



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 09:35 PM EDT

PDB ID : 5ZLH
Title : Crystal structure of Mn-ProtoporphyrinIX-reconstituted P450BM3
Authors : Omura, K.; Aiba, Y.; Onoda, H.; Sugimoto, H.; Shoji, O.; Watanabe, Y.
Deposited on : 2018-03-28
Resolution : 3.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

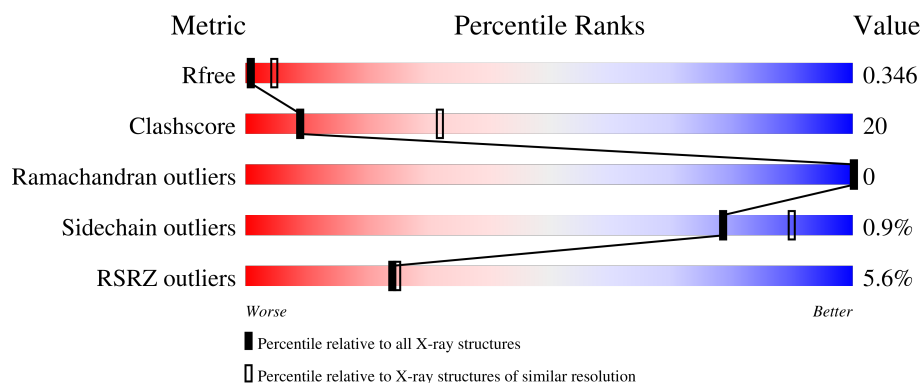
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	455	<div> <div>4%</div> <div>58%</div> <div>41%</div> <div>..</div> </div>
1	B	455	<div> <div>5%</div> <div>65%</div> <div>33%</div> <div>..</div> </div>
1	C	455	<div> <div>4%</div> <div>58%</div> <div>41%</div> <div>.</div> </div>
1	D	455	<div> <div>9%</div> <div>59%</div> <div>40%</div> <div>.</div> </div>

2 Entry composition [i](#)

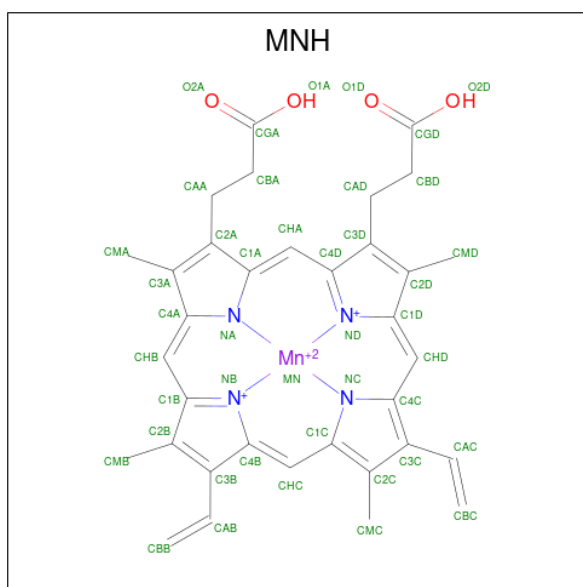
There are 2 unique types of molecules in this entry. The entry contains 14722 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional cytochrome P450/NADPH-P450 reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	452	Total	C	N	O	S	0	0	0
			3646	2329	619	681	17			
1	B	449	Total	C	N	O	S	0	0	0
			3621	2313	616	676	16			
1	C	452	Total	C	N	O	S	0	0	0
			3646	2329	619	681	17			
1	D	451	Total	C	N	O	S	0	0	0
			3637	2324	618	678	17			

- Molecule 2 is MANGANESE PROTOPORPHYRIN IX (three-letter code: MNH) (formula: $C_{34}H_{32}MnN_4O_4$).



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

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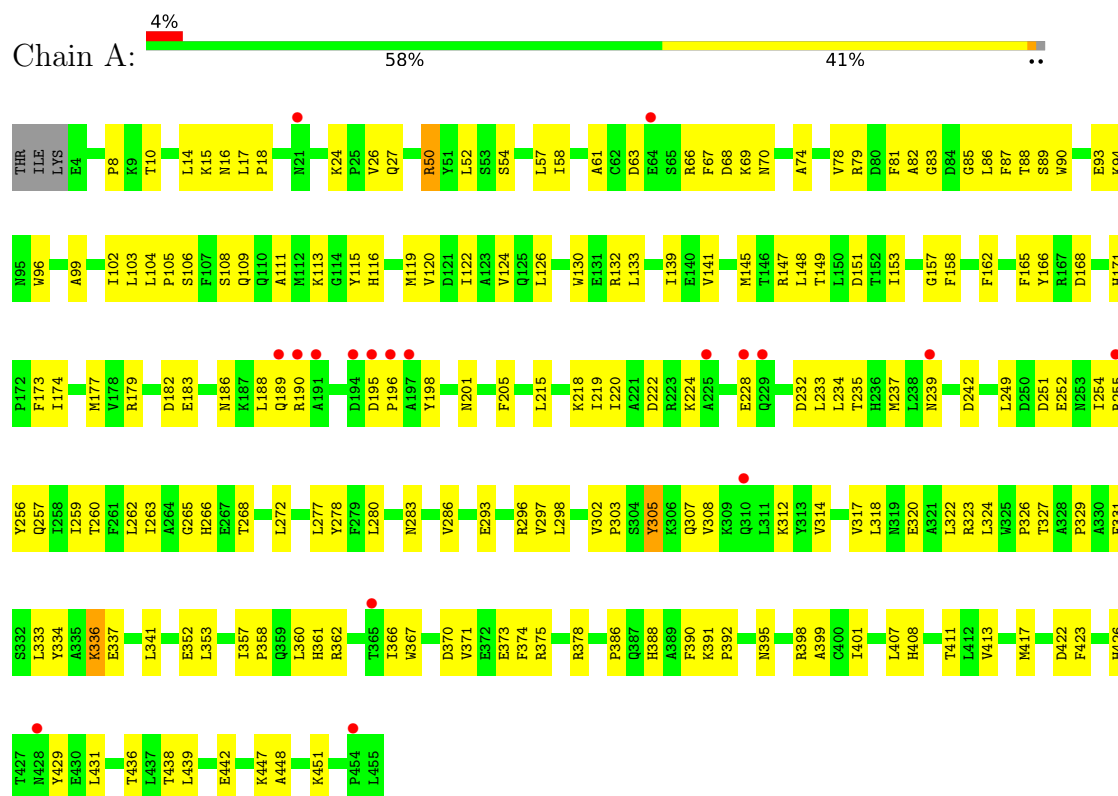
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	Mn	N	O	0	0
			43	34	1	4	4		
2	D	1	Total	C	Mn	N	O	0	0
			43	34	1	4	4		

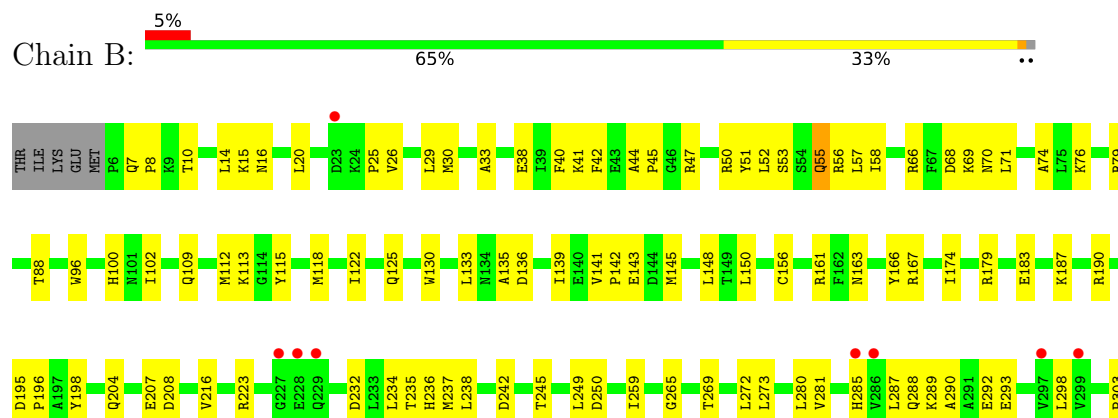
3 Residue-property plots [i](#)

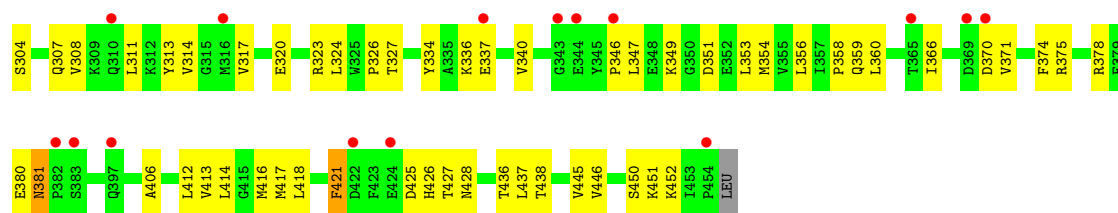
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

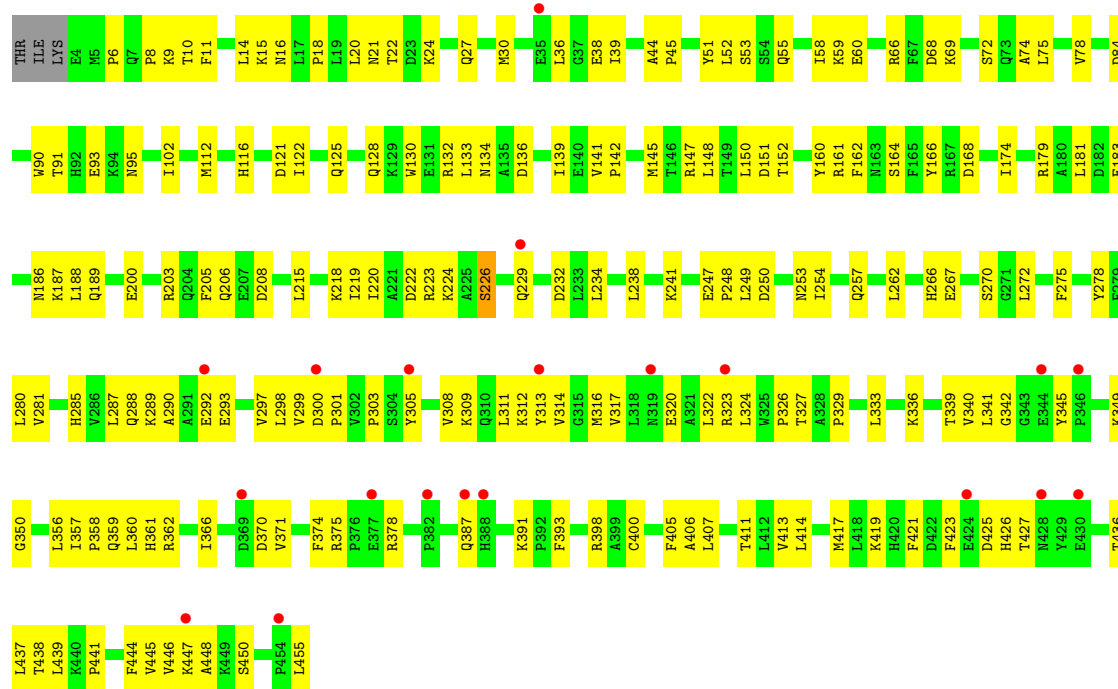


- Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase

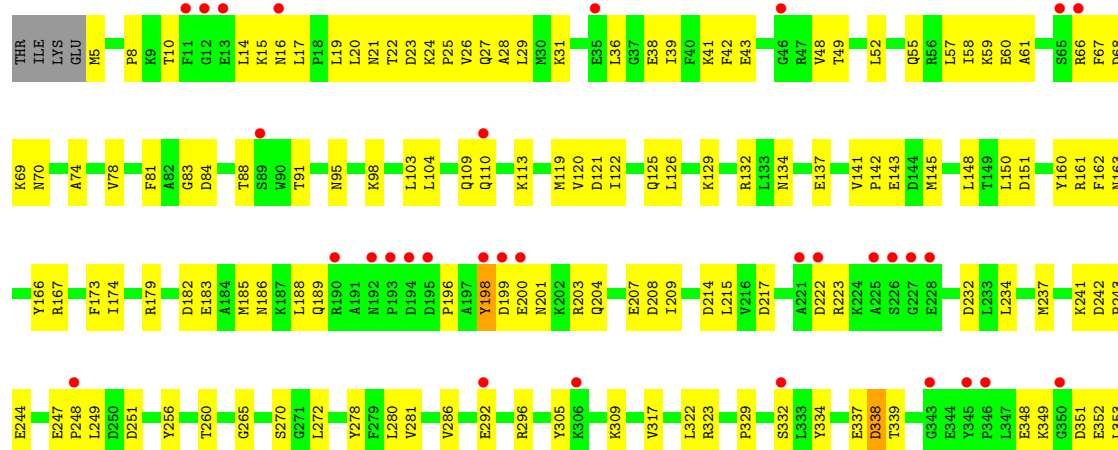


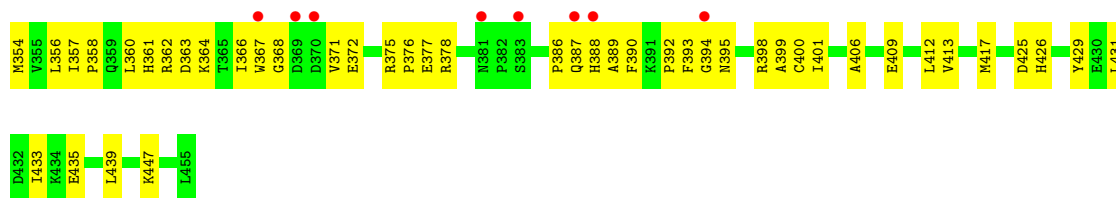


• Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase



• Molecule 1: Bifunctional cytochrome P450/NADPH-P450 reductase





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	104.76Å 155.32Å 208.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.93 – 3.40 19.93 – 3.40	Depositor EDS
% Data completeness (in resolution range)	95.2 (19.93-3.40) 95.2 (19.93-3.40)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 3.44Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.310 , 0.346 0.310 , 0.346	Depositor DCC
R_{free} test set	1147 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 13.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	14722	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.30	0/3731	0.48	0/5045
1	B	0.29	0/3706	0.49	0/5011
1	C	0.31	0/3731	0.48	0/5045
1	D	0.29	0/3722	0.48	0/5033
All	All	0.30	0/14890	0.48	0/20134

