



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2026 – 12:00 AM JST

PDB ID : 7W7D / pdb_00007w7d
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)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The 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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

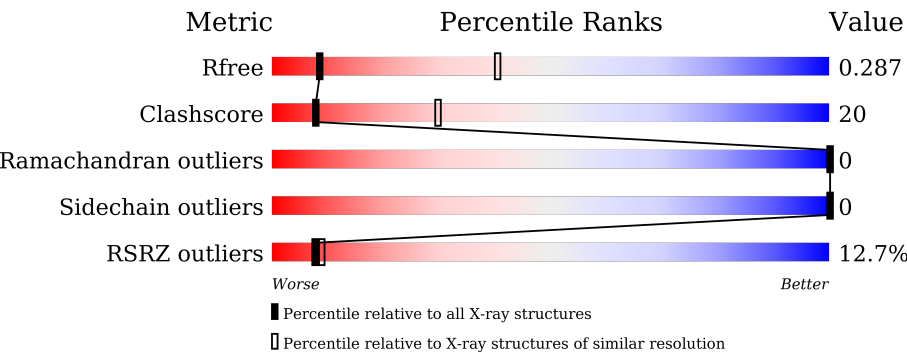
1 Overall quality at a glance i

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}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	231	13% 61% 33% 6%
1	C	231	10% 65% 30% 6%
1	E	231	13% 60% 34% 6%
1	G	231	13% 68% 29% •
1	I	231	6% 56% 40% •
1	K	231	11% 60% 35% 5%

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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

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

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

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

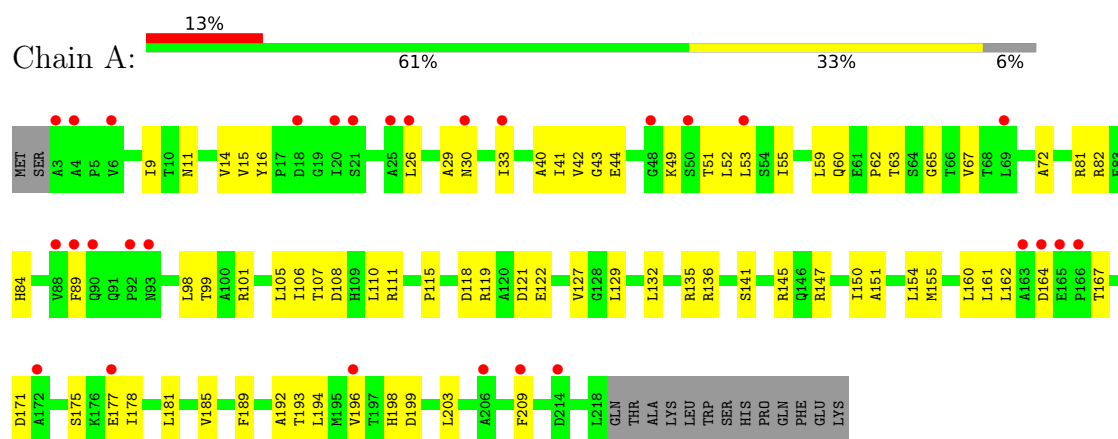
- # HEM

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

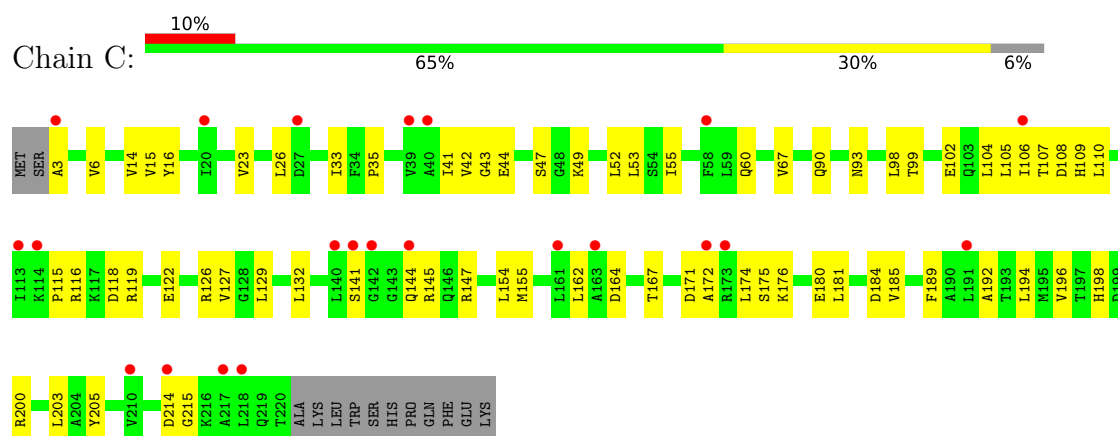
3 Residue-property plots [i](#)

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 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.

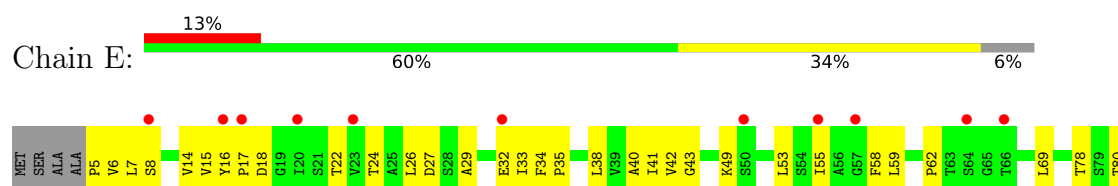
- Molecule 1: Putative ABC transport system, ATP-binding protein

