WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jun 27, 2023 – 07:17 pm BST

PDB ID	:	8A3F
Title	:	Proline Racemase (ProR) from the Gram-positive bacterium Acetoanaerobium sticklandii from isotropic tetragonal data at 3.15 A
Authors	:	Najmudin, S.; Pan, X.-S.; McAuley, K.E.; Fisher, L.M.; Sanderson, M.R.
Deposited on	:	2022-06-08
Resolution	:	3.15 Å(reported)

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

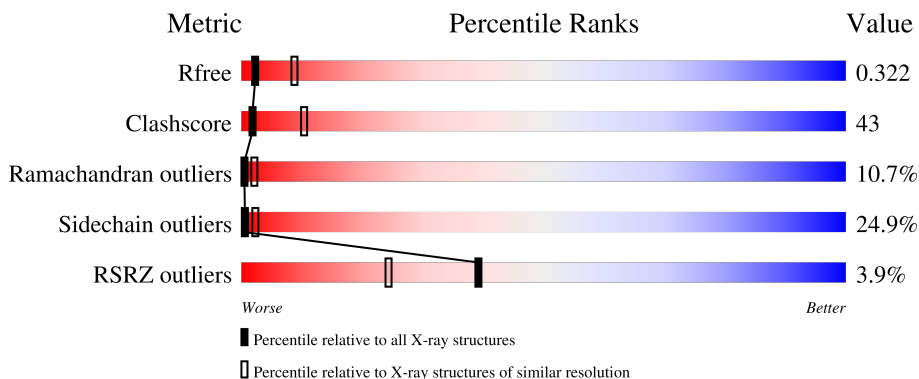|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.33
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.33

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 3.15 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	Percentile Ranks	Value
Rfree		0.322
Clashscore		43
Ramachandran outliers		10.7%
Sidechain outliers		24.9%
RSRZ outliers		3.9%

Worse   *Better*

▌ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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% 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	AAA	343	% 41% 41% 14% • •
1	BBB	343	7% 34% 41% 18% 6% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PYC	BBB	401	-	-	X	-

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 10400 atoms, of which 5214 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 Proline racemase A (AsProR).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	335	Total	C	H	N	O	S	71	0	0
			5188	1649	2603	421	500	15			
1	BBB	335	Total	C	H	N	O	S	71	0	0
			5188	1649	2603	421	500	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	336	LEU	-	expression tag	UNP E3PTZ4
AAA	337	GLU	-	expression tag	UNP E3PTZ4
AAA	338	HIS	-	expression tag	UNP E3PTZ4
AAA	339	HIS	-	expression tag	UNP E3PTZ4
AAA	340	HIS	-	expression tag	UNP E3PTZ4
AAA	341	HIS	-	expression tag	UNP E3PTZ4
AAA	342	HIS	-	expression tag	UNP E3PTZ4
AAA	343	HIS	-	expression tag	UNP E3PTZ4
BBB	336	LEU	-	expression tag	UNP E3PTZ4
BBB	337	GLU	-	expression tag	UNP E3PTZ4
BBB	338	HIS	-	expression tag	UNP E3PTZ4
BBB	339	HIS	-	expression tag	UNP E3PTZ4
BBB	340	HIS	-	expression tag	UNP E3PTZ4
BBB	341	HIS	-	expression tag	UNP E3PTZ4
BBB	342	HIS	-	expression tag	UNP E3PTZ4
BBB	343	HIS	-	expression tag	UNP E3PTZ4

- Molecule 2 is PYRROLE-2-CARBOXYLATE (three-letter code: PYC) (formula: $C_5H_4NO_2$) (labeled as "Ligand of Interest" by depositor).

PYC

N6

C5

C2

C1

O8

O⁻

H
N

C4

C3

O7

O
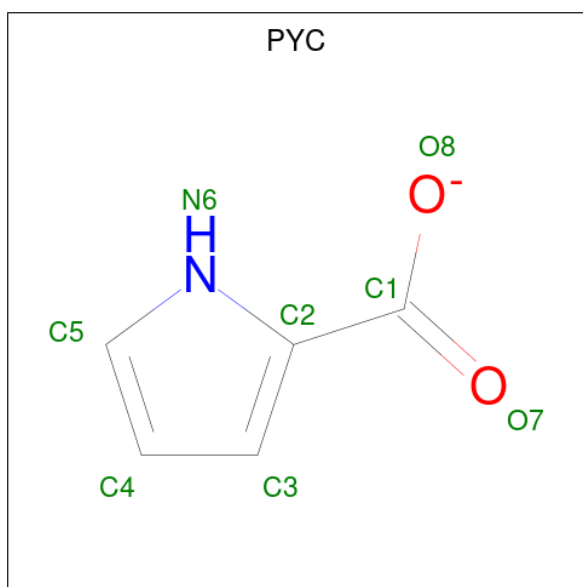
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	H	N	O	0	0
			12	5	4	1	2		
2	BBB	1	Total	C	H	N	O	0	0
			12	5	4	1	2		

3 Residue-property plots ⓘ

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 o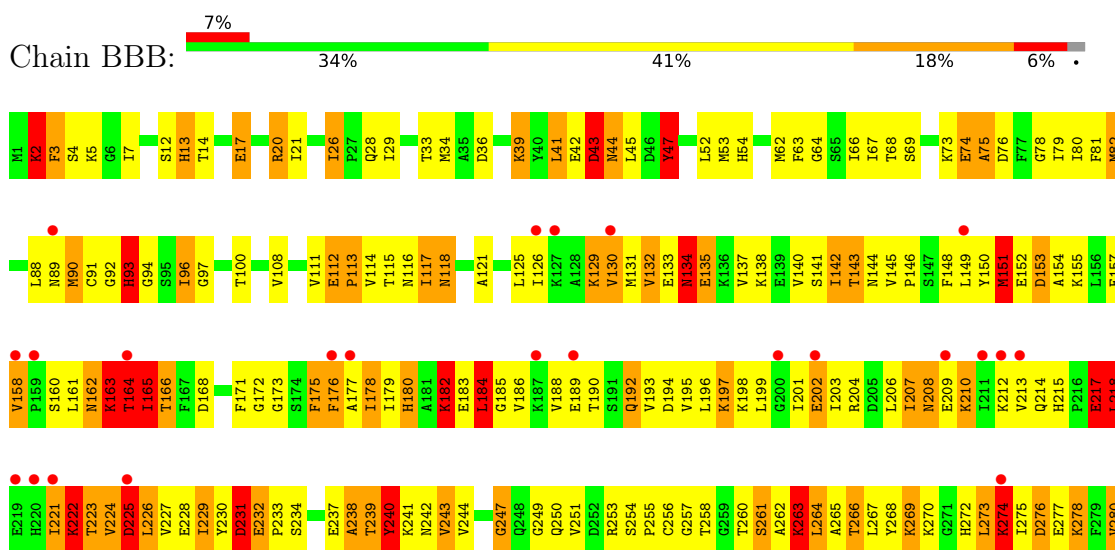utlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 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: Proline racemase A (AsProR)

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Y281 E282 S283 I284 T285 M288 F289 K290 G291 R292 V293 L294 T297 K298 V299 G300 E301 F302 D303 A304 I305 I306 P307 T310 A313 F321 V322 I323 D324 P325 E326 D327 P328 L329 K330 Y331 G332 F333 T334 V335 LEU GLU HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	109.72Å　　109.72Å　　104.99Å 90.00°　　　90.00°　　　90.00°	Depositor
Resolution (Å)	77.71　–　3.15 77.59　–　3.15	Depositor EDS
% Data completeness (in resolution range)	100.0 (77.71-3.15) 100.0 (77.59-3.15)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.68 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.266　,　0.330 0.265　,　0.322	Depositor DCC
R_{free} test set	690 reflections (5.96%)	wwPDB-VP
Wilson B-factor (Å^2)	101.1	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 90.9	EDS
L-test for twinning[2]	$< |L| > = 0.44, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.048 for -h,-l,-k 0.029 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10400	wwPDB-VP
Average B, all atoms (Å^2)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.20% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

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

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	AAA	0.66	0/2634	0.85	0/3556
1	BBB	0.67	0/2634	0.96	3/3556 (0.1%)
All	All	0.67	0/5268	0.91	3/7112 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	AAA	0	8
1	BBB	0	9
All	All	0	17

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BBB	164	THR	CB-CA-C	-21.61	53.25	111.60
1	BBB	164	THR	N-CA-C	10.09	138.25	111.00
1	BBB	164	THR	N-CA-CB	-9.68	91.90	110.30

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	121	ALA	Peptide
1	AAA	208	ASN	Peptide
1	AAA	209	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	AAA	272	HIS	Peptide
1	AAA	273	LEU	Peptide
1	AAA	29	ILE	Peptide
1	AAA	47	TYR	Peptide
1	AAA	60	ASN	Peptide
1	BBB	163	LYS	Peptide
1	BBB	184	LEU	Peptide
1	BBB	2	LYS	Peptide
1	BBB	223	THR	Peptide
1	BBB	224	VAL	Peptide
1	BBB	225	ASP	Peptide
1	BBB	238	ALA	Peptide
1	BBB	278	LYS	Peptide
1	BBB	47	TYR	Peptide

5.2 Too-close contacts ⓘ

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	AAA	2585	2603	2593	166	1
1	BBB	2585	2603	2592	276	2
2	AAA	8	4	4	2	0
2	BBB	8	4	4	4	0
All	All	5186	5214	5193	442	2

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 43.