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	3646	0	3611	168	0
1	B	3621	0	3586	126	0
1	C	3646	0	3611	171	0
1	D	3637	0	3605	157	0
2	A	43	0	30	10	0
2	B	43	0	30	7	0
2	C	43	0	30	2	0
2	D	43	0	30	5	0
All	All	14722	0	14533	592	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (592) 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:A:69:LYS:HD3	1:A:398:ARG:HH11	1.14	1.12
1:C:128:GLN:HG2	1:C:132:ARG:HH12	1.17	1.06
1:C:128:GLN:CG	1:C:132:ARG:HH12	1.69	1.05
1:C:128:GLN:HG2	1:C:132:ARG:NH1	1.72	1.04
1:A:362:ARG:HA	1:A:371:VAL:HG11	1.47	0.93
1:A:69:LYS:HE3	2:A:500:MNH:O1A	1.71	0.91
1:A:69:LYS:HD3	1:A:398:ARG:NH1	1.85	0.90
1:D:387:GLN:O	1:D:388:HIS:ND1	2.08	0.85
1:B:421:PHE:HB3	1:B:450:SER:HA	1.64	0.80
1:D:16:ASN:HD21	1:D:42:PHE:HA	1.48	0.77
1:D:74:ALA:HB2	1:D:188:LEU:HD11	1.65	0.77
1:C:122:ILE:HG22	1:C:148:LEU:HD12	1.65	0.77
1:A:63:ASP:HB3	1:A:66:ARG:HB2	1.67	0.76
1:A:69:LYS:CD	1:A:398:ARG:HH11	1.94	0.76
1:C:329:PRO:HG3	1:C:439:LEU:HG	1.66	0.76
1:C:162:PHE:HZ	1:C:262:LEU:HD21	1.50	0.75
1:A:94:LYS:H	1:A:94:LYS:HD2	1.52	0.75
1:D:70:ASN:HB2	1:D:334:TYR:HB3	1.68	0.74
1:D:58:ILE:HD12	1:D:360:LEU:HD13	1.67	0.74
1:A:120:VAL:HG11	1:A:302:VAL:HG23	1.69	0.74
1:C:362:ARG:HA	1:C:371:VAL:HG11	1.67	0.73
1:A:102:ILE:HD11	1:A:249:LEU:HG	1.70	0.73
1:C:223:ARG:NH2	1:C:232:ASP:OD2	2.21	0.73
1:D:26:VAL:HG21	1:D:329:PRO:HB2	1.69	0.73
1:A:183:GLU:HB2	1:A:205:PHE:CZ	2.25	0.72
1:C:311:LEU:HD13	1:C:314:VAL:HG21	1.71	0.72
1:A:24:LYS:HE3	1:C:250:ASP:HB3	1.71	0.71
1:A:69:LYS:HE3	2:A:500:MNH:CGA	2.19	0.71
1:B:323:ARG:HH22	1:B:371:VAL:HA	1.55	0.71
1:C:147:ARG:NH2	1:C:168:ASP:O	2.23	0.71
1:A:109:GLN:HG3	1:A:113:LYS:HE3	1.73	0.71
1:A:85:GLY:HA3	1:A:260:THR:HG21	1.72	0.71
1:D:69:LYS:HB2	1:D:398:ARG:HG3	1.72	0.71
1:B:223:ARG:NH2	1:B:232:ASP:OD2	2.25	0.70
1:A:329:PRO:HG3	1:A:439:LEU:HG	1.73	0.70
1:B:290:ALA:HB1	1:B:418:LEU:HD13	1.73	0.70
1:C:406:ALA:HB2	2:C:500:MNH:HMC2	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ALA:HB3	1:B:359:GLN:OE1	1.93	0.69
1:C:84:ASP:OD2	1:C:95:ASN:ND2	2.25	0.69
1:C:162:PHE:HZ	1:C:262:LEU:CD2	2.05	0.69
1:B:370:ASP:OD2	1:B:375:ARG:NH2	2.25	0.69
1:C:22:THR:HG23	1:C:24:LYS:H	1.58	0.68
1:C:128:GLN:HG3	1:C:132:ARG:HH12	1.56	0.68
1:C:370:ASP:OD2	1:C:375:ARG:NH1	2.25	0.68
1:C:301:PRO:HA	1:C:419:LYS:HE2	1.75	0.67
1:D:337:GLU:HG3	1:D:338:ASP:H	1.59	0.67
1:D:375:ARG:HE	1:D:377:GLU:HB2	1.60	0.67
1:C:285:HIS:O	1:C:288:GLN:NE2	2.27	0.67
1:D:121:ASP:OD2	1:D:161:ARG:NH2	2.25	0.67
1:A:79:ARG:HG2	1:A:88:THR:HG22	1.74	0.67
1:D:84:ASP:OD2	1:D:95:ASN:ND2	2.27	0.67
1:D:59:LYS:HB2	1:D:388:HIS:CD2	2.29	0.67
1:D:98:LYS:HD2	1:D:249:LEU:HD23	1.77	0.67
1:A:10:THR:HB	1:A:15:LYS:HA	1.76	0.66
1:B:74:ALA:HB1	1:B:437:LEU:HD11	1.76	0.66
1:C:122:ILE:HA	1:C:125:GLN:HB2	1.75	0.66
1:A:122:ILE:HD12	1:A:151:ASP:HB3	1.78	0.66
1:B:281:VAL:HG11	1:B:425:ASP:HB2	1.78	0.66
1:C:222:ASP:OD1	1:C:223:ARG:N	2.28	0.66
1:C:280:LEU:HB3	1:C:287:LEU:HD21	1.77	0.66
1:D:49:THR:HG22	1:D:352:GLU:HG2	1.78	0.65
1:C:324:LEU:O	1:C:362:ARG:NH1	2.27	0.65
1:B:293:GLU:OE1	1:B:313:TYR:N	2.25	0.65
1:D:21:ASN:HA	1:D:189:GLN:HG2	1.79	0.65
1:A:179:ARG:O	1:A:182:ASP:HB2	1.97	0.65
1:D:66:ARG:HD2	1:D:339:THR:HG21	1.79	0.64
1:B:33:ALA:HB2	1:B:40:PHE:HE1	1.61	0.64
1:C:148:LEU:HD21	1:C:413:VAL:HG21	1.78	0.64
1:A:90:TRP:HB2	1:A:93:GLU:HB2	1.79	0.64
1:B:356:LEU:HD23	1:B:358:PRO:HD2	1.79	0.64
1:C:179:ARG:NH1	1:C:208:ASP:OD1	2.31	0.64
1:D:367:TRP:HD1	1:D:378:ARG:HD3	1.63	0.64
1:A:86:LEU:HB2	2:A:500:MNH:HAD1	1.78	0.63
1:C:249:LEU:HD23	1:C:253:ASN:OD1	1.97	0.63
1:C:121:ASP:OD2	1:D:132:ARG:NH1	2.29	0.63
1:D:247:GLU:HG2	1:D:248:PRO:HD2	1.81	0.63
1:A:86:LEU:HD12	1:A:96:TRP:CD1	2.34	0.63
1:C:139:ILE:HG12	1:C:446:VAL:O	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ARG:HD3	1:A:198:TYR:CE2	2.34	0.62
1:B:232:ASP:O	1:B:236:HIS:ND1	2.33	0.62
1:C:128:GLN:CG	1:C:132:ARG:NH1	2.43	0.62
1:D:162:PHE:O	1:D:167:ARG:NH1	2.26	0.61
1:C:44:ALA:HB1	1:C:45:PRO:HD2	1.81	0.61
1:D:8:PRO:HB2	1:D:19:LEU:HD11	1.83	0.61
1:D:137:GLU:O	1:D:447:LYS:NZ	2.34	0.61
1:A:85:GLY:O	1:A:89:SER:N	2.33	0.61
1:A:366:ILE:HG23	1:A:386:PRO:HG2	1.83	0.61
1:D:292:GLU:O	1:D:296:ARG:HG3	2.01	0.60
1:C:21:ASN:HA	1:C:189:GLN:OE1	2.02	0.60
1:D:59:LYS:HB2	1:D:388:HIS:NE2	2.17	0.60
1:D:27:GLN:HG3	1:D:435:GLU:OE2	2.02	0.60
1:B:30:MET:HA	1:B:359:GLN:OE1	2.01	0.59
1:A:327:THR:O	1:A:329:PRO:HD3	2.02	0.59
1:C:66:ARG:HH21	1:C:339:THR:HB	1.68	0.59
1:C:130:TRP:CE2	1:C:139:ILE:HD12	2.37	0.59
1:C:262:LEU:O	1:C:266:HIS:ND1	2.25	0.59
1:C:74:ALA:HB2	1:C:188:LEU:HD11	1.83	0.59
1:B:145:MET:HE1	1:B:273:LEU:HD22	1.84	0.59
1:C:223:ARG:HA	1:C:226:SER:HB3	1.85	0.59
1:A:57:LEU:HD22	1:A:341:LEU:HG	1.84	0.59
1:B:187:LYS:HG2	1:B:190:ARG:HH12	1.67	0.59
1:B:375:ARG:HG3	1:B:378:ARG:HB2	1.85	0.59
1:D:55:GLN:OE1	1:D:360:LEU:HD11	2.03	0.59
1:B:122:ILE:HG22	1:B:148:LEU:HD12	1.85	0.58
1:C:102:ILE:HD12	1:C:249:LEU:CD1	2.33	0.58
1:D:196:PRO:HA	1:D:199:ASP:HB3	1.85	0.58
1:A:69:LYS:CD	1:A:398:ARG:HE	2.17	0.58
1:A:86:LEU:CB	2:A:500:MNH:HAD1	2.33	0.58
1:A:153:ILE:HD12	1:A:265:GLY:HA3	1.86	0.58
1:A:320:GLU:OE2	1:A:323:ARG:NH2	2.29	0.58
1:C:393:PHE:O	1:C:400:CYS:N	2.36	0.58
1:D:280:LEU:HD21	1:D:317:VAL:HG11	1.84	0.58
1:A:52:LEU:HD12	1:A:353:LEU:HD13	1.85	0.58
1:B:356:LEU:HD22	1:B:359:GLN:HG3	1.84	0.58
1:C:141:VAL:HB	1:C:444:PHE:HD2	1.68	0.58
1:C:132:ARG:HG2	1:D:161:ARG:NH1	2.18	0.58
1:C:281:VAL:HG12	1:C:425:ASP:HB2	1.85	0.58
1:D:305:TYR:HB2	1:D:309:LYS:NZ	2.19	0.58
1:A:86:LEU:HD12	1:A:96:TRP:HD1	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:GLU:OE1	1:B:56:ARG:NH2	2.37	0.57
1:B:421:PHE:HA	1:B:451:LYS:HG3	1.86	0.57
1:C:241:LYS:HG2	1:C:248:PRO:HG3	1.86	0.57
1:D:27:GLN:OE1	1:D:433:ILE:HB	2.04	0.57
1:C:39:ILE:HD11	1:C:345:TYR:CE2	2.40	0.57
1:C:142:PRO:HD3	1:C:444:PHE:HB3	1.87	0.57
1:D:241:LYS:HD2	1:D:248:PRO:HD3	1.87	0.57
1:D:348:GLU:N	1:D:351:ASP:OD2	2.38	0.57
1:A:70:ASN:HB2	1:A:334:TYR:HB3	1.87	0.56
1:C:223:ARG:HE	1:C:234:LEU:HD23	1.70	0.56
1:C:250:ASP:O	1:C:254:ILE:HG13	2.05	0.56
1:B:150:LEU:HD22	1:B:174:ILE:HD11	1.87	0.56
1:D:183:GLU:OE1	1:D:201:ASN:HB3	2.06	0.56
1:C:414:LEU:HA	1:C:417:MET:HE2	1.88	0.56
1:B:55:GLN:HG3	1:B:366:ILE:HD13	1.88	0.56
1:B:285:HIS:NE2	1:B:289:LYS:HE3	2.21	0.56
1:C:58:ILE:HD12	1:C:360:LEU:HD13	1.86	0.56
1:A:69:LYS:HD3	1:A:398:ARG:HE	1.69	0.56
1:B:52:LEU:HD11	1:B:57:LEU:HB2	1.88	0.56
1:C:55:GLN:HB3	1:C:366:ILE:HD11	1.87	0.56
1:D:60:GLU:HB3	1:D:66:ARG:NH2	2.20	0.56
1:D:179:ARG:NH1	1:D:208:ASP:OD1	2.39	0.56
1:A:86:LEU:HB3	2:A:500:MNH:CGD	2.35	0.56
1:B:406:ALA:HB2	2:B:500:MNH:HMC2	1.88	0.56
1:C:421:PHE:HD1	1:C:450:SER:HA	1.71	0.56
1:B:320:GLU:OE1	1:B:323:ARG:HD3	2.07	0.55
1:C:320:GLU:OE1	1:C:323:ARG:NE	2.35	0.55
1:A:69:LYS:HD3	1:A:398:ARG:CZ	2.36	0.55
1:A:116:HIS:HA	1:A:119:MET:SD	2.46	0.55
1:A:79:ARG:HG2	1:A:88:THR:CG2	2.37	0.55
1:C:297:VAL:HG11	1:C:311:LEU:HB3	1.88	0.55
1:C:417:MET:HB3	1:C:423:PHE:HZ	1.71	0.55
1:B:58:ILE:HG21	1:B:360:LEU:HD22	1.89	0.55
1:D:26:VAL:HG21	1:D:329:PRO:CB	2.35	0.55
1:A:157:GLY:O	1:A:233:LEU:HB2	2.07	0.55
1:D:329:PRO:HB3	1:D:439:LEU:HD13	1.89	0.55
1:D:272:LEU:HD13	1:D:322:LEU:HG	1.89	0.55
1:D:361:HIS:HA	1:D:367:TRP:CZ3	2.41	0.54
1:B:71:LEU:O	1:B:76:LYS:NZ	2.37	0.54
1:B:10:THR:HG23	1:B:15:LYS:HA	1.90	0.54
1:C:132:ARG:CB	1:D:161:ARG:HD3	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:GLU:HB3	1:D:48:VAL:HG13	1.88	0.54
1:B:20:LEU:HD21	1:B:29:LEU:HD21	1.89	0.54
1:B:183:GLU:O	1:B:187:LYS:HG3	2.06	0.54
1:A:132:ARG:NH2	1:B:125:GLN:OE1	2.41	0.54
1:D:52:LEU:HD11	1:D:353:LEU:HD11	1.90	0.54
1:C:20:LEU:O	1:C:189:GLN:NE2	2.40	0.54
1:A:148:LEU:HA	1:A:165:PHE:HE1	1.71	0.54
1:A:293:GLU:OE2	1:A:312:LYS:N	2.38	0.54
1:D:60:GLU:HB3	1:D:66:ARG:HH22	1.72	0.54
1:B:427:THR:HG21	1:B:445:VAL:HG23	1.90	0.54
1:C:132:ARG:HG2	1:D:161:ARG:CZ	2.38	0.54
1:A:201:ASN:HB3	1:A:205:PHE:HE2	1.73	0.53
1:B:427:THR:O	1:B:428:ASN:OD1	2.26	0.53
1:C:181:LEU:HD22	1:C:437:LEU:HD12	1.90	0.53
1:A:24:LYS:HD3	1:A:27:GLN:OE1	2.09	0.53
1:A:108:SER:H	1:A:111:ALA:HB3	1.73	0.53
1:A:336:LYS:NZ	1:A:337:GLU:OE2	2.40	0.53
1:B:356:LEU:CD2	1:B:359:GLN:H	2.22	0.53
1:D:20:LEU:HD21	1:D:29:LEU:HG	1.90	0.53
1:D:60:GLU:OE1	1:D:66:ARG:NH2	2.41	0.53
1:A:133:LEU:HD23	1:B:163:ASN:ND2	2.24	0.53
1:B:190:ARG:HD3	1:B:198:TYR:CZ	2.44	0.53
1:C:74:ALA:O	1:C:78:VAL:HG23	2.09	0.53
1:A:395:ASN:N	1:A:399:ALA:HB2	2.24	0.53
1:A:413:VAL:O	1:A:417:MET:HG3	2.09	0.53
1:C:290:ALA:O	1:C:293:GLU:HB3	2.08	0.53
1:A:24:LYS:CE	1:C:250:ASP:HB3	2.38	0.53
1:C:298:LEU:HD22	1:C:303:PRO:HB3	1.89	0.53
1:C:134:ASN:OD1	1:D:160:TYR:CE1	2.62	0.53
1:C:220:ILE:O	1:C:224:LYS:HG2	2.09	0.53
1:A:82:ALA:HB1	1:A:260:THR:HG22	1.91	0.53
1:A:17:LEU:HD11	1:A:188:LEU:O	2.08	0.52
1:A:220:ILE:O	1:A:224:LYS:HB2	2.08	0.52
1:B:298:LEU:HD11	1:B:311:LEU:HD11	1.91	0.52
1:A:262:LEU:O	1:A:266:HIS:ND1	2.42	0.52
1:B:33:ALA:HB2	1:B:40:PHE:CE1	2.43	0.52
