



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 07:42 AM EDT

PDB ID : 5UIT
Title : Crystal structure of IRAK4 in complex with compound 14
Authors : Han, S.; Chang, J.S.
Deposited on : 2017-01-14
Resolution : 1.84 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.37.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

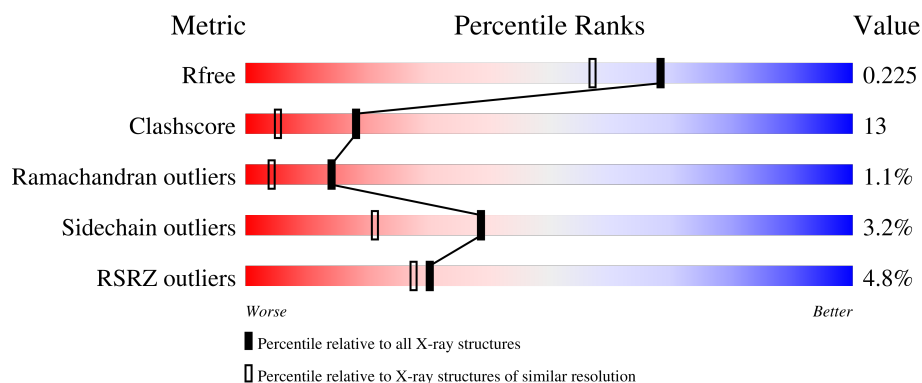
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.84 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}	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	A	323	<div> <div>4%</div> <div>72%</div> <div>15%</div> <div>•</div> <div>11%</div> </div>
1	B	323	<div> <div>4%</div> <div>68%</div> <div>18%</div> <div>•</div> <div>12%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5048 atoms, of which 42 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	A	286	Total	C	N	O	P	S	0	0	0
			2256	1414	379	447	2	14			
1	B	285	Total	C	N	O	P	S	0	0	0
			2246	1409	378	443	2	14			

There are 32 discrepancies between the modelled and reference sequences:

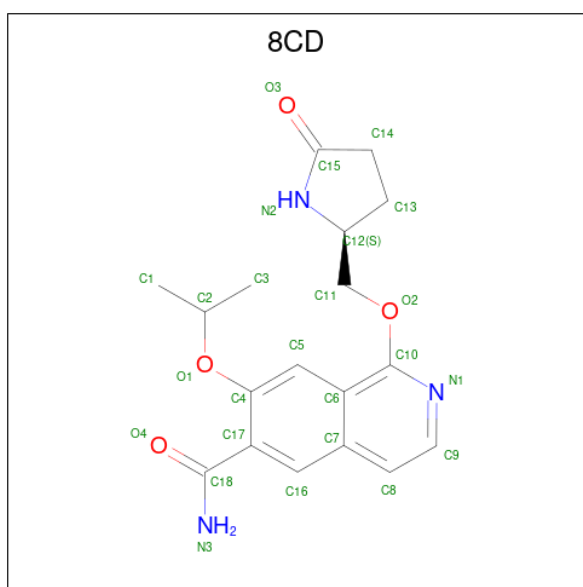
Chain	Residue	Modelled	Actual	Comment	Reference
A	138	MET	-	initiating methionine	UNP Q9NWZ3
A	139	HIS	-	expression tag	UNP Q9NWZ3
A	140	HIS	-	expression tag	UNP Q9NWZ3
A	141	HIS	-	expression tag	UNP Q9NWZ3
A	142	HIS	-	expression tag	UNP Q9NWZ3
A	143	HIS	-	expression tag	UNP Q9NWZ3
A	144	HIS	-	expression tag	UNP Q9NWZ3
A	145	GLY	-	expression tag	UNP Q9NWZ3
A	146	GLY	-	expression tag	UNP Q9NWZ3
A	147	GLU	-	expression tag	UNP Q9NWZ3
A	148	ASN	-	expression tag	UNP Q9NWZ3
A	149	LEU	-	expression tag	UNP Q9NWZ3
A	150	TYR	-	expression tag	UNP Q9NWZ3
A	151	PHE	-	expression tag	UNP Q9NWZ3
A	152	GLN	-	expression tag	UNP Q9NWZ3
A	153	GLY	-	expression tag	UNP Q9NWZ3
B	138	MET	-	initiating methionine	UNP Q9NWZ3
B	139	HIS	-	expression tag	UNP Q9NWZ3
B	140	HIS	-	expression tag	UNP Q9NWZ3
B	141	HIS	-	expression tag	UNP Q9NWZ3
B	142	HIS	-	expression tag	UNP Q9NWZ3
B	143	HIS	-	expression tag	UNP Q9NWZ3
B	144	HIS	-	expression tag	UNP Q9NWZ3
B	145	GLY	-	expression tag	UNP Q9NWZ3
B	146	GLY	-	expression tag	UNP Q9NWZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	147	GLU	-	expression tag	UNP Q9NWZ3
B	148	ASN	-	expression tag	UNP Q9NWZ3
B	149	LEU	-	expression tag	UNP Q9NWZ3
B	150	TYR	-	expression tag	UNP Q9NWZ3
B	151	PHE	-	expression tag	UNP Q9NWZ3
B	152	GLN	-	expression tag	UNP Q9NWZ3
B	153	GLY	-	expression tag	UNP Q9NWZ3

