Full wwPDB X-ray Structure Validation Report (i)

Dec 19, 2023 – 03:43 PM EST

PDB ID	:	1J36
Title	:	Crystal Structure of Drosophila AnCE
Authors	:	Kim, H.M.; Shin, D.R.; Yoo, O.J.; Lee, H.; Lee, J.-O.
Deposited on	:	2003-01-20
Resolution	:	2.40 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 (i) 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 (1)) were used in the production of this report:

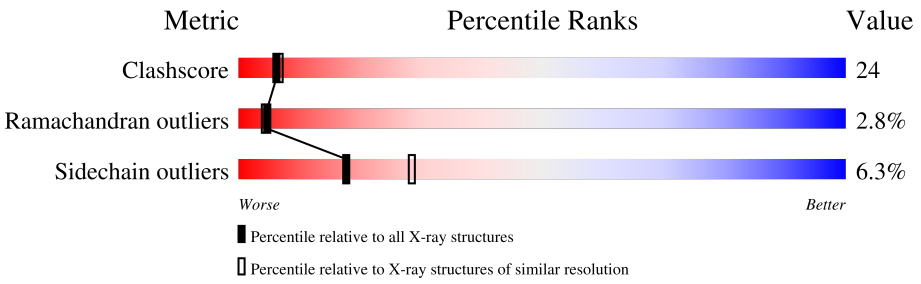
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	607	58% 35% 5% •
1	B	607	57% 36% 6% •

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10263 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 angiotensin converting enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	598	4900	3135	819	926	20	154	0	0
1	B	598	4900	3135	819	926	20	154	0	0

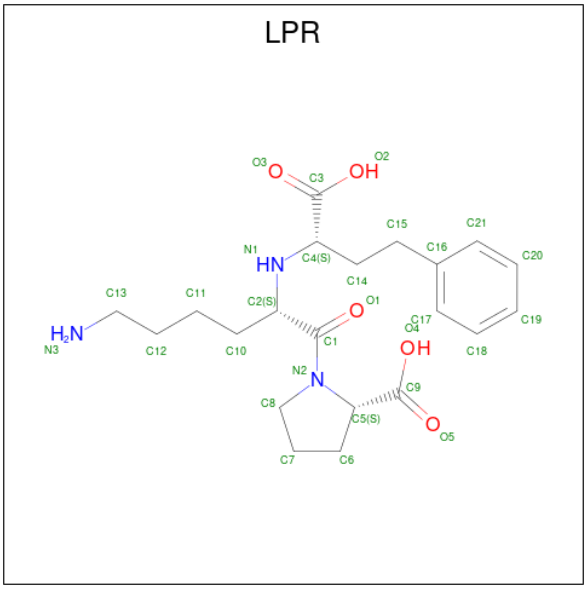
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	51	ARG	GLY	conflict	UNP Q10714
A	53	ALA	ASN	conflict	UNP Q10714
A	607	ILE	THR	conflict	UNP Q10714
A	616	HIS	-	expression tag	UNP Q10714
A	617	HIS	-	expression tag	UNP Q10714
A	618	HIS	-	expression tag	UNP Q10714
A	619	HIS	-	expression tag	UNP Q10714
A	620	HIS	-	expression tag	UNP Q10714
B	51	ARG	GLY	conflict	UNP Q10714
B	53	ALA	ASN	conflict	UNP Q10714
B	607	ILE	THR	conflict	UNP Q10714
B	616	HIS	-	expression tag	UNP Q10714
B	617	HIS	-	expression tag	UNP Q10714
B	618	HIS	-	expression tag	UNP Q10714
B	619	HIS	-	expression tag	UNP Q10714
B	620	HIS	-	expression tag	UNP Q10714

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	1	1	1	0	0
2	B	1	1	1	0	0

- Molecule 3 is [N2-[(S)-1-CARBOXY-3-PHENYLPROPYL]-L-LYSYL-L-PROLINE (three-letter code: LPR) (formula: $C_{21}H_{31}N_3O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	29	21	3	5	0	0
			Total	C	N	O		
3	B	1	29	21	3	5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	196	196	196	0	0
			Total	O		
4	B	207	207	207	0	0

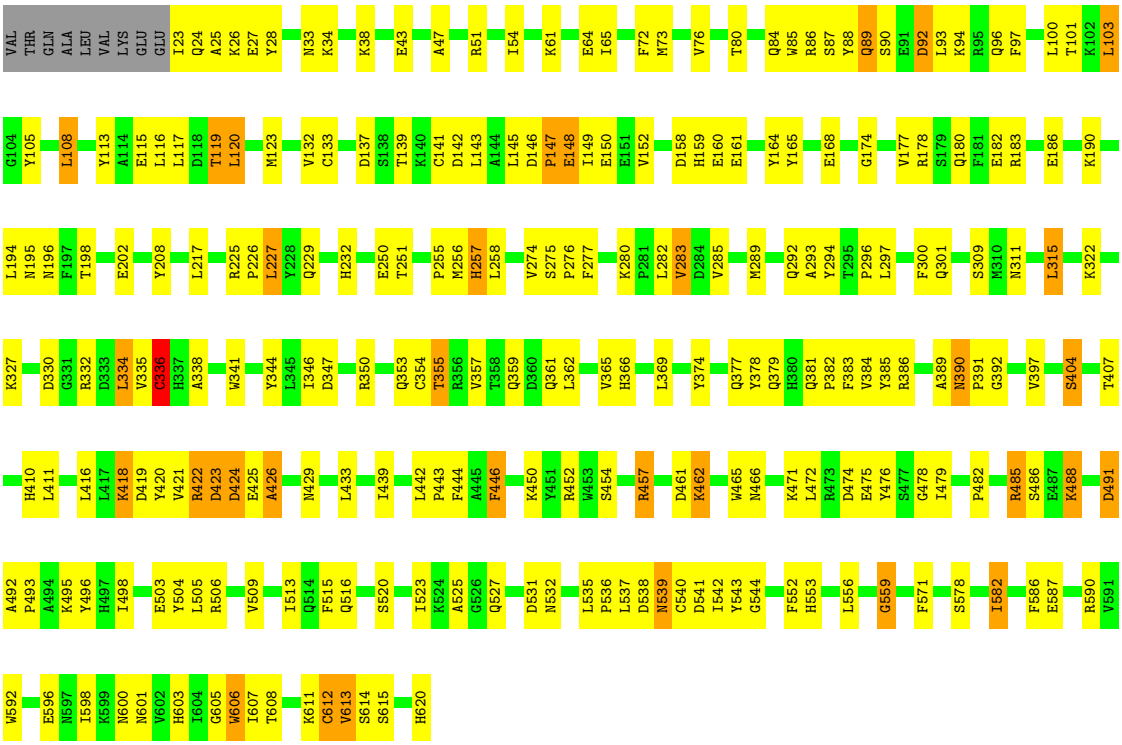
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

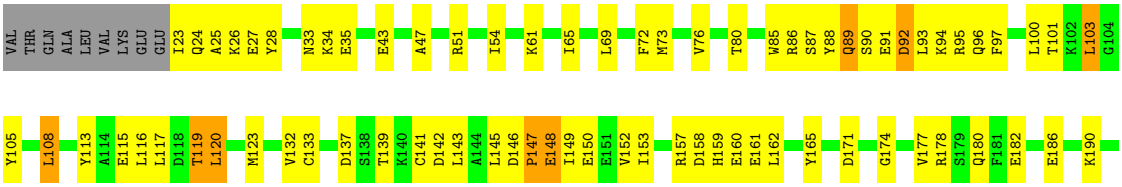
• Molecule 1: angiotensin converting enzyme

