



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:07 PM GMT

PDB ID : 4BLC
Title : THE STRUCTURE OF ORTHORHOMBIC CRYSTALS OF BEEF LIVER CATALASE
Authors : Ko, T.P.; Day, J.; Malkin, A.; McPherson, A.
Deposited on : 1998-09-27
Resolution : 2.30 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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

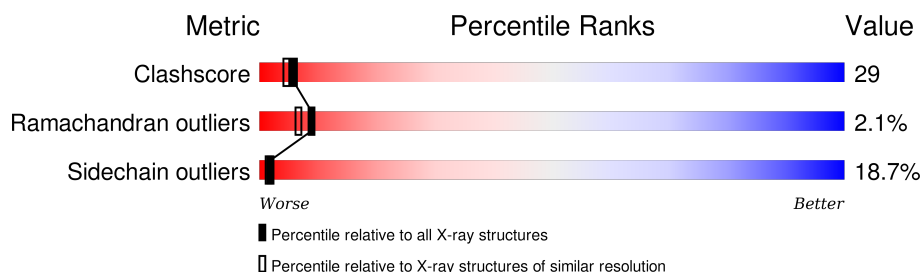
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	506	 56% 36% 6% •
1	B	506	 38% 45% 15% ••
1	C	506	 44% 41% 13% ••
1	D	506	 47% 42% 10% •

2 Entry composition [i](#)

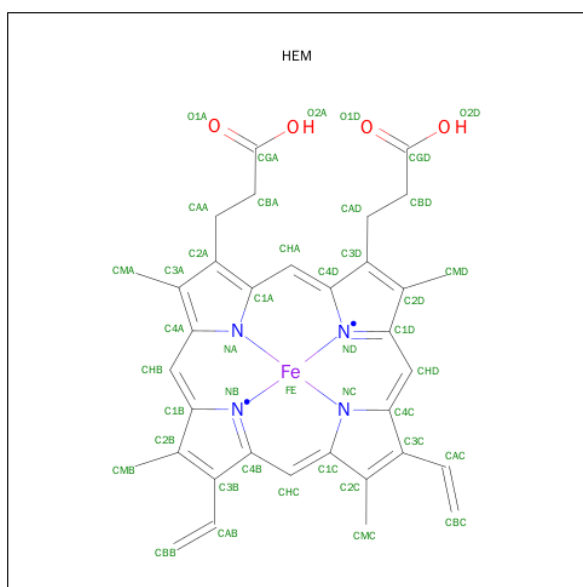
There are 4 unique types of molecules in this entry. The entry contains 16816 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN (CATALASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			
1	B	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			
1	C	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			
1	D	499	Total	C	N	O	S	0	0	0
			4017	2548	715	740	14			

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



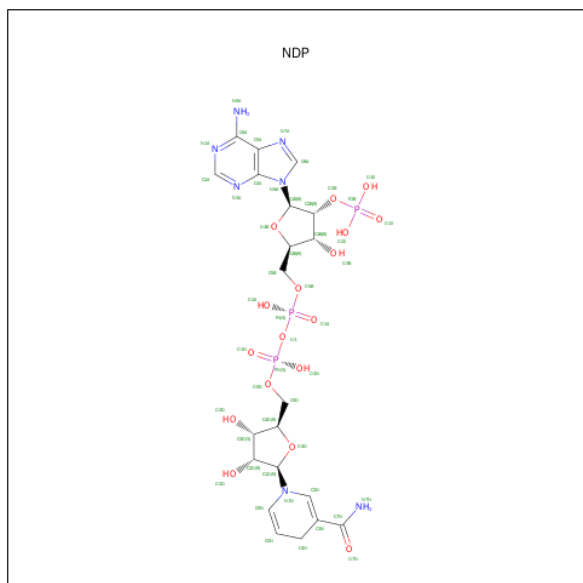
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	
			43	34	1	4	4	0
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

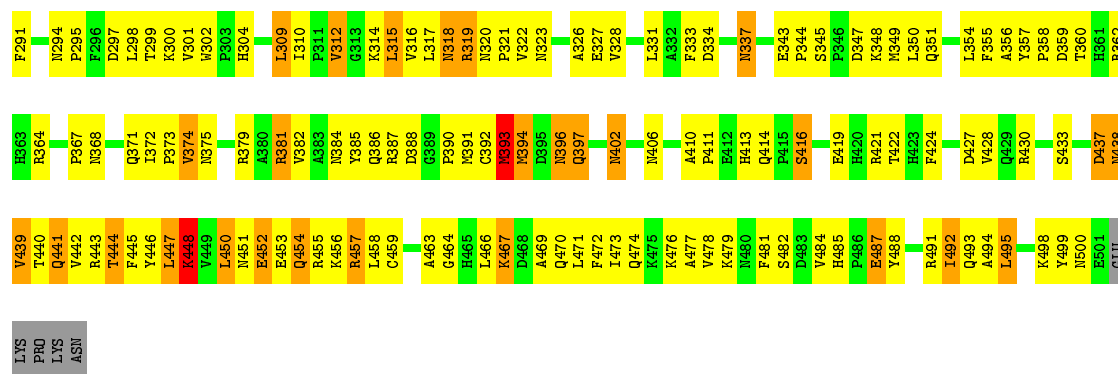
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	119	Total	O	0	0
			119	119		
4	B	89	Total	O	0	0
			89	89		
4	C	83	Total	O	0	0
			83	83		

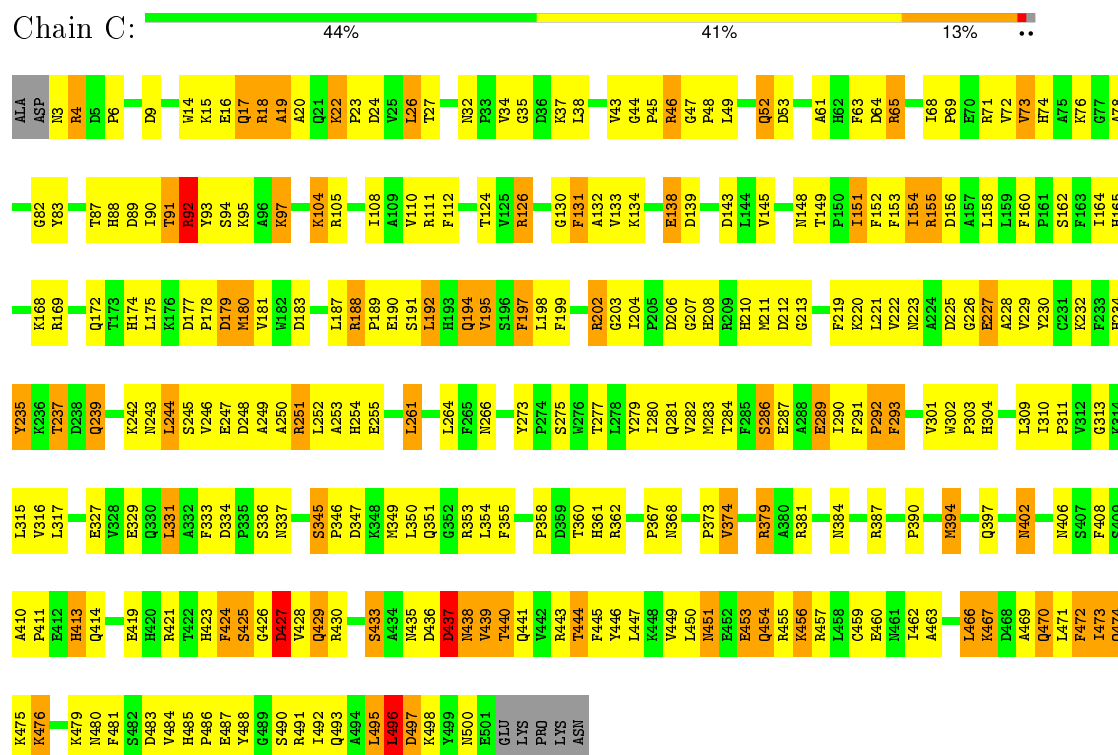
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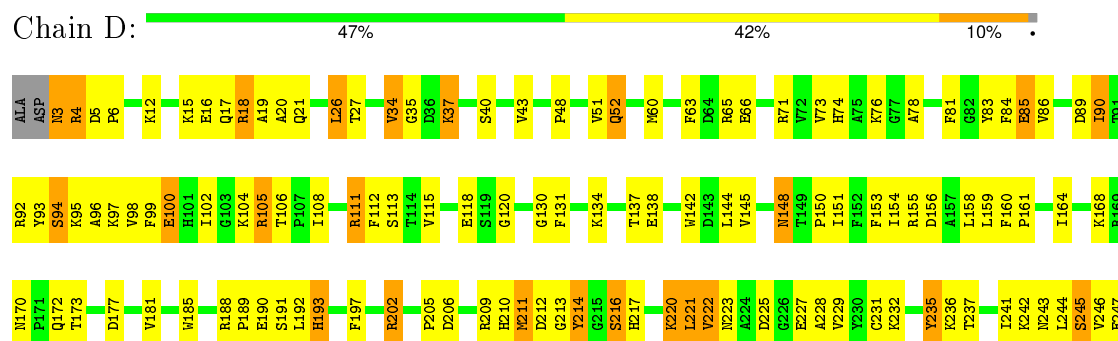
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	93	Total	O	0	0
			93	93		



• Molecule 1: PROTEIN (CATALASE)



• Molecule 1: PROTEIN (CATALASE)





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.80 Å 140.60 Å 232.40 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30	Depositor
% Data completeness (in resolution range)	87.5 (20.00-2.30)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.205 , 0.273	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16816	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

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, NDP

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	0.41	0/4137	0.62	0/5619
1	B	0.39	0/4137	0.59	0/5619
1	C	0.39	0/4137	0.60	0/5619
1	D	0.41	0/4137	0.60	0/5619
All	All	0.40	0/16548	0.60	0/22476

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	4017	0	3839	171	0
1	B	4017	0	3839	305	0
1	C	4017	0	3839	273	0
1	D	4017	0	3839	253	0
2	A	43	0	30	5	0
2	B	43	0	30	0	0
2	C	43	0	30	4	0
2	D	43	0	30	2	0
3	A	48	0	26	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	26	4	0
3	C	48	0	26	2	0
3	D	48	0	26	1	0
4	A	119	0	0	8	0
4	B	89	0	0	16	0
4	C	83	0	0	8	0
4	D	93	0	0	10	0
All	All	16816	0	15580	917	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 29.