- Molecule 2 is 1-{[(2S)-5-oxopyrrolidin-2-yl]methoxy}-7-[(propan-2-yl)oxy]isoquinoline-6-carboxamide (three-letter code: 8CD) (formula: C₁₈H₂₁N₃O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	21	0
			46	18	21	3	4		
2	B	1	Total	C	H	N	O	21	0
			46	18	21	3	4		

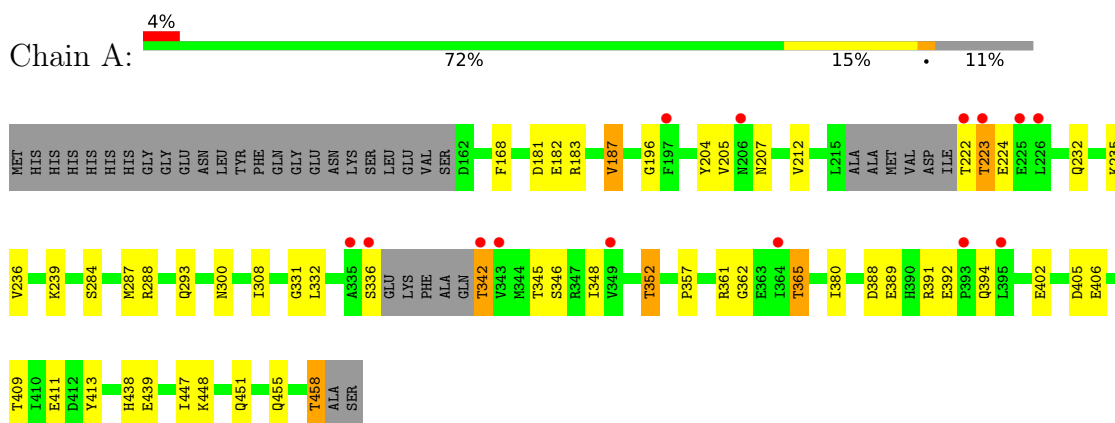
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	234	Total	O	0	0
			234	234		
3	B	220	Total	O	0	0
			220	220		

