



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:14 PM GMT

PDB ID : 1JBQ
Title : STRUCTURE OF HUMAN CYSTATHIONINE BETA-SYNTHASE: A
UNIQUE PYRIDOXAL 5'-PHOSPHATE DEPENDENT HEMEPROTEIN
Authors : Meier, M.; Janosik, M.; Kery, V.; Kraus, J.P.; Burkhard, P.
Deposited on : 2001-06-06
Resolution : 2.60 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

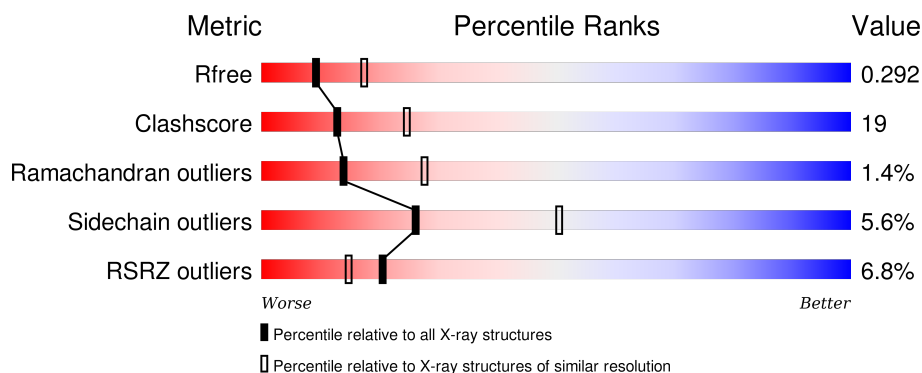
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	435	<div> <div>3%</div> <div> <div></div> <div>51%</div> <div>26%</div> <div>•</div> <div>20%</div> </div> </div>
1	B	435	<div> <div>9%</div> <div> <div></div> <div>51%</div> <div>26%</div> <div>•</div> <div>20%</div> </div> </div>
1	C	435	<div> <div>6%</div> <div> <div></div> <div>50%</div> <div>27%</div> <div>•</div> <div>20%</div> </div> </div>
1	D	435	<div> <div>7%</div> <div> <div></div> <div>50%</div> <div>27%</div> <div>•</div> <div>20%</div> </div> </div>
1	E	435	<div> <div>4%</div> <div> <div></div> <div>52%</div> <div>25%</div> <div>•</div> <div>20%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	435	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a small red segment at the beginning labeled '4%', followed by a green segment labeled '53%', a yellow segment labeled '25%', and a small grey segment at the end labeled '20%'. A small black dot is visible on the yellow segment.

2 Entry composition [i](#)

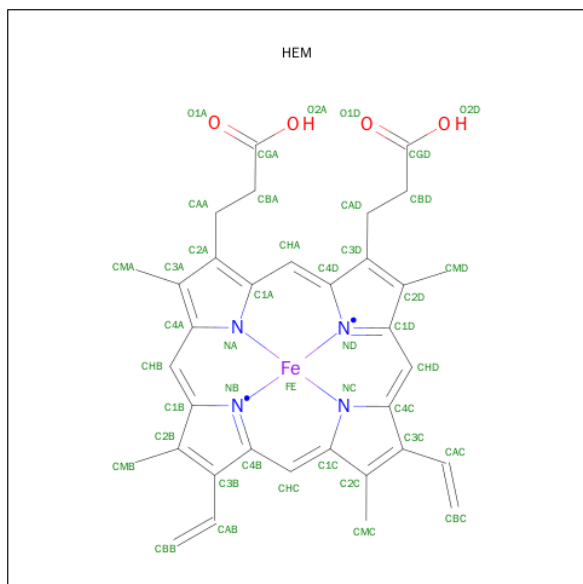
There are 4 unique types of molecules in this entry. The entry contains 16522 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called CYSTATHIONINE BETA-SYNTHASE.

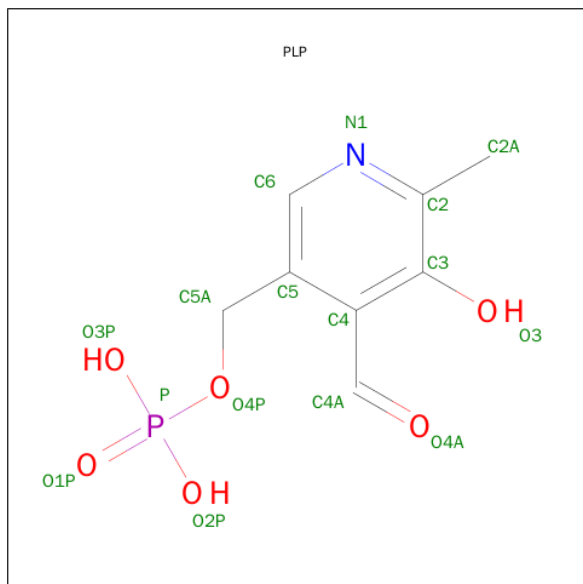
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	348	Total	C	N	O	S	0	0	0
			2667	1678	469	503	17			
1	B	348	Total	C	N	O	S	0	0	0
			2667	1678	469	503	17			
1	C	348	Total	C	N	O	S	0	0	0
			2667	1678	469	503	17			
1	D	348	Total	C	N	O	S	0	0	0
			2667	1678	469	503	17			
1	E	350	Total	C	N	O	S	0	0	0
			2685	1689	472	507	17			
1	F	348	Total	C	N	O	S	0	0	0
			2667	1678	469	503	17			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	F	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).

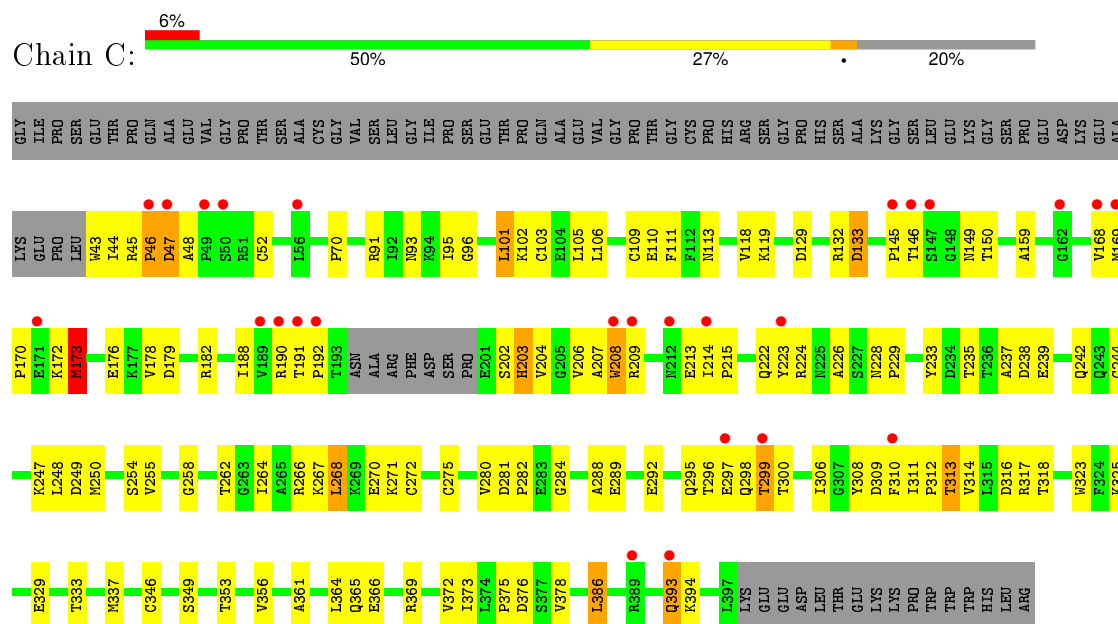


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
3	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

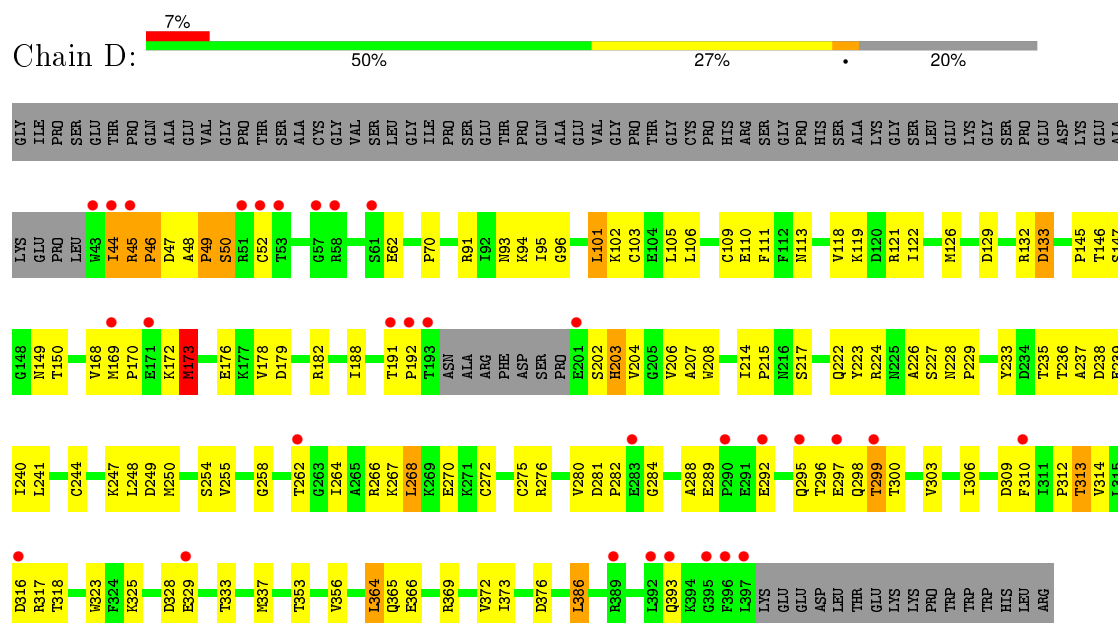
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total 22	O 22	0	0
4	B	30	Total 30	O 30	0	0
4	C	25	Total 25	O 25	0	0
4	D	24	Total 24	O 24	0	0
4	E	31	Total 31	O 31	0	0
4	F	22	Total 22	O 22	0	0

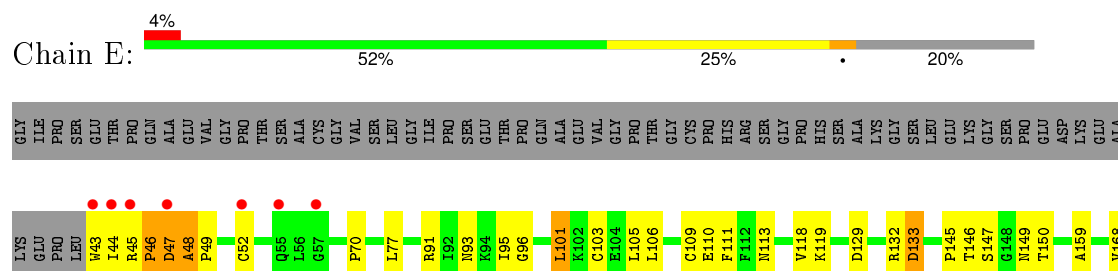
- Molecule 1: CYSTATHIONINE BETA-SYNTHASE