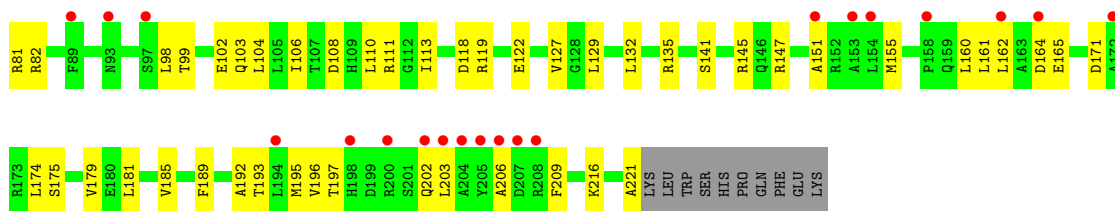


- Molecule 1: Putative ABC transport system, ATP-binding protein

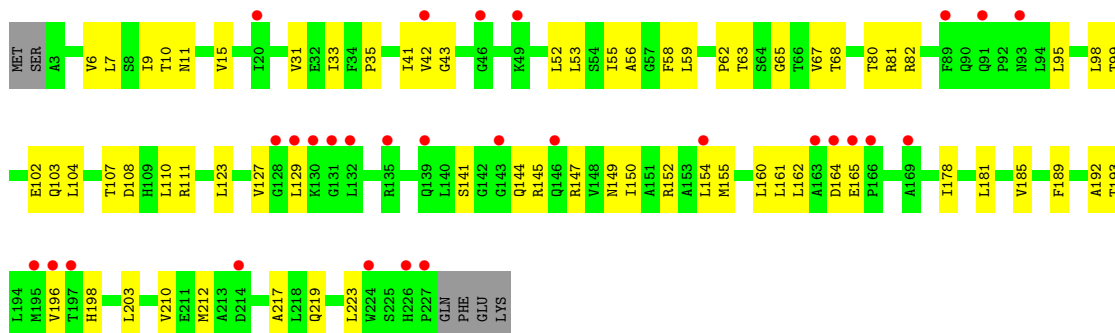


- Molecule 1: Putative ABC transport system, ATP-binding protein

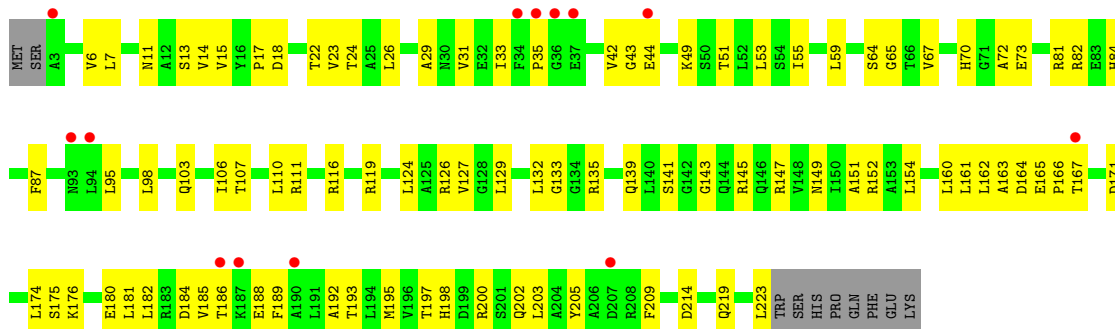




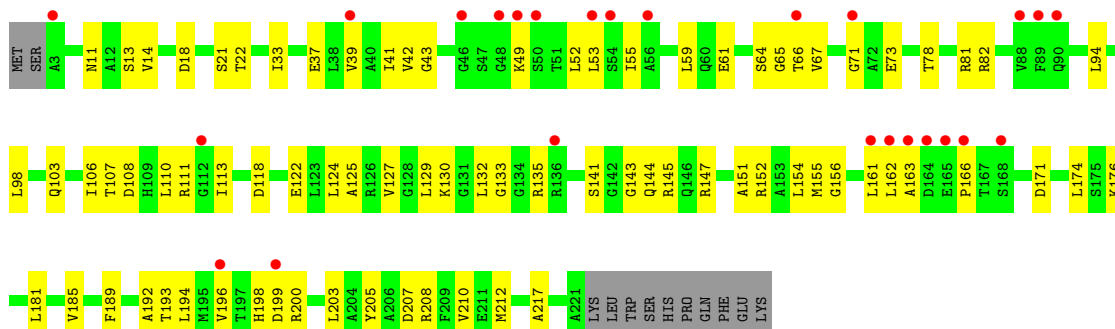
- Molecule 1: Putative ABC transport system, ATP-binding protein



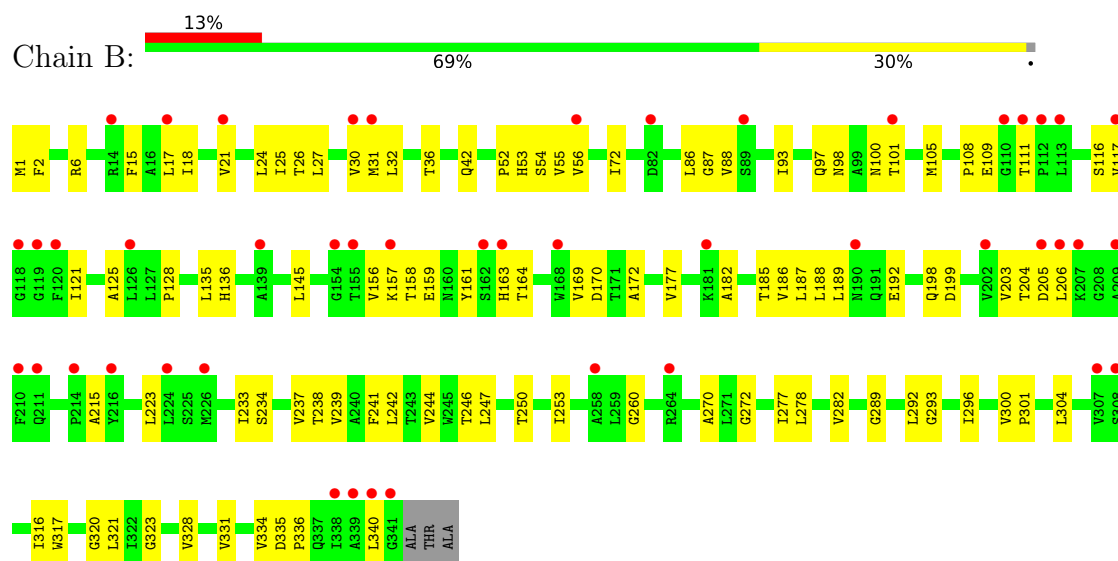
- Molecule 1: Putative ABC transport system, ATP-binding protein



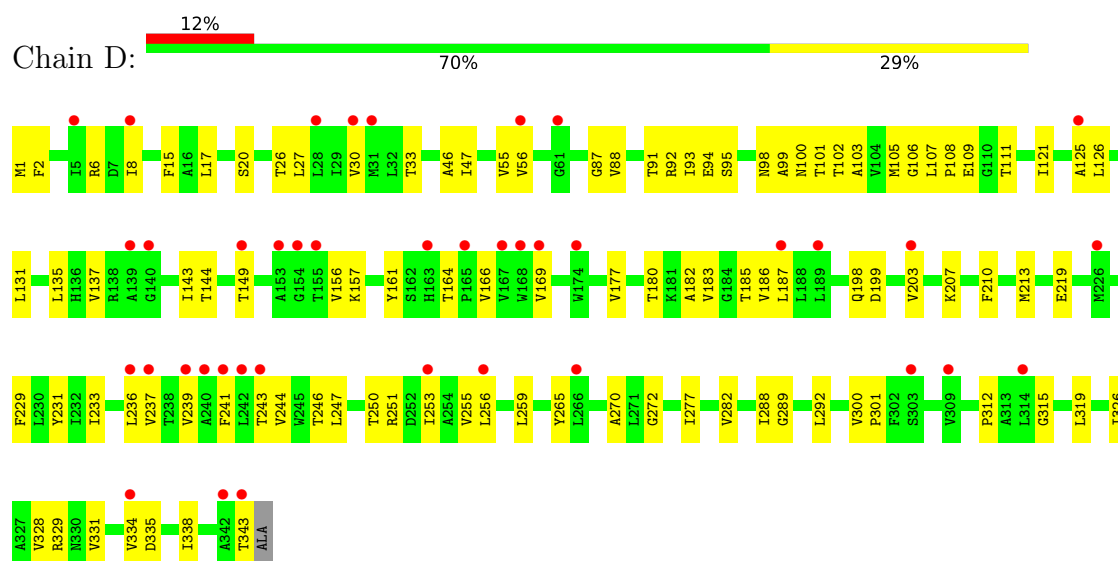
- Molecule 1: Putative ABC transport system, ATP-binding protein



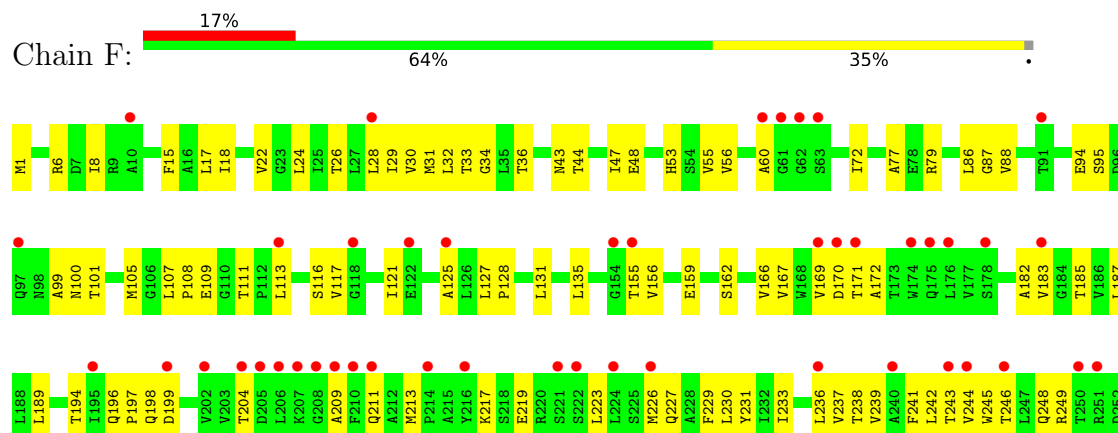
• Molecule 2: Putative ABC transport system integral membrane protein



