



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:25 AM UTC

PDB ID : 9HB7 / pdb_00009hb7
Title : Crystal structure of human tryptophan hydroxylase 2 in complex with inhibitor AG-01-128
Authors : Schuetz, A.; Gogolin, A.; Pfeifer, J.; Mallow, K.; Nazare, M.; Specker, E.; Heinemann, U.
Deposited on : 2024-11-05
Resolution : 2.96 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

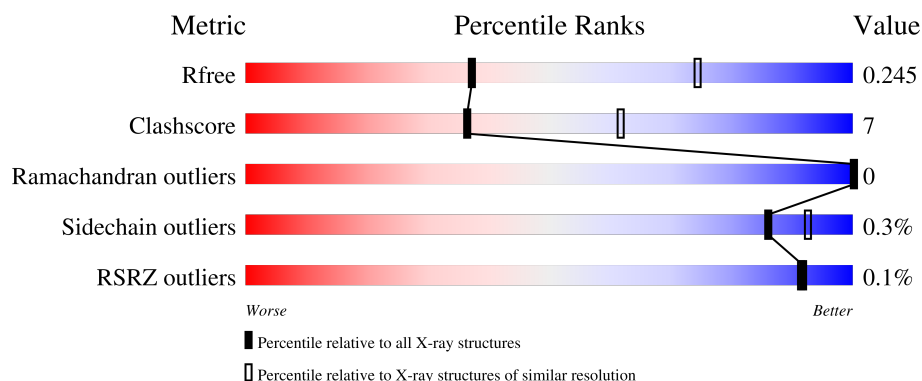
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 2.96 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	372	 77% 14% • 8%
1	B	372	 67% 21% • 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5498 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 Tryptophan 5-hydroxylase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2764	1769	460	519	16			
1	B	329	Total	C	N	O	S	0	0	0
			2670	1712	445	498	15			

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	MET	-	initiating methionine	UNP Q8IWU9
A	120	LYS	-	expression tag	UNP Q8IWU9
A	121	HIS	-	expression tag	UNP Q8IWU9
A	122	HIS	-	expression tag	UNP Q8IWU9
A	123	HIS	-	expression tag	UNP Q8IWU9
A	124	HIS	-	expression tag	UNP Q8IWU9
A	125	HIS	-	expression tag	UNP Q8IWU9
A	126	HIS	-	expression tag	UNP Q8IWU9
A	127	HIS	-	expression tag	UNP Q8IWU9
A	128	GLY	-	expression tag	UNP Q8IWU9
A	129	ALA	-	expression tag	UNP Q8IWU9
A	130	ALA	-	expression tag	UNP Q8IWU9
A	131	GLY	-	expression tag	UNP Q8IWU9
A	132	THR	-	expression tag	UNP Q8IWU9
A	133	SER	-	expression tag	UNP Q8IWU9
A	134	LEU	-	expression tag	UNP Q8IWU9
A	135	TYR	-	expression tag	UNP Q8IWU9
A	136	LYS	-	expression tag	UNP Q8IWU9
A	137	LYS	-	expression tag	UNP Q8IWU9
A	138	ALA	-	expression tag	UNP Q8IWU9
A	139	GLY	-	expression tag	UNP Q8IWU9
A	140	GLU	-	expression tag	UNP Q8IWU9
A	141	ASN	-	expression tag	UNP Q8IWU9
A	142	LEU	-	expression tag	UNP Q8IWU9
A	143	TYR	-	expression tag	UNP Q8IWU9