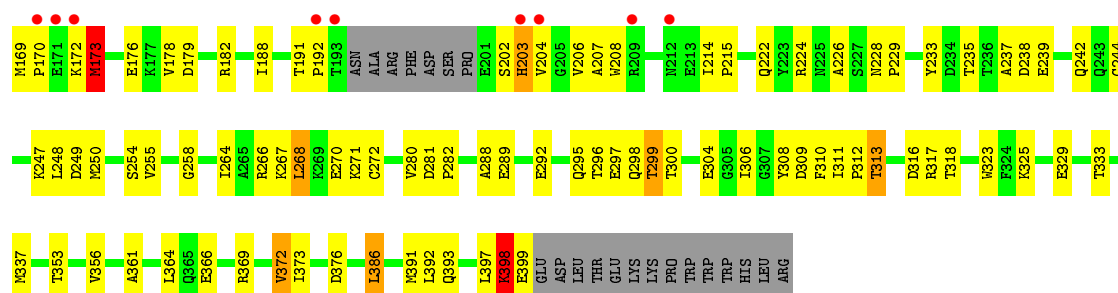


- Molecule 1: CYSTATHIONINE BETA-SYNTHASE

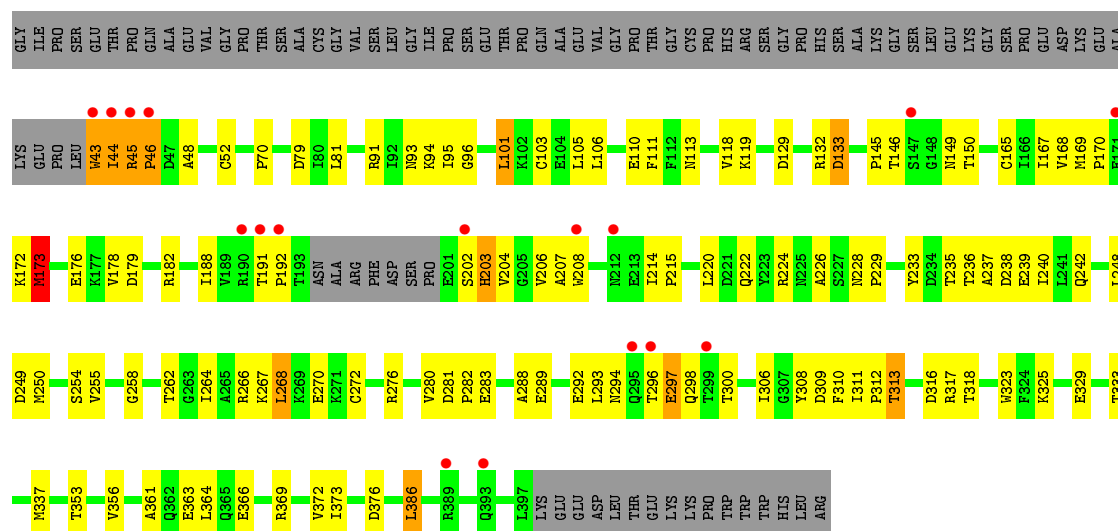


- Molecule 1: CYSTATHIONINE BETA-SYNTHASE





• Molecule 1: CYSTATHIONINE BETA-SYNTHASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	144.52Å 144.52Å 108.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.34 – 2.60 43.34 – 2.60	Depositor EDS
% Data completeness (in resolution range)	82.3 (43.34-2.60) 82.3 (43.34-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.49 (at 2.61Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.257 , 0.296 0.255 , 0.292	Depositor DCC
R_{free} test set	3219 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.110	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.9	EDS
Estimated twinning fraction	0.000 for -h,-k,l 0.036 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 66710 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	16522	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 43.39 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.7767e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

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	0.39	0/2715	0.67	1/3672 (0.0%)
1	B	0.38	0/2715	0.65	0/3672
1	C	0.39	0/2715	0.65	0/3672
1	D	0.37	0/2715	0.66	1/3672 (0.0%)
1	E	0.38	0/2733	0.67	0/3695
1	F	0.38	0/2715	0.66	0/3672
All	All	0.38	0/16308	0.66	2/22055 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	ILE	N-CA-C	-8.54	87.93	111.00
1	D	44	ILE	N-CA-C	-7.01	92.06	111.00

