:33:ILE:HD11	1:A:194:LEU:HG	1.87	0.57
2:L:36:THR:HA	2:L:223:LEU:HD13	1.86	0.57
2:D:288:ILE:O	2:D:292:LEU:HD13	2.05	0.57
1:E:111:ARG:HH12	1:E:113:ILE:HD11	1.70	0.57
2:F:26:THR:O	2:F:30:VAL:HG23	2.04	0.57
2:L:26:THR:O	2:L:30:VAL:HG23	2.05	0.57
1:C:127:VAL:O	1:C:127:VAL:HG12	2.03	0.57
1:E:59:LEU:HD13	2:F:340:LEU:CD1	2.33	0.57
1:I:18:ASP:HB2	1:I:23:VAL:HG23	1.86	0.57
1:A:185:VAL:HG13	1:A:189:PHE:CD2	2.40	0.57
2:D:55:VAL:CG1	2:D:186:VAL:HG11	2.34	0.57
1:I:127:VAL:HG13	1:I:181:LEU:CD2	2.28	0.57
2:B:42:GLN:HG3	2:B:163:HIS:HA	1.85	0.57
1:E:14:VAL:HG23	1:E:55:ILE:HD11	1.87	0.57
2:D:156:VAL:HG12	2:D:157:LYS:N	2.17	0.56
2:H:8:ILE:HA	2:H:15:PHE:CE2	2.40	0.56
1:C:127:VAL:CG1	1:C:147:ARG:HB3	2.34	0.56
2:F:238:THR:O	2:F:242:LEU:HD23	2.05	0.56
2:H:36:THR:HG22	2:H:223:LEU:CD1	2.32	0.56
2:L:335:ASP:OD1	2:L:338:ILE:HG12	2.05	0.56
1:C:26:LEU:CD2	1:C:55:ILE:HD12	2.35	0.56
2:F:26:THR:HG22	2:F:316:ILE:HG21	1.88	0.56
1:G:102:GLU:OE2	2:H:6:ARG:NH1	2.37	0.56
1:G:127:VAL:O	1:G:127:VAL:HG12	2.06	0.56
1:K:141:SER:OG	1:K:144:GLN:HG3	2.05	0.56
2:L:161:TYR:O	2:L:164:THR:OG1	2.20	0.56
3:F:401:HEM:HBB1	2:H:301:PRO:HD2	1.87	0.56
2:B:55:VAL:O	2:B:204:THR:HG22	2.05	0.56
2:B:125:ALA:HA	2:B:169:VAL:HG12	1.88	0.56
1:E:160:LEU:HD12	1:E:192:ALA:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:328:VAL:HG13	2:H:331:VAL:CG2	2.35	0.56
1:I:55:ILE:HG22	1:I:67:VAL:HG21	1.86	0.56
1:I:203:LEU:HB3	1:I:209:PHE:CE1	2.40	0.56
1:C:141:SER:O	1:C:145:ARG:HG3	2.04	0.56
2:D:94:GLU:HB3	2:D:144:THR:HB	1.87	0.56
2:F:233:ILE:O	2:F:237:VAL:HG23	2.06	0.56
2:D:328:VAL:HG12	2:D:328:VAL:O	2.06	0.56
1:I:185:VAL:HG13	1:I:189:PHE:CD2	2.41	0.56
2:J:74:GLU:HG2	2:J:183:VAL:HG13	1.87	0.56
1:K:53:LEU:HD11	1:K:162:LEU:HB3	1.87	0.56
1:I:98:LEU:HD11	1:I:106:ILE:HD12	1.88	0.56
2:L:270:ALA:HB3	2:L:328:VAL:HG11	1.87	0.56
2:J:86:LEU:O	2:J:185:THR:HG22	2.05	0.56
2:J:119:GLY:O	2:J:120:PHE:HD1	1.88	0.56
2:J:205:ASP:OD1	2:J:206:LEU:N	2.36	0.56
2:L:14:ARG:O	2:L:18:ILE:HG13	2.06	0.56
1:A:59:LEU:HD12	2:B:340:LEU:HD11	1.87	0.55
1:A:127:VAL:O	1:A:127:VAL:HG12	2.06	0.55
2:F:127:LEU:HD23	2:F:167:VAL:HG13	1.87	0.55
1:A:33:ILE:HG22	1:A:192:ALA:HB1	1.89	0.55
2:B:328:VAL:O	2:B:331:VAL:HG12	2.07	0.55
1:C:42:VAL:CG1	1:C:200:ARG:HE	2.20	0.55
1:G:141:SER:O	1:G:145:ARG:HG3	2.06	0.55
2:D:233:ILE:O	2:D:237:VAL:HG23	2.06	0.55
1:A:11:ASN:O	1:A:65:GLY:HA3	2.06	0.55
1:I:171:ASP:OD1	1:I:174:LEU:HB2	2.06	0.55
1:K:127:VAL:CG1	1:K:147:ARG:HB3	2.36	0.55
1:K:127:VAL:HG12	1:K:127:VAL:O	2.06	0.55
2:H:55:VAL:CG1	2:H:209:ALA:HB2	2.37	0.55
1:A:41:ILE:HD13	1:A:52:LEU:HD23	1.89	0.55
1:A:141:SER:O	1:A:145:ARG:HG3	2.07	0.55
2:B:86:LEU:O	2:B:185:THR:HG22	2.07	0.55
1:A:42:VAL:HG21	1:A:203:LEU:HD21	1.88	0.55
1:C:104:LEU:CB	1:C:155:MET:HG3	2.35	0.55
1:E:49:LYS:HD2	1:E:196:VAL:HG13	1.89	0.55
2:F:17:LEU:HD21	2:H:239:VAL:HG12	1.89	0.55
2:F:328:VAL:O	2:F:331:VAL:HG12	2.07	0.55
1:E:7:LEU:HD23	1:E:33:ILE:HD13	1.88	0.55
2:F:43:ASN:OD1	2:F:162:SER:HA	2.07	0.55
1:G:161:LEU:O	1:G:193:THR:HA	2.07	0.55
2:H:88:VAL:HG11	2:H:161:TYR:CZ	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:326:ILE:O	2:L:329:ARG:NH1	2.37	0.55
1:C:15:VAL:HA	1:C:23:VAL:O	2.07	0.55
1:G:123:LEU:CD1	1:G:155:MET:HA	2.37	0.55
2:J:328:VAL:HG13	2:J:331:VAL:CG2	2.37	0.55
2:L:328:VAL:HG13	2:L:331:VAL:CG2	2.37	0.55
1:A:53:LEU:CD2	1:A:164:ASP:HB2	2.36	0.54
2:D:335:ASP:OD1	2:D:338:ILE:HG13	2.07	0.54
2:L:317:TRP:CH2	2:L:321:LEU:HD11	2.41	0.54
1:E:132:LEU:HD22	1:E:135:ARG:NE	2.22	0.54
2:F:29:ILE:HD13	2:F:231:TYR:CE1	2.42	0.54
1:I:7:LEU:HB3	1:I:33:ILE:HG22	1.87	0.54
1:A:160:LEU:HD12	1:A:192:ALA:O	2.07	0.54
1:G:31:VAL:HA	1:G:219:GLN:NE2	2.22	0.54
2:L:233:ILE:O	2:L:237:VAL:HG23	2.07	0.54
2:F:32:LEU:HD13	2:H:226:MET:CE	2.37	0.54
2:H:55:VAL:HG11	2:H:209:ALA:CB	2.38	0.54
1:K:33:ILE:HG22	1:K:192:ALA:HB1	1.88	0.54
1:K:42:VAL:HG11	1:K:200:ARG:HE	1.72	0.54
2:L:245:TRP:NE1	2:L:249:ARG:HD2	2.22	0.54
1:C:16:TYR:HE1	1:C:60:GLN:HE22	1.54	0.54
1:E:59:LEU:CD1	2:F:340:LEU:HD11	2.36	0.54
2:F:219:GLU:HG3	3:F:401:HEM:C1C	2.42	0.54
2:H:72:ILE:O	2:H:182:ALA:HB1	2.08	0.54
1:A:16:TYR:OH	1:A:51:THR:HG23	2.07	0.54
2:B:54:SER:HB3	2:B:203:VAL:HG13	1.90	0.54
1:C:53:LEU:HD21	1:C:164:ASP:HB2	1.90	0.54
2:D:186:VAL:HG12	2:D:187:LEU:N	2.23	0.54
2:L:88:VAL:HG22	2:L:105:MET:HG2	1.89	0.54
1:A:26:LEU:HD11	1:A:29:ALA:HB2	1.90	0.54
1:C:154:LEU:HD11	1:C:185:VAL:HG11	1.90	0.54
2:D:186:VAL:HG12	2:D:187:LEU:H	1.73	0.54
2:D:241:PHE:O	2:D:244:VAL:HG12	2.08	0.54
1:E:58:PHE:CE2	1:E:80:THR:HG21	2.43	0.54
1:E:195:MET:HG2	1:E:197:THR:CG2	2.38	0.54
2:F:26:THR:HG22	2:F:316:ILE:HD13	1.88	0.54
1:G:15:VAL:H	1:G:63:THR:HG21	1.72	0.54
2:L:239:VAL:HG22	2:L:323:GLY:O	2.08	0.54
1:E:127:VAL:CG1	1:E:147:ARG:HB3	2.38	0.54
3:F:401:HEM:CBA	2:H:215:ALA:HB2	2.38	0.54
2:H:8:ILE:HA	2:H:15:PHE:HE2	1.73	0.54
2:H:137:VAL:HG13	2:H:141:ASP:CB	2.38	0.54