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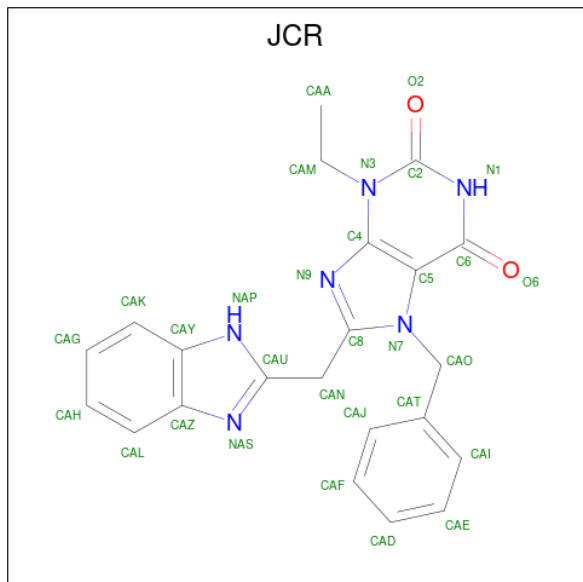
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Chain	Residue	Modelled	Actual	Comment	Reference
A	144	PHE	-	expression tag	UNP Q8IWU9
A	145	GLN	-	expression tag	UNP Q8IWU9
A	146	GLY	-	expression tag	UNP Q8IWU9
A	147	SER	-	expression tag	UNP Q8IWU9
B	119	MET	-	initiating methionine	UNP Q8IWU9
B	120	LYS	-	expression tag	UNP Q8IWU9
B	121	HIS	-	expression tag	UNP Q8IWU9
B	122	HIS	-	expression tag	UNP Q8IWU9
B	123	HIS	-	expression tag	UNP Q8IWU9
B	124	HIS	-	expression tag	UNP Q8IWU9
B	125	HIS	-	expression tag	UNP Q8IWU9
B	126	HIS	-	expression tag	UNP Q8IWU9
B	127	HIS	-	expression tag	UNP Q8IWU9
B	128	GLY	-	expression tag	UNP Q8IWU9
B	129	ALA	-	expression tag	UNP Q8IWU9
B	130	ALA	-	expression tag	UNP Q8IWU9
B	131	GLY	-	expression tag	UNP Q8IWU9
B	132	THR	-	expression tag	UNP Q8IWU9
B	133	SER	-	expression tag	UNP Q8IWU9
B	134	LEU	-	expression tag	UNP Q8IWU9
B	135	TYR	-	expression tag	UNP Q8IWU9
B	136	LYS	-	expression tag	UNP Q8IWU9
B	137	LYS	-	expression tag	UNP Q8IWU9
B	138	ALA	-	expression tag	UNP Q8IWU9
B	139	GLY	-	expression tag	UNP Q8IWU9
B	140	GLU	-	expression tag	UNP Q8IWU9
B	141	ASN	-	expression tag	UNP Q8IWU9
B	142	LEU	-	expression tag	UNP Q8IWU9
B	143	TYR	-	expression tag	UNP Q8IWU9
B	144	PHE	-	expression tag	UNP Q8IWU9
B	145	GLN	-	expression tag	UNP Q8IWU9
B	146	GLY	-	expression tag	UNP Q8IWU9
B	147	SER	-	expression tag	UNP Q8IWU9

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

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

- Molecule 3 is 8-(1 {H}-benzimidazol-2-ylmethyl)-3-ethyl-7-(phenylmethyl)purine-2,6-dione (CCD ID: JCR) (formula: C₂₂H₂₀N₆O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			30	22	6	2		
3	B	1	Total	C	N	O	0	0
			30	22	6	2		

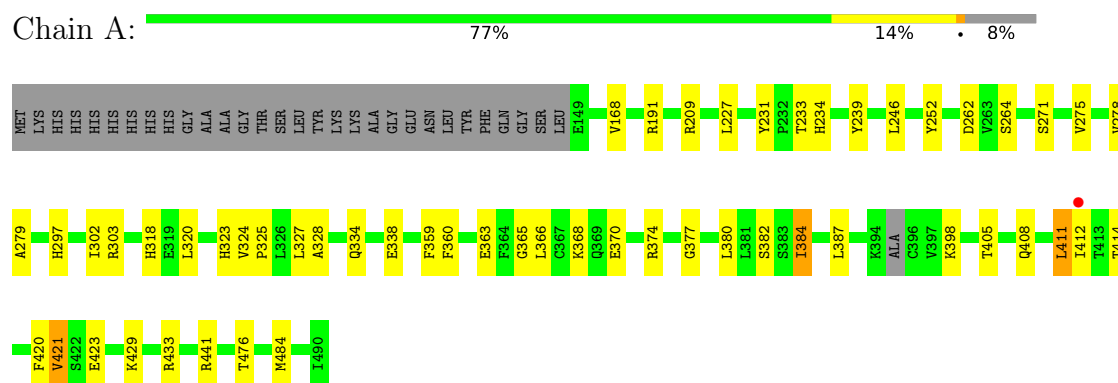
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	1	Total	O	0	0
			1	1		

