



Full wwPDB X-ray Structure Validation Report ⓘ

May 7, 2026 – 11:32 AM EDT

PDB ID : 7PB3 / pdb_00007pb3
Title : Structural and Functional analysis of the Proline Racemase (ProR) from the Gram-positive bacterium *Acetoanaerobium sticklandii*
Authors : Najmudin, S.; Pan, X.-S.; McAuley, K.E.; Fisher, L.M.; Sanderson, M.R.
Deposited on : 2021-07-30
Resolution : 2.84 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

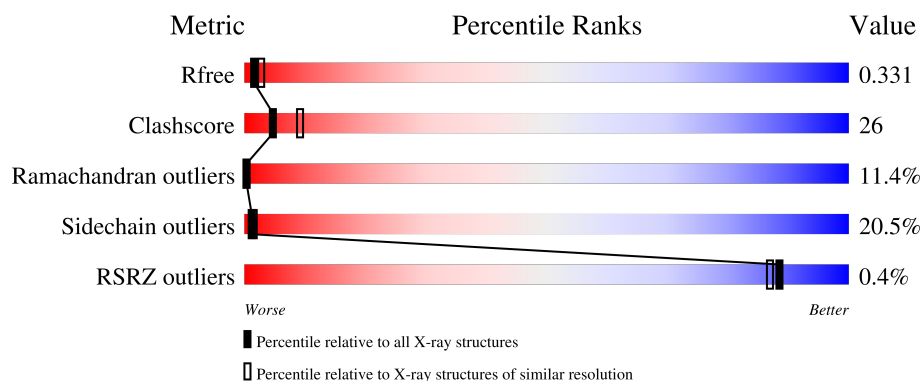
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.84 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}	180053	1520 (2.86-2.82)
Clashscore	190562	1559 (2.86-2.82)
Ramachandran outliers	187476	1517 (2.86-2.82)
Sidechain outliers	187428	1518 (2.86-2.82)
RSRZ outliers	180081	1521 (2.86-2.82)

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	AAA	343	 47% 34% 15% . .
1	BBB	343	 45% 37% 13% . .

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.

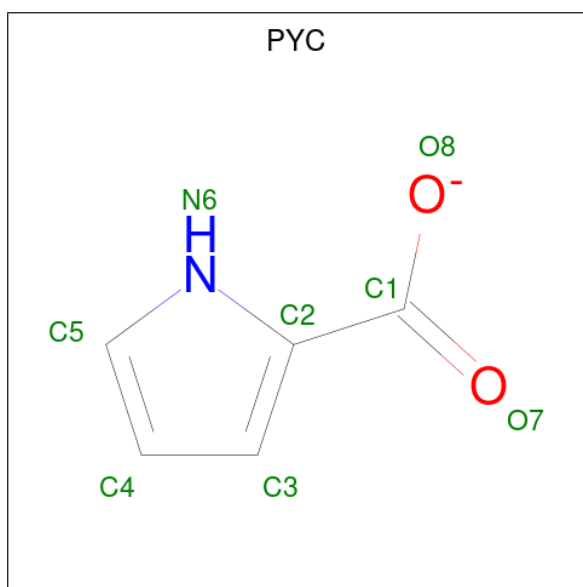
- Molecule 1 is a protein called Proline racemase A (AsProR).

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 (CCD ID: PYC) (formula: $C_5H_4NO_2$) (labeled as "Ligand of Interest" by depositor).

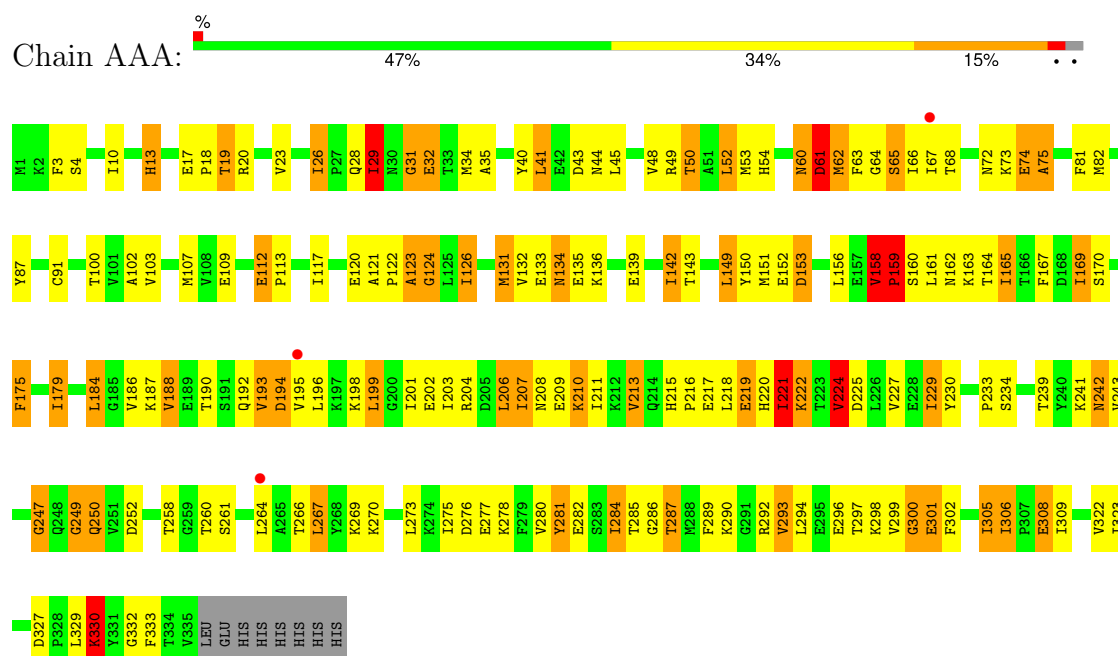


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	H	N	O	0	0
			12	5	4	1	2		
2	BBB	1	Total	C	H	N	O	0	0
			12	5	4	1	2		