All (917) 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:D:223:ASN:HD21	1:D:227:GLU:HB3	0.98	1.12
1:A:451:ASN:H	1:A:454:GLN:HE21	1.06	1.01
1:D:223:ASN:ND2	1:D:227:GLU:HB3	1.79	0.98
1:B:169:ARG:HH11	1:B:169:ARG:HG2	1.30	0.95
1:B:457:ARG:HH11	1:B:457:ARG:HB2	1.28	0.95
1:C:251:ARG:HD2	1:C:255:GLU:HG3	1.50	0.93
1:A:92:ARG:HB3	1:A:92:ARG:HH11	1.33	0.93
1:B:457:ARG:NH1	1:B:457:ARG:HB2	1.82	0.92
1:D:291:PHE:HD1	1:D:293:PHE:H	1.17	0.92
1:D:85:GLU:HG2	1:D:105:ARG:HG3	1.52	0.92
1:C:402:ASN:HD22	1:C:402:ASN:H	1.09	0.90
1:B:4:ARG:HH22	1:C:470:GLN:HE21	1.21	0.89
1:C:466:LEU:HD12	1:C:466:LEU:O	1.74	0.88
1:C:485:HIS:CE1	1:C:487:GLU:HB3	2.08	0.87
1:B:100:GLU:HB3	1:B:104:LYS:HG3	1.56	0.86
1:B:129:ARG:HB2	1:B:148:ASN:ND2	1.90	0.85
1:B:406:ASN:HD21	1:B:410:ALA:HB3	1.40	0.85
1:C:438:ASN:N	1:C:438:ASN:HD22	1.71	0.85
1:B:148:ASN:HD22	1:B:211:MET:CE	1.90	0.84
1:C:487:GLU:O	1:C:491:ARG:HG3	1.77	0.84
1:B:223:ASN:HD21	1:B:227:GLU:HB2	1.42	0.82
1:A:353:ARG:HG3	2:A:507:HEM:HBB2	1.62	0.82
1:B:454:GLN:HA	1:B:457:ARG:NH1	1.95	0.81
1:A:43:VAL:O	1:A:47:GLY:HA3	1.78	0.81
1:D:347:ASP:HB3	1:D:350:LEU:HB3	1.63	0.81
1:D:170:ASN:ND2	1:D:172:GLN:H	1.77	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:451:ASN:N	1:A:454:GLN:HE21	1.78	0.81
1:C:151:ILE:HD12	1:C:194:GLN:HG2	1.62	0.81
1:B:495:LEU:H	1:B:495:LEU:HD23	1.46	0.81
1:A:487:GLU:O	1:A:491:ARG:HG3	1.81	0.79
1:A:451:ASN:H	1:A:454:GLN:NE2	1.80	0.79
1:D:221:LEU:HD11	1:D:231:CYS:HB3	1.64	0.79
1:B:223:ASN:ND2	1:B:227:GLU:HB2	1.99	0.78
1:B:178:PRO:HD3	4:B:762:HOH:O	1.83	0.78
1:C:406:ASN:HD21	1:C:410:ALA:HB3	1.47	0.78
1:C:476:LYS:HB3	1:C:476:LYS:NZ	1.98	0.78
1:D:284:THR:OG1	1:D:287:GLU:HG2	1.83	0.78
1:B:241:ILE:HG22	1:B:242:LYS:H	1.47	0.77
1:A:485:HIS:HD2	1:A:487:GLU:H	1.28	0.77
1:D:202:ARG:NH1	1:D:241:ILE:HG21	1.99	0.77
1:B:37:LYS:HE3	1:B:59:GLU:OE2	1.84	0.77
1:B:191:SER:O	1:B:195:VAL:HG23	1.85	0.77
1:D:244:LEU:HD21	1:D:248:ASP:HB2	1.67	0.76
1:C:488:TYR:O	1:C:492:ILE:HG12	1.86	0.76
1:A:35:GLY:HA2	1:C:414:GLN:O	1.86	0.75
1:B:304:HIS:HD2	1:B:309:LEU:HD21	1.51	0.75
1:A:36:ASP:HA	1:C:413:HIS:ND1	2.01	0.75
1:C:110:VAL:HG22	1:C:133:VAL:HG22	1.67	0.75
1:C:210:HIS:HB3	1:C:242:LYS:H	1.52	0.75
1:C:222:VAL:HG22	1:C:228:ALA:HB2	1.68	0.75
1:C:244:LEU:HD13	1:C:248:ASP:HB3	1.69	0.74
1:D:145:VAL:O	2:D:507:HEM:HBC2	1.88	0.74
1:C:78:ALA:HB2	1:C:261:LEU:HD22	1.68	0.74
1:C:191:SER:O	1:C:195:VAL:HG23	1.87	0.73
1:A:223:ASN:ND2	1:A:227:GLU:HB2	2.03	0.73
1:B:182:TRP:O	1:B:186:SER:HB3	1.88	0.72
1:A:223:ASN:HD21	1:A:227:GLU:HB2	1.54	0.72
1:B:122:ALA:HB2	1:B:257:PRO:HB3	1.71	0.72
1:B:414:GLN:HE21	1:B:416:SER:CB	2.03	0.72
1:B:89:ASP:HB2	1:B:102:ILE:HD11	1.72	0.72
1:B:78:ALA:HB2	1:B:261:LEU:HG	1.71	0.72
1:B:6:PRO:HG2	1:B:266:ASN:OD1	1.89	0.71
1:D:170:ASN:HD22	1:D:173:THR:H	1.39	0.71
1:D:78:ALA:HB2	1:D:261:LEU:HG	1.72	0.71
1:C:491:ARG:O	1:C:495:LEU:HD12	1.90	0.71
1:B:241:ILE:HG22	1:B:242:LYS:N	2.06	0.71
1:C:72:VAL:HG13	1:C:73:VAL:HG22	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:ARG:H	1:A:148:ASN:ND2	1.88	0.71
1:B:241:ILE:O	1:B:242:LYS:HB2	1.91	0.70
1:B:281:GLN:OE1	1:B:302:TRP:HB2	1.89	0.70
1:C:183:ASP:O	1:C:187:LEU:HG	1.90	0.70
1:D:137:THR:HA	1:D:379:ARG:HH21	1.56	0.70
1:C:301:VAL:HG22	1:C:441:GLN:OE1	1.90	0.70
1:B:190:GLU:HA	1:B:438:ASN:HB3	1.74	0.70
1:D:286:SER:O	1:D:290:ILE:HD12	1.91	0.70
1:C:189:PRO:O	1:C:192:LEU:HG	1.92	0.70
1:C:289:GLU:HG2	4:C:898:HOH:O	1.92	0.70
1:B:112:PHE:HA	1:B:130:GLY:O	1.91	0.69
1:C:402:ASN:HD22	1:C:402:ASN:N	1.84	0.69
1:A:82:GLY:HA3	1:A:316:VAL:O	1.92	0.69
1:B:126:ARG:HE	1:B:199:PHE:HA	1.58	0.69
1:D:367:PRO:HG2	1:D:390:PRO:HG2	1.72	0.69
1:D:84:PHE:O	1:D:105:ARG:HA	1.92	0.69
1:C:74:HIS:O	1:C:111:ARG:NH2	2.24	0.69
1:A:92:ARG:CB	1:A:92:ARG:HH11	2.04	0.69
1:C:273:TYR:HB3	1:C:317:LEU:O	1.93	0.69
1:D:387:ARG:HH11	1:D:387:ARG:HG2	1.56	0.68
1:D:367:PRO:HG2	1:D:390:PRO:CG	2.23	0.68
1:A:425:SER:HA	1:B:424:PHE:O	1.93	0.68
1:A:209:ARG:HG2	1:A:274:PRO:HB3	1.74	0.68
1:D:221:LEU:HD11	1:D:231:CYS:SG	2.33	0.68
1:C:232:LYS:HB2	1:C:281:GLN:HB2	1.76	0.68
1:C:438:ASN:ND2	1:C:438:ASN:N	2.41	0.68
1:B:37:LYS:O	1:C:158:LEU:HD13	1.93	0.68
1:A:51:VAL:HG13	1:B:49:LEU:O	1.93	0.68
4:A:718:HOH:O	1:D:363:HIS:HD2	1.77	0.68
1:D:364:ARG:HD2	4:D:1022:HOH:O	1.93	0.67
1:C:92:ARG:HH11	1:C:92:ARG:HG3	1.59	0.67
1:B:264:LEU:O	1:B:264:LEU:HD12	1.95	0.67
1:B:148:ASN:HD22	1:B:211:MET:HE2	1.59	0.67
1:A:94:SER:HB2	1:A:221:LEU:HD22	1.77	0.67
1:C:251:ARG:HG2	1:C:251:ARG:HH11	1.59	0.67
1:B:301:VAL:H	1:B:441:GLN:NE2	1.92	0.67
1:B:100:GLU:HB2	1:B:104:LYS:HZ3	1.59	0.67
1:B:301:VAL:H	1:B:441:GLN:HE22	1.41	0.67
1:B:454:GLN:HA	1:B:457:ARG:HH12	1.58	0.66
1:C:471:LEU:HA	1:C:474:GLN:HG3	1.75	0.66
1:B:47:GLY:HA2	1:C:424:PHE:CE1	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:787:HOH:O	1:C:44:GLY:HA2	1.94	0.66
1:B:414:GLN:HE21	1:B:416:SER:HB2	1.61	0.66
1:D:383:ALA:HB1	1:D:411:PRO:HG3	1.78	0.66
1:D:220:LYS:HE3	1:D:343:GLU:HB2	1.78	0.66
1:B:169:ARG:HH11	1:B:169:ARG:CG	2.06	0.66
1:B:360:THR:HG23	1:C:64:ASP:O	1.95	0.66
1:C:6:PRO:HD2	1:C:266:ASN:OD1	1.95	0.65
1:B:273:TYR:HB3	1:B:317:LEU:O	1.96	0.65
1:D:221:LEU:HD11	1:D:231:CYS:CB	2.26	0.65
1:C:470:GLN:O	1:C:473:ILE:HB	1.96	0.65
1:D:18:ARG:HB3	4:D:841:HOH:O	1.97	0.65
1:D:94:SER:HB2	1:D:221:LEU:HB3	1.79	0.65
1:A:280:ILE:HG23	1:A:312:VAL:HG21	1.77	0.65
1:B:220:LYS:C	1:B:221:LEU:HD23	2.16	0.65
1:D:287:GLU:HA	1:D:290:ILE:HB	1.78	0.65
1:A:419:GLU:OE2	1:B:430:ARG:NH1	2.30	0.65
1:A:170:ASN:HB3	1:A:173:THR:OG1	1.96	0.65
1:D:83:TYR:CE1	1:D:85:GLU:HG3	2.32	0.65
1:B:318:ASN:N	1:B:318:ASN:HD22	1.95	0.64
1:D:223:ASN:HD21	1:D:227:GLU:CB	1.93	0.64
1:C:402:ASN:H	1:C:402:ASN:ND2	1.90	0.64
1:A:471:LEU:HA	1:A:474:GLN:HG3	1.79	0.64
1:D:284:THR:HG23	1:D:287:GLU:OE2	1.98	0.64
1:B:97:LYS:HB3	1:B:138:GLU:OE1	1.97	0.64
1:D:487:GLU:HA	1:D:490:SER:OG	1.97	0.64
1:A:485:HIS:CD2	1:A:487:GLU:H	2.12	0.64
1:C:347:ASP:HB3	1:C:350:LEU:HB3	1.79	0.64
1:A:333:PHE:O	1:A:361:HIS:HE1	1.81	0.64
1:A:15:LYS:HD2	4:A:936:HOH:O	1.98	0.64
1:C:331:LEU:HD13	1:C:333:PHE:CZ	2.33	0.64
1:A:95:LYS:HG2	1:A:222:VAL:O	1.98	0.64
1:A:43:VAL:HG13	1:A:48:PRO:HD2	1.81	0.63
1:C:221:LEU:O	1:C:228:ALA:HA	1.98	0.63
1:D:347:ASP:HB3	1:D:350:LEU:CB	2.27	0.63
1:C:410:ALA:HB1	1:C:411:PRO:HD2	1.80	0.63
1:D:285:PHE:HD1	1:D:285:PHE:H	1.46	0.63
1:D:76:LYS:O	1:D:113:SER:HB2	1.99	0.63
1:A:18:ARG:HG2	4:A:935:HOH:O	1.98	0.63
1:C:451:ASN:OD1	1:C:454:GLN:HG2	1.99	0.63
1:A:498:LYS:HD2	4:A:725:HOH:O	1.97	0.63
1:B:41:LEU:HB3	1:B:53:ASP:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:15:LYS:HD3	1:D:408:PHE:HA	1.80	0.63
1:D:338:MET:CE	1:D:342:ILE:HG22	2.29	0.63
1:C:154:ILE:HG13	1:C:349:MET:CE	2.29	0.62
1:C:445:PHE:O	1:C:450:LEU:HB2	1.99	0.62
1:B:391:MET:HE2	1:D:365:LEU:O	1.98	0.62
1:A:25:VAL:HG13	1:C:414:GLN:HG2	1.80	0.62
1:A:347:ASP:HB3	1:A:350:LEU:HB3	1.80	0.62
1:B:447:LEU:O	1:B:448:LYS:HB2	1.98	0.62
1:B:321:PRO:HG2	4:C:996:HOH:O	2.00	0.62
1:D:63:PHE:O	1:D:66:GLU:HG3	2.00	0.62
1:D:404:TYR:CD1	1:D:405:PRO:HA	2.34	0.62
1:C:4:ARG:HD3	1:C:9:ASP:OD1	2.00	0.62
1:B:466:LEU:CD2	1:B:474:GLN:HG2	2.30	0.62
1:B:304:HIS:CD2	1:B:309:LEU:HD21	2.32	0.62
1:D:445:PHE:HA	1:D:449:VAL:CG2	2.30	0.62
1:B:229:VAL:HG23	1:B:284:THR:HA	1.81	0.62
1:A:451:ASN:N	1:A:454:GLN:NE2	2.43	0.61
1:B:43:VAL:O	1:B:47:GLY:HA3	2.00	0.61
1:B:38:LEU:HG	1:D:413:HIS:CE1	2.35	0.61
1:C:165:HIS:HB3	1:D:402:ASN:ND2	2.15	0.61
1:D:154:ILE:HG13	1:D:349:MET:CE	2.31	0.61
1:A:414:GLN:O	1:C:35:GLY:HA2	1.99	0.61
1:D:156:ASP:OD1	1:D:158:LEU:HB2	2.01	0.61
1:C:451:ASN:H	1:C:454:GLN:HE21	1.48	0.61
1:C:358:PRO:O	1:C:362:ARG:HG3	2.00	0.61
1:C:437:ASP:OD2	1:C:440:THR:HB	2.00	0.61
1:D:244:LEU:CD2	1:D:248:ASP:HB2	2.31	0.61
1:B:318:ASN:ND2	1:B:318:ASN:N	2.49	0.61
1:B:142:TRP:CZ2	1:B:144:LEU:HD23	2.36	0.61
1:C:485:HIS:NE2	1:C:487:GLU:HB3	2.16	0.61
1:C:251:ARG:HG3	1:C:252:LEU:N	2.16	0.61
1:C:138:GLU:HA	1:C:379:ARG:O	2.01	0.61
1:B:397:GLN:HG2	4:B:835:HOH:O	2.00	0.61
1:B:160:PHE:O	1:B:164:ILE:HG12	2.01	0.61
1:A:148:ASN:H	1:A:148:ASN:HD22	1.49	0.60
1:C:425:SER:HB2	1:D:425:SER:OG	2.01	0.60
1:C:26:LEU:HD21	1:C:37:LYS:HD3	1.83	0.60
1:D:170:ASN:ND2	1:D:173:THR:H	1.98	0.60
1:C:213:GLY:HA3	1:C:235:TYR:CE2	2.36	0.60
1:C:329:GLU:OE1	1:C:329:GLU:HA	2.01	0.60
1:A:43:VAL:CG1	1:A:48:PRO:HD2	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:235:TYR:HA	1:C:277:THR:O	2.00	0.60
1:C:252:LEU:HA	1:C:255:GLU:HB2	1.83	0.60
1:A:197:PHE:HD2	4:A:1043:HOH:O	1.83	0.60
1:B:88:HIS:HB2	1:B:312:VAL:HA	1.82	0.60
1:B:323:ASN:O	1:B:327:GLU:HG3	2.01	0.60
1:B:205:PRO:HG3	1:B:211:MET:HE3	1.84	0.60
1:A:160:PHE:HB3	1:A:161:PRO:HD3	1.84	0.60
1:A:206:ASP:O	1:A:210:HIS:HD2	1.85	0.60
1:C:89:ASP:OD1	1:C:91:THR:HB	2.02	0.59
1:D:338:MET:HE3	1:D:342:ILE:HG22	1.82	0.59
1:C:351:GLN:O	1:C:354:LEU:HB2	2.01	0.59
1:D:150:PRO:HB3	1:D:214:TYR:CD2	2.37	0.59
1:A:97:LYS:O	1:A:100:GLU:HB2	2.02	0.59
1:D:170:ASN:HD22	1:D:172:GLN:H	1.51	0.59
1:A:150:PRO:HG3	3:A:1102:NDP:H41N	1.83	0.59
1:D:222:VAL:HG11	1:D:420:HIS:HB2	1.84	0.59
1:C:153:PHE:HZ	1:C:198:LEU:HD22	1.67	0.59
1:C:154:ILE:HG13	1:C:349:MET:HE1	1.84	0.59
1:D:455:ARG:HD2	1:D:491:ARG:HH12	1.67	0.59
1:C:476:LYS:HZ3	1:C:476:LYS:HB3	1.67	0.59
1:C:437:ASP:C	1:C:438:ASN:HD22	2.06	0.59
1:C:197:PHE:HB2	4:C:1074:HOH:O	2.03	0.59
1:B:351:GLN:HE22	1:D:52:GLN:HG3	1.68	0.59
1:D:83:TYR:HE1	1:D:85:GLU:HG3	1.67	0.59
1:B:4:ARG:NH2	1:C:470:GLN:HE21	1.94	0.59
1:B:206:ASP:OD2	1:B:244:LEU:HD21	2.03	0.58
1:C:72:VAL:HG11	2:C:507:HEM:HMA3	1.84	0.58
1:C:374:VAL:HG13	4:C:752:HOH:O	2.03	0.58
1:B:98:VAL:HG13	1:B:99:PHE:CD1	2.38	0.58
1:B:34:VAL:HG13	1:B:55:VAL:HG11	1.84	0.58
1:D:432:ASN:ND2	1:D:432:ASN:C	2.57	0.58
1:B:402:ASN:HD22	1:B:402:ASN:C	2.06	0.58
1:B:495:LEU:CD2	1:B:495:LEU:H	2.17	0.58
1:B:322:VAL:O	1:C:172:GLN:HG3	2.03	0.58
1:A:42:THR:HG22	1:A:49:LEU:HA	1.85	0.58
1:C:327:GLU:HA	1:C:374:VAL:HG11	1.86	0.58
1:C:284:THR:OG1	1:C:287:GLU:HG3	2.02	0.58
1:B:232:LYS:O	1:B:280:ILE:HA	2.04	0.58
1:C:188:ARG:HD3	1:C:190:GLU:OE2	2.04	0.58