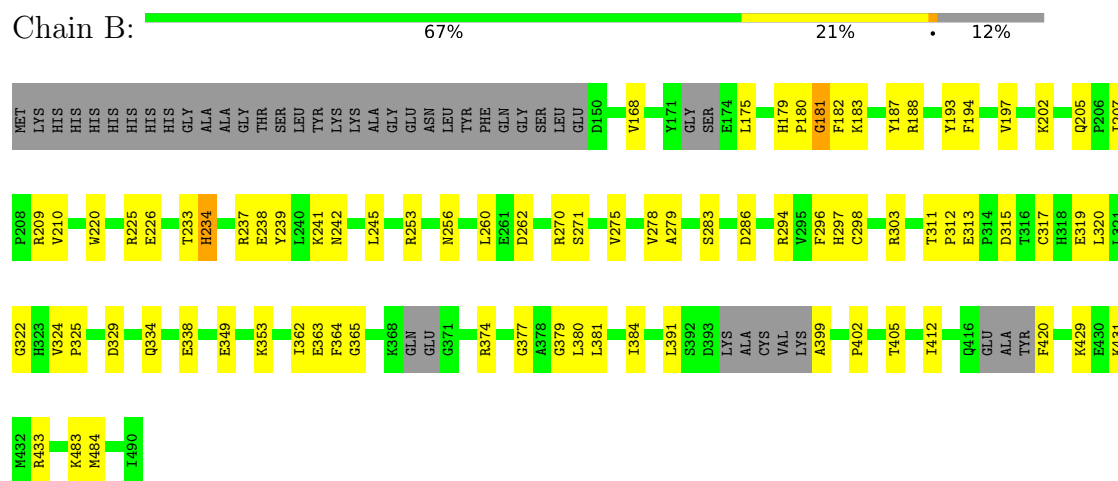
3 Residue-property plots

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 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: Tryptophan 5-hydroxylase 2



• Molecule 1: Tryptophan 5-hydroxylase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	101.14Å 94.65Å 88.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.32 – 2.96 47.32 – 2.96	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.32-2.96) 99.6 (47.32-2.96)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.205 , 0.244 0.210 , 0.245	Depositor DCC
R_{free} test set	918 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	85.5	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 69.7	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	0.95	EDS
Total number of atoms	5498	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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: JCR, FE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.36	0/2833	0.82	5/3831 (0.1%)
1	B	0.38	0/2735	0.90	11/3696 (0.3%)
All	All	0.37	0/5568	0.86	16/7527 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	412	ILE	N-CA-C	6.81	117.60	110.72
1	B	234	HIS	N-CA-C	6.35	121.81	113.30
1	B	181	GLY	N-CA-C	5.88	119.79	112.73
1	B	412	ILE	N-CA-C	5.73	115.92	110.53
1	B	362	ILE	N-CA-C	5.54	116.27	110.62
1	B	311	THR	CA-C-N	5.49	124.83	118.85
1	B	311	THR	C-N-CA	5.49	124.83	118.85
1	A	320	LEU	N-CA-C	5.38	117.23	111.36
1	B	324	VAL	CB-CA-C	-5.29	108.67	113.70
1	A	324	VAL	CB-CA-C	-5.25	108.71	113.70
1	B	329	ASP	CA-C-N	5.23	125.28	119.32
1	B	329	ASP	C-N-CA	5.23	125.28	119.32
1	B	320	LEU	N-CA-C	5.14	116.97	111.36
1	B	384	ILE	N-CA-C	5.12	115.34	110.42
1	A	405	THR	N-CA-C	5.12	116.94	111.36
1	A	421	VAL	N-CA-C	5.11	116.07	108.46

There are no chirality outliers.

There are no planarity outliers.

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	A	2764	0	2693	33	0
1	B	2670	0	2602	47	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	30	0	0	0	0
3	B	30	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	5498	0	5295	78	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 7.