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	2667	0	2691	108	0
1	B	2667	0	2691	103	0
1	C	2667	0	2691	108	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2667	0	2691	114	0
1	E	2685	0	2710	96	0
1	F	2667	0	2691	107	0
2	A	43	0	30	4	0
2	B	43	0	30	2	0
2	C	43	0	30	2	0
2	D	43	0	30	3	0
2	E	43	0	30	2	0
2	F	43	0	30	3	0
3	A	15	0	7	1	0
3	B	15	0	7	1	0
3	C	15	0	7	1	0
3	D	15	0	7	1	0
3	E	15	0	7	1	0
3	F	15	0	7	1	0
4	A	22	0	0	4	0
4	B	30	0	0	2	0
4	C	25	0	0	6	0
4	D	24	0	0	7	0
4	E	31	0	0	2	0
4	F	22	0	0	0	0
All	All	16522	0	16387	628	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 (628) 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:296:THR:HG22	1:E:298:GLN:H	1.30	0.94
1:A:296:THR:HG22	1:A:298:GLN:H	1.33	0.93
1:C:296:THR:HG22	1:C:298:GLN:H	1.32	0.92
1:D:296:THR:HG22	1:D:298:GLN:H	1.33	0.92
1:B:296:THR:HG22	1:B:298:GLN:H	1.33	0.91
1:C:129:ASP:HA	1:C:132:ARG:HH12	1.33	0.91
1:E:129:ASP:HA	1:E:132:ARG:HH12	1.35	0.90
1:F:129:ASP:HA	1:F:132:ARG:HH12	1.37	0.90
1:B:129:ASP:HA	1:B:132:ARG:HH12	1.34	0.90
1:D:129:ASP:HA	1:D:132:ARG:HH12	1.35	0.89
1:A:129:ASP:HA	1:A:132:ARG:HH12	1.35	0.89
1:F:43:TRP:NE1	1:F:45:ARG:HG3	1.89	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:398:LYS:HG3	1:E:399:GLU:H	1.40	0.86
1:D:224:ARG:HG2	1:D:313:THR:HG21	1.58	0.86
1:B:224:ARG:HG2	1:B:313:THR:HG21	1.58	0.85
1:C:129:ASP:HA	1:C:132:ARG:NH1	1.91	0.84
1:C:224:ARG:HG2	1:C:313:THR:HG21	1.59	0.84
1:B:224:ARG:HG2	1:B:313:THR:CG2	2.08	0.84
1:F:224:ARG:HG2	1:F:313:THR:CG2	2.09	0.83
1:E:191:THR:HG21	1:E:203:HIS:HA	1.61	0.82
1:A:129:ASP:HA	1:A:132:ARG:NH1	1.94	0.82
1:D:224:ARG:HG2	1:D:313:THR:CG2	2.08	0.82
1:B:191:THR:HG21	1:B:203:HIS:HA	1.62	0.82
1:B:129:ASP:HA	1:B:132:ARG:NH1	1.95	0.81
1:E:129:ASP:HA	1:E:132:ARG:NH1	1.96	0.81
1:F:129:ASP:HA	1:F:132:ARG:NH1	1.96	0.81
1:C:224:ARG:HG2	1:C:313:THR:CG2	2.10	0.81
1:C:191:THR:HG21	1:C:203:HIS:HA	1.62	0.81
1:D:191:THR:HG21	1:D:203:HIS:HA	1.61	0.81
1:F:224:ARG:HG2	1:F:313:THR:HG21	1.62	0.80
1:D:129:ASP:HA	1:D:132:ARG:NH1	1.95	0.80
1:E:224:ARG:HG2	1:E:313:THR:HG21	1.64	0.80
1:B:304:GLU:HG3	4:B:1017:HOH:O	1.82	0.80
1:F:191:THR:HG21	1:F:203:HIS:HA	1.62	0.79
1:A:191:THR:HG21	1:A:203:HIS:HA	1.64	0.79
1:E:224:ARG:HG2	1:E:313:THR:CG2	2.14	0.78
1:A:224:ARG:HG2	1:A:313:THR:HG21	1.64	0.78
1:A:224:ARG:HG2	1:A:313:THR:CG2	2.14	0.78
1:D:118:VAL:O	4:D:1022:HOH:O	2.01	0.77
1:C:316:ASP:OD2	1:C:318:THR:HB	1.85	0.76
1:C:310:PHE:HA	4:C:1003:HOH:O	1.84	0.76
1:A:44:ILE:HG22	1:A:45:ARG:N	2.02	0.75
1:A:316:ASP:OD2	1:A:318:THR:HB	1.86	0.75
1:C:393:GLN:HG3	1:C:394:LYS:N	2.01	0.75
1:E:46:PRO:O	1:E:313:THR:HG22	1.86	0.74
1:D:121:ARG:N	4:D:1022:HOH:O	2.20	0.74
1:A:46:PRO:O	1:A:313:THR:HG22	1.88	0.74
1:D:281:ASP:O	1:D:325:LYS:HA	1.88	0.73
1:E:271:LYS:HD2	4:E:1009:HOH:O	1.89	0.73
1:A:281:ASP:O	1:A:325:LYS:HA	1.89	0.72
1:F:297:GLU:HG3	1:F:298:GLN:H	1.52	0.72
1:C:281:ASP:O	1:C:325:LYS:HA	1.89	0.72
1:F:316:ASP:OD2	1:F:318:THR:HB	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:281:ASP:O	1:F:325:LYS:HA	1.91	0.71
1:C:45:ARG:HD2	1:C:47:ASP:OD2	1.90	0.71
1:B:281:ASP:O	1:B:325:LYS:HA	1.90	0.71
1:E:316:ASP:OD2	1:E:318:THR:HB	1.89	0.71
1:B:316:ASP:OD2	1:B:318:THR:HB	1.91	0.69
1:E:281:ASP:O	1:E:325:LYS:HA	1.92	0.69
1:F:266:ARG:O	1:F:270:GLU:HG3	1.93	0.69
1:A:44:ILE:CG2	1:A:45:ARG:N	2.56	0.69
1:C:266:ARG:O	1:C:270:GLU:HG3	1.92	0.69
1:A:44:ILE:CG2	1:A:45:ARG:H	2.06	0.69
1:B:145:PRO:O	1:B:146:THR:HB	1.91	0.69
1:F:43:TRP:CE2	1:F:45:ARG:HG3	2.27	0.68
1:A:118:VAL:HG11	4:A:1019:HOH:O	1.92	0.68
1:D:316:ASP:OD2	1:D:318:THR:HB	1.91	0.68
1:D:173:MET:HA	1:D:173:MET:CE	2.23	0.68
1:B:266:ARG:O	1:B:270:GLU:HG3	1.93	0.68
1:A:299:THR:HG22	1:A:300:THR:HG23	1.75	0.67
1:B:43:TRP:C	1:B:44:ILE:HD12	2.14	0.67
1:A:296:THR:HG22	1:A:297:GLU:N	2.10	0.67
1:F:283:GLU:HB3	1:F:296:THR:HG21	1.75	0.67
1:D:266:ARG:O	1:D:270:GLU:HG3	1.94	0.67
1:C:296:THR:HG22	1:C:297:GLU:N	2.10	0.67
1:F:48:ALA:O	1:F:313:THR:HB	1.95	0.66
1:A:266:ARG:O	1:A:270:GLU:HG3	1.96	0.66
1:E:299:THR:HG22	1:E:300:THR:HG23	1.75	0.66
1:E:296:THR:HG22	1:E:297:GLU:N	2.10	0.66
1:D:296:THR:HG22	1:D:297:GLU:N	2.11	0.66
1:B:296:THR:HG22	1:B:297:GLU:N	2.10	0.66
1:C:299:THR:HG22	1:C:300:THR:HG23	1.76	0.66
1:D:299:THR:HG22	1:D:300:THR:HG23	1.77	0.65
1:F:44:ILE:HG22	1:F:224:ARG:CD	2.27	0.64
1:F:296:THR:HG22	1:F:297:GLU:HG2	1.80	0.64
1:F:173:MET:HA	1:F:173:MET:CE	2.28	0.64
1:E:266:ARG:O	1:E:270:GLU:HG3	1.96	0.64
1:C:46:PRO:O	1:C:313:THR:HG22	1.97	0.64
1:B:299:THR:HG22	1:B:300:THR:HG23	1.78	0.63
1:A:44:ILE:HG22	1:A:45:ARG:H	1.64	0.62
1:C:179:ASP:HB3	1:D:386:LEU:HD13	1.81	0.62
1:F:46:PRO:O	1:F:313:THR:HG22	1.99	0.62
1:A:289:GLU:OE2	1:A:317:ARG:HB3	2.00	0.62
1:A:296:THR:HG21	1:A:298:GLN:HG2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:173:MET:HA	1:E:173:MET:CE	2.30	0.61
1:F:353:THR:HG22	1:F:372:VAL:CG2	2.30	0.61
1:B:46:PRO:O	1:B:313:THR:HG22	2.00	0.61
1:A:179:ASP:HB3	1:B:386:LEU:HD13	1.82	0.61
1:E:296:THR:HG21	1:E:298:GLN:HG2	1.83	0.61
1:C:233:TYR:CE1	1:C:267:LYS:HE3	2.36	0.61
1:C:103:CYS:HB3	1:C:364:LEU:HB3	1.83	0.61
1:A:232:HIS:NE2	4:A:1020:HOH:O	2.29	0.61
1:E:91:ARG:HD2	1:E:93:ASN:OD1	2.02	0.60
1:D:91:ARG:HD2	1:D:93:ASN:OD1	2.02	0.60
1:B:296:THR:HG21	1:B:298:GLN:HG2	1.83	0.60
1:F:280:VAL:HG22	1:F:356:VAL:HG21	1.84	0.60
1:B:91:ARG:HD2	1:B:93:ASN:OD1	2.00	0.60
1:D:46:PRO:O	1:D:313:THR:HG22	2.02	0.60
1:D:121:ARG:HG2	4:D:1020:HOH:O	2.01	0.60
1:F:103:CYS:HB3	1:F:364:LEU:HB3	1.84	0.60
1:B:233:TYR:CE1	1:B:267:LYS:HE3	2.36	0.60
1:E:129:ASP:O	1:E:133:ASP:HB2	2.02	0.60
1:A:48:ALA:O	1:A:313:THR:HB	2.02	0.60
1:E:386:LEU:HD13	1:F:179:ASP:HB3	1.84	0.59
1:C:223:TYR:HE1	4:C:1005:HOH:O	1.84	0.59
1:A:57:GLY:N	4:A:1022:HOH:O	2.34	0.59
1:D:233:TYR:CE1	1:D:267:LYS:HE3	2.36	0.59
1:C:296:THR:HG21	1:C:298:GLN:HG2	1.83	0.59
1:D:353:THR:HG22	1:D:372:VAL:CG2	2.32	0.59
1:C:173:MET:HA	1:C:173:MET:CE	2.31	0.59
1:F:129:ASP:O	1:F:133:ASP:HB2	2.02	0.59
1:D:103:CYS:HB3	1:D:364:LEU:HB3	1.85	0.59
1:D:296:THR:HG21	1:D:298:GLN:HG2	1.84	0.59
1:A:393:GLN:HG3	1:A:394:LYS:N	2.18	0.59
1:A:353:THR:HG22	1:A:372:VAL:CG2	2.33	0.59
1:B:353:THR:HG22	1:B:372:VAL:HG22	1.83	0.59
1:E:310:PHE:O	1:E:312:PRO:HD3	2.03	0.59
1:A:103:CYS:HB3	1:A:364:LEU:HB3	1.85	0.59
1:E:179:ASP:HB3	1:F:386:LEU:HD13	1.84	0.59
1:E:103:CYS:HB3	1:E:364:LEU:HB3	1.85	0.59
1:B:353:THR:HG22	1:B:372:VAL:CG2	2.33	0.58
1:B:310:PHE:O	1:B:312:PRO:HD3	2.03	0.58
1:B:103:CYS:HB3	1:B:364:LEU:HB3	1.85	0.58
1:F:110:GLU:HG2	1:F:118:VAL:CB	2.34	0.58
1:D:353:THR:HG22	1:D:372:VAL:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:PHE:O	1:C:312:PRO:HD3	2.03	0.58
1:B:264:ILE:HG22	1:B:268:LEU:HD22	1.86	0.58
1:A:149:ASN:ND2	3:A:1001:PLP:H2A1	2.18	0.58
1:C:48:ALA:O	1:C:313:THR:HB	2.02	0.58
1:E:233:TYR:CE1	1:E:267:LYS:HE3	2.39	0.58
1:E:353:THR:HG22	1:E:372:VAL:CG2	2.34	0.58
1:C:281:ASP:OD2	1:C:282:PRO:HD2	2.03	0.58
1:E:110:GLU:HG2	1:E:118:VAL:CB	2.33	0.58
1:C:353:THR:HG22	1:C:372:VAL:CG2	2.33	0.58
1:A:353:THR:HG22	1:A:372:VAL:HG22	1.86	0.58
1:A:173:MET:CE	1:A:173:MET:HA	2.34	0.57
1:D:110:GLU:HG2	1:D:118:VAL:CB	2.34	0.57
1:D:237:ALA:HB2	1:D:264:ILE:HA	1.86	0.57
1:B:45:ARG:HH12	1:B:48:ALA:HA	1.70	0.57
1:E:119:LYS:HD2	1:E:150:THR:OG1	2.04	0.57
1:A:264:ILE:HG22	1:A:268:LEU:HD22	1.87	0.57
1:B:110:GLU:HG2	1:B:118:VAL:CB	2.34	0.57
1:C:129:ASP:O	1:C:133:ASP:HB2	2.05	0.57
1:B:237:ALA:HB2	1:B:264:ILE:HA	1.87	0.57
1:F:310:PHE:O	1:F:312:PRO:HD3	2.04	0.57
1:F:353:THR:HG22	1:F:372:VAL:HG22	1.85	0.57
1:A:310:PHE:O	1:A:312:PRO:HD3	2.04	0.57
1:C:106:LEU:HD11	1:C:369:ARG:HD2	1.86	0.57
1:C:95:ILE:HG23	1:C:337:MET:CE	2.35	0.56
1:E:237:ALA:HB2	1:E:264:ILE:HA	1.87	0.56
1:C:296:THR:CG2	1:C:298:GLN:HG2	2.35	0.56
1:C:248:LEU:HD23	1:C:250:MET:H	1.69	0.56
1:A:255:VAL:HG13	1:A:258:GLY:HA2	1.88	0.56
1:E:106:LEU:HD11	1:E:369:ARG:HD2	1.86	0.56
1:E:110:GLU:HG2	1:E:118:VAL:HB	1.88	0.56
1:F:149:ASN:ND2	3:F:1001:PLP:H2A1	2.19	0.56
1:B:296:THR:CG2	1:B:298:GLN:HG2	2.36	0.56
1:D:129:ASP:O	1:D:133:ASP:HB2	2.06	0.56
1:E:353:THR:HG22	1:E:372:VAL:HG22	1.86	0.56
1:E:296:THR:CG2	1:E:298:GLN:HG2	2.35	0.56
1:D:149:ASN:ND2	3:D:1001:PLP:H2A1	2.20	0.56
1:C:264:ILE:HG22	1:C:268:LEU:HD22	1.86	0.56
1:A:110:GLU:HG2	1:A:118:VAL:CB	2.35	0.56
1:D:172:LYS:HD2	1:D:172:LYS:N	2.21	0.56
1:F:172:LYS:HD2	1:F:172:LYS:N	2.21	0.56
1:F:281:ASP:OD2	1:F:282:PRO:HD2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:281:ASP:OD2	1:E:282:PRO:HD2	2.06	0.56
1:B:129:ASP:O	1:B:133:ASP:HB2	2.06	0.56
1:D:119:LYS:C	4:D:1022:HOH:O	2.43	0.56
1:A:386:LEU:HD13	1:B:179:ASP:HB3	1.88	0.56
1:C:110:GLU:HG2	1:C:118:VAL:CB	2.36	0.55
1:B:268:LEU:O	1:B:272:CYS:N	2.40	0.55
1:E:172:LYS:HD2	1:E:172:LYS:N	2.21	0.55
1:F:264:ILE:HG22	1:F:268:LEU:HD22	1.89	0.55
1:A:129:ASP:O	1:A:133:ASP:HB2	2.06	0.55
1:D:264:ILE:HG22	1:D:268:LEU:HD22	1.87	0.55
1:F:91:ARG:HD2	1:F:93:ASN:OD1	2.07	0.55
1:A:248:LEU:HD23	1:A:250:MET:H	1.72	0.55
1:F:106:LEU:HD11	1:F:369:ARG:HD2	1.88	0.55
1:B:172:LYS:N	1:B:172:LYS:HD2	2.21	0.55
1:D:296:THR:CG2	1:D:298:GLN:HG2	2.36	0.55
1:B:173:MET:CE	1:B:173:MET:HA	2.36	0.55
1:A:172:LYS:N	1:A:172:LYS:HD2	2.22	0.55
1:A:296:THR:CG2	1:A:298:GLN:HG2	2.36	0.55
1:C:119:LYS:HD2	1:C:150:THR:OG1	2.06	0.55
1:A:280:VAL:HG22	1:A:356:VAL:HG21	1.89	0.55
1:A:106:LEU:HD11	1:A:369:ARG:HD2	1.88	0.55
1:B:228:ASN:HB3	1:B:229:PRO:CD	2.37	0.55
1:F:235:THR:O	1:F:239:GLU:HG3	2.07	0.54
1:D:228:ASN:HB3	1:D:229:PRO:CD	2.37	0.54
1:B:106:LEU:HD11	1:B:369:ARG:HD2	1.89	0.54
1:C:172:LYS:N	1:C:172:LYS:HD2	2.22	0.54