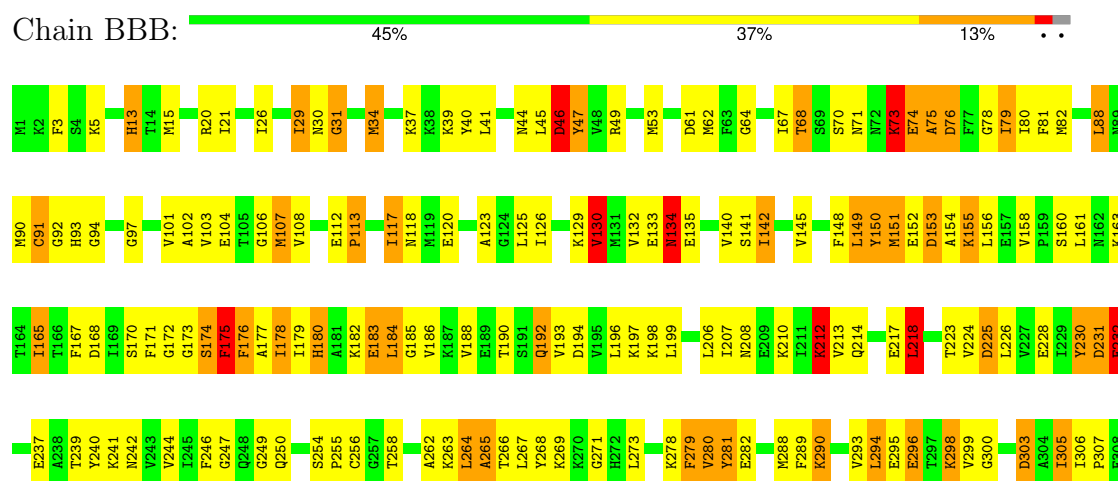
3 Residue-property plots [i](#)

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: Proline racemase A (AsProR)



• Molecule 1: Proline racemase A (AsProR)



I309	T310	G311	G312	G317	V322	I323	D327	P328	L329	K330	Y331	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	109.04Å 109.04Å 105.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	77.22 – 2.84 77.10 – 2.84	Depositor EDS
% Data completeness (in resolution range)	61.4 (77.22-2.84) 61.4 (77.10-2.84)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.31 (at 2.86Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.251 , 0.330 0.250 , 0.331	Depositor DCC
R_{free} test set	542 reflections (5.35%)	wwPDB-VP
Wilson B-factor (Å ²)	117.6	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 98.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for -h,-l,-k 0.016 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10400	wwPDB-VP
Average B, all atoms (Å ²)	134.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.57% 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

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	1.03	0/2634	1.40	1/3556 (0.0%)
1	BBB	1.05	0/2634	1.42	2/3556 (0.1%)
All	All	1.04	0/5268	1.41	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	1
1	BBB	0	3
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	175	PHE	CA-CB-CG	-5.73	108.07	113.80
1	BBB	317	GLY	CA-C-O	-5.52	118.16	122.52
1	AAA	61	ASP	CB-CA-C	5.22	120.81	110.42

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	158	VAL	Peptide
1	BBB	232	GLU	Peptide
1	BBB	273	LEU	Peptide

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Mol	Chain	Res	Type	Group
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	126	0
1	BBB	2585	2603	2593	142	0
2	AAA	8	4	4	2	0
2	BBB	8	4	4	1	0
All	All	5186	5214	5194	268	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 26.