1:B:130:TRP:HA	1:B:133:LEU:HG	1.90	0.52
1:C:39:ILE:HG23	1:C:52:LEU:HD23	1.91	0.52
1:C:293:GLU:O	1:C:297:VAL:N	2.39	0.52
1:A:268:THR:HA	1:A:327:THR:HG21	1.91	0.52
1:B:288:GLN:O	1:B:292:GLU:HG3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:THR:HG23	1:C:15:LYS:HA	1.90	0.52
1:A:54:SER:O	1:A:58:ILE:HG12	2.10	0.52
1:C:186:ASN:O	1:C:189:GLN:HB2	2.09	0.52
1:B:380:GLU:O	1:B:381:ASN:ND2	2.28	0.52
1:C:39:ILE:HA	1:C:51:TYR:O	2.09	0.52
1:A:85:GLY:HA2	1:A:257:GLN:OE1	2.10	0.52
1:A:177:MET:SD	1:A:266:HIS:NE2	2.83	0.52
1:A:228:GLU:N	1:A:228:GLU:OE1	2.43	0.52
1:A:86:LEU:HB2	2:A:500:MNH:HMD1	1.92	0.51
1:A:86:LEU:HD11	1:A:99:ALA:HB3	1.92	0.51
1:A:251:ASP:HA	1:A:254:ILE:HD12	1.93	0.51
1:C:407:LEU:O	1:C:411:THR:HG23	2.10	0.51
1:A:69:LYS:HD3	1:A:398:ARG:NE	2.25	0.51
1:A:358:PRO:HB2	1:A:362:ARG:HH12	1.75	0.51
1:B:337:GLU:HA	1:B:349:LYS:HE2	1.91	0.51
1:C:68:ASP:OD2	1:C:91:THR:HG21	2.11	0.51
1:C:288:GLN:HG2	1:C:289:LYS:H	1.76	0.51
1:B:96:TRP:O	1:B:100:HIS:HB3	2.11	0.51
1:D:242:ASP:OD1	1:D:243:PRO:HD2	2.10	0.51
1:A:74:ALA:O	1:A:78:VAL:HG23	2.10	0.51
1:B:450:SER:O	1:B:452:LYS:NZ	2.44	0.51
1:C:38:GLU:HA	1:C:53:SER:HB2	1.93	0.51
1:D:91:THR:OG1	1:D:398:ARG:NH1	2.42	0.51
1:D:199:ASP:OD1	1:D:200:GLU:N	2.43	0.51
1:A:219:ILE:HG22	1:A:234:LEU:HD22	1.93	0.51
1:D:214:ASP:O	1:D:217:ASP:HB2	2.11	0.51
1:A:14:LEU:HB3	1:A:18:PRO:HD3	1.90	0.51
1:D:366:ILE:HG23	1:D:386:PRO:HG2	1.93	0.51
1:A:183:GLU:HB2	1:A:205:PHE:CE1	2.45	0.51
1:D:126:LEU:HD22	1:D:148:LEU:HD13	1.91	0.51
1:B:187:LYS:HG2	1:B:190:ARG:NH1	2.25	0.51
1:C:132:ARG:HB3	1:D:161:ARG:HD3	1.92	0.51
1:D:323:ARG:HH22	1:D:371:VAL:HA	1.75	0.50
1:A:232:ASP:O	1:A:235:THR:OG1	2.24	0.50
1:A:251:ASP:N	1:A:251:ASP:OD1	2.44	0.50
1:A:388:HIS:ND1	1:A:391:LYS:HD2	2.26	0.50
1:C:39:ILE:HG23	1:C:52:LEU:HA	1.93	0.50
1:C:125:GLN:C	1:C:128:GLN:HE22	2.15	0.50
1:D:110:GLN:O	1:D:113:LYS:HE2	2.11	0.50
1:B:66:ARG:O	1:B:336:LYS:N	2.39	0.50
1:D:119:MET:SD	1:D:409:GLU:HB3	2.52	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ASP:OD2	1:B:167:ARG:HB3	2.12	0.50
1:C:116:HIS:HE1	1:C:308:VAL:HG21	1.77	0.50
1:C:313:TYR:HA	1:C:316:MET:HG2	1.93	0.50
1:D:19:LEU:HB2	1:D:42:PHE:HE2	1.75	0.50
1:B:53:SER:HB3	1:B:359:GLN:NE2	2.26	0.50
1:C:324:LEU:HD11	1:C:374:PHE:HA	1.94	0.50
1:C:370:ASP:OD1	1:C:370:ASP:N	2.40	0.50
1:C:151:ASP:OD1	1:C:162:PHE:HB2	2.12	0.50
1:A:68:ASP:HB3	1:A:334:TYR:CE1	2.47	0.50
1:B:68:ASP:OD1	1:B:69:LYS:N	2.45	0.50
1:C:200:GLU:OE1	1:C:200:GLU:N	2.42	0.50
1:A:83:GLY:HA3	1:A:256:TYR:CE2	2.46	0.50
1:A:102:ILE:HG22	1:A:242:ASP:HA	1.93	0.50
1:C:417:MET:HB3	1:C:423:PHE:CZ	2.47	0.50
1:D:19:LEU:HD12	1:D:42:PHE:CE2	2.47	0.50
1:C:39:ILE:CG2	1:C:52:LEU:HD23	2.41	0.49
1:A:116:HIS:HB3	1:A:305:TYR:HD2	1.77	0.49
1:B:265:GLY:HA2	2:B:500:MNH:CMC	2.43	0.49
1:C:301:PRO:HB2	1:C:455:LEU:HD12	1.95	0.49
1:D:109:GLN:OE1	1:D:309:LYS:HE3	2.12	0.49
1:D:375:ARG:HB3	1:D:378:ARG:NH1	2.28	0.49
1:A:168:ASP:OD1	1:B:167:ARG:HG2	2.13	0.49
1:A:367:TRP:CZ2	1:A:390:PHE:HB2	2.47	0.49
1:C:60:GLU:OE1	1:C:342:GLY:N	2.42	0.49
1:D:182:ASP:OD1	1:D:186:ASN:ND2	2.45	0.49
1:A:26:VAL:HG11	1:A:329:PRO:HB3	1.94	0.49
1:A:352:GLU:OE1	1:A:352:GLU:N	2.43	0.49
1:A:429:TYR:OH	1:A:442:GLU:O	2.28	0.49
1:B:29:LEU:HD13	1:B:51:TYR:CE2	2.47	0.49
1:C:341:LEU:O	1:C:345:TYR:HB2	2.13	0.49
1:D:390:PHE:CZ	1:D:392:PRO:HG3	2.47	0.49
1:C:69:LYS:HA	1:C:333:LEU:HD23	1.94	0.49
1:B:109:GLN:O	1:B:113:LYS:HG3	2.13	0.49
1:B:320:GLU:HG3	1:B:374:PHE:CE1	2.48	0.49
1:C:426:HIS:CD2	1:C:447:LYS:HE3	2.47	0.49
1:D:256:TYR:O	1:D:260:THR:OG1	2.26	0.49
1:A:83:GLY:HA3	1:A:256:TYR:CD2	2.48	0.49
1:A:87:PHE:HA	2:A:500:MNH:HAD2	1.94	0.49
1:A:232:ASP:OD1	1:A:233:LEU:N	2.45	0.49
1:A:331:PHE:HE1	1:A:333:LEU:HD11	1.78	0.48
1:A:407:LEU:O	1:A:411:THR:OG1	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:TYR:HE2	1:D:129:LYS:HB2	1.78	0.48
1:A:115:TYR:O	1:A:119:MET:HG3	2.13	0.48
1:A:272:LEU:HD13	1:A:322:LEU:HD13	1.96	0.48
1:B:356:LEU:CD2	1:B:358:PRO:HD2	2.44	0.48
1:C:11:PHE:CD1	1:C:18:PRO:HG2	2.48	0.48
1:D:83:GLY:O	1:D:88:THR:OG1	2.32	0.48
1:B:216:VAL:HG21	1:B:259:ILE:HG13	1.94	0.48
1:D:141:VAL:O	1:D:145:MET:HG2	2.13	0.48
1:C:122:ILE:HD13	1:C:152:THR:HA	1.96	0.48
1:C:298:LEU:HD23	1:C:298:LEU:HA	1.65	0.48
1:D:150:LEU:HD22	1:D:174:ILE:HD11	1.94	0.48
1:A:168:ASP:OD1	1:B:167:ARG:CG	2.62	0.48
1:A:367:TRP:HZ2	1:A:390:PHE:HB2	1.78	0.48
1:A:293:GLU:OE1	1:A:296:ARG:NH2	2.46	0.48
1:D:204:GLN:O	1:D:207:GLU:HB3	2.14	0.48
1:C:147:ARG:HG2	1:C:164:SER:HB3	1.96	0.48
1:D:357:ILE:HG22	1:D:361:HIS:HE1	1.79	0.48
1:A:66:ARG:HA	1:A:336:LYS:HE2	1.96	0.47
1:A:190:ARG:HD3	1:A:198:TYR:CZ	2.49	0.47
1:A:111:ALA:HB1	1:A:115:TYR:HE2	1.79	0.47
1:B:232:ASP:OD1	1:B:232:ASP:N	2.45	0.47
1:B:234:LEU:O	1:B:238:LEU:HG	2.13	0.47
1:C:125:GLN:HA	1:C:128:GLN:HE22	1.79	0.47
1:C:326:PRO:HG3	1:C:357:ILE:HG22	1.95	0.47
1:D:69:LYS:HD3	1:D:398:ARG:CZ	2.43	0.47
1:A:8:PRO:HG2	1:A:16:ASN:ND2	2.30	0.47
1:B:436:THR:C	1:B:438:THR:H	2.15	0.47
1:C:267:GLU:OE2	1:C:438:THR:OG1	2.31	0.47
1:D:337:GLU:HA	1:D:349:LYS:HB2	1.96	0.47
1:D:367:TRP:CD1	1:D:378:ARG:HD3	2.46	0.47
1:B:195:ASP:OD1	1:B:196:PRO:HD2	2.15	0.47
1:A:102:ILE:CD1	1:A:249:LEU:HG	2.44	0.47
1:B:324:LEU:HD12	1:B:374:PHE:HD1	1.79	0.47
1:D:223:ARG:NH2	1:D:232:ASP:OD2	2.47	0.47
1:A:141:VAL:O	1:A:145:MET:HG2	2.14	0.47
1:B:20:LEU:HG	1:B:42:PHE:CZ	2.50	0.47
1:C:90:TRP:HB2	1:C:93:GLU:HG3	1.97	0.47
1:D:392:PRO:HG2	1:D:393:PHE:CD2	2.50	0.47
1:D:429:TYR:HE2	1:D:431:LEU:HD12	1.80	0.47
1:B:412:LEU:O	1:B:416:MET:HG3	2.14	0.47
1:C:222:ASP:O	1:C:226:SER:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:23:ASP:O	1:D:25:PRO:HD3	2.13	0.47
1:D:98:LYS:HG2	1:D:242:ASP:HB2	1.96	0.47
1:A:162:PHE:CE2	1:A:215:LEU:HD21	2.50	0.47
1:B:139:ILE:HG12	1:B:446:VAL:O	2.15	0.47
1:C:427:THR:HG21	1:C:445:VAL:HG23	1.96	0.47
1:A:218:LYS:HG2	1:B:136:ASP:OD2	2.15	0.47
1:A:303:PRO:HA	1:A:307:GLN:OE1	2.14	0.47
1:D:332:SER:HA	1:D:354:MET:HA	1.97	0.47
1:D:81:PHE:HB3	1:D:209:ILE:HG12	1.97	0.47
1:D:103:LEU:HD21	1:D:237:MET:HG2	1.97	0.47
1:D:148:LEU:HD21	1:D:413:VAL:HG21	1.96	0.47
1:A:422:ASP:OD1	1:A:451:LYS:NZ	2.49	0.46
1:B:51:TYR:CE2	1:B:354:MET:HG2	2.50	0.46
1:A:86:LEU:HD22	1:A:257:GLN:HE22	1.80	0.46
1:C:66:ARG:NH2	1:C:340:VAL:O	2.46	0.46
1:D:25:PRO:HD2	1:D:435:GLU:OE1	2.15	0.46
1:A:61:ALA:HA	1:A:67:PHE:CD1	2.51	0.46
1:A:132:ARG:O	1:B:161:ARG:HD2	2.15	0.46
1:B:190:ARG:HD3	1:B:198:TYR:CE2	2.50	0.46
1:C:30:MET:O	1:C:359:GLN:NE2	2.48	0.46
1:C:58:ILE:HG21	1:C:360:LEU:HD22	1.97	0.46
1:C:278:TYR:HA	1:C:444:PHE:CZ	2.51	0.46
1:D:281:VAL:HG11	1:D:425:ASP:HB2	1.98	0.46
1:D:366:ILE:HB	1:D:367:TRP:CE3	2.50	0.46
1:A:58:ILE:HG13	1:A:360:LEU:HD13	1.97	0.46
1:B:326:PRO:HD2	1:B:358:PRO:HG3	1.98	0.46
1:C:8:PRO:HD2	1:C:16:ASN:HD21	1.81	0.46
1:D:14:LEU:O	1:D:14:LEU:HG	2.15	0.46
1:A:102:ILE:HD11	1:A:249:LEU:CG	2.44	0.46
1:B:356:LEU:HD22	1:B:359:GLN:CG	2.45	0.46
1:C:141:VAL:O	1:C:145:MET:HG2	2.15	0.46
1:C:288:GLN:O	1:C:292:GLU:HG3	2.14	0.46
1:D:426:HIS:ND1	1:D:447:LYS:HG3	2.31	0.46
1:B:58:ILE:HD12	1:B:360:LEU:HD13	1.98	0.46
1:B:96:TRP:NE1	2:B:500:MNH:O2D	2.31	0.46
1:C:24:LYS:HB2	1:C:27:GLN:HB3	1.98	0.46
1:D:20:LEU:HD22	1:D:25:PRO:CB	2.46	0.46
1:A:126:LEU:HA	1:A:165:PHE:CE2	2.50	0.46
1:A:158:PHE:HB3	1:A:219:ILE:HG21	1.98	0.46
1:A:263:ILE:HA	1:A:266:HIS:CE1	2.50	0.46
1:B:340:VAL:HG12	1:B:346:PRO:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:GLN:HA	1:B:207:GLU:HB3	1.98	0.46
1:B:311:LEU:HB3	1:B:314:VAL:HG22	1.97	0.46
1:B:370:ASP:OD1	1:B:370:ASP:N	2.47	0.46
1:C:183:GLU:HG2	1:C:205:PHE:CD1	2.51	0.46
1:D:305:TYR:HB2	1:D:309:LYS:HZ3	1.79	0.46
1:C:162:PHE:CE2	1:C:215:LEU:HD21	2.50	0.46
1:A:171:HIS:H	1:A:174:ILE:HD12	1.82	0.45
1:B:428:ASN:OD1	1:B:428:ASN:O	2.35	0.45
1:D:185:MET:O	1:D:188:LEU:HB2	2.16	0.45
1:A:133:LEU:HD23	1:B:163:ASN:HD21	1.80	0.45
1:D:366:ILE:C	1:D:368:GLY:H	2.19	0.45
1:B:234:LEU:HA	1:B:237:MET:HE2	1.97	0.45
1:B:380:GLU:C	1:B:381:ASN:HD22	2.14	0.45
1:B:414:LEU:HG	1:B:418:LEU:HD11	1.97	0.45
1:C:121:ASP:CG	1:D:132:ARG:HH12	2.16	0.45
1:C:280:LEU:HD11	1:C:317:VAL:HG13	1.97	0.45
1:C:305:TYR:CE2	1:C:309:LYS:HD2	2.52	0.45
1:D:143:GLU:OE1	1:D:143:GLU:N	2.48	0.45
1:D:417:MET:HB2	1:D:417:MET:HE2	1.89	0.45
1:A:120:VAL:O	1:A:124:VAL:HG23	2.17	0.45
1:B:370:ASP:OD1	1:B:378:ARG:NH2	2.50	0.45
1:C:132:ARG:CA	1:D:161:ARG:HD3	2.46	0.45
1:C:436:THR:O	1:C:437:LEU:HB2	2.16	0.45
1:D:160:TYR:HD1	1:D:222:ASP:OD2	1.99	0.45
1:D:223:ARG:HH22	1:D:234:LEU:HB3	1.82	0.45
1:A:298:LEU:HD23	1:A:303:PRO:HG3	1.99	0.45
1:A:326:PRO:HD2	1:A:358:PRO:HB3	1.97	0.45
2:A:500:MNH:HMB1	2:A:500:MNH:HBB1	1.98	0.45
1:C:91:THR:HB	1:C:398:ARG:NH1	2.31	0.45
1:C:166:TYR:CE2	1:D:129:LYS:HB2	2.51	0.45
1:C:203:ARG:HA	1:C:206:GLN:HE21	1.82	0.45
1:C:400:CYS:SG	2:C:500:MNH:C1C	3.00	0.45
1:A:104:LEU:HD13	1:A:401:ILE:HD12	1.97	0.45
1:D:244:GLU:OE1	1:D:244:GLU:N	2.49	0.45
1:A:102:ILE:CG2	1:A:242:ASP:HA	2.47	0.45
1:A:436:THR:C	1:A:438:THR:H	2.18	0.45