1:C:353:THR:HG22	1:C:372:VAL:HG22	1.88	0.54
1:E:264:ILE:HG22	1:E:268:LEU:HD22	1.90	0.54
1:C:349:SER:HB3	4:C:1009:HOH:O	2.08	0.54
1:A:296:THR:HG22	1:A:297:GLU:H	1.73	0.54
1:E:149:ASN:ND2	3:E:1001:PLP:H2A1	2.22	0.54
1:A:233:TYR:CE1	1:A:267:LYS:HE3	2.42	0.54
1:D:310:PHE:O	1:D:312:PRO:HD3	2.06	0.54
1:B:248:LEU:HD23	1:B:249:ASP:N	2.23	0.53
1:A:228:ASN:HB3	1:A:229:PRO:CD	2.37	0.53
1:D:49:PRO:O	1:D:50:SER:O	2.26	0.53
1:C:237:ALA:HB2	1:C:264:ILE:HA	1.89	0.53
1:E:248:LEU:HD23	1:E:250:MET:H	1.72	0.53
1:D:296:THR:HG22	1:D:297:GLU:H	1.74	0.53
1:B:95:ILE:HG23	1:B:337:MET:CE	2.38	0.53
1:E:289:GLU:OE2	1:E:317:ARG:HB3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:248:LEU:HD23	1:F:250:MET:H	1.73	0.53
1:C:129:ASP:CA	1:C:132:ARG:HH12	2.14	0.53
1:A:281:ASP:OD2	1:A:282:PRO:HD2	2.09	0.53
1:D:235:THR:O	1:D:239:GLU:HG3	2.09	0.53
1:F:233:TYR:CE1	1:F:267:LYS:HE3	2.43	0.53
1:D:48:ALA:O	1:D:313:THR:HB	2.09	0.53
1:C:268:LEU:O	1:C:272:CYS:N	2.42	0.53
1:D:281:ASP:OD2	1:D:282:PRO:HD2	2.09	0.52
1:F:145:PRO:HB3	1:F:207:ALA:HB2	1.92	0.52
1:C:248:LEU:HD23	1:C:249:ASP:N	2.25	0.52
1:C:110:GLU:HG3	1:C:113:ASN:ND2	2.25	0.52
1:E:296:THR:HG22	1:E:297:GLU:H	1.74	0.52
1:B:147:SER:HB3	1:B:169:MET:SD	2.49	0.52
1:B:281:ASP:OD2	1:B:282:PRO:HD2	2.09	0.52
1:B:149:ASN:ND2	3:B:1001:PLP:H2A1	2.24	0.52
1:C:296:THR:HG22	1:C:297:GLU:H	1.72	0.52
1:F:119:LYS:HD2	1:F:150:THR:OG1	2.10	0.52
1:C:149:ASN:ND2	3:C:1001:PLP:H2A1	2.25	0.52
1:C:255:VAL:HG13	1:C:258:GLY:HA2	1.90	0.52
1:A:237:ALA:HB2	1:A:264:ILE:HA	1.92	0.52
1:B:248:LEU:HD23	1:B:250:MET:H	1.73	0.52
1:D:248:LEU:HD23	1:D:250:MET:H	1.74	0.52
1:A:91:ARG:HD2	1:A:93:ASN:OD1	2.10	0.52
1:F:110:GLU:HG2	1:F:118:VAL:HB	1.91	0.52
1:B:145:PRO:HB3	1:B:207:ALA:HB2	1.92	0.52
1:C:91:ARG:HD2	1:C:93:ASN:OD1	2.09	0.52
1:D:254:SER:HA	1:D:280:VAL:HB	1.92	0.52
1:B:296:THR:HG22	1:B:297:GLU:H	1.75	0.52
1:B:203:HIS:CD2	1:B:204:VAL:HG23	2.45	0.52
1:C:145:PRO:HB3	1:C:207:ALA:HB2	1.92	0.52
1:E:304:GLU:HG3	4:E:1016:HOH:O	2.09	0.52
1:C:386:LEU:HD13	1:D:179:ASP:HB3	1.91	0.52
1:C:329:GLU:O	1:C:333:THR:HG23	2.10	0.51
1:F:255:VAL:HG13	1:F:258:GLY:HA2	1.92	0.51
1:B:110:GLU:HG2	1:B:118:VAL:HB	1.92	0.51
1:C:228:ASN:HB3	1:C:229:PRO:CD	2.41	0.51
1:D:236:THR:O	1:D:240:ILE:HG13	2.11	0.51
1:B:109:CYS:HB3	1:B:111:PHE:CE2	2.45	0.51
1:D:106:LEU:HD11	1:D:369:ARG:HD2	1.91	0.51
1:F:224:ARG:HG2	1:F:313:THR:HG23	1.89	0.51
1:F:203:HIS:CD2	1:F:204:VAL:HG23	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:147:SER:HB3	1:D:169:MET:HB2	1.92	0.51
1:E:235:THR:O	1:E:239:GLU:HG3	2.11	0.51
1:E:95:ILE:HG23	1:E:337:MET:CE	2.40	0.51
1:E:398:LYS:HG3	1:E:399:GLU:N	2.18	0.51
1:A:203:HIS:CD2	1:A:204:VAL:HG23	2.46	0.51
1:D:121:ARG:HB2	4:D:1022:HOH:O	2.11	0.51
1:B:254:SER:HA	1:B:280:VAL:HB	1.93	0.51
1:E:203:HIS:CD2	1:E:204:VAL:HG23	2.46	0.51
1:C:203:HIS:CD2	1:C:204:VAL:HG23	2.46	0.51
1:A:268:LEU:O	1:A:272:CYS:N	2.41	0.51
1:B:376:ASP:HB2	4:B:1028:HOH:O	2.11	0.51
1:E:268:LEU:O	1:E:272:CYS:N	2.41	0.51
1:D:248:LEU:HD23	1:D:249:ASP:N	2.26	0.51
1:B:255:VAL:HG13	1:B:258:GLY:HA2	1.93	0.51
1:E:228:ASN:HB3	1:E:229:PRO:CD	2.40	0.51
1:B:329:GLU:O	1:B:333:THR:HG23	2.11	0.50
1:E:145:PRO:HB3	1:E:207:ALA:HB2	1.92	0.50
1:B:119:LYS:HD2	1:B:150:THR:OG1	2.11	0.50
1:F:95:ILE:HG23	1:F:337:MET:CE	2.41	0.50
1:D:119:LYS:HD2	1:D:150:THR:OG1	2.10	0.50
1:F:296:THR:CG2	1:F:297:GLU:HG2	2.41	0.50
1:F:110:GLU:HG3	1:F:113:ASN:ND2	2.27	0.50
1:D:329:GLU:O	1:D:333:THR:HG23	2.11	0.50
1:F:228:ASN:HB3	1:F:229:PRO:CD	2.41	0.50
1:A:95:ILE:HG23	1:A:337:MET:CE	2.41	0.50
1:D:288:ALA:HA	1:D:323:TRP:CD2	2.46	0.50
1:A:110:GLU:HG2	1:A:118:VAL:HG23	1.93	0.50
1:A:262:THR:HG23	1:A:316:ASP:HB3	1.93	0.50
1:E:329:GLU:O	1:E:333:THR:HG23	2.12	0.50
1:E:254:SER:HA	1:E:280:VAL:HB	1.94	0.50
1:C:132:ARG:NH1	1:C:132:ARG:HB3	2.27	0.50
1:D:203:HIS:CD2	1:D:204:VAL:HG23	2.46	0.50
1:F:296:THR:HG22	1:F:297:GLU:N	2.25	0.50
1:F:268:LEU:O	1:F:272:CYS:N	2.43	0.50
1:F:169:MET:HE2	1:F:188:ILE:HG23	1.94	0.50
1:C:150:THR:OG1	1:C:222:GLN:NE2	2.45	0.50
1:F:292:GLU:O	1:F:294:ASN:N	2.45	0.50
1:D:110:GLU:HG2	1:D:118:VAL:HB	1.94	0.49
1:A:288:ALA:HA	1:A:323:TRP:CD2	2.46	0.49
1:D:255:VAL:HG13	1:D:258:GLY:HA2	1.93	0.49
1:D:110:GLU:HG3	1:D:113:ASN:ND2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:237:ALA:HB2	1:F:264:ILE:HA	1.94	0.49
1:C:254:SER:HA	1:C:280:VAL:HB	1.94	0.49
1:E:255:VAL:HG13	1:E:258:GLY:HA2	1.93	0.49
1:D:147:SER:HB2	1:D:173:MET:CG	2.43	0.49
1:D:169:MET:HE2	1:D:188:ILE:HG23	1.93	0.49
1:F:288:ALA:HB3	1:F:294:ASN:HD21	1.77	0.49
1:D:45:ARG:HD2	1:D:47:ASP:OD1	2.12	0.49
1:D:110:GLU:HG2	1:D:118:VAL:HG23	1.94	0.49
1:A:119:LYS:HD2	1:A:150:THR:OG1	2.13	0.49
1:B:280:VAL:HG22	1:B:356:VAL:HG21	1.94	0.49
1:B:393:GLN:HG3	1:B:394:LYS:N	2.26	0.49
1:B:178:VAL:O	1:B:182:ARG:HG3	2.13	0.49
1:B:132:ARG:NH1	1:B:132:ARG:HB3	2.28	0.49
1:A:329:GLU:O	1:A:333:THR:HG23	2.12	0.49
1:A:292:GLU:O	1:A:295:GLN:HG3	2.13	0.49
1:A:248:LEU:HD23	1:A:249:ASP:N	2.27	0.49
1:D:145:PRO:HB3	1:D:207:ALA:HB2	1.94	0.49
1:D:95:ILE:HG12	1:D:337:MET:CE	2.42	0.49
1:D:70:PRO:HG2	1:D:238:ASP:HB3	1.95	0.49
1:A:110:GLU:HG3	1:A:113:ASN:ND2	2.28	0.49
1:F:44:ILE:HG22	1:F:224:ARG:HD2	1.94	0.48
1:C:110:GLU:HG2	1:C:118:VAL:HB	1.95	0.48
1:C:43:TRP:HA	1:C:208:TRP:CE2	2.47	0.48
1:A:110:GLU:HG2	1:A:118:VAL:HB	1.95	0.48
1:C:289:GLU:OE2	1:C:317:ARG:HB3	2.12	0.48
1:F:132:ARG:NH1	1:F:132:ARG:HB3	2.28	0.48
1:D:147:SER:CB	1:D:173:MET:HG2	2.43	0.48
1:D:129:ASP:CA	1:D:132:ARG:HH12	2.18	0.48
1:F:276:ARG:CZ	1:F:363:GLU:OE2	2.62	0.48
1:A:169:MET:HE2	1:A:188:ILE:HG23	1.95	0.48
1:D:254:SER:HB2	1:D:306:ILE:HG21	1.95	0.48
1:E:296:THR:HG21	1:E:298:GLN:CG	2.43	0.48
1:B:44:ILE:N	1:B:44:ILE:HD12	2.29	0.48
1:B:254:SER:HB2	1:B:306:ILE:HG21	1.95	0.48
1:A:109:CYS:HB3	1:A:111:PHE:CE2	2.49	0.48
1:A:145:PRO:HB3	1:A:207:ALA:HB2	1.95	0.48
1:E:168:VAL:HG12	1:E:203:HIS:HB2	1.96	0.48
1:D:264:ILE:CD1	1:D:373:ILE:HD11	2.43	0.48
1:B:110:GLU:HG3	1:B:113:ASN:ND2	2.29	0.48
1:E:248:LEU:HD23	1:E:249:ASP:N	2.28	0.48
1:C:271:LYS:NZ	4:C:1019:HOH:O	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:CYS:HB3	1:D:111:PHE:CE2	2.49	0.48
1:E:132:ARG:NH1	1:E:132:ARG:HB3	2.28	0.48
1:D:173:MET:HE2	1:D:173:MET:HA	1.96	0.48
1:A:254:SER:HA	1:A:280:VAL:HB	1.96	0.48
1:E:280:VAL:HG22	1:E:356:VAL:HG21	1.96	0.48
1:C:169:MET:HE2	1:C:188:ILE:HG23	1.94	0.48
1:C:296:THR:HG21	1:C:298:GLN:CG	2.43	0.47
1:B:110:GLU:HG2	1:B:118:VAL:HG23	1.96	0.47
1:B:296:THR:CG2	1:B:297:GLU:N	2.77	0.47
1:A:129:ASP:CA	1:A:132:ARG:HH12	2.18	0.47
1:E:173:MET:HA	1:E:173:MET:HE3	1.96	0.47
1:C:288:ALA:HA	1:C:323:TRP:CD2	2.49	0.47
1:C:292:GLU:O	1:C:295:GLN:HG3	2.15	0.47
1:B:223:TYR:O	1:B:314:VAL:HG13	2.14	0.47
1:D:280:VAL:HG22	1:D:356:VAL:HG21	1.97	0.47
1:A:296:THR:CG2	1:A:297:GLU:N	2.77	0.47
1:C:296:THR:CG2	1:C:297:GLU:N	2.77	0.47
1:F:264:ILE:CD1	1:F:373:ILE:HD11	2.44	0.47
1:A:132:ARG:NH1	1:A:132:ARG:HB3	2.29	0.47
1:C:110:GLU:HG2	1:C:118:VAL:HG23	1.96	0.47
1:D:289:GLU:OE2	1:D:317:ARG:HB3	2.14	0.47
1:B:292:GLU:O	1:B:295:GLN:HG3	2.15	0.47
1:D:132:ARG:NH1	1:D:132:ARG:HB3	2.29	0.47
1:C:45:ARG:O	1:C:45:ARG:HG3	2.14	0.47
1:F:248:LEU:HD23	1:F:249:ASP:N	2.29	0.47
1:B:235:THR:O	1:B:239:GLU:HG3	2.14	0.47
1:A:254:SER:HB2	1:A:306:ILE:HG21	1.96	0.47
1:C:375:PRO:HD2	4:C:1009:HOH:O	2.15	0.47
1:F:178:VAL:O	1:F:182:ARG:HG3	2.15	0.47
1:E:288:ALA:HA	1:E:323:TRP:CD2	2.50	0.47
1:B:48:ALA:O	1:B:313:THR:HB	2.14	0.47
1:D:168:VAL:HG12	1:D:203:HIS:HB2	1.97	0.47
1:B:264:ILE:CD1	1:B:373:ILE:HD11	2.45	0.47
1:E:296:THR:CG2	1:E:297:GLU:N	2.77	0.47
1:C:224:ARG:HG2	1:C:313:THR:HG23	1.94	0.47
1:F:297:GLU:CG	1:F:298:GLN:H	2.22	0.47
1:B:150:THR:OG1	1:B:222:GLN:NE2	2.48	0.47
1:F:43:TRP:HE1	1:F:45:ARG:HG3	1.72	0.46
1:D:268:LEU:O	1:D:272:CYS:N	2.44	0.46
1:F:44:ILE:HG21	1:F:224:ARG:CZ	2.45	0.46
1:B:224:ARG:HG2	1:B:313:THR:HG23	1.92	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:95:ILE:HG12	1:F:337:MET:HE3	1.96	0.46
1:C:52:CYS:HA	2:C:501:HEM:C1A	2.50	0.46
1:E:44:ILE:HG22	1:E:224:ARG:HD2	1.97	0.46
1:B:147:SER:HB3	1:B:169:MET:CB	2.45	0.46
1:C:254:SER:HB2	1:C:306:ILE:HG21	1.96	0.46
1:C:159:ALA:O	1:D:94:LYS:NZ	2.48	0.46
1:D:224:ARG:HG2	1:D:313:THR:HG23	1.93	0.46
1:D:147:SER:HB2	1:D:173:MET:HG3	1.96	0.46
1:F:150:THR:OG1	1:F:222:GLN:NE2	2.48	0.46
1:B:296:THR:HG21	1:B:298:GLN:CG	2.44	0.46
1:F:168:VAL:HG12	1:F:203:HIS:HB2	1.97	0.46
1:E:366:GLU:HG2	1:E:366:GLU:H	1.52	0.46
1:C:284:GLY:HA2	1:C:298:GLN:O	2.16	0.46
1:A:226:ALA:HA	2:A:501:HEM:HMD2	1.98	0.46
1:D:296:THR:HG21	1:D:298:GLN:CG	2.45	0.46
1:F:297:GLU:HG3	1:F:298:GLN:N	2.25	0.46
1:E:52:CYS:HA	2:E:501:HEM:C1A	2.50	0.46
1:A:296:THR:HG21	1:A:298:GLN:CG	2.45	0.46
1:F:173:MET:HA	1:F:173:MET:HE2	1.95	0.46
1:C:353:THR:CG2	1:C:372:VAL:HG22	2.46	0.46
1:F:276:ARG:NH1	1:F:363:GLU:OE2	2.49	0.46
1:E:111:PHE:HB3	1:E:376:ASP:C	2.36	0.46
1:E:110:GLU:HG3	1:E:113:ASN:ND2	2.31	0.46
1:F:329:GLU:O	1:F:333:THR:HG23	2.15	0.46
1:A:178:VAL:O	1:A:182:ARG:HG3	2.15	0.46
1:C:96:GLY:O	1:C:101:LEU:HB2	2.16	0.46
1:C:111:PHE:HB3	1:C:376:ASP:C	2.37	0.46
1:F:353:THR:CG2	1:F:372:VAL:HG22	2.46	0.46
1:F:70:PRO:HG2	1:F:238:ASP:HB3	1.98	0.46
1:E:202:SER:O	1:E:206:VAL:HG23	2.16	0.46
1:E:292:GLU:O	1:E:295:GLN:HG3	2.16	0.45
1:B:366:GLU:H	1:B:366:GLU:HG2	1.54	0.45
1:D:150:THR:OG1	1:D:222:GLN:NE2	2.50	0.45
1:C:280:VAL:HG22	1:C:356:VAL:HG21	1.98	0.45
1:D:95:ILE:HG12	1:D:337:MET:HE3	1.98	0.45
1:F:289:GLU:OE2	1:F:317:ARG:HD3	2.16	0.45
1:C:366:GLU:HG2	1:C:366:GLU:H	1.57	0.45