All (268) 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:174:SER:O	1:BBB:175:PHE:O	1.87	0.92
1:AAA:199:LEU:HD22	1:AAA:203:ILE:HD11	1.57	0.86
1:BBB:290:LYS:HB3	1:BBB:310:THR:OG1	1.81	0.81
1:AAA:72:ASN:HD22	1:AAA:75:ALA:HB2	1.47	0.77
1:BBB:207:ILE:O	1:BBB:207:ILE:HG22	1.84	0.77
1:BBB:228:GLU:CG	1:BBB:242:ASN:HD21	1.97	0.77
1:AAA:206:LEU:HD23	1:AAA:206:LEU:C	2.15	0.70
1:BBB:106:GLY:O	1:BBB:108:VAL:N	2.23	0.70
1:BBB:175:PHE:CE2	1:BBB:226:LEU:HB2	2.26	0.70
1:BBB:228:GLU:HG2	1:BBB:242:ASN:HD21	1.56	0.70
1:BBB:29:ILE:HG21	1:BBB:41:LEU:HD21	1.75	0.68
1:BBB:242:ASN:HB3	1:BBB:281:TYR:CE1	2.29	0.67
1:AAA:150:TYR:CD2	1:AAA:151:MET:HG2	2.29	0.67
1:BBB:217:GLU:HG3	1:BBB:218:LEU:HD22	1.77	0.67
1:BBB:192:GLN:CD	1:BBB:196:LEU:HD11	2.21	0.66
1:BBB:184:LEU:HD12	1:BBB:184:LEU:H	1.61	0.66
1:AAA:323:ILE:HG13	1:AAA:323:ILE:O	1.96	0.65
1:AAA:53:MET:HE3	1:AAA:82:MET:HG3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:141:SER:OG	1:BBB:310:THR:HG22	1.97	0.64
1:BBB:178:ILE:HD11	1:BBB:230:TYR:CD2	2.32	0.64
1:AAA:285:THR:O	1:AAA:287:THR:N	2.30	0.64
1:AAA:29:ILE:HD13	1:AAA:40:TYR:CD2	2.33	0.64
1:BBB:265:ALA:O	1:BBB:267:LEU:N	2.32	0.63
1:AAA:258:THR:HG22	2:AAA:401:PYC:O8	1.99	0.63
1:BBB:174:SER:C	1:BBB:175:PHE:O	2.42	0.63
1:AAA:53:MET:HE1	1:AAA:64:GLY:HA3	1.81	0.63
1:AAA:208:ASN:O	1:AAA:210:LYS:HE2	1.99	0.63
1:BBB:327:ASP:O	1:BBB:330:LYS:NZ	2.30	0.63
1:AAA:126:ILE:HB	1:AAA:142:ILE:HD11	1.79	0.62
1:BBB:141:SER:CB	1:BBB:310:THR:HG22	2.29	0.62
1:AAA:175:PHE:HB3	1:AAA:224:VAL:HA	1.80	0.62
1:BBB:73:LYS:O	1:BBB:75:ALA:N	2.32	0.62
1:AAA:184:LEU:HD23	1:AAA:186:VAL:HG23	1.81	0.62
1:BBB:108:VAL:HG21	1:BBB:117:ILE:HG12	1.82	0.62
1:AAA:196:LEU:CD2	1:AAA:243:VAL:HG21	2.30	0.61
1:AAA:169:ILE:HD11	1:AAA:175:PHE:CD2	2.35	0.61
1:AAA:48:VAL:O	1:AAA:52:LEU:HD12	2.00	0.61
1:AAA:203:ILE:HA	1:AAA:206:LEU:HD22	1.82	0.60
1:BBB:192:GLN:NE2	1:BBB:196:LEU:HD11	2.16	0.60
1:AAA:35:ALA:N	1:AAA:122:PRO:HG3	2.17	0.60
1:AAA:190:THR:O	1:AAA:193:VAL:HG22	2.02	0.60
1:AAA:299:VAL:O	1:AAA:301:GLU:N	2.35	0.60
1:BBB:232:GLU:HA	1:BBB:240:TYR:HA	1.82	0.60
1:BBB:293:VAL:HG12	1:BBB:294:LEU:H	1.66	0.60
1:AAA:188:VAL:CG1	1:AAA:229:ILE:HD11	2.32	0.59
1:BBB:45:LEU:O	1:BBB:47:TYR:N	2.35	0.59
1:BBB:91:CYS:SG	1:BBB:94:GLY:N	2.76	0.59
1:AAA:329:LEU:O	1:AAA:332:GLY:N	2.36	0.59
1:BBB:170:SER:HB2	1:BBB:176:PHE:CE2	2.37	0.58
1:BBB:172:GLY:HA3	1:BBB:262:ALA:HB2	1.84	0.58
1:BBB:179:ILE:HD12	1:BBB:183:GLU:OE2	2.04	0.58
1:BBB:91:CYS:O	1:BBB:93:HIS:N	2.36	0.58
1:BBB:226:LEU:HD13	1:BBB:246:PHE:HB3	1.84	0.57
1:BBB:88:LEU:HD12	1:BBB:90:MET:O	2.04	0.57
1:AAA:300:GLY:O	1:AAA:301:GLU:HG2	2.05	0.57
1:BBB:148:PHE:C	1:BBB:149:LEU:HD13	2.30	0.57
1:AAA:258:THR:N	2:AAA:401:PYC:O8	2.36	0.56
1:BBB:53:MET:HE3	1:BBB:82:MET:HG3	1.87	0.56
1:AAA:29:ILE:C	1:AAA:29:ILE:HD12	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:149:LEU:HD13	1:BBB:149:LEU:N	2.20	0.56
1:BBB:207:ILE:O	1:BBB:207:ILE:CG2	2.52	0.56
1:BBB:39:LYS:HG3	1:BBB:40:TYR:N	2.19	0.56
1:BBB:29:ILE:HD11	1:BBB:68:THR:HG23	1.87	0.56
1:AAA:133:GLU:O	1:AAA:135:GLU:N	2.39	0.56
1:AAA:158:VAL:HG13	1:AAA:159:PRO:N	2.22	0.55
1:AAA:65:SER:OG	1:AAA:66:ILE:N	2.40	0.55
1:AAA:158:VAL:O	1:AAA:160:SER:N	2.40	0.55
1:AAA:196:LEU:HD22	1:AAA:243:VAL:HG21	1.89	0.55
1:BBB:15:MET:HE3	1:BBB:312:GLY:O	2.06	0.55
1:BBB:293:VAL:HG13	1:BBB:307:PRO:HA	1.89	0.54
1:AAA:121:ALA:N	1:AAA:122:PRO:HA	2.21	0.54
1:BBB:180:HIS:HA	1:BBB:230:TYR:CE1	2.42	0.54
1:BBB:130:VAL:O	1:BBB:130:VAL:CG2	2.55	0.54
1:AAA:131:MET:SD	1:AAA:131:MET:N	2.81	0.54
1:BBB:53:MET:HE1	1:BBB:64:GLY:HA3	1.90	0.54
1:AAA:215:HIS:N	1:AAA:221:ILE:HD11	2.22	0.54
1:BBB:112:GLU:HB2	1:BBB:113:PRO:HD3	1.90	0.54
1:BBB:293:VAL:HG11	1:BBB:305:ILE:HB	1.89	0.54
1:AAA:50:THR:HG22	1:AAA:54:HIS:CE1	2.43	0.54
1:BBB:133:GLU:O	1:BBB:135:GLU:N	2.36	0.53
1:AAA:327:ASP:O	1:AAA:330:LYS:NZ	2.27	0.53
1:BBB:176:PHE:CD1	1:BBB:176:PHE:C	2.86	0.53
1:BBB:70:SER:O	1:BBB:120:GLU:OE1	2.27	0.53
1:BBB:184:LEU:HD23	1:BBB:199:LEU:HD23	1.91	0.53
1:AAA:121:ALA:HB3	1:AAA:123:ALA:N	2.23	0.53
1:AAA:142:ILE:HD13	1:AAA:143:THR:N	2.23	0.53
1:AAA:229:ILE:HG13	1:AAA:243:VAL:HG22	1.90	0.53
1:BBB:262:ALA:O	1:BBB:265:ALA:HB3	2.09	0.52
1:AAA:61:ASP:HA	1:AAA:250:GLN:HB2	1.92	0.52
1:BBB:241:LYS:HG2	1:BBB:282:GLU:HB2	1.92	0.52
1:BBB:246:PHE:O	1:BBB:250:GLN:N	2.43	0.52
1:AAA:158:VAL:HB	1:AAA:163:LYS:HD2	1.90	0.52
1:BBB:230:TYR:CD1	1:BBB:230:TYR:C	2.88	0.52
1:BBB:184:LEU:HD12	1:BBB:184:LEU:N	2.26	0.51
1:BBB:212:LYS:CB	1:BBB:223:THR:HB	2.40	0.51
1:AAA:289:PHE:HB3	1:AAA:309:ILE:HD11	1.93	0.51
1:AAA:122:PRO:O	1:AAA:124:GLY:N	2.43	0.51
1:BBB:176:PHE:HD1	1:BBB:177:ALA:N	2.09	0.51
1:BBB:264:LEU:HD21	1:BBB:307:PRO:HB3	1.92	0.51
1:AAA:3:PHE:CE2	1:AAA:322:VAL:HG21	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:194:ASP:O	1:BBB:197:LYS:HG2	2.11	0.51
1:AAA:45:LEU:O	1:AAA:48:VAL:HG22	2.11	0.50
1:AAA:53:MET:HE1	1:AAA:64:GLY:CA	2.40	0.50
1:AAA:196:LEU:HD23	1:AAA:243:VAL:HG21	1.93	0.50
1:BBB:258:THR:HG22	2:BBB:401:PYC:C1	2.42	0.50
1:BBB:231:ASP:O	1:BBB:232:GLU:HB2	2.11	0.50
1:BBB:20:ARG:NE	1:BBB:62:MET:HE2	2.26	0.50
1:BBB:155:LYS:O	1:BBB:167:PHE:CE2	2.65	0.50
1:BBB:125:LEU:C	1:BBB:125:LEU:HD23	2.37	0.50
1:BBB:67:ILE:HG21	1:BBB:107:MET:HE1	1.94	0.50
1:BBB:184:LEU:HD22	1:BBB:186:VAL:HG13	1.94	0.50
1:AAA:195:VAL:O	1:AAA:198:LYS:HG2	2.12	0.50
1:AAA:60:ASN:C	1:AAA:60:ASN:HD22	2.20	0.49
1:AAA:213:VAL:O	1:AAA:222:LYS:HG3	2.12	0.49
1:BBB:68:THR:N	1:BBB:78:GLY:O	2.44	0.49
1:BBB:184:LEU:HD11	1:BBB:186:VAL:HG22	1.94	0.49
1:BBB:230:TYR:C	1:BBB:230:TYR:HD1	2.21	0.49
1:AAA:275:ILE:HA	1:AAA:293:VAL:O	2.12	0.49
1:BBB:183:GLU:OE2	1:BBB:184:LEU:HG	2.12	0.49
1:AAA:188:VAL:HG13	1:AAA:229:ILE:HD11	1.94	0.49
1:AAA:193:VAL:HG23	1:AAA:194:ASP:H	1.77	0.49
1:AAA:221:ILE:HD13	1:AAA:222:LYS:H	1.77	0.49
1:BBB:232:GLU:HG2	1:BBB:240:TYR:CD2	2.47	0.49
1:BBB:130:VAL:HG12	1:BBB:140:VAL:HG22	1.95	0.49
1:BBB:41:LEU:O	1:BBB:46:ASP:N	2.38	0.49
1:BBB:268:TYR:OH	1:BBB:303:ASP:O	2.28	0.49
1:BBB:141:SER:CA	1:BBB:310:THR:HG22	2.43	0.49
1:BBB:329:LEU:HD12	1:BBB:329:LEU:N	2.27	0.49
1:AAA:72:ASN:HD22	1:AAA:75:ALA:CB	2.23	0.49
1:AAA:190:THR:HA	1:AAA:193:VAL:HG13	1.94	0.49
1:BBB:81:PHE:CD1	1:BBB:91:CYS:HB3	2.48	0.49
1:AAA:175:PHE:CB	1:AAA:224:VAL:HA	2.42	0.48
1:BBB:76:ASP:OD2	1:BBB:118:ASN:N	2.42	0.48
1:AAA:247:GLY:C	1:AAA:249:GLY:H	2.21	0.48
1:BBB:228:GLU:HG3	1:BBB:242:ASN:HD21	1.76	0.48
1:AAA:260:THR:HG22	1:AAA:281:TYR:CD2	2.49	0.48
