



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:40 AM UTC

PDB ID : 8BR5 / pdb_00008br5
Title : Discovery of IRAK4 Inhibitor 41
Authors : Schafer, M.; Bothe, U.; Schmidt, N.; Gunther, J.; Nubbemeyer, R.; Siebene-
icher, H.; Ring, S.; Boemer, U.; Peters, M.; Denner, K.; Himmel, H.; Sutter,
A.; Terebesi, I.; Lange, M.; Wenger, A.M.; Guimond, N.; Thaler, T.; Platzek,
J.; Eberspaecher, U.; Steuber, H.; Steinmeyer, A.; Zollner, T.M.
Deposited on : 2022-11-22
Resolution : 2.70 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](#) ①) 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

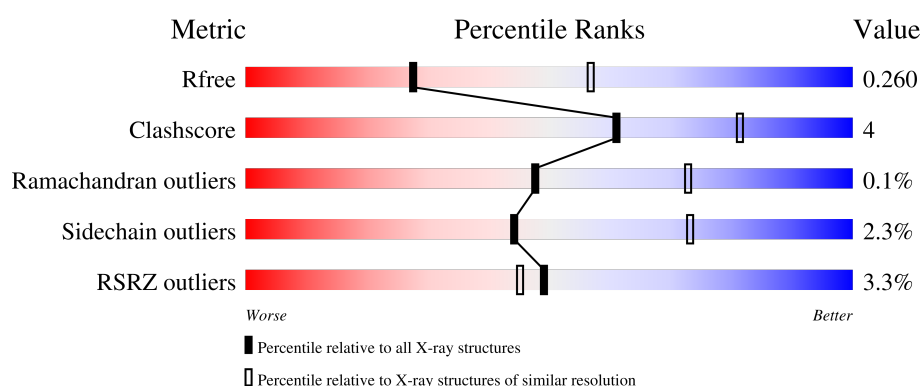
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	299	3% 87% 7% 5%
1	BBB	299	4% 88% 7%
1	CCC	299	2% 81% 14% 5%
1	DDD	299	3% 83% 11% 5%

2 Entry composition [i](#)

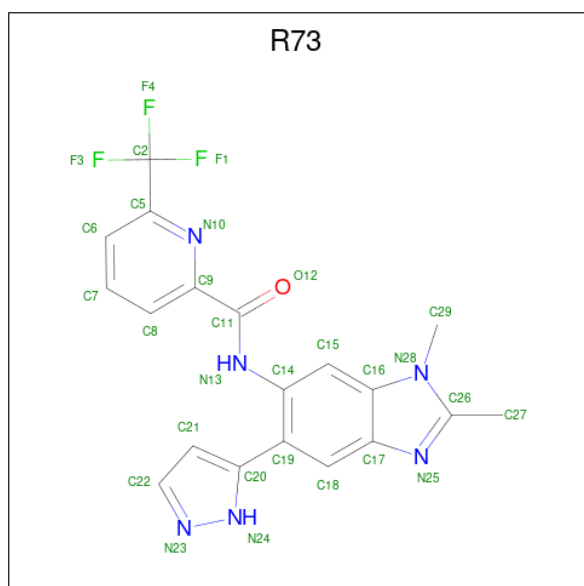
There are 3 unique types of molecules in this entry. The entry contains 9350 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	285	Total	C	N	O	P	S	0	5	0
			2304	1440	388	459	3	14			
1	BBB	286	Total	C	N	O	P	S	0	0	0
			2261	1415	381	448	3	14			
1	CCC	284	Total	C	N	O	P	S	0	0	0
			2256	1413	379	447	3	14			
1	DDD	285	Total	C	N	O	P	S	0	1	0
			2268	1419	382	450	3	14			

- Molecule 2 is {N}-[2,3-dimethyl-6-(1 {H}-pyrazol-5-yl)benzimidazol-5-yl]-6-(trifluoromethyl)pyridine-2-carboxamide (CCD ID: R73) (formula: C₁₉H₁₅F₃N₆O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	F	N	O	0	0
			29	19	3	6	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	BBB	1	Total	C	F	N	O	0	0
			29	19	3	6	1		
2	CCC	1	Total	C	F	N	O	0	0
			29	19	3	6	1		
2	DDD	1	Total	C	F	N	O	0	0
			29	19	3	6	1		

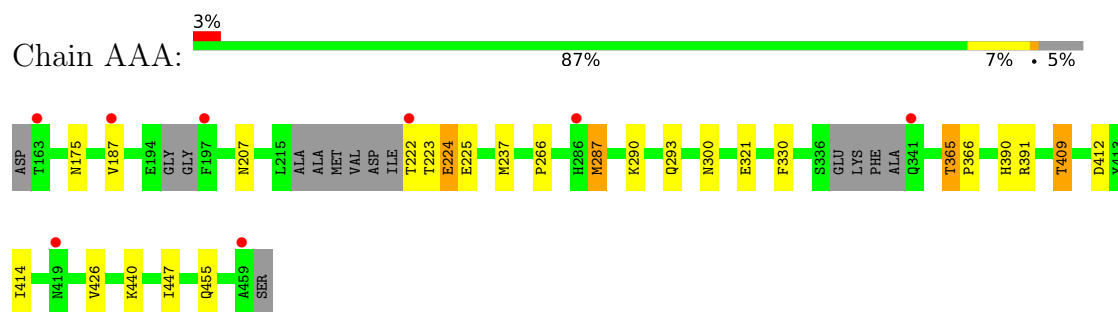
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	48	Total	O	0	0
			48	48		
3	BBB	26	Total	O	0	0
			26	26		
3	CCC	34	Total	O	0	0
			34	34		
3	DDD	37	Total	O	0	0
			37	37		

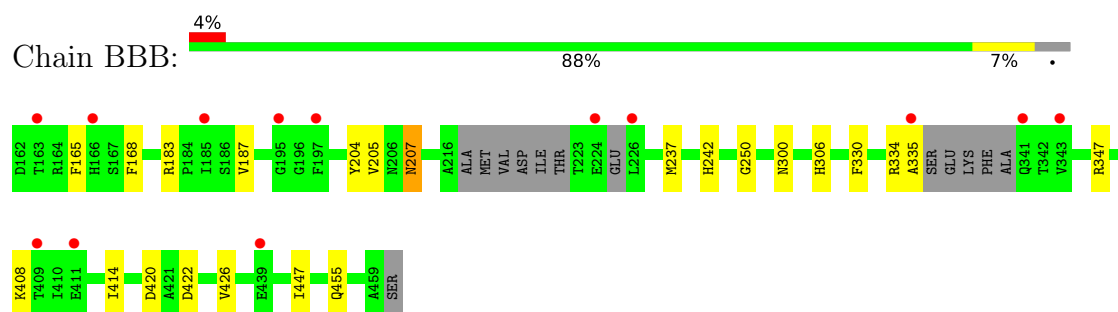
3 Residue-property plots [i](#)

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.