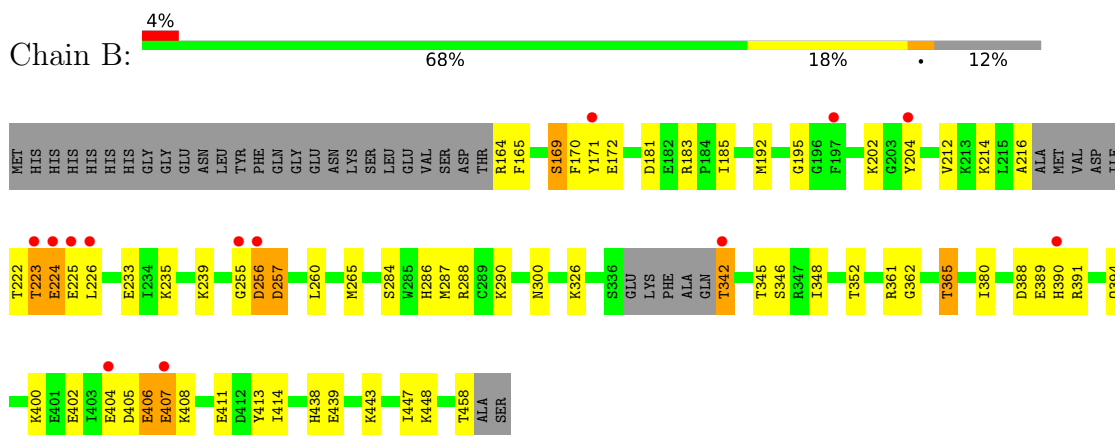
3 Residue-property plots

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: Interleukin-1 receptor-associated kinase 4



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



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	91.14Å 118.58Å 139.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	59.29 – 1.84 59.29 – 1.84	Depositor EDS
% Data completeness (in resolution range)	89.7 (59.29-1.84) 90.2 (59.29-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 1.84Å)	Xtriage
Refinement program	BUSTER 2.9.6	Depositor
R, R_{free}	0.181 , 0.218 0.184 , 0.225	Depositor DCC
R_{free} test set	3010 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.6	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	0.96	EDS
Total number of atoms	5048	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.99% 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: 8CD, TPO, SEP

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	0.47	0/2271	0.59	0/3060
1	B	0.53	0/2261	0.61	0/3046
All	All	0.50	0/4532	0.60	0/6106

There are no bond length outliers.

There are no bond angle outliers.

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	2256	0	2215	55	0
1	B	2246	0	2208	65	1
2	A	25	21	0	0	0
2	B	25	21	0	0	0
3	A	234	0	0	12	0
3	B	220	0	0	7	0
All	All	5006	42	4423	120	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 13.