1:BBB:175:PHE:HE2	1:BBB:226:LEU:N	2.12	0.48
1:AAA:41:LEU:HD13	1:AAA:87:TYR:CE2	2.48	0.48
1:BBB:3:PHE:HB3	1:BBB:322:VAL:HB	1.96	0.48
1:BBB:175:PHE:C	1:BBB:175:PHE:CD2	2.91	0.48
1:BBB:306:ILE:N	1:BBB:306:ILE:HD12	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:49:ARG:HD3	1:AAA:87:TYR:CZ	2.49	0.48
1:AAA:292:ARG:HG2	1:AAA:308:GLU:HG3	1.95	0.47
1:AAA:192:GLN:O	1:AAA:193:VAL:C	2.57	0.47
1:BBB:293:VAL:HG11	1:BBB:305:ILE:CG1	2.44	0.47
1:BBB:91:CYS:SG	1:BBB:91:CYS:O	2.72	0.47
1:BBB:150:TYR:CD2	1:BBB:213:VAL:HG11	2.49	0.47
1:AAA:169:ILE:HD13	1:AAA:170:SER:N	2.29	0.47
1:AAA:204:ARG:HB2	1:AAA:227:VAL:HG23	1.96	0.47
1:AAA:49:ARG:HA	1:AAA:82:MET:HE2	1.96	0.47
1:AAA:206:LEU:HD23	1:AAA:207:ILE:N	2.29	0.47
1:AAA:293:VAL:HG23	1:AAA:305:ILE:CD1	2.44	0.47
1:BBB:142:ILE:N	1:BBB:309:ILE:O	2.42	0.47
1:BBB:178:ILE:HD13	1:BBB:179:ILE:N	2.29	0.47
1:BBB:151:MET:SD	1:BBB:151:MET:C	2.98	0.47
1:AAA:193:VAL:HG23	1:AAA:194:ASP:N	2.30	0.46
1:BBB:34:MET:HE3	1:BBB:80:ILE:HD11	1.97	0.46
1:BBB:148:PHE:CE2	1:BBB:171:PHE:CD2	3.03	0.46
1:AAA:20:ARG:NH1	1:AAA:52:LEU:O	2.48	0.46
1:BBB:241:LYS:CG	1:BBB:282:GLU:HB2	2.46	0.46
1:AAA:102:ALA:HA	1:AAA:107:MET:HE3	1.98	0.46
1:BBB:184:LEU:HD13	1:BBB:185:GLY:N	2.31	0.46
1:BBB:46:ASP:HB2	1:BBB:47:TYR:CG	2.50	0.46
1:BBB:263:LYS:HD2	1:BBB:281:TYR:CE2	2.51	0.46
1:BBB:118:ASN:HB3	1:BBB:125:LEU:HD21	1.97	0.46
1:BBB:152:GLU:O	1:BBB:153:ASP:HB2	2.15	0.46
1:BBB:183:GLU:N	1:BBB:183:GLU:OE1	2.49	0.46
1:AAA:149:LEU:HD23	1:AAA:266:THR:HB	1.98	0.45
1:AAA:179:ILE:O	1:AAA:229:ILE:HA	2.16	0.45
1:BBB:140:VAL:O	1:BBB:310:THR:HA	2.16	0.45
1:BBB:226:LEU:HD12	1:BBB:244:VAL:CG1	2.47	0.45
1:AAA:290:LYS:HD2	1:AAA:290:LYS:N	2.30	0.45
1:BBB:79:ILE:HD11	1:BBB:81:PHE:CE2	2.52	0.45
1:AAA:188:VAL:O	1:AAA:188:VAL:HG23	2.17	0.45
1:AAA:193:VAL:HA	1:AAA:196:LEU:HD13	1.99	0.45
1:AAA:229:ILE:HD12	1:AAA:230:TYR:N	2.31	0.45
1:AAA:234:SER:H	1:AAA:241:LYS:HE2	1.82	0.45
1:AAA:17:GLU:OE1	1:AAA:252:ASP:HA	2.16	0.45
1:AAA:61:ASP:O	1:AAA:62:MET:O	2.35	0.45
1:BBB:196:LEU:HD12	1:BBB:196:LEU:H	1.82	0.45
1:AAA:242:ASN:HB3	1:AAA:281:TYR:CE1	2.52	0.45
1:BBB:13:HIS:O	1:BBB:13:HIS:CG	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:26:ILE:HD13	1:AAA:26:ILE:H	1.82	0.44
1:AAA:112:GLU:O	1:AAA:132:VAL:CG2	2.65	0.44
1:AAA:216:PRO:HB3	1:AAA:301:GLU:HG2	1.98	0.44
1:BBB:3:PHE:C	1:BBB:5:LYS:H	2.25	0.44
1:BBB:30:ASN:O	1:BBB:31:GLY:O	2.35	0.44
1:BBB:141:SER:HA	1:BBB:310:THR:HG22	1.99	0.44
1:BBB:74:GLU:O	1:BBB:75:ALA:HB2	2.17	0.44
1:AAA:10:ILE:CD1	1:AAA:23:VAL:HG21	2.47	0.44
1:AAA:160:SER:HA	1:AAA:161:LEU:HA	1.71	0.44
1:AAA:261:SER:HA	1:AAA:264:LEU:CD2	2.48	0.44
1:BBB:15:MET:HG3	1:BBB:289:PHE:CE1	2.52	0.44
1:AAA:179:ILE:HD13	1:AAA:229:ILE:HA	1.99	0.44
1:BBB:101:VAL:O	1:BBB:102:ALA:C	2.61	0.44
1:BBB:172:GLY:CA	1:BBB:262:ALA:HB2	2.47	0.44
1:BBB:242:ASN:HB3	1:BBB:281:TYR:HE1	1.79	0.44
1:AAA:13:HIS:HA	1:AAA:18:PRO:HA	1.99	0.44
1:AAA:158:VAL:HG12	1:AAA:163:LYS:HE3	1.99	0.44
1:AAA:195:VAL:HG22	1:AAA:196:LEU:HD12	1.99	0.44
1:BBB:178:ILE:CD1	1:BBB:230:TYR:CD2	3.00	0.43
1:AAA:175:PHE:HB3	1:AAA:224:VAL:HG12	2.00	0.43
1:AAA:195:VAL:O	1:AAA:199:LEU:HB2	2.18	0.43
1:AAA:156:LEU:CB	1:AAA:164:THR:HG23	2.47	0.43
1:AAA:220:HIS:CG	1:AAA:221:ILE:N	2.87	0.43
1:BBB:264:LEU:C	1:BBB:265:ALA:O	2.62	0.43
1:BBB:34:MET:HE1	1:BBB:68:THR:HB	2.00	0.43
1:AAA:48:VAL:HG23	1:AAA:49:ARG:N	2.34	0.43
1:AAA:192:GLN:O	1:AAA:195:VAL:HG22	2.18	0.43
1:AAA:220:HIS:CD2	1:AAA:221:ILE:N	2.87	0.43
1:BBB:37:LYS:O	1:BBB:40:TYR:HB3	2.19	0.43
1:AAA:53:MET:HE1	1:AAA:64:GLY:N	2.34	0.43
1:BBB:279:PHE:CD1	1:BBB:279:PHE:C	2.96	0.43
1:AAA:284:ILE:HG23	1:AAA:285:THR:HG23	2.01	0.42
1:BBB:61:ASP:HA	1:BBB:250:GLN:HB2	2.00	0.42
1:BBB:237:GLU:O	1:BBB:280:VAL:HG21	2.19	0.42
1:BBB:323:ILE:HG23	1:BBB:330:LYS:HB2	2.00	0.42
1:AAA:66:ILE:HD11	1:AAA:82:MET:SD	2.59	0.42
1:BBB:134:ASN:HB2	1:BBB:135:GLU:OE1	2.19	0.42
1:BBB:21:ILE:HD13	1:BBB:101:VAL:HG21	2.01	0.42
1:BBB:176:PHE:C	1:BBB:176:PHE:HD1	2.28	0.42
1:BBB:145:VAL:HG11	1:BBB:173:GLY:HA2	2.00	0.42
1:BBB:207:ILE:C	1:BBB:208:ASN:HD22	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:242:ASN:CB	1:BBB:281:TYR:CE1	3.01	0.42
1:AAA:112:GLU:OE1	1:AAA:134:ASN:O	2.37	0.42
1:BBB:79:ILE:HD11	1:BBB:81:PHE:CZ	2.54	0.42
1:AAA:151:MET:O	1:AAA:152:GLU:HB3	2.19	0.42
1:AAA:217:GLU:C	1:AAA:219:GLU:H	2.27	0.42
1:AAA:220:HIS:O	1:AAA:221:ILE:C	2.63	0.42
1:BBB:184:LEU:CD1	1:BBB:186:VAL:HG22	2.49	0.42
1:AAA:31:GLY:O	1:AAA:32:GLU:CB	2.67	0.42
1:AAA:267:LEU:O	1:AAA:269:LYS:N	2.53	0.42
1:BBB:247:GLY:C	1:BBB:249:GLY:H	2.26	0.42
1:AAA:44:ASN:CB	1:AAA:45:LEU:HD12	2.49	0.42
1:AAA:229:ILE:HD12	1:AAA:229:ILE:C	2.45	0.42
1:BBB:254:SER:HB2	1:BBB:289:PHE:CE2	2.55	0.42
1:AAA:19:THR:HA	1:AAA:63:PHE:O	2.20	0.42
1:BBB:49:ARG:HA	1:BBB:82:MET:HE2	2.02	0.41
1:AAA:179:ILE:CD1	1:AAA:229:ILE:HG22	2.50	0.41
1:AAA:187:LYS:O	1:AAA:192:GLN:NE2	2.53	0.41
1:BBB:176:PHE:CE1	1:BBB:178:ILE:HB	2.55	0.41
1:AAA:221:ILE:HG12	1:AAA:222:LYS:N	2.35	0.41
1:BBB:44:ASN:N	1:BBB:46:ASP:OD1	2.53	0.41
1:AAA:229:ILE:CG1	1:AAA:243:VAL:HG22	2.50	0.41
1:AAA:305:ILE:HD13	1:AAA:306:ILE:N	2.35	0.41
1:BBB:103:VAL:HG13	1:BBB:104:GLU:N	2.36	0.41
1:AAA:34:MET:HG2	1:AAA:120:GLU:O	2.21	0.41
1:BBB:3:PHE:O	1:BBB:323:ILE:O	2.38	0.41
1:BBB:279:PHE:C	1:BBB:279:PHE:HD1	2.28	0.41
1:AAA:26:ILE:HD13	1:AAA:26:ILE:N	2.36	0.41
1:AAA:34:MET:HB3	1:AAA:122:PRO:HB3	2.02	0.41
1:AAA:260:THR:HG22	1:AAA:281:TYR:CG	2.56	0.41
1:BBB:172:GLY:O	1:BBB:258:THR:OG1	2.30	0.41
1:BBB:295:GLU:C	1:BBB:296:GLU:HG3	2.45	0.41
1:AAA:215:HIS:H	1:AAA:221:ILE:HD11	1.86	0.41
1:AAA:44:ASN:HB3	1:AAA:45:LEU:HD12	2.03	0.40
1:AAA:221:ILE:CD1	1:AAA:222:LYS:H	2.34	0.40
1:AAA:233:PRO:HA	1:AAA:241:LYS:HG3	2.02	0.40
1:BBB:152:GLU:O	1:BBB:153:ASP:CB	2.69	0.40
1:BBB:160:SER:HA	1:BBB:161:LEU:HA	1.73	0.40
1:BBB:226:LEU:HD12	1:BBB:244:VAL:HG12	2.03	0.40
1:BBB:130:VAL:O	1:BBB:130:VAL:HG23	2.21	0.40
1:BBB:133:GLU:C	1:BBB:134:ASN:ND2	2.79	0.40
1:BBB:175:PHE:CZ	1:BBB:225:ASP:N	2.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:190:THR:N	1:AAA:284:ILE:HD11	2.36	0.40
1:BBB:255:PRO:HD2	1:BBB:289:PHE:CD2	2.56	0.40
1:AAA:81:PHE:CD2	1:AAA:91:CYS:HB3	2.55	0.40
1:AAA:241:LYS:HA	1:AAA:282:GLU:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	333/343 (97%)	237 (71%)	57 (17%)	39 (12%)	0	0
1	BBB	333/343 (97%)	242 (73%)	54 (16%)	37 (11%)	0	0
All	All	666/686 (97%)	479 (72%)	111 (17%)	76 (11%)	0	0