All (442) 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:BBB:155:LYS:HE3	1:BBB:164:THR:HG22	1.28	1.15
1:BBB:273:LEU:HD21	1:BBB:277:GLU:HB3	1.43	1.00
1:AAA:5:LYS:HB2	1:AAA:323:ILE:HD11	1.41	0.99
1:BBB:229:ILE:O	1:BBB:242:ASN:HB2	1.63	0.97
1:BBB:178:ILE:HG12	1:BBB:230:TYR:HE1	1.33	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:178:ILE:HG12	1:BBB:230:TYR:CE1	2.04	0.92
1:BBB:114:VAL:HG12	1:BBB:131:MET:HA	1.53	0.88
1:BBB:238:ALA:HA	1:BBB:280:VAL:HG22	1.57	0.86
1:AAA:199:LEU:O	1:AAA:203:ILE:HD12	1.75	0.86
1:BBB:2:LYS:HE3	1:BBB:3:PHE:CD1	2.12	0.84
1:AAA:184:LEU:HD23	1:AAA:199:LEU:HD11	1.61	0.83
1:AAA:34:MET:HG2	1:AAA:120:GLU:O	1.79	0.82
1:AAA:203:ILE:HA	1:AAA:206:LEU:HD22	1.61	0.82
1:BBB:193:VAL:HG12	1:BBB:196:LEU:HD22	1.63	0.78
1:BBB:228:GLU:OE2	1:BBB:263:LYS:NZ	2.17	0.78
1:AAA:184:LEU:HD13	1:AAA:185:GLY:N	2.00	0.77
1:BBB:240:TYR:HE2	1:BBB:281:TYR:HA	1.50	0.77
1:BBB:273:LEU:CD2	1:BBB:277:GLU:HB3	2.15	0.77
1:BBB:155:LYS:CE	1:BBB:164:THR:HG22	2.12	0.76
1:BBB:240:TYR:OH	1:BBB:281:TYR:CD1	2.38	0.76
1:AAA:192:GLN:O	1:AAA:196:LEU:HD12	1.87	0.75
1:AAA:170:SER:OG	1:AAA:266:THR:HG22	1.88	0.74
1:BBB:2:LYS:NZ	1:BBB:3:PHE:HA	2.03	0.74
1:BBB:130:VAL:HG13	1:BBB:140:VAL:CG2	2.17	0.74
1:AAA:169:ILE:HG12	1:AAA:176:PHE:O	1.88	0.73
1:BBB:243:VAL:HG11	1:BBB:284:ILE:HG13	1.70	0.73
1:BBB:29:ILE:HG12	1:BBB:41:LEU:HD21	1.70	0.73
1:BBB:155:LYS:HE3	1:BBB:164:THR:CG2	2.15	0.73
1:AAA:208:ASN:O	1:AAA:209:GLU:HG3	1.88	0.73
1:AAA:41:LEU:HD23	1:AAA:87:TYR:CE1	2.23	0.72
1:AAA:21:ILE:HG23	1:AAA:67:ILE:HD13	1.73	0.71
1:AAA:181:ALA:HA	1:AAA:184:LEU:HD11	1.72	0.71
1:AAA:206:LEU:HD23	1:AAA:206:LEU:C	2.11	0.71
1:AAA:306:ILE:HG23	1:AAA:306:ILE:O	1.90	0.71
1:BBB:81:PHE:CD1	1:BBB:91:CYS:SG	2.83	0.71
1:AAA:260:THR:HG22	1:AAA:281:TYR:CD2	2.26	0.70
1:AAA:121:ALA:HB3	1:AAA:122:PRO:C	2.11	0.70
1:AAA:253:ARG:O	1:AAA:285:THR:HG22	1.91	0.70
1:BBB:115:THR:O	1:BBB:130:VAL:HG23	1.90	0.70
1:AAA:207:ILE:O	1:AAA:210:LYS:HB3	1.92	0.70
1:BBB:91:CYS:SG	1:BBB:91:CYS:O	2.49	0.70
1:AAA:14:THR:OG1	1:AAA:93:HIS:HB2	1.92	0.70
1:AAA:48:VAL:O	1:AAA:52:LEU:HD23	1.93	0.69
1:AAA:199:LEU:HD23	1:AAA:200:GLY:N	2.08	0.69
1:BBB:215:HIS:NE2	1:BBB:218:LEU:HB2	2.07	0.69
1:BBB:265:ALA:O	1:BBB:266:THR:HG23	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:215:HIS:HE2	1:BBB:218:LEU:HB2	1.58	0.69
1:BBB:264:LEU:HD11	1:BBB:307:PRO:HG3	1.75	0.69
1:AAA:184:LEU:CD2	1:AAA:186:VAL:HG13	2.23	0.68
1:BBB:2:LYS:HZ2	1:BBB:3:PHE:HA	1.57	0.68
1:BBB:264:LEU:HD11	1:BBB:307:PRO:CG	2.22	0.68
1:BBB:264:LEU:HD23	1:BBB:265:ALA:N	2.09	0.68
1:BBB:2:LYS:HZ2	1:BBB:3:PHE:HD1	1.42	0.68
1:AAA:91:CYS:SG	1:AAA:93:HIS:CE1	2.88	0.67
1:BBB:93:HIS:ND1	1:BBB:93:HIS:C	2.46	0.67
1:BBB:53:MET:HE2	1:BBB:82:MET:SD	2.35	0.67
1:BBB:164:THR:OG1	1:BBB:165:ILE:CG2	2.43	0.67
1:BBB:239:THR:O	1:BBB:240:TYR:O	2.13	0.67
1:BBB:100:THR:HG23	1:BBB:137:VAL:HG11	1.77	0.67
1:BBB:204:ARG:HD2	1:BBB:225:ASP:HA	1.77	0.66
1:BBB:268:TYR:O	1:BBB:269:LYS:NZ	2.26	0.66
1:BBB:243:VAL:CG1	1:BBB:284:ILE:HG13	2.26	0.66
1:BBB:130:VAL:HG13	1:BBB:140:VAL:HG23	1.78	0.66
1:BBB:260:THR:HG22	1:BBB:281:TYR:CD1	2.30	0.66
1:AAA:233:PRO:HA	1:AAA:241:LYS:HG2	1.78	0.66
1:BBB:79:ILE:HD13	1:BBB:81:PHE:CE1	2.31	0.66
1:BBB:2:LYS:HD2	1:BBB:3:PHE:N	2.11	0.65
1:BBB:184:LEU:HD13	1:BBB:185:GLY:H	1.61	0.65
1:BBB:240:TYR:CE2	1:BBB:281:TYR:HA	2.31	0.65
1:AAA:217:GLU:HB2	1:AAA:218:LEU:HD22	1.76	0.65
1:BBB:176:PHE:CZ	1:BBB:263:LYS:HG2	2.30	0.65
1:BBB:21:ILE:HG23	1:BBB:67:ILE:HD13	1.77	0.65
1:AAA:207:ILE:O	1:AAA:211:ILE:HD12	1.96	0.65
1:BBB:2:LYS:CE	1:BBB:324:ASP:HA	2.27	0.64
1:BBB:272:HIS:O	1:BBB:273:LEU:HB3	1.97	0.64
1:BBB:2:LYS:CE	1:BBB:3:PHE:CD1	2.82	0.63
1:BBB:233:PRO:HG3	1:BBB:239:THR:C	2.18	0.63
1:BBB:240:TYR:OH	1:BBB:281:TYR:CE1	2.48	0.63
1:BBB:222:LYS:HA	1:BBB:222:LYS:HE3	1.79	0.63
1:AAA:243:VAL:HG11	1:AAA:284:ILE:HB	1.79	0.63
1:BBB:2:LYS:CD	1:BBB:324:ASP:HA	2.28	0.63
1:BBB:2:LYS:NZ	1:BBB:3:PHE:HD1	1.97	0.63
1:BBB:2:LYS:HZ3	1:BBB:323:ILE:C	2.02	0.62
1:AAA:156:LEU:HD21	1:AAA:164:THR:O	1.98	0.62
1:BBB:176:PHE:CZ	1:BBB:263:LYS:CG	2.83	0.62
1:BBB:207:ILE:HD12	1:BBB:224:VAL:HG11	1.82	0.61
1:BBB:273:LEU:O	1:BBB:274:LYS:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:65:SER:OG	1:AAA:80:ILE:O	2.15	0.61
1:AAA:302:PHE:CE1	1:AAA:303:ASP:O	2.53	0.61
1:BBB:194:ASP:HA	1:BBB:197:LYS:HD3	1.81	0.61
1:BBB:324:ASP:HB3	1:BBB:327:ASP:HB2	1.82	0.61
1:AAA:184:LEU:HD22	1:AAA:186:VAL:HG13	1.83	0.61
1:BBB:275:ILE:HA	1:BBB:293:VAL:HG11	1.83	0.61
1:BBB:90:MET:SD	1:BBB:91:CYS:N	2.74	0.61
1:BBB:164:THR:OG1	1:BBB:165:ILE:HG22	2.00	0.61
1:BBB:188:VAL:HG23	1:BBB:188:VAL:O	2.01	0.60
1:BBB:247:GLY:O	1:BBB:250:GLN:HG2	2.01	0.60
1:BBB:151:MET:HE3	1:BBB:152:GLU:O	2.02	0.60
1:BBB:2:LYS:HD3	1:BBB:324:ASP:HA	1.83	0.60
1:AAA:45:LEU:HD23	1:AAA:45:LEU:N	2.16	0.60
1:BBB:227:VAL:HG22	1:BBB:228:GLU:H	1.65	0.60
1:BBB:263:LYS:O	1:BBB:266:THR:OG1	2.19	0.59
1:BBB:2:LYS:HD2	1:BBB:3:PHE:HA	1.84	0.59
1:BBB:165:ILE:HD11	1:BBB:182:LYS:HD3	1.85	0.59
1:AAA:299:VAL:O	1:AAA:301:GLU:N	2.36	0.59
1:AAA:245:ILE:HD11	1:AAA:251:VAL:HG12	1.83	0.59
1:BBB:2:LYS:NZ	1:BBB:323:ILE:C	2.56	0.59
1:BBB:66:ILE:O	1:BBB:79:ILE:HA	2.03	0.58
1:BBB:5:LYS:HE2	1:BBB:7:ILE:HD11	1.84	0.58
1:BBB:283:SER:OG	1:BBB:285:THR:HG22	2.03	0.58
1:BBB:229:ILE:HD13	1:BBB:230:TYR:N	2.18	0.58
1:BBB:2:LYS:HE2	1:BBB:324:ASP:CB	2.34	0.58
1:BBB:151:MET:O	1:BBB:151:MET:HG3	2.03	0.58
1:BBB:290:LYS:HB3	1:BBB:310:THR:OG1	2.03	0.58
1:AAA:184:LEU:H	1:AAA:184:LEU:HD12	1.69	0.58
1:BBB:116:ASN:O	1:BBB:117:ILE:HD13	2.04	0.58
1:AAA:3:PHE:O	1:AAA:323:ILE:O	2.22	0.57
1:BBB:264:LEU:HD23	1:BBB:265:ALA:H	1.66	0.57
1:BBB:176:PHE:CZ	1:BBB:178:ILE:HG22	2.39	0.57
1:AAA:188:VAL:O	1:AAA:188:VAL:HG23	2.05	0.57
1:AAA:253:ARG:O	1:AAA:285:THR:CG2	2.51	0.57
1:BBB:2:LYS:CE	1:BBB:3:PHE:HD1	2.17	0.57
1:AAA:275:ILE:HA	1:AAA:293:VAL:HB	1.86	0.57
1:AAA:187:LYS:O	1:AAA:192:GLN:NE2	2.38	0.57
1:BBB:164:THR:OG1	1:BBB:165:ILE:HG23	2.05	0.57
1:BBB:260:THR:HG22	1:BBB:281:TYR:CE1	2.40	0.57
1:BBB:164:THR:O	1:BBB:165:ILE:HG23	2.05	0.56
1:BBB:176:PHE:CE1	1:BBB:263:LYS:HG3	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:2:LYS:HD2	1:BBB:3:PHE:CA	2.35	0.56
1:BBB:198:LYS:HG3	1:BBB:199:LEU:HD12	1.87	0.56
1:AAA:218:LEU:HD22	1:AAA:218:LEU:N	2.20	0.56
1:BBB:189:GLU:H	1:BBB:192:GLN:HE22	1.53	0.56
1:BBB:276:ASP:H	1:BBB:293:VAL:CG1	2.18	0.56
1:BBB:195:VAL:HG13	1:BBB:196:LEU:HD12	1.87	0.56
1:BBB:217:GLU:HG3	1:BBB:218:LEU:HD22	1.87	0.56
1:BBB:273:LEU:HD11	1:BBB:277:GLU:HB2	1.87	0.56
1:AAA:111:VAL:HG13	1:AAA:115:THR:HG23	1.87	0.56
1:AAA:29:ILE:HG13	1:AAA:40:TYR:HD2	1.71	0.56
1:AAA:41:LEU:O	1:AAA:43:ASP:N	2.39	0.56
1:BBB:17:GLU:H	1:BBB:253:ARG:HB2	1.70	0.56
1:BBB:178:ILE:CG1	1:BBB:230:TYR:CE1	2.86	0.55
1:AAA:68:THR:OG1	1:AAA:69:SER:N	2.40	0.55
1:BBB:125:LEU:C	1:BBB:125:LEU:HD23	2.26	0.55
1:AAA:131:MET:SD	1:AAA:131:MET:N	2.79	0.55
1:BBB:39:LYS:O	1:BBB:42:GLU:O	2.25	0.55
1:BBB:111:VAL:O	1:BBB:112:GLU:HB2	2.06	0.55
1:AAA:45:LEU:N	1:AAA:45:LEU:CD2	2.70	0.55