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Atom-1	**Atom-2**	**Interatomic distance (Å)**	**Clash overlap (Å)**
2:F:270:ALA:HB3	2:F:328:VAL:HG11	1.89	0.54
1:I:95:LEU:O	1:I:103:GLN:NE2	2.41	0.54
2:J:113:LEU:HD21	2:J:121:ILE:HD11	1.89	0.54
2:J:343:THR:O	2:L:341:GLY:HA3	2.08	0.54
2:L:15:PHE:CD1	2:L:277:ILE:HG13	2.43	0.54
1:A:33:ILE:HD11	1:A:194:LEU:CG	2.38	0.53
2:B:1:MET:HE2	2:B:272:GLY:HA3	1.90	0.53
1:I:141:SER:O	1:I:145:ARG:HG3	2.08	0.53
1:A:49:LYS:HB3	1:A:196:VAL:HG13	1.89	0.53
1:G:141:SER:OG	1:G:144:GLN:HG3	2.08	0.53
2:L:47:ILE:HG13	2:L:213:MET:HE2	1.90	0.53
1:C:171:ASP:OD1	1:C:174:LEU:HD12	2.08	0.53
2:F:194:THR:O	2:F:194:THR:HG22	2.08	0.53
1:G:11:ASN:O	1:G:65:GLY:HA3	2.08	0.53
1:I:82:ARG:HB2	2:J:260:GLY:HA3	1.89	0.53
1:G:15:VAL:H	1:G:63:THR:CG2	2.20	0.53
2:J:80:TRP:HA	2:J:195:ILE:HD12	1.90	0.53
2:L:67:PHE:HD2	2:L:161:TYR:HH	1.54	0.53
1:A:53:LEU:HD21	1:A:164:ASP:HB2	1.91	0.53
1:A:161:LEU:O	1:A:193:THR:HA	2.08	0.53
2:J:302:PHE:CE2	2:J:304:LEU:HD13	2.43	0.53
1:G:95:LEU:HD12	1:G:98:LEU:CD1	2.37	0.53
2:H:36:THR:HG22	2:H:223:LEU:HB3	1.91	0.53
1:I:161:LEU:O	1:I:193:THR:HA	2.07	0.53
2:J:127:LEU:HD23	2:J:167:VAL:HG13	1.89	0.53
2:J:161:TYR:O	2:J:164:THR:OG1	2.23	0.53
1:K:41:ILE:HD13	1:K:52:LEU:HD23	1.90	0.53
2:L:191:GLN:HG2	2:L:192:GLU:H	1.74	0.53
2:F:1:MET:HE2	2:F:272:GLY:HA3	1.91	0.53
2:J:26:THR:HG21	2:J:282:VAL:HG22	1.91	0.53
2:B:97:GLN:HG3	2:B:136:HIS:HB2	1.91	0.53
1:E:108:ASP:OD1	1:E:113:ILE:HD11	2.08	0.53
2:J:55:VAL:HG13	2:J:186:VAL:CG1	2.38	0.53
1:A:40:ALA:O	1:A:209:PHE:HA	2.09	0.53
2:L:56:VAL:HB	2:L:187:LEU:HB2	1.91	0.53
1:A:119:ARG:HH12	1:A:155:MET:HA	1.73	0.52
1:C:107:THR:O	1:C:110:LEU:HG	2.08	0.52
2:D:27:LEU:HD12	2:D:289:GLY:CA	2.39	0.52
2:D:300:VAL:CG1	2:D:301:PRO:HD2	2.40	0.52
1:E:141:SER:O	1:E:145:ARG:HG3	2.09	0.52
1:I:126:ARG:NH2	1:I:184:ASP:OD2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:22:VAL:O	2:J:26:THR:HG23	2.08	0.52
2:F:72:ILE:O	2:F:182:ALA:HB1	2.09	0.52
2:B:52:PRO:HD2	2:B:206:LEU:HD13	1.91	0.52
2:H:27:LEU:HD12	2:H:289:GLY:CA	2.40	0.52
1:K:200:ARG:CA	1:K:203:LEU:HD13	2.39	0.52
2:B:335:ASP:OD1	2:B:336:PRO:HD2	2.09	0.52
2:D:87:GLY:O	2:D:105:MET:HA	2.10	0.52
2:F:328:VAL:O	2:F:328:VAL:HG12	2.10	0.52
1:I:214:ASP:OD1	1:K:171:ASP:HB2	2.10	0.52
1:G:10:THR:HG21	1:K:73:GLU:HG2	1.92	0.52
2:L:18:ILE:HG12	2:L:241:PHE:CD1	2.44	0.52
1:E:127:VAL:HG12	1:E:127:VAL:O	2.10	0.52
1:E:127:VAL:HG13	1:E:181:LEU:CD2	2.40	0.52
1:G:41:ILE:HB	1:G:196:VAL:HG22	1.92	0.52
2:B:53:HIS:CD2	2:B:192:GLU:HA	2.45	0.52
2:D:27:LEU:HD12	2:D:289:GLY:HA2	1.92	0.52
2:L:251:ARG:NH1	2:L:341:GLY:O	2.41	0.51
1:A:55:ILE:CG2	1:A:67:VAL:HG21	2.40	0.51
2:B:239:VAL:HG12	2:D:17:LEU:HD21	1.93	0.51
1:C:118:ASP:O	1:C:122:GLU:HG3	2.10	0.51
2:D:95:SER:HB2	2:D:137:VAL:CG1	2.40	0.51
2:J:98:ASN:HB2	2:J:135:LEU:HA	1.91	0.51
2:B:26:THR:O	2:B:30:VAL:HG23	2.10	0.51
2:B:205:ASP:OD1	2:B:206:LEU:N	2.42	0.51
1:C:127:VAL:HG13	1:C:181:LEU:CD2	2.37	0.51
1:I:180:GLU:HG2	1:I:205:TYR:CE2	2.45	0.51
2:B:278:LEU:HD13	2:B:320:GLY:HA3	1.93	0.51
1:E:108:ASP:OD1	1:E:111:ARG:NH2	2.37	0.51
2:F:109:GLU:HA	2:F:121:ILE:HG22	1.92	0.51
1:A:89:PHE:HD1	2:B:340:LEU:HD23	1.75	0.51
2:B:108:PRO:HD2	2:B:111:THR:HG21	1.91	0.51
1:G:53:LEU:CD2	1:G:164:ASP:HB2	2.41	0.51
2:J:27:LEU:HD12	2:J:289:GLY:HA2	1.93	0.51
2:L:29:ILE:HD11	2:L:230:LEU:CB	2.40	0.51
2:J:55:VAL:CG1	2:J:186:VAL:HG11	2.41	0.51
1:K:127:VAL:O	1:K:147:ARG:HD3	2.10	0.51
1:C:93:ASN:OD1	2:D:251:ARG:NH2	2.36	0.51
2:D:93:ILE:N	2:D:100:ASN:O	2.34	0.51
2:F:241:PHE:CE1	2:H:244:VAL:HG21	2.46	0.51
2:F:253:ILE:HD13	2:F:331:VAL:HG23	1.93	0.51
1:G:52:LEU:HA	1:G:55:ILE:HG22	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:229:PHE:O	2:H:233:ILE:HG13	2.10	0.51
2:B:156:VAL:CG1	2:B:157:LYS:H	2.24	0.51
2:F:236:LEU:HD12	2:H:24:LEU:HD12	1.91	0.51
2:H:27:LEU:HD12	2:H:289:GLY:HA2	1.91	0.51
1:A:44:GLU:HA	1:A:198:HIS:NE2	2.25	0.51
2:B:270:ALA:HB3	2:B:328:VAL:CG1	2.40	0.51
2:F:271:LEU:HD21	2:F:325:THR:CG2	2.42	0.51
1:G:154:LEU:HD11	1:G:185:VAL:HG11	1.93	0.51
2:D:107:LEU:HB3	2:D:108:PRO:HD2	1.92	0.50
2:D:143:ILE:O	2:D:149:THR:HA	2.11	0.50
2:F:270:ALA:CB	2:F:328:VAL:HG11	2.40	0.50
2:J:95:SER:HB3	2:J:135:LEU:HD13	1.91	0.50
2:B:238:THR:O	2:B:242:LEU:HD23	2.10	0.50
1:I:154:LEU:HD11	1:I:185:VAL:CG1	2.37	0.50
1:A:185:VAL:HG13	1:A:189:PHE:HD2	1.77	0.50
2:B:328:VAL:O	2:B:328:VAL:HG12	2.11	0.50
2:D:46:ALA:HB2	2:D:166:VAL:HG21	1.93	0.50
1:K:141:SER:O	1:K:145:ARG:HG3	2.11	0.50
1:K:212:MET:HG2	1:K:217:ALA:HA	1.93	0.50
2:L:191:GLN:HG2	2:L:192:GLU:N	2.26	0.50
2:B:247:LEU:O	2:B:250:THR:HG23	2.11	0.50
1:G:165:GLU:OE2	1:G:198:HIS:NE2	2.45	0.50
1:A:33:ILE:HD11	1:A:194:LEU:HD21	1.93	0.50
1:I:51:THR:O	1:I:55:ILE:HG12	2.11	0.50
1:E:161:LEU:O	1:E:193:THR:HA	2.12	0.50
2:F:116:SER:OG	2:F:159:GLU:OE2	2.30	0.50
2:F:244:VAL:CG1	2:H:244:VAL:HG12	2.39	0.50
2:H:42:GLN:CG	2:H:163:HIS:HA	2.40	0.50
2:H:197:PRO:HB2	2:H:201:GLU:HB2	1.93	0.50
1:I:49:LYS:HE3	1:I:198:HIS:NE2	2.27	0.50
1:I:124:LEU:CD1	1:I:133:GLY:HA2	2.41	0.50
2:J:47:ILE:HG13	2:J:213:MET:CE	2.41	0.50
2:J:233:ILE:O	2:J:237:VAL:HG23	2.11	0.50
2:F:229:PHE:O	2:F:233:ILE:HG13	2.12	0.50
1:I:127:VAL:CG1	1:I:147:ARG:HB3	2.41	0.50
1:K:185:VAL:HG13	1:K:189:PHE:CD2	2.47	0.50
2:B:242:LEU:O	2:B:246:THR:HG23	2.12	0.50
1:C:35:PRO:HB2	1:K:66:THR:HG22	1.93	0.50
1:G:59:LEU:HD23	1:G:81:ARG:HD3	1.94	0.50
2:H:85:PRO:HD2	2:H:108:PRO:CG	2.42	0.50
2:L:26:THR:HG22	2:L:316:ILE:CD1	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:109:GLU:HA	2:L:121:ILE:HG22	1.94	0.50
1:A:55:ILE:HD12	1:A:62:PRO:HG3	1.93	0.50
2:F:105:MET:SD	2:F:166:VAL:HG11	2.52	0.50
2:L:223:LEU:O	2:L:227:GLN:HG3	2.12	0.50
2:D:91:THR:HG21	2:D:177:VAL:CG1	2.41	0.49
2:F:31:MET:SD	2:F:292:LEU:HD23	2.51	0.49
1:A:44:GLU:HA	1:A:198:HIS:HE2	1.76	0.49
1:C:49:LYS:HB3	1:C:196:VAL:CG1	2.43	0.49
2:D:46:ALA:CB	2:D:166:VAL:HG21	2.41	0.49
2:J:300:VAL:HG13	2:J:301:PRO:HD2	1.94	0.49
1:A:127:VAL:HG21	1:A:151:ALA:HB2	1.94	0.49
2:B:32:LEU:O	2:B:36:THR:HG23	2.11	0.49
1:E:78:THR:HA	1:E:81:ARG:CZ	2.42	0.49
1:E:42:VAL:CG2	1:E:203:LEU:HD21	2.41	0.49
2:F:36:THR:CG2	2:F:223:LEU:HB3	2.42	0.49
2:H:49:ALA:O	2:H:114:PRO:HB3	2.11	0.49
2:H:79:ARG:HH22	2:H:198:GLN:CD	2.15	0.49
1:I:127:VAL:HG12	1:I:127:VAL:O	2.11	0.49
2:L:271:LEU:HD21	2:L:325:THR:HG22	1.94	0.49
1:A:49:LYS:HB3	1:A:196:VAL:CG1	2.42	0.49
2:B:2:PHE:O	2:B:6:ARG:NH1	2.44	0.49
2:L:95:SER:OG	2:L:135:LEU:HD22	2.12	0.49
1:A:127:VAL:HG11	1:A:147:ARG:O	2.13	0.49
2:B:239:VAL:HG22	2:B:323:GLY:O	2.11	0.49
2:H:328:VAL:HG12	2:H:328:VAL:O	2.11	0.49
2:F:125:ALA:CA	2:F:169:VAL:HG12	2.39	0.49
2:F:304:LEU:HD21	2:F:309:VAL:HG21	1.95	0.49
1:K:108:ASP:OD1	1:K:113:ILE:HD11	2.12	0.49
2:F:31:MET:O	2:F:302:PHE:HE1	1.95	0.49
2:H:125:ALA:CB	2:H:169:VAL:HG12	2.43	0.49
1:I:18:ASP:OD2	1:K:141:SER:HB2	2.12	0.49
2:L:300:VAL:HG13	2:L:301:PRO:HD2	1.94	0.49
1:C:42:VAL:HG21	1:C:203:LEU:HD11	1.94	0.49
2:D:100:ASN:OD1	2:D:101:THR:N	2.41	0.49
2:H:145:LEU:HG	2:H:177:VAL:HG11	1.95	0.49
1:A:9:ILE:O	1:A:30:ASN:HA	2.13	0.48
1:E:53:LEU:CD2	1:E:164:ASP:HB2	2.43	0.48
2:J:108:PRO:HD2	2:J:111:THR:HG21	1.94	0.48
1:I:198:HIS:O	1:K:198:HIS:HE1	1.96	0.48
1:K:41:ILE:HD11	1:K:194:LEU:HD22	1.95	0.48
1:A:33:ILE:HD11	1:A:194:LEU:CD2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:198:GLN:HG2	2:D:199:ASP:N	2.28	0.48
2:F:290:ALA:HA	2:F:304:LEU:HD11	1.94	0.48
1:A:129:LEU:HD22	1:A:132:LEU:HD12	1.96	0.48
2:B:156:VAL:CG1	2:B:157:LYS:N	2.73	0.48
2:B:317:TRP:CZ3	2:B:321:LEU:HD11	2.48	0.48
2:F:47:ILE:HD12	2:F:213:MET:CE	2.44	0.48
2:F:107:LEU:HB3	2:F:108:PRO:HD2	1.95	0.48
2:H:300:VAL:CG1	2:H:301:PRO:HD2	2.43	0.48
2:J:21:VAL:CG1	2:J:237:VAL:HG11	2.44	0.48
2:B:15:PHE:HB3	2:B:277:ILE:HD12	1.96	0.48
2:F:8:ILE:HA	2:F:15:PHE:CE2	2.48	0.48
2:F:241:PHE:HD2	2:F:242:LEU:HD22	1.78	0.48
1:K:37:GLU:HA	1:K:207:ASP:OD2	2.14	0.48
1:K:49:LYS:HB3	1:K:196:VAL:HG13	1.96	0.48
1:K:129:LEU:HD11	1:K:147:ARG:HB2	1.95	0.48
1:C:185:VAL:HG13	1:C:189:PHE:CD2	2.47	0.48
1:E:41:ILE:HG22	1:E:49:LYS:HB3	1.96	0.48
2:F:239:VAL:O	2:F:243:THR:HG23	2.14	0.48
2:J:112:PRO:HA	2:J:120:PHE:CD1	2.48	0.48
2:J:328:VAL:HG12	2:J:328:VAL:O	2.14	0.48
2:D:8:ILE:HG12	2:D:15:PHE:CE2	2.49	0.48
2:F:8:ILE:HA	2:F:15:PHE:CD2	2.49	0.48
2:F:128:PRO:HG2	2:F:131:LEU:HB3	1.96	0.48
1:K:59:LEU:CD1	2:L:340:LEU:HD11	2.44	0.48
2:B:36:THR:HG22	2:B:223:LEU:CB	2.41	0.48
1:G:59:LEU:HD13	2:H:340:LEU:HD11	1.93	0.48
2:J:290:ALA:HB2	2:J:309:VAL:HG21	1.94	0.48
2:L:26:THR:OG1	2:L:285:GLY:HA3	2.14	0.48
1:A:53:LEU:CD1	1:A:162:LEU:HB3	2.34	0.48
1:I:185:VAL:HG13	1:I:189:PHE:CE2	2.49	0.48
2:J:34:GLY:HA3	2:J:302:PHE:CE1	2.49	0.48
2:J:55:VAL:HG13	2:J:186:VAL:HG11	1.96	0.48
2:J:186:VAL:CG1	2:J:187:LEU:N	2.77	0.48
1:K:78:THR:HG23	1:K:81:ARG:NH2	2.29	0.48
1:C:53:LEU:CD2	1:C:164:ASP:HB2	2.44	0.47
2:H:183:VAL:HG12	2:H:183:VAL:O	2.14	0.47
1:I:18:ASP:HB2	1:I:23:VAL:CG2	2.43	0.47
2:J:108:PRO:O	2:J:111:THR:HG23	2.14	0.47
2:L:54:SER:HB3	2:L:203:VAL:CG1	2.43	0.47
1:E:175:SER:O	1:E:179:VAL:HG23	2.14	0.47
1:I:165:GLU:HG2	1:I:197:THR:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:53:HIS:HB2	2:J:190:ASN:O	2.13	0.47
2:J:141:ASP:O	2:J:152:VAL:HG23	2.13	0.47
1:K:59:LEU:HD13	2:L:340:LEU:HD11	1.95	0.47
2:B:25:ILE:HG21	2:B:234:SER:HB3	1.95	0.47
2:F:1:MET:CE	2:F:272:GLY:HA3	2.44	0.47
2:F:127:LEU:O	2:F:155:THR:HA	2.15	0.47