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	32	GLU
1	AAA	62	MET
1	AAA	75	ALA
1	AAA	123	ALA
1	AAA	134	ASN
1	AAA	153	ASP
1	AAA	159	PRO
1	AAA	218	LEU
1	AAA	222	LYS
1	AAA	270	LYS
1	AAA	286	GLY
1	AAA	300	GLY
1	BBB	31	GLY
1	BBB	46	ASP

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Mol	Chain	Res	Type
1	BBB	73	LYS
1	BBB	74	GLU
1	BBB	75	ALA
1	BBB	113	PRO
1	BBB	153	ASP
1	BBB	155	LYS
1	BBB	175	PHE
1	BBB	188	VAL
1	BBB	193	VAL
1	BBB	218	LEU
1	BBB	265	ALA
1	AAA	29	ILE
1	AAA	31	GLY
1	AAA	61	ASP
1	AAA	124	GLY
1	AAA	165	ILE
1	AAA	193	VAL
1	AAA	224	VAL
1	AAA	247	GLY
1	AAA	277	GLU
1	AAA	296	GLU
1	AAA	301	GLU
1	BBB	92	GLY
1	BBB	107	MET
1	BBB	156	LEU
1	BBB	163	LYS
1	BBB	165	ILE
1	BBB	210	LYS
1	BBB	212	LYS
1	BBB	266	THR
1	BBB	296	GLU
1	BBB	300	GLY
1	AAA	74	GLU
1	AAA	113	PRO
1	AAA	162	ASN
1	AAA	167	PHE
1	AAA	188	VAL
1	AAA	219	GLU
1	AAA	221	ILE
1	AAA	267	LEU
1	BBB	76	ASP
1	BBB	134	ASN