• Molecule 2: Putative ABC transport system integral membrane protein

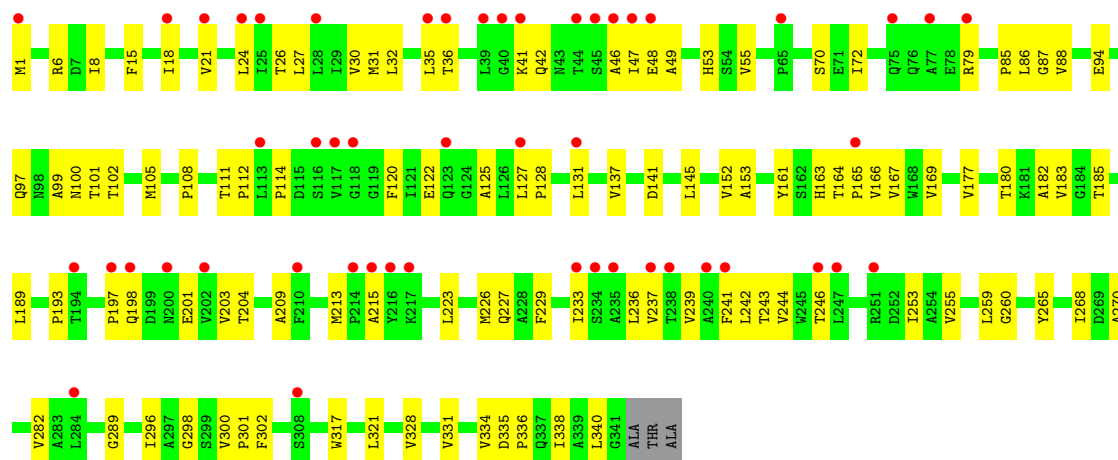


• Molecule 2: Putative ABC transport system integral membrane protein

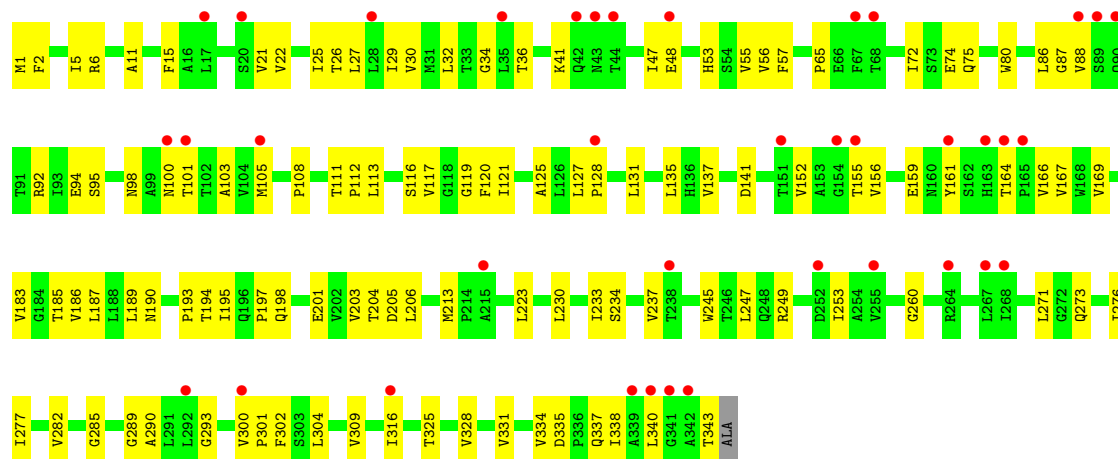




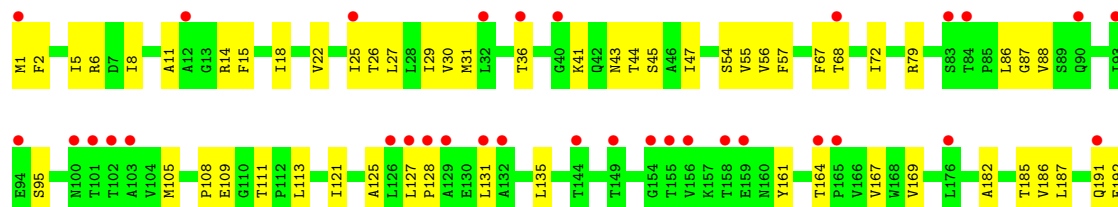
• Molecule 2: Putative ABC transport system integral membrane protein

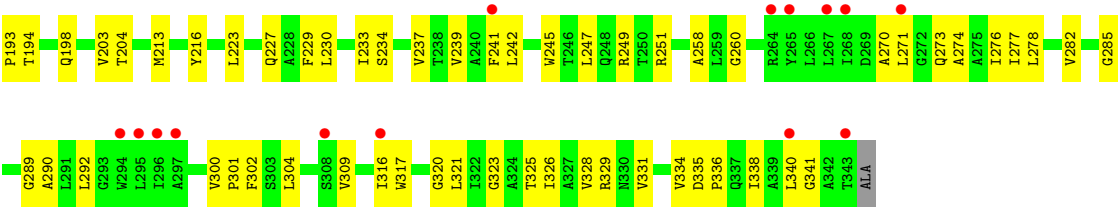


• Molecule 2: Putative ABC transport system integral membrane protein



• Molecule 2: Putative ABC transport system integral membrane protein





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 – 3.40	Depositor EDS
% Data completeness (in resolution range)	97.6 (49.29-3.40) 85.5 (49.29-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.53 (at 3.25Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.255 , 0.285 0.257 , 0.287	Depositor DCC
R_{free} test set	2948 reflections (1.94%)	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)	0.26 , 72.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.12	0/1637	0.27	0/2216
1	C	0.13	0/1653	0.28	0/2238
1	E	0.09	0/1648	0.26	0/2230
1	G	0.13	0/1716	0.29	0/2325
1	I	0.14	0/1671	0.28	0/2263
1	K	0.16	0/1658	0.30	0/2245
2	B	0.12	0/2556	0.25	0/3495
2	D	0.09	0/2568	0.21	0/3512
2	F	0.11	0/2561	0.24	0/3502
2	H	0.08	0/2556	0.21	0/3495
2	J	0.10	0/2568	0.23	0/3512
2	L	0.11	0/2568	0.24	0/3512
All	All	0.11	0/25360	0.25	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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1618	0	1664	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1634	0	1679	74	0
1	E	1629	0	1675	75	0
1	G	1693	0	1737	62	0
1	I	1652	0	1697	87	0
1	K	1639	0	1684	80	0
2	B	2510	0	2588	94	0
2	D	2522	0	2600	88	0
2	F	2515	0	2593	123	0
2	H	2510	0	2588	108	0
2	J	2522	0	2600	94	0
2	L	2522	0	2600	95	0
3	D	43	30	30	7	0
3	F	43	30	30	9	0
All	All	25052	60	25765	1004	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 20.