1:D:488:TYR:O	1:D:492:ILE:HD12	2.04	0.58
1:D:108:ILE:HA	1:D:134:LYS:O	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:GLU:OE1	1:D:329:GLU:HA	2.02	0.58
1:C:446:TYR:CE1	1:C:455:ARG:HG2	2.39	0.57
1:D:280:ILE:HG12	1:D:281:GLN:N	2.19	0.57
1:D:415:PRO:O	1:D:418:LEU:HD12	2.04	0.57
1:A:147:ASN:ND2	2:A:507:HEM:HAC	2.20	0.57
1:C:291:PHE:CD1	1:C:292:PRO:HD2	2.40	0.57
1:B:159:LEU:HD21	1:C:38:LEU:HD22	1.85	0.57
1:A:437:ASP:OD2	1:A:440:THR:HB	2.05	0.57
1:B:491:ARG:O	1:B:495:LEU:HD23	2.05	0.57
1:B:82:GLY:HA3	1:B:316:VAL:O	2.04	0.57
1:C:162:SER:HG	1:D:404:TYR:H	1.48	0.57
1:B:223:ASN:C	1:B:225:ASP:H	2.08	0.57
1:A:15:LYS:HD3	1:C:408:PHE:HA	1.87	0.57
1:D:213:GLY:HA3	1:D:235:TYR:CD2	2.39	0.57
1:D:220:LYS:NZ	1:D:343:GLU:OE1	2.37	0.57
1:D:95:LYS:HG2	1:D:222:VAL:O	2.05	0.57
1:D:212:ASP:HB2	1:D:214:TYR:CE1	2.40	0.57
1:C:462:ILE:HD13	1:C:481:PHE:HE2	1.70	0.57
1:B:148:ASN:HD22	1:B:211:MET:HE1	1.70	0.57
1:D:217:HIS:CE1	1:D:298:LEU:HD22	2.40	0.57
1:D:237:THR:HA	1:D:276:TRP:CD1	2.39	0.57
1:C:287:GLU:HA	1:C:290:ILE:CD1	2.35	0.57
1:D:108:ILE:HD13	1:D:315:LEU:HD22	1.86	0.57
1:D:97:LYS:O	1:D:100:GLU:HB2	2.05	0.57
1:A:52:GLN:HB2	4:C:907:HOH:O	2.03	0.57
1:C:462:ILE:HD13	1:C:481:PHE:CE2	2.40	0.57
1:D:177:ASP:O	1:D:181:VAL:HG23	2.05	0.57
1:D:160:PHE:HB3	1:D:161:PRO:HD3	1.87	0.56
1:C:251:ARG:NH1	1:C:251:ARG:HG2	2.20	0.56
1:C:287:GLU:HA	1:C:290:ILE:HD11	1.88	0.56
1:C:462:ILE:HG21	1:C:481:PHE:HE2	1.69	0.56
1:B:18:ARG:HD2	1:D:409:SER:O	2.05	0.56
1:C:208:HIS:HA	1:C:211:MET:CE	2.35	0.56
1:B:372:ILE:HB	1:B:375:ASN:HD22	1.70	0.56
1:C:178:PRO:HA	1:C:181:VAL:HB	1.87	0.56
1:B:279:TYR:HB3	1:B:309:LEU:HB3	1.87	0.56
1:B:294:ASN:HA	1:C:46:ARG:HH12	1.70	0.56
1:A:446:TYR:OH	1:A:487:GLU:HG2	2.06	0.56
1:B:430:ARG:HH22	1:C:53:ASP:CG	2.08	0.56
1:B:455:ARG:HG3	1:B:455:ARG:HH11	1.71	0.56
1:C:110:VAL:HG13	1:C:132:ALA:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:LEU:HD23	1:B:466:LEU:O	2.06	0.56
1:A:284:THR:OG1	1:A:287:GLU:HG3	2.05	0.56
1:C:207:GLY:HA3	4:C:919:HOH:O	2.05	0.56
1:A:335:PRO:HD2	4:A:712:HOH:O	2.05	0.55
1:A:367:PRO:HG3	1:C:65:ARG:HD3	1.89	0.55
1:D:18:ARG:HD3	4:D:887:HOH:O	2.06	0.55
1:C:223:ASN:HD21	1:C:227:GLU:HB3	1.72	0.55
1:D:93:TYR:CE1	1:D:282:VAL:HG11	2.42	0.55
1:A:485:HIS:HD2	1:A:487:GLU:N	2.01	0.55
1:B:126:ARG:HH11	1:B:126:ARG:HB2	1.71	0.55
1:C:169:ARG:HD3	1:C:174:HIS:CE1	2.41	0.55
1:B:382:VAL:O	1:B:382:VAL:HG13	2.05	0.55
1:A:232:LYS:HB2	1:A:281:GLN:HB2	1.88	0.55
1:B:160:PHE:CE1	1:B:164:ILE:HD11	2.42	0.55
1:A:384:ASN:HA	1:C:26:LEU:HD13	1.89	0.55
1:C:97:LYS:O	1:C:104:LYS:NZ	2.39	0.55
1:B:491:ARG:O	1:B:494:ALA:HB3	2.06	0.55
1:B:388:ASP:H	1:B:396:ASN:HD21	1.53	0.55
1:B:495:LEU:HD23	1:B:495:LEU:N	2.20	0.55
1:B:334:ASP:O	1:B:337:ASN:HB2	2.07	0.55
1:B:38:LEU:HD21	1:D:404:TYR:CD2	2.42	0.55
1:A:254:HIS:ND1	1:A:255:GLU:N	2.55	0.55
1:B:283:MET:HB2	1:B:302:TRP:CH2	2.42	0.55
1:B:317:LEU:C	1:B:318:ASN:HD22	2.11	0.55
1:C:443:ARG:C	1:C:445:PHE:H	2.10	0.55
1:D:26:LEU:O	1:D:34:VAL:HG13	2.06	0.54
1:C:206:ASP:HB2	1:C:244:LEU:HD23	1.89	0.54
1:D:211:MET:O	1:D:237:THR:HB	2.08	0.54
1:D:447:LEU:HD11	1:D:485:HIS:CD2	2.42	0.54
1:D:498:LYS:HB3	4:D:1084:HOH:O	2.05	0.54
1:B:208:HIS:O	1:B:211:MET:HG2	2.07	0.54
1:C:169:ARG:HH11	1:C:169:ARG:HG2	1.73	0.54
1:A:485:HIS:CD2	1:A:487:GLU:HB3	2.43	0.54
1:B:241:ILE:CG2	1:B:242:LYS:H	2.20	0.54
1:B:439:VAL:O	1:B:442:VAL:N	2.38	0.54
1:C:195:VAL:O	1:C:199:PHE:HD1	1.91	0.54
1:B:294:ASN:HB3	1:B:297:ASP:HB2	1.89	0.54
1:A:72:VAL:HG13	1:A:73:VAL:HG22	1.90	0.54
1:B:4:ARG:HH22	1:C:470:GLN:NE2	1.99	0.54
1:C:91:THR:HG22	1:C:92:ARG:N	2.21	0.54
1:C:112:PHE:HA	1:C:130:GLY:O	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:SER:HA	1:C:222:VAL:O	2.07	0.54
1:D:285:PHE:CD1	1:D:285:PHE:N	2.75	0.54
1:B:95:LYS:HB3	1:B:224:ALA:HB2	1.89	0.54
1:A:148:ASN:N	1:A:148:ASN:HD22	2.05	0.54
1:B:160:PHE:N	1:B:161:PRO:HD2	2.23	0.54
1:B:464:GLY:O	1:B:467:LYS:HE3	2.07	0.54
1:B:101:HIS:O	1:B:104:LYS:HB2	2.07	0.54
1:B:221:LEU:HD23	1:B:221:LEU:N	2.23	0.54
1:C:444:THR:HG21	4:C:801:HOH:O	2.07	0.54
1:C:22:LYS:HD3	1:C:23:PRO:HD2	1.90	0.54
1:B:76:LYS:HD3	1:B:121:SER:O	2.07	0.54
1:C:206:ASP:HB3	1:C:242:LYS:HG2	1.89	0.53
1:C:453:GLU:O	1:C:456:LYS:HB3	2.08	0.53
1:C:281:GLN:OE1	1:C:302:TRP:HB2	2.09	0.53
1:D:73:VAL:O	1:D:74:HIS:HB2	2.08	0.53
1:C:406:ASN:ND2	1:C:410:ALA:HB3	2.19	0.53
1:C:310:ILE:HD12	1:C:310:ILE:N	2.24	0.53
1:B:357:TYR:HB2	1:B:358:PRO:HD3	1.91	0.53
1:D:437:ASP:HA	4:D:827:HOH:O	2.07	0.53
1:B:169:ARG:CG	1:B:169:ARG:NH1	2.69	0.53
1:C:466:LEU:HD12	1:C:469:ALA:HB3	1.91	0.53
1:C:446:TYR:O	1:C:455:ARG:HD3	2.08	0.53
1:A:73:VAL:O	1:A:74:HIS:HB2	2.09	0.53
1:B:138:GLU:H	1:B:138:GLU:CD	2.12	0.53
1:C:493:GLN:HA	1:C:496:LEU:HD23	1.90	0.53
1:D:445:PHE:HA	1:D:449:VAL:HG23	1.89	0.53
1:C:88:HIS:ND1	1:C:311:PRO:HB2	2.24	0.53
1:B:153:PHE:CE2	1:B:194:GLN:HG3	2.43	0.53
1:D:439:VAL:HG23	1:D:440:THR:N	2.24	0.53
1:A:141:ASN:O	1:A:337:ASN:HB3	2.09	0.53
1:D:471:LEU:O	1:D:475:LYS:HG3	2.09	0.53
4:B:998:HOH:O	1:D:386:GLN:HA	2.08	0.53
1:B:456:LYS:HB2	1:B:491:ARG:NH2	2.23	0.53
1:A:280:ILE:HG23	1:A:312:VAL:CG2	2.37	0.53
1:D:34:VAL:HG21	1:D:37:LYS:HB2	1.89	0.53
1:B:4:ARG:HD2	1:B:8:SER:HB2	1.90	0.53
1:A:424:PHE:CE2	1:D:48:PRO:HD3	2.43	0.53
1:D:432:ASN:C	1:D:432:ASN:HD22	2.12	0.53
1:B:322:VAL:C	1:C:172:GLN:HG3	2.29	0.53
1:C:245:SER:OG	1:C:248:ASP:HB2	2.09	0.52
1:B:235:TYR:CD1	1:B:235:TYR:N	2.77	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:PRO:HD2	1:D:266:ASN:OD1	2.09	0.52
1:C:108:ILE:HD13	1:C:315:LEU:HD22	1.91	0.52
1:C:145:VAL:CG1	1:C:353:ARG:HH22	2.22	0.52
1:B:485:HIS:CE1	1:B:487:GLU:HB3	2.44	0.52
1:B:201:ASP:O	1:B:243:ASN:ND2	2.42	0.52
1:C:440:THR:HG22	1:C:441:GLN:N	2.25	0.52
1:D:327:GLU:O	1:D:331:LEU:HG	2.09	0.52
1:A:215:GLY:O	1:A:216:SER:HB2	2.08	0.52
1:D:164:ILE:HG22	1:D:168:LYS:HD2	1.91	0.52
1:B:327:GLU:O	1:B:374:VAL:HG11	2.10	0.52
1:D:401:PRO:HA	4:D:995:HOH:O	2.09	0.52
1:A:402:ASN:HD22	1:A:402:ASN:C	2.12	0.52
1:B:368:ASN:O	1:B:371:GLN:HB2	2.09	0.52
1:B:64:ASP:HB3	1:C:360:THR:HB	1.91	0.52
1:B:100:GLU:HB2	1:B:104:LYS:NZ	2.24	0.52
1:C:49:LEU:HG	1:D:51:VAL:HG21	1.92	0.52
1:B:110:VAL:HG11	1:B:131:PHE:HE1	1.74	0.52
1:B:164:ILE:O	1:B:168:LYS:HG3	2.09	0.52
1:B:36:ASP:HB3	1:C:430:ARG:HD2	1.92	0.52
1:B:280:ILE:CD1	1:B:282:VAL:HG22	2.40	0.52
1:C:462:ILE:HG21	1:C:481:PHE:CE2	2.45	0.52
1:A:36:ASP:OD2	1:A:39:ASN:HB2	2.09	0.51
1:D:232:LYS:HB2	1:D:281:GLN:HG3	1.90	0.51
1:C:479:LYS:HG3	1:C:480:ASN:N	2.23	0.51
1:D:478:VAL:HG21	1:D:493:GLN:OE1	2.10	0.51
1:C:449:VAL:HG21	3:C:1302:NDP:O4D	2.10	0.51
1:D:12:LYS:O	1:D:16:GLU:HG3	2.10	0.51
1:C:291:PHE:CG	1:C:292:PRO:HD2	2.45	0.51
1:C:239:GLN:HE22	1:C:275:SER:H	1.56	0.51
1:C:19:ALA:O	1:C:20:ALA:HB3	2.09	0.51
1:C:463:ALA:O	1:C:467:LYS:HB3	2.10	0.51
1:B:205:PRO:HA	1:B:243:ASN:HA	1.92	0.51
1:A:37:LYS:NZ	1:D:158:LEU:HD22	2.24	0.51
1:C:73:VAL:O	1:C:74:HIS:HB2	2.09	0.51
1:A:424:PHE:CD2	1:D:48:PRO:HD3	2.46	0.51
1:A:446:TYR:OH	1:A:491:ARG:HD2	2.11	0.51
1:D:447:LEU:HD11	1:D:485:HIS:HD2	1.75	0.51
1:A:92:ARG:NH1	1:A:92:ARG:H	2.08	0.51
1:C:303:PRO:HA	3:C:1302:NDP:O2N	2.11	0.51
1:A:385:TYR:HE1	1:C:26:LEU:HD22	1.75	0.51
1:D:277:THR:HB	1:D:279:TYR:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:LYS:C	1:C:158:LEU:HD13	2.31	0.51
1:A:66:GLU:HG2	1:C:387:ARG:O	2.10	0.51
1:D:267:ALA:O	1:D:272:ASN:HB3	2.10	0.51
1:B:444:THR:O	1:B:448:LYS:HB3	2.10	0.51
1:A:472:PHE:HA	1:A:475:LYS:HD3	1.93	0.51
1:C:394:MET:HA	1:C:394:MET:HE3	1.93	0.51
1:B:495:LEU:CD2	1:B:495:LEU:N	2.74	0.51
1:C:34:VAL:HG21	1:C:37:LYS:HB2	1.92	0.51
1:B:331:LEU:HD13	1:B:333:PHE:CZ	2.46	0.51
1:A:276:TRP:HB2	1:A:315:LEU:HD12	1.92	0.51
1:D:202:ARG:HB3	4:D:1019:HOH:O	2.11	0.50
1:A:213:GLY:HA3	1:A:235:TYR:CE2	2.46	0.50
1:A:411:PRO:HA	1:C:24:ASP:O	2.10	0.50
1:B:198:LEU:O	1:B:203:GLY:HA3	2.10	0.50
1:A:88:HIS:CD2	1:A:311:PRO:HG2	2.46	0.50
1:D:188:ARG:HB3	1:D:190:GLU:OE1	2.11	0.50
1:A:139:ASP:O	1:C:32:ASN:HA	2.11	0.50
1:B:221:LEU:HD21	1:B:231:CYS:SG	2.51	0.50
1:C:449:VAL:HG12	1:C:449:VAL:O	2.11	0.50
1:D:443:ARG:NE	1:D:484:VAL:O	2.44	0.50
1:D:74:HIS:O	1:D:111:ARG:NH2	2.44	0.50
1:B:11:MET:HB3	1:D:408:PHE:CE2	2.47	0.50
1:D:213:GLY:HA3	1:D:235:TYR:CE2	2.46	0.50
1:B:450:LEU:HD22	1:B:454:GLN:HG3	1.92	0.50
4:B:787:HOH:O	1:C:45:PRO:HD3	2.12	0.50
1:C:225:ASP:HB2	4:C:895:HOH:O	2.10	0.50
1:B:248:ASP:O	1:B:251:ARG:HB3	2.11	0.50
1:C:61:ALA:O	1:C:65:ARG:HG3	2.11	0.50
1:D:296:PHE:CE1	1:D:346:PRO:HD2	2.45	0.50
1:C:124:THR:O	1:C:249:ALA:HB1	2.12	0.50
1:C:487:GLU:HA	1:C:490:SER:HB3	1.94	0.50
1:B:155:ARG:HD2	4:B:1005:HOH:O	2.12	0.50
1:D:60:MET:CE	1:D:63:PHE:HD2	2.24	0.50
1:D:282:VAL:HG12	1:D:283:MET:N	2.26	0.50
1:A:445:PHE:HA	1:A:449:VAL:CG2	2.42	0.50
1:B:386:GLN:C	1:B:387:ARG:HG2	2.32	0.50
1:D:284:THR:HG23	1:D:287:GLU:CD	2.32	0.50
1:B:430:ARG:NH2	1:C:53:ASP:OD2	2.44	0.50
1:D:153:PHE:HE2	1:D:185:TRP:CZ2	2.30	0.50
1:B:301:VAL:CG2	1:B:441:GLN:HE22	2.25	0.50
1:D:367:PRO:CG	1:D:390:PRO:HG2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:LEU:HD21	1:B:474:GLN:HA	1.94	0.50
1:C:177:ASP:OD1	1:C:179:ASP:HB2	2.12	0.49
1:C:451:ASN:H	1:C:454:GLN:NE2	2.09	0.49
1:D:441:GLN:HA	1:D:444:THR:CG2	2.42	0.49
1:A:182:TRP:O	1:A:186:SER:HB3	2.12	0.49
1:C:466:LEU:CD1	1:C:469:ALA:HB3	2.42	0.49
1:B:301:VAL:HG22	1:B:441:GLN:HE22	1.77	0.49
1:C:287:GLU:O	1:C:290:ILE:HG12	2.12	0.49
1:D:279:TYR:C	1:D:280:ILE:HG22	2.32	0.49
1:D:440:THR:O	1:D:444:THR:HG22	2.11	0.49
1:D:205:PRO:HA	1:D:243:ASN:HA	1.94	0.49
1:B:207:GLY:HA3	4:B:763:HOH:O	2.11	0.49
1:B:442:VAL:O	1:B:445:PHE:HB3	2.13	0.49
1:C:26:LEU:HD12	1:C:27:THR:N	2.28	0.49
1:C:334:ASP:OD1	1:C:361:HIS:ND1	2.45	0.49
1:D:106:THR:O	1:D:108:ILE:HG23	2.12	0.49
1:A:357:TYR:HB2	1:A:358:PRO:HD3	1.95	0.49
1:A:87:THR:HG23	1:A:313:GLY:HA2	1.95	0.49
1:B:148:ASN:CB	1:B:211:MET:HE2	2.42	0.49
1:A:120:GLY:H	1:D:120:GLY:H	1.60	0.49
1:A:108:ILE:HA	1:A:134:LYS:O	2.12	0.49
1:B:169:ARG:HG2	1:B:169:ARG:NH1	2.09	0.49
1:D:112:PHE:HA	1:D:130:GLY:O	2.13	0.49