2:B:500:MNH:HMB1	2:B:500:MNH:HBB1	1.98	0.45
1:B:269:THR:OG1	2:B:500:MNH:HMC3	2.17	0.45
1:C:413:VAL:O	1:C:417:MET:HG3	2.16	0.45
1:A:147:ARG:HD3	1:A:165:PHE:HA	1.99	0.44
1:C:30:MET:HE3	1:C:359:GLN:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:ARG:NE	1:D:125:GLN:OE1	2.50	0.44
1:A:183:GLU:HB2	1:A:205:PHE:CE2	2.52	0.44
1:A:168:ASP:CG	1:B:167:ARG:HB3	2.38	0.44
1:B:250:ASP:OD1	1:B:250:ASP:N	2.43	0.44
1:B:413:VAL:O	1:B:417:MET:HG3	2.18	0.44
1:D:20:LEU:HD22	1:D:25:PRO:HB2	2.00	0.44
1:A:108:SER:N	1:A:111:ALA:HB3	2.33	0.44
1:A:370:ASP:O	1:A:378:ARG:NH2	2.49	0.44
1:C:6:PRO:HB2	1:C:36:LEU:HB3	1.98	0.44
1:C:148:LEU:HD22	1:C:413:VAL:HG11	2.00	0.44
1:C:323:ARG:HA	1:C:361:HIS:ND1	2.32	0.44
1:D:16:ASN:HB2	1:D:19:LEU:HD11	1.99	0.44
1:D:27:GLN:O	1:D:31:LYS:HG2	2.17	0.44
1:D:406:ALA:HB2	2:D:500:MNH:HHC	2.00	0.44
1:A:222:ASP:OD2	1:B:135:ALA:HB3	2.16	0.44
1:B:50:ARG:NH2	1:B:351:ASP:OD2	2.50	0.44
1:B:179:ARG:NE	1:B:208:ASP:OD1	2.49	0.44
1:B:285:HIS:CE1	1:B:289:LYS:HE3	2.52	0.44
1:C:272:LEU:HD13	1:C:322:LEU:HG	2.00	0.44
1:C:288:GLN:HG2	1:C:289:LYS:N	2.32	0.44
1:D:223:ARG:NH2	1:D:234:LEU:HB3	2.33	0.44
1:A:320:GLU:HG3	1:A:374:PHE:CD1	2.53	0.44
1:C:312:LYS:HA	1:C:312:LYS:HD3	1.71	0.44
1:C:336:LYS:O	1:C:349:LYS:HG3	2.18	0.44
1:C:102:ILE:CD1	1:C:249:LEU:CD1	2.96	0.44
1:C:166:TYR:HA	1:D:166:TYR:HA	2.00	0.44
1:C:229:GLN:HA	1:C:229:GLN:OE1	2.18	0.44
1:D:357:ILE:HG21	1:D:392:PRO:HA	1.99	0.44
1:A:195:ASP:OD1	1:A:196:PRO:HD2	2.17	0.44
1:C:69:LYS:HD3	1:C:398:ARG:CZ	2.47	0.44
1:C:161:ARG:HD3	1:D:132:ARG:HB3	2.00	0.43
1:A:278:TYR:OH	1:A:431:LEU:HB2	2.18	0.43
1:B:69:LYS:NZ	2:B:500:MNH:O1A	2.38	0.43
1:B:406:ALA:HB2	2:B:500:MNH:HHC	2.00	0.43
1:A:103:LEU:O	1:A:106:SER:OG	2.24	0.43
1:A:297:VAL:HG12	1:A:298:LEU:HD12	2.00	0.43
1:B:242:ASP:HB3	1:B:245:THR:OG1	2.19	0.43
1:B:336:LYS:HE3	1:B:336:LYS:HB2	1.88	0.43
1:B:426:HIS:CD2	1:B:427:THR:HG23	2.53	0.43
1:C:132:ARG:HA	1:D:161:ARG:CD	2.48	0.43
1:D:8:PRO:HB2	1:D:19:LEU:CD1	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:243:PRO:HG2	1:D:244:GLU:OE1	2.18	0.43
1:A:130:TRP:CD2	1:A:139:ILE:HD13	2.54	0.43
1:A:195:ASP:OD1	1:C:350:GLY:HA3	2.19	0.43
1:A:308:VAL:HG11	1:A:408:HIS:ND1	2.32	0.43
1:A:323:ARG:O	1:A:361:HIS:ND1	2.47	0.43
1:A:358:PRO:O	1:A:362:ARG:NH1	2.49	0.43
1:D:39:ILE:HD11	1:D:57:LEU:HB3	2.00	0.43
1:A:201:ASN:HB3	1:A:205:PHE:CE2	2.52	0.43
1:A:353:LEU:HD12	1:A:353:LEU:O	2.19	0.43
1:A:390:PHE:CZ	1:A:392:PRO:HG3	2.52	0.43
1:B:115:TYR:HD1	1:B:156:CYS:HB3	1.83	0.43
1:B:356:LEU:HD22	1:B:359:GLN:H	1.82	0.43
1:C:224:LYS:NZ	1:C:238:LEU:HD13	2.33	0.43
1:D:55:GLN:CB	1:D:366:ILE:HD11	2.49	0.43
1:D:203:ARG:HG3	1:D:204:GLN:N	2.34	0.43
1:A:283:ASN:O	1:A:286:VAL:HG22	2.18	0.43
1:A:324:LEU:HD23	1:A:324:LEU:HA	1.74	0.43
1:B:14:LEU:O	1:B:45:PRO:HD3	2.19	0.43
1:B:272:LEU:N	1:B:327:THR:HG21	2.34	0.43
1:D:22:THR:HG21	1:D:28:ALA:HB2	1.99	0.43
1:A:50:ARG:HD2	1:A:352:GLU:O	2.19	0.43
1:A:426:HIS:CD2	1:A:447:LYS:HG3	2.54	0.43
1:B:112:MET:HA	1:B:115:TYR:HD2	1.84	0.43
1:D:265:GLY:HA2	2:D:500:MNH:C2C	2.49	0.43
1:A:86:LEU:HD22	1:A:86:LEU:H	1.83	0.43
1:B:8:PRO:HG2	1:B:16:ASN:ND2	2.34	0.43
1:B:26:VAL:O	1:B:30:MET:HG3	2.18	0.43
1:B:298:LEU:HD23	1:B:303:PRO:HB3	2.00	0.43
1:C:38:GLU:O	1:C:53:SER:N	2.51	0.43
1:D:173:PHE:HB2	1:D:215:LEU:HD22	1.99	0.43
1:B:347:LEU:HD21	1:B:353:LEU:HD11	2.01	0.42
1:C:215:LEU:O	1:C:219:ILE:HG13	2.19	0.42
1:D:120:VAL:HG12	1:D:412:LEU:HD21	2.01	0.42
1:D:122:ILE:HD12	1:D:151:ASP:HB3	2.01	0.42
1:D:196:PRO:HB3	1:D:199:ASP:OD2	2.19	0.42
1:D:413:VAL:O	1:D:417:MET:HG3	2.19	0.42
1:B:143:GLU:OE1	1:B:143:GLU:N	2.46	0.42
1:D:141:VAL:HB	1:D:142:PRO:HD3	2.01	0.42
1:D:400:CYS:HB2	2:D:500:MNH:NA	2.33	0.42
1:A:280:LEU:HD21	1:A:317:VAL:HG11	2.01	0.42
1:D:38:GLU:OE1	1:D:38:GLU:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:THR:O	1:A:153:ILE:HG22	2.20	0.42
1:A:277:LEU:HD11	1:A:423:PHE:CE2	2.54	0.42
1:B:102:ILE:HD12	1:B:249:LEU:HD13	2.02	0.42
1:C:160:TYR:CE1	1:D:134:ASN:ND2	2.88	0.42
1:D:198:TYR:HB2	1:D:201:ASN:ND2	2.35	0.42
1:A:116:HIS:HB3	1:A:305:TYR:CD2	2.53	0.42
1:A:252:GLU:O	1:A:255:ARG:HG2	2.19	0.42
1:B:70:ASN:HB2	1:B:334:TYR:HD1	1.84	0.42
1:D:203:ARG:HG3	1:D:204:GLN:H	1.85	0.42
1:D:362:ARG:NH2	1:D:372:GLU:OE2	2.52	0.42
1:A:370:ASP:HB2	1:A:373:GLU:HG3	2.02	0.42
1:C:293:GLU:OE1	1:C:311:LEU:HB2	2.19	0.42
1:C:326:PRO:HD2	1:C:358:PRO:HG3	2.01	0.42
1:D:52:LEU:HD21	1:D:353:LEU:HD11	2.00	0.42
1:D:357:ILE:HD13	1:D:392:PRO:HA	2.02	0.42
1:A:126:LEU:HD22	1:A:148:LEU:HD13	2.02	0.42
1:B:289:LYS:HB2	1:B:313:TYR:CZ	2.55	0.42
1:B:308:VAL:HG21	1:B:412:LEU:HD12	2.02	0.42
1:C:72:SER:HB2	1:C:75:LEU:HD13	2.02	0.42
1:D:68:ASP:HB3	1:D:334:TYR:CE2	2.54	0.42
1:D:247:GLU:HG2	1:D:248:PRO:CD	2.48	0.42
1:D:278:TYR:CZ	1:D:431:LEU:HD13	2.54	0.42
1:A:111:ALA:HB1	1:A:115:TYR:CE2	2.54	0.42
1:B:280:LEU:HD22	1:B:287:LEU:HA	2.02	0.42
1:C:102:ILE:HD12	1:C:249:LEU:HD11	2.00	0.42
1:C:14:LEU:HG	1:C:18:PRO:HD3	2.02	0.42
1:C:133:LEU:HD23	1:D:163:ASN:HD21	1.85	0.42
1:C:316:MET:SD	1:C:316:MET:N	2.93	0.42
1:C:423:PHE:CD2	1:C:448:ALA:HB2	2.55	0.42
1:A:173:PHE:CD1	1:A:215:LEU:HD23	2.54	0.42
1:A:314:VAL:HG12	1:A:411:THR:HG22	2.02	0.42
1:B:44:ALA:HB3	1:B:47:ARG:HG3	2.02	0.42
1:C:51:TYR:HB3	1:C:356:LEU:HD11	2.02	0.42
1:C:247:GLU:HA	1:C:248:PRO:HD3	1.65	0.42
1:D:61:ALA:HA	1:D:67:PHE:CD2	2.55	0.42
1:D:272:LEU:HD22	2:D:500:MNH:HBB2	2.01	0.42
1:A:148:LEU:HD21	1:A:413:VAL:HG21	2.01	0.41
1:B:324:LEU:HD23	1:B:324:LEU:HA	1.77	0.41
1:C:183:GLU:O	1:C:187:LYS:HG3	2.19	0.41
1:C:253:ASN:O	1:C:257:GLN:HG2	2.20	0.41
1:D:8:PRO:HG3	1:D:36:LEU:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:LEU:HD23	1:D:20:LEU:HA	1.84	0.41
1:D:363:ASP:OD1	1:D:364:LYS:N	2.53	0.41
1:A:308:VAL:HG11	1:A:408:HIS:HD1	1.85	0.41
1:A:318:LEU:HD12	1:A:411:THR:HG23	2.02	0.41
1:C:58:ILE:HD13	1:C:360:LEU:HD22	2.02	0.41
1:C:60:GLU:HB3	1:C:66:ARG:NH1	2.36	0.41
1:C:112:MET:HE1	1:C:405:PHE:HA	2.02	0.41
1:C:387:GLN:O	1:C:391:LYS:HE2	2.20	0.41
1:D:74:ALA:O	1:D:78:VAL:HG23	2.19	0.41
1:D:281:VAL:CG1	1:D:425:ASP:HB2	2.50	0.41
1:C:398:ARG:HD2	1:C:398:ARG:HA	1.72	0.41
1:D:272:LEU:CD2	2:D:500:MNH:HBB2	2.49	0.41
1:A:166:TYR:HA	1:B:166:TYR:HA	2.02	0.41
1:A:186:ASN:O	1:A:189:GLN:HG2	2.21	0.41
1:D:5:MET:HG2	1:D:41:LYS:HE3	2.03	0.41
1:D:14:LEU:HG	1:D:17:LEU:HB3	2.03	0.41
1:D:366:ILE:HD13	1:D:389:ALA:HB1	2.02	0.41
1:A:24:LYS:HE3	1:C:250:ASP:CB	2.45	0.41
1:B:52:LEU:HG	1:B:58:ILE:CG1	2.51	0.41
1:C:55:GLN:O	1:C:59:LYS:HG2	2.20	0.41
1:C:234:LEU:O	1:C:238:LEU:HG	2.20	0.41
1:C:375:ARG:HD3	1:C:378:ARG:NH2	2.35	0.41
1:A:104:LEU:N	1:A:105:PRO:HD2	2.34	0.41
1:C:132:ARG:HA	1:D:161:ARG:HD3	2.02	0.41
1:C:272:LEU:N	1:C:327:THR:HG21	2.34	0.41
1:C:299:VAL:HG23	1:C:300:ASP:OD1	2.21	0.41
1:A:268:THR:HB	2:A:500:MNH:CBB	2.50	0.41
1:B:79:ARG:HG3	1:B:88:THR:HB	2.03	0.41
1:B:304:SER:HB3	1:B:307:GLN:HG3	2.02	0.41
1:C:9:LYS:HD3	1:C:9:LYS:HA	1.90	0.41
1:D:16:ASN:HB2	1:D:19:LEU:CD1	2.51	0.41
1:D:38:GLU:HB3	1:D:57:LEU:HD12	2.03	0.41
1:B:141:VAL:HB	1:B:142:PRO:HD3	2.03	0.41
1:C:136:ASP:OD1	1:C:136:ASP:N	2.49	0.41
1:C:150:LEU:HD22	1:C:174:ILE:HD11	2.02	0.41
1:C:275:PHE:CE2	1:C:441:PRO:HD3	2.56	0.41
1:C:301:PRO:HG3	1:C:455:LEU:C	2.42	0.41
1:B:7:GLN:HG3	1:B:41:LYS:O	2.20	0.41
1:D:24:LYS:HD3	1:D:27:GLN:CD	2.42	0.41
1:D:286:VAL:HG11	1:D:376:PRO:HG2	2.03	0.40
1:B:223:ARG:NH1	1:B:235:THR:OG1	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:THR:HG23	1:D:15:LYS:O	2.19	0.40
1:D:68:ASP:O	1:D:334:TYR:N	2.40	0.40
1:D:104:LEU:HA	1:D:401:ILE:HD11	2.02	0.40
1:D:356:LEU:HD12	1:D:358:PRO:HD2	2.02	0.40
1:A:69:LYS:CE	2:A:500:MNH:CGA	2.94	0.40
1:A:149:THR:HB	1:A:266:HIS:HA	2.02	0.40
1:A:324:LEU:O	1:A:362:ARG:NH2	2.55	0.40
1:B:118:MET:SD	1:B:156:CYS:HA	2.62	0.40
1:C:218:LYS:HA	1:C:218:LYS:HD3	1.83	0.40
1:A:81:PHE:O	1:A:259:ILE:HG21	2.21	0.40
1:A:375:ARG:HG3	1:A:378:ARG:HG3	2.03	0.40
1:A:422:ASP:O	1:A:448:ALA:HA	2.21	0.40
1:B:204:GLN:O	1:B:207:GLU:HB3	2.22	0.40
1:B:280:LEU:HB3	1:B:287:LEU:HD13	2.04	0.40
1:B:313:TYR:O	1:B:317:VAL:HG23	2.22	0.40
1:A:237:MET:HB3	1:A:254:ILE:HG23	2.03	0.40
1:A:357:ILE:HG22	1:A:361:HIS:CE1	2.57	0.40
1:B:20:LEU:HD22	1:B:25:PRO:HB2	2.04	0.40
1:C:162:PHE:CZ	1:C:262:LEU:CD2	2.94	0.40
1:C:249:LEU:CD2	1:C:253:ASN:OD1	2.67	0.40
1:D:55:GLN:HG2	1:D:366:ILE:HD11	2.04	0.40
1:D:394:GLY:HA3	1:D:399:ALA:HA	2.03	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	450/455 (99%)	436 (97%)	14 (3%)	0	100	100
1	B	447/455 (98%)	439 (98%)	8 (2%)	0	100	100
1	C	450/455 (99%)	423 (94%)	27 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	449/455 (99%)	421 (94%)	28 (6%)	0	100	100
All	All	1796/1820 (99%)	1719 (96%)	77 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	396/399 (99%)	392 (99%)	4 (1%)	76	88
1	B	393/399 (98%)	390 (99%)	3 (1%)	81	91
1	C	396/399 (99%)	394 (100%)	2 (0%)	88	94
1	D	395/399 (99%)	390 (99%)	5 (1%)	69	84
All	All	1580/1596 (99%)	1566 (99%)	14 (1%)	78	90