2:H:112:PRO:HA	2:H:120:PHE:CD1	2.48	0.47
1:I:135:ARG:NH2	1:I:139:GLN:O	2.46	0.47
1:I:203:LEU:HD22	1:I:209:PHE:CE1	2.50	0.47
2:L:245:TRP:NE1	2:L:273:GLN:OE1	2.47	0.47
1:K:33:ILE:HD11	1:K:194:LEU:CG	2.45	0.47
1:C:127:VAL:HG11	1:C:147:ARG:O	2.14	0.47
2:D:183:VAL:HG12	2:D:183:VAL:O	2.14	0.47
2:B:233:ILE:O	2:B:237:VAL:HG23	2.14	0.47
2:D:125:ALA:CA	2:D:169:VAL:HG12	2.40	0.47
2:B:241:PHE:HD2	2:B:242:LEU:HD22	1.80	0.47
1:C:26:LEU:HD22	1:C:55:ILE:HD12	1.96	0.47
1:E:118:ASP:O	1:E:122:GLU:HG3	2.15	0.47
1:E:171:ASP:OD1	1:E:174:LEU:HB2	2.14	0.47
2:F:8:ILE:HG12	2:F:15:PHE:CD2	2.49	0.47
2:J:29:ILE:CG1	2:J:230:LEU:HB3	2.45	0.47
2:J:194:THR:HG22	2:J:194:THR:O	2.15	0.47
2:J:253:ILE:HD13	2:J:331:VAL:HG13	1.97	0.47
2:L:245:TRP:O	2:L:249:ARG:HG3	2.14	0.47
1:A:98:LEU:HD11	1:A:106:ILE:HD12	1.97	0.47
2:H:122:GLU:OE1	2:H:153:ALA:HB1	2.13	0.47
2:J:95:SER:OG	2:J:135:LEU:HB3	2.15	0.47
2:F:15:PHE:HA	2:F:18:ILE:HG22	1.97	0.47
2:F:34:GLY:HA3	2:F:302:PHE:CZ	2.50	0.47
1:G:6:VAL:CG2	1:G:35:PRO:HG3	2.45	0.47
2:H:242:LEU:O	2:H:246:THR:HG23	2.15	0.47
1:I:127:VAL:HG11	1:I:147:ARG:O	2.14	0.47
2:J:127:LEU:O	2:J:155:THR:HA	2.14	0.47
2:L:108:PRO:O	2:L:111:THR:HG23	2.15	0.47
2:B:24:LEU:HD12	2:D:236:LEU:HD12	1.97	0.47
2:B:100:ASN:OD1	2:B:101:THR:N	2.47	0.47
2:B:170:ASP:OD2	2:B:172:ALA:HB3	2.15	0.47
2:L:194:THR:HG22	2:L:194:THR:O	2.15	0.47
1:C:180:GLU:HG2	1:C:205:TYR:CE2	2.49	0.46
1:I:163:ALA:O	1:I:195:MET:HA	2.15	0.46
2:B:21:VAL:CG2	2:D:236:LEU:HB3	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:161:TYR:O	2:D:164:THR:OG1	2.33	0.46
2:L:1:MET:HE3	2:L:5:ILE:HD11	1.97	0.46
2:L:128:PRO:HG2	2:L:131:LEU:HB3	1.97	0.46
2:B:145:LEU:HD23	2:B:177:VAL:HG21	1.98	0.46
2:D:247:LEU:O	2:D:250:THR:HG23	2.14	0.46
2:F:128:PRO:HG2	2:F:131:LEU:CB	2.45	0.46
2:F:245:TRP:NE1	2:F:273:GLN:OE1	2.40	0.46
1:G:7:LEU:HD21	1:G:56:ALA:HB1	1.96	0.46
2:H:15:PHE:HA	2:H:18:ILE:HG22	1.97	0.46
2:H:36:THR:HG21	2:H:223:LEU:HB3	1.97	0.46
2:J:88:VAL:HG11	2:J:161:TYR:CE2	2.49	0.46
2:J:335:ASP:OD1	2:J:338:ILE:HG13	2.14	0.46
1:E:42:VAL:HG12	1:E:43:GLY:N	2.30	0.46
2:J:103:ALA:HB2	2:J:164:THR:OG1	2.16	0.46
2:L:290:ALA:HB2	2:L:309:VAL:HG21	1.97	0.46
2:F:8:ILE:HG12	2:F:15:PHE:CE2	2.51	0.46
2:B:253:ILE:HG22	2:B:334:VAL:HG11	1.97	0.46
2:D:102:THR:HG21	2:D:131:LEU:HD22	1.97	0.46
2:F:87:GLY:O	2:F:105:MET:HA	2.15	0.46
1:I:53:LEU:HD21	1:I:164:ASP:HB2	1.96	0.46
1:C:6:VAL:CG2	1:C:35:PRO:HG3	2.45	0.46
1:C:99:THR:OG1	1:C:102:GLU:HG3	2.16	0.46
1:E:38:LEU:HD21	1:E:195:MET:HE1	1.97	0.46
2:H:18:ILE:HD13	2:H:241:PHE:CD1	2.51	0.46
2:H:47:ILE:HD12	2:H:213:MET:HE2	1.97	0.46
2:J:21:VAL:HG11	2:J:237:VAL:HG11	1.98	0.46
2:J:80:TRP:HH2	2:J:201:GLU:CD	2.19	0.46
2:D:1:MET:HE1	2:D:272:GLY:HA3	1.97	0.46
2:F:95:SER:CB	2:F:135:LEU:HB3	2.45	0.46
1:G:58:PHE:O	1:G:81:ARG:NH1	2.48	0.46
1:K:163:ALA:HB1	1:K:166:PRO:HG3	1.98	0.46
2:L:1:MET:CE	2:L:5:ILE:HD11	2.45	0.46
2:B:26:THR:HG22	2:B:316:ILE:HD13	1.97	0.46
2:B:72:ILE:O	2:B:182:ALA:HB1	2.16	0.46
1:I:14:VAL:CG2	1:I:55:ILE:HD11	2.45	0.46
2:J:271:LEU:HD21	2:J:325:THR:HG22	1.98	0.46
2:J:334:VAL:HG13	2:J:334:VAL:O	2.16	0.46
1:K:118:ASP:O	1:K:122:GLU:HG3	2.16	0.46
1:A:154:LEU:CD1	1:A:185:VAL:HG11	2.44	0.46
1:I:149:ASN:ND2	1:I:152:ARG:HH21	2.13	0.46
2:J:245:TRP:O	2:J:249:ARG:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:21:SER:OG	1:K:22:THR:N	2.49	0.46
1:E:41:ILE:CG2	1:E:49:LYS:HB3	2.46	0.45
2:F:100:ASN:OD1	2:F:101:THR:N	2.48	0.45
2:H:46:ALA:HB2	2:H:166:VAL:HG21	1.98	0.45
1:I:129:LEU:HD11	1:I:147:ARG:HB2	1.98	0.45
1:I:198:HIS:HB3	1:K:198:HIS:ND1	2.31	0.45
1:K:33:ILE:CG2	1:K:192:ALA:HB1	2.46	0.45
1:A:55:ILE:HD13	1:A:60:GLN:O	2.16	0.45
1:C:26:LEU:HD23	1:C:55:ILE:HD12	1.97	0.45
1:G:185:VAL:HG13	1:G:189:PHE:HD2	1.81	0.45
1:C:90:GLN:HA	1:C:164:ASP:O	2.16	0.45
1:C:41:ILE:HG13	1:C:194:LEU:HD11	1.97	0.45
2:D:47:ILE:HD12	2:D:213:MET:HE3	1.99	0.45
1:E:26:LEU:HD22	1:E:55:ILE:HD12	1.98	0.45
1:E:185:VAL:HG13	1:E:189:PHE:CD1	2.52	0.45
1:G:149:ASN:ND2	1:G:152:ARG:HH21	2.15	0.45
1:G:210:VAL:CG1	1:G:217:ALA:HB1	2.46	0.45
1:C:106:ILE:HD13	2:D:256:LEU:HD21	1.98	0.45
2:D:229:PHE:O	2:D:233:ILE:HG13	2.17	0.45
1:E:111:ARG:HH12	1:E:113:ILE:CD1	2.29	0.45
2:H:53:HIS:N	2:H:189:LEU:O	2.49	0.45
1:K:14:VAL:HG21	1:K:55:ILE:HD11	1.96	0.45
2:L:27:LEU:HD12	2:L:289:GLY:CA	2.46	0.45
2:L:55:VAL:HG13	2:L:204:THR:HG22	1.98	0.45
1:A:14:VAL:CG2	1:A:55:ILE:HD11	2.47	0.45
2:D:246:THR:HG21	2:D:328:VAL:HG22	1.99	0.45
2:J:337:GLN:HG3	2:J:337:GLN:O	2.17	0.45
2:L:11:ALA:O	2:L:15:PHE:HD2	1.98	0.45
1:A:82:ARG:HB2	2:B:260:GLY:HA3	1.99	0.45
1:K:125:ALA:CB	1:K:130:LYS:HB2	2.47	0.45
2:L:55:VAL:HG13	2:L:204:THR:CG2	2.46	0.45
2:F:55:VAL:HG13	2:F:204:THR:CG2	2.47	0.45
2:F:86:LEU:O	2:F:185:THR:N	2.39	0.45
2:F:170:ASP:OD2	2:F:172:ALA:HB3	2.17	0.45
2:H:18:ILE:HD13	2:H:241:PHE:CG	2.52	0.45
2:H:94:GLU:CG	2:H:99:ALA:HB2	2.38	0.45
2:J:245:TRP:NE1	2:J:273:GLN:OE1	2.50	0.45
2:F:22:VAL:O	2:F:26:THR:HG23	2.17	0.45
2:F:300:VAL:CG1	2:F:301:PRO:HD2	2.47	0.45
1:G:68:THR:HG21	1:K:71:GLY:HA2	1.97	0.45
1:A:82:ARG:NH1	2:B:260:GLY:O	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LEU:HD22	1:A:115:PRO:HB3	1.99	0.45
2:F:304:LEU:C	2:F:304:LEU:HD23	2.37	0.45
2:J:128:PRO:HG2	2:J:131:LEU:HB3	1.99	0.45
1:K:171:ASP:OD1	1:K:174:LEU:HB2	2.17	0.45
1:A:42:VAL:HG21	1:A:203:LEU:HD11	1.98	0.44
2:D:109:GLU:HA	2:D:121:ILE:HG22	1.98	0.44
1:E:5:PRO:HB3	1:E:34:PHE:CE2	2.53	0.44
2:H:100:ASN:OD1	2:H:101:THR:N	2.47	0.44
2:J:245:TRP:NE1	2:J:249:ARG:HD2	2.32	0.44
2:L:22:VAL:O	2:L:26:THR:HG23	2.17	0.44
1:A:59:LEU:HD23	1:A:81:ARG:HD3	1.98	0.44
1:A:132:LEU:HD22	1:A:135:ARG:CZ	2.47	0.44
2:F:32:LEU:HD13	2:H:226:MET:HE2	1.99	0.44
2:H:102:THR:OG1	2:H:165:PRO:O	2.35	0.44
2:L:328:VAL:O	2:L:328:VAL:HG12	2.16	0.44
1:A:167:THR:HB	1:A:175:SER:CB	2.46	0.44
2:B:88:VAL:HG11	2:B:161:TYR:CZ	2.52	0.44
2:F:107:LEU:O	2:F:171:THR:N	2.51	0.44
2:F:242:LEU:O	2:F:246:THR:HG23	2.17	0.44
2:L:334:VAL:HG13	2:L:334:VAL:O	2.17	0.44
1:A:44:GLU:OE1	1:A:198:HIS:NE2	2.39	0.44
1:A:99:THR:HG22	1:A:136:ARG:HG2	2.00	0.44
1:C:41:ILE:CG1	1:C:194:LEU:HD11	2.47	0.44
2:D:207:LYS:HA	2:D:210:PHE:CD2	2.52	0.44
2:H:55:VAL:HG13	2:H:204:THR:CG2	2.48	0.44
1:I:116:ARG:CZ	1:I:119:ARG:HD3	2.47	0.44
1:I:203:LEU:HD13	1:I:223:LEU:HD22	2.00	0.44
1:C:33:ILE:CD1	1:C:194:LEU:HB2	2.47	0.44
2:D:2:PHE:O	2:D:6:ARG:NH1	2.49	0.44
2:D:255:VAL:O	2:D:259:LEU:HG	2.18	0.44
1:E:165:GLU:HG3	1:E:196:VAL:HG12	2.00	0.44
1:K:124:LEU:CD1	1:K:133:GLY:HA2	2.47	0.44
1:A:118:ASP:O	1:A:122:GLU:HG3	2.17	0.44
2:B:31:MET:CE	2:B:292:LEU:HB2	2.47	0.44
2:F:243:THR:HG23	2:F:327:ALA:CB	2.47	0.44
2:J:87:GLY:HA2	2:J:185:THR:HG22	2.00	0.44
2:J:98:ASN:HB3	2:J:135:LEU:HD23	1.99	0.44
2:L:25:ILE:HG21	2:L:234:SER:HB3	2.00	0.44
1:A:15:VAL:H	1:A:63:THR:HG21	1.83	0.44
2:B:87:GLY:O	2:B:105:MET:HA	2.18	0.44
1:C:23:VAL:O	1:C:23:VAL:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:172:ALA:O	1:C:176:LYS:HG3	2.17	0.44
2:F:88:VAL:HB	2:F:185:THR:HG21	1.98	0.44
2:L:72:ILE:HG13	2:L:187:LEU:HG	2.00	0.44
2:L:185:THR:HG23	2:L:186:VAL:HG13	2.00	0.44
1:E:195:MET:HG2	1:E:197:THR:HG23	2.00	0.44
2:F:263:LYS:HD3	2:F:332:THR:CG2	2.48	0.44
1:G:52:LEU:C	1:G:55:ILE:HG22	2.38	0.44
2:L:192:GLU:HG3	2:L:193:PRO:HD2	1.99	0.44
1:A:199:ASP:HB2	1:C:44:GLU:OE2	2.18	0.44
2:B:300:VAL:CG1	2:B:301:PRO:HD2	2.48	0.44
1:C:105:LEU:HB3	1:C:115:PRO:HB3	1.99	0.44
1:C:126:ARG:HH22	1:C:184:ASP:HB3	1.83	0.44
1:G:110:LEU:HA	2:H:265:TYR:CE2	2.53	0.44
2:H:128:PRO:HG2	2:H:131:LEU:HB2	1.99	0.44
1:I:107:THR:O	1:I:111:ARG:HG3	2.18	0.44
2:J:72:ILE:HG13	2:J:187:LEU:HG	2.00	0.44
1:K:33:ILE:HD11	1:K:194:LEU:HD21	1.99	0.44
2:L:242:LEU:HD11	2:L:274:ALA:HB1	2.00	0.44
1:E:53:LEU:HD21	1:E:164:ASP:HB2	2.00	0.43
3:F:401:HEM:CBC	2:H:223:LEU:HD21	2.48	0.43
1:G:150:ILE:HD11	1:G:178:ILE:HG23	2.00	0.43
1:I:126:ARG:HH22	1:I:184:ASP:CG	2.21	0.43
1:K:42:VAL:HG21	1:K:203:LEU:HD21	1.99	0.43
1:I:42:VAL:HG12	1:I:43:GLY:N	2.33	0.43
1:K:154:LEU:HD21	1:K:185:VAL:CG1	2.45	0.43
2:B:109:GLU:HA	2:B:121:ILE:HG22	2.00	0.43
2:B:116:SER:OG	2:B:159:GLU:OE2	2.35	0.43
2:B:198:GLN:HG2	2:B:199:ASP:N	2.33	0.43
2:F:198:GLN:HG2	2:F:199:ASP:N	2.32	0.43
1:G:129:LEU:HD11	1:G:147:ARG:HB2	1.99	0.43
1:E:15:VAL:CG2	1:E:24:THR:HG22	2.43	0.43
1:G:9:ILE:HG23	1:G:67:VAL:HG22	2.00	0.43
1:I:70:HIS:HA	1:I:73:GLU:OE2	2.18	0.43
2:J:56:VAL:CG2	2:J:189:LEU:HD11	2.49	0.43
2:L:27:LEU:HD12	2:L:289:GLY:HA2	2.00	0.43
2:L:54:SER:HB3	2:L:203:VAL:HG13	1.99	0.43
1:A:107:THR:O	1:A:110:LEU:HG	2.19	0.43
2:B:185:THR:HG23	2:B:186:VAL:HG22	2.01	0.43
2:D:126:LEU:HB3	2:D:156:VAL:CG2	2.49	0.43
2:D:334:VAL:HG13	2:D:334:VAL:O	2.17	0.43
2:F:243:THR:HG23	2:F:327:ALA:HB1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:239:VAL:O	2:H:243:THR:HG23	2.18	0.43
1:I:72:ALA:HB2	1:I:84:HIS:CD2	2.53	0.43
1:I:165:GLU:CG	1:I:197:THR:HA	2.49	0.43
2:J:27:LEU:HD12	2:J:289:GLY:CA	2.49	0.43
1:K:132:LEU:HD13	1:K:135:ARG:NE	2.34	0.43
2:D:300:VAL:HG13	2:D:301:PRO:HD2	1.99	0.43
2:F:29:ILE:HD13	2:F:231:TYR:HD1	1.82	0.43
2:F:95:SER:HB2	2:F:135:LEU:HB3	1.99	0.43
2:F:245:TRP:O	2:F:248:GLN:HB3	2.19	0.43
1:G:42:VAL:HG12	1:G:43:GLY:N	2.34	0.43
1:A:105:LEU:HB3	1:A:115:PRO:HB3	2.00	0.43
2:B:15:PHE:HA	2:B:18:ILE:HG22	1.99	0.43
1:C:167:THR:HB	1:C:175:SER:HB3	2.01	0.43
2:F:244:VAL:HG12	2:H:244:VAL:CG1	2.44	0.43
2:H:86:LEU:HD21	2:H:105:MET:CE	2.49	0.43
1:K:210:VAL:CG1	1:K:217:ALA:HB1	2.49	0.43