1:E:391:MET:HB3	1:E:397:LEU:HB2	1.99	0.45
1:E:119:LYS:HG3	1:E:149:ASN:HB2	1.97	0.45
1:A:264:ILE:CD1	1:A:373:ILE:HD11	2.46	0.45
1:E:70:PRO:HG2	1:E:238:ASP:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:PRO:O	1:D:146:THR:HB	2.17	0.45
1:B:52:CYS:HA	2:B:501:HEM:C1A	2.51	0.45
1:D:178:VAL:O	1:D:182:ARG:HG3	2.16	0.45
1:C:132:ARG:HB3	1:C:132:ARG:CZ	2.46	0.45
1:A:52:CYS:HA	2:A:501:HEM:C1A	2.52	0.45
1:D:111:PHE:HB3	1:D:376:ASP:C	2.36	0.45
1:C:178:VAL:O	1:C:182:ARG:HG3	2.17	0.45
1:A:119:LYS:HG3	1:A:149:ASN:HB2	1.99	0.45
1:D:70:PRO:HG3	1:D:235:THR:HA	1.98	0.45
1:D:292:GLU:O	1:D:295:GLN:HG3	2.17	0.45
1:F:254:SER:HA	1:F:280:VAL:HB	1.99	0.45
1:D:353:THR:CG2	1:D:372:VAL:HG22	2.46	0.45
1:B:70:PRO:HG2	1:B:238:ASP:HB3	1.99	0.45
1:B:288:ALA:HA	1:B:323:TRP:CD2	2.52	0.45
1:A:235:THR:O	1:A:239:GLU:HG3	2.16	0.45
1:D:96:GLY:O	1:D:101:LEU:HB2	2.16	0.45
1:F:298:GLN:HG3	1:F:300:THR:O	2.17	0.45
1:B:262:THR:HG23	1:B:316:ASP:HB3	1.99	0.45
1:B:353:THR:CG2	1:B:372:VAL:HG22	2.46	0.45
1:C:119:LYS:HG3	1:C:149:ASN:HB2	1.98	0.45
1:E:70:PRO:HG3	1:E:235:THR:HA	1.99	0.45
1:D:202:SER:O	1:D:206:VAL:HG23	2.17	0.45
1:E:169:MET:HE2	1:E:188:ILE:HG23	1.98	0.45
1:E:178:VAL:O	1:E:182:ARG:HG3	2.17	0.45
1:C:264:ILE:CD1	1:C:373:ILE:HD11	2.47	0.45
1:C:168:VAL:HG12	1:C:203:HIS:HB2	1.99	0.44
1:D:122:ILE:N	4:D:1022:HOH:O	2.26	0.44
1:F:296:THR:CG2	1:F:297:GLU:N	2.80	0.44
1:E:48:ALA:HA	1:E:49:PRO:HD2	1.79	0.44
1:F:236:THR:O	1:F:240:ILE:HG13	2.17	0.44
1:F:262:THR:HG23	1:F:316:ASP:HB3	2.00	0.44
1:E:353:THR:CG2	1:E:372:VAL:HG22	2.48	0.44
1:E:264:ILE:CD1	1:E:373:ILE:HD11	2.47	0.44
1:C:70:PRO:HG3	1:C:235:THR:HA	1.99	0.44
1:F:111:PHE:HB3	1:F:376:ASP:C	2.37	0.44
1:B:147:SER:OG	1:B:173:MET:CG	2.65	0.44
1:F:95:ILE:HG12	1:F:337:MET:CE	2.47	0.44
1:F:52:CYS:HA	2:F:501:HEM:C1A	2.52	0.44
1:E:43:TRP:O	1:E:44:ILE:HG12	2.16	0.44
1:D:262:THR:HG23	1:D:316:ASP:HB3	1.99	0.44
1:C:361:ALA:O	1:C:364:LEU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:PHE:HB3	1:A:376:ASP:C	2.37	0.44
1:D:52:CYS:HA	2:D:501:HEM:C1A	2.52	0.44
1:F:96:GLY:O	1:F:101:LEU:HB2	2.17	0.44
1:A:168:VAL:HG12	1:A:203:HIS:HB2	1.99	0.44
1:C:262:THR:HG23	1:C:316:ASP:HB3	1.99	0.44
1:B:169:MET:HE2	1:B:188:ILE:HG23	1.99	0.44
1:C:235:THR:O	1:C:239:GLU:HG3	2.17	0.44
1:B:168:VAL:HG12	1:B:203:HIS:HB2	1.99	0.44
1:F:254:SER:HB2	1:F:306:ILE:HG21	1.99	0.44
1:B:308:TYR:HD2	1:B:310:PHE:O	2.01	0.44
1:F:110:GLU:CG	1:F:118:VAL:HA	2.48	0.44
1:B:132:ARG:CZ	1:B:132:ARG:HB3	2.47	0.44
1:D:110:GLU:CG	1:D:118:VAL:HA	2.48	0.44
1:F:145:PRO:O	1:F:146:THR:HB	2.18	0.44
1:C:214:ILE:HA	1:C:215:PRO:HD3	1.91	0.44
1:A:70:PRO:HG2	1:A:238:ASP:HB3	2.00	0.44
1:F:226:ALA:HA	2:F:501:HEM:HMD2	1.99	0.44
1:E:150:THR:OG1	1:E:222:GLN:NE2	2.51	0.44
1:C:95:ILE:HG23	1:C:337:MET:HE3	1.99	0.44
1:E:109:CYS:HB3	1:E:111:PHE:CE2	2.53	0.44
1:F:311:ILE:CD1	1:F:317:ARG:NH1	2.81	0.44
1:A:132:ARG:HB3	1:A:132:ARG:CZ	2.47	0.43
1:A:353:THR:CG2	1:A:372:VAL:HG22	2.47	0.43
1:F:110:GLU:HG2	1:F:118:VAL:HG23	2.00	0.43
1:D:95:ILE:HG23	1:D:337:MET:CE	2.47	0.43
1:C:271:LYS:HE3	4:C:1014:HOH:O	2.18	0.43
1:C:209:ARG:O	1:C:213:GLU:HG3	2.18	0.43
1:A:77:LEU:N	1:A:77:LEU:HD12	2.32	0.43
1:D:295:GLN:O	1:D:296:THR:OG1	2.34	0.43
1:F:119:LYS:HG3	1:F:149:ASN:HB2	2.00	0.43
1:E:254:SER:HB2	1:E:306:ILE:HG21	1.99	0.43
1:E:47:ASP:O	1:E:48:ALA:HB3	2.18	0.43
1:C:308:TYR:HD2	1:C:310:PHE:O	2.02	0.43
1:A:70:PRO:HG3	1:A:235:THR:HA	1.99	0.43
1:F:220:LEU:HA	1:F:220:LEU:HD23	1.79	0.43
1:D:296:THR:CG2	1:D:297:GLU:N	2.77	0.43
1:F:129:ASP:CA	1:F:132:ARG:HH12	2.19	0.43
1:E:397:LEU:HD22	1:E:398:LYS:H	1.82	0.43
1:B:248:LEU:HD22	1:B:275:CYS:SG	2.58	0.43
1:E:311:ILE:HD13	1:E:317:ARG:CZ	2.49	0.43
1:F:288:ALA:HA	1:F:323:TRP:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:PRO:HG2	1:C:238:ASP:HB3	2.00	0.43
1:F:101:LEU:HD12	1:F:101:LEU:HA	1.90	0.43
1:A:202:SER:O	1:A:206:VAL:HG23	2.18	0.43
1:D:132:ARG:CZ	1:D:132:ARG:HB3	2.48	0.43
1:D:44:ILE:O	1:D:45:ARG:O	2.37	0.43
1:B:214:ILE:HA	1:B:215:PRO:HD3	1.89	0.43
1:A:308:TYR:HD2	1:A:310:PHE:O	2.02	0.43
1:A:96:GLY:O	1:A:101:LEU:HB2	2.18	0.43
1:C:202:SER:O	1:C:206:VAL:HG23	2.18	0.43
1:F:132:ARG:HB3	1:F:132:ARG:CZ	2.48	0.43
1:D:119:LYS:HG3	1:D:149:ASN:HB2	1.99	0.43
1:C:44:ILE:O	1:C:45:ARG:C	2.57	0.43
1:C:109:CYS:HB3	1:C:111:PHE:CE2	2.54	0.43
1:B:289:GLU:OE2	1:B:317:ARG:HB3	2.18	0.43
1:E:132:ARG:CZ	1:E:132:ARG:HB3	2.49	0.43
1:C:223:TYR:O	1:C:314:VAL:HG13	2.19	0.43
1:D:241:LEU:HD21	1:D:268:LEU:HD12	2.01	0.43
1:A:95:ILE:HG12	1:A:337:MET:CE	2.48	0.43
1:F:311:ILE:HD13	1:F:317:ARG:NH1	2.33	0.43
1:B:111:PHE:HB3	1:B:376:ASP:C	2.40	0.43
1:C:226:ALA:HA	2:C:501:HEM:HMD2	2.01	0.43
1:B:303:VAL:HG22	1:B:328:ASP:OD2	2.19	0.43
1:B:110:GLU:CG	1:B:118:VAL:HA	2.49	0.42
1:D:226:ALA:HA	2:D:501:HEM:HMD2	2.00	0.42
1:B:202:SER:O	1:B:206:VAL:HG23	2.19	0.42
1:F:366:GLU:H	1:F:366:GLU:HG2	1.56	0.42
1:B:96:GLY:O	1:B:101:LEU:HB2	2.19	0.42
1:B:119:LYS:HG3	1:B:149:ASN:HB2	2.00	0.42
1:C:311:ILE:HD13	1:C:317:ARG:CZ	2.48	0.42
1:B:70:PRO:HG3	1:B:235:THR:HA	2.02	0.42
1:D:62:GLU:O	2:D:501:HEM:HMB1	2.19	0.42
1:A:126:MET:HG2	1:A:227:SER:HB2	2.01	0.42
1:A:44:ILE:HD12	1:A:44:ILE:HA	1.66	0.42
1:A:110:GLU:CG	1:A:118:VAL:HA	2.49	0.42
1:B:373:ILE:O	1:B:375:PRO:HD3	2.19	0.42
1:D:101:LEU:HD12	1:D:101:LEU:HA	1.88	0.42
1:E:244:CYS:HB3	1:E:247:LYS:O	2.20	0.42
1:F:44:ILE:HA	1:F:44:ILE:HD13	1.65	0.42
1:F:44:ILE:HG22	1:F:224:ARG:HD3	2.02	0.42
1:A:311:ILE:HD13	1:A:317:ARG:CZ	2.49	0.42
1:B:95:ILE:HG12	1:B:337:MET:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:ILE:O	1:A:99:PHE:HD1	2.03	0.42
1:A:110:GLU:HG2	1:A:118:VAL:CG2	2.49	0.42
1:F:70:PRO:HG3	1:F:235:THR:HA	2.01	0.42
1:E:96:GLY:O	1:E:101:LEU:HB2	2.19	0.42
1:D:126:MET:HG2	1:D:227:SER:HB2	2.00	0.42
1:C:95:ILE:HG12	1:C:337:MET:CE	2.49	0.42
1:C:110:GLU:CG	1:C:118:VAL:HA	2.50	0.42
1:A:233:TYR:CD1	1:A:267:LYS:HB2	2.54	0.42
1:D:121:ARG:CA	4:D:1022:HOH:O	2.65	0.42
1:D:233:TYR:CD1	1:D:267:LYS:HB2	2.55	0.42
1:A:150:THR:OG1	1:A:222:GLN:NE2	2.53	0.42
1:A:229:PRO:O	2:A:501:HEM:HBC1	2.20	0.42
1:D:366:GLU:HG2	1:D:366:GLU:H	1.55	0.42
1:E:77:LEU:N	1:E:77:LEU:HD12	2.35	0.42
1:A:244:CYS:HB3	1:A:247:LYS:O	2.20	0.42
1:A:295:GLN:O	1:A:296:THR:OG1	2.35	0.42
1:D:110:GLU:HG2	1:D:118:VAL:CG2	2.49	0.42
1:B:43:TRP:HD1	1:B:208:TRP:CE3	2.37	0.42
1:B:44:ILE:N	1:B:44:ILE:CD1	2.83	0.42
1:C:311:ILE:CD1	1:C:317:ARG:NH1	2.83	0.42
1:A:346:CYS:O	1:A:378:VAL:CG1	2.68	0.42
1:E:147:SER:HB2	1:E:173:MET:CG	2.50	0.41
1:B:241:LEU:HD21	1:B:268:LEU:HD12	2.02	0.41
1:F:308:TYR:HD2	1:F:310:PHE:O	2.02	0.41
1:C:173:MET:HA	1:C:173:MET:HE2	2.02	0.41
1:A:173:MET:HE3	1:A:177:LYS:NZ	2.35	0.41
1:F:79:ASP:OD1	1:F:81:LEU:N	2.53	0.41
1:B:190:ARG:NH1	1:B:190:ARG:HG3	2.35	0.41
1:E:110:GLU:CG	1:E:118:VAL:HA	2.50	0.41
1:E:311:ILE:CD1	1:E:317:ARG:NH1	2.83	0.41
1:D:223:TYR:O	1:D:314:VAL:HG13	2.20	0.41
1:F:202:SER:O	1:F:206:VAL:HG23	2.20	0.41
1:A:220:LEU:HA	1:A:220:LEU:HD23	1.84	0.41
1:F:45:ARG:O	1:F:224:ARG:HD2	2.20	0.41
1:B:110:GLU:HG2	1:B:118:VAL:CG2	2.51	0.41
1:F:311:ILE:HD13	1:F:317:ARG:CZ	2.50	0.41
1:D:268:LEU:HA	1:D:268:LEU:HD12	1.90	0.41
1:E:129:ASP:CA	1:E:132:ARG:HH12	2.19	0.41
1:E:392:LEU:HD23	1:E:397:LEU:O	2.21	0.41
1:A:224:ARG:HG2	1:A:313:THR:HG23	1.98	0.41
1:C:102:LYS:NZ	1:C:365:GLN:HA	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:45:ARG:HB2	1:F:45:ARG:HE	1.30	0.41
1:D:147:SER:CB	1:D:173:MET:CG	2.99	0.41
1:A:373:ILE:O	1:A:375:PRO:HD3	2.21	0.41
1:A:261:ILE:O	1:A:265:ALA:CB	2.69	0.41
1:E:308:TYR:HD2	1:E:310:PHE:O	2.02	0.41
1:C:248:LEU:HD22	1:C:275:CYS:SG	2.61	0.41
1:A:62:GLU:O	2:A:501:HEM:HMB1	2.21	0.41
1:B:95:ILE:O	1:B:99:PHE:HD1	2.04	0.41
1:C:145:PRO:O	1:C:146:THR:HB	2.21	0.41
1:A:95:ILE:HG12	1:A:337:MET:HE3	2.02	0.41
1:B:226:ALA:HA	2:B:501:HEM:HMD2	2.02	0.41
1:D:214:ILE:HB	1:D:217:SER:OG	2.20	0.41
1:F:165:CYS:SG	1:F:167:ILE:CD1	3.09	0.41
1:C:346:CYS:O	1:C:378:VAL:CG1	2.69	0.41
1:A:366:GLU:H	1:A:366:GLU:HG2	1.60	0.41
1:A:97:LYS:HG2	4:A:1006:HOH:O	2.21	0.41
1:D:102:LYS:HE3	1:D:365:GLN:HA	2.02	0.41
1:E:214:ILE:HA	1:E:215:PRO:HD3	1.89	0.41
1:C:110:GLU:HG2	1:C:118:VAL:HA	2.02	0.40
1:E:159:ALA:O	1:F:94:LYS:NZ	2.51	0.40
1:B:295:GLN:O	1:B:296:THR:OG1	2.34	0.40
1:A:311:ILE:CD1	1:A:317:ARG:NH1	2.85	0.40
1:E:361:ALA:O	1:E:364:LEU:HB2	2.22	0.40
1:D:272:CYS:O	1:D:275:CYS:HB2	2.22	0.40
1:E:145:PRO:O	1:E:146:THR:HB	2.21	0.40
1:C:101:LEU:HD12	1:C:101:LEU:HA	1.86	0.40
1:D:284:GLY:HA2	1:D:298:GLN:O	2.22	0.40
1:F:361:ALA:O	1:F:364:LEU:HB2	2.21	0.40
1:A:303:VAL:HG22	1:A:328:ASP:OD2	2.21	0.40
1:C:244:CYS:HB3	1:C:247:LYS:O	2.22	0.40
1:F:214:ILE:HA	1:F:215:PRO:HD3	1.91	0.40
1:E:110:GLU:HG2	1:E:118:VAL:HG23	2.03	0.40
1:E:226:ALA:HA	2:E:501:HEM:HMD2	2.02	0.40
1:D:244:CYS:HB3	1:D:247:LYS:O	2.21	0.40
1:A:284:GLY:HA2	1:A:298:GLN:O	2.21	0.40
1:B:110:GLU:HG2	1:B:118:VAL:HA	2.04	0.40
1:F:226:ALA:HA	2:F:501:HEM:CMD	2.52	0.40
1:B:214:ILE:HB	1:B:217:SER:OG	2.21	0.40
1:D:214:ILE:HA	1:D:215:PRO:HD3	1.90	0.40
1:B:261:ILE:O	1:B:265:ALA:CB	2.70	0.40
1:D:303:VAL:HG22	1:D:328:ASP:OD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:ARG:NH1	1:C:190:ARG:HG3	2.37	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	344/435 (79%)	325 (94%)	16 (5%)	3 (1%)	21	42
1	B	344/435 (79%)	319 (93%)	19 (6%)	6 (2%)	11	22
1	C	344/435 (79%)	323 (94%)	18 (5%)	3 (1%)	21	42
1	D	344/435 (79%)	319 (93%)	19 (6%)	6 (2%)	11	22
1	E	346/435 (80%)	321 (93%)	19 (6%)	6 (2%)	11	22
1	F	344/435 (79%)	322 (94%)	17 (5%)	5 (2%)	13	26
All	All	2066/2610 (79%)	1929 (93%)	108 (5%)	29 (1%)	14	28