1:AAA:61:ASP:HA	1:AAA:250:GLN:HB2	1.89	0.55
1:BBB:233:PRO:HA	1:BBB:241:LYS:HB3	1.89	0.55
1:AAA:14:THR:HG21	1:AAA:93:HIS:O	2.07	0.55
1:BBB:260:THR:HG22	1:BBB:281:TYR:CG	2.42	0.55
1:BBB:26:ILE:O	1:BBB:26:ILE:HG12	2.06	0.54
1:BBB:43:ASP:O	1:BBB:45:LEU:N	2.40	0.54
1:AAA:49:ARG:HD3	1:AAA:87:TYR:CZ	2.41	0.54
1:BBB:214:GLN:NE2	1:BBB:221:ILE:HD13	2.22	0.54
1:BBB:255:PRO:HG2	1:BBB:289:PHE:CG	2.43	0.54
1:AAA:181:ALA:HA	1:AAA:184:LEU:CD1	2.37	0.54
1:AAA:221:ILE:HG12	1:AAA:222:LYS:H	1.72	0.54
1:AAA:333:PHE:CZ	1:AAA:335:VAL:HG22	2.42	0.54
1:BBB:2:LYS:HD3	1:BBB:325:PRO:HD2	1.90	0.54
1:BBB:193:VAL:HA	1:BBB:196:LEU:HD13	1.89	0.54
1:BBB:240:TYR:HE2	1:BBB:281:TYR:CA	2.20	0.54
1:BBB:153:ASP:CG	1:BBB:166:THR:HG21	2.28	0.54
1:AAA:190:THR:HA	1:AAA:193:VAL:HG13	1.90	0.54
1:AAA:112:GLU:O	1:AAA:132:VAL:O	2.26	0.53
1:BBB:257:GLY:N	2:BBB:401:PYC:O8	2.41	0.53
1:AAA:20:ARG:HD3	1:AAA:321:PHE:CE2	2.44	0.53
1:AAA:32:GLU:HG3	1:AAA:33:THR:H	1.73	0.53
1:AAA:79:ILE:HD12	1:AAA:81:PHE:CZ	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:197:LYS:O	1:AAA:201:ILE:HG13	2.09	0.53
1:BBB:20:ARG:HD3	1:BBB:321:PHE:CE2	2.43	0.53
1:AAA:126:ILE:HD13	1:AAA:126:ILE:H	1.72	0.53
1:BBB:297:THR:HG22	1:BBB:299:VAL:HG12	1.91	0.53
1:AAA:112:GLU:HB3	1:AAA:113:PRO:CD	2.39	0.53
1:BBB:2:LYS:HE2	1:BBB:324:ASP:HB2	1.91	0.53
1:BBB:88:LEU:HD21	2:BBB:401:PYC:H31	1.90	0.53
1:BBB:240:TYR:CE1	1:BBB:242:ASN:CG	2.82	0.53
1:AAA:156:LEU:HD11	1:AAA:164:THR:HG22	1.90	0.52
1:AAA:103:VAL:HG23	1:AAA:117:ILE:HD11	1.91	0.52
1:AAA:111:VAL:HG21	1:AAA:114:VAL:O	2.08	0.52
1:AAA:234:SER:N	1:AAA:241:LYS:HE2	2.23	0.52
1:AAA:198:LYS:HA	1:AAA:201:ILE:HD11	1.90	0.52
1:BBB:168:ASP:HB3	1:BBB:178:ILE:CG2	2.39	0.52
1:AAA:245:ILE:CD1	1:AAA:251:VAL:HG12	2.40	0.52
1:BBB:53:MET:HE3	1:BBB:64:GLY:N	2.25	0.52
1:BBB:148:PHE:CE1	1:BBB:171:PHE:HB2	2.44	0.52
1:AAA:215:HIS:HB3	1:AAA:221:ILE:HG13	1.91	0.52
1:BBB:192:GLN:H	1:BBB:192:GLN:HE21	1.58	0.52
1:BBB:240:TYR:CE2	1:BBB:281:TYR:CG	2.98	0.52
1:BBB:240:TYR:CD1	1:BBB:241:LYS:N	2.77	0.52
1:BBB:179:ILE:HG23	1:BBB:183:GLU:HG2	1.92	0.52
1:BBB:74:GLU:O	1:BBB:75:ALA:HB2	2.09	0.52
1:BBB:176:PHE:CZ	1:BBB:178:ILE:CG2	2.93	0.52
1:BBB:163:LYS:O	1:BBB:164:THR:HB	1.96	0.52
1:AAA:198:LYS:O	1:AAA:201:ILE:HD12	2.10	0.51
1:AAA:235:ASN:OD1	1:AAA:237:GLU:HB2	2.10	0.51
1:BBB:79:ILE:HD11	1:BBB:81:PHE:CZ	2.45	0.51
1:BBB:210:LYS:HA	1:BBB:212:LYS:HD3	1.92	0.51
1:BBB:134:ASN:CG	1:BBB:135:GLU:N	2.64	0.51
1:AAA:199:LEU:HD23	1:AAA:199:LEU:C	2.31	0.51
1:AAA:12:SER:OG	1:AAA:19:THR:HB	2.10	0.51
1:BBB:239:THR:HG22	1:BBB:280:VAL:O	2.11	0.51
1:BBB:146:PRO:HB3	1:BBB:306:ILE:HD11	1.92	0.51
1:BBB:229:ILE:O	1:BBB:242:ASN:CB	2.49	0.51
1:BBB:290:LYS:HB3	1:BBB:310:THR:HG1	1.75	0.51
1:BBB:260:THR:CG2	1:BBB:281:TYR:CD1	2.94	0.51
1:BBB:267:LEU:HD11	1:BBB:273:LEU:HD22	1.92	0.51
1:AAA:17:GLU:H	1:AAA:253:ARG:HB2	1.76	0.51
1:AAA:20:ARG:HG3	1:AAA:62:MET:HE1	1.92	0.51
1:AAA:192:GLN:O	1:AAA:195:VAL:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:133:GLU:O	1:BBB:135:GLU:N	2.40	0.51
1:BBB:263:LYS:NZ	1:BBB:281:TYR:OH	2.42	0.51
1:AAA:65:SER:CB	1:AAA:80:ILE:O	2.59	0.50
1:AAA:150:TYR:HB3	1:AAA:169:ILE:HD13	1.92	0.50
1:BBB:266:THR:N	1:BBB:269:LYS:HZ1	2.09	0.50
1:BBB:268:TYR:CE1	1:BBB:305:ILE:HG23	2.46	0.50
1:AAA:14:THR:HG22	1:AAA:313:ALA:HB2	1.93	0.50
1:AAA:165:ILE:HG12	1:AAA:166:THR:H	1.77	0.50
1:BBB:20:ARG:HG3	1:BBB:62:MET:HE1	1.93	0.50
1:AAA:21:ILE:CG2	1:AAA:67:ILE:HD13	2.41	0.50
1:AAA:46:ASP:O	1:AAA:47:TYR:HD1	1.93	0.50
1:AAA:158:VAL:N	1:AAA:159:PRO:CD	2.75	0.50
1:AAA:241:LYS:HB3	1:AAA:282:GLU:HB3	1.93	0.50
1:BBB:176:PHE:CE2	1:BBB:178:ILE:HB	2.47	0.50
1:AAA:111:VAL:HG21	1:AAA:114:VAL:C	2.32	0.50
1:AAA:221:ILE:HD13	1:AAA:222:LYS:HD3	1.93	0.50
1:BBB:20:ARG:HG3	1:BBB:62:MET:CE	2.41	0.50
1:BBB:184:LEU:HD13	1:BBB:185:GLY:N	2.25	0.50
1:BBB:201:ILE:CD1	1:BBB:204:ARG:CZ	2.90	0.50
1:BBB:218:LEU:N	1:BBB:218:LEU:HD13	2.27	0.49
1:BBB:2:LYS:HE3	1:BBB:3:PHE:CE1	2.47	0.49
1:BBB:118:ASN:HB3	1:BBB:125:LEU:HD21	1.94	0.49
1:BBB:177:ALA:HB3	1:BBB:227:VAL:HG23	1.93	0.49
1:BBB:275:ILE:CG2	1:BBB:276:ASP:N	2.76	0.49
1:AAA:150:TYR:CD2	1:AAA:151:MET:HG2	2.48	0.49
1:AAA:239:THR:OG1	1:AAA:240:TYR:N	2.41	0.49
1:BBB:150:TYR:OH	1:BBB:213:VAL:HG21	2.12	0.49
1:BBB:199:LEU:HA	1:BBB:202:GLU:HG2	1.93	0.49
1:BBB:197:LYS:O	1:BBB:201:ILE:HG22	2.13	0.49
1:AAA:306:ILE:O	1:AAA:306:ILE:CG2	2.60	0.49
1:AAA:196:LEU:HA	1:AAA:199:LEU:HD22	1.94	0.49
1:AAA:203:ILE:O	1:AAA:207:ILE:HG23	2.12	0.49
1:AAA:283:SER:OG	1:AAA:285:THR:HG22	2.12	0.49
1:BBB:45:LEU:N	1:BBB:45:LEU:HD22	2.27	0.49
1:BBB:188:VAL:HG11	1:BBB:229:ILE:HD12	1.95	0.49
1:BBB:108:VAL:HG21	1:BBB:117:ILE:HD11	1.95	0.49
1:BBB:151:MET:CE	1:BBB:154:ALA:HB2	2.42	0.49
1:BBB:168:ASP:HB3	1:BBB:178:ILE:HD12	1.94	0.48
1:BBB:175:PHE:HD2	1:BBB:221:ILE:HG13	1.78	0.48
1:BBB:179:ILE:CG2	1:BBB:183:GLU:HG2	2.43	0.48
1:BBB:266:THR:H	1:BBB:269:LYS:HZ1	1.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:238:ALA:HB2	1:AAA:288:MET:SD	2.53	0.48
1:BBB:267:LEU:O	1:BBB:272:HIS:O	2.31	0.48
1:AAA:96:ILE:HG22	1:AAA:313:ALA:HB2	1.96	0.48
1:BBB:33:THR:O	1:BBB:36:ASP:OD1	2.32	0.48
1:BBB:88:LEU:HD23	1:BBB:91:CYS:HB3	1.95	0.48
1:AAA:258:THR:HG22	2:AAA:401:PYC:O7	2.13	0.48
1:BBB:168:ASP:HB3	1:BBB:178:ILE:HG23	1.96	0.48
1:AAA:156:LEU:HD13	1:AAA:165:ILE:O	2.14	0.48
1:AAA:299:VAL:HG22	1:AAA:301:GLU:OE1	2.14	0.48
1:BBB:208:ASN:HA	1:BBB:223:THR:HG21	1.95	0.48
1:BBB:231:ASP:O	1:BBB:232:GLU:O	2.32	0.48
1:BBB:81:PHE:CE2	1:BBB:90:MET:HA	2.49	0.47
1:BBB:176:PHE:CZ	1:BBB:263:LYS:HG3	2.48	0.47
1:BBB:188:VAL:CG2	1:BBB:241:LYS:HD2	2.44	0.47
1:BBB:112:GLU:CB	1:BBB:113:PRO:HD3	2.44	0.47
1:BBB:145:VAL:HG21	1:BBB:173:GLY:HA2	1.96	0.47
1:AAA:237:GLU:O	1:AAA:280:VAL:HG21	2.14	0.47
1:AAA:5:LYS:HB2	1:AAA:323:ILE:CD1	2.30	0.47
1:AAA:133:GLU:O	1:AAA:135:GLU:N	2.46	0.47
1:BBB:3:PHE:O	1:BBB:323:ILE:O	2.32	0.47
1:BBB:162:ASN:ND2	1:BBB:164:THR:OG1	2.46	0.47
1:BBB:240:TYR:CD1	1:BBB:240:TYR:C	2.87	0.47
1:AAA:92:GLY:N	2:AAA:401:PYC:O7	2.48	0.47
1:AAA:34:MET:C	1:AAA:122:PRO:HB3	2.34	0.47
1:BBB:63:PHE:CD1	1:BBB:64:GLY:N	2.83	0.47
1:BBB:283:SER:OG	1:BBB:284:ILE:N	2.47	0.47
1:AAA:14:THR:HG22	1:AAA:313:ALA:CB	2.45	0.47
1:AAA:65:SER:OG	1:AAA:66:ILE:N	2.47	0.47
1:BBB:142:ILE:HD12	1:BBB:143:THR:N	2.30	0.47
1:BBB:223:THR:HG22	1:BBB:224:VAL:HG22	1.97	0.47
1:AAA:165:ILE:HD13	1:AAA:165:ILE:H	1.79	0.47
1:BBB:112:GLU:OE1	1:BBB:112:GLU:HA	2.15	0.47
1:AAA:207:ILE:HD13	1:AAA:208:ASN:N	2.30	0.46
1:BBB:74:GLU:O	1:BBB:75:ALA:CB	2.63	0.46
1:BBB:275:ILE:HG23	1:BBB:276:ASP:N	2.30	0.46
1:AAA:47:TYR:CD1	1:AAA:50:THR:HG21	2.51	0.46
1:AAA:161:LEU:HD22	1:AAA:162:ASN:N	2.30	0.46
1:AAA:221:ILE:HG12	1:AAA:222:LYS:N	2.29	0.46
1:BBB:111:VAL:HG21	1:BBB:114:VAL:C	2.36	0.46
1:BBB:155:LYS:HB2	1:BBB:166:THR:HA	1.95	0.46
1:BBB:158:VAL:CG1	1:BBB:163:LYS:O	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:290:LYS:HD2	1:AAA:290:LYS:N	2.31	0.46
1:BBB:100:THR:HG21	1:BBB:313:ALA:O	2.16	0.46
1:BBB:240:TYR:HE1	1:BBB:242:ASN:CG	2.18	0.46
1:BBB:96:ILE:HG22	1:BBB:313:ALA:HB2	1.96	0.46