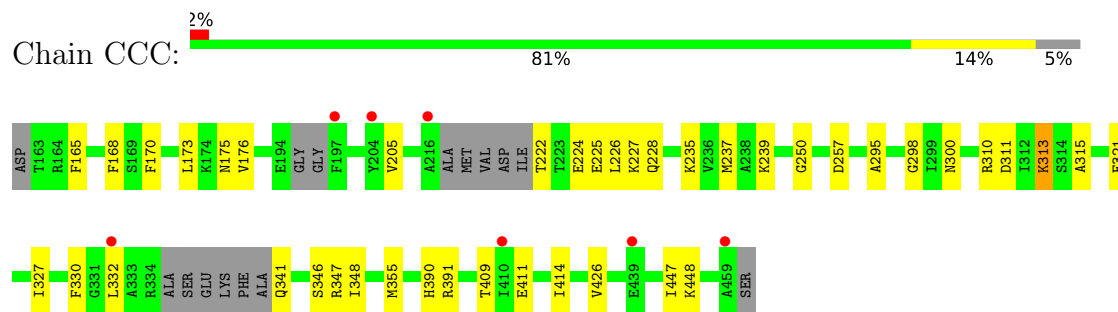
- Molecule 1: Interleukin-1 receptor-associated kinase 4



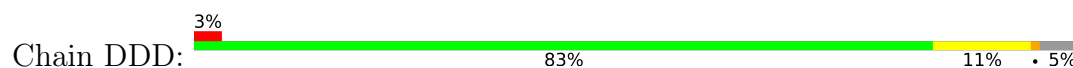
- Molecule 1: Interleukin-1 receptor-associated kinase 4

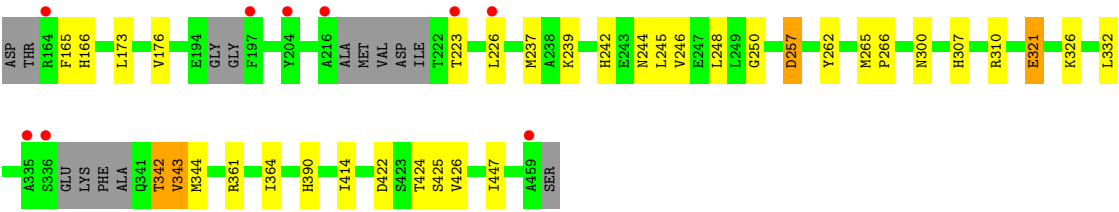


- Molecule 1: Interleukin-1 receptor-associated kinase 4



- Molecule 1: Interleukin-1 receptor-associated kinase 4





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	143.21Å 141.20Å 87.92Å 90.00° 124.46° 90.00°	Depositor
Resolution (Å)	90.58 – 2.70 90.58 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (90.58-2.70) 99.8 (90.58-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.215 , 0.254 0.219 , 0.260	Depositor DCC
R_{free} test set	746 reflections (1.88%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9350	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, R73, TPO

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	0.99	0/2310	1.49	2/3109 (0.1%)
1	BBB	1.00	0/2263	1.48	2/3045 (0.1%)
1	CCC	0.99	0/2258	1.48	0/3039
1	DDD	0.99	0/2270	1.49	1/3055 (0.0%)
All	All	0.99	0/9101	1.48	5/12248 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	242	HIS	CA-C-N	5.45	127.84	120.38
1	BBB	242	HIS	C-N-CA	5.45	127.84	120.38
1	AAA	175	ASN	CA-C-N	5.27	127.90	120.42
1	AAA	175	ASN	C-N-CA	5.27	127.90	120.42
1	DDD	257	ASP	CB-CA-C	5.05	118.46	109.72

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	AAA	2304	0	2251	14	0
1	BBB	2261	0	2219	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CCC	2256	0	2217	25	1
1	DDD	2268	0	2224	23	1
2	AAA	29	0	0	1	0
2	BBB	29	0	0	1	0
2	CCC	29	0	0	1	0
2	DDD	29	0	0	1	0
3	AAA	48	0	0	0	0
3	BBB	26	0	0	0	0
3	CCC	34	0	0	0	0
3	DDD	37	0	0	0	0
All	All	9350	0	8911	76	1

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 4.

All (76) 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:CCC:311:ASP:HB2	1:CCC:332:LEU:HD11	1.61	0.82
1:DDD:343:VAL:HG13	1:DDD:364:ILE:HB	1.78	0.66
1:AAA:287:MET:HE1	1:AAA:290:LYS:HD3	1.80	0.64
1:AAA:390:HIS:O	1:CCC:391:ARG:HA	1.98	0.63
1:CCC:313:LYS:HD2	1:CCC:315:ALA:HB3	1.80	0.62
1:DDD:422:ASP:OD1	1:DDD:425:SER:OG	2.15	0.61
1:AAA:391:ARG:HA	1:CCC:390:HIS:O	2.00	0.61
1:DDD:237:MET:HE2	1:DDD:262:TYR:HE1	1.65	0.60
1:DDD:266:PRO:HG2	1:DDD:321:GLU:HG2	1.83	0.60
2:CCC:501:R73:N24	2:CCC:501:R73:N13	2.49	0.60
1:CCC:332:LEU:H	1:CCC:332:LEU:HD23	1.68	0.58
2:BBB:501:R73:N24	2:BBB:501:R73:N13	2.47	0.58
1:DDD:237:MET:HE2	1:DDD:262:TYR:CE1	2.40	0.57
1:AAA:266:PRO:HG2	1:AAA:321[B]:GLU:HG2	1.87	0.57
1:CCC:224:GLU:O	1:CCC:228:GLN:HG2	2.07	0.55
1:BBB:334:ARG:O	1:BBB:335:ALA:HB3	2.07	0.54
1:BBB:168:PHE:CE1	1:BBB:205:VAL:HG11	2.42	0.54
1:DDD:237:MET:HE3	1:DDD:248:LEU:HB2	1.89	0.54
1:DDD:310:ARG:HD3	1:DDD:332:LEU:O	2.08	0.53
1:CCC:168:PHE:HE2	1:CCC:205:VAL:HG11	1.74	0.53
1:DDD:237:MET:HE3	1:DDD:248:LEU:N	2.24	0.53
1:AAA:224:GLU:H	1:AAA:224:GLU:CD	2.16	0.53
2:DDD:501:R73:N24	2:DDD:501:R73:N13	2.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:168:PHE:CE2	1:CCC:205:VAL:HG11	2.45	0.52
1:CCC:310:ARG:HD3	1:CCC:332:LEU:O	2.10	0.52
1:AAA:222:THR:HB	1:AAA:225:GLU:HB2	1.92	0.51
1:BBB:300:ASN:HA	1:BBB:447:ILE:HG21	1.94	0.50
1:BBB:204:TYR:CE1	1:BBB:207:ASN:HA	2.46	0.50
1:CCC:235:LYS:O	1:CCC:239:LYS:HG3	2.12	0.49
1:AAA:300:ASN:HA	1:AAA:447:ILE:HG21	1.94	0.49
1:CCC:347:ARG:HA	1:CCC:347:ARG:NH2	2.27	0.49
1:DDD:300:ASN:HA	1:DDD:447:ILE:HG21	1.94	0.49
1:CCC:348:ILE:HD12	1:CCC:348:ILE:N	2.28	0.48
1:CCC:237:MET:HE3	1:CCC:330:PHE:CE1	2.49	0.48
1:CCC:332:LEU:H	1:CCC:332:LEU:CD2	2.26	0.48
1:CCC:300:ASN:HA	1:CCC:447:ILE:HG21	1.94	0.47
1:AAA:293[B]:GLN:OE1	1:AAA:455:GLN:HG3	2.14	0.47
1:CCC:347:ARG:HA	1:CCC:347:ARG:CZ	2.44	0.47
1:CCC:222:THR:HB	1:CCC:225:GLU:HB2	1.95	0.47
1:AAA:207:ASN:O	1:BBB:420:ASP:HA	2.14	0.47
1:BBB:168:PHE:HE1	1:BBB:205:VAL:HG11	1.79	0.46
1:CCC:165:PHE:HB3	1:CCC:250:GLY:HA2	1.97	0.46
1:CCC:298:GLY:HA3	1:CCC:327:ILE:CD1	2.46	0.45
2:AAA:501:R73:N13	2:AAA:501:R73:N24	2.64	0.45
1:BBB:237:MET:HE3	1:BBB:330:PHE:CE2	2.52	0.45
1:DDD:342:TPO:O	1:DDD:343:VAL:HB	2.17	0.45
1:AAA:409:THR:HG22	1:AAA:412:ASP:CG	2.42	0.45
1:BBB:165:PHE:HB3	1:BBB:250:GLY:HA2	1.98	0.44
1:CCC:170:PHE:HE2	1:CCC:257:ASP:HB2	1.82	0.44
1:BBB:237:MET:HA	1:BBB:237:MET:HE2	2.00	0.44
1:CCC:237:MET:HA	1:CCC:237:MET:HE2	2.00	0.43
1:BBB:306:HIS:O	1:BBB:335:ALA:HA	2.18	0.43
1:AAA:237:MET:HE3	1:AAA:330:PHE:CE2	2.54	0.43
1:DDD:244:ASN:C	1:DDD:245:LEU:HD12	2.44	0.43
1:DDD:165:PHE:HB3	1:DDD:250:GLY:HA2	2.01	0.43
1:BBB:347:ARG:CZ	1:BBB:347:ARG:HA	2.49	0.42
1:DDD:342:TPO:C	1:DDD:343:VAL:HG12	2.50	0.42
1:CCC:414:ILE:HG12	1:CCC:426:VAL:HG11	2.01	0.42
1:CCC:173:LEU:HA	1:CCC:176:VAL:HG22	2.02	0.42
1:AAA:237:MET:HE2	1:AAA:237:MET:HA	2.01	0.42
1:DDD:237:MET:HE1	1:DDD:246:VAL:HG23	2.01	0.41
1:DDD:226:LEU:HD23	1:DDD:226:LEU:HA	1.88	0.41
1:CCC:295:ALA:O	1:CCC:327:ILE:HD11	2.20	0.41
1:DDD:239:LYS:HD3	1:DDD:307:HIS:CE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:414:ILE:CD1	1:AAA:426:VAL:HG11	2.49	0.41
1:BBB:408:LYS:HE3	1:DDD:390:HIS:NE2	2.35	0.41
1:DDD:265:MET:SD	1:DDD:326:LYS:HD2	2.60	0.41
1:CCC:226:LEU:HD23	1:CCC:226:LEU:HA	1.91	0.41
1:DDD:173:LEU:HA	1:DDD:176:VAL:HG22	2.03	0.41
1:AAA:365:THR:HG22	1:AAA:366:PRO:HD2	2.02	0.41
1:BBB:183:ARG:HB3	1:BBB:187:VAL:CG2	2.51	0.41
1:DDD:237:MET:HE3	1:DDD:248:LEU:H	1.83	0.41
1:DDD:242:HIS:HB3	1:DDD:245:LEU:HD13	2.03	0.41
1:DDD:343:VAL:HG22	1:DDD:344:MET:N	2.36	0.41
1:BBB:414:ILE:CD1	1:BBB:426:VAL:HG11	2.51	0.41
1:DDD:414:ILE:CD1	1:DDD:426:VAL:HG11	2.51	0.40