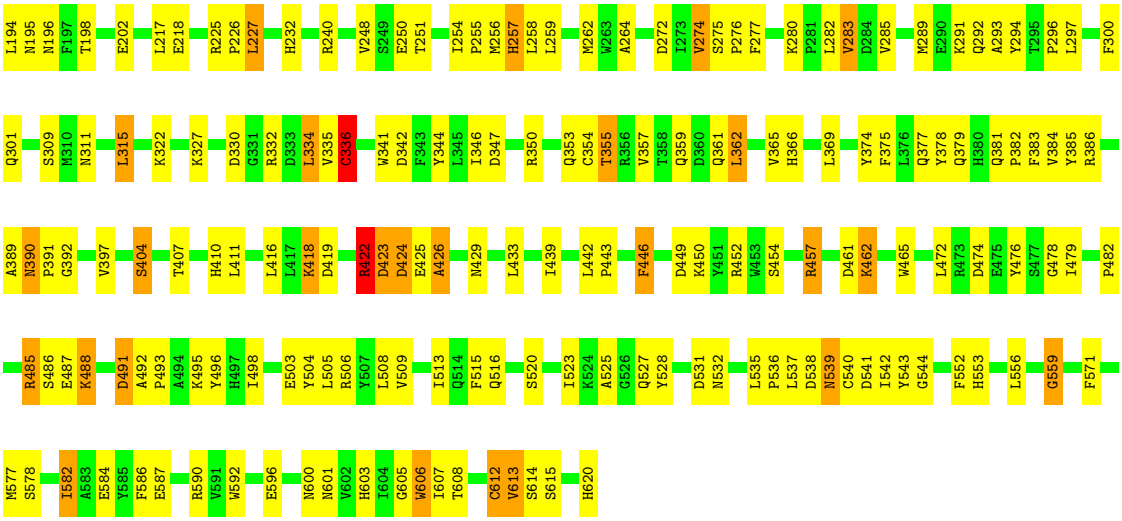
Chain A: 58% 35% 5%



• Molecule 1: angiotensin converting enzyme

Chain B: 57% 36% 6%




L194 N195 N196 F197 T198 E202 L217 E218 R225 P226 L227 H232 R240 V248 S249 E250 T251 I254 P255 M256 H257 L258 L259 M262 W263 A264 D272 I273 V274 S275 P276 F277 K280 P281 L282 V283 D284 V285 M289 E290 K291 Q292 A293 Y294 T295 P296 L297 F300
Q301 S309 M310 N311 L315 K322 K327 D330 G331 R332 D333 L334 V335 C336 W341 D342 F343 Y344 L345 I346 D347 R350 Q353 C354 T355 R356 V357 T358 Q359 D360 Q361 L362 V365 H366 L369 Y374 F375 L376 Q377 Y378 Q379 H380 Q381 P382 F383 V384 Y385 R386
A389 N390 P391 G392 V397 S404 T407 H410 L411 L416 L417 K418 D419 R422 D423 D424 E425 A426 N429 L433 I439 L442 P443 F446 D449 K450 Y451 R452 W453 S454 R457 D461 K462 W465 L472 R473 D474 E475 Y476 S477 G478 I479 P482
R485 S486 E487 K488 D491 A492 P493 A494 K495 Y496 H497 I498 E503 Y504 L505 R506 Y507 L508 V509 I513 Q514 F515 Q516 S520 I523 K524 A525 G526 Q527 Y528 D531 N532 L535 P536 L537 D538 N539 C540 D541 I542 Y543 G544 F552 H553 L556 G559 F571
M577 S578 I582 A583 E584 Y585 F586 E587 R590 V591 W592 E596 N600 N601 V602 H603 I604 G605 W606 I607 T608 C612 V613 S614 S615 H620

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	94.91Å 121.22Å 94.74Å 90.00° 99.39° 90.00°	Depositor
Resolution (Å)	20.00 – 2.40	Depositor
% Data completeness (in resolution range)	92.2 (20.00-2.40)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.234 , 0.280	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10263	wwPDB-VP
Average B, all atoms (Å^2)	23.0	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: ZN, LPR

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	0.45	0/5031	0.67	3/6814 (0.0%)
1	B	0.46	0/5031	0.67	3/6814 (0.0%)
All	All	0.46	0/10062	0.67	6/13628 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	336	CYS	CA-CB-SG	-5.85	103.47	114.00
1	A	457	ARG	N-CA-C	-5.68	95.65	111.00
1	B	457	ARG	N-CA-C	-5.57	95.96	111.00
1	B	336	CYS	CA-CB-SG	-5.35	104.36	114.00
1	B	491	ASP	N-CA-C	5.17	124.97	111.00
1	A	491	ASP	N-CA-C	5.12	124.83	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4900	0	4696	217	0
1	B	4900	0	4696	240	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
3	A	29	0	29	1	0
3	B	29	0	29	1	0
4	A	196	0	0	10	0
4	B	207	0	0	31	0
All	All	10263	0	9450	458	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 24.