1:BBB:273:LEU:HD11	1:BBB:277:GLU:CB	2.46	0.46
1:AAA:266:THR:O	1:AAA:270:LYS:HB2	2.16	0.46
1:BBB:149:LEU:C	1:BBB:149:LEU:HD13	2.36	0.46
1:BBB:264:LEU:CD1	1:BBB:307:PRO:HB3	2.45	0.46
1:AAA:45:LEU:HB3	1:AAA:48:VAL:HG22	1.97	0.46
1:AAA:47:TYR:CE1	1:AAA:50:THR:HG21	2.51	0.46
1:BBB:20:ARG:HD3	1:BBB:321:PHE:HE2	1.80	0.46
1:BBB:111:VAL:HG13	1:BBB:115:THR:HG23	1.97	0.46
1:BBB:172:GLY:HA3	1:BBB:262:ALA:HB2	1.98	0.46
1:AAA:176:PHE:CZ	1:AAA:259:GLY:HA2	2.51	0.46
1:BBB:192:GLN:CD	1:BBB:193:VAL:H	2.19	0.46
1:BBB:179:ILE:O	1:BBB:230:TYR:CD1	2.69	0.46
1:BBB:180:HIS:ND1	1:BBB:182:LYS:HG3	2.31	0.46
1:BBB:226:LEU:CD1	1:BBB:244:VAL:HG11	2.46	0.45
1:AAA:187:LYS:HG3	1:AAA:192:GLN:HE22	1.80	0.45
1:AAA:216:PRO:HG2	1:AAA:301:GLU:OE1	2.17	0.45
1:BBB:164:THR:O	1:BBB:165:ILE:CG2	2.63	0.45
1:BBB:164:THR:HG23	1:BBB:165:ILE:O	2.17	0.45
1:BBB:329:LEU:CD1	1:BBB:329:LEU:N	2.79	0.45
1:AAA:150:TYR:O	1:AAA:169:ILE:HG23	2.16	0.45
1:BBB:41:LEU:HD23	1:BBB:80:ILE:HD13	1.97	0.45
1:BBB:158:VAL:HG12	1:BBB:163:LYS:O	2.17	0.45
1:BBB:276:ASP:N	1:BBB:293:VAL:CG1	2.79	0.45
1:BBB:34:MET:CE	1:BBB:78:GLY:HA3	2.46	0.45
1:BBB:79:ILE:CD1	1:BBB:81:PHE:CE1	2.98	0.45
1:BBB:175:PHE:CD2	1:BBB:221:ILE:HG13	2.51	0.45
1:BBB:214:GLN:NE2	1:BBB:215:HIS:ND1	2.61	0.45
1:BBB:241:LYS:HB3	1:BBB:282:GLU:OE2	2.17	0.45
1:BBB:324:ASP:HB3	1:BBB:327:ASP:CB	2.45	0.45
1:AAA:169:ILE:HD13	1:AAA:169:ILE:C	2.37	0.45
1:AAA:220:HIS:CE1	1:AAA:221:ILE:HG22	2.52	0.45
1:BBB:88:LEU:HD12	1:BBB:89:ASN:H	1.82	0.45
1:AAA:80:ILE:HG22	1:AAA:81:PHE:N	2.32	0.45
1:BBB:76:ASP:CG	1:BBB:117:ILE:HD12	2.36	0.45
1:BBB:150:TYR:CZ	1:BBB:213:VAL:HG21	2.51	0.45
1:BBB:41:LEU:HD13	1:BBB:41:LEU:HA	1.89	0.45
1:BBB:176:PHE:HA	1:BBB:226:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:188:VAL:HG12	1:BBB:196:LEU:HD21	1.98	0.45
1:AAA:20:ARG:HD3	1:AAA:321:PHE:HE2	1.81	0.45
1:AAA:180:HIS:CG	1:AAA:180:HIS:O	2.69	0.45
1:BBB:275:ILE:HG23	1:BBB:276:ASP:H	1.79	0.45
1:AAA:31:GLY:O	1:AAA:37:LYS:HG2	2.16	0.44
1:AAA:78:GLY:O	1:AAA:79:ILE:HG22	2.17	0.44
1:AAA:158:VAL:N	1:AAA:159:PRO:HD3	2.31	0.44
1:BBB:233:PRO:HG3	1:BBB:239:THR:CA	2.46	0.44
1:BBB:240:TYR:O	1:BBB:282:GLU:OE2	2.35	0.44
1:AAA:68:THR:HG21	1:AAA:80:ILE:HD11	1.99	0.44
1:AAA:122:PRO:O	1:AAA:123:ALA:C	2.55	0.44
1:AAA:182:LYS:CD	1:AAA:183:GLU:N	2.80	0.44
1:BBB:28:GLN:C	1:BBB:29:ILE:HD12	2.37	0.44
1:BBB:203:ILE:N	1:BBB:203:ILE:HD13	2.33	0.44
1:AAA:166:THR:O	1:AAA:183:GLU:CD	2.55	0.44
1:AAA:333:PHE:CD1	1:AAA:333:PHE:C	2.91	0.44
1:BBB:2:LYS:NZ	1:BBB:324:ASP:N	2.65	0.44
1:AAA:4:SER:OG	1:AAA:5:LYS:N	2.50	0.44
1:AAA:161:LEU:HD13	1:AAA:161:LEU:C	2.37	0.44
1:BBB:42:GLU:C	1:BBB:43:ASP:O	2.56	0.44
1:BBB:92:GLY:O	2:BBB:401:PYC:C1	2.65	0.44
1:BBB:129:LYS:HG3	1:BBB:141:SER:OG	2.17	0.44
1:BBB:144:ASN:ND2	1:BBB:261:SER:HB3	2.33	0.44
1:BBB:26:ILE:HG12	1:BBB:29:ILE:HD11	2.00	0.44
1:AAA:165:ILE:HD13	1:AAA:165:ILE:N	2.33	0.44
1:BBB:130:VAL:HG12	1:BBB:137:VAL:HG23	2.00	0.44
1:AAA:195:VAL:HA	1:AAA:198:LYS:HG2	2.00	0.44
1:AAA:245:ILE:HD13	1:AAA:251:VAL:HA	2.00	0.44
1:BBB:164:THR:C	1:BBB:165:ILE:CG2	2.87	0.44
1:AAA:292:ARG:HG3	1:AAA:308:GLU:HG3	2.00	0.44
1:BBB:112:GLU:HB2	1:BBB:113:PRO:HD3	1.99	0.44
1:BBB:221:ILE:HD13	1:BBB:222:LYS:N	2.33	0.44
1:BBB:4:SER:OG	1:BBB:5:LYS:N	2.50	0.43
1:BBB:241:LYS:CB	1:BBB:282:GLU:OE2	2.66	0.43
1:AAA:149:LEU:HD13	1:AAA:150:TYR:N	2.32	0.43
1:BBB:240:TYR:CE1	1:BBB:242:ASN:N	2.87	0.43
1:BBB:298:LYS:O	1:BBB:299:VAL:HG13	2.18	0.43
1:AAA:184:LEU:H	1:AAA:184:LEU:CD1	2.30	0.43
1:AAA:261:SER:HA	1:AAA:264:LEU:HD11	1.99	0.43
1:BBB:2:LYS:CE	1:BBB:324:ASP:CA	2.94	0.43
1:BBB:240:TYR:HE1	1:BBB:242:ASN:N	2.15	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:41:LEU:HD23	1:BBB:80:ILE:CD1	2.48	0.43
1:BBB:227:VAL:O	1:BBB:244:VAL:HG13	2.18	0.43
1:BBB:267:LEU:O	1:BBB:267:LEU:HD13	2.19	0.43
1:BBB:171:PHE:O	1:BBB:262:ALA:HB2	2.18	0.43
1:BBB:193:VAL:HG12	1:BBB:196:LEU:HD13	2.00	0.43
1:AAA:121:ALA:HB3	1:AAA:123:ALA:N	2.33	0.43
1:AAA:206:LEU:C	1:AAA:206:LEU:CD2	2.85	0.43
1:BBB:232:GLU:HA	1:BBB:233:PRO:HD3	1.92	0.43
1:AAA:323:ILE:O	1:AAA:323:ILE:HG12	2.19	0.43
1:BBB:111:VAL:HG23	1:BBB:112:GLU:N	2.34	0.43
1:BBB:240:TYR:CE2	1:BBB:281:TYR:CD2	3.07	0.43
1:AAA:176:PHE:HZ	1:AAA:258:THR:HG23	1.83	0.42
1:BBB:130:VAL:O	1:BBB:132:VAL:HG12	2.18	0.42
1:BBB:79:ILE:CD1	1:BBB:81:PHE:CZ	3.02	0.42
1:AAA:164:THR:HG21	1:AAA:183:GLU:O	2.20	0.42
1:AAA:293:VAL:C	1:AAA:294:LEU:HD12	2.40	0.42
1:AAA:333:PHE:O	1:AAA:334:THR:CB	2.67	0.42
1:BBB:233:PRO:HG3	1:BBB:240:TYR:N	2.34	0.42
1:AAA:264:LEU:HA	1:AAA:267:LEU:HB2	2.00	0.42
1:BBB:96:ILE:HG22	1:BBB:97:GLY:N	2.34	0.42
1:BBB:155:LYS:HD3	1:BBB:155:LYS:C	2.40	0.42
1:BBB:260:THR:HG22	1:BBB:281:TYR:CD2	2.55	0.42
1:AAA:111:VAL:CG2	1:AAA:114:VAL:C	2.88	0.42
1:BBB:230:TYR:O	1:BBB:231:ASP:HB3	2.19	0.42
1:AAA:20:ARG:HG3	1:AAA:62:MET:CE	2.49	0.42
1:AAA:149:LEU:HD13	1:AAA:149:LEU:C	2.40	0.42
1:BBB:264:LEU:HD11	1:BBB:307:PRO:CB	2.50	0.42
1:AAA:150:TYR:HB3	1:AAA:169:ILE:CD1	2.49	0.42
1:AAA:119:MET:HB2	1:AAA:126:ILE:HD11	2.00	0.42
1:BBB:152:GLU:O	1:BBB:153:ASP:CB	2.68	0.42
1:AAA:158:VAL:H	1:AAA:159:PRO:HD3	1.85	0.41
1:AAA:112:GLU:HA	1:AAA:112:GLU:OE1	2.20	0.41
1:BBB:45:LEU:HA	1:BBB:47:TYR:CE1	2.55	0.41
1:BBB:275:ILE:HG13	1:BBB:293:VAL:HG21	2.02	0.41
1:BBB:54:HIS:HB2	1:BBB:332:GLY:CA	2.50	0.41
1:BBB:68:THR:OG1	1:BBB:69:SER:N	2.53	0.41
1:BBB:131:MET:CE	1:BBB:138:LYS:HG2	2.50	0.41
1:BBB:2:LYS:CD	1:BBB:3:PHE:HA	2.50	0.41
1:BBB:21:ILE:N	1:BBB:21:ILE:HD12	2.35	0.41
1:BBB:76:ASP:OD2	1:BBB:117:ILE:HD12	2.20	0.41
1:BBB:240:TYR:HE1	1:BBB:242:ASN:CB	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:260:THR:CG2	1:BBB:281:TYR:CE1	3.03	0.41
1:BBB:176:PHE:HE2	1:BBB:178:ILE:HB	1.85	0.41
1:BBB:189:GLU:O	1:BBB:192:GLN:NE2	2.53	0.41
1:BBB:258:THR:OG1	2:BBB:401:PYC:C1	2.68	0.41
1:BBB:264:LEU:HD11	1:BBB:307:PRO:HB3	2.02	0.41
1:BBB:54:HIS:HB2	1:BBB:332:GLY:HA2	2.02	0.41
1:BBB:179:ILE:C	1:BBB:230:TYR:CE1	2.94	0.41
1:BBB:168:ASP:CB	1:BBB:178:ILE:HD12	2.50	0.41
1:BBB:239:THR:O	1:BBB:240:TYR:CD2	2.74	0.41
1:AAA:203:ILE:HA	1:AAA:206:LEU:CD2	2.40	0.41
1:BBB:144:ASN:ND2	1:BBB:145:VAL:HG22	2.36	0.41
1:AAA:35:ALA:O	1:AAA:38:LYS:HB3	2.21	0.41
1:AAA:224:VAL:HG22	1:AAA:224:VAL:O	2.21	0.41
1:AAA:284:ILE:HG23	1:AAA:285:THR:N	2.36	0.41
1:BBB:273:LEU:HD23	1:BBB:274:LYS:N	2.36	0.41
1:AAA:82:MET:HB3	1:AAA:87:TYR:CE1	2.56	0.40
1:AAA:111:VAL:O	1:AAA:113:PRO:HD2	2.21	0.40
1:AAA:54:HIS:HB2	1:AAA:332:GLY:HA2	2.03	0.40
1:AAA:55:GLU:HB3	1:AAA:56:PRO:HA	2.03	0.40
1:AAA:22:VAL:HB	1:AAA:66:ILE:HG13	2.04	0.40
1:BBB:188:VAL:HA	1:BBB:193:VAL:CG1	2.51	0.40
1:BBB:52:LEU:CD2	1:BBB:321:PHE:CD2	3.05	0.40
1:AAA:50:THR:HA	1:AAA:54:HIS:ND1	2.36	0.40
1:AAA:104:GLU:OE1	1:AAA:136:LYS:HD2	2.21	0.40
1:AAA:110:MET:O	1:AAA:110:MET:CG	2.68	0.40
1:BBB:242:ASN:OD1	1:BBB:242:ASN:C	2.60	0.40
1:BBB:260:THR:HG22	1:BBB:281:TYR:CZ	2.57	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:69:SER:HB2	1:BBB:69:SER:HG[7_555]	1.29	0.31
1:BBB:13:HIS:HE2	1:BBB:327:ASP:OD1[8_555]	1.56	0.04