All (120) 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:A:284:SER:H	1:A:287:MET:HE3	1.04	1.12
1:A:389:GLU:HA	1:A:394:GLN:HE21	0.99	1.08
1:A:389:GLU:HA	1:A:394:GLN:NE2	1.73	1.04
1:B:406:GLU:O	1:B:407:GLU:HB2	1.25	1.01
1:B:406:GLU:O	1:B:407:GLU:CB	2.09	1.01
1:B:257:ASP:HA	3:B:639:HOH:O	1.63	0.96
1:A:361:ARG:HD2	3:A:762:HOH:O	1.68	0.93
1:A:284:SER:N	1:A:287:MET:HE3	1.85	0.90
1:A:284:SER:H	1:A:287:MET:CE	1.85	0.87
1:B:170:PHE:CE2	1:B:257:ASP:HB3	2.09	0.87
1:B:389:GLU:HA	1:B:394:GLN:HE21	1.44	0.83
1:B:400:LYS:O	1:B:404:GLU:HG3	1.78	0.83
1:B:195:GLY:HA3	3:B:753:HOH:O	1.84	0.78
1:B:405:ASP:O	1:B:406:GLU:O	2.03	0.77
1:B:388:ASP:O	1:B:394:GLN:HG2	1.87	0.75
1:B:181:ASP:OD2	1:B:183:ARG:HD3	1.88	0.73
1:A:224:GLU:HB3	3:A:672:HOH:O	1.88	0.73
1:A:287:MET:HE1	3:A:706:HOH:O	1.86	0.73
1:B:389:GLU:HA	1:B:394:GLN:NE2	2.02	0.73
1:B:402:GLU:OE2	1:B:413:TYR:OH	2.07	0.70
1:A:409:THR:HG22	1:A:411:GLU:H	1.56	0.69
1:B:342:THR:HB	1:B:365:THR:HB	1.76	0.67
1:A:409:THR:HG22	1:A:411:GLU:N	2.10	0.67
1:B:224:GLU:HG2	1:B:225:GLU:N	2.10	0.66
1:B:222:THR:O	1:B:223:THR:OG1	2.07	0.66
1:A:438:HIS:ND1	3:A:601:HOH:O	2.29	0.65
1:A:389:GLU:CA	1:A:394:GLN:HE21	1.92	0.65
1:B:235:LYS:HZ3	1:B:239:LYS:NZ	1.95	0.65
1:B:235:LYS:NZ	1:B:239:LYS:NZ	2.44	0.65
1:A:388:ASP:HB3	1:A:391:ARG:HB3	1.78	0.64
1:A:293:GLN:HE22	1:A:458:THR:HG21	1.62	0.64
1:A:222:THR:O	1:A:223:THR:OG1	2.15	0.63
1:B:255:GLY:O	1:B:256:ASP:HB2	1.99	0.62
1:A:448:LYS:HB2	3:A:655:HOH:O	1.99	0.61
1:B:257:ASP:OD2	1:B:257:ASP:N	2.33	0.61
1:B:439:GLU:CD	1:B:439:GLU:H	2.03	0.60
1:B:183:ARG:HD2	3:B:646:HOH:O	2.00	0.60
1:B:405:ASP:C	1:B:406:GLU:O	2.38	0.60
1:B:407:GLU:O	1:B:408:LYS:HG2	2.02	0.60
1:A:187:VAL:HG23	1:A:187:VAL:O	2.02	0.59
1:B:235:LYS:HZ3	1:B:239:LYS:HZ2	1.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:ILE:HG12	1:B:362:GLY:HA2	1.84	0.59
1:B:235:LYS:NZ	1:B:239:LYS:HZ1	2.01	0.58
1:B:170:PHE:CE2	1:B:257:ASP:CB	2.86	0.57
1:A:235:LYS:HZ3	1:A:239:LYS:HZ2	1.52	0.56
1:B:235:LYS:HZ1	1:B:239:LYS:HZ1	1.51	0.56
1:A:394:GLN:HG3	3:A:631:HOH:O	2.04	0.56
1:A:168:PHE:HE2	1:A:205:VAL:HG11	1.69	0.56
1:B:214:LYS:NZ	3:B:604:HOH:O	2.38	0.56
1:A:181:ASP:OD2	1:A:183:ARG:HD3	2.05	0.56
1:B:181:ASP:OD2	1:B:183:ARG:CD	2.54	0.55
1:B:164:ARG:HG3	1:B:165:PHE:H	1.70	0.55
1:A:222:THR:HG22	1:A:223:THR:N	2.22	0.55
1:A:284:SER:CB	1:A:287:MET:HE3	2.37	0.54
1:B:216:ALA:C	1:B:226:LEU:HD21	2.29	0.54
1:A:455:GLN:NE2	3:A:603:HOH:O	2.41	0.53
1:A:284:SER:OG	1:A:287:MET:HE3	2.08	0.53
1:B:405:ASP:O	1:B:406:GLU:C	2.47	0.53
1:B:411:GLU:OE2	1:B:414:ILE:HD12	2.09	0.53
1:A:409:THR:CG2	1:A:411:GLU:HB2	2.39	0.52
1:B:216:ALA:O	1:B:226:LEU:HD22	2.08	0.52