All (458) 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:B:26:LYS:HE2	1:B:93:LEU:HD21	1.39	1.03
1:B:479:ILE:HA	4:B:947:HOH:O	1.57	1.01
1:A:26:LYS:HE2	1:A:93:LEU:HD21	1.40	0.98
1:B:347:ASP:H	1:B:379:GLN:NE2	1.68	0.92
1:A:347:ASP:H	1:A:379:GLN:NE2	1.67	0.91
1:B:89:GLN:H	1:B:89:GLN:NE2	1.69	0.91
1:A:89:GLN:H	1:A:89:GLN:NE2	1.69	0.91
1:B:143:LEU:HD22	1:B:148:GLU:HG2	1.57	0.85
1:B:347:ASP:H	1:B:379:GLN:HE22	1.21	0.84
1:B:92:ASP:O	1:B:96:GLN:HG3	1.77	0.84
1:A:143:LEU:HD22	1:A:148:GLU:HG2	1.58	0.84
1:A:92:ASP:O	1:A:96:GLN:HG3	1.77	0.83
1:A:347:ASP:H	1:A:379:GLN:HE22	1.20	0.83
1:B:26:LYS:CE	1:B:93:LEU:HD21	2.09	0.82
1:A:365:VAL:O	1:A:369:LEU:HD23	1.78	0.82
1:B:418:LYS:HE3	1:B:418:LYS:H	1.43	0.81
1:A:418:LYS:HE3	1:A:418:LYS:H	1.43	0.81
1:A:26:LYS:CE	1:A:93:LEU:HD21	2.11	0.80
1:A:322:LYS:HB3	1:A:350:ARG:HD3	1.65	0.79
1:B:322:LYS:HB3	1:B:350:ARG:HD3	1.63	0.78
1:A:389:ALA:O	1:A:390:ASN:HB3	1.83	0.77
1:B:365:VAL:O	1:B:369:LEU:HD23	1.85	0.77
1:B:133:CYS:HA	1:B:141:CYS:HA	1.67	0.76
1:B:423:ASP:O	1:B:424:ASP:HB2	1.86	0.75
1:B:418:LYS:HE3	1:B:418:LYS:N	2.01	0.75
1:B:153:ILE:HD11	4:B:979:HOH:O	1.85	0.74
1:A:89:GLN:H	1:A:89:GLN:HE21	1.33	0.74
1:A:418:LYS:HE3	1:A:418:LYS:N	2.01	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:389:ALA:O	1:B:390:ASN:HB3	1.86	0.74
1:A:133:CYS:HA	1:A:141:CYS:HA	1.69	0.74
1:A:488:LYS:HZ2	1:A:488:LYS:HB2	1.54	0.73
1:A:423:ASP:O	1:A:424:ASP:HB2	1.87	0.73
1:B:479:ILE:HD12	4:B:947:HOH:O	1.89	0.73
1:B:256:MET:O	1:B:257:HIS:ND1	2.21	0.73
1:B:85:TRP:HA	1:B:88:TYR:CD1	2.24	0.73
1:A:613:VAL:HG23	1:A:614:SER:N	2.04	0.72
1:A:256:MET:O	1:A:257:HIS:ND1	2.21	0.72
1:B:254:ILE:HB	4:B:947:HOH:O	1.88	0.72
1:B:89:GLN:H	1:B:89:GLN:HE21	1.34	0.71
1:A:85:TRP:HA	1:A:88:TYR:CD1	2.25	0.71
1:B:613:VAL:HG23	1:B:614:SER:N	2.04	0.71
1:A:275:SER:OG	1:A:282:LEU:HD11	1.90	0.71
1:B:251:THR:HG22	1:B:603:HIS:CD2	2.25	0.71
1:B:227:LEU:O	1:B:227:LEU:HD23	1.91	0.70
1:A:227:LEU:HD23	1:A:227:LEU:O	1.91	0.70
1:B:275:SER:OG	1:B:282:LEU:HD11	1.91	0.70
1:B:285:VAL:CG1	1:B:416:LEU:HB3	2.21	0.70
1:B:541:ASP:O	1:B:543:TYR:N	2.26	0.69
1:A:285:VAL:CG1	1:A:416:LEU:HB3	2.23	0.69
1:A:251:THR:HG22	1:A:603:HIS:CD2	2.27	0.69
1:A:541:ASP:O	1:A:543:TYR:N	2.26	0.68
1:A:418:LYS:HG2	1:A:419:ASP:H	1.59	0.68
1:B:418:LYS:HG2	1:B:419:ASP:H	1.58	0.68
1:A:474:ASP:O	1:A:606:TRP:CZ3	2.48	0.67
1:B:513:ILE:HD12	1:B:516:GLN:HB2	1.76	0.67
1:A:174:GLY:HA2	1:A:493:PRO:HB2	1.76	0.66
1:A:513:ILE:HD12	1:A:516:GLN:HB2	1.77	0.66
1:A:355:THR:HA	1:A:361:GLN:OE1	1.95	0.66
1:B:355:THR:HA	1:B:361:GLN:OE1	1.95	0.66
1:B:255:PRO:HB2	1:B:258:LEU:HD12	1.78	0.66
3:B:802:LPR:H112	3:B:802:LPR:H8C1	1.78	0.66
1:B:174:GLY:HA2	1:B:493:PRO:HB2	1.78	0.66
1:B:262:MET:HE1	4:B:979:HOH:O	1.95	0.66
1:B:488:LYS:HB2	1:B:488:LYS:NZ	2.11	0.65
1:B:330:ASP:OD2	1:B:332:ARG:HD3	1.97	0.65
1:A:330:ASP:OD2	1:A:332:ARG:HD3	1.95	0.65
1:B:486:SER:HB2	1:B:614:SER:HA	1.79	0.65
1:B:327:LYS:HB2	1:B:354:CYS:SG	2.37	0.65
1:A:72:PHE:O	1:A:76:VAL:HG23	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:801:LPR:H8C1	3:A:801:LPR:H112	1.77	0.64
1:B:72:PHE:O	1:B:76:VAL:HG23	1.97	0.64
1:B:474:ASP:O	1:B:606:TRP:CZ3	2.50	0.64
1:B:488:LYS:HB2	1:B:488:LYS:HZ2	1.62	0.64
1:A:255:PRO:HB2	1:A:258:LEU:HD12	1.78	0.64
1:A:132:VAL:HG22	1:A:149:ILE:HD11	1.80	0.64
1:A:486:SER:HB2	1:A:614:SER:HA	1.80	0.63
1:A:73:MET:HB3	1:A:103:LEU:HD11	1.81	0.63
1:A:327:LYS:HB2	1:A:354:CYS:SG	2.39	0.63
1:B:143:LEU:CD2	1:B:148:GLU:HG2	2.28	0.63
1:B:334:LEU:HD22	1:B:335:VAL:C	2.19	0.63
1:A:527:GLN:HB3	1:A:540:CYS:CB	2.29	0.63
1:B:334:LEU:HD21	1:B:336:CYS:SG	2.39	0.63
1:A:123:MET:HG2	1:A:177:VAL:HG21	1.81	0.63
1:B:257:HIS:ND1	1:B:482:PRO:HB3	2.14	0.63
1:B:527:GLN:HB3	1:B:540:CYS:CB	2.29	0.63
1:A:105:TYR:O	1:A:108:LEU:HB2	1.98	0.62
1:B:105:TYR:O	1:B:108:LEU:HB2	1.99	0.62
1:B:113:TYR:CE2	1:B:117:LEU:HD11	2.34	0.62
1:B:73:MET:HB3	1:B:103:LEU:HD11	1.80	0.62
1:B:385:TYR:O	1:B:559:GLY:O	2.16	0.62
1:A:488:LYS:HB2	1:A:488:LYS:NZ	2.15	0.62
1:A:334:LEU:HD22	1:A:335:VAL:C	2.20	0.62
1:A:541:ASP:C	1:A:543:TYR:H	2.04	0.61
1:B:582:ILE:HG22	1:B:586:PHE:HE2	1.65	0.61
1:B:123:MET:HG2	1:B:177:VAL:HG21	1.82	0.61
1:B:178:ARG:HH11	1:B:178:ARG:HG2	1.65	0.61
1:B:509:VAL:HG13	4:B:1006:HOH:O	2.01	0.61
1:A:190:LYS:O	1:A:194:LEU:HD23	2.01	0.61
1:B:277:PHE:H	1:B:429:ASN:HD21	1.49	0.61
1:B:297:LEU:HG	1:B:301:GLN:NE2	2.16	0.61
1:A:277:PHE:H	1:A:429:ASN:HD21	1.48	0.60
1:A:115:GLU:O	1:A:119:THR:HG23	2.01	0.60
1:A:582:ILE:HG22	1:A:586:PHE:HE2	1.66	0.60
1:A:377:GLN:HE22	1:A:553:HIS:CD2	2.19	0.60
1:B:541:ASP:C	1:B:543:TYR:H	2.05	0.60
1:A:43:GLU:HA	1:A:65:ILE:HG21	1.84	0.60
1:A:257:HIS:ND1	1:A:482:PRO:HB3	2.17	0.59
1:B:254:ILE:N	4:B:947:HOH:O	2.34	0.59
1:B:285:VAL:HG13	1:B:416:LEU:HB3	1.82	0.59
1:B:72:PHE:HB3	4:B:980:HOH:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:LEU:HD21	1:A:336:CYS:SG	2.43	0.59
1:A:113:TYR:CE2	1:A:117:LEU:HD11	2.37	0.59
1:A:385:TYR:O	1:A:559:GLY:O	2.21	0.59
1:B:190:LYS:O	1:B:194:LEU:HD23	2.01	0.59
1:A:152:VAL:HG11	1:A:165:TYR:CD2	2.37	0.59
1:B:145:LEU:O	1:B:150:GLU:HB2	2.03	0.59
1:B:254:ILE:O	4:B:947:HOH:O	2.17	0.59
1:B:132:VAL:HG22	1:B:149:ILE:HD11	1.85	0.58
1:A:51:ARG:HD2	1:A:341:TRP:CH2	2.38	0.58
1:B:51:ARG:HD2	1:B:341:TRP:CH2	2.38	0.58
1:A:296:PRO:HB3	1:A:355:THR:OG1	2.04	0.58
1:B:115:GLU:O	1:B:119:THR:HG23	2.02	0.58
1:A:297:LEU:HG	1:A:301:GLN:NE2	2.17	0.58
1:A:362:LEU:O	1:A:366:HIS:HD2	1.86	0.58
1:B:362:LEU:O	1:B:366:HIS:HD2	1.87	0.58
1:A:285:VAL:HG13	1:A:416:LEU:HB3	1.84	0.58
1:B:296:PRO:HB3	1:B:355:THR:OG1	2.04	0.58
1:B:582:ILE:HG22	1:B:586:PHE:CE2	2.39	0.58
1:B:377:GLN:HE22	1:B:553:HIS:CD2	2.21	0.58
1:A:516:GLN:NE2	1:A:578:SER:H	2.02	0.57
1:A:178:ARG:HG2	1:A:178:ARG:HH11	1.68	0.57
1:B:43:GLU:HA	1:B:65:ILE:HG21	1.85	0.57
1:A:598:ILE:CD1	1:B:35:GLU:HG2	2.35	0.57
1:A:51:ARG:HD2	1:A:341:TRP:HH2	1.70	0.57
1:A:582:ILE:HG22	1:A:586:PHE:CE2	2.40	0.57
1:B:505:LEU:HG	4:B:1006:HOH:O	2.04	0.57
1:A:146:ASP:HB3	1:A:147:PRO:CD	2.35	0.56
1:B:51:ARG:HD2	1:B:341:TRP:HH2	1.70	0.56
1:B:95:ARG:HB2	4:B:810:HOH:O	2.05	0.56
1:A:145:LEU:O	1:A:150:GLU:HB2	2.04	0.56
1:B:274:VAL:HG13	1:B:274:VAL:O	2.05	0.56
1:A:33:ASN:ND2	1:A:384:VAL:H	2.03	0.56
1:A:452:ARG:NH2	1:A:504:TYR:HB2	2.21	0.56
1:B:162:LEU:HD12	4:B:924:HOH:O	2.04	0.56
1:B:449:ASP:HB2	4:B:919:HOH:O	2.04	0.56
1:B:607:ILE:HD12	1:B:608:THR:H	1.71	0.56
1:A:607:ILE:HD12	1:A:608:THR:H	1.71	0.56
1:B:146:ASP:HB3	1:B:147:PRO:CD	2.36	0.55
1:B:54:ILE:HG13	1:B:334:LEU:HA	1.87	0.55
1:A:143:LEU:CD2	1:A:148:GLU:HG2	2.31	0.55
1:B:527:GLN:HE21	1:B:540:CYS:HA	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:VAL:HG11	1:B:416:LEU:HB3	1.88	0.55