All (1) 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:CCC:355:MET:O	1:DDD:361:ARG:NH2[4_445]	2.01	0.19

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	279/299 (93%)	268 (96%)	11 (4%)	0	100	100
1	BBB	275/299 (92%)	263 (96%)	12 (4%)	0	100	100
1	CCC	273/299 (91%)	264 (97%)	9 (3%)	0	100	100
1	DDD	275/299 (92%)	265 (96%)	9 (3%)	1 (0%)	30	54
All	All	1102/1196 (92%)	1060 (96%)	41 (4%)	1 (0%)	48	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	DDD	343	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	AAA	253/257 (98%)	246 (97%)	7 (3%)	38	68
1	BBB	246/257 (96%)	243 (99%)	3 (1%)	63	84
1	CCC	247/257 (96%)	239 (97%)	8 (3%)	34	64
1	DDD	248/257 (96%)	243 (98%)	5 (2%)	48	76
All	All	994/1028 (97%)	971 (98%)	23 (2%)	44	73

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	187	VAL
1	AAA	223	THR
1	AAA	224	GLU
1	AAA	287	MET
1	AAA	365	THR
1	AAA	409	THR
1	AAA	440	LYS
1	BBB	207	ASN
1	BBB	422	ASP
1	BBB	455	GLN
1	CCC	175	ASN
1	CCC	227	LYS
1	CCC	313	LYS
1	CCC	321	GLU
1	CCC	341	GLN
1	CCC	409	THR
1	CCC	411	GLU
1	CCC	448	LYS
1	DDD	166	HIS
1	DDD	223	THR
1	DDD	257	ASP

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Mol	Chain	Res	Type
1	DDD	321	GLU
1	DDD	424	THR

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 ⓘ

12 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	SEP	CCC	346	1	8,9,10	0.64	0	7,12,14	1.00	1 (14%)
1	TPO	DDD	342	1	8,10,11	0.89	0	10,14,16	1.02	1 (10%)
1	TPO	DDD	345	1	8,10,11	0.88	0	10,14,16	0.74	0
1	SEP	BBB	346	1	8,9,10	0.63	0	7,12,14	0.70	0
1	TPO	BBB	345	1	8,10,11	0.64	0	10,14,16	0.86	0
1	TPO	CCC	342	1	8,10,11	0.77	0	10,14,16	0.81	0
1	TPO	CCC	345	1	8,10,11	0.77	0	10,14,16	0.81	0
1	SEP	DDD	346	1	8,9,10	0.60	0	7,12,14	0.69	0
1	TPO	AAA	342	1	8,10,11	0.63	0	10,14,16	0.80	0
1	TPO	BBB	342	1	8,10,11	0.80	0	10,14,16	0.76	0
1	TPO	AAA	345	1	8,10,11	0.87	0	10,14,16	0.73	0
1	SEP	AAA	346	1	8,9,10	0.60	0	7,12,14	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
1	SEP	CCC	346	1	-	2/6/8/10	-
1	TPO	DDD	342	1	-	2/9/11/13	-
1	TPO	DDD	345	1	-	3/9/11/13	-
1	SEP	BBB	346	1	-	2/6/8/10	-
1	TPO	BBB	345	1	-	3/9/11/13	-
1	TPO	CCC	342	1	-	1/9/11/13	-
1	TPO	CCC	345	1	-	4/9/11/13	-
1	SEP	DDD	346	1	-	2/6/8/10	-
1	TPO	AAA	342	1	-	2/9/11/13	-
1	TPO	BBB	342	1	-	0/9/11/13	-
1	TPO	AAA	345	1	-	3/9/11/13	-
1	SEP	AAA	346	1	-	2/6/8/10	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	DDD	342	TPO	O-C-CA	-2.10	119.36	124.77
1	CCC	346	SEP	OG-CB-CA	2.03	110.12	108.14