All (1004) 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
2:L:31:MET:HE1	2:L:292:LEU:HD23	1.36	1.03
2:D:1:MET:HE1	2:D:272:GLY:HA3	1.41	1.02
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
2:F:1:MET:HE2	2:F:272:GLY:HA3	1.49	0.94
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:H:86:LEU:HD21	2:H:105:MET:HE2	1.52	0.92
2:B:253:ILE:HD13	2:B:331:VAL:HG23	1.52	0.92
2:B:1:MET:HE1	2:B:272:GLY:HA3	1.52	0.91
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:I:176:LYS:NZ	1:I:205:TYR:OH	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:F:1:MET:HE2	2:F:272:GLY:CA	2.19	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:L:1:MET:HE1	2:L:276:ILE:HD11	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:D:1:MET:HE1	2:D:272:GLY:CA	2.22	0.68
2:B:1:MET:HE1	2:B:272:GLY:CA	2.22	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
2:H:47:ILE:HD12	2:H:213:MET:HE3	1.74	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: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
2:L:1:MET:HE3	2:L:5:ILE:HD11	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:1:MET:CE	2:D:272:GLY:HA3	2.22	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:1:MET:CE	2:B:272:GLY:HA3	2.26	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:K:108:ASP:OD2	1:K:155:MET:HE3	2.01	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
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:F:47:ILE:HD12	2:F:213:MET:HE3	1.84	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
2:H:1:MET:HE2	2:H:268:ILE:CG2	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:L:31:MET:CE	2:L:292:LEU:HD23	2.25	0.55
2:D:233:ILE:O	2:D:237:VAL:HG23	2.06	0.55
1:G:127:VAL:O	1:G:127:VAL:HG12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:E:38:LEU:HD21	1:E:195:MET:HE2	1.87	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
2:H:79:ARG:HH22	2:H:198:GLN:CD	2.15	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:186:VAL:HG12	2:D:187:LEU:N	2.23	0.54
2:F:32:LEU:HD13	2:H:226:MET:HE1	1.88	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
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:47:ILE:HD12	2:D:213:MET:HE3	1.91	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
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: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:J:161:TYR:O	2:J:164:THR:OG1	2.23	0.52
2:L:1:MET:HE1	2:L:276:ILE:CD1	2.39	0.51
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:E:127:VAL:HG12	1:E:127:VAL:O	2.10	0.51
1:I:180:GLU:HG2	1:I:205:TYR:CE2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:J:80:TRP:HH2	2:J:201:GLU:CD	2.19	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
1:I:176:LYS:HZ2	1:I:205:TYR:HH	1.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:F:304:LEU:C	2:F:304:LEU:HD23	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:328:VAL:HG12	2:H:328:VAL:O	2.11	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:G:52:LEU:C	1:G:55:ILE:HG22	2.38	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
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:I:126:ARG:HH22	1:I:184:ASP:CG	2.21	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
1:C:109:HIS:HD1	2:D:265:TYR:HE2	1.60	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:47:ILE:HD12	2:F:213:MET:CE	2.44	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:L:1:MET:HE3	2:L:5:ILE:CD1	2.43	0.46
2:B:21:VAL:CG2	2:D:236:LEU:HB3	2.43	0.46
2:D:161:TYR:O	2:D:164:THR:OG1	2.33	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:18:ILE:HD13	2:H:241:PHE:CD1	2.51	0.46
2:J:21:VAL:HG11	2:J:237:VAL:HG11	1.98	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: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
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
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
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
2:B:161:TYR:O	2:B:164:THR:OG1	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:108:ASP:OD2	1:A:155:MET:HE3	2.17	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:H:161:TYR:O	2:H:164:THR:OG1	2.35	0.45
2:J:245:TRP:NE1	2:J:273:GLN:OE1	2.50	0.45
2:J:334:VAL:HG13	2:J:334:VAL:O	2.16	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
1:A:105:LEU:HD22	1:A:115:PRO:HB3	1.99	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: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
1:K:21:SER:OG	1:K:22:THR:N	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:J:1:MET:HE3	2:J:5:ILE:HD11	1.99	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: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:L:334:VAL:HG13	2:L:334:VAL:O	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:1:MET:HE2	2:H:268:ILE:HG21	1.98	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:1:MET:CE	2:L:5:ILE:HD11	2.45	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
2:H:239:VAL:O	2:H:243:THR:HG23	2.18	0.43
2:H:296:ILE:C	2:H:298:GLY:H	2.26	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
1:A:44:GLU:CD	1:A:198:HIS:HE2	2.26	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:J:198:GLN:H	2:J:201:GLU:CD	2.26	0.43
1:K:210:VAL:CG1	1:K:217:ALA:HB1	2.49	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:110:LEU:C	1:E:110:LEU:HD12	2.44	0.43
2:H:70:SER:OG	2:H:185:THR:O	2.28	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: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:1:MET:HE1	2:J:276:ILE:HD11	2.01	0.42
2:J:197:PRO:HB2	2:J:201:GLU:HB2	2.01	0.42
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
2:B:304:LEU:C	2:B:304:LEU:HD23	2.45	0.42
2:D:17:LEU:O	2:D:20:SER:OG	2.38	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
1:K:73:GLU:H	1:K:73:GLU:CD	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:226:MET:HE1	2:H:226:MET:SD	2.60	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: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
2:L:68:THR:O	2:L:68:THR:HG22	2.19	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
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:110:LEU:C	1:G:110:LEU:HD12	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:110:LEU:HD12	1:I:110:LEU:C	2.45	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: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: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
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:C:110:LEU:C	1:C:110:LEU:HD12	2.46	0.41
1:E:104:LEU:O	1:E:155:MET:HG2	2.21	0.41
2:F:44:THR:OG1	2:F:48:GLU:OE2	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:108:ASP:CG	1:E:113:ILE:HD11	2.46	0.40
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
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:L:44:THR:HA	2:L:213:MET:HE1	2.02	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: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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	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
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 [i](#)

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%)	174 (100%)	0	100	100
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%)	174 (100%)	0	100	100
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%)	2636 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
2	B	97	GLN
2	B	123	GLN
1	C	149	ASN
2	D	53	HIS
2	D	97	GLN
2	D	191	GLN
1	E	11	ASN
1	E	157	ASN
2	F	42	GLN
2	F	53	HIS
2	F	90	GLN
2	F	97	GLN
2	H	53	HIS
1	I	11	ASN
1	I	60	GLN
1	I	149	ASN
2	J	90	GLN
2	J	98	ASN

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Mol	Chain	Res	Type
2	J	136	HIS
2	J	200	ASN
1	K	198	HIS
1	K	219	GLN
2	L	90	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	F	401	2	50,50,50	1.39	8 (16%)	66,82,82	1.39	11 (16%)
3	HEM	D	401	2	50,50,50	1.42	8 (16%)	66,82,82	1.38	8 (12%)

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	F	401	2	-	4/14/54/54	-
3	HEM	D	401	2	-	5/14/54/54	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	401	HEM	FE-NA	3.60	2.07	1.95
3	D	401	HEM	FE-ND	3.59	2.06	1.94
3	F	401	HEM	FE-NC	3.48	2.06	1.95
3	F	401	HEM	FE-NB	3.32	2.05	1.94
3	F	401	HEM	FE-ND	3.25	2.04	1.94
3	D	401	HEM	FE-NC	3.21	2.06	1.95
3	D	401	HEM	FE-NB	3.13	2.04	1.94
3	F	401	HEM	FE-NA	2.92	2.05	1.95
3	D	401	HEM	CAB-C3B	2.54	1.54	1.47
3	F	401	HEM	CAC-C3C	2.46	1.54	1.47
3	F	401	HEM	CAB-C3B	2.44	1.54	1.47
3	D	401	HEM	CAC-C3C	2.40	1.54	1.47
3	F	401	HEM	CMB-C2B	2.24	1.55	1.50
3	F	401	HEM	CMC-C2C	2.21	1.55	1.50
3	D	401	HEM	CMB-C2B	2.20	1.55	1.50
3	D	401	HEM	CMC-C2C	2.17	1.55	1.50

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	401	HEM	C1B-NB-C4B	3.29	108.47	105.07
3	F	401	HEM	C1B-NB-C4B	3.16	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	D	401	HEM	C4C-NC-C1C	3.05	108.33	105.35
3	F	401	HEM	C4A-NA-C1A	2.97	108.25	105.35
3	F	401	HEM	C4C-NC-C1C	2.96	108.25	105.35
3	D	401	HEM	C4A-NA-C1A	2.87	108.16	105.35
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	C2A-C1A-NA	-2.28	107.60	110.15
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	F	401	HEM	CMC-C2C-C1C	-2.12	120.97	124.71
3	F	401	HEM	CBC-CAC-C3C	-2.08	117.28	127.62
3	D	401	HEM	C2A-C1A-NA	-2.05	107.86	110.15
3	F	401	HEM	CHC-C4B-NB	2.04	126.64	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	401	HEM	CBB-CAB-C3B	-2.02	117.55	127.62
3	D	401	HEM	CHD-C4C-NC	2.02	126.63	124.44

There are no chirality outliers.