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	333/343 (97%)	242 (73%)	63 (19%)	28 (8%)	1	4
1	BBB	333/343 (97%)	235 (71%)	55 (16%)	43 (13%)	0	1
All	All	666/686 (97%)	477 (72%)	118 (18%)	71 (11%)	0	2

All (71) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	42	GLU
1	AAA	62	MET
1	AAA	112	GLU
1	AAA	121	ALA
1	AAA	221	ILE
1	AAA	272	HIS
1	AAA	275	ILE
1	AAA	300	GLY
1	AAA	333	PHE
1	AAA	334	THR
1	BBB	75	ALA
1	BBB	112	GLU
1	BBB	153	ASP
1	BBB	157	GLU
1	BBB	158	VAL
1	BBB	164	THR
1	BBB	175	PHE
1	BBB	232	GLU
1	BBB	239	THR
1	BBB	240	TYR
1	BBB	273	LEU
1	BBB	274	LYS
1	BBB	299	VAL
1	AAA	41	LEU
1	AAA	47	TYR

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Mol	Chain	Res	Type
1	AAA	61	ASP
1	AAA	134	ASN
1	AAA	151	MET
1	AAA	213	VAL
1	AAA	247	GLY
1	AAA	276	ASP
1	AAA	301	GLU
1	BBB	3	PHE
1	BBB	43	ASP
1	BBB	151	MET
1	BBB	162	ASN
1	BBB	163	LYS
1	BBB	165	ILE
1	BBB	184	LEU
1	BBB	208	ASN
1	BBB	247	GLY
1	BBB	266	THR
1	AAA	2	LYS
1	AAA	79	ILE
1	AAA	123	ALA
1	BBB	2	LYS
1	BBB	47	TYR
1	BBB	113	PRO
1	BBB	160	SER
1	BBB	217	GLU
1	AAA	113	PRO
1	AAA	152	GLU
1	AAA	153	ASP
1	AAA	160	SER
1	BBB	93	HIS
1	BBB	94	GLY
1	BBB	134	ASN
1	BBB	222	LYS
1	BBB	231	ASP
1	BBB	256	CYS
1	BBB	276	ASP
1	AAA	165	ILE
1	BBB	17	GLU
1	BBB	182	LYS
1	BBB	218	LEU
1	BBB	44	ASN
1	BBB	121	ALA