1:B:152:VAL:HG11	1:B:165:TYR:CD2	2.41	0.55
1:B:280:LYS:HG3	1:B:425:GLU:O	2.07	0.55
1:B:259:LEU:HB2	4:B:804:HOH:O	2.07	0.55
1:A:256:MET:O	1:A:257:HIS:CB	2.55	0.55
1:A:274:VAL:HG13	1:A:274:VAL:O	2.06	0.55
1:B:516:GLN:NE2	1:B:578:SER:H	2.04	0.55
1:A:47:ALA:O	1:A:51:ARG:HG3	2.06	0.54
1:B:256:MET:O	1:B:257:HIS:CB	2.54	0.54
1:A:255:PRO:HB2	1:A:258:LEU:CD1	2.37	0.54
1:B:180:GLN:HB3	4:B:932:HOH:O	2.07	0.54
1:A:285:VAL:H	1:A:359:GLN:NE2	2.06	0.54
1:B:346:ILE:HD11	4:B:890:HOH:O	2.06	0.54
1:B:97:PHE:O	1:B:101:THR:HG23	2.08	0.54
1:A:527:GLN:HE21	1:A:540:CYS:HA	1.72	0.54
1:B:527:GLN:HB3	1:B:540:CYS:HB3	1.88	0.54
1:A:527:GLN:HB3	1:A:540:CYS:HB3	1.88	0.54
1:A:285:VAL:HG11	1:A:416:LEU:HB3	1.88	0.54
1:B:285:VAL:H	1:B:359:GLN:NE2	2.06	0.54
1:A:280:LYS:HG3	1:A:425:GLU:O	2.08	0.54
1:B:26:LYS:HB3	4:B:838:HOH:O	2.08	0.54
1:B:254:ILE:CA	4:B:947:HOH:O	2.55	0.53
1:B:255:PRO:HB2	1:B:258:LEU:CD1	2.39	0.53
1:A:198:THR:HB	1:A:202:GLU:HG3	1.90	0.53
1:A:89:GLN:H	1:A:89:GLN:CD	2.08	0.53
1:A:347:ASP:N	1:A:379:GLN:HE22	1.99	0.53
1:B:452:ARG:NH2	1:B:504:TYR:HB2	2.24	0.53
1:A:418:LYS:HG2	1:A:419:ASP:N	2.24	0.53
1:B:423:ASP:HB2	1:B:426:ALA:CB	2.39	0.53
1:A:300:PHE:HE2	1:A:355:THR:HG21	1.74	0.52
1:B:33:ASN:ND2	1:B:384:VAL:H	2.06	0.52
1:B:34:LYS:HB2	1:B:34:LYS:NZ	2.23	0.52
1:B:264:ALA:HB2	4:B:804:HOH:O	2.07	0.52
1:B:418:LYS:HG2	1:B:419:ASP:N	2.23	0.52
1:A:423:ASP:HB2	1:A:426:ALA:CB	2.40	0.52
1:B:23:ILE:HG12	1:B:24:GLN:H	1.75	0.52
1:B:334:LEU:HD22	1:B:335:VAL:N	2.24	0.52
1:A:54:ILE:HG13	1:A:334:LEU:HA	1.90	0.52
1:A:76:VAL:O	1:A:80:THR:HG23	2.10	0.52
1:B:69:LEU:HD12	4:B:980:HOH:O	2.10	0.52
1:B:488:LYS:HZ3	1:B:615:SER:HB2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:GLN:HB3	1:B:540:CYS:HB2	1.91	0.52
1:B:198:THR:HB	1:B:202:GLU:HG3	1.92	0.52
1:B:614:SER:O	1:B:615:SER:HB3	2.08	0.52
1:A:346:ILE:O	1:A:347:ASP:HB2	2.09	0.52
1:A:34:LYS:HB2	1:A:34:LYS:NZ	2.25	0.52
1:B:291:LYS:HE2	4:B:1002:HOH:O	2.10	0.52
1:B:300:PHE:HE2	1:B:355:THR:HG21	1.74	0.52
1:A:520:SER:HB2	1:A:571:PHE:HE2	1.75	0.52
1:A:23:ILE:HG12	1:A:24:GLN:H	1.75	0.51
1:A:123:MET:HG2	1:A:177:VAL:CG2	2.40	0.51
1:B:76:VAL:O	1:B:80:THR:HG23	2.09	0.51
1:B:439:ILE:HD11	1:B:586:PHE:CD2	2.45	0.51
1:A:85:TRP:C	1:A:87:SER:H	2.13	0.51
1:B:47:ALA:O	1:B:51:ARG:HG3	2.10	0.51
1:A:390:ASN:OD1	1:A:392:GLY:N	2.43	0.51
1:B:283:VAL:HG23	1:B:283:VAL:O	2.10	0.51
1:B:346:ILE:O	1:B:347:ASP:HB2	2.10	0.51
1:B:532:ASN:HD22	1:B:535:LEU:HD12	1.75	0.51
1:A:527:GLN:HB3	1:A:540:CYS:HB2	1.92	0.51
1:B:327:LYS:CB	1:B:354:CYS:SG	2.98	0.51
1:A:444:PHE:HA	4:A:813:HOH:O	2.11	0.51
1:B:85:TRP:C	1:B:87:SER:H	2.13	0.51
1:A:439:ILE:HD11	1:A:586:PHE:CG	2.46	0.51
1:A:488:LYS:HZ2	1:A:488:LYS:CB	2.21	0.51
1:B:347:ASP:N	1:B:379:GLN:HE22	2.00	0.51
1:A:515:PHE:CD2	1:A:582:ILE:HG23	2.45	0.51
1:B:353:GLN:CG	1:B:355:THR:HG22	2.41	0.51
1:A:474:ASP:O	1:A:606:TRP:CH2	2.63	0.50
1:B:439:ILE:HD11	1:B:586:PHE:CG	2.46	0.50
1:B:474:ASP:O	1:B:606:TRP:CH2	2.64	0.50
1:B:535:LEU:N	1:B:536:PRO:CD	2.74	0.50
1:B:407:THR:HB	1:B:539:ASN:HD22	1.76	0.50
1:B:509:VAL:O	1:B:513:ILE:HG22	2.11	0.50
1:B:330:ASP:OD1	1:B:332:ARG:HD3	2.11	0.50
1:A:148:GLU:CD	1:A:148:GLU:H	2.15	0.50
1:A:535:LEU:N	1:A:536:PRO:CD	2.74	0.50
1:B:488:LYS:HZ2	1:B:488:LYS:CB	2.23	0.50
1:A:439:ILE:HD11	1:A:586:PHE:CD2	2.47	0.50
1:B:515:PHE:CD2	1:B:582:ILE:HG23	2.47	0.50
1:B:422:ARG:O	1:B:423:ASP:C	2.50	0.50
1:A:334:LEU:HD22	1:A:335:VAL:N	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:GLU:OE2	1:A:590:ARG:NH2	2.45	0.50
1:B:330:ASP:CG	1:B:332:ARG:HD3	2.31	0.50
1:A:327:LYS:CB	1:A:354:CYS:SG	3.00	0.50
1:B:587:GLU:OE2	1:B:590:ARG:NH2	2.45	0.50
1:B:277:PHE:CZ	1:B:425:GLU:HB3	2.47	0.49
1:A:330:ASP:CG	1:A:332:ARG:HD3	2.31	0.49
1:A:488:LYS:HZ3	1:A:615:SER:HB2	1.77	0.49
1:A:488:LYS:NZ	1:A:615:SER:HB2	2.27	0.49
1:B:146:ASP:HB3	1:B:147:PRO:HD3	1.95	0.49
1:B:251:THR:HG22	1:B:603:HIS:CG	2.47	0.49
1:A:159:HIS:CE1	1:A:160:GLU:HG2	2.48	0.49
1:A:180:GLN:N	1:A:180:GLN:OE1	2.46	0.49
1:B:123:MET:HG2	1:B:177:VAL:CG2	2.41	0.49
1:A:33:ASN:HD22	1:A:383:PHE:HB3	1.77	0.49
1:A:277:PHE:CZ	1:A:425:GLU:HB3	2.47	0.49
1:A:283:VAL:O	1:A:283:VAL:HG23	2.12	0.49
1:A:532:ASN:HD22	1:A:535:LEU:HD12	1.77	0.49
1:A:146:ASP:HB3	1:A:147:PRO:HD3	1.95	0.49
1:A:353:GLN:CG	1:A:355:THR:HG22	2.42	0.49
1:A:454:SER:O	1:A:457:ARG:O	2.30	0.49
1:A:492:ALA:O	1:A:498:ILE:HG13	2.13	0.49
1:B:251:THR:HG22	1:B:603:HIS:NE2	2.28	0.49
1:A:407:THR:HB	1:A:539:ASN:HD22	1.78	0.49
1:B:159:HIS:CE1	1:B:160:GLU:HG2	2.48	0.49
1:B:520:SER:HB2	1:B:571:PHE:HE2	1.78	0.49
1:A:97:PHE:O	1:A:101:THR:HG23	2.13	0.49
1:A:344:TYR:HA	1:A:386:ARG:NH2	2.27	0.49
1:B:462:LYS:HA	1:B:465:TRP:CD1	2.47	0.49
1:A:85:TRP:HA	1:A:88:TYR:CG	2.48	0.49
1:B:218:GLU:HG2	4:B:990:HOH:O	2.13	0.49
1:B:256:MET:O	1:B:257:HIS:HB3	2.12	0.49
1:B:390:ASN:OD1	1:B:392:GLY:N	2.42	0.49
1:B:454:SER:O	1:B:457:ARG:O	2.31	0.48
1:B:85:TRP:HA	1:B:88:TYR:CG	2.48	0.48
1:A:422:ARG:O	1:A:423:ASP:C	2.50	0.48
1:A:611:LYS:HB2	4:A:899:HOH:O	2.13	0.48
1:A:596:GLU:OE2	1:A:600:ASN:ND2	2.47	0.48
1:B:344:TYR:HA	1:B:386:ARG:NH2	2.28	0.48
1:B:225:ARG:HB3	1:B:226:PRO:HD3	1.96	0.48
1:B:612:CYS:O	1:B:612:CYS:SG	2.72	0.48
1:A:256:MET:O	1:A:257:HIS:HB3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ASP:OD1	1:A:332:ARG:HD3	2.13	0.47
1:A:392:GLY:HA3	1:A:509:VAL:CG2	2.44	0.47
1:B:148:GLU:CD	1:B:148:GLU:H	2.17	0.47
1:B:492:ALA:O	1:B:498:ILE:HG13	2.14	0.47
1:A:462:LYS:HA	1:A:465:TRP:CD1	2.49	0.47
1:B:182:GLU:O	1:B:186:GLU:HG3	2.14	0.47
1:A:116:LEU:O	1:A:120:LEU:HB2	2.14	0.47
1:A:276:PRO:HB3	1:A:592:TRP:CH2	2.48	0.47
1:B:423:ASP:HB2	1:B:426:ALA:HB3	1.96	0.47
1:A:294:TYR:CE1	1:A:416:LEU:HD11	2.49	0.47
1:A:614:SER:O	1:A:615:SER:HB3	2.15	0.47
1:B:89:GLN:H	1:B:89:GLN:CD	2.08	0.47
1:B:143:LEU:HD21	4:B:898:HOH:O	2.14	0.47
1:B:177:VAL:HG22	1:B:180:GLN:HB2	1.97	0.47
1:B:285:VAL:HG11	1:B:416:LEU:HD13	1.95	0.47
1:B:541:ASP:C	1:B:543:TYR:N	2.67	0.47
1:B:620:HIS:CG	1:B:620:HIS:OXT	2.68	0.47
1:B:180:GLN:OE1	1:B:180:GLN:N	2.48	0.47
1:B:276:PRO:HB3	1:B:592:TRP:CH2	2.50	0.47
1:B:315:LEU:HD21	1:B:369:LEU:HD11	1.97	0.47
1:B:442:LEU:HB2	1:B:443:PRO:CD	2.45	0.47
1:A:523:ILE:O	1:A:525:ALA:O	2.32	0.47
1:B:294:TYR:CE1	1:B:416:LEU:HD11	2.50	0.47
1:A:446:PHE:O	1:A:450:LYS:HG3	2.15	0.46
1:B:158:ASP:HB3	1:B:161:GLU:HB3	1.96	0.46
1:B:446:PHE:O	1:B:450:LYS:HG3	2.15	0.46
1:A:251:THR:HG22	1:A:603:HIS:CG	2.50	0.46
1:B:116:LEU:O	1:B:120:LEU:HB2	2.15	0.46
1:B:322:LYS:CB	1:B:350:ARG:HD3	2.41	0.46
1:A:225:ARG:HB3	1:A:226:PRO:HD3	1.98	0.46
1:A:285:VAL:HG12	1:A:285:VAL:O	2.16	0.46
1:B:523:ILE:O	1:B:525:ALA:O	2.34	0.46
1:B:596:GLU:OE2	1:B:600:ASN:ND2	2.49	0.46
1:A:137:ASP:OD1	1:A:139:THR:HB	2.15	0.46