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ARG
1	A	239	ASN
1	A	305	TYR
1	A	336	LYS
1	B	55	GLN
1	B	381	ASN
1	B	421	PHE
1	C	226	SER
1	C	270	SER
1	D	198	TYR
1	D	251	ASP
1	D	270	SER
1	D	338	ASP
1	D	395	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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$
2	MNH	C	500	1	36,50,50	2.59	14 (38%)	34,82,82	2.65	11 (32%)
2	MNH	D	500	1	36,50,50	2.57	13 (36%)	34,82,82	2.64	9 (26%)
2	MNH	A	500	1	36,50,50	2.61	14 (38%)	34,82,82	2.71	10 (29%)
2	MNH	B	500	1	36,50,50	2.62	14 (38%)	34,82,82	2.71	11 (32%)

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
2	MNH	C	500	1	-	2/12/114/114	-
2	MNH	D	500	1	-	2/12/114/114	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	MNH	A	500	1	-	2/12/114/114	-
2	MNH	B	500	1	-	6/12/114/114	-

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	500	MNH	CHB-C1B	6.24	1.48	1.37
2	C	500	MNH	CHB-C1B	6.20	1.48	1.37
2	D	500	MNH	CHB-C1B	6.12	1.48	1.37
2	B	500	MNH	CHB-C1B	6.05	1.47	1.37
2	A	500	MNH	CHA-C4D	6.04	1.47	1.37
2	D	500	MNH	CHC-C4B	5.99	1.47	1.37
2	B	500	MNH	CHA-C4D	5.93	1.47	1.37
2	C	500	MNH	CHA-C4D	5.91	1.47	1.37
2	B	500	MNH	CHC-C4B	5.91	1.47	1.37
2	C	500	MNH	CHC-C4B	5.84	1.47	1.37
2	B	500	MNH	CHD-C1D	5.79	1.47	1.37
2	A	500	MNH	CHD-C1D	5.79	1.47	1.37
2	D	500	MNH	CHD-C1D	5.70	1.47	1.37
2	D	500	MNH	CHA-C4D	5.69	1.47	1.37
2	A	500	MNH	CHC-C4B	5.69	1.47	1.37
2	C	500	MNH	CHD-C1D	5.69	1.47	1.37
2	D	500	MNH	CHC-C1C	3.56	1.48	1.40
2	A	500	MNH	O2A-CGA	3.49	1.33	1.22
2	B	500	MNH	CHD-C4C	3.48	1.47	1.40
2	D	500	MNH	O2A-CGA	3.47	1.33	1.22
2	D	500	MNH	O1D-CGD	3.46	1.33	1.22
2	B	500	MNH	O2A-CGA	3.46	1.33	1.22
2	C	500	MNH	O2A-CGA	3.46	1.33	1.22
2	A	500	MNH	O1D-CGD	3.45	1.33	1.22
2	B	500	MNH	CHC-C1C	3.45	1.47	1.40
2	B	500	MNH	O1D-CGD	3.43	1.33	1.22
2	A	500	MNH	CHA-C1A	3.41	1.47	1.40
2	B	500	MNH	CHA-C1A	3.40	1.47	1.40
2	C	500	MNH	O1D-CGD	3.39	1.33	1.22
2	C	500	MNH	CHA-C1A	3.35	1.47	1.40
2	C	500	MNH	CHC-C1C	3.34	1.47	1.40
2	C	500	MNH	CHD-C4C	3.32	1.47	1.40
2	A	500	MNH	CHB-C4A	3.30	1.47	1.40
2	D	500	MNH	CHD-C4C	3.30	1.47	1.40
2	A	500	MNH	CHD-C4C	3.28	1.47	1.40
2	A	500	MNH	CHC-C1C	3.24	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	MNH	CHB-C4A	3.23	1.47	1.40
2	B	500	MNH	CHB-C4A	3.23	1.47	1.40
2	D	500	MNH	CHA-C1A	3.15	1.47	1.40
2	A	500	MNH	C4B-C3B	-3.10	1.40	1.45
2	D	500	MNH	CHB-C4A	3.07	1.47	1.40
2	C	500	MNH	C4B-C3B	-2.91	1.41	1.45
2	B	500	MNH	C4B-C3B	-2.81	1.41	1.45
2	D	500	MNH	C4B-C3B	-2.64	1.41	1.45
2	C	500	MNH	O1A-CGA	-2.48	1.22	1.30
2	A	500	MNH	O2D-CGD	-2.47	1.22	1.30
2	B	500	MNH	O1A-CGA	-2.47	1.22	1.30
2	D	500	MNH	O1A-CGA	-2.43	1.22	1.30
2	B	500	MNH	O2D-CGD	-2.42	1.22	1.30
2	D	500	MNH	O2D-CGD	-2.42	1.22	1.30
2	C	500	MNH	O2D-CGD	-2.41	1.22	1.30
2	A	500	MNH	O1A-CGA	-2.35	1.22	1.30
2	A	500	MNH	C1B-NB	-2.21	1.33	1.36
2	B	500	MNH	C1B-NB	-2.07	1.33	1.36
2	C	500	MNH	C1B-NB	-2.01	1.33	1.36