2:L:68:THR:O	2:L:68:THR:HG22	2.19	0.43
2:L:127:LEU:HD23	2:L:167:VAL:HG13	2.01	0.43
1:A:72:ALA:HB2	1:A:84:HIS:CD2	2.53	0.43
1:C:6:VAL:HG23	1:C:35:PRO:HG3	2.00	0.43
1:C:42:VAL:HG12	1:C:43:GLY:N	2.33	0.43
1:C:129:LEU:HD22	1:C:132:LEU:HD12	2.00	0.43
2:D:94:GLU:HA	2:D:99:ALA:CB	2.49	0.43
1:E:15:VAL:HG13	1:E:24:THR:HG22	2.00	0.43
1:E:99:THR:O	1:E:103:GLN:HG2	2.18	0.43
2:J:185:THR:HG23	2:J:186:VAL:HG23	2.01	0.43
2:B:15:PHE:CD1	2:B:277:ILE:HG13	2.54	0.42
2:D:94:GLU:N	2:D:144:THR:O	2.41	0.42
2:F:236:LEU:HB3	2:H:21:VAL:CG2	2.49	0.42
2:J:1:MET:HE1	2:J:5:ILE:HD11	2.00	0.42
2:J:57:PHE:CE1	2:J:204:THR:HG21	2.53	0.42
2:L:55:VAL:HG13	2:L:57:PHE:HE1	1.84	0.42
1:E:38:LEU:HD21	1:E:195:MET:CE	2.49	0.42
2:F:94:GLU:HG3	2:F:99:ALA:HB2	1.99	0.42
2:J:75:GLN:OE1	2:J:75:GLN:N	2.48	0.42
2:J:135:LEU:HB2	2:J:137:VAL:HG22	2.01	0.42
2:L:79:ARG:NH1	2:L:198:GLN:HB2	2.32	0.42
1:A:198:HIS:O	1:A:198:HIS:ND1	2.52	0.42
2:B:72:ILE:HG13	2:B:187:LEU:HG	2.01	0.42
2:D:219:GLU:HG3	3:D:401:HEM:CHC	2.50	0.42
2:J:197:PRO:HB2	2:J:201:GLU:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:44:THR:HG22	2:L:213:MET:SD	2.60	0.42
2:B:27:LEU:HD12	2:B:289:GLY:CA	2.49	0.42
2:B:86:LEU:HD22	2:B:188:LEU:HD11	2.01	0.42
2:B:253:ILE:HG21	2:B:331:VAL:HG23	2.01	0.42
2:D:33:THR:HG21	2:D:312:PRO:HG2	2.01	0.42
2:D:56:VAL:O	2:D:186:VAL:HG13	2.19	0.42
2:D:277:ILE:HD13	2:D:277:ILE:HA	1.91	0.42
1:E:16:TYR:CD2	1:E:18:ASP:OD1	2.72	0.42
2:H:317:TRP:CH2	2:H:321:LEU:HD11	2.54	0.42
1:I:6:VAL:CG2	1:I:35:PRO:HG3	2.49	0.42
1:C:33:ILE:HD11	1:C:194:LEU:HD13	2.01	0.42
2:D:239:VAL:O	2:D:243:THR:HG23	2.20	0.42
1:E:132:LEU:HD22	1:E:135:ARG:CZ	2.48	0.42
1:G:210:VAL:HG13	1:G:217:ALA:HB1	2.01	0.42
1:I:154:LEU:HD21	1:I:185:VAL:HG11	2.00	0.42
2:L:229:PHE:O	2:L:233:ILE:HG13	2.19	0.42
1:E:6:VAL:HG23	1:E:35:PRO:HG3	2.00	0.42
2:F:53:HIS:HB3	2:F:189:LEU:O	2.20	0.42
1:G:59:LEU:HD23	1:G:81:ARG:CD	2.50	0.42
2:J:247:LEU:HD23	2:J:247:LEU:HA	1.90	0.42
2:D:92:ARG:HA	2:D:101:THR:HA	2.02	0.42
2:F:223:LEU:O	2:F:227:GLN:HG3	2.19	0.42
2:H:31:MET:HA	2:H:302:PHE:HE2	1.84	0.42
2:J:41:LYS:NZ	2:J:48:GLU:OE1	2.47	0.42
2:L:258:ALA:HA	2:L:336:PRO:HB2	2.00	0.42
2:D:88:VAL:HB	2:D:185:THR:HG21	2.02	0.42
2:F:125:ALA:CB	2:F:169:VAL:HG12	2.50	0.42
1:E:14:VAL:H	1:E:26:LEU:HB3	1.84	0.42
1:G:107:THR:O	1:G:110:LEU:HG	2.19	0.42
2:H:338:ILE:HG22	2:H:338:ILE:O	2.20	0.42
1:I:44:GLU:OE1	1:K:199:ASP:OD1	2.38	0.42
1:I:53:LEU:CD2	1:I:164:ASP:HB2	2.50	0.42
1:K:94:LEU:HB3	1:K:103:GLN:NE2	2.34	0.42
1:K:161:LEU:O	1:K:193:THR:HA	2.20	0.42
1:A:181:LEU:O	1:A:185:VAL:HG23	2.19	0.42
2:D:87:GLY:O	2:D:106:GLY:N	2.44	0.42
2:F:32:LEU:HD13	2:H:226:MET:HE1	2.00	0.42
2:F:77:ALA:HB2	2:F:183:VAL:HG21	2.02	0.42
2:L:43:ASN:HD22	2:L:216:TYR:HA	1.85	0.42
1:A:42:VAL:HG12	1:A:43:GLY:N	2.35	0.41
1:A:150:ILE:HD11	1:A:178:ILE:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:LEU:HD11	1:E:106:ILE:HD12	2.02	0.41
2:F:29:ILE:HD11	2:F:230:LEU:HB3	2.01	0.41
2:F:56:VAL:HB	2:F:187:LEU:HB2	2.02	0.41
2:F:334:VAL:O	2:F:334:VAL:HG13	2.19	0.41
1:G:154:LEU:HD21	1:G:185:VAL:HG11	2.02	0.41
1:I:202:GLN:OE1	1:I:202:GLN:HA	2.20	0.41
2:J:11:ALA:O	2:J:15:PHE:HD2	2.02	0.41
2:J:105:MET:SD	2:J:166:VAL:HG11	2.60	0.41
2:D:103:ALA:HB2	2:D:164:THR:OG1	2.20	0.41
2:F:302:PHE:HE2	2:F:304:LEU:HB2	1.83	0.41
1:I:200:ARG:HG2	1:I:203:LEU:HD11	2.02	0.41
2:L:2:PHE:O	2:L:6:ARG:NH1	2.53	0.41
1:A:15:VAL:H	1:A:63:THR:CG2	2.33	0.41
1:A:101:ARG:HD3	1:A:121:ASP:OD1	2.21	0.41
2:D:231:TYR:OH	2:D:312:PRO:HB3	2.20	0.41
1:E:82:ARG:NH1	2:F:260:GLY:O	2.49	0.41
1:G:160:LEU:HD12	1:G:192:ALA:O	2.20	0.41
1:I:6:VAL:HG23	1:I:35:PRO:HG3	2.01	0.41
2:J:36:THR:CG2	2:J:223:LEU:HB3	2.50	0.41
1:K:39:VAL:HG22	1:K:208:ARG:HG3	2.01	0.41
1:K:154:LEU:HD11	1:K:185:VAL:HG11	2.01	0.41
2:B:21:VAL:HG22	2:D:236:LEU:HB3	2.02	0.41
2:B:108:PRO:O	2:B:111:THR:HG23	2.20	0.41
1:C:42:VAL:HG11	1:C:200:ARG:HE	1.83	0.41
1:E:40:ALA:O	1:E:209:PHE:HA	2.21	0.41
2:L:31:MET:HE1	2:L:292:LEU:HB3	2.03	0.41
2:L:41:LYS:O	2:L:45:SER:HB3	2.21	0.41
2:L:113:LEU:HD21	2:L:121:ILE:CD1	2.46	0.41
1:E:129:LEU:CD2	1:E:132:LEU:HD12	2.46	0.41
1:I:141:SER:OG	1:K:18:ASP:OD2	2.38	0.41
1:K:110:LEU:HD12	1:K:111:ARG:HD3	2.01	0.41
1:E:33:ILE:CG2	1:E:192:ALA:HB1	2.50	0.41
2:F:60:ALA:HB1	2:H:97:GLN:O	2.21	0.41
2:F:332:THR:O	2:F:332:THR:HG22	2.21	0.41
1:G:127:VAL:O	1:G:147:ARG:HD3	2.21	0.41
1:G:127:VAL:HG12	1:G:147:ARG:HD3	2.02	0.41
2:H:47:ILE:HD12	2:H:213:MET:HE3	2.03	0.41
2:J:55:VAL:CG1	2:J:186:VAL:CG1	2.98	0.41
2:J:277:ILE:HD13	2:J:277:ILE:HA	1.90	0.41
1:K:127:VAL:CG1	1:K:127:VAL:O	2.69	0.41
1:A:198:HIS:ND1	1:C:198:HIS:CE1	2.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:98:ASN:HB2	2:B:135:LEU:HA	2.03	0.41
2:D:88:VAL:HG22	2:D:105:MET:HG2	2.01	0.41
2:D:126:LEU:HB3	2:D:156:VAL:HG23	2.02	0.41
2:F:249:ARG:HB2	2:F:253:ILE:HD11	2.02	0.41
1:G:58:PHE:CE2	1:G:80:THR:HG21	2.56	0.41
1:I:18:ASP:HB3	1:I:23:VAL:HG23	2.02	0.41
2:J:98:ASN:CB	2:J:135:LEU:HD23	2.51	0.41
2:B:117:VAL:O	2:B:156:VAL:HG13	2.21	0.41
2:B:328:VAL:O	2:B:328:VAL:CG1	2.69	0.41
1:E:104:LEU:O	1:E:155:MET:HG2	2.21	0.41
2:F:253:ILE:HG21	2:F:331:VAL:HG23	2.02	0.41
1:I:163:ALA:HB1	1:I:166:PRO:HG3	2.02	0.41
1:I:167:THR:HB	1:I:175:SER:CB	2.45	0.41
1:K:11:ASN:O	1:K:65:GLY:HA3	2.20	0.41
1:A:16:TYR:HE1	1:A:60:GLN:NE2	2.10	0.41
2:B:244:VAL:HG12	2:D:244:VAL:HG22	2.03	0.41
2:B:300:VAL:HG13	2:B:301:PRO:HD2	2.03	0.41
1:C:105:LEU:HD22	1:C:115:PRO:CB	2.51	0.41
1:C:109:HIS:ND1	2:D:265:TYR:HE2	2.19	0.41
2:D:93:ILE:HD11	2:D:143:ILE:HD12	2.03	0.41
1:G:104:LEU:HD23	1:G:152:ARG:HA	2.03	0.41
2:L:72:ILE:O	2:L:182:ALA:HB1	2.21	0.41
2:L:192:GLU:CG	2:L:193:PRO:HD2	2.51	0.41
2:L:247:LEU:HD23	2:L:247:LEU:HA	1.86	0.41
2:B:53:HIS:N	2:B:189:LEU:O	2.53	0.41
1:C:33:ILE:HG22	1:C:192:ALA:HB1	2.01	0.41
1:G:212:MET:SD	1:G:217:ALA:HB2	2.60	0.41
1:I:17:PRO:HA	1:I:22:THR:HA	2.03	0.41
2:J:300:VAL:HG12	2:J:301:PRO:HD2	2.03	0.41
1:K:176:LYS:HE3	1:K:205:TYR:OH	2.21	0.41
2:J:57:PHE:CD2	2:J:65:PRO:HB2	2.56	0.40
1:K:107:THR:O	1:K:110:LEU:HG	2.21	0.40
1:K:107:THR:HG21	1:K:152:ARG:HG3	2.02	0.40
2:L:26:THR:HG21	2:L:282:VAL:HA	2.01	0.40
1:A:82:ARG:CG	1:A:111:ARG:HG2	2.51	0.40
1:C:109:HIS:ND1	2:D:2:PHE:HB2	2.36	0.40
2:F:28:LEU:HD11	2:H:226:MET:HG3	2.02	0.40
2:F:33:THR:HA	2:F:227:GLN:OE1	2.20	0.40
2:F:302:PHE:HE2	2:F:304:LEU:CD1	2.25	0.40
2:H:24:LEU:HD23	2:H:24:LEU:HA	1.96	0.40
2:H:255:VAL:O	2:H:259:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:26:LEU:HD11	1:I:29:ALA:HB2	2.03	0.40
2:J:2:PHE:O	2:J:6:ARG:NH1	2.55	0.40
2:J:100:ASN:OD1	2:J:101:THR:N	2.51	0.40
1:E:179:VAL:HG21	1:E:202:GLN:HG2	2.04	0.40
2:H:300:VAL:HG13	2:H:301:PRO:HD2	2.04	0.40
1:K:42:VAL:HG12	1:K:43:GLY:N	2.36	0.40
1:K:132:LEU:HD13	1:K:135:ARG:HE	1.86	0.40
2:B:93:ILE:HG22	2:B:100:ASN:O	2.21	0.40
2:B:334:VAL:O	2:B:334:VAL:HG13	2.22	0.40
2:F:55:VAL:HG11	2:F:209:ALA:HB2	2.04	0.40
1:G:52:LEU:O	1:G:55:ILE:CG2	2.66	0.40
2:L:321:LEU:O	2:L:325:THR:HG23	2.22	0.40
2:H:79:ARG:HH22	2:H:198:GLN:NE2	2.20	0.40
2:H:334:VAL:O	2:H:334:VAL:HG13	2.21	0.40
1:I:59:LEU:HD13	2:J:340:LEU:HD11	2.00	0.40
2:L:128:PRO:HG2	2:L:131:LEU:CB	2.52	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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	214/231 (93%)	211 (99%)	3 (1%)	0	100	100
1	C	216/231 (94%)	212 (98%)	4 (2%)	0	100	100
1	E	215/231 (93%)	212 (99%)	3 (1%)	0	100	100
1	G	223/231 (96%)	220 (99%)	3 (1%)	0	100	100
1	I	219/231 (95%)	217 (99%)	2 (1%)	0	100	100
1	K	217/231 (94%)	214 (99%)	3 (1%)	0	100	100
2	B	339/344 (98%)	333 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	341/344 (99%)	334 (98%)	7 (2%)	0	100	100
2	F	340/344 (99%)	335 (98%)	5 (2%)	0	100	100
2	H	339/344 (98%)	331 (98%)	8 (2%)	0	100	100
2	J	341/344 (99%)	333 (98%)	8 (2%)	0	100	100
2	L	341/344 (99%)	335 (98%)	6 (2%)	0	100	100
All	All	3345/3450 (97%)	3287 (98%)	58 (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 X-ray entries followed by that with respect to entries of similar resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	172/186 (92%)	172 (100%)	0	100	100
1	C	174/186 (94%)	173 (99%)	1 (1%)	86	94
1	E	174/186 (94%)	174 (100%)	0	100	100
1	G	180/186 (97%)	180 (100%)	0	100	100
1	I	175/186 (94%)	175 (100%)	0	100	100
1	K	174/186 (94%)	173 (99%)	1 (1%)	86	94
2	B	264/265 (100%)	264 (100%)	0	100	100
2	D	265/265 (100%)	265 (100%)	0	100	100
2	F	264/265 (100%)	264 (100%)	0	100	100
2	H	264/265 (100%)	264 (100%)	0	100	100
2	J	265/265 (100%)	265 (100%)	0	100	100
2	L	265/265 (100%)	265 (100%)	0	100	100
All	All	2636/2706 (97%)	2634 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	149	ASN
1	K	111	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	149	ASN
1	I	149	ASN
1	K	198	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	HEM	D	401	2	41,50,50	1.43	5 (12%)	45,82,82	1.59	8 (17%)
3	HEM	F	401	2	41,50,50	1.39	4 (9%)	45,82,82	1.61	9 (20%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	HEM	D	401	2	-	5/12/54/54	-
3	HEM	F	401	2	-	4/12/54/54	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	HEM	C3C-C2C	-3.99	1.34	1.40
3	F	401	HEM	C3C-C2C	-3.71	1.35	1.40
3	F	401	HEM	C3C-CAC	3.09	1.54	1.47
3	D	401	HEM	C3C-CAC	3.01	1.54	1.47
3	D	401	HEM	CAB-C3B	2.53	1.54	1.47
3	F	401	HEM	CAB-C3B	2.44	1.54	1.47
3	F	401	HEM	CMB-C2B	2.24	1.55	1.50
3	D	401	HEM	CAA-C2A	2.21	1.55	1.52
3	D	401	HEM	CMB-C2B	2.20	1.55	1.50