1:B:41:LEU:CB	1:B:53:ASP:HB2	2.43	0.49
1:B:40:SER:O	1:C:430:ARG:HA	2.12	0.49
1:B:51:VAL:HG23	1:B:52:GLN:N	2.27	0.49
1:B:492:ILE:HG22	1:B:493:GLN:N	2.28	0.49
1:B:128:PRO:O	1:B:129:ARG:HD2	2.12	0.49
1:B:97:LYS:HD2	1:B:138:GLU:HB2	1.95	0.49
1:C:155:ARG:HD2	1:C:433:SER:HB2	1.94	0.49
1:C:88:HIS:CE1	1:C:311:PRO:HB2	2.47	0.49
1:B:406:ASN:ND2	1:B:410:ALA:HB3	2.20	0.49
1:B:391:MET:HE2	1:D:365:LEU:C	2.32	0.49
1:D:442:VAL:CG1	1:D:484:VAL:HG11	2.43	0.49
1:D:442:VAL:O	1:D:445:PHE:HB3	2.13	0.49
1:C:293:PHE:CD1	1:C:293:PHE:N	2.72	0.49
1:C:223:ASN:HD21	1:C:227:GLU:CB	2.26	0.49
1:D:439:VAL:HG23	1:D:440:THR:H	1.78	0.49
1:B:275:SER:HA	1:B:315:LEU:O	2.13	0.49
1:C:423:HIS:HA	1:D:427:ASP:HA	1.94	0.49
1:D:357:TYR:O	1:D:360:THR:HG22	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:VAL:HG23	1:D:104:LYS:O	2.12	0.48
1:B:456:LYS:HB2	1:B:491:ARG:HH22	1.78	0.48
1:B:241:ILE:CG2	1:B:242:LYS:N	2.76	0.48
1:B:11:MET:HE1	1:C:180:MET:HG2	1.95	0.48
1:B:328:VAL:O	1:B:331:LEU:HB2	2.12	0.48
1:C:126:ARG:HB2	1:C:126:ARG:CZ	2.42	0.48
1:C:208:HIS:HA	1:C:211:MET:HE1	1.95	0.48
1:D:471:LEU:O	1:D:474:GLN:HB2	2.13	0.48
1:B:367:PRO:HG2	1:B:390:PRO:CG	2.43	0.48
1:A:54:VAL:HG11	1:C:336:SER:HB2	1.95	0.48
1:C:197:PHE:O	1:C:197:PHE:HD1	1.95	0.48
1:D:85:GLU:O	1:D:313:GLY:HA3	2.13	0.48
1:C:402:ASN:N	1:C:402:ASN:ND2	2.55	0.48
1:B:127:ASP:O	1:B:129:ARG:NH1	2.45	0.48
1:D:244:LEU:HD23	1:D:245:SER:N	2.29	0.48
1:B:440:THR:O	1:B:444:THR:HG23	2.14	0.48
1:B:439:VAL:O	1:B:442:VAL:HG23	2.14	0.48
1:B:402:ASN:ND2	1:B:402:ASN:C	2.66	0.48
1:B:205:PRO:HB3	4:B:1001:HOH:O	2.13	0.48
1:B:201:ASP:HB3	1:B:243:ASN:HD22	1.79	0.48
1:B:452:GLU:HB2	1:B:455:ARG:NH2	2.28	0.48
1:C:476:LYS:HZ2	1:C:476:LYS:HB3	1.78	0.48
1:A:37:LYS:O	1:D:158:LEU:HD22	2.13	0.48
1:D:338:MET:HE2	1:D:342:ILE:C	2.33	0.48
1:D:491:ARG:O	1:D:495:LEU:HD12	2.14	0.48
1:B:463:ALA:O	1:B:467:LYS:HG2	2.14	0.48
1:B:17:GLN:HG2	4:B:1026:HOH:O	2.14	0.48
1:D:397:GLN:HE21	1:D:397:GLN:HB2	1.54	0.48
1:B:100:GLU:CB	1:B:104:LYS:HG3	2.38	0.48
1:A:419:GLU:CD	1:A:419:GLU:H	2.17	0.48
1:A:18:ARG:HG2	1:A:18:ARG:HH11	1.77	0.48
1:B:326:ALA:O	1:B:374:VAL:HG21	2.12	0.48
1:A:97:LYS:HG2	1:A:100:GLU:OE1	2.13	0.48
1:D:86:VAL:HB	1:D:102:ILE:HA	1.95	0.48
1:A:324:TYR:CE1	1:A:328:VAL:HG11	2.49	0.48
1:B:206:ASP:HB2	1:B:244:LEU:HG	1.95	0.48
1:D:387:ARG:NH1	1:D:387:ARG:HG2	2.27	0.48
1:D:81:PHE:HZ	1:D:327:GLU:HB3	1.79	0.48
1:C:310:ILE:HD12	1:C:310:ILE:H	1.79	0.48
1:B:319:ARG:O	1:B:319:ARG:HD2	2.14	0.48
1:D:291:PHE:CE1	1:D:293:PHE:HB2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:ILE:HG13	1:D:349:MET:HE2	1.95	0.47
1:C:94:SER:OG	1:C:221:LEU:HD22	2.14	0.47
1:C:345:SER:O	1:C:347:ASP:N	2.47	0.47
1:D:235:TYR:CD1	1:D:235:TYR:N	2.81	0.47
1:B:396:ASN:HB3	1:D:323:ASN:ND2	2.28	0.47
1:A:248:ASP:O	1:A:251:ARG:N	2.46	0.47
1:B:472:PHE:CE2	1:B:473:ILE:HG13	2.49	0.47
1:C:202:ARG:HA	1:C:243:ASN:ND2	2.28	0.47
1:D:298:LEU:HD23	1:D:349:MET:HG3	1.96	0.47
1:B:125:VAL:HG22	1:B:126:ARG:N	2.28	0.47
1:C:126:ARG:O	1:C:126:ARG:HG3	2.13	0.47
1:B:297:ASP:HB3	1:B:300:LYS:HG3	1.95	0.47
1:C:439:VAL:HG12	1:C:484:VAL:HA	1.95	0.47
1:C:480:ASN:O	1:C:484:VAL:HG23	2.15	0.47
1:A:464:GLY:O	1:A:467:LYS:HD3	2.14	0.47
1:A:42:THR:O	1:D:431:PHE:HE1	1.97	0.47
1:D:212:ASP:OD1	1:D:237:THR:HG22	2.14	0.47
1:A:402:ASN:C	1:A:402:ASN:ND2	2.68	0.47
1:B:176:LYS:HG2	4:B:800:HOH:O	2.13	0.47
1:D:265:PHE:CD1	1:D:320:ASN:ND2	2.83	0.47
1:B:229:VAL:CG2	1:B:284:THR:HA	2.43	0.47
1:B:351:GLN:O	1:B:354:LEU:HB2	2.14	0.47
1:D:19:ALA:N	4:D:841:HOH:O	2.47	0.47
1:B:135:PHE:HB2	1:B:142:TRP:HB3	1.95	0.47
1:D:279:TYR:O	1:D:280:ILE:HG22	2.14	0.47
1:C:444:THR:HG22	1:C:444:THR:O	2.14	0.47
1:D:74:HIS:CE1	1:D:115:VAL:HG22	2.49	0.47
1:A:357:TYR:O	1:A:360:THR:HG22	2.14	0.47
1:A:60:MET:HB3	1:D:355:PHE:HE2	1.79	0.47
1:D:65:ARG:HG3	1:D:65:ARG:HH11	1.79	0.47
1:A:147:ASN:CG	2:A:507:HEM:HAC	2.34	0.47
1:C:151:ILE:CD1	1:C:194:GLN:HG2	2.41	0.47
1:B:264:LEU:C	1:B:264:LEU:HD12	2.34	0.47
1:B:270:THR:O	1:B:272:ASN:N	2.48	0.47
1:A:271:GLY:HA2	1:A:273:TYR:CE1	2.50	0.47
1:B:235:TYR:HA	1:B:277:THR:O	2.15	0.47
1:A:277:THR:OG1	1:A:314:LYS:NZ	2.48	0.47
1:D:500:ASN:C	1:D:501:GLU:HG3	2.34	0.47
1:B:46:ARG:HD2	4:B:1056:HOH:O	2.15	0.47
1:D:443:ARG:HG3	1:D:484:VAL:O	2.15	0.47
1:A:177:ASP:HB3	1:A:180:MET:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:PHE:CE2	1:D:173:THR:HG22	2.50	0.47
1:D:245:SER:HB3	1:D:248:ASP:OD2	2.15	0.47
1:D:214:TYR:N	1:D:214:TYR:CD1	2.83	0.47
1:B:95:LYS:HG3	1:B:222:VAL:O	2.15	0.47
1:A:467:LYS:HG2	1:A:468:ASP:N	2.30	0.47
1:B:71:ARG:HH11	1:B:71:ARG:HG3	1.80	0.47
1:D:148:ASN:C	1:D:148:ASN:ND2	2.68	0.47
1:A:381:ARG:HH11	1:A:381:ARG:HG2	1.80	0.46
1:B:5:ASP:HB2	1:B:6:PRO:HD2	1.96	0.46
1:B:485:HIS:CE1	1:B:487:GLU:HG2	2.50	0.46
1:D:154:ILE:HG13	1:D:349:MET:HE1	1.96	0.46
1:C:349:MET:HE3	2:C:507:HEM:HBB1	1.98	0.46
1:B:145:VAL:HG22	1:B:333:PHE:HB3	1.97	0.46
1:A:50:LEU:HD12	1:B:48:PRO:HB2	1.98	0.46
1:D:210:HIS:HB3	1:D:242:LYS:H	1.81	0.46
1:C:446:TYR:OH	1:C:488:TYR:HA	2.15	0.46
1:B:19:ALA:HB3	1:B:21:GLN:HG3	1.97	0.46
1:C:219:PHE:O	1:C:230:TYR:HA	2.15	0.46
1:A:155:ARG:NH2	1:A:438:ASN:OD1	2.49	0.46
1:B:268:ILE:HB	1:B:320:ASN:HD21	1.80	0.46
1:D:142:TRP:HA	1:D:337:ASN:O	2.14	0.46
1:C:367:PRO:HG2	1:C:390:PRO:CG	2.46	0.46
1:D:476:LYS:O	1:D:480:ASN:OD1	2.34	0.46
1:B:155:ARG:NH2	1:B:438:ASN:OD1	2.46	0.46
1:C:156:ASP:OD1	1:C:158:LEU:HB2	2.15	0.46
1:A:51:VAL:HG11	1:B:49:LEU:HD13	1.98	0.46
1:C:283:MET:HE2	1:C:291:PHE:CD1	2.51	0.46
1:B:359:ASP:O	1:B:362:ARG:HB2	2.16	0.46
1:B:254:HIS:ND1	1:C:254:HIS:ND1	2.64	0.46
1:C:244:LEU:HD11	1:C:252:LEU:HD12	1.98	0.46
1:C:459:CYS:SG	1:C:492:ILE:HD13	2.54	0.46
1:B:280:ILE:O	1:B:280:ILE:HG13	2.15	0.46
1:D:209:ARG:HB2	4:D:1020:HOH:O	2.15	0.46
1:D:71:ARG:HG3	4:D:1078:HOH:O	2.15	0.46
1:C:428:VAL:O	1:C:429:GLN:HB3	2.15	0.46
1:C:250:ALA:O	1:C:253:ALA:HB3	2.16	0.46
1:B:419:GLU:CD	1:B:419:GLU:H	2.19	0.46
1:D:118:GLU:N	1:D:118:GLU:OE1	2.44	0.46
1:C:446:TYR:O	1:C:447:LEU:HD23	2.16	0.46
1:D:455:ARG:HD2	1:D:491:ARG:NH1	2.29	0.46
1:C:239:GLN:H	1:C:239:GLN:CD	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:PRO:HD2	1:D:340:PRO:HD3	1.98	0.46
1:D:369:TYR:O	1:D:372:ILE:HG13	2.16	0.46
1:A:42:THR:HG22	1:A:48:PRO:O	2.16	0.46
1:D:284:THR:O	1:D:288:ALA:N	2.48	0.46
1:B:209:ARG:HG2	1:B:274:PRO:CG	2.46	0.46
1:B:35:GLY:O	1:D:413:HIS:HB3	2.16	0.46
1:D:492:ILE:HA	1:D:495:LEU:HD12	1.98	0.46
1:D:189:PRO:C	1:D:191:SER:H	2.19	0.46
1:D:217:HIS:HE1	1:D:298:LEU:HD22	1.81	0.46
1:D:96:ALA:HB3	1:D:99:PHE:CD2	2.51	0.46
1:B:393:MET:HB3	1:B:394:MET:H	1.55	0.46
1:C:459:CYS:SG	1:C:492:ILE:CD1	3.04	0.45
1:B:202:ARG:HG2	1:B:202:ARG:HH11	1.80	0.45
1:C:92:ARG:HH11	1:C:92:ARG:CG	2.27	0.45
1:D:153:PHE:CE2	1:D:185:TRP:CZ2	3.05	0.45
1:C:212:ASP:OD1	1:C:237:THR:HG22	2.16	0.45
1:D:202:ARG:HH11	1:D:241:ILE:HG21	1.78	0.45
1:B:281:GLN:HB2	1:B:302:TRP:CE3	2.51	0.45
1:B:73:VAL:HG11	1:B:164:ILE:HD12	1.98	0.45
1:B:16:GLU:C	1:B:18:ARG:H	2.19	0.45
1:C:82:GLY:HA3	1:C:316:VAL:O	2.16	0.45
1:C:90:ILE:O	1:C:93:TYR:HB2	2.16	0.45
1:D:410:ALA:HB1	1:D:411:PRO:HD2	1.98	0.45
1:D:334:ASP:OD1	1:D:361:HIS:ND1	2.49	0.45
1:B:381:ARG:HH11	1:B:381:ARG:CG	2.29	0.45
1:B:273:TYR:HA	1:B:274:PRO:HD3	1.78	0.45
1:B:316:VAL:HG12	1:B:318:ASN:ND2	2.31	0.45
1:A:304:HIS:HB2	3:A:1102:NDP:O2A	2.17	0.45
1:D:3:ASN:HB2	1:D:4:ARG:H	1.62	0.45
1:C:446:TYR:HE2	1:C:485:HIS:ND1	2.15	0.45
1:B:452:GLU:OE2	1:B:491:ARG:NH2	2.50	0.45
1:D:475:LYS:HG3	1:D:475:LYS:H	1.53	0.45
1:C:220:LYS:HA	1:C:229:VAL:O	2.17	0.45
1:A:4:ARG:HD3	1:A:9:ASP:OD1	2.16	0.45
1:B:67:ARG:HB2	4:B:753:HOH:O	2.15	0.45
1:C:251:ARG:HG3	1:C:252:LEU:H	1.80	0.45
1:B:223:ASN:HD21	1:B:227:GLU:CD	2.20	0.45
1:B:16:GLU:O	1:B:18:ARG:N	2.49	0.45
1:D:343:GLU:HB3	1:D:344:PRO:HD2	1.99	0.45
1:D:98:VAL:HG13	1:D:99:PHE:CD1	2.52	0.45
1:A:280:ILE:HG13	1:A:280:ILE:O	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:480:ASN:O	1:C:483:ASP:HB2	2.16	0.45
1:B:287:GLU:O	1:B:290:ILE:N	2.44	0.45
1:B:451:ASN:O	1:B:451:ASN:OD1	2.35	0.45
1:A:39:ASN:OD1	1:D:432:ASN:HA	2.17	0.45
1:C:179:ASP:O	1:C:183:ASP:HB2	2.17	0.45
1:C:280:ILE:O	1:C:280:ILE:HG13	2.17	0.45
1:D:228:ALA:HB2	1:D:420:HIS:CE1	2.52	0.45
1:D:63:PHE:HA	1:D:66:GLU:HG3	1.98	0.45
1:B:110:VAL:HG11	1:B:131:PHE:CE1	2.52	0.45
1:D:71:ARG:HG3	1:D:71:ARG:HH11	1.82	0.45
1:A:329:GLU:HA	1:A:329:GLU:OE1	2.16	0.45
1:D:271:GLY:HA2	1:D:273:TYR:CE1	2.52	0.45
1:A:156:ASP:OD1	1:A:158:LEU:HB2	2.17	0.45
1:B:155:ARG:NH1	1:B:299:THR:OG1	2.50	0.45
1:B:38:LEU:HG	1:D:413:HIS:HE1	1.81	0.45
1:C:126:ARG:HA	1:C:204:ILE:HG12	1.98	0.45
1:B:280:ILE:HD12	1:B:282:VAL:HG22	1.99	0.45
1:B:345:SER:C	1:B:347:ASP:H	2.19	0.45
1:D:331:LEU:HD23	1:D:331:LEU:HA	1.81	0.45
1:C:148:ASN:HA	1:C:212:ASP:O	2.16	0.45
1:A:470:GLN:HG3	1:D:4:ARG:NH2	2.32	0.45
1:B:90:ILE:O	1:B:93:TYR:HB2	2.17	0.45
1:B:92:ARG:H	1:B:92:ARG:HG3	1.43	0.45
1:A:24:ASP:N	1:A:24:ASP:OD1	2.50	0.45
1:D:291:PHE:CD1	1:D:292:PRO:HD2	2.52	0.44
1:C:73:VAL:HB	1:C:74:HIS:HD2	1.81	0.44
1:A:499:TYR:C	1:A:501:GLU:H	2.21	0.44
1:A:498:LYS:O	1:A:501:GLU:N	2.49	0.44
1:B:364:ARG:HD3	4:B:961:HOH:O	2.17	0.44
1:B:166:SER:HA	1:B:180:MET:HE3	1.99	0.44
1:C:14:TRP:O	1:C:18:ARG:HB2	2.17	0.44
1:B:298:LEU:HD23	1:B:349:MET:HE2	1.99	0.44
1:C:52:GLN:HB3	1:C:52:GLN:HE21	1.52	0.44
1:B:283:MET:SD	1:B:288:ALA:HA	2.58	0.44
1:B:278:LEU:O	1:B:312:VAL:HG13	2.17	0.44
1:B:218:THR:O	1:B:345:SER:HB3	2.18	0.44
1:D:206:ASP:HB3	1:D:242:LYS:HG2	1.99	0.44
1:A:422:THR:O	1:B:428:VAL:HG22	2.16	0.44
1:C:446:TYR:CE2	1:C:485:HIS:ND1	2.86	0.44
1:C:154:ILE:HG12	1:C:154:ILE:H	1.68	0.44
1:C:73:VAL:HG11	1:C:164:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:VAL:HG23	1:B:424:PHE:HD1	1.82	0.44
1:A:273:TYR:HA	1:A:274:PRO:HD3	1.86	0.44
1:A:273:TYR:HB3	1:A:317:LEU:O	2.17	0.44
1:A:445:PHE:HB2	3:A:1102:NDP:O2D	2.17	0.44
1:C:155:ARG:NH2	1:C:190:GLU:HB3	2.32	0.44
1:C:481:PHE:HD1	1:C:481:PHE:N	2.16	0.44
1:B:477:ALA:O	1:B:481:PHE:CD2	2.70	0.44
1:B:202:ARG:HD3	3:B:1202:NDP:C6A	2.48	0.44
1:D:90:ILE:HD11	1:D:99:PHE:CG	2.52	0.44