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	500	MNH	CHA-C4D-ND	7.81	127.75	120.84
2	B	500	MNH	CHA-C4D-ND	7.49	127.47	120.84
2	A	500	MNH	CHD-C1D-ND	7.44	127.42	120.84
2	C	500	MNH	CHA-C4D-ND	7.24	127.25	120.84
2	B	500	MNH	CHD-C1D-ND	7.15	127.17	120.84
2	D	500	MNH	CHD-C1D-ND	7.03	127.06	120.84
2	A	500	MNH	CHA-C4D-ND	6.96	127.00	120.84
2	C	500	MNH	CHD-C1D-ND	6.92	126.96	120.84
2	A	500	MNH	CHC-C4B-NB	6.51	126.60	120.84
2	C	500	MNH	CHC-C4B-NB	6.50	126.59	120.84
2	D	500	MNH	CHC-C4B-NB	6.10	126.24	120.84
2	B	500	MNH	CHC-C4B-NB	5.93	126.08	120.84
2	A	500	MNH	CHB-C1B-NB	-4.77	116.61	120.84
2	B	500	MNH	CHB-C1B-NB	-4.29	117.04	120.84
2	C	500	MNH	CHB-C1B-NB	-3.83	117.45	120.84
2	B	500	MNH	CMA-C3A-C2A	3.71	131.94	124.94
2	C	500	MNH	C1B-CHB-C4A	3.63	128.49	118.67
2	A	500	MNH	C1B-CHB-C4A	3.62	128.45	118.67
2	D	500	MNH	C1B-CHB-C4A	3.52	128.20	118.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	MNH	CBA-CAA-C2A	-3.48	106.73	112.60
2	B	500	MNH	C1B-CHB-C4A	3.44	127.98	118.67
2	D	500	MNH	CBA-CAA-C2A	-3.29	107.05	112.60
2	D	500	MNH	CHB-C1B-NB	-3.23	117.98	120.84
2	A	500	MNH	CHC-C4B-C3B	-3.06	121.77	126.66
2	C	500	MNH	CHC-C4B-C3B	-2.84	122.13	126.66
2	D	500	MNH	CHC-C4B-C3B	-2.68	122.38	126.66
2	B	500	MNH	CHC-C4B-C3B	-2.68	122.39	126.66
2	A	500	MNH	CAD-CBD-CGD	-2.66	107.88	113.60
2	A	500	MNH	C3D-C4D-ND	-2.51	109.46	115.01
2	B	500	MNH	CBA-CAA-C2A	2.43	116.70	112.60
2	B	500	MNH	C3D-C4D-ND	-2.41	109.70	115.01
2	A	500	MNH	CBA-CAA-C2A	-2.27	108.78	112.60
2	D	500	MNH	C3D-C4D-ND	-2.25	110.05	115.01
2	C	500	MNH	O2D-CGD-CBD	2.23	121.18	114.03
2	C	500	MNH	C3D-C4D-ND	-2.21	110.14	115.01
2	C	500	MNH	C4D-C3D-C2D	-2.17	105.19	113.64
2	B	500	MNH	C4D-C3D-C2D	-2.12	105.40	113.64
2	D	500	MNH	C4D-C3D-C2D	-2.07	105.59	113.64
2	C	500	MNH	CBD-CAD-C3D	-2.06	106.96	112.62
2	A	500	MNH	C4D-C3D-C2D	-2.04	105.69	113.64
2	B	500	MNH	CAA-C2A-C3A	2.02	133.06	127.25

There are no chirality outliers.

All (12) torsion outliers are listed below:

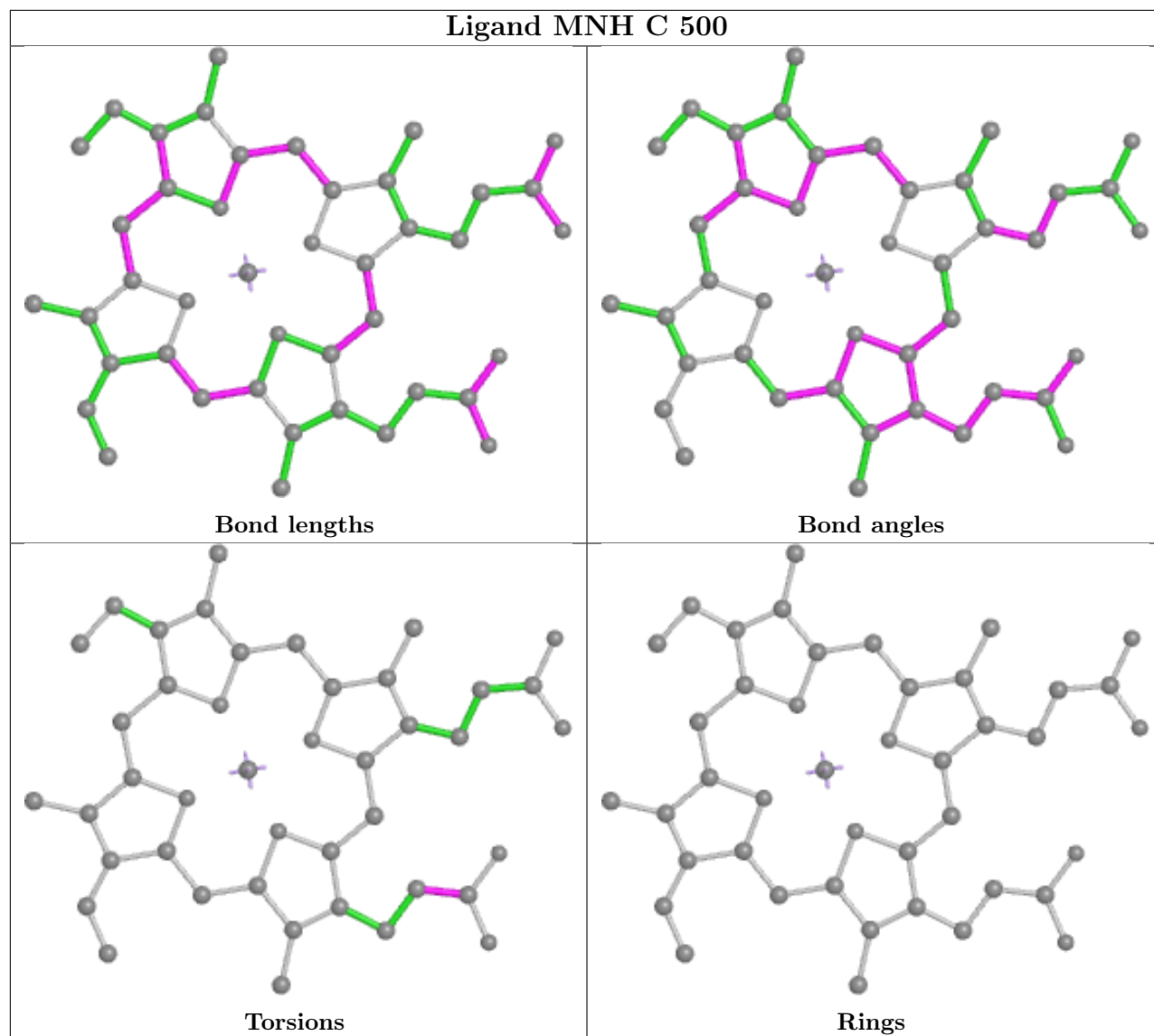
Mol	Chain	Res	Type	Atoms
2	B	500	MNH	C3A-C2A-CAA-CBA
2	B	500	MNH	C1A-C2A-CAA-CBA
2	B	500	MNH	CAA-CBA-CGA-O1A
2	B	500	MNH	CAA-CBA-CGA-O2A
2	A	500	MNH	CAD-CBD-CGD-O1D
2	D	500	MNH	CAD-CBD-CGD-O2D
2	B	500	MNH	C2A-CAA-CBA-CGA
2	A	500	MNH	CAD-CBD-CGD-O2D
2	D	500	MNH	CAD-CBD-CGD-O1D
2	B	500	MNH	C3D-CAD-CBD-CGD
2	C	500	MNH	CAD-CBD-CGD-O1D
2	C	500	MNH	CAD-CBD-CGD-O2D