All (9) torsion outliers are listed below:

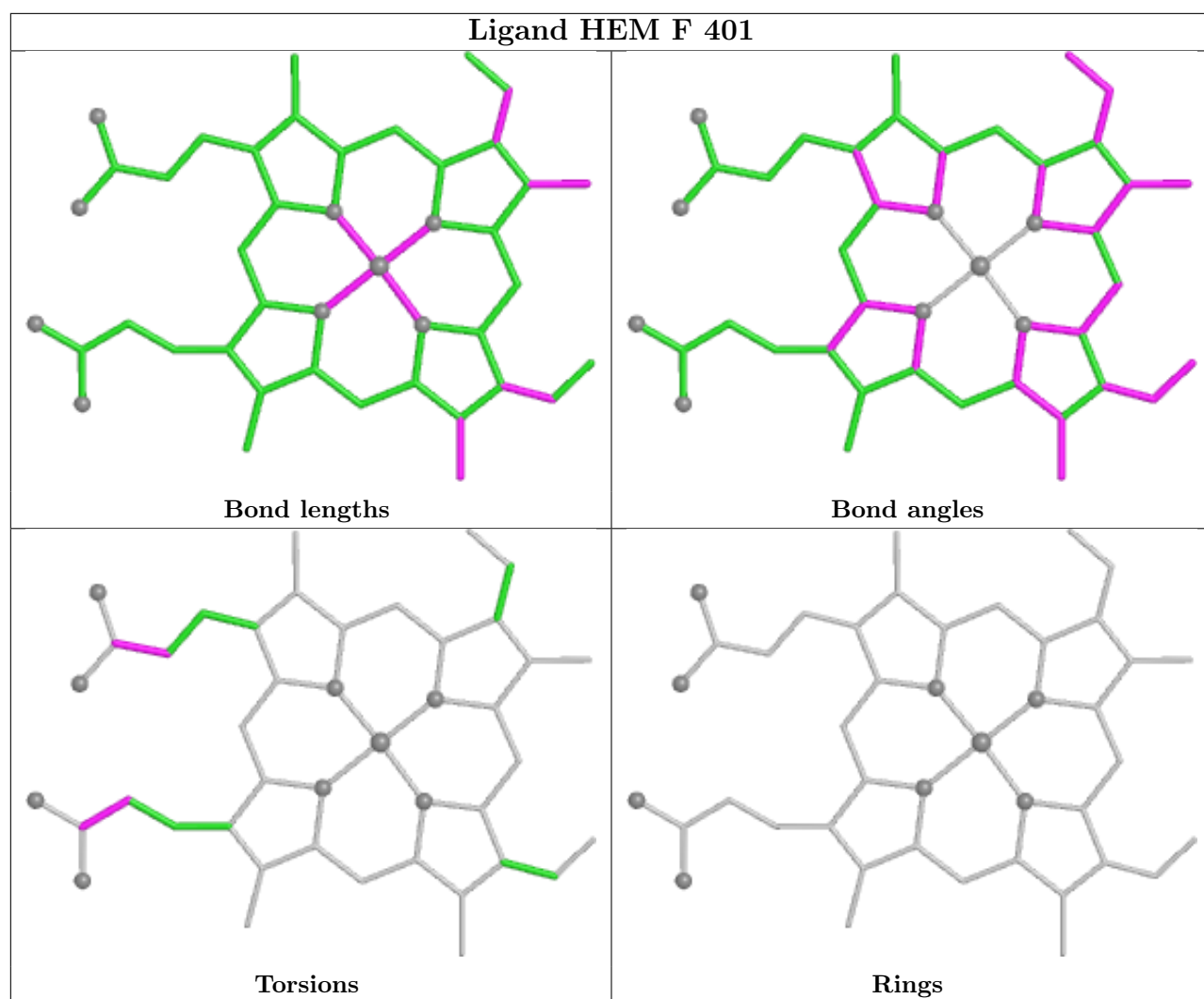
Mol	Chain	Res	Type	Atoms
3	D	401	HEM	C2A-CAA-CBA-CGA
3	F	401	HEM	CAA-CBA-CGA-O1A
3	D	401	HEM	CAA-CBA-CGA-O2A
3	D	401	HEM	CAD-CBD-CGD-O2D
3	D	401	HEM	CAD-CBD-CGD-O1D
3	F	401	HEM	CAA-CBA-CGA-O2A
3	D	401	HEM	CAA-CBA-CGA-O1A
3	F	401	HEM	CAD-CBD-CGD-O2D
3	F	401	HEM	CAD-CBD-CGD-O1D

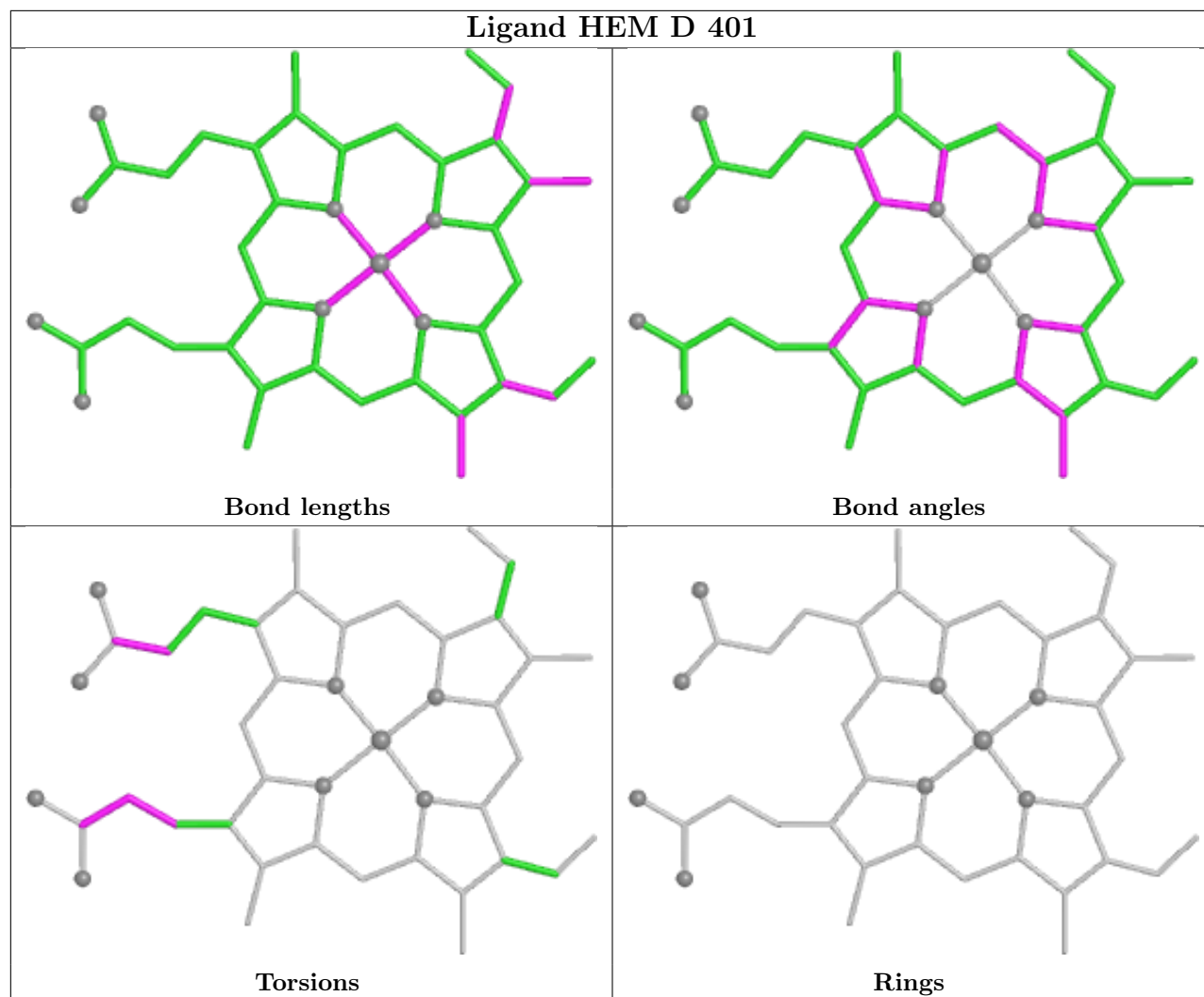
There are no ring outliers.