1:B:309:SER:O	1:B:544:GLY:HA2	2.16	0.46
1:A:552:PHE:O	1:A:556:LEU:HG	2.16	0.46
1:A:177:VAL:HG22	1:A:180:GLN:HB2	1.98	0.45
1:A:541:ASP:C	1:A:543:TYR:N	2.67	0.45
1:B:72:PHE:HD2	4:B:980:HOH:O	1.99	0.45
1:B:91:GLU:HB2	4:B:810:HOH:O	2.15	0.45
1:B:541:ASP:O	1:B:541:ASP:OD2	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:442:LEU:HB2	1:A:443:PRO:CD	2.46	0.45
1:A:256:MET:O	1:A:257:HIS:CG	2.70	0.45
1:B:137:ASP:OD1	1:B:139:THR:HB	2.16	0.45
1:B:250:GLU:HA	1:B:250:GLU:OE1	2.17	0.45
1:A:158:ASP:HB3	1:A:161:GLU:HB3	1.98	0.45
1:A:250:GLU:OE1	1:A:250:GLU:HA	2.16	0.45
1:A:285:VAL:HG12	1:A:289:MET:HG3	1.99	0.45
1:A:620:HIS:CG	1:A:620:HIS:OXT	2.70	0.45
1:B:33:ASN:HD22	1:B:383:PHE:HB3	1.80	0.45
1:B:217:LEU:CD1	1:B:505:LEU:HD21	2.47	0.45
1:A:182:GLU:O	1:A:186:GLU:HG3	2.15	0.45
1:A:423:ASP:HB2	1:A:426:ALA:HB3	1.97	0.45
1:A:183:ARG:HD3	4:A:964:HOH:O	2.16	0.45
1:A:485:ARG:HD3	1:A:491:ASP:OD2	2.17	0.45
1:B:285:VAL:HG12	1:B:285:VAL:O	2.16	0.45
1:A:24:GLN:HB3	4:A:833:HOH:O	2.17	0.45
1:A:251:THR:HG22	1:A:603:HIS:NE2	2.32	0.45
1:A:285:VAL:HG11	1:A:416:LEU:HD13	1.97	0.45
1:B:285:VAL:HG12	1:B:289:MET:HG3	1.99	0.45
1:A:382:PRO:O	1:A:383:PHE:C	2.55	0.45
1:B:552:PHE:O	1:B:556:LEU:HG	2.17	0.45
1:A:315:LEU:HD21	1:A:369:LEU:HD11	1.98	0.45
1:A:450:LYS:HE2	1:A:476:TYR:CZ	2.52	0.45
1:A:541:ASP:O	1:A:541:ASP:OD2	2.35	0.45
1:B:487:GLU:HB2	4:B:814:HOH:O	2.17	0.45
1:A:94:LYS:CB	1:A:94:LYS:NZ	2.80	0.45
1:A:495:LYS:O	1:A:496:TYR:C	2.55	0.45
1:A:61:LYS:O	1:A:65:ILE:HG12	2.17	0.44
1:A:137:ASP:C	1:A:139:THR:H	2.19	0.44
1:A:410:HIS:HB2	1:A:541:ASP:CG	2.37	0.44
1:A:25:ALA:O	1:A:28:TYR:HB3	2.17	0.44
1:A:404:SER:OG	1:A:541:ASP:O	2.34	0.44
1:A:292:GLN:O	1:A:293:ALA:HB3	2.16	0.44
1:B:171:ASP:OD1	1:B:485:ARG:NH2	2.35	0.44
1:B:251:THR:HG22	1:B:603:HIS:CE1	2.52	0.44
1:A:27:GLU:HB2	4:A:833:HOH:O	2.17	0.44
1:A:178:ARG:HD2	4:A:844:HOH:O	2.16	0.44
1:A:357:VAL:HG23	1:A:357:VAL:O	2.18	0.44
1:A:478:GLY:O	1:A:479:ILE:HD12	2.18	0.44
1:A:276:PRO:HD2	1:A:429:ASN:ND2	2.32	0.44
1:B:256:MET:O	1:B:257:HIS:CG	2.69	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:GLN:HE22	1:A:578:SER:H	1.64	0.44
1:B:137:ASP:C	1:B:139:THR:H	2.21	0.44
1:B:274:VAL:O	1:B:274:VAL:CG1	2.65	0.43
1:B:327:LYS:HG3	1:B:354:CYS:SG	2.58	0.43
1:A:195:ASN:O	1:A:196:ASN:HB2	2.18	0.43
1:B:613:VAL:CG2	1:B:614:SER:N	2.72	0.43
1:A:217:LEU:CD1	1:A:505:LEU:HD21	2.49	0.43
1:B:410:HIS:HB2	1:B:541:ASP:CG	2.39	0.43
1:B:25:ALA:O	1:B:28:TYR:HB3	2.17	0.43
1:B:353:GLN:HG2	1:B:355:THR:HG22	2.00	0.43
1:A:64:GLU:HB2	4:A:860:HOH:O	2.17	0.43
1:A:143:LEU:HD22	1:A:148:GLU:CG	2.41	0.43
1:A:421:VAL:HG22	4:A:944:HOH:O	2.18	0.43
1:B:257:HIS:CE1	1:B:482:PRO:HB3	2.53	0.43
1:B:292:GLN:O	1:B:293:ALA:HB3	2.19	0.43
1:B:495:LYS:O	1:B:496:TYR:C	2.57	0.43
1:B:227:LEU:C	1:B:227:LEU:CD2	2.87	0.43
1:B:377:GLN:HG3	1:B:556:LEU:HD12	2.00	0.43
1:B:381:GLN:HE21	1:B:382:PRO:HD2	1.83	0.43
1:A:164:TYR:CZ	1:A:168:GLU:HG3	2.54	0.43
1:B:61:LYS:O	1:B:65:ILE:HG12	2.19	0.43
1:B:357:VAL:HG23	1:B:357:VAL:O	2.18	0.43
1:A:506:ARG:O	1:A:509:VAL:CG2	2.67	0.43
1:A:23:ILE:HG12	1:A:24:GLN:N	2.33	0.43
1:B:327:LYS:CG	1:B:354:CYS:SG	3.07	0.43
1:A:227:LEU:C	1:A:227:LEU:CD2	2.88	0.42
1:A:229:GLN:HG2	4:A:831:HOH:O	2.19	0.42
1:A:334:LEU:N	1:A:334:LEU:CD1	2.82	0.42
1:B:227:LEU:HD23	1:B:227:LEU:C	2.40	0.42
1:A:471:LYS:O	1:A:475:GLU:HG3	2.19	0.42
1:B:147:PRO:HG2	1:B:148:GLU:H	1.85	0.42
1:B:227:LEU:O	1:B:227:LEU:CD2	2.65	0.42
1:B:488:LYS:NZ	1:B:615:SER:HB2	2.34	0.42
1:B:505:LEU:HD12	4:B:919:HOH:O	2.19	0.42
1:A:274:VAL:O	1:A:274:VAL:CG1	2.66	0.42
1:A:353:GLN:HG2	1:A:355:THR:HG22	2.01	0.42
1:A:509:VAL:O	1:A:513:ILE:HG22	2.19	0.42
1:B:382:PRO:O	1:B:383:PHE:C	2.56	0.42
1:B:528:TYR:OH	1:B:584:GLU:OE1	2.34	0.42
1:A:208:TYR:CE1	1:A:391:PRO:HD2	2.54	0.42
1:A:289:MET:O	1:A:294:TYR:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:PRO:HD2	1:B:429:ASN:ND2	2.33	0.42
1:B:478:GLY:O	1:B:479:ILE:HD12	2.19	0.42
1:A:309:SER:O	1:A:544:GLY:HA2	2.19	0.42
1:B:23:ILE:HG12	1:B:24:GLN:N	2.33	0.42
1:B:195:ASN:O	1:B:196:ASN:HB2	2.19	0.42
1:A:466:ASN:ND2	1:A:491:ASP:H	2.17	0.42
1:B:178:ARG:HH11	1:B:178:ARG:CG	2.31	0.42
1:B:450:LYS:HE2	1:B:476:TYR:CZ	2.55	0.42
1:A:612:CYS:O	1:A:612:CYS:SG	2.75	0.42
1:B:27:GLU:HG3	4:B:838:HOH:O	2.19	0.42
1:B:254:ILE:CB	4:B:947:HOH:O	2.57	0.42
1:B:605:GLY:C	1:B:606:TRP:CD1	2.93	0.42
1:B:157:ARG:NH1	1:B:272:ASP:OD2	2.52	0.42
1:A:327:LYS:CG	1:A:354:CYS:SG	3.08	0.41
1:A:381:GLN:HE21	1:A:382:PRO:HD2	1.85	0.41
1:B:294:TYR:O	1:B:357:VAL:HG11	2.20	0.41
1:B:297:LEU:HG	1:B:301:GLN:HE21	1.85	0.41
1:A:227:LEU:HD23	1:A:227:LEU:C	2.40	0.41
1:A:327:LYS:HG3	1:A:354:CYS:SG	2.59	0.41
1:B:416:LEU:HD23	1:B:416:LEU:HA	1.89	0.41
1:B:508:LEU:HD12	1:B:508:LEU:O	2.20	0.41
1:A:285:VAL:HG21	1:A:411:LEU:HD13	2.02	0.41
1:A:410:HIS:HD2	1:A:541:ASP:OD1	2.03	0.41
1:B:94:LYS:NZ	1:B:94:LYS:CB	2.84	0.41
1:B:285:VAL:HG21	1:B:411:LEU:HD13	2.02	0.41
1:B:342:ASP:HB2	1:B:375:PHE:CE1	2.55	0.41
1:A:94:LYS:HZ3	1:A:94:LYS:HB3	1.85	0.41
1:A:257:HIS:CE1	1:A:482:PRO:HB3	2.55	0.41
1:A:613:VAL:HG23	1:A:615:SER:H	1.85	0.41
1:B:24:GLN:HB3	4:B:838:HOH:O	2.20	0.41
1:B:147:PRO:HG2	1:B:148:GLU:OE1	2.20	0.41
1:B:232:HIS:CE1	1:B:606:TRP:CD1	3.08	0.41
1:A:377:GLN:HE22	1:A:553:HIS:HD2	1.67	0.41
1:A:377:GLN:HG3	1:A:556:LEU:HD12	2.02	0.41
1:B:485:ARG:HD3	1:B:491:ASP:OD2	2.21	0.41
1:B:506:ARG:O	1:B:509:VAL:CG2	2.68	0.41
1:B:509:VAL:HB	1:B:577:MET:HE1	2.03	0.41
1:B:613:VAL:HG23	1:B:615:SER:H	1.86	0.41
1:A:420:TYR:HA	4:A:944:HOH:O	2.20	0.41
1:B:142:ASP:C	1:B:142:ASP:OD1	2.59	0.41
1:B:240:ARG:HA	1:B:248:VAL:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LYS:HB2	1:A:38:LYS:HE2	1.90	0.41
1:B:165:TYR:C	4:B:979:HOH:O	2.59	0.41
1:B:404:SER:OG	1:B:541:ASP:O	2.39	0.41
1:B:423:ASP:HB2	1:B:426:ALA:HB2	2.03	0.41
1:A:96:GLN:HE21	1:A:96:GLN:HB3	1.66	0.40
1:A:611:LYS:HD3	1:A:611:LYS:HA	1.89	0.40
1:A:142:ASP:OD1	1:A:142:ASP:C	2.60	0.40
1:A:251:THR:HG22	1:A:603:HIS:CE1	2.57	0.40
1:A:423:ASP:HB2	1:A:426:ALA:HB2	2.03	0.40
1:A:605:GLY:C	1:A:606:TRP:CD1	2.95	0.40
1:A:84:GLN:O	1:A:84:GLN:HG3	2.22	0.40
1:A:334:LEU:HD22	1:A:334:LEU:C	2.42	0.40
1:A:338:ALA:HB2	1:A:353:GLN:HG3	2.03	0.40
1:A:389:ALA:O	1:A:390:ASN:CB	2.57	0.40
1:B:113:TYR:O	1:B:117:LEU:HG	2.21	0.40
1:B:275:SER:HA	1:B:276:PRO:HD3	1.87	0.40
1:B:390:ASN:HA	1:B:391:PRO:HD3	1.95	0.40
1:B:334:LEU:N	1:B:334:LEU:CD1	2.84	0.40
1:B:392:GLY:HA3	1:B:509:VAL:CG2	2.52	0.40
1:A:232:HIS:CE1	1:A:606:TRP:CD1	3.09	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	596/607 (98%)	541 (91%)	39 (6%)	16 (3%)	5 5
1	B	596/607 (98%)	537 (90%)	42 (7%)	17 (3%)	4 4
All	All	1192/1214 (98%)	1078 (90%)	81 (7%)	33 (3%)	5 4