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Mol	Chain	Res	Type
1	BBB	183	GLU
1	BBB	231	ASP
1	AAA	4	SER
1	AAA	100	THR
1	AAA	209	GLU
1	AAA	276	ASP
1	BBB	130	VAL
1	BBB	256	CYS
1	BBB	298	LYS
1	BBB	331	TYR
1	AAA	330	LYS
1	BBB	154	ALA
1	BBB	232	GLU
1	BBB	299	VAL
1	AAA	297	THR
1	BBB	123	ALA
1	BBB	271	GLY
1	AAA	158	VAL
1	AAA	249	GLY
1	BBB	97	GLY

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	AAA	285/293 (97%)	222 (78%)	63 (22%)	1	1
1	BBB	285/293 (97%)	231 (81%)	54 (19%)	1	2
All	All	570/586 (97%)	453 (80%)	117 (20%)	1	1

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	13	HIS
1	AAA	19	THR
1	AAA	26	ILE

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Mol	Chain	Res	Type
1	AAA	28	GLN
1	AAA	29	ILE
1	AAA	41	LEU
1	AAA	43	ASP
1	AAA	50	THR
1	AAA	52	LEU
1	AAA	60	ASN
1	AAA	65	SER
1	AAA	67	ILE
1	AAA	68	THR
1	AAA	73	LYS
1	AAA	74	GLU
1	AAA	103	VAL
1	AAA	109	GLU
1	AAA	112	GLU
1	AAA	117	ILE
1	AAA	126	ILE
1	AAA	131	MET
1	AAA	136	LYS
1	AAA	139	GLU
1	AAA	142	ILE
1	AAA	149	LEU
1	AAA	153	ASP
1	AAA	159	PRO
1	AAA	165	ILE
1	AAA	169	ILE
1	AAA	175	PHE
1	AAA	179	ILE
1	AAA	184	LEU
1	AAA	194	ASP
1	AAA	199	LEU
1	AAA	201	ILE
1	AAA	202	GLU
1	AAA	206	LEU
1	AAA	207	ILE
1	AAA	210	LYS
1	AAA	211	ILE
1	AAA	213	VAL
1	AAA	221	ILE
1	AAA	224	VAL
1	AAA	225	ASP
1	AAA	229	ILE

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Mol	Chain	Res	Type
1	AAA	239	THR
1	AAA	242	ASN
1	AAA	250	GLN
1	AAA	273	LEU
1	AAA	278	LYS
1	AAA	280	VAL
1	AAA	281	TYR
1	AAA	284	ILE
1	AAA	287	THR
1	AAA	293	VAL
1	AAA	294	LEU
1	AAA	298	LYS
1	AAA	302	PHE
1	AAA	305	ILE
1	AAA	306	ILE
1	AAA	308	GLU
1	AAA	330	LYS
1	AAA	333	PHE
1	BBB	13	HIS
1	BBB	26	ILE
1	BBB	29	ILE
1	BBB	34	MET
1	BBB	46	ASP
1	BBB	68	THR
1	BBB	71	ASN
1	BBB	73	LYS
1	BBB	79	ILE
1	BBB	88	LEU
1	BBB	91	CYS
1	BBB	117	ILE
1	BBB	126	ILE
1	BBB	129	LYS
1	BBB	130	VAL
1	BBB	132	VAL
1	BBB	134	ASN
1	BBB	142	ILE
1	BBB	149	LEU
1	BBB	150	TYR
1	BBB	151	MET
1	BBB	158	VAL
1	BBB	165	ILE
1	BBB	168	ASP