2 monomers are involved in 16 short contacts:

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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%)	0.70	29 (13%) 7 8	110, 140, 164, 193	0
1	C	218/231 (94%)	0.57	22 (10%) 12 12	98, 137, 164, 180	0
1	E	217/231 (93%)	0.74	31 (14%) 6 8	126, 193, 245, 288	0
1	G	225/231 (97%)	0.82	29 (12%) 7 9	102, 149, 223, 263	0
1	I	221/231 (95%)	0.33	13 (5%) 28 22	102, 130, 156, 170	0
1	K	219/231 (94%)	0.58	25 (11%) 10 10	90, 122, 151, 225	0
2	B	341/344 (99%)	0.79	46 (13%) 7 8	108, 153, 213, 268	0
2	D	343/344 (99%)	0.80	40 (11%) 9 10	115, 203, 284, 307	0
2	F	342/344 (99%)	0.83	57 (16%) 4 6	128, 160, 221, 310	0
2	H	341/344 (99%)	0.83	50 (14%) 6 7	144, 202, 253, 283	0
2	J	343/344 (99%)	0.69	38 (11%) 10 11	108, 190, 244, 279	0
2	L	343/344 (99%)	0.76	47 (13%) 6 8	112, 168, 218, 251	0
All	All	3369/3450 (97%)	0.72	427 (12%) 8 9	90, 158, 240, 310	0

All (427) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	164	ASP	9.8
2	B	154	GLY	9.1
1	G	164	ASP	8.6
1	G	196	VAL	8.5
2	H	241	PHE	7.7
1	A	18	ASP	7.4
2	D	154	GLY	7.4
1	A	164	ASP	7.4
2	F	207	LYS	6.7
2	B	155	THR	6.6
2	B	112	PRO	6.5

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Mol	Chain	Res	Type	RSRZ
2	B	163	HIS	6.4
2	L	101	THR	6.3
2	D	243	THR	6.2
2	D	149	THR	6.1
2	H	48	GLU	6.1
2	L	264	ARG	6.0
2	J	163	HIS	6.0
2	D	240	ALA	6.0
1	G	165	GLU	6.0
2	L	94	GLU	5.9
1	E	203	LEU	5.9
2	F	202	VAL	5.8
2	L	154	GLY	5.8
1	K	50	SER	5.7
2	L	127	LEU	5.7
2	L	295	LEU	5.7
2	H	46	ALA	5.6
1	E	204	ALA	5.5
1	G	135	ARG	5.4
2	F	178	SER	5.4
2	B	190	ASN	5.4
2	F	154	GLY	5.4
1	G	163	ALA	5.3
2	J	101	THR	5.3
2	L	267	LEU	5.3
1	I	36	GLY	5.2
2	B	207	LYS	5.2
2	L	158	THR	5.2
2	L	128	PRO	5.2
2	L	155	THR	5.1
1	A	90	GLN	5.1
2	F	199	ASP	5.1
2	B	118	GLY	5.0
1	C	214	ASP	5.0
1	E	205	TYR	5.0
1	C	39	VAL	4.9
1	G	139	GLN	4.9
2	B	339	ALA	4.9
1	G	132	LEU	4.9
1	C	144	GLN	4.8
2	F	211	GLN	4.8
1	E	20	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	K	165	GLU	4.8
2	J	90	GLN	4.7
1	I	187	LYS	4.7
2	L	93	ILE	4.7
1	C	142	GLY	4.7
1	K	162	LEU	4.7
2	H	251	ARG	4.7
2	D	239	VAL	4.7
2	F	240	ALA	4.6
1	G	93	ASN	4.6
2	D	256	LEU	4.6
1	G	128	GLY	4.6
1	K	163	ALA	4.5
2	J	215	ALA	4.5
2	L	268	ILE	4.5
2	B	340	LEU	4.5
1	A	89	PHE	4.4
2	H	233	ILE	4.4
2	L	102	THR	4.4
1	G	197	THR	4.4
1	K	53	LEU	4.3
2	F	342	ALA	4.3
2	J	300	VAL	4.3
1	G	195	MET	4.3
2	H	44	THR	4.3
2	F	62	GLY	4.3
1	E	97	SER	4.3
2	H	216	TYR	4.2
1	C	161	LEU	4.2
2	H	246	THR	4.2
2	J	100	ASN	4.2
2	B	113	LEU	4.2
2	B	211	GLN	4.2
2	F	226	MET	4.1
2	H	28	LEU	4.1
2	B	139	ALA	4.1
1	E	16	TYR	4.0
1	K	89	PHE	4.0
2	L	144	THR	4.0
2	B	117	VAL	4.0
2	D	241	PHE	4.0
2	J	44	THR	4.0

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Mol	Chain	Res	Type	RSRZ
2	F	298	GLY	3.9
1	C	113	ILE	3.9
1	E	200	ARG	3.9
2	H	198	GLN	3.9
2	L	316	ILE	3.9
2	L	129	ALA	3.9
2	H	47	ILE	3.9
2	J	48	GLU	3.8
2	L	100	ASN	3.8
1	K	90	GLN	3.8
2	D	168	TRP	3.8
1	C	114	LYS	3.8
2	J	341	GLY	3.8
1	C	3	ALA	3.8
1	C	141	SER	3.8
1	G	49	LYS	3.8
2	F	204	THR	3.8
2	D	155	THR	3.8
2	B	338	ILE	3.7
1	E	198	HIS	3.7
1	E	32	GLU	3.7
1	G	130	LYS	3.7
1	K	49	LYS	3.7
2	B	14	ARG	3.7
1	E	202	GLN	3.6
2	L	1	MET	3.6
2	J	340	LEU	3.6
2	F	175	GLN	3.6
2	F	210	PHE	3.6
1	E	194	LEU	3.6
1	E	50	SER	3.6
1	A	163	ALA	3.6
1	K	3	ALA	3.6
2	H	237	VAL	3.6
1	K	168	SER	3.6
1	C	173	ARG	3.5
2	F	208	GLY	3.5
1	G	129	LEU	3.5
2	J	164	THR	3.5
2	D	30	VAL	3.5
1	G	91	GLN	3.4
2	F	205	ASP	3.4