1:A:278:LEU:HD23	1:A:312:VAL:HB	1.99	0.44
1:C:481:PHE:CD1	1:C:481:PHE:N	2.85	0.44
1:A:76:LYS:HD3	1:A:121:SER:O	2.17	0.44
1:A:291:PHE:HD2	1:A:293:PHE:O	2.00	0.44
1:D:5:ASP:OD1	1:D:5:ASP:N	2.50	0.44
1:A:322:VAL:O	1:D:172:GLN:HB2	2.17	0.44
1:D:284:THR:O	1:D:288:ALA:HB2	2.18	0.44
1:D:150:PRO:HB3	1:D:214:TYR:HD2	1.80	0.44
1:A:235:TYR:CD1	1:A:235:TYR:N	2.85	0.44
1:B:237:THR:OG1	1:B:239:GLN:NE2	2.51	0.44
1:B:252:LEU:HD23	1:B:259:TYR:CD2	2.53	0.44
1:C:17:GLN:HE21	1:C:17:GLN:HB3	1.61	0.44
1:A:37:LYS:HZ2	1:D:158:LEU:HD22	1.82	0.44
1:B:283:MET:CE	1:B:295:PRO:HB3	2.48	0.44
1:B:36:ASP:C	1:B:36:ASP:OD1	2.56	0.44
1:D:281:GLN:HG2	1:D:309:LEU:HD12	2.00	0.44
1:B:16:GLU:O	1:B:19:ALA:N	2.46	0.44
1:B:245:SER:O	1:B:248:ASP:N	2.51	0.44
1:C:143:ASP:HB2	1:C:334:ASP:O	2.18	0.44
1:B:162:SER:O	1:B:165:HIS:HB2	2.18	0.44
1:D:220:LYS:HB3	1:D:343:GLU:HB2	2.00	0.44
1:A:216:SER:HB3	1:A:298:LEU:HD11	1.99	0.44
1:B:251:ARG:HG2	1:B:251:ARG:NH1	2.33	0.44
1:B:69:PRO:HD3	1:C:69:PRO:HG3	2.00	0.44
1:C:110:VAL:HG11	1:C:131:PHE:HE1	1.83	0.44
1:C:110:VAL:HG11	1:C:131:PHE:CE1	2.53	0.44
1:A:221:LEU:O	1:A:228:ALA:HA	2.17	0.44
1:D:228:ALA:HB1	1:D:285:PHE:HZ	1.82	0.44
1:C:168:LYS:HB3	1:C:169:ARG:H	1.71	0.44
1:B:245:SER:O	1:B:246:VAL:C	2.55	0.44
1:C:470:GLN:CB	1:C:473:ILE:HD12	2.48	0.43
1:B:55:VAL:CG2	1:C:430:ARG:NH2	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ARG:CG	1:B:18:ARG:HH11	2.30	0.43
1:D:291:PHE:HE1	1:D:293:PHE:HB2	1.83	0.43
1:B:382:VAL:O	1:B:382:VAL:CG1	2.66	0.43
1:B:467:LYS:HD3	1:B:499:TYR:CD1	2.54	0.43
1:A:155:ARG:NH1	1:A:297:ASP:OD2	2.51	0.43
1:C:419:GLU:H	1:C:419:GLU:CD	2.22	0.43
1:D:151:ILE:HD13	1:D:193:HIS:CD2	2.53	0.43
1:A:74:HIS:HA	1:A:114:THR:O	2.18	0.43
1:B:37:LYS:O	1:C:158:LEU:HB3	2.19	0.43
1:C:154:ILE:CD1	1:C:160:PHE:HA	2.48	0.43
1:D:442:VAL:HB	1:D:484:VAL:HG13	2.00	0.43
1:B:26:LEU:HD22	1:D:385:TYR:HE1	1.83	0.43
1:D:391:MET:C	1:D:393:MET:HE2	2.38	0.43
1:A:343:GLU:HB3	1:A:344:PRO:CD	2.48	0.43
1:D:301:VAL:O	1:D:303:PRO:HD3	2.18	0.43
1:B:142:TRP:HA	1:B:337:ASN:O	2.19	0.43
1:A:436:ASP:O	1:A:437:ASP:O	2.36	0.43
1:A:343:GLU:HB3	1:A:344:PRO:HD2	2.00	0.43
1:A:496:LEU:O	1:A:497:ASP:C	2.57	0.43
1:C:337:ASN:HD22	1:C:337:ASN:HA	1.70	0.43
1:D:85:GLU:OE2	1:D:105:ARG:NH1	2.52	0.43
1:C:232:LYS:O	1:C:280:ILE:HA	2.18	0.43
1:B:218:THR:OG1	1:B:232:LYS:HE3	2.19	0.43
1:B:358:PRO:HD3	4:B:965:HOH:O	2.19	0.43
1:C:15:LYS:O	1:C:15:LYS:HG2	2.19	0.43
1:A:451:ASN:C	1:A:451:ASN:OD1	2.57	0.43
1:B:220:LYS:HB3	1:B:343:GLU:HB2	2.01	0.43
1:C:291:PHE:HD2	1:C:293:PHE:O	2.01	0.43
1:A:50:LEU:C	1:A:52:GLN:N	2.71	0.43
1:D:210:HIS:CG	1:D:242:LYS:HB3	2.54	0.43
1:C:43:VAL:O	1:C:47:GLY:HA3	2.18	0.43
1:D:381:ARG:HG2	1:D:381:ARG:HH11	1.84	0.43
1:B:414:GLN:O	1:D:35:GLY:HA2	2.18	0.43
1:C:445:PHE:HD1	1:C:449:VAL:HB	1.83	0.43
1:C:169:ARG:HG2	1:C:169:ARG:NH1	2.33	0.43
1:C:426:GLY:O	1:C:427:ASP:O	2.37	0.43
1:C:466:LEU:HD12	1:C:466:LEU:C	2.38	0.43
1:B:11:MET:HE3	1:B:11:MET:HB2	1.92	0.43
1:A:100:GLU:HB3	1:A:104:LYS:HE3	2.01	0.43
1:A:445:PHE:HA	1:A:449:VAL:HG23	2.01	0.43
1:C:496:LEU:O	1:C:500:ASN:OD1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:VAL:CG2	1:B:52:GLN:N	2.82	0.43
1:B:193:HIS:HB2	4:B:941:HOH:O	2.19	0.43
1:B:236:LYS:HG2	1:B:236:LYS:H	1.45	0.43
1:D:241:ILE:O	1:D:241:ILE:HG22	2.19	0.43
1:C:282:VAL:HG12	1:C:283:MET:N	2.33	0.43
1:B:26:LEU:O	1:B:34:VAL:HG23	2.19	0.42
1:B:212:ASP:OD1	1:B:236:LYS:HA	2.19	0.42
1:D:170:ASN:HD22	1:D:172:GLN:N	2.16	0.42
1:B:437:ASP:HA	4:B:1007:HOH:O	2.18	0.42
1:B:466:LEU:HD23	1:B:474:GLN:HG2	2.01	0.42
1:C:202:ARG:O	1:C:204:ILE:N	2.53	0.42
1:C:239:GLN:CD	1:C:239:GLN:N	2.73	0.42
1:B:386:GLN:O	1:B:387:ARG:HG2	2.19	0.42
1:A:279:TYR:HA	1:A:310:ILE:O	2.20	0.42
1:C:191:SER:C	1:C:195:VAL:HG23	2.39	0.42
1:A:501:GLU:HA	1:A:501:GLU:OE1	2.19	0.42
1:A:281:GLN:HG3	1:A:309:LEU:HD13	2.02	0.42
1:A:235:TYR:HA	1:A:277:THR:O	2.20	0.42
1:D:189:PRO:C	1:D:191:SER:N	2.71	0.42
1:A:160:PHE:CD1	2:A:507:HEM:HAB	2.55	0.42
1:D:220:LYS:HZ3	1:D:420:HIS:HD2	1.67	0.42
1:D:60:MET:CE	1:D:63:PHE:CD2	3.01	0.42
1:C:22:LYS:CD	1:C:23:PRO:HD2	2.50	0.42
1:A:391:MET:HE2	1:C:368:ASN:HB2	2.01	0.42
1:C:286:SER:O	1:C:289:GLU:N	2.53	0.42
1:D:220:LYS:HB2	1:D:344:PRO:O	2.20	0.42
1:A:169:ARG:HD2	1:A:174:HIS:CE1	2.55	0.42
1:A:18:ARG:HG3	1:A:18:ARG:H	1.58	0.42
1:C:433:SER:C	1:C:435:ASN:H	2.22	0.42
1:C:108:ILE:HA	1:C:134:LYS:O	2.20	0.42
1:B:262:ARG:HB3	1:C:175:LEU:HD11	2.00	0.42
1:A:209:ARG:CG	1:A:274:PRO:HB3	2.46	0.42
1:D:442:VAL:HB	1:D:484:VAL:CG1	2.49	0.42
1:D:279:TYR:C	1:D:280:ILE:CG2	2.87	0.42
1:B:95:LYS:H	1:B:95:LYS:HG3	1.50	0.42
1:A:139:ASP:HB3	1:A:340:PRO:HD2	2.02	0.42
1:B:74:HIS:O	1:B:111:ARG:NH2	2.53	0.42
1:A:430:ARG:HA	1:D:40:SER:O	2.19	0.42
1:D:415:PRO:HA	1:D:418:LEU:CD1	2.50	0.42
1:B:169:ARG:HD3	1:B:174:HIS:CE1	2.55	0.42
1:D:217:HIS:HD1	1:D:347:ASP:CG	2.22	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:LYS:O	1:D:96:ALA:C	2.58	0.42
1:D:76:LYS:O	1:D:113:SER:CB	2.67	0.42
1:C:290:ILE:O	1:C:291:PHE:C	2.57	0.42
1:B:347:ASP:HB3	1:B:350:LEU:HB3	2.01	0.42
1:B:355:PHE:CD2	1:B:356:ALA:N	2.88	0.42
1:A:393:MET:O	1:A:394:MET:HB2	2.19	0.42
1:C:43:VAL:CG1	1:C:48:PRO:HD2	2.50	0.42
1:C:472:PHE:HA	1:C:475:LYS:HG3	2.02	0.42
1:D:20:ALA:O	1:D:21:GLN:C	2.58	0.42
1:B:279:TYR:HA	1:B:310:ILE:O	2.20	0.41
1:B:122:ALA:CB	1:B:257:PRO:HB3	2.44	0.41
1:B:414:GLN:HG2	1:B:416:SER:OG	2.20	0.41
1:B:231:CYS:HA	1:B:281:GLN:O	2.20	0.41
1:B:126:ARG:HA	1:B:204:ILE:HG12	2.02	0.41
1:C:180:MET:HB3	1:D:403:TYR:CE1	2.55	0.41
1:B:268:ILE:HB	1:B:320:ASN:ND2	2.35	0.41
1:A:406:ASN:HD21	1:A:410:ALA:HB3	1.85	0.41
1:A:72:VAL:CG1	2:A:507:HEM:HMA1	2.50	0.41
1:D:221:LEU:HD21	1:D:231:CYS:SG	2.60	0.41
1:A:223:ASN:OD1	1:A:223:ASN:C	2.59	0.41
1:B:26:LEU:HD13	1:D:384:ASN:HA	2.00	0.41
1:D:391:MET:O	1:D:393:MET:HE2	2.19	0.41
1:A:296:PHE:CD1	1:A:346:PRO:HD2	2.55	0.41
1:A:350:LEU:O	1:A:353:ARG:HB2	2.21	0.41
1:D:104:LYS:NZ	1:D:138:GLU:OE1	2.54	0.41
1:A:374:VAL:HB	4:A:929:HOH:O	2.20	0.41
1:D:170:ASN:ND2	1:D:172:GLN:N	2.58	0.41
1:B:304:HIS:HB2	3:B:1202:NDP:O2A	2.21	0.41
1:B:94:SER:HB3	1:B:221:LEU:HD13	2.02	0.41
1:B:158:LEU:O	1:C:37:LYS:NZ	2.54	0.41
1:C:284:THR:HG23	1:C:287:GLU:OE2	2.20	0.41
1:D:296:PHE:CD1	1:D:346:PRO:HD2	2.55	0.41
1:C:87:THR:OG1	1:C:313:GLY:HA2	2.19	0.41
1:A:20:ALA:O	1:A:21:GLN:C	2.59	0.41
1:C:71:ARG:HH11	1:C:71:ARG:HG3	1.86	0.41
1:B:223:ASN:C	1:B:225:ASP:N	2.74	0.41
1:C:90:ILE:O	1:C:91:THR:C	2.59	0.41
1:A:173:THR:O	1:A:174:HIS:HB3	2.20	0.41
1:B:16:GLU:C	1:B:18:ARG:N	2.73	0.41
1:D:148:ASN:C	1:D:148:ASN:HD22	2.23	0.41
1:D:189:PRO:O	1:D:192:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:TYR:CD1	1:C:83:TYR:C	2.94	0.41
1:C:72:VAL:HG12	2:C:507:HEM:HAA2	2.03	0.41
1:B:430:ARG:NH2	1:C:53:ASP:CG	2.73	0.41
1:C:126:ARG:HD3	1:C:198:LEU:HG	2.02	0.41
1:C:496:LEU:O	1:C:498:LYS:N	2.53	0.41
1:B:393:MET:HG3	1:D:373:PRO:HD3	2.03	0.41
1:A:26:LEU:CD1	1:C:384:ASN:HA	2.50	0.41
1:C:460:GLU:HG2	1:C:495:LEU:HD21	2.03	0.41
1:B:439:VAL:HG12	1:B:484:VAL:HG22	2.02	0.41
1:B:221:LEU:O	1:B:228:ALA:HA	2.21	0.41
1:A:423:HIS:HA	1:B:427:ASP:HA	2.03	0.41
1:A:444:THR:HG21	4:A:972:HOH:O	2.21	0.41
1:C:63:PHE:C	1:C:63:PHE:CD1	2.94	0.41
1:B:410:ALA:HB1	1:B:411:PRO:HD2	2.02	0.41
1:C:152:PHE:HA	1:C:194:GLN:HG3	2.02	0.41
1:B:301:VAL:HB	3:B:1202:NDP:N7N	2.36	0.41
1:A:39:ASN:C	1:D:158:LEU:HD12	2.40	0.41
1:B:188:ARG:HA	1:B:189:PRO:HD2	1.91	0.41
1:C:232:LYS:HG3	1:C:302:TRP:CE3	2.56	0.41
1:D:93:TYR:CZ	1:D:282:VAL:HG21	2.56	0.41
1:D:440:THR:HG22	1:D:441:GLN:N	2.35	0.41
1:A:237:THR:HA	1:A:276:TRP:CD1	2.56	0.41
1:B:290:ILE:O	1:B:291:PHE:C	2.59	0.41
1:A:14:TRP:O	1:A:17:GLN:HB3	2.21	0.41
1:B:107:PRO:HD2	1:B:379:ARG:HE	1.85	0.41
1:A:404:TYR:CD1	1:A:405:PRO:HA	2.56	0.41
1:B:343:GLU:HB3	1:B:344:PRO:HD2	2.02	0.41
1:B:209:ARG:HG2	1:B:274:PRO:HB3	2.03	0.41
1:C:347:ASP:O	1:C:350:LEU:HB3	2.21	0.41
1:B:327:GLU:O	1:B:331:LEU:HG	2.21	0.41
1:D:93:TYR:CE1	1:D:282:VAL:HG21	2.56	0.41
1:D:450:LEU:HD21	3:D:1402:NDP:N6A	2.36	0.41
1:D:496:LEU:HD23	1:D:496:LEU:HA	1.94	0.41
1:B:445:PHE:HD1	3:B:1202:NDP:HO2N	1.70	0.40
1:C:72:VAL:CG1	2:C:507:HEM:HMA3	2.50	0.40
1:D:442:VAL:HG12	1:D:484:VAL:HG11	2.03	0.40
1:C:172:GLN:HB3	1:C:172:GLN:HE21	1.69	0.40
1:B:10:GLN:HE21	1:C:172:GLN:NE2	2.19	0.40
1:B:118:GLU:O	1:B:121:SER:HB3	2.21	0.40
1:B:381:ARG:HH11	1:B:381:ARG:HB2	1.86	0.40
1:A:430:ARG:HG2	1:A:430:ARG:HH11	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:HIS:O	1:C:279:TYR:N	2.43	0.40
1:D:160:PHE:CD1	2:D:507:HEM:HAB	2.56	0.40
1:C:89:ASP:CG	1:C:91:THR:HB	2.41	0.40
1:D:220:LYS:HE3	1:D:343:GLU:CB	2.48	0.40
1:C:310:ILE:HA	1:C:311:PRO:HD3	1.96	0.40
1:D:331:LEU:HD13	1:D:333:PHE:CZ	2.56	0.40
1:A:355:PHE:O	1:A:358:PRO:HD2	2.21	0.40
1:B:469:ALA:HB1	1:B:473:ILE:HG21	2.04	0.40
1:D:378:TYR:C	1:D:380:ALA:H	2.24	0.40
1:B:446:TYR:CZ	1:B:455:ARG:HD2	2.56	0.40
1:B:439:VAL:HG23	1:B:440:THR:H	1.86	0.40
1:D:145:VAL:CG1	1:D:353:ARG:NH2	2.85	0.40
1:B:188:ARG:HB3	1:B:190:GLU:OE2	2.21	0.40
1:A:291:PHE:HA	1:A:292:PRO:HD3	1.88	0.40
1:A:370:LEU:HD23	1:A:370:LEU:HA	1.89	0.40
1:C:264:LEU:HD12	1:C:264:LEU:O	2.21	0.40
1:D:488:TYR:CE1	1:D:492:ILE:HD11	2.56	0.40
1:B:55:VAL:HG21	1:C:430:ARG:NH2	2.36	0.40
1:A:155:ARG:HD3	1:A:297:ASP:OD1	2.21	0.40
1:C:384:ASN:OD1	1:C:397:GLN:NE2	2.55	0.40
1:B:384:ASN:HB2	1:B:385:TYR:H	1.66	0.40
1:B:205:PRO:O	1:B:244:LEU:HD12	2.22	0.40
1:D:345:SER:C	1:D:347:ASP:H	2.25	0.40
1:B:447:LEU:O	1:B:448:LYS:HE2	2.21	0.40
1:A:428:VAL:HG23	1:B:424:PHE:CD1	2.56	0.40
1:D:228:ALA:HB1	1:D:285:PHE:CZ	2.56	0.40
1:C:22:LYS:HD3	1:C:23:PRO:CD	2.50	0.40
1:D:499:TYR:O	1:D:501:GLU:HG3	2.22	0.40
1:D:189:PRO:HG3	1:D:480:ASN:ND2	2.37	0.40
1:D:414:GLN:O	1:D:416:SER:N	2.53	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	497/506 (98%)	442 (89%)	50 (10%)	5 (1%)	19	21
1	B	497/506 (98%)	423 (85%)	58 (12%)	16 (3%)	5	3
1	C	497/506 (98%)	417 (84%)	65 (13%)	15 (3%)	5	3
1	D	497/506 (98%)	442 (89%)	49 (10%)	6 (1%)	16	16
All	All	1988/2024 (98%)	1724 (87%)	222 (11%)	42 (2%)	9	7