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	401	HEM	CMC-C2C-C3C	3.53	131.29	124.68
3	D	401	HEM	C1B-NB-C4B	3.29	108.47	105.07
3	F	401	HEM	C1B-NB-C4B	3.15	108.33	105.07
3	D	401	HEM	C4D-ND-C1D	3.13	108.31	105.07
3	F	401	HEM	C4D-ND-C1D	3.07	108.24	105.07
3	F	401	HEM	C4B-CHC-C1C	2.72	126.14	122.56
3	D	401	HEM	CMC-C2C-C3C	2.70	129.72	124.68
3	D	401	HEM	C4B-CHC-C1C	2.62	126.01	122.56
3	F	401	HEM	C4C-CHD-C1D	2.48	125.83	122.56
3	D	401	HEM	C4C-CHD-C1D	2.47	125.82	122.56
3	D	401	HEM	CMB-C2B-C1B	-2.37	121.43	125.04
3	D	401	HEM	C3D-C4D-ND	-2.36	107.54	110.17
3	F	401	HEM	C3D-C4D-ND	-2.28	107.63	110.17
3	F	401	HEM	CMB-C2B-C1B	-2.24	121.63	125.04
3	D	401	HEM	C2C-C3C-C4C	2.11	108.37	106.90
3	F	401	HEM	CHC-C4B-NB	2.02	126.63	124.43
3	F	401	HEM	CBB-CAB-C3B	-2.02	117.55	127.62