All (78) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:ILE:HG21	1:B:260:LEU:HB2	1.68	0.75
1:B:182:PHE:HB2	1:B:188:ARG:HH21	1.60	0.67
1:B:182:PHE:HA	1:B:188:ARG:HE	1.61	0.66
1:B:220:TRP:NE1	1:B:256:ASN:O	2.30	0.65
1:A:365:GLY:H	1:A:377:GLY:HA3	1.64	0.62
1:B:238:GLU:O	1:B:242:ASN:ND2	2.33	0.62
1:B:363:GLU:O	1:B:379:GLY:N	2.30	0.61
1:A:168:VAL:HG21	1:A:279:ALA:HB3	1.87	0.57
1:A:264:SER:HB2	1:A:275:VAL:HG22	1.88	0.56
1:A:233:THR:HG23	1:A:234:HIS:ND1	2.21	0.55
1:A:338:GLU:OE2	1:A:433:ARG:NH2	2.40	0.55
1:A:227:LEU:HB3	1:A:231:TYR:CZ	2.44	0.52
1:A:366:LEU:O	1:A:421:VAL:HA	2.10	0.51
1:A:476:THR:OG1	1:B:433:ARG:NH1	2.44	0.50
1:B:234:HIS:CD2	1:B:391:LEU:HD12	2.46	0.50
1:B:283:SER:OG	1:B:286:ASP:OD1	2.21	0.50
1:B:402:PRO:HG3	1:B:431:LYS:O	2.12	0.50
1:A:368:LYS:HD3	1:A:423:GLU:OE1	2.12	0.49
1:B:193:TYR:O	1:B:197:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:ARG:NH1	1:B:226:GLU:OE2	2.46	0.49
1:B:233:THR:O	1:B:374:ARG:NH1	2.46	0.49
1:B:405:THR:HG23	1:B:420:PHE:CZ	2.48	0.48
1:B:209:ARG:NH2	1:B:262:ASP:OD1	2.45	0.48
1:A:227:LEU:HD23	1:A:384:ILE:CG2	2.44	0.47
1:A:359:PHE:O	1:A:363:GLU:HB2	2.14	0.47
1:B:233:THR:C	1:B:374:ARG:NH1	2.74	0.46
1:B:202:LYS:HB2	1:B:205:GLN:NE2	2.29	0.46
1:B:194:PHE:CE1	1:B:210:VAL:HG11	2.51	0.46
1:A:441:ARG:O	1:B:483:LYS:HD3	2.16	0.46
1:B:168:VAL:HG21	1:B:279:ALA:HB3	1.97	0.46
1:B:245:LEU:HD23	1:B:270:ARG:NH2	2.31	0.45
1:B:179:HIS:HE1	1:B:187:TYR:HE2	1.63	0.45
1:A:334:GLN:O	1:A:338:GLU:HG2	2.16	0.45
1:B:207:ILE:HD11	1:B:275:VAL:O	2.17	0.45
1:B:241:LYS:O	1:B:245:LEU:HD13	2.17	0.45
1:B:237:ARG:O	1:B:241:LYS:HG2	2.17	0.45
1:B:312:PRO:HG2	1:B:313:GLU:OE1	2.17	0.45
1:B:365:GLY:H	1:B:377:GLY:HA3	1.82	0.45
1:A:191:ARG:HA	1:A:191:ARG:HD2	1.75	0.44
1:A:318:HIS:ND1	1:A:382:SER:OG	2.37	0.44
1:A:398:LYS:O	1:A:420:PHE:HA	2.18	0.44
1:B:364:PHE:HD1	1:B:380:LEU:HD23	1.82	0.44
1:B:180:PRO:HA	1:B:183:LYS:HD2	2.00	0.44
1:B:338:GLU:HG3	1:B:429:LYS:HG3	1.99	0.44
1:B:349:GLU:O	1:B:353:LYS:HG3	2.18	0.44
1:A:429:LYS:NZ	1:A:433:ARG:HH21	2.16	0.43
1:B:253:ARG:HG3	1:B:256:ASN:HB2	2.01	0.43
1:B:303:ARG:NH2	1:B:317:CYS:HB2	2.33	0.43
1:B:334:GLN:HB3	1:B:429:LYS:NZ	2.33	0.43
1:B:315:ASP:O	1:B:319:GLU:HG2	2.18	0.43
1:A:271:SER:HB3	1:A:328:ALA:O	2.18	0.43
1:B:175:LEU:HD13	1:B:181:GLY:HA3	2.01	0.43
1:A:246:LEU:HB3	1:A:252:TYR:CD1	2.53	0.43
1:A:302:ILE:HG22	1:A:303:ARG:O	2.19	0.43
1:A:380:LEU:O	1:A:387:LEU:HB2	2.18	0.43
1:B:322:GLY:HA2	1:B:381:LEU:HB2	2.00	0.43
1:A:370:GLU:HG2	1:A:370:GLU:O	2.18	0.43
1:B:239:TYR:CE2	1:B:381:LEU:HD13	2.53	0.43
1:B:484:MET:HE3	1:B:484:MET:HB2	1.78	0.42
1:A:233:THR:HA	1:A:374:ARG:HH12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:TYR:CE1	1:A:325:PRO:HG2	2.55	0.42
1:A:484:MET:HE3	1:A:484:MET:HB2	1.86	0.42
1:A:278:VAL:HB	1:A:297:HIS:HB3	2.02	0.42
1:B:239:TYR:CE2	1:B:325:PRO:HG2	2.55	0.42
1:A:411:LEU:HD23	1:A:414:THR:HB	2.02	0.42
1:A:239:TYR:HE1	1:A:325:PRO:HG2	1.85	0.42
1:A:209:ARG:NH2	1:A:262:ASP:OD1	2.35	0.42
1:A:227:LEU:HD23	1:A:384:ILE:HG23	2.02	0.41
1:B:399:ALA:O	1:B:420:PHE:HD2	2.02	0.41
1:B:303:ARG:HH21	1:B:317:CYS:HB2	1.84	0.41
1:B:275:VAL:HG12	1:B:296:PHE:HB3	2.03	0.41
1:A:365:GLY:H	1:A:377:GLY:CA	2.31	0.41
1:B:179:HIS:HE1	1:B:187:TYR:CE2	2.38	0.41
1:B:278:VAL:HG12	1:B:298:CYS:O	2.20	0.41
1:B:278:VAL:HB	1:B:297:HIS:HB3	2.02	0.40
1:A:360:PHE:CE2	1:A:408:GLN:HB3	2.56	0.40
1:B:271:SER:O	1:B:294:ARG:NH1	2.51	0.40
1:A:323:HIS:O	1:A:327:LEU:HG	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	A	337/372 (91%)	334 (99%)	3 (1%)	0	100	100
1	B	319/372 (86%)	317 (99%)	2 (1%)	0	100	100
All	All	656/744 (88%)	651 (99%)	5 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	303/326 (93%)	301 (99%)	2 (1%)	76	87
1	B	293/326 (90%)	293 (100%)	0	100	100
All	All	596/652 (91%)	594 (100%)	2 (0%)	86	92