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	AAA	345	TPO	N-CA-CB-OG1
1	AAA	345	TPO	O-C-CA-CB
1	AAA	346	SEP	N-CA-CB-OG
1	AAA	346	SEP	C-CA-CB-OG
1	BBB	345	TPO	N-CA-CB-OG1
1	BBB	345	TPO	O-C-CA-CB
1	BBB	346	SEP	N-CA-CB-OG
1	BBB	346	SEP	C-CA-CB-OG
1	CCC	345	TPO	N-CA-CB-OG1
1	CCC	345	TPO	O-C-CA-CB
1	CCC	346	SEP	N-CA-CB-OG
1	CCC	346	SEP	C-CA-CB-OG
1	DDD	345	TPO	N-CA-CB-OG1
1	DDD	345	TPO	O-C-CA-CB
1	DDD	346	SEP	N-CA-CB-OG
1	DDD	346	SEP	C-CA-CB-OG

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Mol	Chain	Res	Type	Atoms
1	DDD	342	TPO	CG2-CB-OG1-P
1	CCC	345	TPO	CB-OG1-P-O1P
1	AAA	342	TPO	CB-OG1-P-O2P
1	AAA	345	TPO	CA-CB-OG1-P
1	CCC	345	TPO	CA-CB-OG1-P
1	DDD	345	TPO	CA-CB-OG1-P
1	CCC	342	TPO	CB-OG1-P-O2P
1	AAA	342	TPO	O-C-CA-CB
1	DDD	342	TPO	O-C-CA-CB
1	BBB	345	TPO	CB-OG1-P-O1P

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	DDD	342	TPO	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	R73	BBB	501	-	32,32,32	2.51	13 (40%)	48,48,48	1.58	9 (18%)
2	R73	DDD	501	-	32,32,32	2.52	13 (40%)	48,48,48	1.50	8 (16%)
2	R73	AAA	501	-	32,32,32	2.53	13 (40%)	48,48,48	1.57	9 (18%)
2	R73	CCC	501	-	32,32,32	2.57	13 (40%)	48,48,48	1.53	10 (20%)

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	R73	BBB	501	-	-	0/18/18/18	0/4/4/4
2	R73	DDD	501	-	-	1/18/18/18	0/4/4/4
2	R73	AAA	501	-	-	4/18/18/18	0/4/4/4
2	R73	CCC	501	-	-	1/18/18/18	0/4/4/4

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	AAA	501	R73	C19-C20	-7.34	1.34	1.47
2	DDD	501	R73	C19-C20	-7.33	1.34	1.47
2	CCC	501	R73	C19-C20	-7.30	1.34	1.47
2	BBB	501	R73	C19-C20	-7.23	1.35	1.47
2	CCC	501	R73	C2-C5	-5.88	1.40	1.50
2	DDD	501	R73	C2-C5	-5.23	1.41	1.50
2	AAA	501	R73	C2-C5	-5.20	1.41	1.50
2	BBB	501	R73	C2-C5	-5.01	1.41	1.50
2	CCC	501	R73	C18-C17	-4.38	1.33	1.40
2	BBB	501	R73	C18-C17	-4.27	1.33	1.40
2	DDD	501	R73	C18-C17	-4.22	1.33	1.40
2	AAA	501	R73	C18-C17	-3.98	1.33	1.40
2	AAA	501	R73	C9-C11	-3.74	1.40	1.50
2	CCC	501	R73	C9-C11	-3.68	1.40	1.50
2	DDD	501	R73	C9-C11	-3.66	1.40	1.50
2	AAA	501	R73	C16-C17	-3.66	1.34	1.40
2	BBB	501	R73	C9-C11	-3.62	1.40	1.50
2	BBB	501	R73	C16-C17	-3.52	1.34	1.40
2	CCC	501	R73	C16-C17	-3.48	1.34	1.40
2	DDD	501	R73	C16-C17	-3.42	1.34	1.40
2	AAA	501	R73	C15-C16	-3.41	1.34	1.39
2	DDD	501	R73	C15-C16	-3.39	1.34	1.39
2	CCC	501	R73	C15-C16	-3.39	1.34	1.39
2	AAA	501	R73	C14-N13	-3.28	1.35	1.41
2	BBB	501	R73	C15-C16	-3.22	1.34	1.39
2	AAA	501	R73	C16-N28	-3.18	1.33	1.39
2	DDD	501	R73	C21-C22	-3.17	1.33	1.39
2	CCC	501	R73	C16-N28	-3.16	1.33	1.39
2	BBB	501	R73	C21-C22	-3.11	1.33	1.39
2	BBB	501	R73	C17-N25	-3.11	1.33	1.39
2	AAA	501	R73	C17-N25	-3.10	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CCC	501	R73	C21-C22	-3.08	1.33	1.39
2	DDD	501	R73	C16-N28	-3.07	1.34	1.39
2	CCC	501	R73	C17-N25	-3.05	1.33	1.39
2	AAA	501	R73	C21-C22	-3.03	1.33	1.39
2	AAA	501	R73	C21-C20	-2.99	1.33	1.38
2	BBB	501	R73	C14-N13	-2.97	1.35	1.41
2	DDD	501	R73	C17-N25	-2.96	1.33	1.39
2	BBB	501	R73	C16-N28	-2.96	1.34	1.39
2	DDD	501	R73	C21-C20	-2.95	1.33	1.38
2	CCC	501	R73	C14-N13	-2.88	1.36	1.41
2	BBB	501	R73	C27-C26	2.88	1.53	1.49
2	CCC	501	R73	C21-C20	-2.84	1.33	1.38
2	BBB	501	R73	C21-C20	-2.80	1.33	1.38
2	CCC	501	R73	C27-C26	2.60	1.53	1.49
2	DDD	501	R73	C14-N13	-2.55	1.36	1.41
2	CCC	501	R73	C26-N28	-2.47	1.32	1.38
2	DDD	501	R73	C27-C26	2.45	1.53	1.49
2	AAA	501	R73	C26-N28	-2.41	1.32	1.38
2	AAA	501	R73	C27-C26	2.36	1.52	1.49
2	DDD	501	R73	C26-N28	-2.28	1.33	1.38
2	BBB	501	R73	C26-N28	-2.13	1.33	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	BBB	501	R73	C2-C5-N10	4.25	119.65	114.60
2	DDD	501	R73	C2-C5-N10	4.05	119.42	114.60
2	AAA	501	R73	C2-C5-N10	3.91	119.25	114.60
2	AAA	501	R73	N28-C26-N25	-3.56	109.74	113.48
2	BBB	501	R73	N28-C26-N25	-3.53	109.77	113.48
2	CCC	501	R73	N28-C26-N25	-3.48	109.83	113.48
2	CCC	501	R73	C2-C5-N10	3.42	118.68	114.60
2	DDD	501	R73	N28-C26-N25	-3.26	110.06	113.48
2	BBB	501	R73	C9-N10-C5	3.16	122.94	118.78
2	CCC	501	R73	C8-C9-N10	-3.12	119.28	122.92
2	DDD	501	R73	C8-C9-N10	-2.96	119.47	122.92
2	CCC	501	R73	C9-N10-C5	2.91	122.61	118.78
2	AAA	501	R73	C9-N10-C5	2.82	122.49	118.78
2	BBB	501	R73	C8-C9-N10	-2.80	119.65	122.92
2	AAA	501	R73	C17-C16-N28	2.75	107.62	105.68
2	DDD	501	R73	C17-C16-N28	2.74	107.61	105.68
2	DDD	501	R73	C9-N10-C5	2.65	122.27	118.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	AAA	501	R73	C8-C9-N10	-2.64	119.84	122.92
2	BBB	501	R73	C6-C5-N10	-2.61	118.77	122.29
2	CCC	501	R73	C29-N28-C16	2.52	128.60	124.59
2	BBB	501	R73	C17-C16-N28	2.50	107.44	105.68
2	BBB	501	R73	C27-C26-N28	2.47	126.09	122.18
2	DDD	501	R73	C11-C9-N10	2.45	121.30	117.43
2	AAA	501	R73	C6-C5-N10	-2.36	119.10	122.29
2	CCC	501	R73	C29-N28-C26	-2.30	123.82	126.85
2	DDD	501	R73	F1-C2-C5	-2.26	108.46	112.43
2	AAA	501	R73	C27-C26-N28	2.25	125.75	122.18
2	CCC	501	R73	F1-C2-C5	-2.18	108.58	112.43
2	CCC	501	R73	F3-C2-C5	-2.10	108.73	112.43
2	AAA	501	R73	C19-C14-N13	-2.10	114.92	118.70
2	CCC	501	R73	C17-C16-N28	2.08	107.15	105.68
2	BBB	501	R73	C19-C14-N13	-2.08	114.96	118.70
2	BBB	501	R73	F3-C2-C5	-2.03	108.86	112.43
2	AAA	501	R73	C19-C20-N24	2.03	125.39	122.65
2	DDD	501	R73	C6-C5-N10	-2.03	119.55	122.29
2	CCC	501	R73	C6-C5-N10	-2.01	119.57	122.29