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Mol	Chain	Res	Type
1	BBB	249	GLY
1	BBB	263	LYS
1	AAA	31	GLY
1	BBB	96	ILE

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	AAA	285/293 (97%)	223 (78%)	62 (22%)	1	5
1	BBB	285/293 (97%)	205 (72%)	80 (28%)	0	1
All	All	570/586 (97%)	428 (75%)	142 (25%)	0	2

All (142) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	7	ILE
1	AAA	13	HIS
1	AAA	15	MET
1	AAA	20	ARG
1	AAA	23	VAL
1	AAA	26	ILE
1	AAA	29	ILE
1	AAA	43	ASP
1	AAA	45	LEU
1	AAA	47	TYR
1	AAA	52	LEU
1	AAA	67	ILE
1	AAA	68	THR
1	AAA	79	ILE
1	AAA	90	MET
1	AAA	115	THR
1	AAA	116	ASN
1	AAA	126	ILE
1	AAA	127	LYS

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Mol	Chain	Res	Type
1	AAA	131	MET
1	AAA	132	VAL
1	AAA	136	LYS
1	AAA	142	ILE
1	AAA	143	THR
1	AAA	156	LEU
1	AAA	161	LEU
1	AAA	165	ILE
1	AAA	166	THR
1	AAA	169	ILE
1	AAA	182	LYS
1	AAA	184	LEU
1	AAA	187	LYS
1	AAA	194	ASP
1	AAA	199	LEU
1	AAA	202	GLU
1	AAA	204	ARG
1	AAA	206	LEU
1	AAA	207	ILE
1	AAA	211	ILE
1	AAA	214	GLN
1	AAA	217	GLU
1	AAA	221	ILE
1	AAA	224	VAL
1	AAA	229	ILE
1	AAA	239	THR
1	AAA	241	LYS
1	AAA	264	LEU
1	AAA	280	VAL
1	AAA	281	TYR
1	AAA	284	ILE
1	AAA	292	ARG
1	AAA	298	LYS
1	AAA	299	VAL
1	AAA	303	ASP
1	AAA	305	ILE
1	AAA	308	GLU
1	AAA	309	ILE
1	AAA	310	THR
1	AAA	319	ASN
1	AAA	323	ILE
1	AAA	330	LYS