1:B:255:GLY:O	1:B:256:ASP:CB	2.57	0.52
1:A:388:ASP:O	1:A:394:GLN:HG2	2.10	0.51
1:B:388:ASP:OD1	1:B:390:HIS:N	2.44	0.50
1:B:164:ARG:HG3	1:B:165:PHE:N	2.27	0.50
1:B:169:SER:N	1:B:172:GLU:OE1	2.27	0.50
1:B:286:HIS:HB2	3:B:745:HOH:O	2.12	0.50
1:B:233:GLU:HG2	1:B:260:LEU:HD13	1.94	0.50
1:A:391:ARG:HG2	1:A:392:GLU:N	2.27	0.49
1:B:216:ALA:C	1:B:226:LEU:CD2	2.81	0.49
1:B:287:MET:HA	1:B:287:MET:CE	2.43	0.49
1:A:293:GLN:HE22	1:A:458:THR:CG2	2.25	0.48
1:A:342:THR:HB	1:A:365:THR:HB	1.95	0.48
1:B:284:SER:O	1:B:288:ARG:HG3	2.14	0.48
1:A:308:ILE:HG13	1:A:336:SER:HB3	1.96	0.48
1:A:357:PRO:HG3	1:A:439:GLU:OE1	2.14	0.48
1:B:185:ILE:HD12	1:B:192:MET:HG2	1.95	0.48
1:B:287:MET:HE1	1:B:290:LYS:HD3	1.95	0.48
1:A:168:PHE:CE2	1:A:205:VAL:HG11	2.49	0.47
1:A:239:LYS:HG3	3:A:646:HOH:O	2.12	0.47
1:B:170:PHE:CD2	1:B:257:ASP:HB2	2.49	0.47
1:A:235:LYS:HZ3	1:A:239:LYS:NZ	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:LYS:NZ	1:A:239:LYS:NZ	2.63	0.47
1:A:232:GLN:O	1:A:236:VAL:HG23	2.15	0.46
1:A:409:THR:HG22	1:A:411:GLU:HB2	1.97	0.46
1:A:288:ARG:HB3	1:A:380:ILE:HG23	1.96	0.46
1:B:265:MET:SD	1:B:326:LYS:HG3	2.56	0.46
1:B:287:MET:HG3	3:B:769:HOH:O	2.15	0.46
1:A:448:LYS:HA	1:A:448:LYS:HD2	1.64	0.46
1:B:287:MET:HA	1:B:287:MET:HE3	1.98	0.45
1:A:448:LYS:HD2	1:A:451:GLN:OE1	2.16	0.45
1:B:171:TYR:C	1:B:171:TYR:CD1	2.89	0.45
1:B:388:ASP:OD1	1:B:388:ASP:C	2.53	0.45
1:A:300:ASN:HA	1:A:447:ILE:HG21	1.99	0.45
1:B:287:MET:HB3	1:B:287:MET:HE2	1.88	0.45
1:A:222:THR:CG2	1:A:223:THR:N	2.80	0.44
1:B:170:PHE:CD2	1:B:257:ASP:CB	3.00	0.44
1:B:388:ASP:O	1:B:394:GLN:CG	2.62	0.44
1:B:287:MET:CE	1:B:290:LYS:HD3	2.47	0.44
1:B:235:LYS:NZ	1:B:239:LYS:HZ2	2.13	0.44
1:A:288:ARG:HB3	1:A:380:ILE:CG2	2.48	0.44
1:A:284:SER:OG	1:A:287:MET:CE	2.66	0.43
1:B:288:ARG:HB3	1:B:380:ILE:CG2	2.48	0.43
1:A:332:LEU:HG	3:A:741:HOH:O	2.18	0.43
1:A:348:ILE:HG12	1:A:362:GLY:HA2	2.01	0.42
1:A:409:THR:CG2	1:A:411:GLU:H	2.29	0.42
1:B:388:ASP:CG	1:B:391:ARG:HB3	2.40	0.42
1:A:405:ASP:O	1:A:406:GLU:HB2	2.20	0.42
1:A:352:THR:HG23	3:A:702:HOH:O	2.18	0.42
1:B:438:HIS:NE2	1:B:443:LYS:HD3	2.35	0.42
1:A:389:GLU:CA	1:A:394:GLN:NE2	2.64	0.42
1:A:394:GLN:CG	3:A:631:HOH:O	2.67	0.42
1:A:331:GLY:HA3	3:A:670:HOH:O	2.20	0.41
1:B:202:LYS:HE2	1:B:204:TYR:OH	2.20	0.41
1:B:300:ASN:HA	1:B:447:ILE:HG21	2.02	0.41
1:B:389:GLU:CA	1:B:394:GLN:HE21	2.24	0.41
1:A:402:GLU:OE2	1:A:413:TYR:OH	2.24	0.41
1:A:204:TYR:CZ	1:A:207:ASN:HA	2.56	0.41
1:B:361:ARG:HD2	3:B:724:HOH:O	2.21	0.40
1:B:402:GLU:O	1:B:406:GLU:O	2.40	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:B:172:GLU:OE2	1:B:172:GLU:OE2[4_555]	1.50	0.70