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Mol	Chain	Res	Type	RSRZ
1	K	196	VAL	3.4
1	I	93	ASN	3.4
2	F	169	VAL	3.4
2	F	170	ASP	3.4
2	J	339	ALA	3.4
2	F	63	SER	3.4
2	H	79	ARG	3.4
1	A	53	LEU	3.3
2	D	5	ILE	3.3
2	H	308	SER	3.3
1	C	218	LEU	3.3
1	E	89	PHE	3.3
2	J	88	VAL	3.3
2	L	265	TYR	3.3
2	F	224	LEU	3.3
1	K	71	GLY	3.3
1	G	166	PRO	3.2
2	J	35	LEU	3.2
1	E	23	VAL	3.2
2	B	82	ASP	3.2
2	H	1	MET	3.2
2	F	171	THR	3.2
1	A	93	ASN	3.2
2	L	165	PRO	3.2
2	H	238	THR	3.2
2	J	155	THR	3.2
1	I	35	PRO	3.1
2	H	116	SER	3.1
2	D	169	VAL	3.1
2	H	214	PRO	3.1
2	F	318	LEU	3.1
2	H	39	LEU	3.1
2	B	101	THR	3.1
2	B	119	GLY	3.1
2	D	303	SER	3.1
2	H	202	VAL	3.1
2	D	167	VAL	3.0
2	F	221	SER	3.0
1	G	20	ILE	3.0
2	F	195	ILE	3.0
2	D	236	LEU	3.0
2	F	209	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	174	TRP	3.0
2	J	268	ILE	3.0
2	D	266	LEU	3.0
2	H	24	LEU	3.0
2	J	17	LEU	3.0
2	B	21	VAL	3.0
2	L	36	THR	3.0
1	C	20	ILE	3.0
2	J	68	THR	3.0
2	F	295	LEU	3.0
2	H	247	LEU	2.9
2	L	297	ALA	2.9
1	A	88	VAL	2.9
2	L	156	VAL	2.9
2	B	210	PHE	2.9
1	C	140	LEU	2.9
2	D	165	PRO	2.9
1	A	172	ALA	2.9
2	J	161	TYR	2.9
2	H	127	LEU	2.9
1	G	227	PRO	2.9
2	H	165	PRO	2.9
2	B	31	MET	2.9
2	F	125	ALA	2.9
2	J	43	ASN	2.9
2	J	342	ALA	2.9
1	I	37	GLU	2.9
2	B	202	VAL	2.9
2	L	83	SER	2.8
1	G	143	GLY	2.8
2	F	28	LEU	2.8
2	F	97	GLN	2.8
1	E	93	ASN	2.8
2	H	200	ASN	2.8
2	B	111	THR	2.8
2	L	343	THR	2.8
1	E	207	ASP	2.8
2	B	341	GLY	2.8
2	F	251	ARG	2.8
2	J	264	ARG	2.8
2	F	183	VAL	2.8
2	F	236	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	165	GLU	2.8
2	D	8	ILE	2.8
1	E	206	ALA	2.7
2	D	125	ALA	2.7
2	L	90	GLN	2.7
2	B	17	LEU	2.7
1	I	44	GLU	2.7
2	H	217	LYS	2.7
1	A	3	ALA	2.7
2	D	203	VAL	2.7
2	B	308	SER	2.7
1	I	3	ALA	2.7
2	F	254	ALA	2.7
1	A	6	VAL	2.7
2	D	334	VAL	2.7
2	F	206	LEU	2.7
2	H	131	LEU	2.7
2	L	164	THR	2.7
1	C	191	LEU	2.7
2	H	113	LEU	2.7
2	L	340	LEU	2.7
1	E	164	ASP	2.7
1	G	226	HIS	2.7
2	F	296	ILE	2.6
1	G	89	PHE	2.6
2	B	181	LYS	2.6
2	F	243	THR	2.6
1	G	224	TRP	2.6
2	D	56	VAL	2.6
2	B	214	PRO	2.6
2	L	241	PHE	2.6
1	G	131	GLY	2.6
2	D	242	LEU	2.6
1	A	92	PRO	2.6
2	F	214	PRO	2.6
1	A	4	ALA	2.6
2	H	25	ILE	2.6
1	G	46	GLY	2.6
2	L	40	GLY	2.6
2	D	139	ALA	2.6
2	H	240	ALA	2.6
2	H	194	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	H	210	PHE	2.5
2	B	126	LEU	2.5
1	A	30	ASN	2.5
2	F	244	VAL	2.5
2	J	252	ASP	2.5
1	C	172	ALA	2.5
2	D	343	THR	2.5
2	L	126	LEU	2.5
1	E	57	GLY	2.5
2	D	61	GLY	2.5
2	H	123	GLN	2.5
2	H	234	SER	2.5
2	J	255	VAL	2.5
1	I	190	ALA	2.5
2	D	153	ALA	2.5
2	B	120	PHE	2.5
1	I	94	LEU	2.5
1	A	206	ALA	2.5
2	J	20	SER	2.5
2	D	140	GLY	2.5
2	H	77	ALA	2.4
2	D	31	MET	2.4
2	F	91	THR	2.4
2	J	28	LEU	2.4
2	J	128	PRO	2.4
2	D	163	HIS	2.4
1	K	88	VAL	2.4
1	A	25	ALA	2.4
2	H	75	GLN	2.4
2	H	18	ILE	2.4
2	B	226	MET	2.4
2	B	264	ARG	2.4
2	H	35	LEU	2.4
2	J	267	LEU	2.4
2	D	237	VAL	2.4
2	F	61	GLY	2.4
1	A	33	ILE	2.4
2	L	132	ALA	2.4
2	H	45	SER	2.4
2	F	155	THR	2.4
2	L	294	TRP	2.4
1	A	166	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	110	GLY	2.4
1	G	169	ALA	2.4
2	B	258	ALA	2.4
1	G	214	ASP	2.4
2	H	118	GLY	2.4
2	F	60	ALA	2.4
2	L	296	ILE	2.4
2	B	206	LEU	2.4
2	B	224	LEU	2.4
2	L	176	LEU	2.4
1	K	39	VAL	2.4
1	K	166	PRO	2.4
2	D	174	TRP	2.4
2	F	246	THR	2.3
2	F	250	THR	2.3
1	C	106	ILE	2.3
2	L	103	ALA	2.3
2	L	191	GLN	2.3
2	L	271	LEU	2.3
1	A	196	VAL	2.3
1	E	158	PRO	2.3
1	K	54	SER	2.3
2	F	277	ILE	2.3
2	H	36	THR	2.3
1	C	40	ALA	2.3
2	H	215	ALA	2.3
2	B	216	TYR	2.3
2	B	205	ASP	2.3
1	A	177	GLU	2.3
2	F	299	SER	2.3
2	H	40	GLY	2.3
1	A	214	ASP	2.3
2	B	168	TRP	2.3
2	J	238	THR	2.3
1	A	209	PHE	2.3
1	I	34	PHE	2.3
1	K	136	ARG	2.3
2	H	21	VAL	2.3
1	E	153	ALA	2.3
1	E	172	ALA	2.3
2	D	189	LEU	2.3
1	C	58	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	B	162	SER	2.3
2	F	216	TYR	2.3
2	B	157	LYS	2.3
1	C	210	VAL	2.3
1	E	17	PRO	2.2
2	D	342	ALA	2.2
2	F	10	ALA	2.2
2	H	235	ALA	2.2
2	J	67	PHE	2.2
2	B	30	VAL	2.2
2	D	253	ILE	2.2
2	L	25	ILE	2.2
1	A	48	GLY	2.2
1	I	167	THR	2.2
2	L	68	THR	2.2
2	L	84	THR	2.2
2	L	149	THR	2.2
1	G	146	GLN	2.2
2	F	122	GLU	2.2
1	K	199	ASP	2.2
1	E	151	ALA	2.2
2	J	154	GLY	2.2
1	E	208	ARG	2.2
1	A	26	LEU	2.2
2	B	209	ALA	2.2
2	H	65	PRO	2.2
1	A	69	LEU	2.2
1	E	162	LEU	2.2
2	J	292	LEU	2.2
1	C	217	ALA	2.2
1	C	27	ASP	2.2
1	A	20	ILE	2.1
1	E	64	SER	2.1
2	D	226	MET	2.1
2	H	41	LYS	2.1
2	F	297	ALA	2.1
2	L	12	ALA	2.1
2	L	308	SER	2.1
1	K	46	GLY	2.1
1	K	112	GLY	2.1
2	B	307	VAL	2.1
1	K	66	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	314	LEU	2.1
1	C	163	ALA	2.1
1	K	56	ALA	2.1
1	A	50	SER	2.1
1	G	154	LEU	2.1
2	F	321	LEU	2.1
1	K	48	GLY	2.1
2	J	165	PRO	2.1
1	E	55	ILE	2.1
1	K	161	LEU	2.1
2	F	176	LEU	2.1
2	L	32	LEU	2.1
2	F	222	SER	2.1
2	J	89	SER	2.1
2	J	42	GLN	2.1
1	A	21	SER	2.0
1	E	8	SER	2.0
2	B	89	SER	2.0
2	J	105	MET	2.0
1	E	66	THR	2.0
2	F	320	GLY	2.0
2	H	197	PRO	2.0
2	L	159	GLU	2.0
1	G	42	VAL	2.0
2	B	56	VAL	2.0
1	E	154	LEU	2.0
2	H	284	LEU	2.0
2	L	131	LEU	2.0
2	J	316	ILE	2.0
1	I	186	THR	2.0
2	J	151	THR	2.0
1	I	207	ASP	2.0
2	F	118	GLY	2.0
2	D	309	VAL	2.0
2	H	117	VAL	2.0
2	D	28	LEU	2.0
2	D	187	LEU	2.0
2	F	113	LEU	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](#)