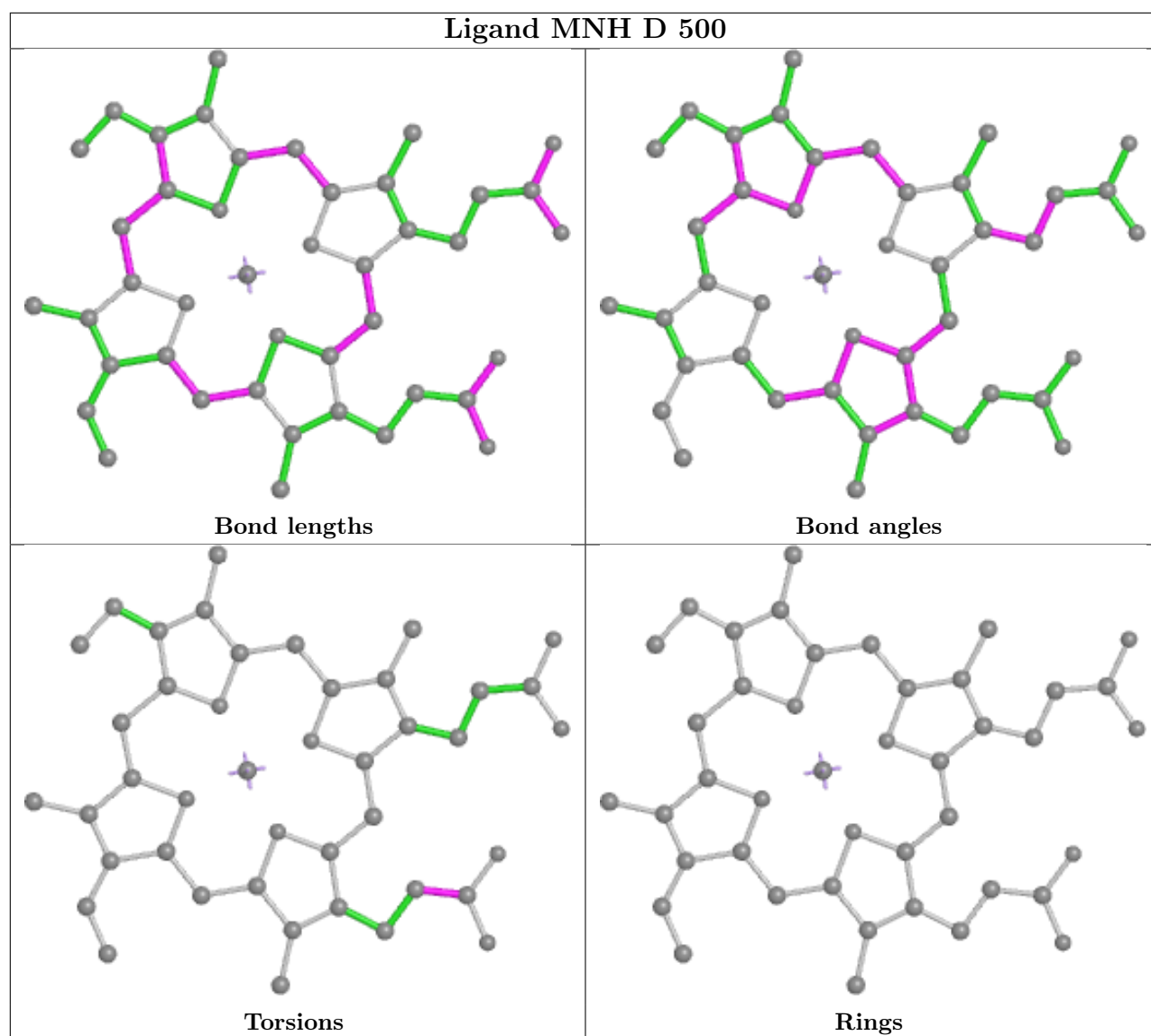
There are no ring outliers.

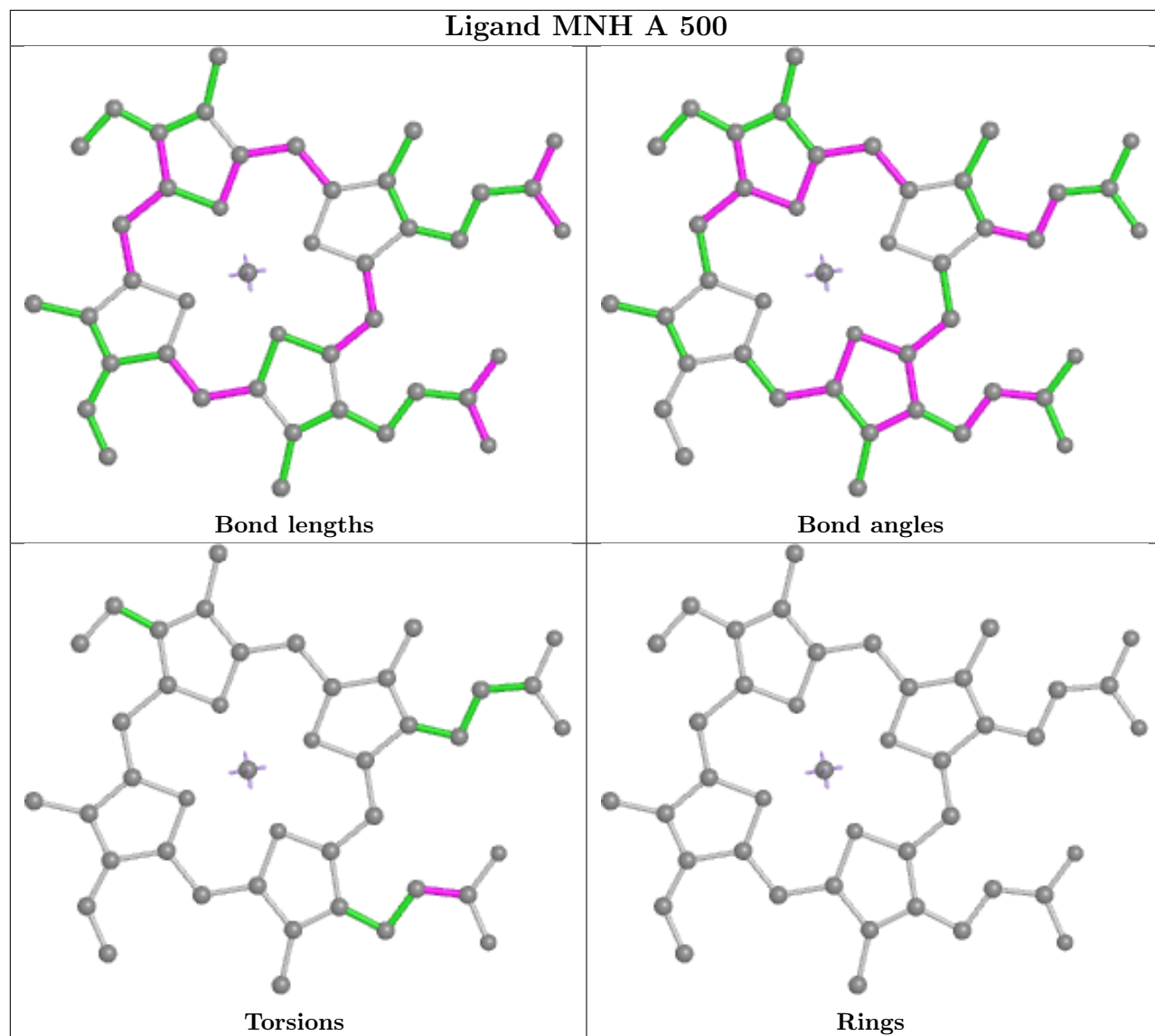
4 monomers are involved in 24 short contacts:

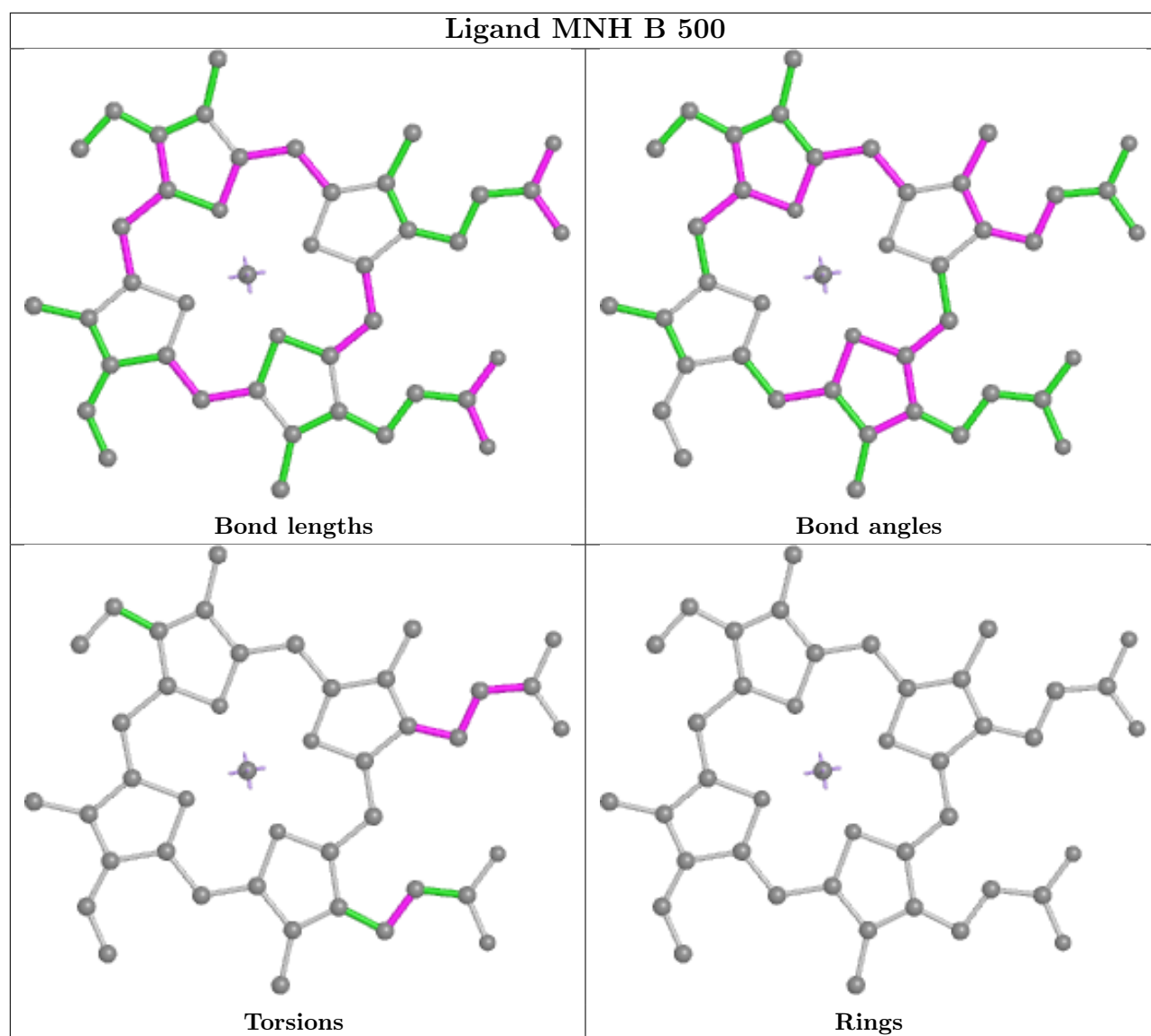
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	500	MNH	2	0
2	D	500	MNH	5	0
2	A	500	MNH	10	0
2	B	500	MNH	7	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	452/455 (99%)	0.58	18 (3%) 38 37	8, 39, 80, 117	0
1	B	449/455 (98%)	0.54	23 (5%) 28 28	8, 38, 74, 115	0
1	C	452/455 (99%)	0.59	20 (4%) 34 34	7, 40, 86, 145	0
1	D	451/455 (99%)	0.78	40 (8%) 9 11	6, 43, 86, 121	0
All	All	1804/1820 (99%)	0.62	101 (5%) 24 25	6, 40, 83, 145	0