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	384	ILE
1	A	411	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	GLN
1	A	242	ASN

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	JCR	B	502	2	34,34,34	2.23	13 (38%)	44,49,49	2.35	11 (25%)
3	JCR	A	502	2	34,34,34	2.22	13 (38%)	44,49,49	2.44	12 (27%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	JCR	B	502	2	-	2/10/10/10	0/5/5/5
3	JCR	A	502	2	-	2/10/10/10	0/5/5/5

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	JCR	CAO-CAT	-6.27	1.40	1.51
3	A	502	JCR	CAO-CAT	-6.20	1.40	1.51
3	B	502	JCR	CAY-CAZ	-4.04	1.34	1.40
3	A	502	JCR	CAY-CAZ	-4.00	1.34	1.40
3	A	502	JCR	CAL-CAZ	-3.98	1.33	1.40
3	B	502	JCR	CAL-CAZ	-3.98	1.33	1.40
3	A	502	JCR	C5-C6	-3.78	1.33	1.43
3	B	502	JCR	CAK-CAY	-3.76	1.33	1.39
3	B	502	JCR	C5-C6	-3.72	1.34	1.43
3	A	502	JCR	CAK-CAY	-3.69	1.33	1.39
3	A	502	JCR	C2-N3	-3.43	1.34	1.39
3	B	502	JCR	C2-N3	-3.41	1.34	1.39
3	A	502	JCR	CAZ-NAS	-3.07	1.33	1.39
3	B	502	JCR	CAZ-NAS	-3.00	1.33	1.39
3	B	502	JCR	CAY-NAP	-2.95	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	JCR	CAY-NAP	-2.75	1.33	1.38
3	B	502	JCR	C8-N7	-2.74	1.32	1.37
3	A	502	JCR	C8-N7	-2.65	1.32	1.37
3	B	502	JCR	C5-N7	-2.57	1.34	1.39
3	A	502	JCR	CAN-C8	2.55	1.53	1.50
3	A	502	JCR	CAN-CAU	2.54	1.53	1.49
3	A	502	JCR	C5-N7	-2.45	1.34	1.39
3	B	502	JCR	CAN-CAU	2.40	1.53	1.49
3	B	502	JCR	C4-N3	-2.32	1.34	1.39
3	B	502	JCR	CAN-C8	2.29	1.53	1.50
3	A	502	JCR	C4-N3	-2.13	1.35	1.39

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	JCR	N3-C4-N9	9.91	130.62	125.53
3	B	502	JCR	N3-C4-N9	9.25	130.28	125.53
3	B	502	JCR	C6-N1-C2	-6.70	118.55	127.34
3	A	502	JCR	C6-N1-C2	-6.63	118.65	127.34
3	A	502	JCR	C5-C6-N1	5.17	120.04	110.94
3	B	502	JCR	C5-C6-N1	4.96	119.68	110.94
3	A	502	JCR	C4-C5-N7	3.93	108.11	104.93
3	A	502	JCR	C5-C4-N9	-3.79	108.13	112.77
3	B	502	JCR	C5-C4-N9	-3.54	108.43	112.77
3	B	502	JCR	C4-C5-N7	3.54	107.79	104.93
3	A	502	JCR	CAO-N7-C5	2.71	131.42	125.53
3	B	502	JCR	CAO-N7-C5	2.65	131.30	125.53
3	B	502	JCR	CAO-N7-C8	-2.55	121.89	126.42
3	A	502	JCR	O6-C6-C5	-2.54	121.37	127.62
3	A	502	JCR	CAO-N7-C8	-2.54	121.91	126.42
3	B	502	JCR	O6-C6-C5	-2.49	121.52	127.62
3	A	502	JCR	CAN-CAU-NAP	2.44	125.25	122.77
3	B	502	JCR	N1-C2-N3	2.23	119.46	115.45
3	A	502	JCR	NAP-CAU-NAS	-2.16	110.09	112.72
3	A	502	JCR	CAZ-CAY-NAP	2.15	108.29	105.71
3	B	502	JCR	NAP-CAU-NAS	-2.15	110.10	112.72
3	B	502	JCR	CAZ-CAY-NAP	2.09	108.22	105.71
3	A	502	JCR	N1-C2-N3	2.07	119.16	115.45

There are no chirality outliers.