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	CCC	501	R73	C14-C19-C20-C21
2	AAA	501	R73	N13-C11-C9-C8
2	AAA	501	R73	O12-C11-C9-C8
2	AAA	501	R73	N13-C11-C9-N10
2	DDD	501	R73	N13-C11-C9-C8
2	AAA	501	R73	O12-C11-C9-N10

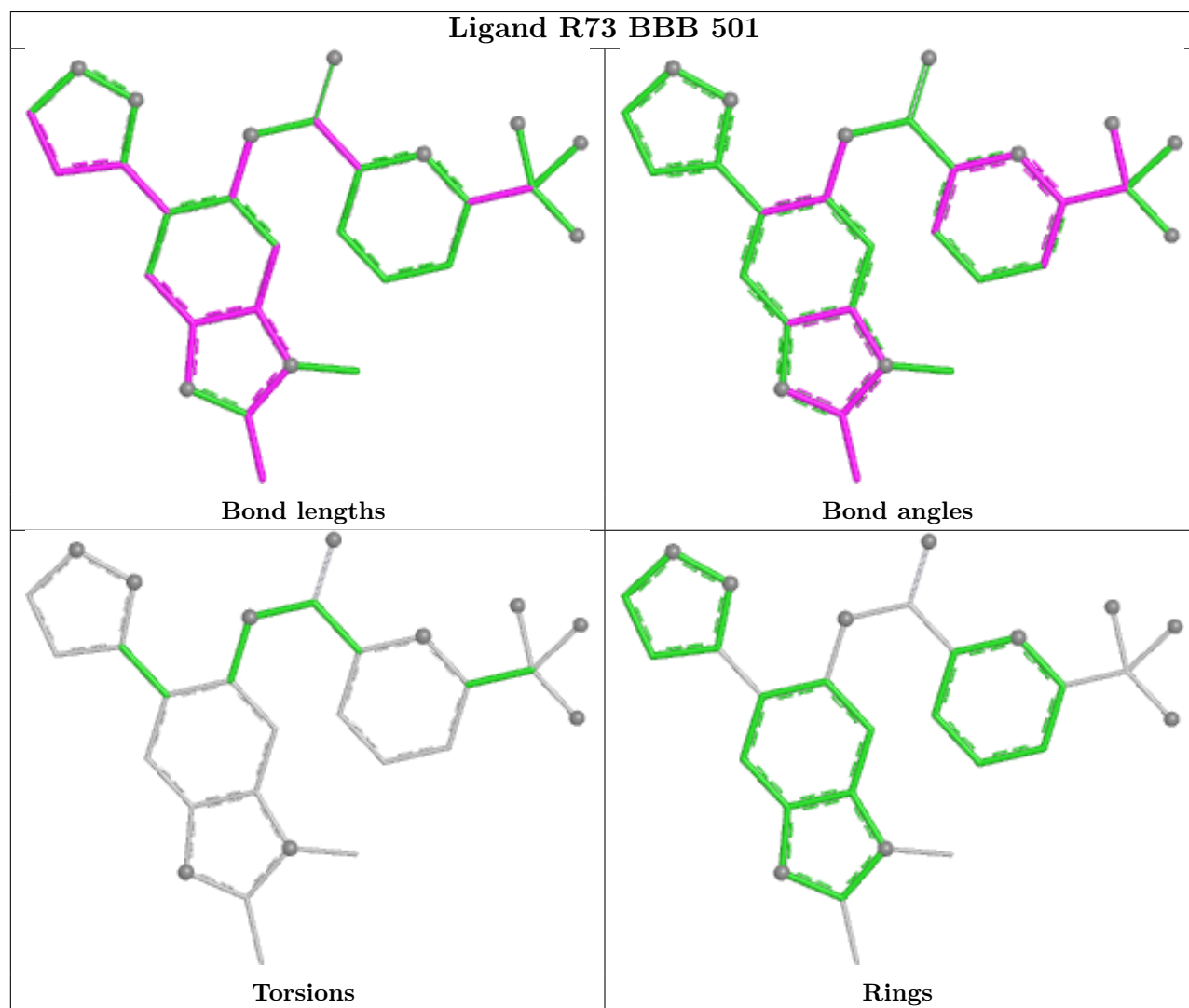
There are no ring outliers.

4 monomers are involved in 4 short contacts:

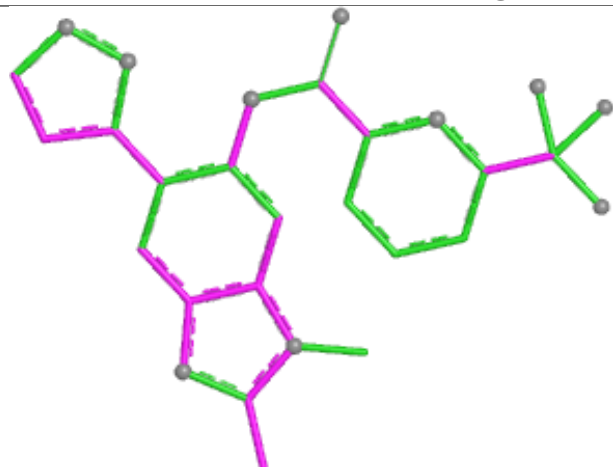
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	501	R73	1	0
2	DDD	501	R73	1	0
2	AAA	501	R73	1	0
2	CCC	501	R73	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

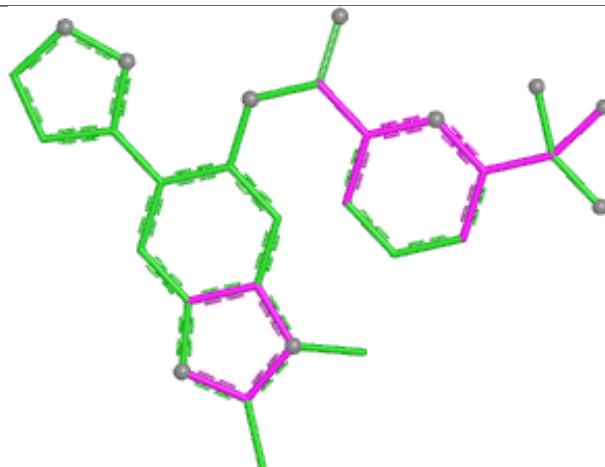
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.