All (42) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ALA
1	A	437	ASP
1	B	124	THR
1	B	242	LYS
1	B	394	MET
1	B	448	LYS
1	C	292	PRO
1	C	427	ASP
1	B	100	GLU
1	B	271	GLY
1	B	348	LYS
1	B	437	ASP
1	C	440	THR
1	C	444	THR
1	C	496	LEU
1	C	497	ASP
1	D	411	PRO
1	D	413	HIS
1	A	21	GLN
1	A	121	SER
1	B	17	GLN
1	B	224	ALA
1	B	241	ILE
1	B	393	MET
1	B	470	GLN
1	C	92	ARG
1	C	226	GLY
1	C	346	PRO
1	C	437	ASP
1	D	437	ASP

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Mol	Chain	Res	Type
1	B	452	GLU
1	C	19	ALA
1	C	203	GLY
1	D	394	MET
1	C	192	LEU
1	D	216	SER
1	A	100	GLU
1	B	19	ALA
1	D	100	GLU
1	C	486	PRO
1	B	373	PRO
1	C	373	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	431/437 (99%)	365 (85%)	66 (15%)	3	3
1	B	431/437 (99%)	332 (77%)	99 (23%)	1	1
1	C	431/437 (99%)	349 (81%)	82 (19%)	2	1
1	D	431/437 (99%)	356 (83%)	75 (17%)	2	2
All	All	1724/1748 (99%)	1402 (81%)	322 (19%)	2	1