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	278/323 (86%)	269 (97%)	7 (2%)	2 (1%)	22	9
1	B	277/323 (86%)	265 (96%)	8 (3%)	4 (1%)	11	3
All	All	555/646 (86%)	534 (96%)	15 (3%)	6 (1%)	14	4

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	406	GLU
1	A	196	GLY
1	A	223	THR
1	B	223	THR
1	B	256	ASP
1	B	407	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	248/279 (89%)	241 (97%)	7 (3%)	43	26
1	B	246/279 (88%)	237 (96%)	9 (4%)	34	16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	494/558 (88%)	478 (97%)	16 (3%)	39	21

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	182	GLU
1	A	187	VAL
1	A	212	VAL
1	A	342	THR
1	A	352	THR
1	A	365	THR
1	A	458	THR
1	B	169	SER
1	B	212	VAL
1	B	224	GLU
1	B	257	ASP
1	B	342	THR
1	B	352	THR
1	B	365	THR
1	B	448	LYS
1	B	458	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	190	ASN
1	A	206	ASN
1	A	293	GLN
1	A	307	HIS
1	A	394	GLN
1	B	190	ASN
1	B	394	GLN
1	B	455	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	A	346	1	8,9,10	0.73	0	8,12,14	3.13	2 (25%)
1	TPO	B	345	1	8,10,11	0.89	1 (12%)	10,14,16	1.60	2 (20%)
1	TPO	A	345	1	8,10,11	0.81	0	10,14,16	1.43	2 (20%)
1	SEP	B	346	1	8,9,10	0.84	0	8,12,14	1.95	2 (25%)

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	A	346	1	-	3/5/8/10	-
1	TPO	B	345	1	-	3/9/11/13	-
1	TPO	A	345	1	-	4/9/11/13	-
1	SEP	B	346	1	-	1/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	345	TPO	CB-CA	2.12	1.58	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	346	SEP	OG-CB-CA	6.83	114.80	108.14
1	A	346	SEP	P-OG-CB	-4.68	105.39	118.30
1	B	346	SEP	P-OG-CB	-4.32	106.40	118.30
1	B	345	TPO	CG2-CB-CA	-3.12	107.01	113.16
1	B	345	TPO	P-OG1-CB	-2.80	114.76	123.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	345	TPO	CG2-CB-CA	-2.67	107.89	113.16
1	A	345	TPO	P-OG1-CB	-2.48	115.72	123.21
1	B	346	SEP	OG-CB-CA	2.38	110.46	108.14

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	O-C-CA-CB
1	A	346	SEP	CB-OG-P-O1P
1	A	346	SEP	CB-OG-P-O2P
1	A	346	SEP	CB-OG-P-O3P
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB
1	B	345	TPO	CB-OG1-P-O1P
1	B	346	SEP	CB-OG-P-O3P
1	A	345	TPO	CB-OG1-P-O2P
1	A	345	TPO	CB-OG1-P-O3P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	8CD	B	501	-	26,27,27	1.11	1 (3%)	35,38,38	1.06	2 (5%)
2	8CD	A	501	-	26,27,27	1.10	1 (3%)	35,38,38	1.24	3 (8%)

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	8CD	B	501	-	-	0/13/22/22	0/3/3/3
2	8CD	A	501	-	-	0/13/22/22	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	8CD	C18-N3	2.59	1.37	1.33
2	A	501	8CD	C18-N3	2.49	1.37	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	8CD	C13-C12-N2	4.56	104.58	102.54
2	B	501	8CD	C13-C12-N2	3.59	104.15	102.54
2	A	501	8CD	O4-C18-N3	-2.70	118.74	122.58
2	B	501	8CD	O4-C18-N3	-2.65	118.82	122.58
2	A	501	8CD	C14-C13-C12	2.05	106.15	104.57

There are no chirality outliers.