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	401	HEM	C2A-CAA-CBA-CGA
3	F	401	HEM	CAA-CBA-CGA-O1A
3	D	401	HEM	CAA-CBA-CGA-O2A
3	D	401	HEM	CAD-CBD-CGD-O2D
3	D	401	HEM	CAD-CBD-CGD-O1D
3	F	401	HEM	CAA-CBA-CGA-O2A
3	D	401	HEM	CAA-CBA-CGA-O1A
3	F	401	HEM	CAD-CBD-CGD-O2D
3	F	401	HEM	CAD-CBD-CGD-O1D

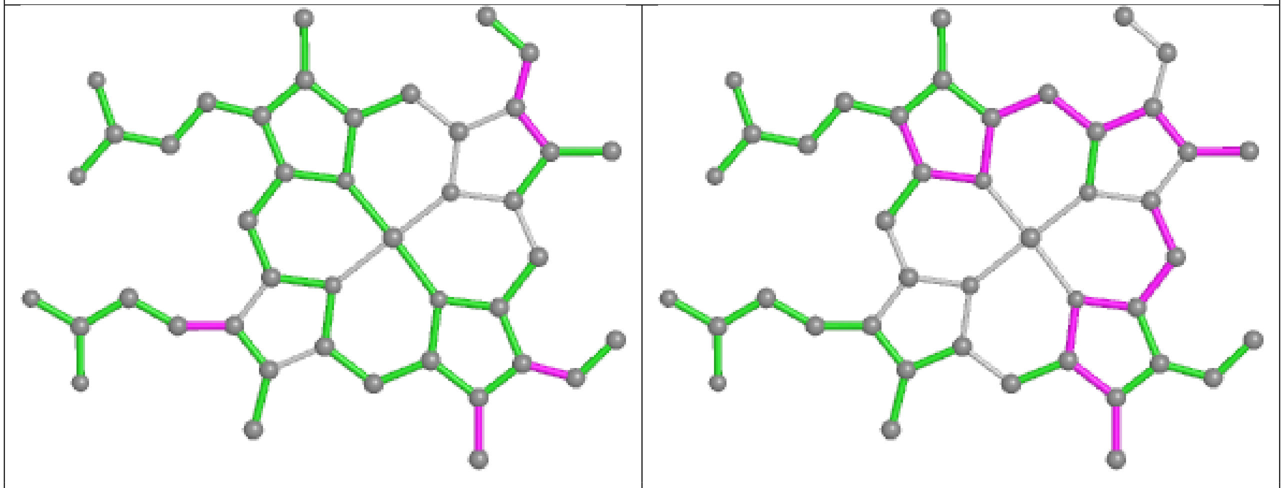
There are no ring outliers.