All (322) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	15	LYS
1	A	18	ARG
1	A	21	GLN
1	A	22	LYS
1	A	24	ASP
1	A	26	LEU
1	A	37	LYS
1	A	40	SER

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Mol	Chain	Res	Type
1	A	41	LEU
1	A	43	VAL
1	A	49	LEU
1	A	65	ARG
1	A	70	GLU
1	A	73	VAL
1	A	92	ARG
1	A	102	ILE
1	A	104	LYS
1	A	105	ARG
1	A	131	PHE
1	A	137	THR
1	A	148	ASN
1	A	149	THR
1	A	155	ARG
1	A	162	SER
1	A	169	ARG
1	A	194	GLN
1	A	196	SER
1	A	197	PHE
1	A	202	ARG
1	A	209	ARG
1	A	229	VAL
1	A	235	TYR
1	A	237	THR
1	A	242	LYS
1	A	247	GLU
1	A	254	HIS
1	A	261	LEU
1	A	263	ASP
1	A	286	SER
1	A	289	GLU
1	A	290	ILE
1	A	309	LEU
1	A	319	ARG
1	A	327	GLU
1	A	374	VAL
1	A	379	ARG
1	A	394	MET
1	A	402	ASN
1	A	407	SER
1	A	413	HIS

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Mol	Chain	Res	Type
1	A	421	ARG
1	A	435	ASN
1	A	448	LYS
1	A	453	GLU
1	A	467	LYS
1	A	471	LEU
1	A	472	PHE
1	A	475	LYS
1	A	476	LYS
1	A	479	LYS
1	A	483	ASP
1	A	488	TYR
1	A	490	SER
1	A	498	LYS
1	A	501	GLU
1	B	3	ASN
1	B	12	LYS
1	B	16	GLU
1	B	17	GLN
1	B	18	ARG
1	B	21	GLN
1	B	26	LEU
1	B	36	ASP
1	B	37	LYS
1	B	41	LEU
1	B	49	LEU
1	B	55	VAL
1	B	59	GLU
1	B	67	ARG
1	B	72	VAL
1	B	73	VAL
1	B	90	ILE
1	B	92	ARG
1	B	94	SER
1	B	95	LYS
1	B	97	LYS
1	B	102	ILE
1	B	121	SER
1	B	124	THR
1	B	126	ARG
1	B	137	THR
1	B	144	LEU

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Mol	Chain	Res	Type
1	B	162	SER
1	B	169	ARG
1	B	186	SER
1	B	193	HIS
1	B	200	SER
1	B	201	ASP
1	B	202	ARG
1	B	220	LYS
1	B	221	LEU
1	B	225	ASP
1	B	229	VAL
1	B	232	LYS
1	B	235	TYR
1	B	236	LYS
1	B	242	LYS
1	B	245	SER
1	B	247	GLU
1	B	248	ASP
1	B	251	ARG
1	B	252	LEU
1	B	255	GLU
1	B	263	ASP
1	B	264	LEU
1	B	272	ASN
1	B	280	ILE
1	B	283	MET
1	B	286	SER
1	B	290	ILE
1	B	309	LEU
1	B	312	VAL
1	B	314	LYS
1	B	315	LEU
1	B	318	ASN
1	B	319	ARG
1	B	337	ASN
1	B	374	VAL
1	B	381	ARG
1	B	392	CYS
1	B	393	MET
1	B	396	ASN
1	B	397	GLN
1	B	402	ASN

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Mol	Chain	Res	Type
1	B	413	HIS
1	B	416	SER
1	B	421	ARG
1	B	422	THR
1	B	433	SER
1	B	438	ASN
1	B	439	VAL
1	B	441	GLN
1	B	443	ARG
1	B	444	THR
1	B	447	LEU
1	B	448	LYS
1	B	450	LEU
1	B	453	GLU
1	B	454	GLN
1	B	457	ARG
1	B	458	LEU
1	B	459	CYS
1	B	467	LYS
1	B	471	LEU
1	B	476	LYS
1	B	478	VAL
1	B	479	LYS
1	B	482	SER
1	B	487	GLU
1	B	488	TYR
1	B	492	ILE
1	B	495	LEU
1	B	498	LYS
1	B	500	ASN
1	C	3	ASN
1	C	4	ARG
1	C	16	GLU
1	C	17	GLN
1	C	18	ARG
1	C	22	LYS
1	C	26	LEU
1	C	46	ARG
1	C	52	GLN
1	C	65	ARG
1	C	68	ILE
1	C	73	VAL

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Mol	Chain	Res	Type
1	C	76	LYS
1	C	91	THR
1	C	92	ARG
1	C	95	LYS
1	C	97	LYS
1	C	104	LYS
1	C	105	ARG
1	C	126	ARG
1	C	131	PHE
1	C	138	GLU
1	C	139	ASP
1	C	149	THR
1	C	151	ILE
1	C	154	ILE
1	C	155	ARG
1	C	179	ASP
1	C	180	MET
1	C	188	ARG
1	C	194	GLN
1	C	195	VAL
1	C	197	PHE
1	C	202	ARG
1	C	227	GLU
1	C	235	TYR
1	C	237	THR
1	C	239	GLN
1	C	244	LEU
1	C	246	VAL
1	C	247	GLU
1	C	251	ARG
1	C	261	LEU
1	C	286	SER
1	C	289	GLU
1	C	293	PHE
1	C	304	HIS
1	C	309	LEU
1	C	331	LEU
1	C	345	SER
1	C	355	PHE
1	C	374	VAL
1	C	379	ARG
1	C	381	ARG

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Mol	Chain	Res	Type
1	C	394	MET
1	C	402	ASN
1	C	413	HIS
1	C	421	ARG
1	C	424	PHE
1	C	425	SER
1	C	427	ASP
1	C	429	GLN
1	C	433	SER
1	C	436	ASP
1	C	437	ASP
1	C	438	ASN
1	C	439	VAL
1	C	451	ASN
1	C	453	GLU
1	C	454	GLN
1	C	456	LYS
1	C	457	ARG
1	C	466	LEU
1	C	467	LYS
1	C	470	GLN
1	C	472	PHE
1	C	473	ILE
1	C	474	GLN
1	C	476	LYS
1	C	495	LEU
1	C	496	LEU
1	C	497	ASP
1	D	3	ASN
1	D	4	ARG
1	D	15	LYS
1	D	17	GLN
1	D	18	ARG
1	D	26	LEU
1	D	27	THR
1	D	34	VAL
1	D	37	LYS
1	D	43	VAL
1	D	52	GLN
1	D	85	GLU
1	D	89	ASP
1	D	90	ILE

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Mol	Chain	Res	Type
1	D	92	ARG
1	D	94	SER
1	D	105	ARG
1	D	111	ARG
1	D	131	PHE
1	D	144	LEU
1	D	148	ASN
1	D	155	ARG
1	D	159	LEU
1	D	193	HIS
1	D	197	PHE
1	D	202	ARG
1	D	211	MET
1	D	214	TYR
1	D	216	SER
1	D	220	LYS
1	D	221	LEU
1	D	222	VAL
1	D	225	ASP
1	D	229	VAL
1	D	235	TYR
1	D	236	LYS
1	D	245	SER
1	D	246	VAL
1	D	247	GLU
1	D	261	LEU
1	D	263	ASP
1	D	275	SER
1	D	280	ILE
1	D	281	GLN
1	D	283	MET
1	D	285	PHE
1	D	289	GLU
1	D	290	ILE
1	D	309	LEU
1	D	314	LYS
1	D	368	ASN
1	D	374	VAL
1	D	379	ARG
1	D	381	ARG
1	D	387	ARG
1	D	394	MET

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Mol	Chain	Res	Type
1	D	397	GLN
1	D	412	GLU
1	D	416	SER
1	D	421	ARG
1	D	432	ASN
1	D	435	ASN
1	D	436	ASP
1	D	443	ARG
1	D	444	THR
1	D	456	LYS
1	D	460	GLU
1	D	467	LYS
1	D	475	LYS
1	D	476	LYS
1	D	479	LYS
1	D	490	SER
1	D	495	LEU
1	D	498	LYS
1	D	501	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	32	ASN
1	A	148	ASN
1	A	167	GLN
1	A	210	HIS
1	A	320	ASN
1	A	337	ASN
1	A	402	ASN
1	A	420	HIS
1	A	429	GLN
1	A	454	GLN
1	A	485	HIS
1	A	500	ASN
1	B	32	ASN
1	B	148	ASN
1	B	167	GLN
1	B	193	HIS
1	B	208	HIS
1	B	243	ASN