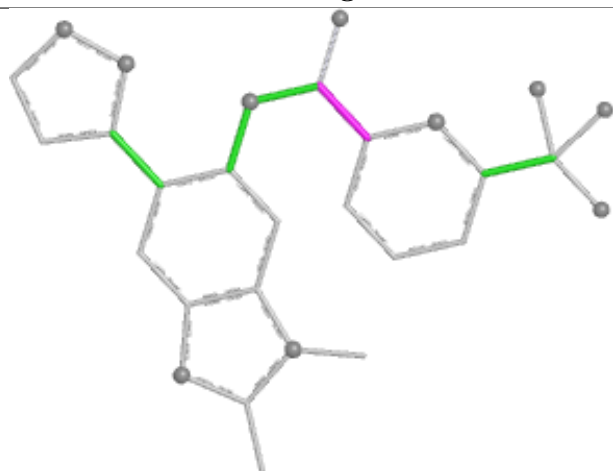
Ligand R73 DDD 501



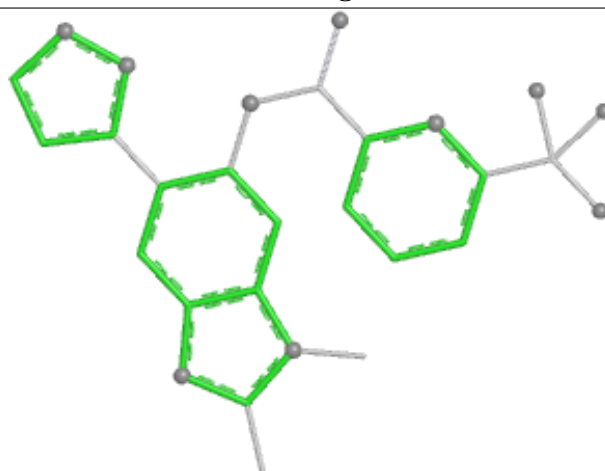
Bond lengths



Bond angles

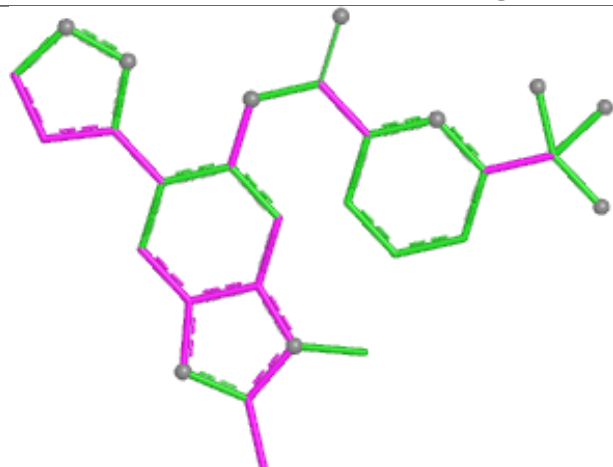


Torsions

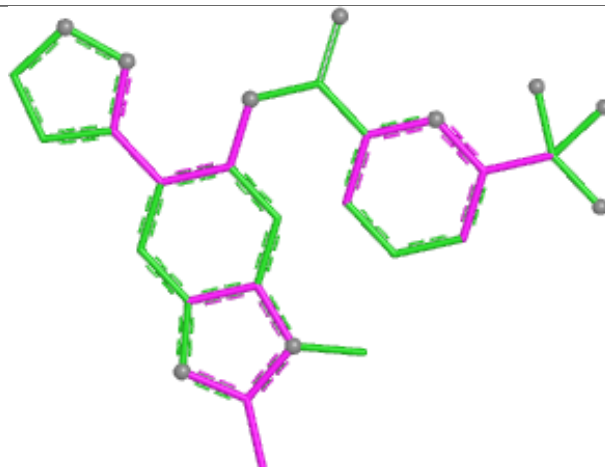


Rings

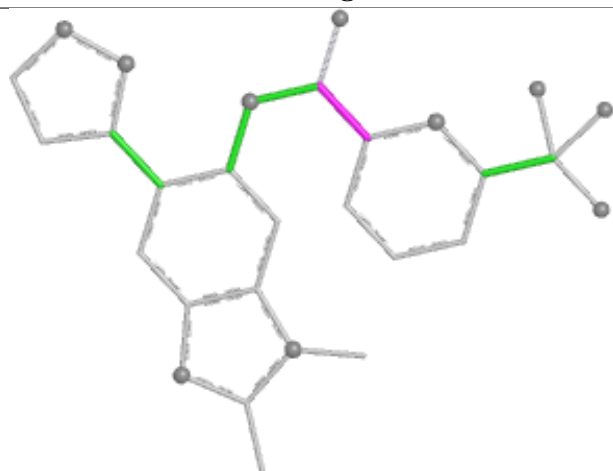
Ligand R73 AAA 501



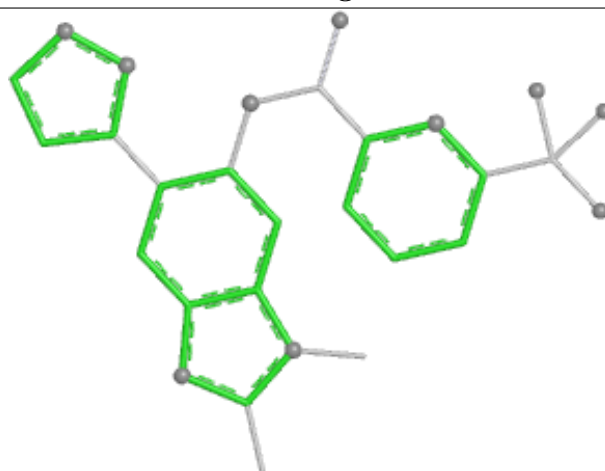
Bond lengths



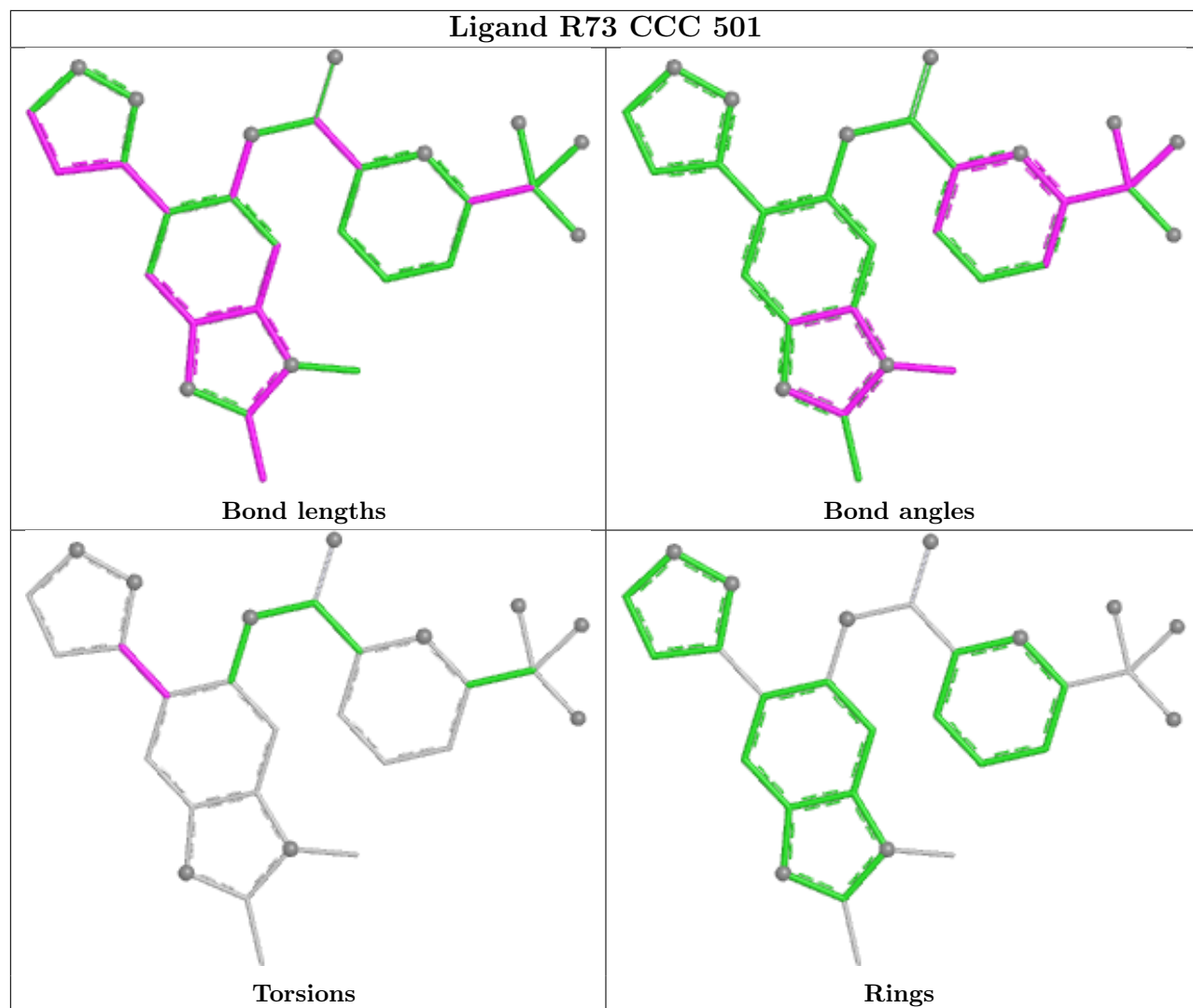
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	282/299 (94%)	0.39	8 (2%) 55 51	23, 55, 93, 119	5 (1%)
1	BBB	283/299 (94%)	0.41	13 (4%) 37 34	33, 60, 103, 136	0
1	CCC	281/299 (93%)	0.41	7 (2%) 58 55	33, 59, 98, 128	0
1	DDD	282/299 (94%)	0.38	9 (3%) 50 46	21, 55, 97, 124	1 (0%)
All	All	1128/1196 (94%)	0.40	37 (3%) 49 45	21, 57, 100, 136	6 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	CCC	197	PHE	4.2
1	BBB	197	PHE	3.7
1	BBB	226	LEU	3.4
1	AAA	197	PHE	3.3
1	BBB	335	ALA	3.3
1	CCC	459	ALA	3.3
1	AAA	187	VAL	3.3
1	AAA	286[A]	HIS	3.2
1	DDD	197	PHE	3.2
1	CCC	439	GLU	3.1
1	AAA	459	ALA	3.0
1	CCC	332	LEU	2.9
1	AAA	419	ASN	2.8
1	BBB	195	GLY	2.6
1	CCC	216	ALA	2.6
1	DDD	336	SER	2.6
1	CCC	410	ILE	2.5
1	DDD	216	ALA	2.5