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	50	SER
1	B	146	THR
1	B	173	MET
1	C	173	MET
1	D	45	ARG
1	D	50	SER
1	D	173	MET
1	E	173	MET
1	F	173	MET
1	A	170	PRO
1	A	173	MET

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Mol	Chain	Res	Type
1	A	192	PRO
1	B	170	PRO
1	B	192	PRO
1	C	192	PRO
1	D	170	PRO
1	D	192	PRO
1	E	170	PRO
1	E	192	PRO
1	F	170	PRO
1	F	192	PRO
1	F	293	LEU
1	C	170	PRO
1	E	47	ASP
1	E	398	LYS
1	F	297	GLU
1	B	49	PRO
1	D	49	PRO
1	E	48	ALA

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	288/362 (80%)	272 (94%)	16 (6%)	26	50
1	B	288/362 (80%)	273 (95%)	15 (5%)	29	54
1	C	288/362 (80%)	272 (94%)	16 (6%)	26	50
1	D	288/362 (80%)	272 (94%)	16 (6%)	26	50
1	E	290/362 (80%)	272 (94%)	18 (6%)	23	45
1	F	288/362 (80%)	272 (94%)	16 (6%)	26	50
All	All	1730/2172 (80%)	1633 (94%)	97 (6%)	26	50