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Mol	Chain	Res	Type
1	B	272	ASN
1	B	318	ASN
1	B	320	ASN
1	B	337	ASN
1	B	396	ASN
1	B	402	ASN
1	B	414	GLN
1	B	435	ASN
1	B	441	GLN
1	C	3	ASN
1	C	17	GLN
1	C	52	GLN
1	C	88	HIS
1	C	172	GLN
1	C	243	ASN
1	C	337	ASN
1	C	402	ASN
1	C	432	ASN
1	C	435	ASN
1	C	438	ASN
1	C	454	GLN
1	C	461	ASN
1	C	470	GLN
1	C	480	ASN
1	D	32	ASN
1	D	52	GLN
1	D	148	ASN
1	D	170	ASN
1	D	193	HIS
1	D	254	HIS
1	D	363	HIS
1	D	368	ASN
1	D	413	HIS
1	D	420	HIS
1	D	432	ASN
1	D	500	ASN

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 ⓘ

8 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	NDP	A	1102	-	42,52,52	1.38	6 (14%)	55,80,80	2.04	10 (18%)
2	HEM	A	507	1	30,50,50	2.91	11 (36%)	24,82,82	2.08	8 (33%)
3	NDP	B	1202	-	42,52,52	1.40	4 (9%)	55,80,80	2.44	14 (25%)
2	HEM	B	507	1	30,50,50	2.55	11 (36%)	24,82,82	2.12	7 (29%)
3	NDP	C	1302	-	42,52,52	1.41	5 (11%)	55,80,80	2.26	14 (25%)
2	HEM	C	507	1	30,50,50	2.50	10 (33%)	24,82,82	1.92	6 (25%)
3	NDP	D	1402	-	42,52,52	1.41	6 (14%)	55,80,80	1.91	9 (16%)
2	HEM	D	507	1	30,50,50	2.70	11 (36%)	24,82,82	2.26	8 (33%)

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	NDP	A	1102	-	-	0/30/77/77	0/5/5/5
2	HEM	A	507	1	-	0/10/54/54	0/0/8/8
3	NDP	B	1202	-	-	0/30/77/77	0/5/5/5
2	HEM	B	507	1	-	0/10/54/54	0/0/8/8
3	NDP	C	1302	-	-	0/30/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	C	507	1	-	0/10/54/54	0/0/8/8
3	NDP	D	1402	-	-	0/30/77/77	0/5/5/5
2	HEM	D	507	1	-	0/10/54/54	0/0/8/8

All (64) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	507	HEM	C3B-C4B	-6.74	1.45	1.51
2	A	507	HEM	C3B-CAB	-6.66	1.38	1.51
2	A	507	HEM	C3C-CAC	-6.41	1.39	1.51
2	D	507	HEM	C2D-C3D	-6.34	1.35	1.54
2	A	507	HEM	C2D-C3D	-6.18	1.36	1.54
2	B	507	HEM	C3B-C4B	-5.75	1.46	1.51
2	B	507	HEM	C2D-C3D	-5.54	1.37	1.54
2	C	507	HEM	C2D-C3D	-5.45	1.38	1.54
2	C	507	HEM	C3B-CAB	-5.36	1.41	1.51
2	D	507	HEM	C3B-CAB	-5.31	1.41	1.51
2	D	507	HEM	C3C-CAC	-5.21	1.41	1.51
2	C	507	HEM	C3C-CAC	-5.11	1.41	1.51
2	B	507	HEM	C3B-CAB	-5.04	1.41	1.51
2	B	507	HEM	C3C-CAC	-5.02	1.41	1.51
2	D	507	HEM	C2C-C1C	-4.81	1.43	1.52
2	D	507	HEM	C3D-C4D	-4.50	1.45	1.51
2	A	507	HEM	C3D-C4D	-4.45	1.45	1.51
2	C	507	HEM	C3B-C4B	-4.27	1.48	1.51
2	D	507	HEM	C3B-C4B	-4.20	1.48	1.51
2	B	507	HEM	C3D-C4D	-4.16	1.46	1.51
2	B	507	HEM	C2C-C1C	-3.73	1.45	1.52
2	A	507	HEM	C2C-C1C	-3.28	1.46	1.52
3	B	1202	NDP	C4N-C5N	-3.23	1.42	1.49
3	C	1302	NDP	C4N-C5N	-3.17	1.42	1.49
2	C	507	HEM	C3D-C4D	-3.11	1.47	1.51
2	C	507	HEM	C2C-C1C	-2.79	1.47	1.52
3	D	1402	NDP	C4N-C5N	-2.78	1.43	1.49
3	A	1102	NDP	C4N-C5N	-2.39	1.43	1.49
2	A	507	HEM	C2B-C1B	-2.08	1.45	1.51
2	B	507	HEM	C2B-C1B	-2.04	1.45	1.51
3	A	1102	NDP	C6N-N1N	2.14	1.43	1.37
3	C	1302	NDP	C6N-N1N	2.19	1.44	1.37
3	D	1402	NDP	C6N-N1N	2.26	1.44	1.37
2	A	507	HEM	CBB-CAB	2.30	1.42	1.29
3	D	1402	NDP	O4B-C1B	2.31	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1102	NDP	C2N-C3N	2.38	1.40	1.34
2	B	507	HEM	C4C-NC	2.45	1.39	1.36
2	D	507	HEM	CHD-C4C	2.45	1.42	1.36
3	A	1102	NDP	O4B-C1B	2.54	1.44	1.41
3	D	1402	NDP	C2N-C3N	2.63	1.41	1.34
2	B	507	HEM	CBB-CAB	2.78	1.45	1.29
2	A	507	HEM	CBC-CAC	2.79	1.45	1.29
3	B	1202	NDP	C2N-C3N	2.81	1.41	1.34
3	C	1302	NDP	C2N-C3N	2.82	1.41	1.34
2	D	507	HEM	CBB-CAB	2.86	1.45	1.29
2	C	507	HEM	CBC-CAC	3.03	1.46	1.29
2	D	507	HEM	CBC-CAC	3.11	1.47	1.29
2	B	507	HEM	CBC-CAC	3.11	1.47	1.29
2	A	507	HEM	C1C-NC	3.21	1.40	1.36
2	C	507	HEM	CBB-CAB	3.22	1.47	1.29
3	B	1202	NDP	P2B-O1X	3.25	1.61	1.51
2	B	507	HEM	C1C-NC	3.32	1.40	1.36
2	D	507	HEM	C1C-NC	3.41	1.40	1.36
3	A	1102	NDP	P2B-O1X	3.49	1.62	1.51
3	C	1302	NDP	P2B-O1X	3.52	1.62	1.51
2	D	507	HEM	C4C-NC	3.70	1.40	1.36
3	D	1402	NDP	P2B-O1X	3.76	1.63	1.51
2	C	507	HEM	C1C-NC	3.96	1.40	1.36
2	A	507	HEM	C4C-NC	4.06	1.41	1.36
2	C	507	HEM	C4C-NC	4.11	1.41	1.36
3	B	1202	NDP	C6N-C5N	4.25	1.41	1.33
3	A	1102	NDP	C6N-C5N	4.33	1.41	1.33
3	D	1402	NDP	C6N-C5N	4.34	1.41	1.33
3	C	1302	NDP	C6N-C5N	4.53	1.42	1.33

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1202	NDP	N3A-C2A-N1A	-11.77	119.88	128.89
3	C	1302	NDP	N3A-C2A-N1A	-10.39	120.94	128.89
3	D	1402	NDP	N3A-C2A-N1A	-9.19	121.86	128.89
3	A	1102	NDP	N3A-C2A-N1A	-9.10	121.93	128.89
3	B	1202	NDP	C1B-N9A-C4A	-4.65	119.93	126.94
3	B	1202	NDP	C4B-O4B-C1B	-4.45	104.83	109.72
3	D	1402	NDP	C1B-N9A-C4A	-3.38	121.84	126.94
3	C	1302	NDP	C1B-N9A-C4A	-2.89	122.58	126.94
3	C	1302	NDP	P2B-O2B-C2B	-2.80	114.86	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1402	NDP	C4N-C5N-C6N	-2.78	118.00	122.58
2	A	507	HEM	CAA-C2A-C1A	-2.57	124.22	127.01
3	C	1302	NDP	C4B-O4B-C1B	-2.52	106.95	109.72
2	A	507	HEM	CBA-CAA-C2A	-2.47	108.10	112.53
3	B	1202	NDP	C4N-C5N-C6N	-2.45	118.55	122.58
3	A	1102	NDP	C1B-N9A-C4A	-2.37	123.37	126.94
2	D	507	HEM	CBA-CAA-C2A	-2.27	108.45	112.53
3	B	1202	NDP	C5D-C4D-C3D	-2.12	106.81	115.21
3	C	1302	NDP	C4N-C5N-C6N	-2.11	119.09	122.58
3	A	1102	NDP	O2B-C2B-C1B	-2.03	102.10	110.02
2	B	507	HEM	C2D-C3D-C4D	2.06	104.99	101.50
2	A	507	HEM	C2D-C3D-C4D	2.13	105.12	101.50
2	D	507	HEM	CMD-C2D-C3D	2.14	123.82	114.35
2	D	507	HEM	C2D-C3D-C4D	2.18	105.19	101.50
3	B	1202	NDP	O5D-C5D-C4D	2.22	117.31	109.12
3	B	1202	NDP	C2A-N1A-C6A	2.25	122.78	118.77
3	C	1302	NDP	O4B-C1B-N9A	2.31	112.94	108.10
2	B	507	HEM	C3B-CAB-CBB	2.32	128.02	124.46
3	D	1402	NDP	C3D-C2D-C1D	2.34	106.10	101.40
3	C	1302	NDP	PN-O3-PA	2.43	139.56	132.73
3	D	1402	NDP	C3B-C2B-C1B	2.45	107.47	102.73
3	C	1302	NDP	O4B-C4B-C3B	2.49	110.16	105.15
3	B	1202	NDP	O4B-C1B-N9A	2.53	113.38	108.10
2	A	507	HEM	CMD-C2D-C3D	2.54	125.61	114.35
3	B	1202	NDP	C4A-C5A-N7A	2.55	111.83	109.48
2	C	507	HEM	C2D-C3D-C4D	2.66	106.01	101.50
2	B	507	HEM	CMD-C2D-C3D	2.68	126.22	114.35
2	C	507	HEM	CMD-C2D-C3D	2.69	126.26	114.35
3	B	1202	NDP	O3X-P2B-O2X	2.82	118.10	107.38
3	D	1402	NDP	C4A-C5A-N7A	2.82	112.08	109.48
3	C	1302	NDP	C4A-C5A-N7A	2.85	112.11	109.48
3	D	1402	NDP	O3X-P2B-O2X	3.12	119.26	107.38
3	A	1102	NDP	O3X-P2B-O2X	3.14	119.35	107.38
3	C	1302	NDP	O3X-P2B-O2X	3.20	119.58	107.38
3	C	1302	NDP	C3B-C2B-C1B	3.26	109.03	102.73
3	A	1102	NDP	C4A-C5A-N7A	3.27	112.49	109.48
2	A	507	HEM	CMB-C2B-C3B	3.27	124.70	116.53
3	A	1102	NDP	C3D-C2D-C1D	3.30	108.03	101.40
2	C	507	HEM	CMB-C2B-C3B	3.33	124.84	116.53
2	C	507	HEM	CMC-C2C-C3C	3.43	125.09	116.53
3	C	1302	NDP	C3D-C2D-C1D	3.44	108.31	101.40
2	D	507	HEM	CMB-C2B-C3B	3.60	125.51	116.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1402	NDP	O4D-C1D-N1N	3.61	115.68	108.07
2	A	507	HEM	CMC-C2C-C3C	3.64	125.61	116.53
3	B	1202	NDP	C3D-C2D-C1D	3.65	108.75	101.40
3	C	1302	NDP	C5N-C4N-C3N	3.67	122.63	112.52
3	A	1102	NDP	O4D-C1D-N1N	3.71	115.91	108.07
2	A	507	HEM	CAD-C3D-C4D	3.76	125.74	112.47
3	A	1102	NDP	C3B-C2B-C1B	3.77	110.03	102.73
2	B	507	HEM	CMB-C2B-C3B	3.80	126.02	116.53
3	B	1202	NDP	PN-O3-PA	3.81	143.42	132.73
3	B	1202	NDP	C5N-C4N-C3N	3.82	123.03	112.52
2	B	507	HEM	CAD-C3D-C4D	3.90	126.22	112.47
2	D	507	HEM	C3C-CAC-CBC	4.04	130.66	124.46
3	A	1102	NDP	C5N-C4N-C3N	4.05	123.69	112.52
3	D	1402	NDP	C5N-C4N-C3N	4.14	123.91	112.52
2	D	507	HEM	CAD-C3D-C4D	4.17	127.17	112.47
2	B	507	HEM	CMC-C2C-C3C	4.31	127.30	116.53
2	C	507	HEM	CAD-C3D-C4D	4.34	127.79	112.47
2	C	507	HEM	CAD-C3D-C2D	4.50	126.15	113.22
3	A	1102	NDP	O4B-C1B-N9A	4.92	118.40	108.10
2	D	507	HEM	CMC-C2C-C3C	4.95	128.89	116.53
3	B	1202	NDP	O4D-C1D-N1N	4.99	118.60	108.07
2	D	507	HEM	CAD-C3D-C2D	5.00	127.58	113.22
2	B	507	HEM	CAD-C3D-C2D	5.41	128.78	113.22
2	A	507	HEM	CAD-C3D-C2D	5.43	128.83	113.22
3	C	1302	NDP	O4D-C1D-N1N	5.61	119.91	108.07

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1102	NDP	3	0
2	A	507	HEM	5	0
3	B	1202	NDP	4	0
3	C	1302	NDP	2	0
2	C	507	HEM	4	0
3	D	1402	NDP	1	0
2	D	507	HEM	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.