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	229	GLN	7.9
1	A	225	ALA	7.8
1	B	228	GLU	5.3
1	B	343	GLY	4.5
1	B	344	GLU	4.5
1	A	191	ALA	4.3
1	D	199	ASP	4.3
1	A	195	ASP	4.1
1	D	110	GLN	4.1
1	D	65	SER	3.8
1	B	346	PRO	3.7
1	A	64	GLU	3.7
1	C	229	GLN	3.7
1	A	194	ASP	3.6
1	D	46	GLY	3.5
1	B	229	GLN	3.4
1	A	189	GLN	3.3
1	B	299	VAL	3.2
1	D	194	ASP	3.2
1	C	319	ASN	3.2
1	A	228	GLU	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	428	ASN	3.1
1	B	369	ASP	3.0
1	D	198	TYR	3.0
1	D	383	SER	3.0
1	D	13	GLU	3.0
1	D	226	SER	3.0
1	D	35	GLU	3.0
1	D	369	ASP	2.9
1	B	297	VAL	2.9
1	C	344	GLU	2.9
1	C	369	ASP	2.9
1	D	228	GLU	2.8
1	D	200	GLU	2.8
1	B	382	PRO	2.7
1	D	11	PHE	2.7
1	D	350	GLY	2.7
1	A	239	ASN	2.7
1	B	370	ASP	2.7
1	A	21	ASN	2.7
1	D	192	ASN	2.7
1	C	323	ARG	2.6
1	D	387	GLN	2.6
1	B	365	THR	2.6
1	C	35	GLU	2.5
1	B	397	GLN	2.5
1	A	196	PRO	2.5
1	C	382	PRO	2.5
1	C	454	PRO	2.5
1	A	428	ASN	2.5
1	D	343	GLY	2.5
1	D	370	ASP	2.5
1	C	292	GLU	2.5
1	A	310	GLN	2.5
1	B	285	HIS	2.5
1	B	383	SER	2.4
1	B	424	GLU	2.4
1	B	286	VAL	2.4
1	B	227	GLY	2.4
1	D	367	TRP	2.4
1	C	387	GLN	2.4
1	D	248	PRO	2.4
1	C	377	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	346	PRO	2.4
1	D	345	TYR	2.3
1	C	424	GLU	2.3
1	B	454	PRO	2.3
1	D	227	GLY	2.3
1	D	381	ASN	2.3
1	D	225	ALA	2.3
1	B	23	ASP	2.3
1	B	422	ASP	2.3
1	C	300	ASP	2.2
1	A	197	ALA	2.2
1	C	388	HIS	2.2
1	D	394	GLY	2.2
1	D	66	ARG	2.2
1	D	12	GLY	2.2
1	D	190	ARG	2.2
1	D	193	PRO	2.2
1	A	190	ARG	2.2
1	D	306	LYS	2.2
1	D	388	HIS	2.2
1	B	337	GLU	2.1
1	D	346	PRO	2.1
1	A	365	THR	2.1
1	C	447	LYS	2.1
1	D	195	ASP	2.1
1	B	316	MET	2.1
1	C	305	TYR	2.1
1	D	292	GLU	2.1
1	A	454	PRO	2.1
1	D	89	SER	2.1
1	D	332	SER	2.1
1	A	255	ARG	2.1
1	B	310	GLN	2.0
1	D	16	ASN	2.0
1	D	221	ALA	2.0
1	D	222	ASP	2.0
1	C	313	TYR	2.0
1	C	430	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

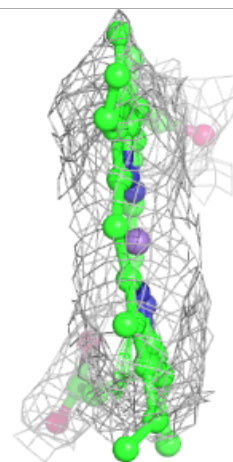
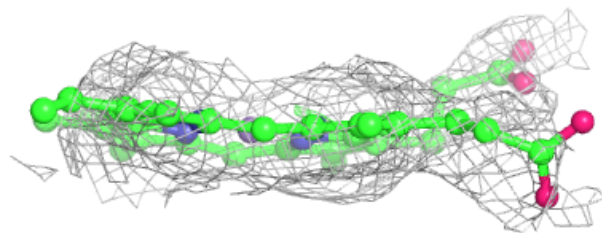
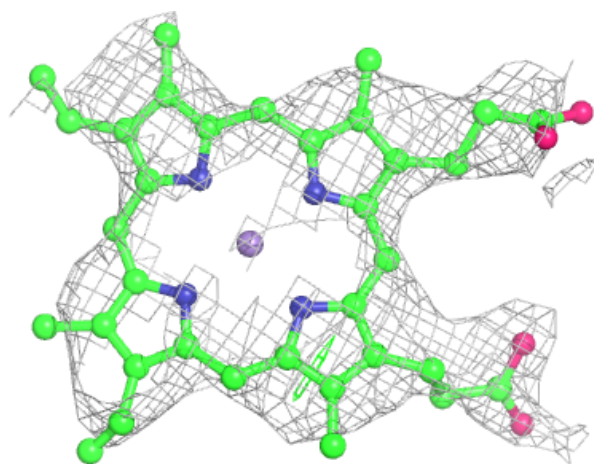
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MNH	B	500	43/43	0.89	0.25	10,18,25,32	0
2	MNH	D	500	43/43	0.89	0.25	11,19,41,59	0
2	MNH	C	500	43/43	0.92	0.20	7,18,35,41	0
2	MNH	A	500	43/43	0.92	0.20	7,19,36,58	0

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

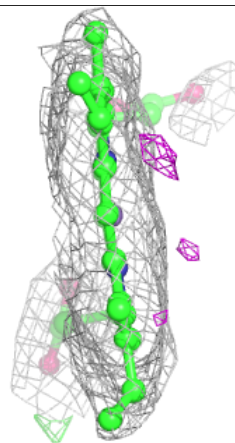
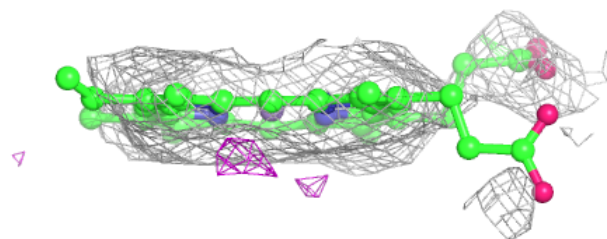
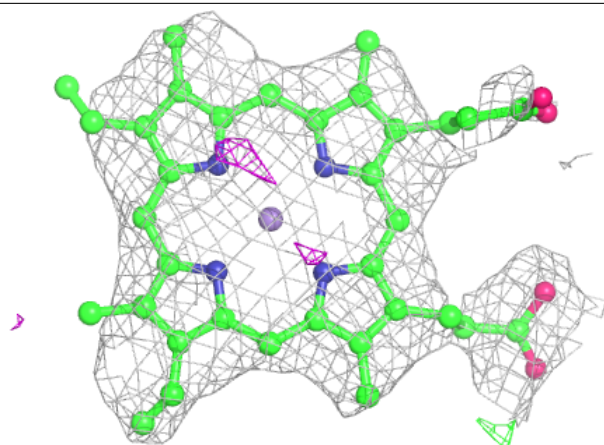
Electron density around MNH B 500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



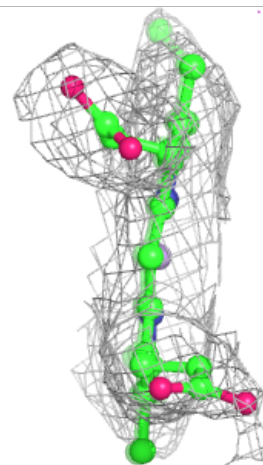
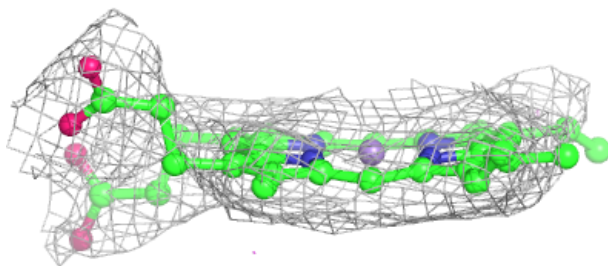
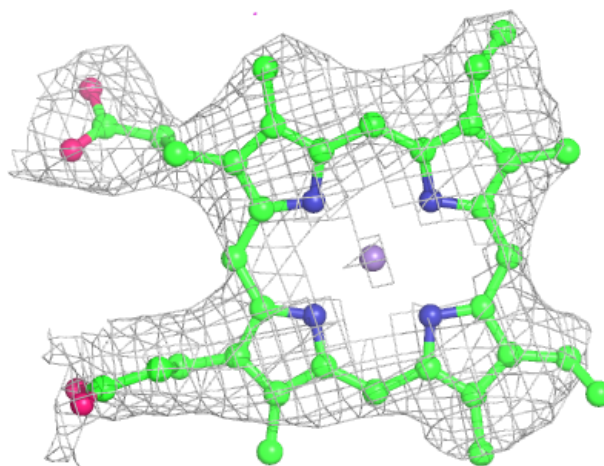
Electron density around MNH D 500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



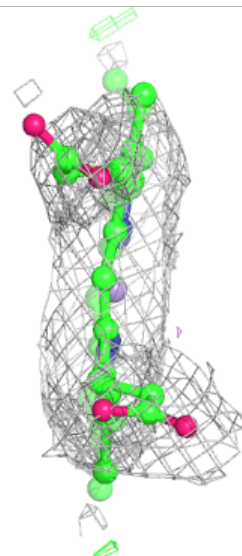
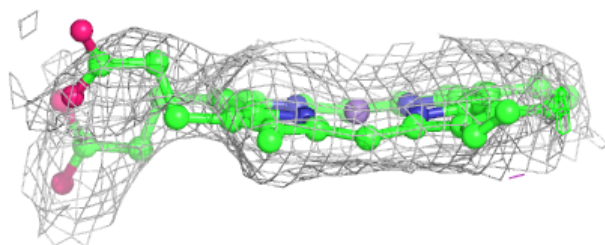
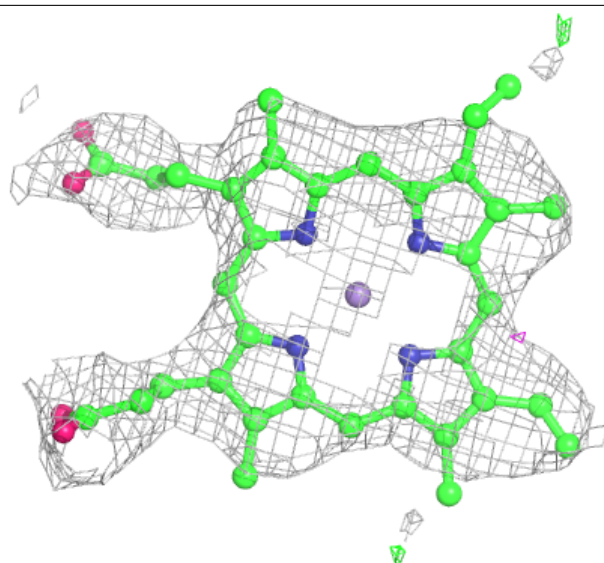
Electron density around MNH C 500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MNH A 500:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.