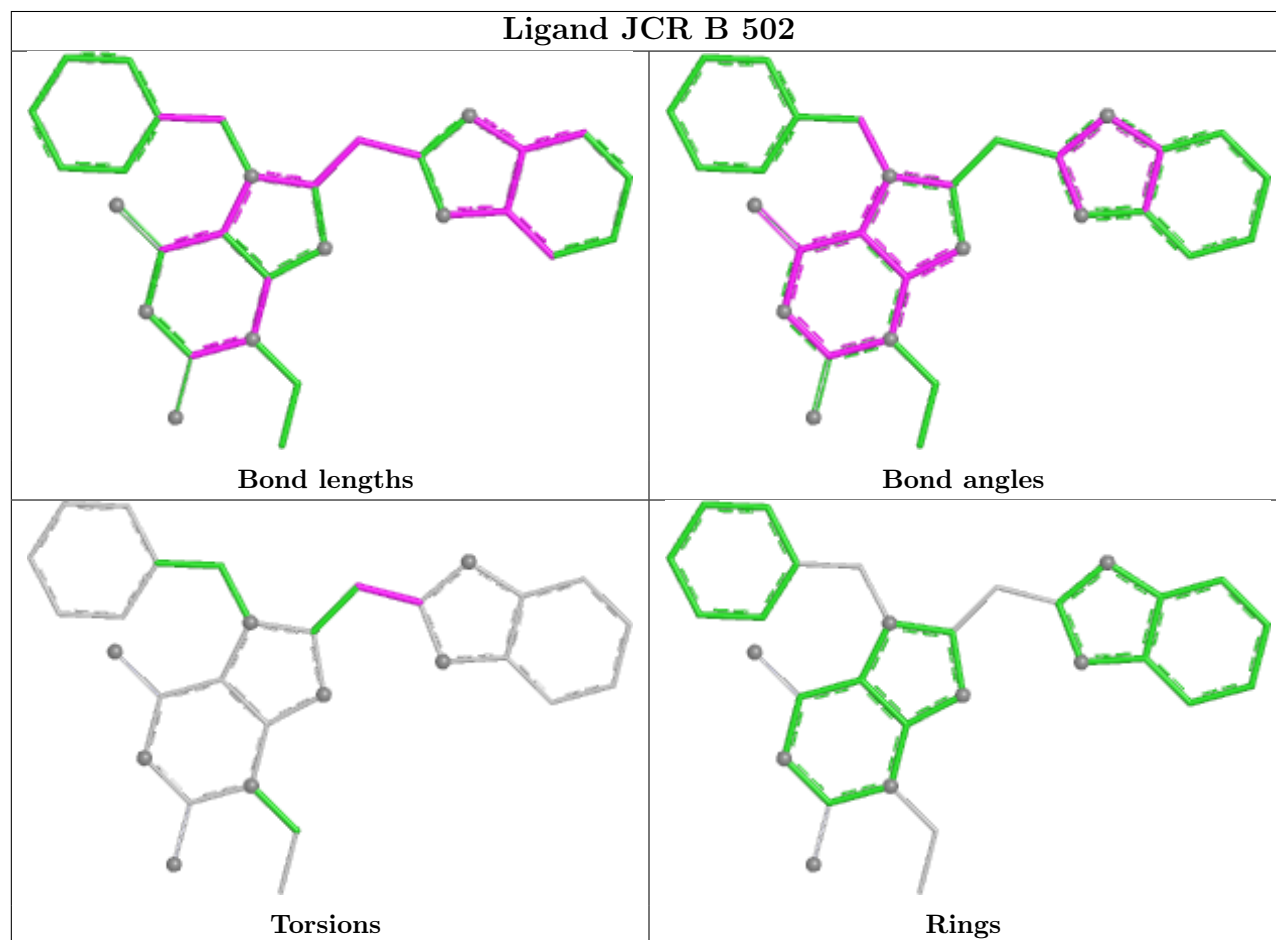
All (4) torsion outliers are listed below:

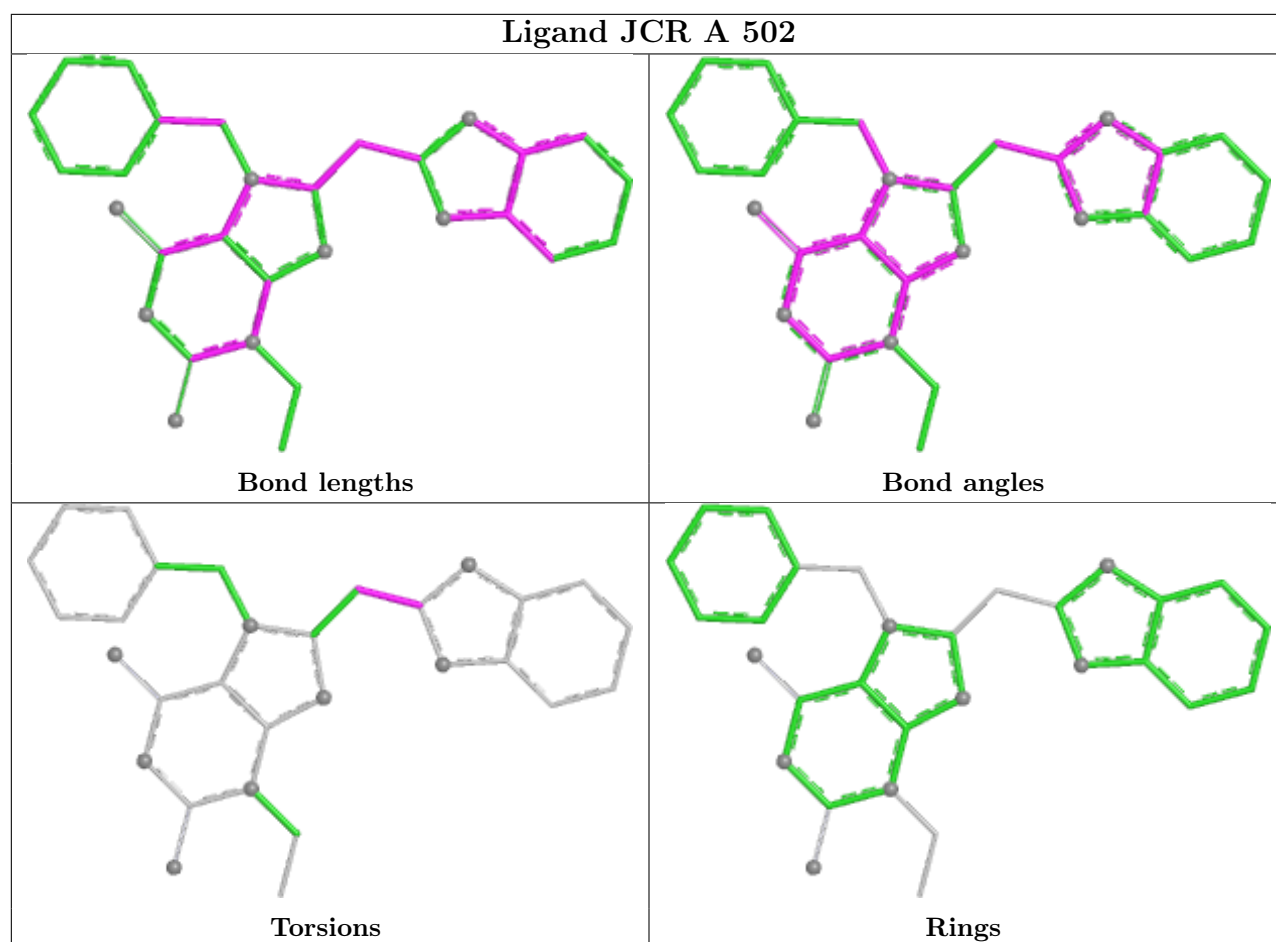
Mol	Chain	Res	Type	Atoms
3	A	502	JCR	C8-CAN-CAU-NAP
3	B	502	JCR	C8-CAN-CAU-NAP
3	A	502	JCR	C8-CAN-CAU-NAS
3	B	502	JCR	C8-CAN-CAU-NAS

There are no ring outliers.

No monomer is involved in short contacts.