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	92	ASP
1	A	147	PRO
1	A	423	ASP
1	A	424	ASP
1	A	542	ILE
1	B	92	ASP
1	B	147	PRO
1	B	423	ASP
1	B	424	ASP
1	B	542	ILE
1	A	257	HIS
1	A	559	GLY
1	B	257	HIS
1	B	559	GLY
1	A	86	ARG
1	A	148	GLU
1	A	283	VAL
1	A	426	ALA
1	B	86	ARG
1	B	148	GLU
1	B	283	VAL
1	B	426	ALA
1	A	538	ASP
1	B	90	SER
1	B	390	ASN
1	B	538	ASP
1	A	90	SER
1	A	390	ASN
1	A	613	VAL
1	B	613	VAL
1	B	422	ARG
1	B	397	VAL
1	A	397	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	522/530 (98%)	490 (94%)	32 (6%)	18	30
1	B	522/530 (98%)	488 (94%)	34 (6%)	17	27
All	All	1044/1060 (98%)	978 (94%)	66 (6%)	18	28

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	GLN
1	A	100	LEU
1	A	103	LEU
1	A	108	LEU
1	A	119	THR
1	A	120	LEU
1	A	227	LEU
1	A	311	ASN
1	A	315	LEU
1	A	334	LEU
1	A	336	CYS
1	A	355	THR
1	A	374	TYR
1	A	378	TYR
1	A	404	SER
1	A	418	LYS
1	A	422	ARG
1	A	433	LEU
1	A	446	PHE
1	A	461	ASP
1	A	462	LYS
1	A	472	LEU
1	A	485	ARG
1	A	488	LYS
1	A	503	GLU
1	A	531	ASP
1	A	537	LEU
1	A	539	ASN
1	A	582	ILE
1	A	601	ASN
1	A	606	TRP
1	A	612	CYS
1	B	89	GLN
1	B	100	LEU
1	B	103	LEU