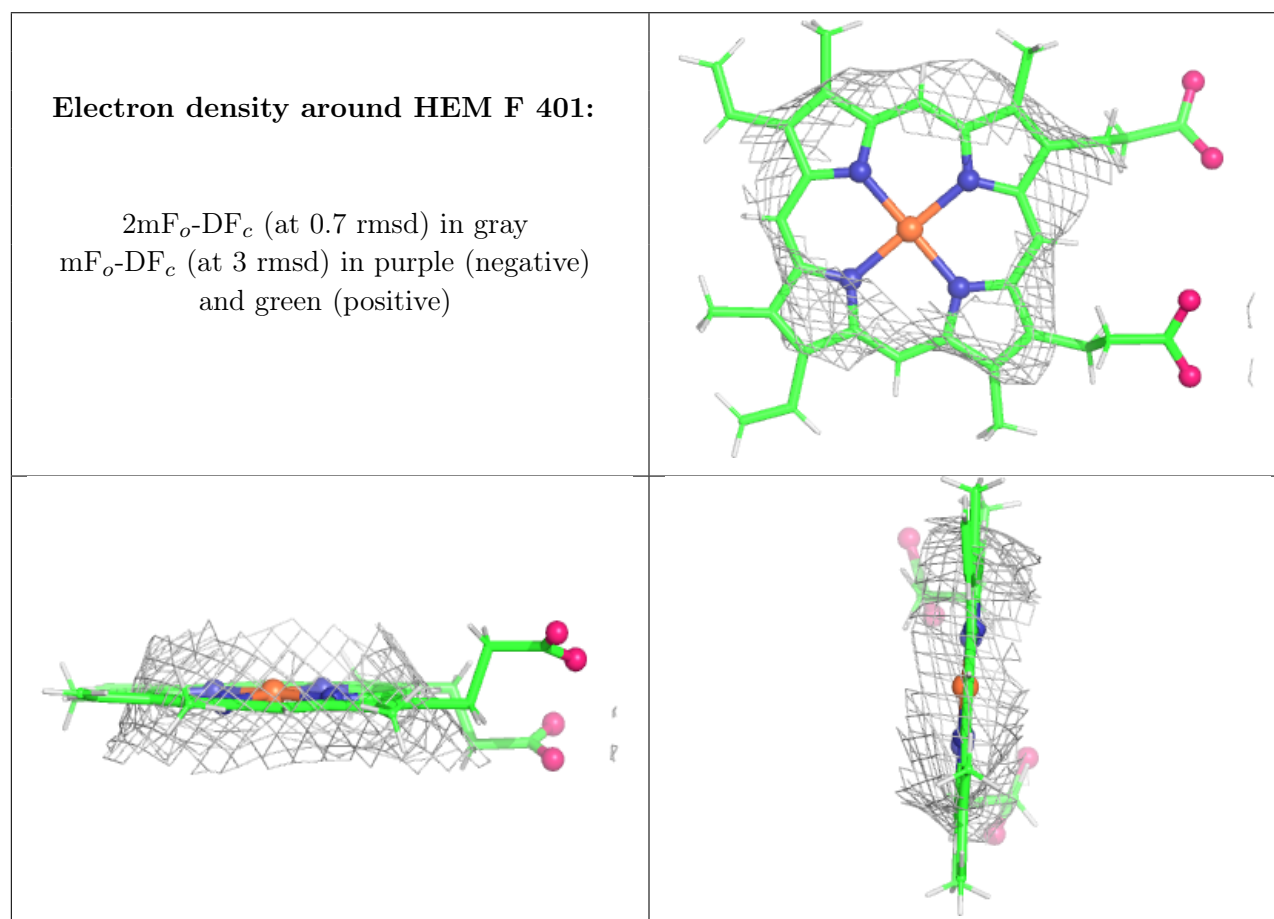
There are no oligosaccharides in this entry.

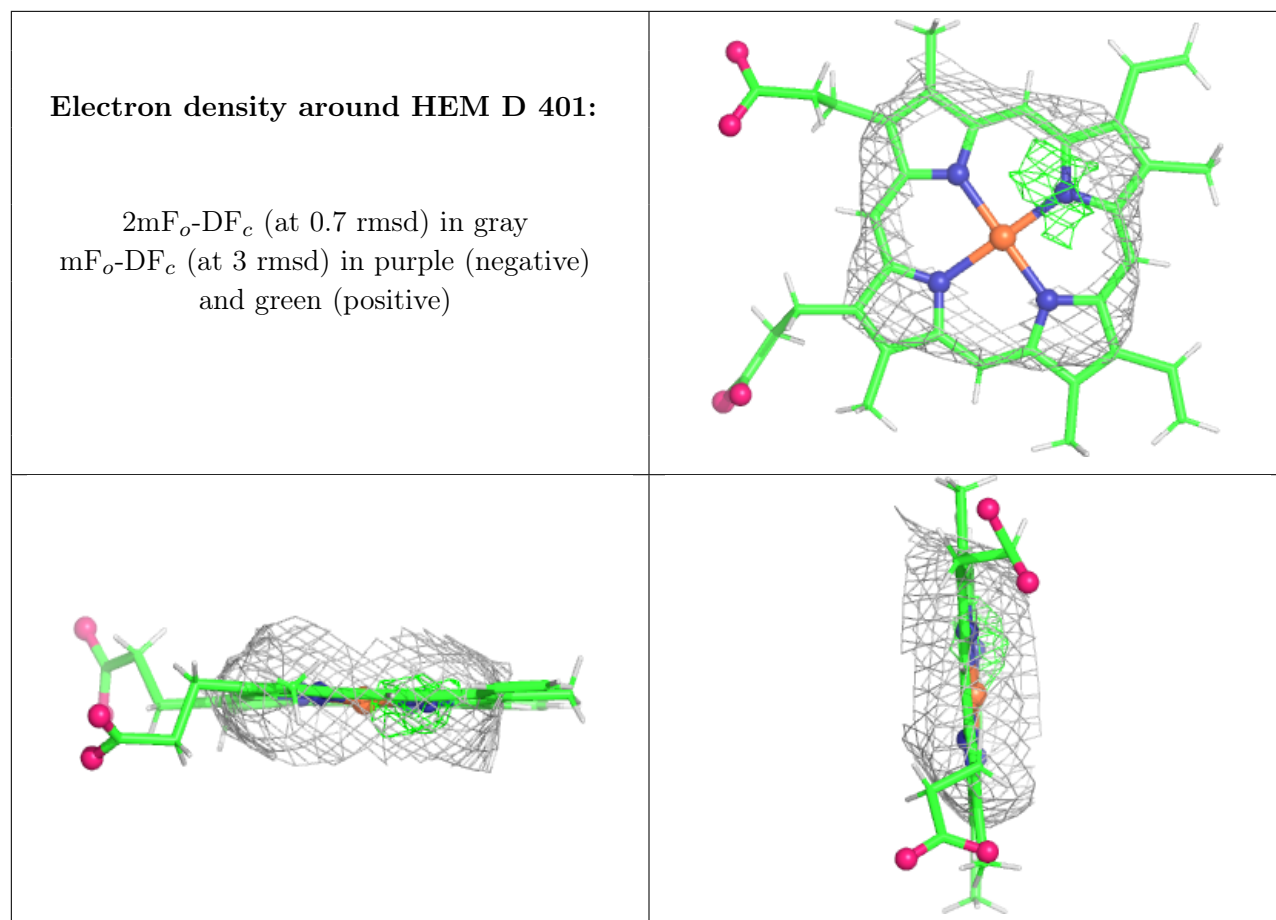
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	HEM	F	401	43/43	0.90	0.19	208,288,288,288	73
3	HEM	D	401	43/43	0.95	0.25	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.