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ILE
1	A	46	PRO
1	A	101	LEU
1	A	105	LEU
1	A	133	ASP
1	A	173	MET
1	A	176	GLU
1	A	203	HIS
1	A	208	TRP
1	A	242	GLN
1	A	268	LEU
1	A	299	THR
1	A	309	ASP
1	A	313	THR
1	A	386	LEU
1	A	393	GLN
1	B	47	ASP
1	B	101	LEU
1	B	105	LEU
1	B	133	ASP
1	B	173	MET
1	B	176	GLU
1	B	203	HIS
1	B	208	TRP
1	B	268	LEU
1	B	299	THR
1	B	309	ASP
1	B	313	THR
1	B	372	VAL
1	B	386	LEU
1	B	393	GLN
1	C	46	PRO
1	C	47	ASP
1	C	101	LEU
1	C	105	LEU
1	C	133	ASP
1	C	173	MET
1	C	176	GLU
1	C	203	HIS
1	C	208	TRP
1	C	242	GLN
1	C	268	LEU
1	C	299	THR

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Mol	Chain	Res	Type
1	C	309	ASP
1	C	313	THR
1	C	386	LEU
1	C	393	GLN
1	D	46	PRO
1	D	101	LEU
1	D	105	LEU
1	D	133	ASP
1	D	173	MET
1	D	176	GLU
1	D	203	HIS
1	D	208	TRP
1	D	268	LEU
1	D	276	ARG
1	D	299	THR
1	D	309	ASP
1	D	313	THR
1	D	364	LEU
1	D	386	LEU
1	D	393	GLN
1	E	45	ARG
1	E	46	PRO
1	E	101	LEU
1	E	105	LEU
1	E	133	ASP
1	E	173	MET
1	E	176	GLU
1	E	203	HIS
1	E	208	TRP
1	E	242	GLN
1	E	268	LEU
1	E	299	THR
1	E	309	ASP
1	E	313	THR
1	E	372	VAL
1	E	386	LEU
1	E	393	GLN
1	E	398	LYS
1	F	43	TRP
1	F	44	ILE
1	F	45	ARG
1	F	46	PRO

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Mol	Chain	Res	Type
1	F	101	LEU
1	F	105	LEU
1	F	133	ASP
1	F	173	MET
1	F	176	GLU
1	F	203	HIS
1	F	208	TRP
1	F	242	GLN
1	F	268	LEU
1	F	309	ASP
1	F	313	THR
1	F	386	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	HIS
1	A	222	GLN
1	A	242	GLN
1	B	203	HIS
1	B	222	GLN
1	B	242	GLN
1	B	341	GLN
1	C	203	HIS
1	C	222	GLN
1	C	242	GLN
1	C	341	GLN
1	D	203	HIS
1	D	222	GLN
1	D	242	GLN
1	D	341	GLN
1	E	203	HIS
1	E	222	GLN
1	E	242	GLN
1	E	393	GLN
1	F	203	HIS
1	F	222	GLN
1	F	242	GLN
1	F	294	ASN
1	F	295	GLN
1	F	393	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

12 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	PLP	A	1001	1	15,15,16	1.35	1 (6%)	21,22,23	1.21	2 (9%)
2	HEM	A	501	1	30,50,50	2.64	9 (30%)	24,82,82	2.90	12 (50%)
3	PLP	B	1001	1	15,15,16	1.24	1 (6%)	21,22,23	1.17	2 (9%)
2	HEM	B	501	1	30,50,50	2.54	10 (33%)	24,82,82	2.87	12 (50%)
3	PLP	C	1001	1	15,15,16	1.24	1 (6%)	21,22,23	1.18	2 (9%)
2	HEM	C	501	1	30,50,50	2.54	8 (26%)	24,82,82	2.93	11 (45%)
3	PLP	D	1001	1	15,15,16	1.35	1 (6%)	21,22,23	1.16	2 (9%)
2	HEM	D	501	1	30,50,50	2.53	8 (26%)	24,82,82	2.89	12 (50%)
3	PLP	E	1001	1	15,15,16	1.83	2 (13%)	21,22,23	1.15	2 (9%)
2	HEM	E	501	1	30,50,50	2.59	8 (26%)	24,82,82	2.95	11 (45%)
3	PLP	F	1001	1	15,15,16	1.37	2 (13%)	21,22,23	1.19	2 (9%)
2	HEM	F	501	1	30,50,50	2.49	10 (33%)	24,82,82	2.93	11 (45%)

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	PLP	A	1001	1	-	0/6/6/8	0/1/1/1
2	HEM	A	501	1	-	0/10/54/54	0/0/8/8
3	PLP	B	1001	1	-	0/6/6/8	0/1/1/1
2	HEM	B	501	1	-	0/10/54/54	0/0/8/8
3	PLP	C	1001	1	-	0/6/6/8	0/1/1/1
2	HEM	C	501	1	-	0/10/54/54	0/0/8/8
3	PLP	D	1001	1	-	0/6/6/8	0/1/1/1
2	HEM	D	501	1	-	0/10/54/54	0/0/8/8
3	PLP	E	1001	1	-	0/6/6/8	0/1/1/1
2	HEM	E	501	1	-	0/10/54/54	0/0/8/8
3	PLP	F	1001	1	-	0/6/6/8	0/1/1/1
2	HEM	F	501	1	-	0/10/54/54	0/0/8/8

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C3B-C4B	-7.65	1.45	1.51
2	E	501	HEM	C3B-C4B	-7.55	1.45	1.51
2	B	501	HEM	C3B-C4B	-7.43	1.45	1.51
2	D	501	HEM	C3B-C4B	-7.30	1.45	1.51
2	F	501	HEM	C3B-C4B	-7.16	1.45	1.51
2	C	501	HEM	C3B-C4B	-7.14	1.45	1.51
2	A	501	HEM	C2D-C3D	-5.93	1.36	1.54
2	E	501	HEM	C2D-C3D	-5.88	1.36	1.54
2	D	501	HEM	C2D-C3D	-5.82	1.37	1.54
2	B	501	HEM	C2D-C3D	-5.82	1.37	1.54
3	E	1001	PLP	C3-C2	-5.80	1.36	1.40
2	C	501	HEM	C2D-C3D	-5.79	1.37	1.54
2	F	501	HEM	C2D-C3D	-5.57	1.37	1.54
2	A	501	HEM	C3D-C4D	-4.76	1.45	1.51
2	E	501	HEM	C3D-C4D	-4.50	1.45	1.51
2	C	501	HEM	C3D-C4D	-4.40	1.45	1.51
2	F	501	HEM	C3D-C4D	-4.27	1.46	1.51
2	D	501	HEM	C3D-C4D	-3.88	1.46	1.51
2	B	501	HEM	C3D-C4D	-3.78	1.46	1.51
3	F	1001	PLP	C3-C2	-3.12	1.38	1.40
3	D	1001	PLP	C3-C2	-3.06	1.38	1.40
3	A	1001	PLP	C3-C2	-3.02	1.38	1.40
2	C	501	HEM	C2C-C1C	-2.75	1.47	1.52
2	B	501	HEM	C2C-C1C	-2.62	1.47	1.52
2	D	501	HEM	C2C-C1C	-2.54	1.47	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HEM	C2C-C1C	-2.49	1.47	1.52
2	F	501	HEM	C2C-C1C	-2.46	1.47	1.52
2	E	501	HEM	C2C-C1C	-2.46	1.47	1.52
3	C	1001	PLP	C3-C2	-2.42	1.39	1.40
3	F	1001	PLP	P-O3P	-2.34	1.46	1.54
3	B	1001	PLP	P-O3P	-2.33	1.46	1.54
3	E	1001	PLP	P-O3P	-2.08	1.47	1.54
2	F	501	HEM	C2B-C1B	-2.05	1.45	1.51
2	B	501	HEM	C2D-C1D	-2.02	1.45	1.51
2	F	501	HEM	C4C-NC	2.04	1.38	1.36
2	B	501	HEM	C3B-CAB	2.09	1.55	1.51
2	B	501	HEM	C3C-CAC	2.27	1.55	1.51
2	F	501	HEM	C3B-CAB	2.33	1.55	1.51
2	A	501	HEM	C4C-NC	2.40	1.39	1.36
2	A	501	HEM	C3B-CAB	2.54	1.56	1.51
2	F	501	HEM	C3C-CAC	2.68	1.56	1.51
2	D	501	HEM	C4C-NC	2.73	1.39	1.36
2	B	501	HEM	C4C-NC	2.76	1.39	1.36
2	D	501	HEM	C3C-CAC	2.76	1.56	1.51
2	C	501	HEM	C4C-NC	2.79	1.39	1.36
2	E	501	HEM	C4C-NC	2.82	1.39	1.36
2	A	501	HEM	C3C-CAC	2.86	1.56	1.51
2	C	501	HEM	C3C-CAC	2.89	1.56	1.51
2	E	501	HEM	C3C-CAC	3.02	1.57	1.51
2	B	501	HEM	CBC-CAC	4.03	1.52	1.29
2	C	501	HEM	CBC-CAC	4.13	1.53	1.29
2	E	501	HEM	CBC-CAC	4.14	1.53	1.29
2	F	501	HEM	CBC-CAC	4.15	1.53	1.29
2	D	501	HEM	CBC-CAC	4.17	1.53	1.29
2	A	501	HEM	CBC-CAC	4.28	1.54	1.29
2	F	501	HEM	CBB-CAB	4.29	1.54	1.29
2	E	501	HEM	CBB-CAB	4.34	1.54	1.29
2	C	501	HEM	CBB-CAB	4.37	1.54	1.29
2	A	501	HEM	CBB-CAB	4.39	1.54	1.29
2	D	501	HEM	CBB-CAB	4.43	1.54	1.29
2	B	501	HEM	CBB-CAB	4.44	1.54	1.29