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Mol	Chain	Res	Type
1	B	108	LEU
1	B	119	THR
1	B	120	LEU
1	B	227	LEU
1	B	274	VAL
1	B	311	ASN
1	B	315	LEU
1	B	334	LEU
1	B	336	CYS
1	B	355	THR
1	B	362	LEU
1	B	374	TYR
1	B	378	TYR
1	B	404	SER
1	B	418	LYS
1	B	422	ARG
1	B	433	LEU
1	B	446	PHE
1	B	461	ASP
1	B	462	LYS
1	B	472	LEU
1	B	485	ARG
1	B	488	LYS
1	B	503	GLU
1	B	531	ASP
1	B	537	LEU
1	B	539	ASN
1	B	582	ILE
1	B	601	ASN
1	B	606	TRP
1	B	612	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	31	ASN
1	A	33	ASN
1	A	41	ASN
1	A	89	GLN
1	A	96	GLN
1	A	266	GLN

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Mol	Chain	Res	Type
1	A	301	GLN
1	A	317	GLN
1	A	359	GLN
1	A	366	HIS
1	A	373	GLN
1	A	377	GLN
1	A	379	GLN
1	A	380	HIS
1	A	381	GLN
1	A	410	HIS
1	A	429	ASN
1	A	466	ASN
1	A	514	GLN
1	A	516	GLN
1	A	527	GLN
1	A	532	ASN
1	A	539	ASN
1	A	600	ASN
1	A	601	ASN
1	A	610	ASN
1	B	24	GLN
1	B	33	ASN
1	B	41	ASN
1	B	84	GLN
1	B	89	GLN
1	B	96	GLN
1	B	301	GLN
1	B	311	ASN
1	B	359	GLN
1	B	366	HIS
1	B	373	GLN
1	B	377	GLN
1	B	379	GLN
1	B	380	HIS
1	B	381	GLN
1	B	410	HIS
1	B	429	ASN
1	B	466	ASN
1	B	514	GLN
1	B	516	GLN
1	B	527	GLN
1	B	532	ASN

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Mol	Chain	Res	Type
1	B	539	ASN
1	B	553	HIS
1	B	601	ASN
1	B	610	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	LPR	A	801	2	30,30,30	1.62	6 (20%)	38,39,39	1.07	3 (7%)
3	LPR	B	802	2	30,30,30	1.64	10 (33%)	38,39,39	1.08	3 (7%)

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	LPR	A	801	2	-	6/30/40/40	0/2/2/2
3	LPR	B	802	2	-	6/30/40/40	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	802	LPR	C7-C6	-3.59	1.36	1.51
3	A	801	LPR	C7-C6	-3.56	1.37	1.51
3	A	801	LPR	O1-C1	2.95	1.27	1.22
3	B	802	LPR	O1-C1	2.71	1.27	1.22
3	B	802	LPR	C17-C16	2.54	1.44	1.38
3	B	802	LPR	C4-N1	2.34	1.53	1.47
3	A	801	LPR	C4-N1	2.34	1.53	1.47
3	B	802	LPR	C5-N2	2.28	1.51	1.47
3	B	802	LPR	C21-C16	2.27	1.43	1.38
3	A	801	LPR	C17-C16	2.26	1.43	1.38
3	A	801	LPR	C5-N2	2.18	1.51	1.47
3	B	802	LPR	C20-C21	2.07	1.43	1.38
3	A	801	LPR	C20-C19	2.07	1.43	1.38
3	B	802	LPR	C20-C19	2.04	1.43	1.38
3	B	802	LPR	C18-C17	2.04	1.43	1.38
3	B	802	LPR	C19-C18	2.00	1.43	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	801	LPR	C2-N1-C4	3.27	122.43	115.52
3	B	802	LPR	C2-N1-C4	3.22	122.35	115.52
3	B	802	LPR	C6-C7-C8	3.11	113.81	104.98
3	A	801	LPR	C6-C7-C8	2.99	113.46	104.98
3	A	801	LPR	C7-C6-C5	2.55	109.52	104.18
3	B	802	LPR	C7-C6-C5	2.52	109.46	104.18

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	LPR	C2-C10-C11-C12
3	B	802	LPR	C2-C10-C11-C12
3	A	801	LPR	O2-C3-C4-N1
3	B	802	LPR	O2-C3-C4-N1
3	B	802	LPR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
3	A	801	LPR	C10-C11-C12-C13
3	B	802	LPR	O3-C3-C4-N1
3	A	801	LPR	C14-C15-C16-C17
3	A	801	LPR	C14-C15-C16-C21
3	B	802	LPR	C14-C15-C16-C17
3	B	802	LPR	C14-C15-C16-C21
3	A	801	LPR	O3-C3-C4-N1

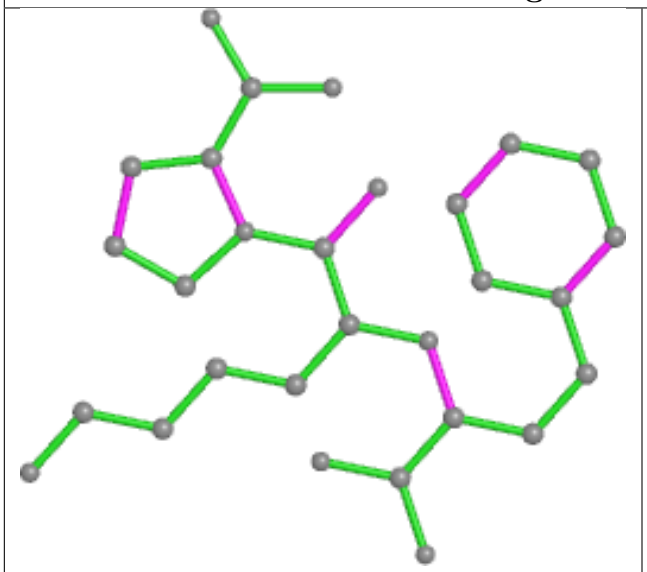
There are no ring outliers.