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Mol	Chain	Res	Type
1	AAA	333	PHE
1	BBB	2	LYS
1	BBB	12	SER
1	BBB	13	HIS
1	BBB	14	THR
1	BBB	20	ARG
1	BBB	26	ILE
1	BBB	39	LYS
1	BBB	41	LEU
1	BBB	43	ASP
1	BBB	44	ASN
1	BBB	73	LYS
1	BBB	74	GLU
1	BBB	82	MET
1	BBB	90	MET
1	BBB	93	HIS
1	BBB	117	ILE
1	BBB	118	ASN
1	BBB	126	ILE
1	BBB	129	LYS
1	BBB	130	VAL
1	BBB	132	VAL
1	BBB	134	ASN
1	BBB	135	GLU
1	BBB	142	ILE
1	BBB	143	THR
1	BBB	151	MET
1	BBB	161	LEU
1	BBB	164	THR
1	BBB	165	ILE
1	BBB	166	THR
1	BBB	176	PHE
1	BBB	178	ILE
1	BBB	180	HIS
1	BBB	182	LYS
1	BBB	184	LEU
1	BBB	186	VAL
1	BBB	190	THR
1	BBB	192	GLN
1	BBB	197	LYS
1	BBB	202	GLU
1	BBB	206	LEU

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Mol	Chain	Res	Type
1	BBB	207	ILE
1	BBB	209	GLU
1	BBB	210	LYS
1	BBB	217	GLU
1	BBB	218	LEU
1	BBB	221	ILE
1	BBB	222	LYS
1	BBB	225	ASP
1	BBB	226	LEU
1	BBB	229	ILE
1	BBB	231	ASP
1	BBB	234	SER
1	BBB	237	GLU
1	BBB	240	TYR
1	BBB	243	VAL
1	BBB	251	VAL
1	BBB	254	SER
1	BBB	261	SER
1	BBB	263	LYS
1	BBB	264	LEU
1	BBB	269	LYS
1	BBB	270	LYS
1	BBB	274	LYS
1	BBB	278	LYS
1	BBB	280	VAL
1	BBB	281	TYR
1	BBB	283	SER
1	BBB	288	MET
1	BBB	290	LYS
1	BBB	292	ARG
1	BBB	294	LEU
1	BBB	299	VAL
1	BBB	301	GLU
1	BBB	303	ASP
1	BBB	305	ILE
1	BBB	310	THR
1	BBB	329	LEU
1	BBB	330	LYS
1	BBB	333	PHE

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 ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	PYC	BBB	401	-	8,8,8	1.96	2 (25%)	8,10,10	1.37	1 (12%)
2	PYC	AAA	401	-	8,8,8	1.68	2 (25%)	8,10,10	1.39	0

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	PYC	BBB	401	-	-	0/2/4/4	0/1/1/1
2	PYC	AAA	401	-	-	0/2/4/4	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	401	PYC	C2-C1	-4.60	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	401	PYC	C2-C1	-3.68	1.45	1.50
2	BBB	401	PYC	O8-C1	-2.95	1.21	1.30
2	AAA	401	PYC	O8-C1	-2.83	1.21	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BBB	401	PYC	O7-C1-C2	-2.01	117.17	121.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	401	PYC	4	0
2	AAA	401	PYC	2	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 PYC BBB 401

Bond lengths

Bond angles

Torsions

Rings

Ligand PYC AAA 401

Bond lengths

Bond angles

Torsions

Rings
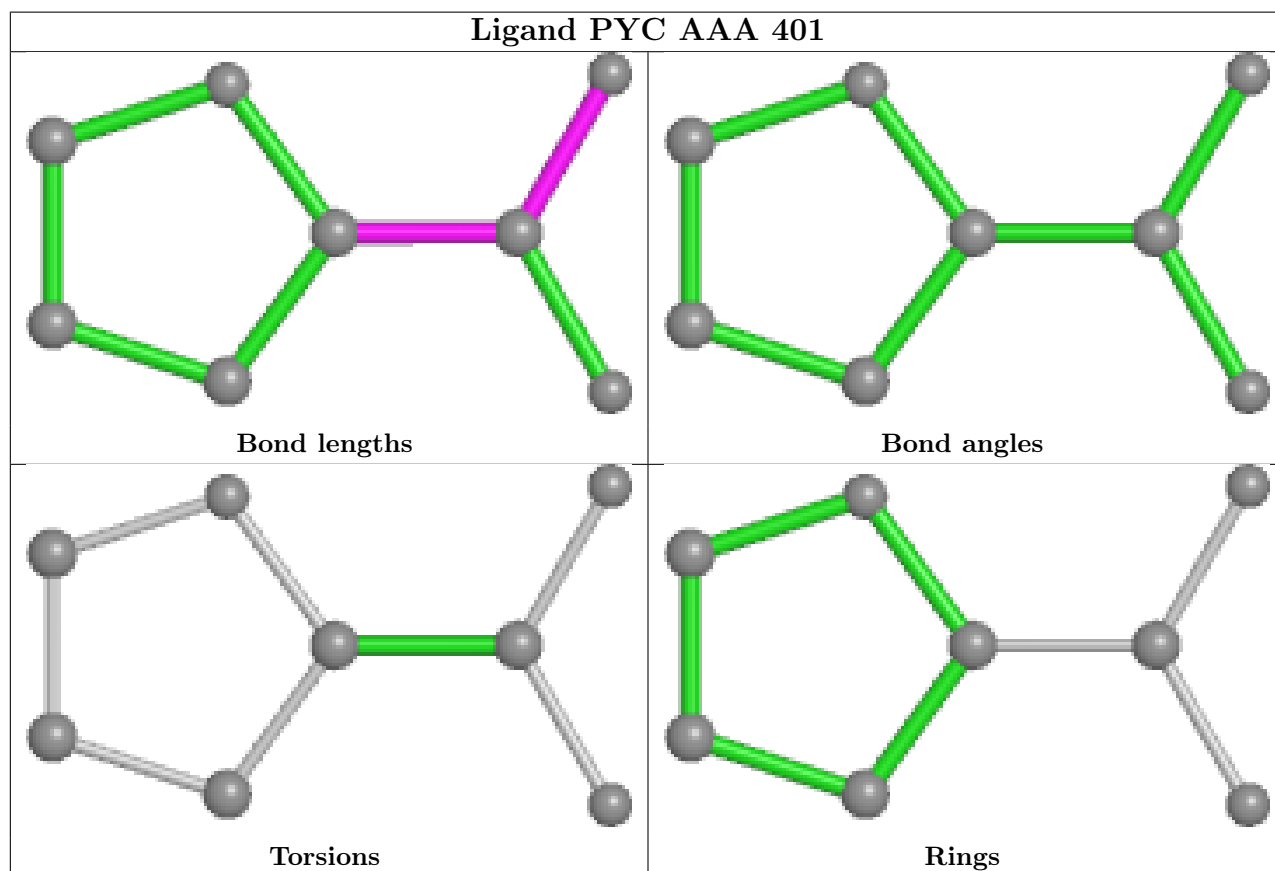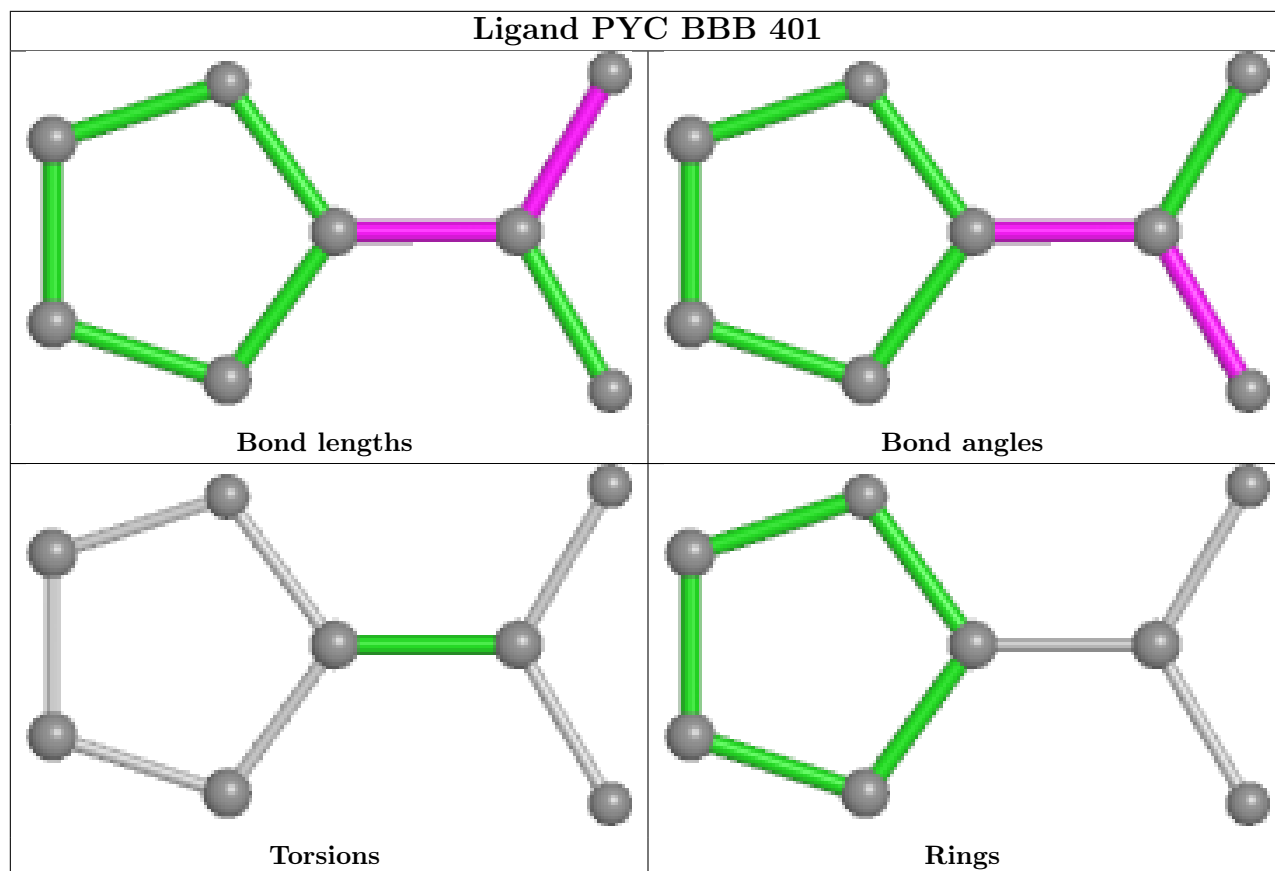
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	AAA	335/343 (97%)	-0.04	3 (0%)	84	75	72, 118, 169, 204	0
1	BBB	335/343 (97%)	0.22	23 (6%)	16	9	74, 138, 240, 277	0
All	All	670/686 (97%)	0.09	26 (3%)	39	24	72, 127, 222, 277	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	159	PRO	5.3
1	BBB	219	GLU	5.0
1	BBB	149	LEU	4.3
1	BBB	187	LYS	4.1
1	BBB	213	VAL	3.8
1	BBB	220	HIS	3.8
1	AAA	248	GLN	3.7
1	AAA	173	GLY	3.5
1	BBB	158	VAL	3.1
1	BBB	212	LYS	2.9
1	BBB	225	ASP	2.8
1	BBB	211	ILE	2.7
1	BBB	126	ILE	2.6
1	BBB	221	ILE	2.6
1	BBB	209	GLU	2.5
1	BBB	200	GLY	2.5
1	BBB	164	THR	2.4
1	BBB	176	PHE	2.4
1	BBB	189	GLU	2.4
1	BBB	89	ASN	2.3
1	BBB	177	ALA	2.3
1	BBB	127	LYS	2.3
1	AAA	151	MET	2.2
1	BBB	274	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	BBB	202	GLU	2.1
1	BBB	130	VAL	2.1