2 monomers are involved in 16 short contacts:

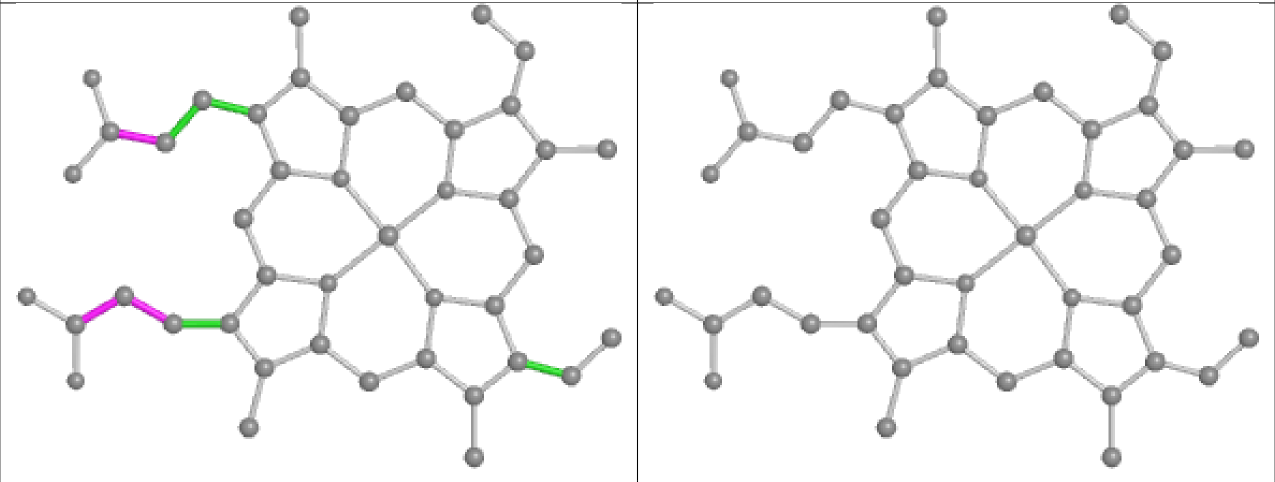
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	HEM	7	0
3	F	401	HEM	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand HEM D 401

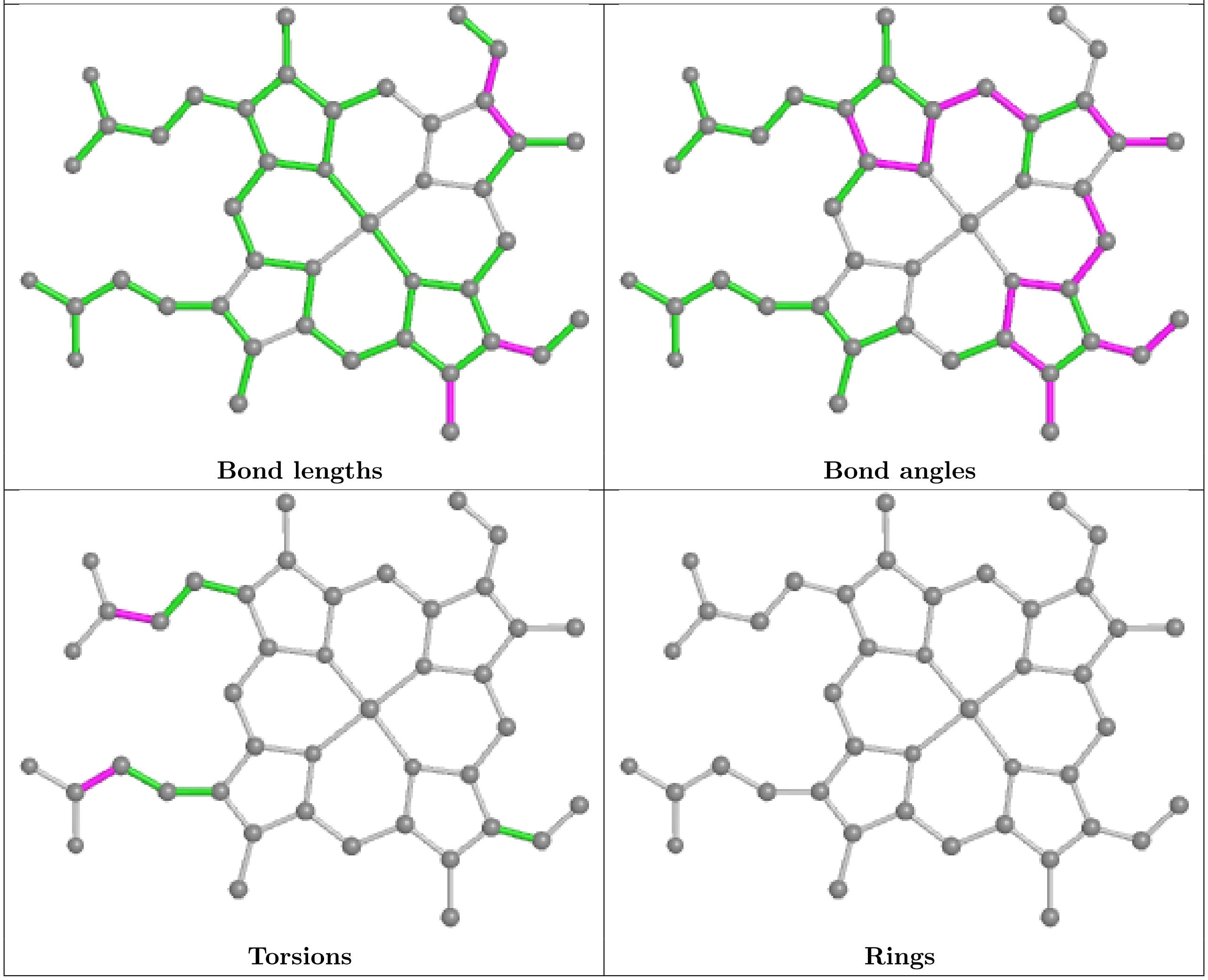


Bond lengths Bond angles



Torsions Rings

Ligand HEM F 401



Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	216/231 (93%)	0.27	5 (2%)	60	59	110, 140, 164, 193	0
1	C	218/231 (94%)	0.22	6 (2%)	53	51	98, 137, 164, 180	0
1	E	217/231 (93%)	0.84	40 (18%)	1	1	126, 193, 245, 288	0
1	G	225/231 (97%)	0.18	9 (4%)	38	37	102, 149, 223, 263	0
1	I	221/231 (95%)	0.12	6 (2%)	54	53	102, 130, 156, 170	0
1	K	219/231 (94%)	-0.02	1 (0%)	91	90	90, 122, 151, 225	0
2	B	341/344 (99%)	0.23	20 (5%)	22	23	108, 153, 213, 268	0
2	D	343/344 (99%)	0.96	64 (18%)	1	1	115, 203, 284, 307	0
2	F	342/344 (99%)	0.32	26 (7%)	13	15	128, 160, 221, 310	0
2	H	341/344 (99%)	0.82	57 (16%)	1	2	144, 202, 253, 283	0
2	J	343/344 (99%)	0.31	28 (8%)	11	13	108, 190, 244, 279	0
2	L	343/344 (99%)	0.41	39 (11%)	5	6	112, 168, 218, 251	0
All	All	3369/3450 (97%)	0.41	301 (8%)	9	11	90, 158, 240, 310	0

All (301) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	154	GLY	12.9
1	E	24	THR	10.7
2	H	154	GLY	10.2
2	H	80	TRP	9.5
2	D	194	THR	8.4
2	D	155	THR	8.2
2	J	100	ASN	8.2
2	F	60	ALA	8.2
2	D	183	VAL	7.7
2	H	155	THR	7.4
2	D	75	GLN	7.1

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Mol	Chain	Res	Type	RSRZ
2	H	79	ARG	6.9
2	L	154	GLY	6.8
2	H	194	THR	6.8
2	D	71	GLU	6.7
2	H	75	GLN	6.6
2	H	78	GLU	6.6
2	H	183	VAL	6.4
2	D	168	TRP	6.3
2	D	78	GLU	6.3
2	H	118	GLY	6.2
1	E	66	THR	6.1
1	E	22	THR	6.1
2	L	191	GLN	6.1
2	D	189	LEU	6.1
2	J	99	ALA	6.0
2	H	193	PRO	5.9
2	D	72	ILE	5.9
2	L	80	TRP	5.8
2	D	80	TRP	5.8
2	D	193	PRO	5.7
1	E	205	TYR	5.7
2	H	109	GLU	5.7
2	H	153	ALA	5.7
2	H	113	LEU	5.6
2	L	157	LYS	5.3
2	L	127	LEU	5.2
1	E	221	ALA	5.2
2	B	202	VAL	5.2
2	H	198	GLN	5.1
2	H	241	PHE	5.1
2	J	101	THR	5.1
1	E	202	GLN	5.0
2	H	195	ILE	5.0
2	F	61	GLY	4.9
2	D	74	GLU	4.9
2	B	154	GLY	4.9
2	H	123	GLN	4.9
1	A	18	ASP	4.9
2	D	56	VAL	4.9
2	L	190	ASN	4.8
2	D	112	PRO	4.8
2	D	57	PHE	4.8