2 monomers are involved in 2 short contacts:

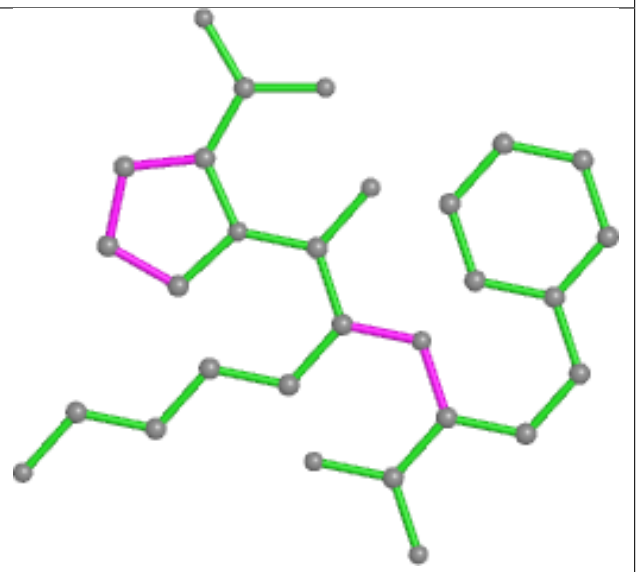
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	LPR	1	0
3	B	802	LPR	1	0

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

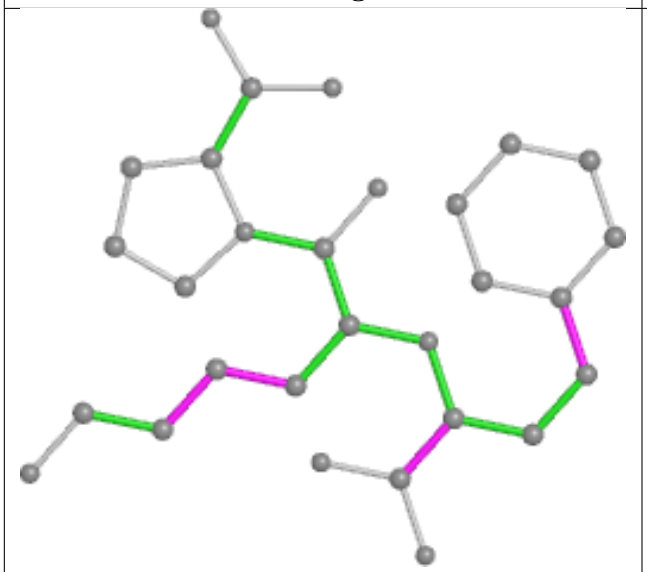
Ligand LPR A 801



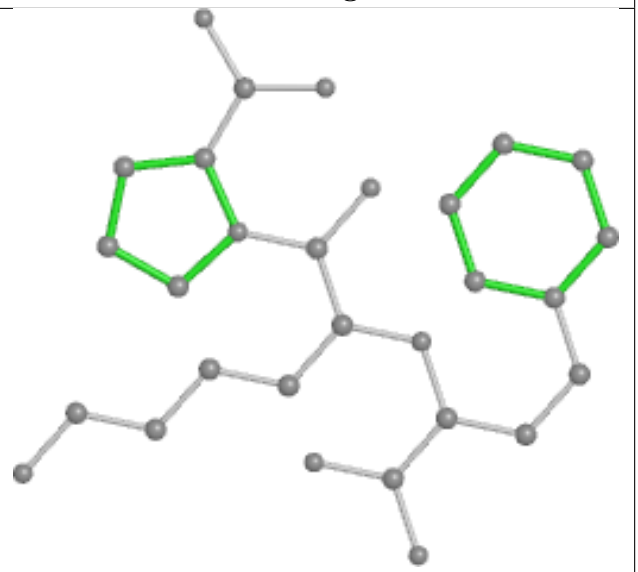
Bond lengths



Bond angles

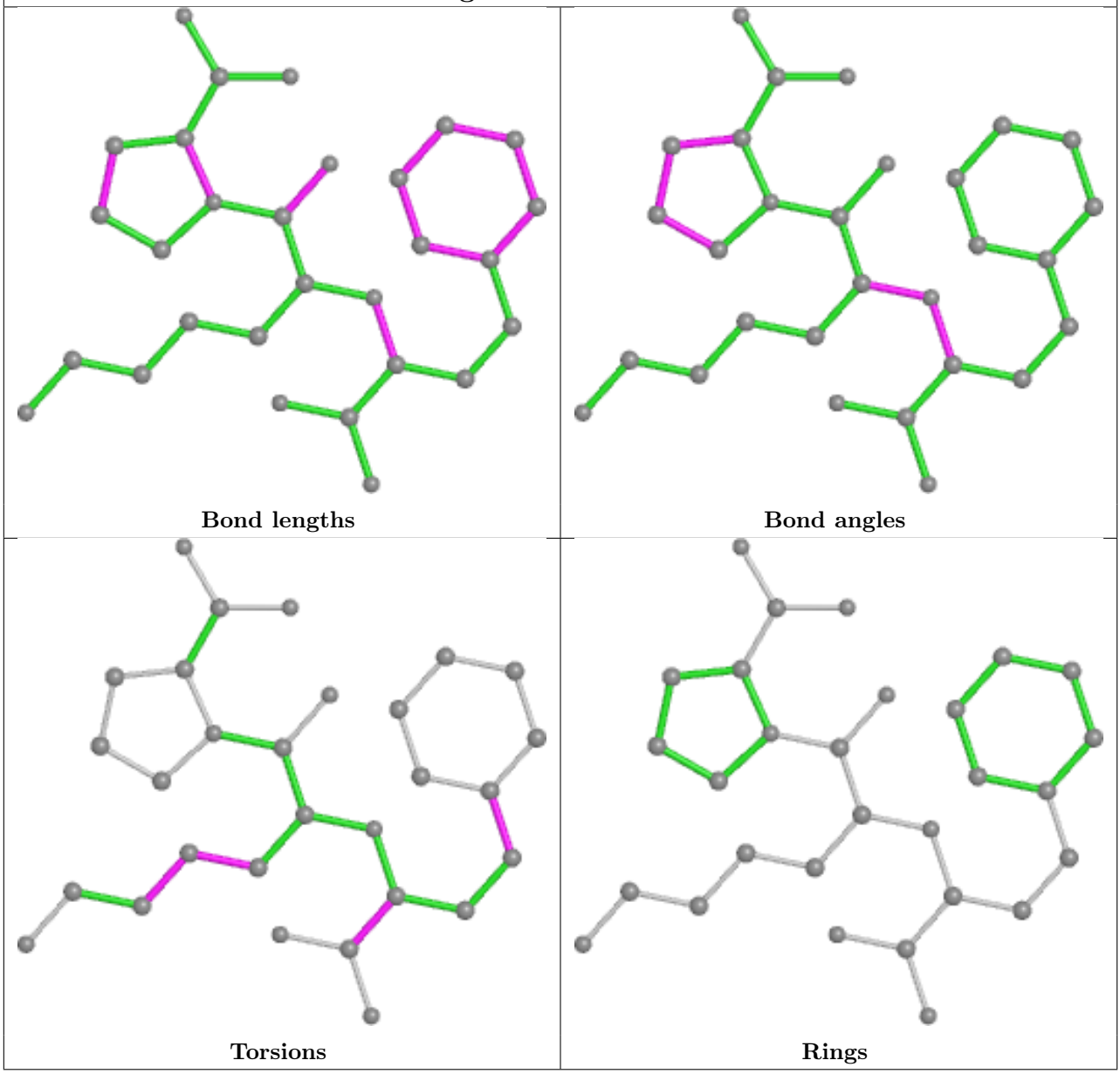


Torsions



Rings

Ligand LPR B 802



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.