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Mol	Chain	Res	Type
1	BBB	174	SER
1	BBB	176	PHE
1	BBB	178	ILE
1	BBB	180	HIS
1	BBB	182	LYS
1	BBB	184	LEU
1	BBB	190	THR
1	BBB	192	GLN
1	BBB	198	LYS
1	BBB	206	LEU
1	BBB	212	LYS
1	BBB	214	GLN
1	BBB	218	LEU
1	BBB	224	VAL
1	BBB	225	ASP
1	BBB	230	TYR
1	BBB	239	THR
1	BBB	264	LEU
1	BBB	269	LYS
1	BBB	278	LYS
1	BBB	279	PHE
1	BBB	280	VAL
1	BBB	281	TYR
1	BBB	288	MET
1	BBB	290	LYS
1	BBB	294	LEU
1	BBB	298	LYS
1	BBB	303	ASP
1	BBB	305	ILE
1	BBB	330	LYS

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 oligosaccharides 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	1.45	1 (12%)	10,10,10	0.85	0
2	PYC	AAA	401	-	8,8,8	1.54	1 (12%)	10,10,10	0.72	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	-	-	0/4/4/4	0/1/1/1
2	PYC	AAA	401	-	-	4/4/4/4	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	401	PYC	O8-C1	-3.63	1.20	1.30
2	BBB	401	PYC	O8-C1	-3.23	1.21	1.30

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	401	PYC	O7-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
2	AAA	401	PYC	O7-C1-C2-N6
2	AAA	401	PYC	O8-C1-C2-C3
2	AAA	401	PYC	O8-C1-C2-N6

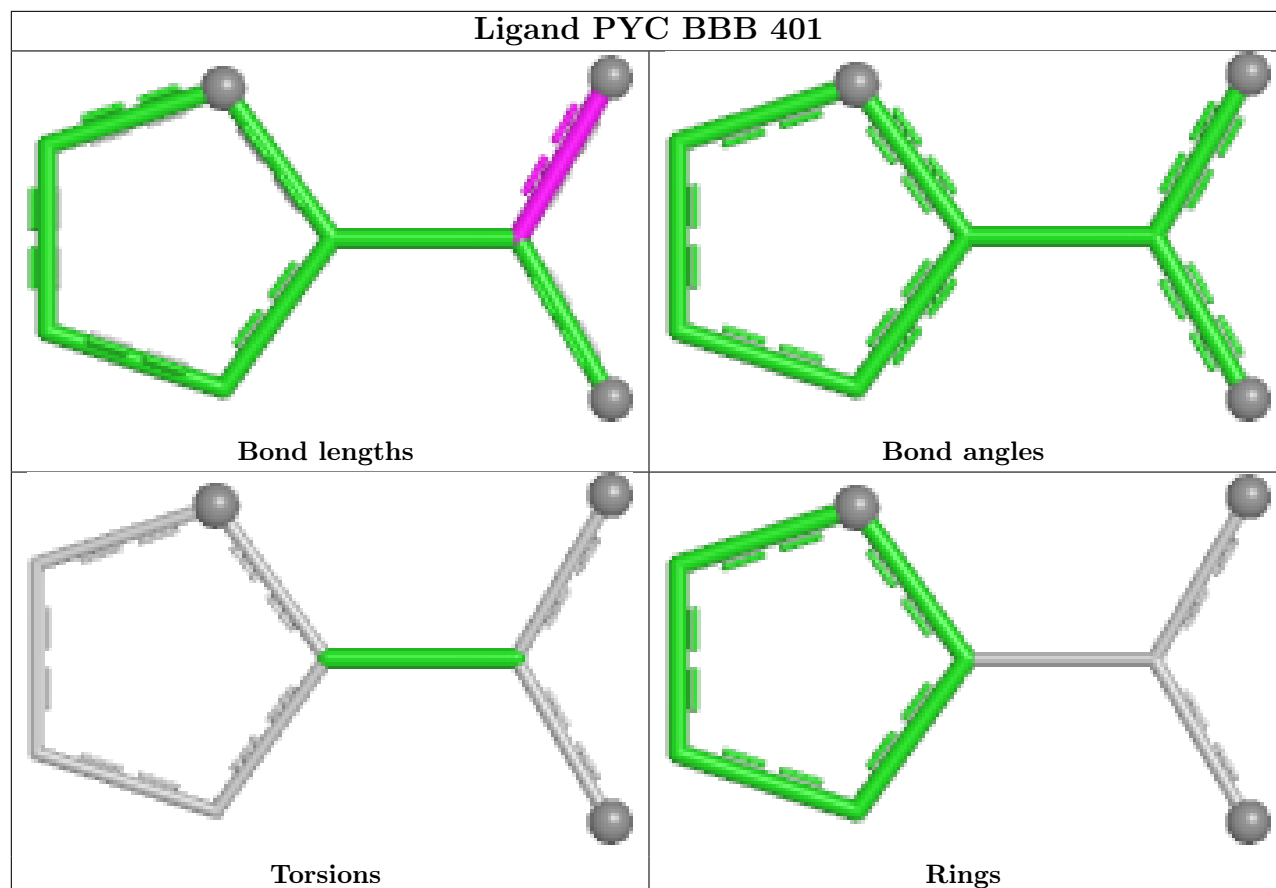
There are no ring outliers.

2 monomers are involved in 3 short contacts:

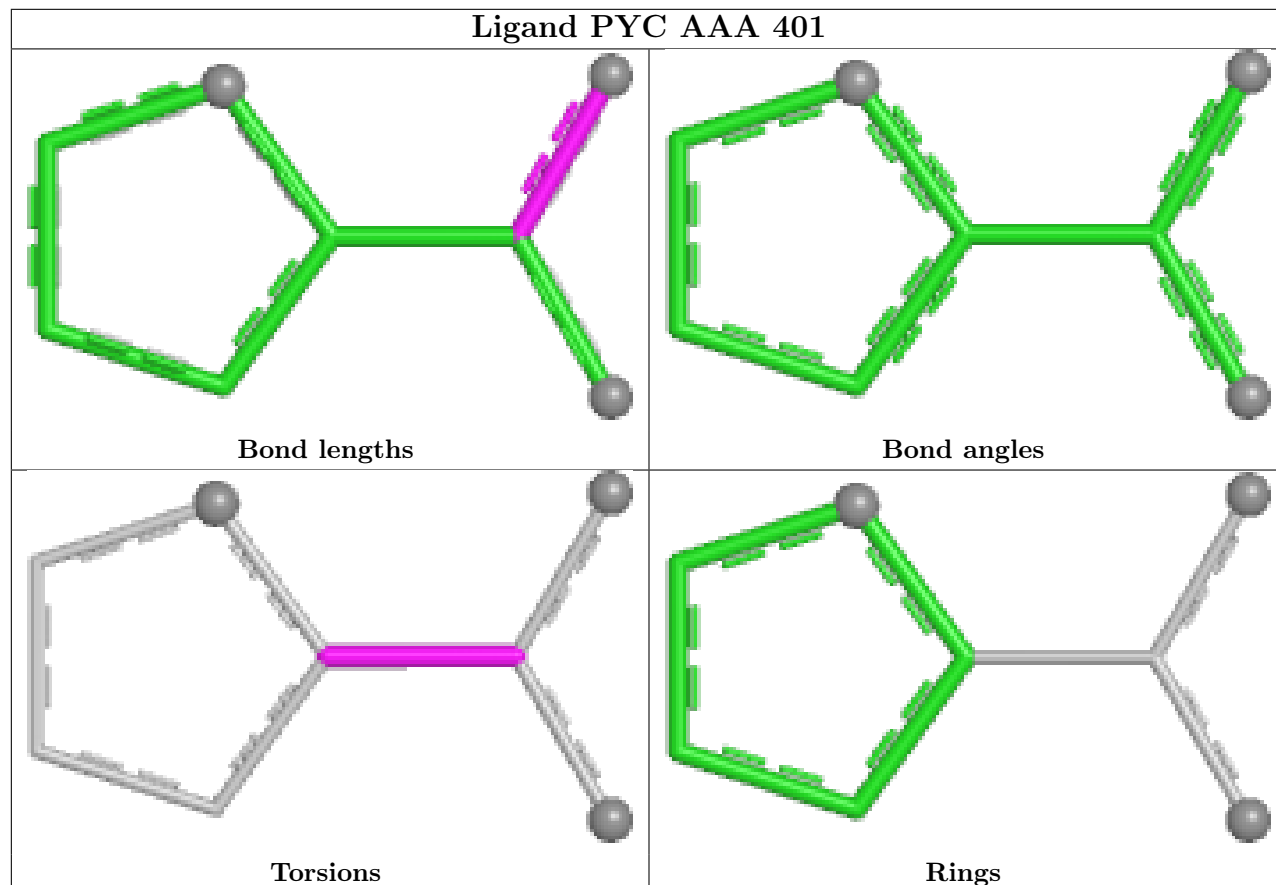
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	401	PYC	1	0
2	AAA	401	PYC	2	0

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 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.

Ligand PYC BBB 401



Ligand PYC AAA 401



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](#)

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%)	-0.41	3 (0%) 81 76	74, 121, 171, 201	0
1	BBB	335/343 (97%)	-0.40	0 100 100	77, 137, 206, 230	0
All	All	670/686 (97%)	-0.41	3 (0%) 88 87	74, 127, 197, 230	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	67	ILE	2.7
1	AAA	195	VAL	2.6
1	AAA	264	LEU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

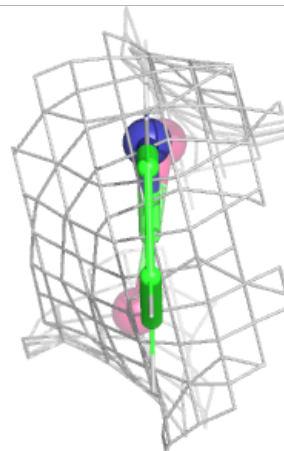
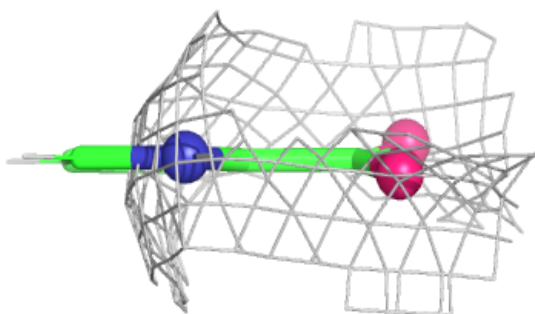
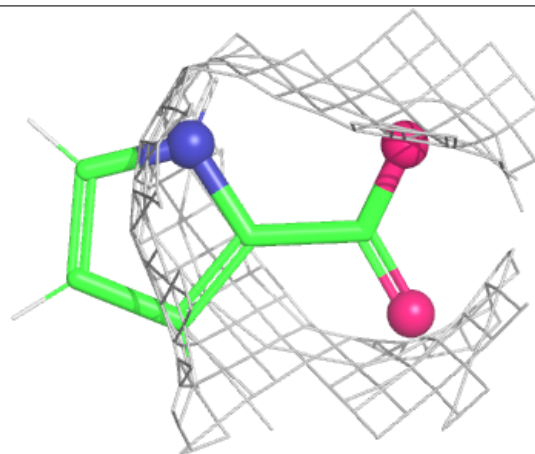
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PYC	BBB	401	8/8	0.90	0.08	154,156,158,159	0
2	PYC	AAA	401	8/8	0.96	0.06	116,123,126,127	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.

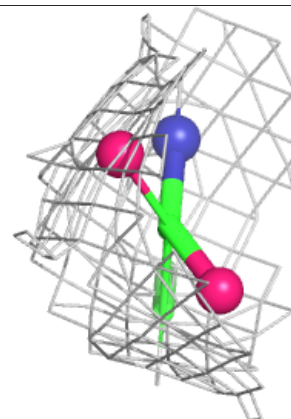
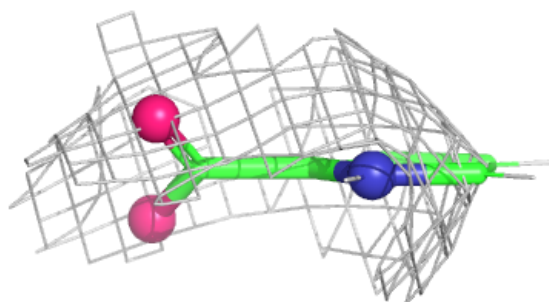
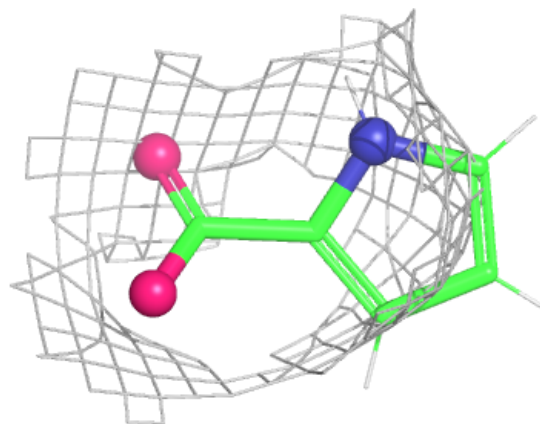
Electron density around PYC BBB 401:

$2mF_o-DF_c$ (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:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.