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 ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(Å^2)	Q<0.9
2	PYC	BBB	401	8/8	0.89	0.30	129,145,148,148	0
2	PYC	AAA	401	8/8	0.91	0.42	114,119,120,120	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 PYC BBB 401:

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

Electron density around PYC AAA 401:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
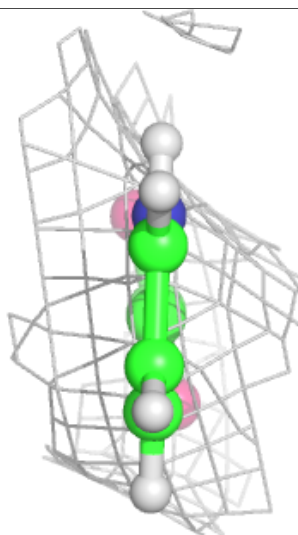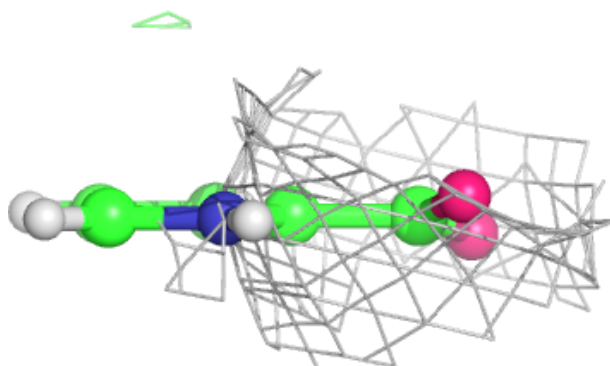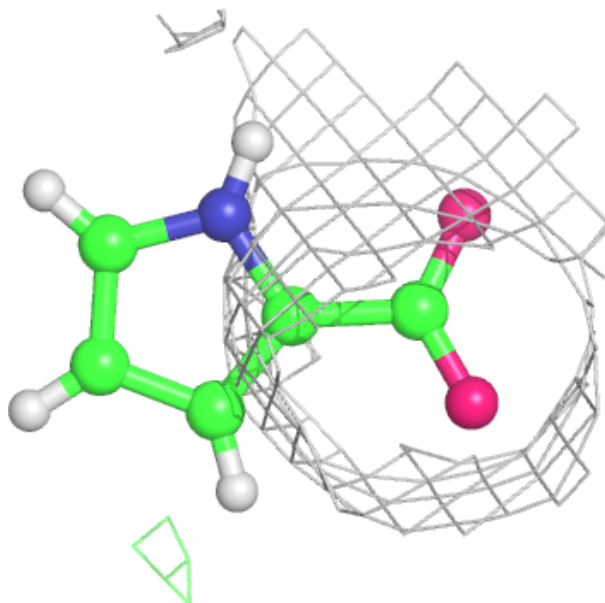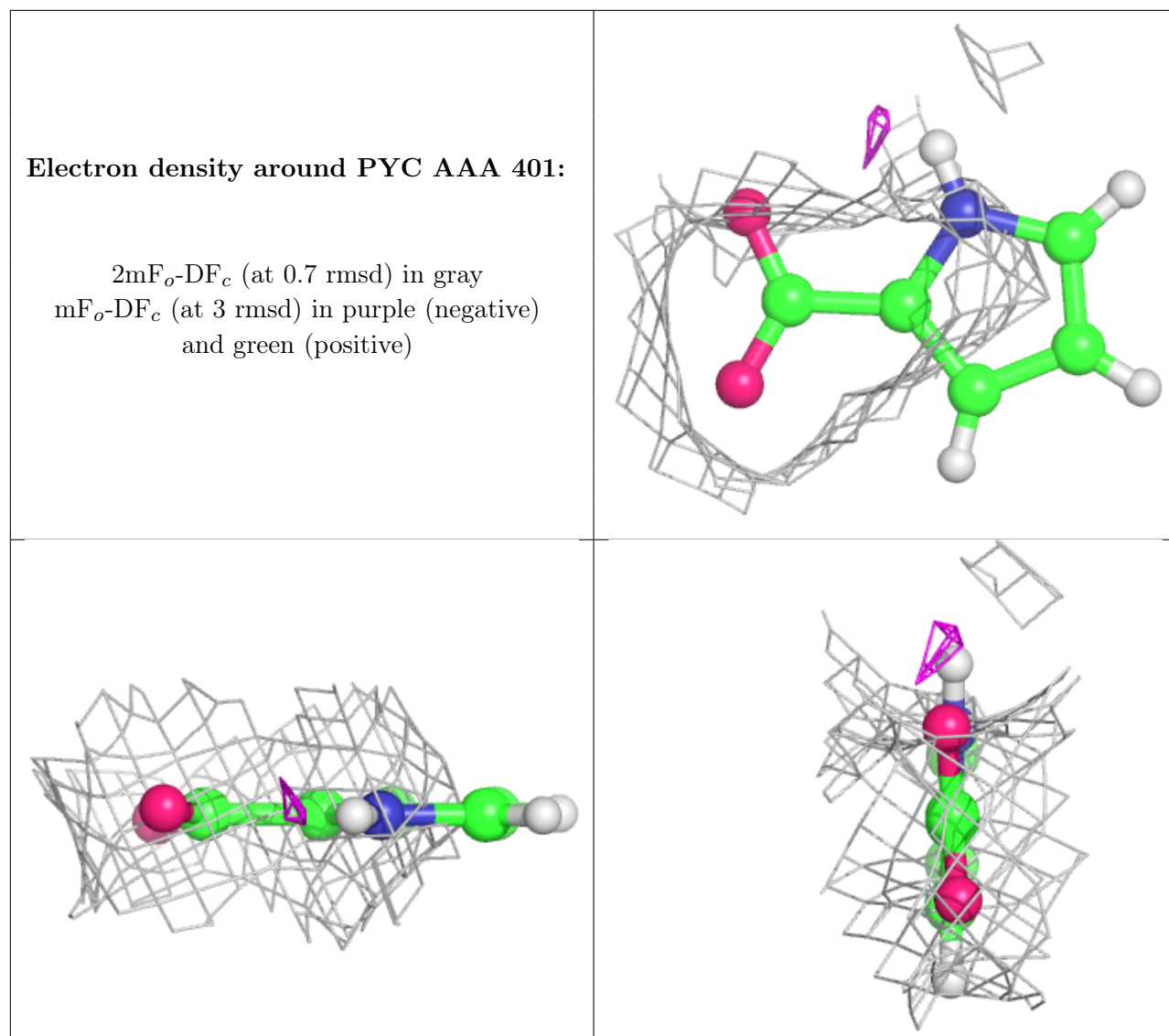
6.5 Other polymers (i)

There are no such residues in this entry.