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	A	341/372 (91%)	-0.30	1 (0%) 90 88	49, 80, 138, 172	0
1	B	329/372 (88%)	-0.11	0 100 100	43, 115, 173, 218	0
All	All	670/744 (90%)	-0.21	1 (0%) 92 91	43, 95, 164, 218	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	412	ILE	2.6

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](#)

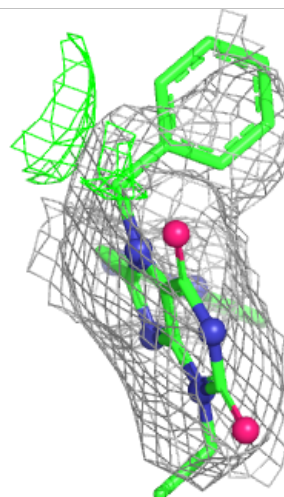
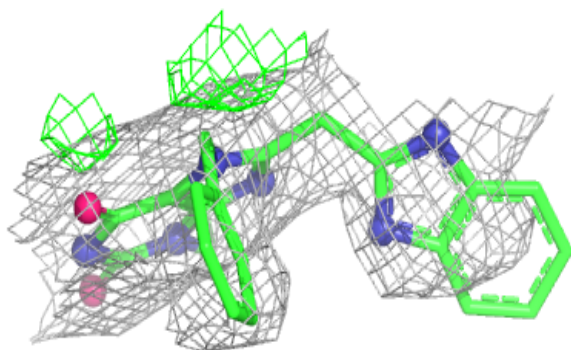
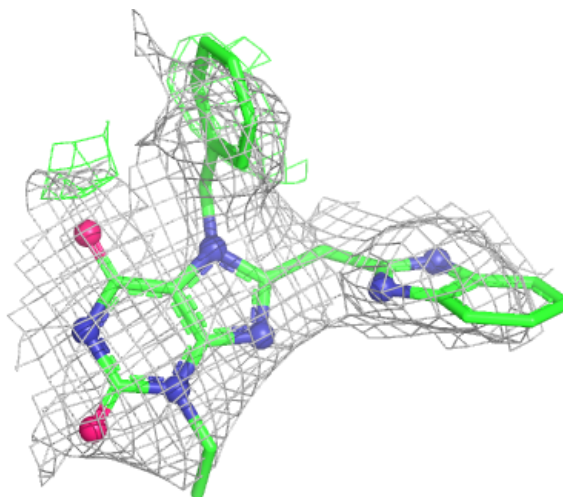
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	JCR	B	502	30/30	0.85	0.14	112,136,156,157	0
3	JCR	A	502	30/30	0.95	0.10	92,107,115,117	0
2	FE	B	501	1/1	0.98	0.03	101,101,101,101	0
2	FE	A	501	1/1	1.00	0.05	80,80,80,80	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.

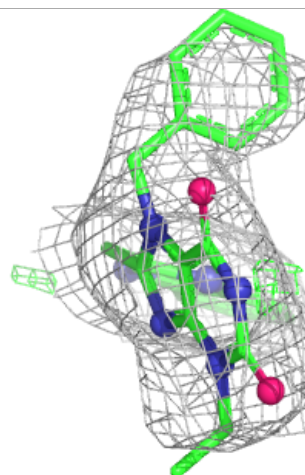
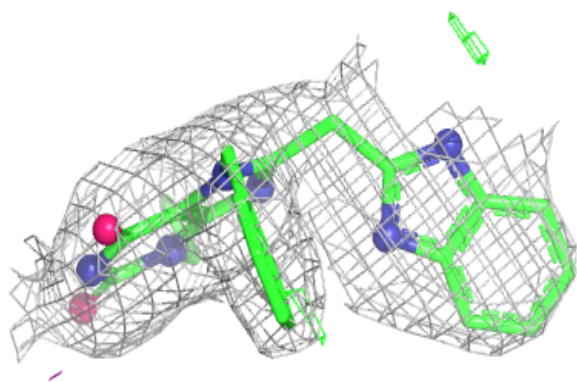
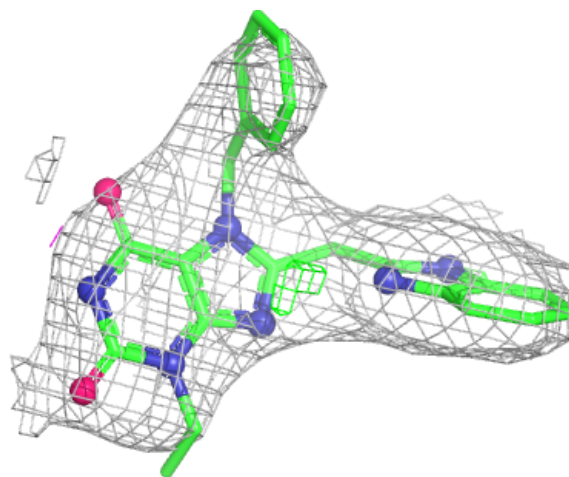
Electron density around JCR B 502:

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



Electron density around JCR A 502:

$2mF_o-DF_c$ (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.