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Mol	Chain	Res	Type	RSRZ
2	D	125	ALA	4.8
2	D	203	VAL	4.7
2	J	91	THR	4.7
2	H	81	LYS	4.6
2	L	297	ALA	4.6
2	D	174	TRP	4.6
2	D	187	LEU	4.6
2	L	194	THR	4.6
2	D	109	GLU	4.5
1	E	207	ASP	4.5
2	H	116	SER	4.4
2	L	189	LEU	4.4
2	J	163	HIS	4.4
1	E	62	PRO	4.4
2	D	195	ILE	4.4
2	H	74	GLU	4.4
1	E	63	THR	4.4
2	F	62	GLY	4.3
2	F	154	GLY	4.3
2	L	82	ASP	4.2
2	L	155	THR	4.2
2	L	81	LYS	4.2
2	L	93	ILE	4.2
2	L	195	ILE	4.2
2	L	1	MET	4.1
1	E	208	ARG	4.1
2	D	123	GLN	4.1
2	J	215	ALA	4.1
2	D	54	SER	4.0
2	D	73	SER	4.0
1	E	203	LEU	4.0
2	B	155	THR	4.0
2	H	117	VAL	4.0
2	D	76	GLN	3.9
2	H	341	GLY	3.9
2	H	197	PRO	3.9
1	E	194	LEU	3.9
2	D	81	LYS	3.9
2	D	126	LEU	3.8
1	C	113	ILE	3.8
1	E	200	ARG	3.8
2	L	168	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
2	D	342	ALA	3.7
2	F	193	PRO	3.7
2	H	77	ALA	3.7
2	F	202	VAL	3.7
2	F	157	LYS	3.7
2	D	169	VAL	3.7
2	L	343	THR	3.7
2	L	126	LEU	3.7
1	E	56	ALA	3.7
1	E	16	TYR	3.6
1	E	220	THR	3.6
2	D	182	ALA	3.6
2	H	82	ASP	3.6
2	D	153	ALA	3.5
1	E	204	ALA	3.5
2	D	127	LEU	3.5
1	E	218	LEU	3.5
2	H	76	GLN	3.5
1	I	74	GLY	3.4
2	L	156	VAL	3.4
2	F	342	ALA	3.4
2	J	90	GLN	3.4
1	I	75	LEU	3.3
2	L	94	GLU	3.3
2	D	202	VAL	3.3
2	L	193	PRO	3.3
2	B	119	GLY	3.3
2	J	193	PRO	3.3
2	L	158	THR	3.3
2	H	238	THR	3.3
2	H	56	VAL	3.3
2	J	44	THR	3.3
1	G	196	VAL	3.3
1	E	39	VAL	3.2
1	E	23	VAL	3.2
2	D	149	THR	3.2
1	G	116	ARG	3.2
2	B	183	VAL	3.2
2	H	203	VAL	3.2
2	H	72	ILE	3.2
2	D	192	GLU	3.2
1	C	114	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	83	SER	3.1
1	E	5	PRO	3.1
2	J	138	ARG	3.1
2	B	211	GLN	3.1
2	H	122	GLU	3.1
2	D	58	THR	3.0
2	J	292	LEU	3.0
2	B	63	SER	3.0
2	F	63	SER	3.0
2	L	12	ALA	3.0
2	H	201	GLU	3.0
2	D	120	PHE	2.9
1	K	71	GLY	2.9
1	C	220	THR	2.9
2	B	201	GLU	2.9
2	D	124	GLY	2.9
1	E	70	HIS	2.9
2	H	85	PRO	2.9
2	H	181	LYS	2.9
2	L	101	THR	2.9
2	D	167	VAL	2.9
2	H	200	ASN	2.9
1	E	57	GLY	2.9
2	B	203	VAL	2.9
2	H	156	VAL	2.9
2	L	128	PRO	2.9
2	J	113	LEU	2.8
2	H	328	VAL	2.8
1	E	32	GLU	2.8
2	J	343	THR	2.8
2	F	192	GLU	2.8
1	I	6	VAL	2.8
2	B	61	GLY	2.8
1	E	40	ALA	2.8
2	L	100	ASN	2.8
2	F	54	SER	2.8
2	B	56	VAL	2.8
1	E	41	ILE	2.7
2	J	288	ILE	2.7
2	B	80	TRP	2.7
1	G	129	LEU	2.7
1	I	3	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	209	PHE	2.7
2	D	214	PRO	2.7
1	C	217	ALA	2.7
2	H	215	ALA	2.7
2	L	78	GLU	2.7
1	I	72	ALA	2.7
2	F	297	ALA	2.7
2	J	125	ALA	2.7
2	L	192	GLU	2.7
2	H	237	VAL	2.7
2	D	85	PRO	2.7
2	F	298	GLY	2.7
2	D	84	THR	2.7
2	D	53	HIS	2.7
1	C	58	PHE	2.6
2	L	183	VAL	2.6
2	L	264	ARG	2.6
1	I	159	GLN	2.6
2	L	165	PRO	2.6
1	E	90	GLN	2.6
1	G	117	LYS	2.6
2	D	110	GLY	2.6
2	H	168	TRP	2.6
2	D	140	GLY	2.6
2	H	199	ASP	2.6
2	H	242	LEU	2.5
2	H	54	SER	2.5
2	H	46	ALA	2.5
2	J	155	THR	2.5
2	L	76	GLN	2.5
2	D	67	PHE	2.5
2	F	183	VAL	2.5
1	E	64	SER	2.5
1	G	224	TRP	2.5
2	J	93	ILE	2.5
2	F	203	VAL	2.5
2	B	118	GLY	2.5
2	F	113	LEU	2.5
2	J	97	GLN	2.5
2	D	201	GLU	2.5
2	D	181	LYS	2.5
2	D	138	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
2	B	59	THR	2.5
1	E	206	ALA	2.5
2	D	188	LEU	2.5
2	B	58	THR	2.4
1	E	65	GLY	2.4
2	J	216	TYR	2.4
2	J	127	LEU	2.4
2	B	62	GLY	2.4
2	J	98	ASN	2.4
1	E	7	LEU	2.4
2	J	183	VAL	2.3
2	L	196	GLN	2.3
2	F	240	ALA	2.3
2	D	243	THR	2.3
1	E	55	ILE	2.3
1	E	14	VAL	2.3
2	D	341	GLY	2.3
2	H	189	LEU	2.3
2	L	125	ALA	2.3
2	L	83	SER	2.3
2	F	118	GLY	2.3
2	F	191	GLN	2.3
2	F	296	ILE	2.3
2	D	173	THR	2.3
2	J	168	TRP	2.3
2	H	192	GLU	2.3
1	E	38	LEU	2.3
2	J	154	GLY	2.3
2	H	246	THR	2.3
2	B	138	ARG	2.3
2	D	79	ARG	2.3
1	E	15	VAL	2.3
1	A	218	LEU	2.2
1	E	10	THR	2.2
1	G	203	LEU	2.2
2	L	129	ALA	2.2
2	D	303	SER	2.2
1	C	161	LEU	2.2
1	E	209	PHE	2.2
2	F	120	PHE	2.2
2	D	115	ASP	2.2
2	B	306	TRP	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	294	TRP	2.2
2	H	125	ALA	2.2
2	F	53	HIS	2.2
2	H	110	GLY	2.2
2	H	157	LYS	2.2
2	D	196	GLN	2.2
2	D	200	ASN	2.1
2	F	195	ILE	2.1
2	J	105	MET	2.1
2	H	126	LEU	2.1
2	H	139	ALA	2.1
1	E	36	GLY	2.1
2	F	340	LEU	2.1
2	L	295	LEU	2.1
1	E	17	PRO	2.1
2	D	108	PRO	2.1
2	L	187	LEU	2.1
2	L	99	ALA	2.1
2	F	156	VAL	2.1
2	H	25	ILE	2.1
1	G	132	LEU	2.1
2	J	50	LEU	2.1
2	B	190	ASN	2.1
2	H	120	PHE	2.1
1	A	67	VAL	2.1
2	H	119	GLY	2.1
2	H	111	THR	2.1
2	J	43	ASN	2.1
1	A	210	VAL	2.1
1	G	163	ALA	2.1
2	D	184	GLY	2.1
2	H	216	TYR	2.0
1	G	227	PRO	2.0
2	B	193	PRO	2.0
2	J	166	VAL	2.0
2	D	70	SER	2.0
2	D	77	ALA	2.0
1	E	195	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

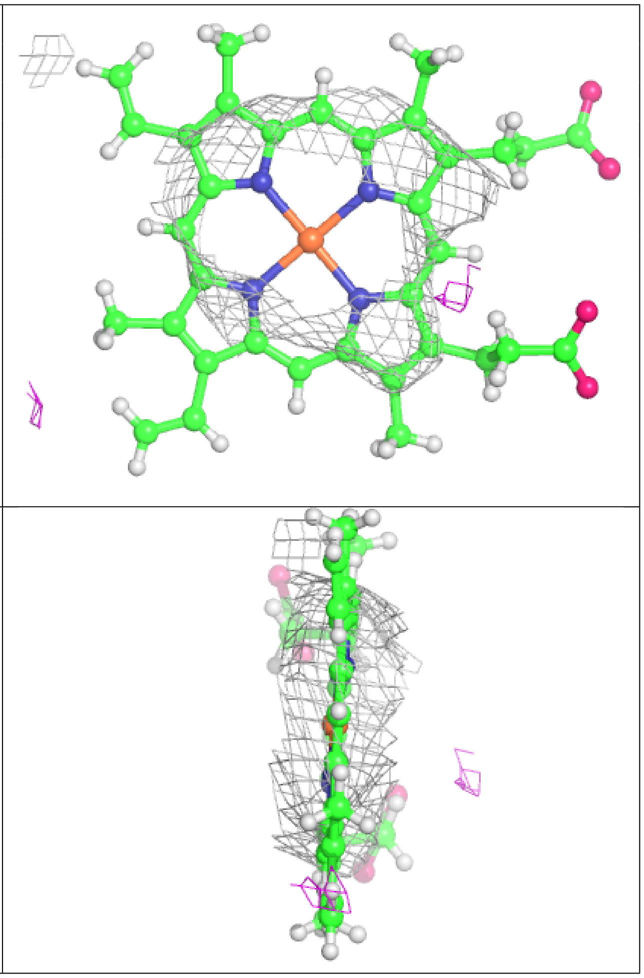
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

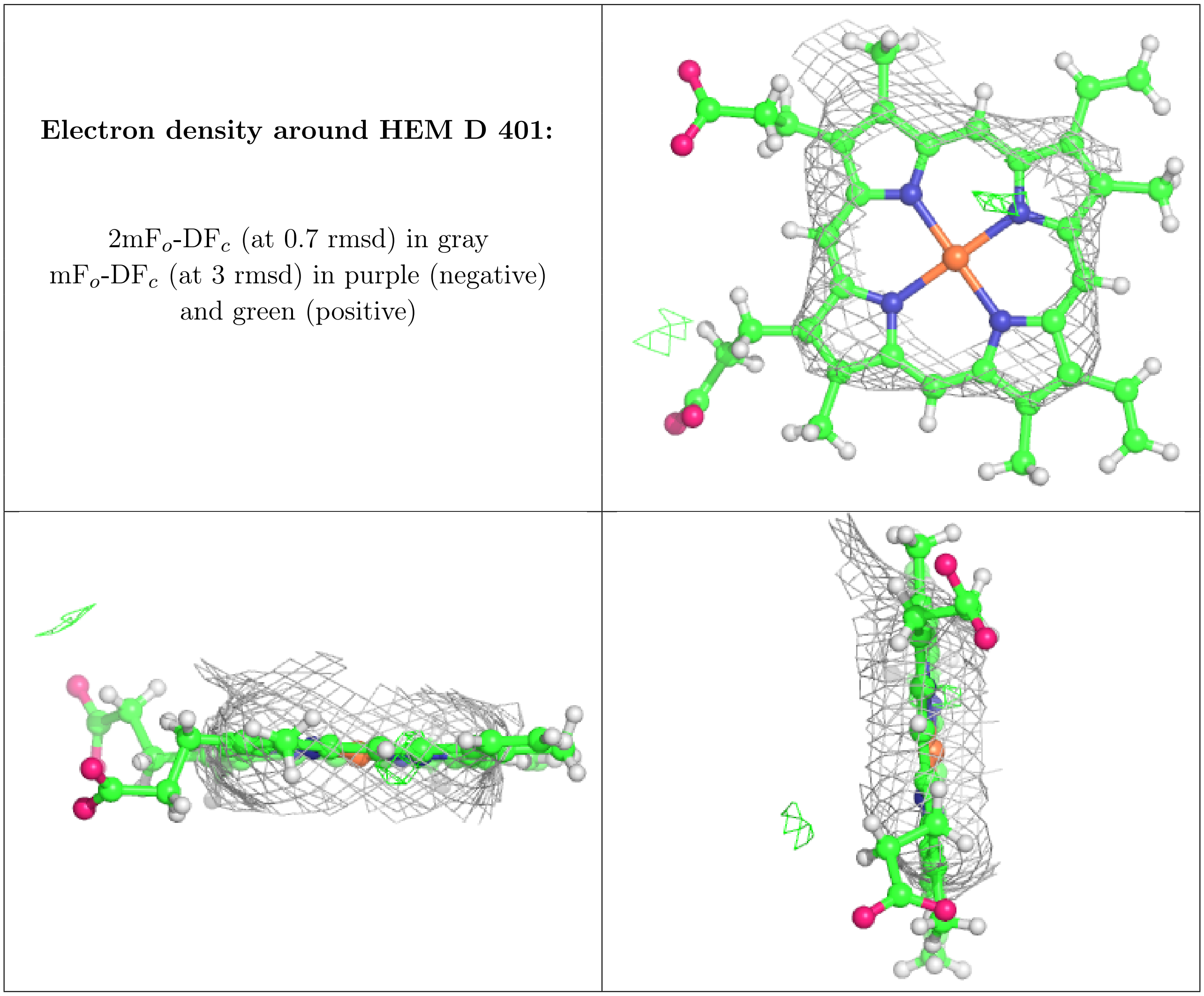
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HEM	F	401	43/43	0.88	0.33	208,288,288,288	73
3	HEM	D	401	43/43	0.92	0.38	208,268,268,268	73

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around HEM F 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around HEM D 401:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.