1	BBB	163	THR	2.4
1	DDD	335	ALA	2.4
1	DDD	204	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	BBB	224	GLU	2.3
1	CCC	204	TYR	2.3
1	DDD	164	ARG	2.3
1	BBB	343	VAL	2.3
1	DDD	459	ALA	2.2
1	BBB	185	ILE	2.2
1	AAA	163	THR	2.2
1	AAA	341	GLN	2.2
1	AAA	222	THR	2.1
1	BBB	409	THR	2.1
1	BBB	411	GLU	2.1
1	BBB	439	GLU	2.1
1	DDD	223	THR	2.1
1	BBB	341	GLN	2.0
1	DDD	226	LEU	2.0
1	BBB	166	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SEP	CCC	346	10/11	0.44	0.12	108,136,156,162	0
1	SEP	AAA	346	10/11	0.57	0.13	82,118,137,142	0
1	TPO	CCC	342	11/12	0.60	0.19	114,129,154,155	0
1	SEP	BBB	346	10/11	0.64	0.11	98,133,149,152	0
1	TPO	AAA	342	11/12	0.66	0.16	88,109,131,132	0
1	SEP	DDD	346	10/11	0.66	0.13	105,109,123,123	0
1	TPO	BBB	342	11/12	0.70	0.18	87,138,168,174	0
1	TPO	DDD	342	11/12	0.78	0.13	116,122,132,133	0
1	TPO	BBB	345	11/12	0.87	0.11	81,94,107,112	0
1	TPO	AAA	345	11/12	0.88	0.12	63,90,97,113	0
1	TPO	CCC	345	11/12	0.90	0.09	74,96,104,108	0
1	TPO	DDD	345	11/12	0.91	0.11	73,80,100,109	0

6.3 Carbohydrates [i](#)

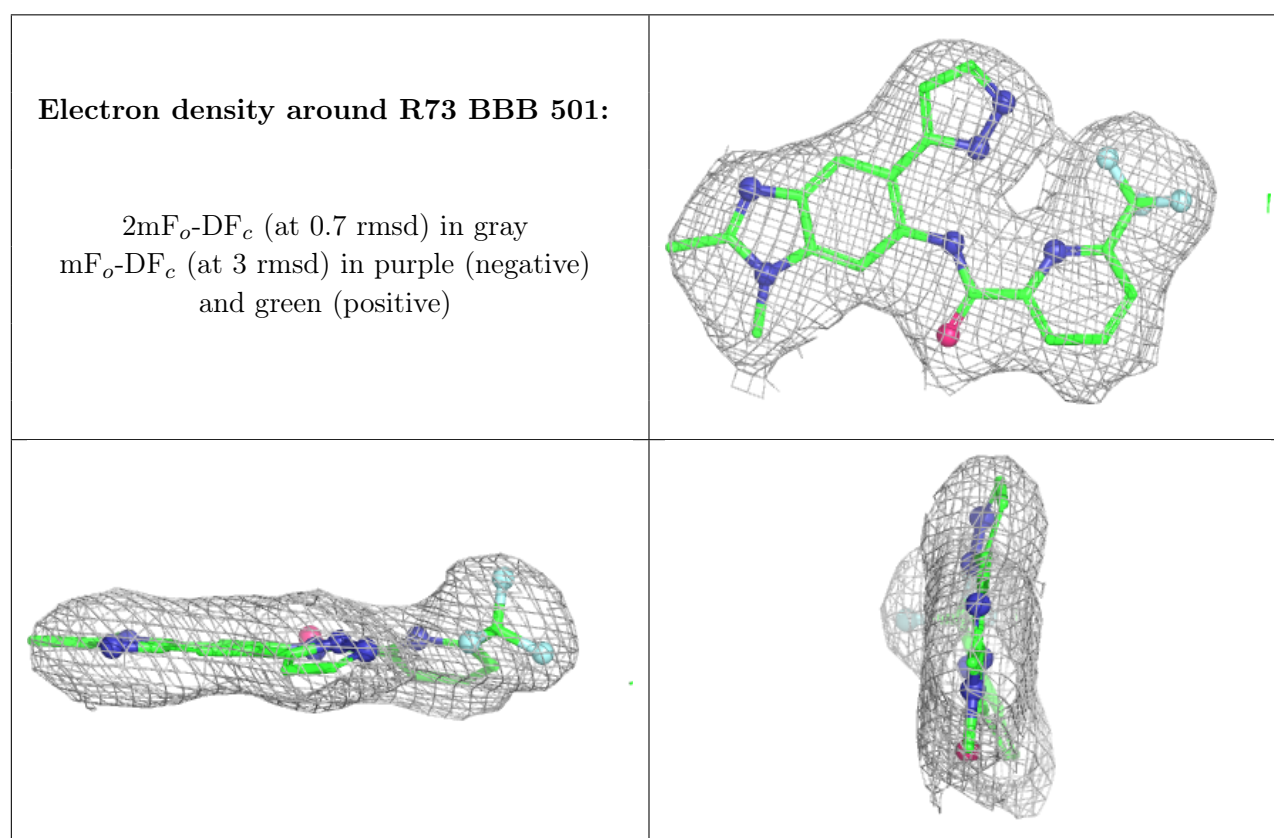
There are no oligosaccharides in this entry.