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C3B-CAB-CBB	-6.11	115.09	124.46
2	C	501	HEM	C3B-CAB-CBB	-6.10	115.11	124.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	501	HEM	C3B-CAB-CBB	-6.06	115.16	124.46
2	F	501	HEM	C3B-CAB-CBB	-5.92	115.38	124.46
2	B	501	HEM	C3B-CAB-CBB	-5.68	115.75	124.46
2	D	501	HEM	C3B-CAB-CBB	-5.59	115.89	124.46
2	F	501	HEM	C3C-CAC-CBC	-4.72	117.21	124.46
2	D	501	HEM	C3C-CAC-CBC	-4.71	117.22	124.46
2	C	501	HEM	C3C-CAC-CBC	-4.63	117.36	124.46
2	E	501	HEM	C3C-CAC-CBC	-4.55	117.47	124.46
2	A	501	HEM	C3C-CAC-CBC	-4.40	117.71	124.46
2	B	501	HEM	C3C-CAC-CBC	-4.39	117.73	124.46
2	E	501	HEM	CAA-C2A-C1A	-3.11	123.63	127.01
2	D	501	HEM	CAA-C2A-C1A	-3.01	123.74	127.01
2	C	501	HEM	CAA-C2A-C1A	-2.99	123.76	127.01
2	A	501	HEM	CAA-C2A-C1A	-2.96	123.80	127.01
2	F	501	HEM	CAA-C2A-C1A	-2.78	123.99	127.01
2	B	501	HEM	CAA-C2A-C1A	-2.74	124.04	127.01
2	C	501	HEM	CMA-C3A-C4A	-2.55	124.15	128.36
2	F	501	HEM	CMA-C3A-C4A	-2.54	124.17	128.36
2	D	501	HEM	CMA-C3A-C4A	-2.50	124.23	128.36
2	B	501	HEM	CMA-C3A-C4A	-2.47	124.28	128.36
2	E	501	HEM	CMA-C3A-C4A	-2.38	124.42	128.36
2	A	501	HEM	CMA-C3A-C4A	-2.15	124.81	128.36
2	B	501	HEM	CBA-CAA-C2A	2.03	116.17	112.53
2	D	501	HEM	CBA-CAA-C2A	2.07	116.24	112.53
2	A	501	HEM	CBA-CAA-C2A	2.14	116.37	112.53
3	E	1001	PLP	O4P-C5A-C5	2.23	112.67	108.99
2	A	501	HEM	C3B-C4B-CHC	2.30	126.40	123.16
3	A	1001	PLP	O4P-C5A-C5	2.38	112.93	108.99
2	E	501	HEM	C3B-C4B-CHC	2.41	126.55	123.16
3	B	1001	PLP	O4P-C5A-C5	2.41	112.98	108.99
2	B	501	HEM	C3B-C4B-CHC	2.43	126.58	123.16
2	D	501	HEM	C3B-C4B-CHC	2.45	126.61	123.16
2	F	501	HEM	C3B-C4B-CHC	2.46	126.62	123.16
3	F	1001	PLP	O4P-C5A-C5	2.49	113.11	108.99
3	D	1001	PLP	O4P-C5A-C5	2.50	113.13	108.99
2	C	501	HEM	C3B-C4B-CHC	2.51	126.69	123.16
3	C	1001	PLP	O4P-C5A-C5	2.65	113.37	108.99
2	B	501	HEM	C2D-C3D-C4D	2.67	106.03	101.50
2	E	501	HEM	C2D-C3D-C4D	2.72	106.11	101.50
2	F	501	HEM	C2D-C3D-C4D	2.74	106.14	101.50
2	D	501	HEM	C2D-C3D-C4D	2.80	106.24	101.50
2	C	501	HEM	C2D-C3D-C4D	2.83	106.30	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HEM	C2D-C3D-C4D	2.94	106.48	101.50
2	A	501	HEM	CMD-C2D-C3D	3.00	127.60	114.35
2	D	501	HEM	CMD-C2D-C3D	3.07	127.95	114.35
3	D	1001	PLP	O3P-P-O1P	3.08	120.49	110.58
2	C	501	HEM	CMD-C2D-C3D	3.09	128.01	114.35
3	A	1001	PLP	O3P-P-O1P	3.09	120.53	110.58
3	F	1001	PLP	O3P-P-O1P	3.11	120.58	110.58
3	E	1001	PLP	O3P-P-O1P	3.11	120.60	110.58
3	C	1001	PLP	O3P-P-O1P	3.12	120.61	110.58
2	B	501	HEM	CMD-C2D-C3D	3.12	128.17	114.35
2	E	501	HEM	CMD-C2D-C3D	3.15	128.30	114.35
2	F	501	HEM	CMD-C2D-C3D	3.17	128.39	114.35
3	B	1001	PLP	O3P-P-O1P	3.22	120.96	110.58
2	C	501	HEM	CAD-C3D-C4D	3.68	125.45	112.47
2	F	501	HEM	CAD-C3D-C4D	3.72	125.58	112.47
2	B	501	HEM	CAD-C3D-C4D	3.72	125.60	112.47
2	D	501	HEM	CAD-C3D-C4D	3.74	125.65	112.47
2	E	501	HEM	CAD-C3D-C4D	3.77	125.75	112.47
2	A	501	HEM	CAD-C3D-C4D	3.77	125.77	112.47
2	D	501	HEM	CMB-C2B-C3B	4.89	128.74	116.53
2	C	501	HEM	CMB-C2B-C3B	4.93	128.83	116.53
2	A	501	HEM	CAD-C3D-C2D	5.06	127.76	113.22
2	F	501	HEM	CMB-C2B-C3B	5.08	129.20	116.53
2	A	501	HEM	CMB-C2B-C3B	5.08	129.21	116.53
2	E	501	HEM	CMB-C2B-C3B	5.09	129.23	116.53
2	B	501	HEM	CMB-C2B-C3B	5.13	129.34	116.53
2	D	501	HEM	CAD-C3D-C2D	5.18	128.11	113.22
2	E	501	HEM	CAD-C3D-C2D	5.19	128.13	113.22
2	C	501	HEM	CAD-C3D-C2D	5.23	128.25	113.22
2	F	501	HEM	CAD-C3D-C2D	5.24	128.29	113.22
2	B	501	HEM	CAD-C3D-C2D	5.27	128.37	113.22
2	B	501	HEM	CMC-C2C-C3C	5.53	130.33	116.53
2	F	501	HEM	CMC-C2C-C3C	5.57	130.43	116.53
2	A	501	HEM	CMC-C2C-C3C	5.69	130.72	116.53
2	C	501	HEM	CMC-C2C-C3C	5.71	130.78	116.53
2	D	501	HEM	CMC-C2C-C3C	5.74	130.87	116.53
2	E	501	HEM	CMC-C2C-C3C	5.85	131.13	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1001	PLP	1	0
2	A	501	HEM	4	0
3	B	1001	PLP	1	0
2	B	501	HEM	2	0
3	C	1001	PLP	1	0
2	C	501	HEM	2	0
3	D	1001	PLP	1	0
2	D	501	HEM	3	0
3	E	1001	PLP	1	0
2	E	501	HEM	2	0
3	F	1001	PLP	1	0
2	F	501	HEM	3	0

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	348/435 (80%)	0.24	15 (4%) 39 31	12, 32, 66, 85	0
1	B	348/435 (80%)	0.65	37 (10%) 8 5	9, 35, 75, 94	0
1	C	348/435 (80%)	0.48	26 (7%) 17 12	15, 36, 72, 87	0
1	D	348/435 (80%)	0.50	31 (8%) 12 8	17, 39, 76, 92	0
1	E	350/435 (80%)	0.18	16 (4%) 36 29	9, 27, 67, 90	0
1	F	348/435 (80%)	0.12	17 (4%) 33 26	9, 26, 67, 89	0
All	All	2090/2610 (80%)	0.36	142 (6%) 20 15	9, 33, 72, 94	0

All (142) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	193	THR	9.9
1	E	193	THR	6.8
1	B	43	TRP	6.3
1	F	147	SER	6.3
1	D	392	LEU	6.2
1	D	43	TRP	6.0
1	C	212	ASN	6.0
1	B	297	GLU	5.7
1	D	44	ILE	5.5
1	C	208	TRP	5.4
1	B	170	PRO	5.3
1	B	212	ASN	5.2
1	D	191	THR	5.2
1	B	192	PRO	5.2
1	B	46	PRO	5.1
1	A	299	THR	5.1
1	D	53	THR	5.0
1	B	191	THR	5.0
1	D	52	CYS	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	47	ASP	4.7
1	E	170	PRO	4.6
1	E	172	LYS	4.6
1	B	311	ILE	4.6
1	B	299	THR	4.4
1	D	193	THR	4.3
1	B	202	SER	4.3
1	E	192	PRO	4.3
1	E	43	TRP	4.3
1	C	192	PRO	4.2
1	B	226	ALA	4.2
1	C	50	SER	4.2
1	A	43	TRP	4.1
1	B	214	ILE	4.1
1	B	171	GLU	4.1
1	B	147	SER	4.1
1	D	292	GLU	4.1
1	B	313	THR	4.0
1	F	43	TRP	4.0
1	F	192	PRO	4.0
1	C	46	PRO	3.9
1	F	389	ARG	3.9
1	D	192	PRO	3.9
1	E	171	GLU	3.8
1	E	44	ILE	3.8
1	C	389	ARG	3.8
1	C	297	GLU	3.8
1	D	171	GLU	3.8
1	A	192	PRO	3.7
1	C	49	PRO	3.7
1	E	57	GLY	3.7
1	A	44	ILE	3.6
1	A	295	GLN	3.6
1	B	209	ARG	3.6
1	F	208	TRP	3.5
1	B	169	MET	3.5
1	B	213	GLU	3.4
1	C	191	THR	3.4
1	A	171	GLU	3.4
1	D	297	GLU	3.4
1	D	299	THR	3.3
1	F	191	THR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	175	SER	3.3
1	F	46	PRO	3.3
1	D	397	LEU	3.3
1	C	393	GLN	3.3
1	B	312	PRO	3.3
1	A	45	ARG	3.3
1	E	203	HIS	3.2
1	B	49	PRO	3.2
1	F	45	ARG	3.1
1	F	190	ARG	3.1
1	D	396	PHE	3.1
1	A	209	ARG	3.1
1	C	190	ARG	3.1
1	D	393	GLN	3.0
1	A	297	GLU	3.0
1	C	299	THR	3.0
1	B	203	HIS	3.0
1	E	212	ASN	3.0
1	E	204	VAL	3.0
1	D	51	ARG	2.9
1	B	172	LYS	2.9
1	C	171	GLU	2.9
1	C	223	TYR	2.9
1	B	290	PRO	2.9
1	A	59	PRO	2.8
1	D	295	GLN	2.8
1	B	296	THR	2.7
1	E	45	ARG	2.7
1	D	57	GLY	2.7
1	B	148	GLY	2.6
1	F	171	GLU	2.6
1	C	147	SER	2.6
1	C	214	ILE	2.6
1	D	389	ARG	2.6
1	D	45	ARG	2.6
1	B	211	LYS	2.6
1	B	48	ALA	2.5
1	E	52	CYS	2.5
1	B	295	GLN	2.5
1	C	168	VAL	2.5
1	F	44	ILE	2.5
1	A	52	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	202	SER	2.5
1	E	55	GLN	2.5
1	B	47	ASP	2.4
1	F	299	THR	2.4
1	E	47	ASP	2.4
1	A	215	PRO	2.4
1	A	293	LEU	2.4
1	E	209	ARG	2.4
1	C	162	GLY	2.3
1	D	201	GLU	2.3
1	C	189	VAL	2.3
1	A	206	VAL	2.3
1	F	212	ASN	2.3
1	D	283	GLU	2.3
1	A	210	LEU	2.3
1	D	290	PRO	2.3
1	B	173	MET	2.2
1	C	169	MET	2.2
1	C	145	PRO	2.2
1	C	56	LEU	2.2
1	B	51	ARG	2.2
1	D	395	GLY	2.2
1	C	209	ARG	2.2
1	D	310	PHE	2.2
1	D	61	SER	2.1
1	C	310	PHE	2.1
1	F	393	GLN	2.1
1	B	87	THR	2.1
1	F	296	THR	2.1
1	C	146	THR	2.1
1	B	292	GLU	2.1
1	D	329	GLU	2.1
1	D	316	ASP	2.1
1	D	169	MET	2.1
1	B	298	GLN	2.1
1	B	145	PRO	2.1
1	F	295	GLN	2.0
1	D	262	THR	2.0
1	D	58	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	PLP	E	1001	15/16	0.97	0.16	0.38	2,12,18,23	0
3	PLP	B	1001	15/16	0.94	0.18	0.19	2,15,25,26	0
2	HEM	C	501	43/43	0.90	0.26	0.19	17,37,49,61	0
2	HEM	D	501	43/43	0.91	0.26	0.15	17,45,54,64	0
2	HEM	F	501	43/43	0.94	0.17	-0.12	5,25,40,51	0
3	PLP	F	1001	15/16	0.97	0.15	-0.18	4,11,17,25	0
3	PLP	C	1001	15/16	0.95	0.17	-0.42	11,22,25,28	0
2	HEM	A	501	43/43	0.91	0.18	-0.44	5,31,43,52	0
3	PLP	D	1001	15/16	0.95	0.15	-0.49	15,22,31,32	0
2	HEM	B	501	43/43	0.89	0.20	-0.62	17,38,45,48	0
3	PLP	A	1001	15/16	0.96	0.14	-0.63	2,19,29,30	0
2	HEM	E	501	43/43	0.95	0.15	-0.94	8,27,42,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.