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.

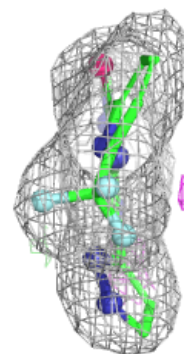
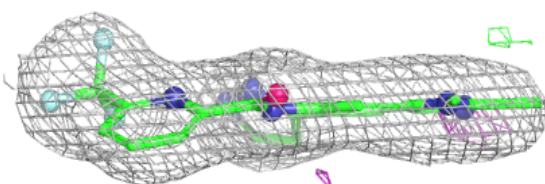
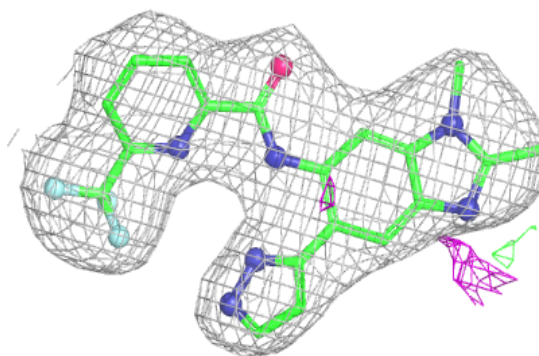
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	R73	BBB	501	29/29	0.94	0.08	39,47,57,60	0
2	R73	AAA	501	29/29	0.95	0.08	34,44,58,60	0
2	R73	DDD	501	29/29	0.95	0.08	39,45,56,57	0
2	R73	CCC	501	29/29	0.96	0.06	36,42,47,53	0

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.

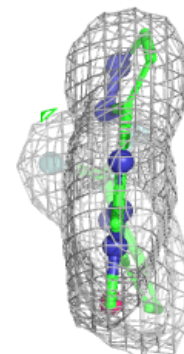
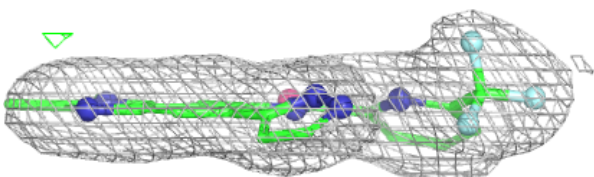
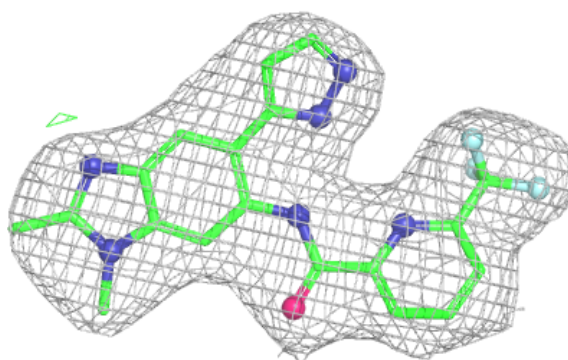


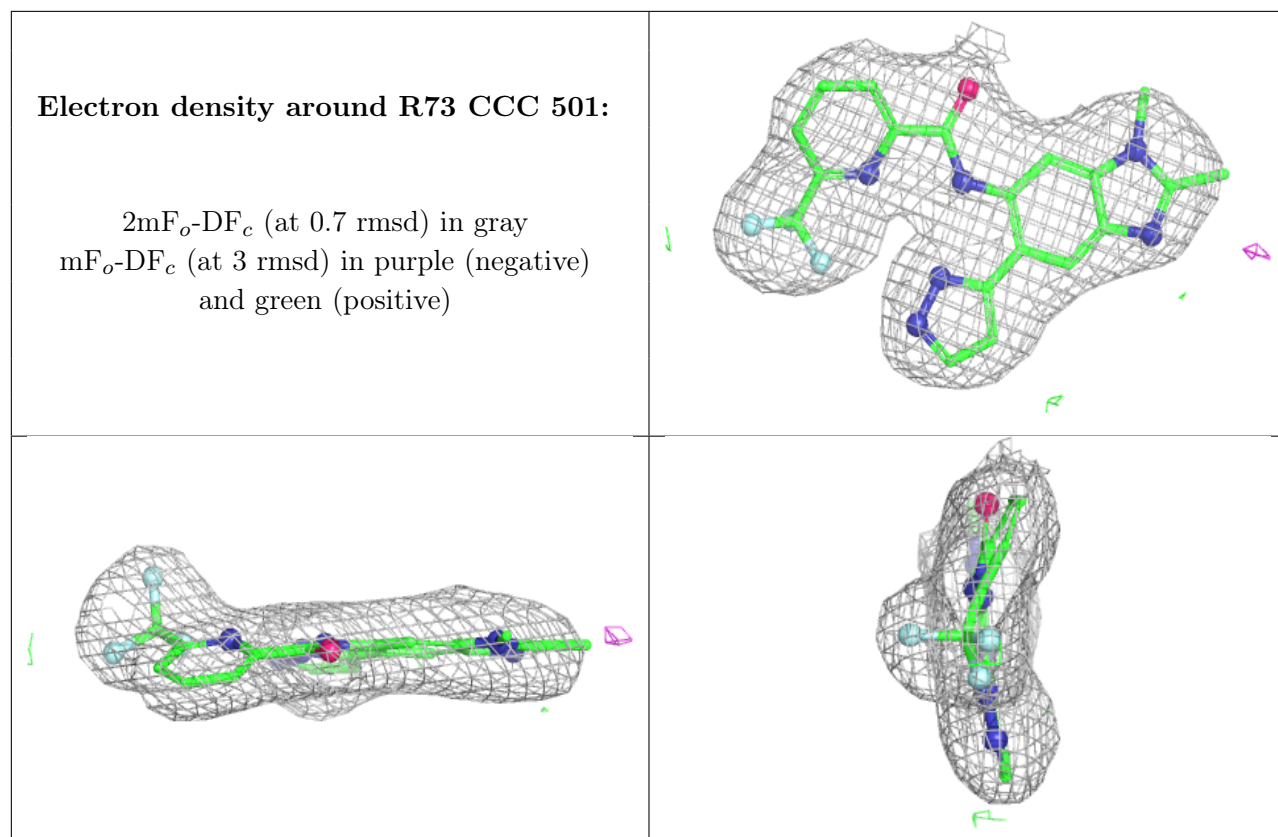
Electron density around R73 AAA 501:

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

**Electron density around R73 DDD 501:**

$2mF_o-DF_c$ (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.