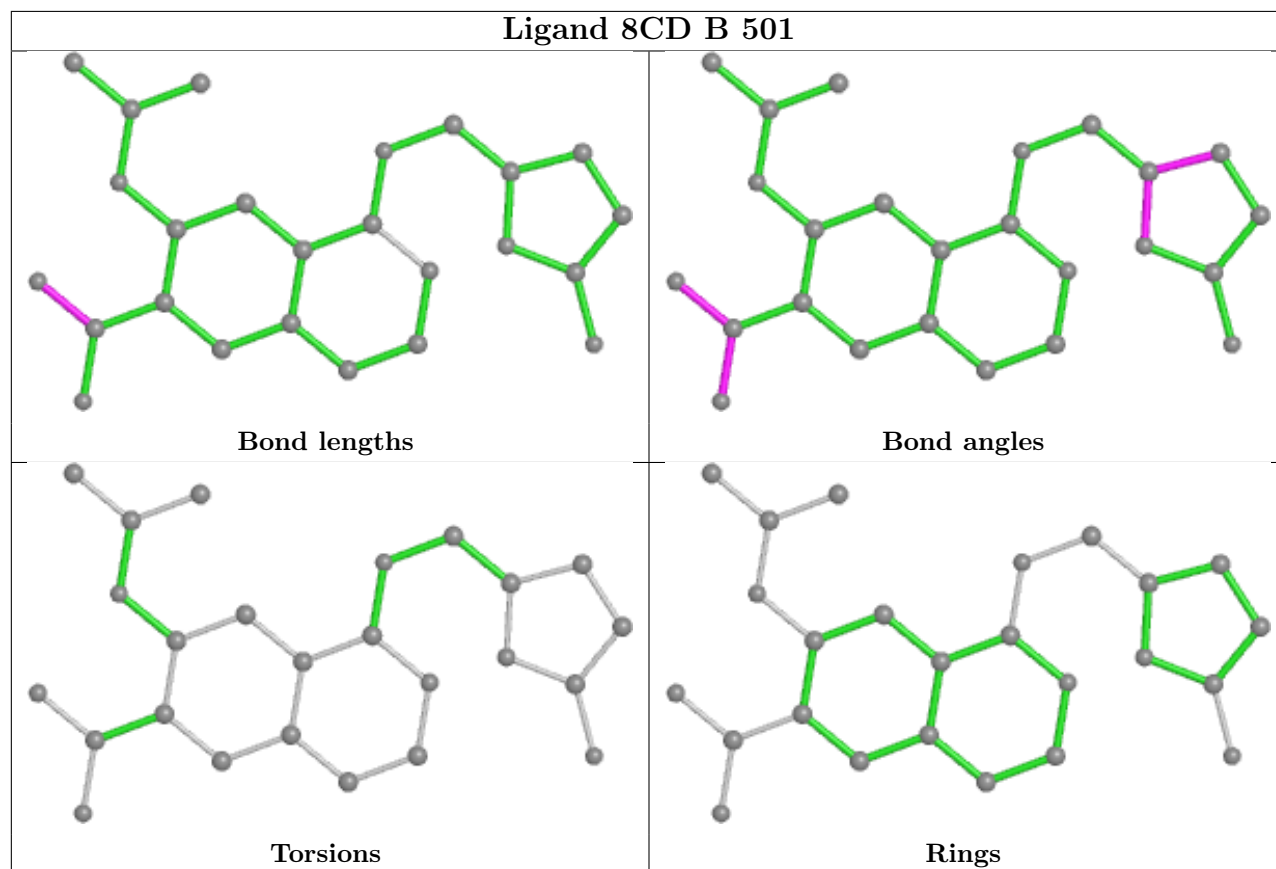
There are no torsion outliers.

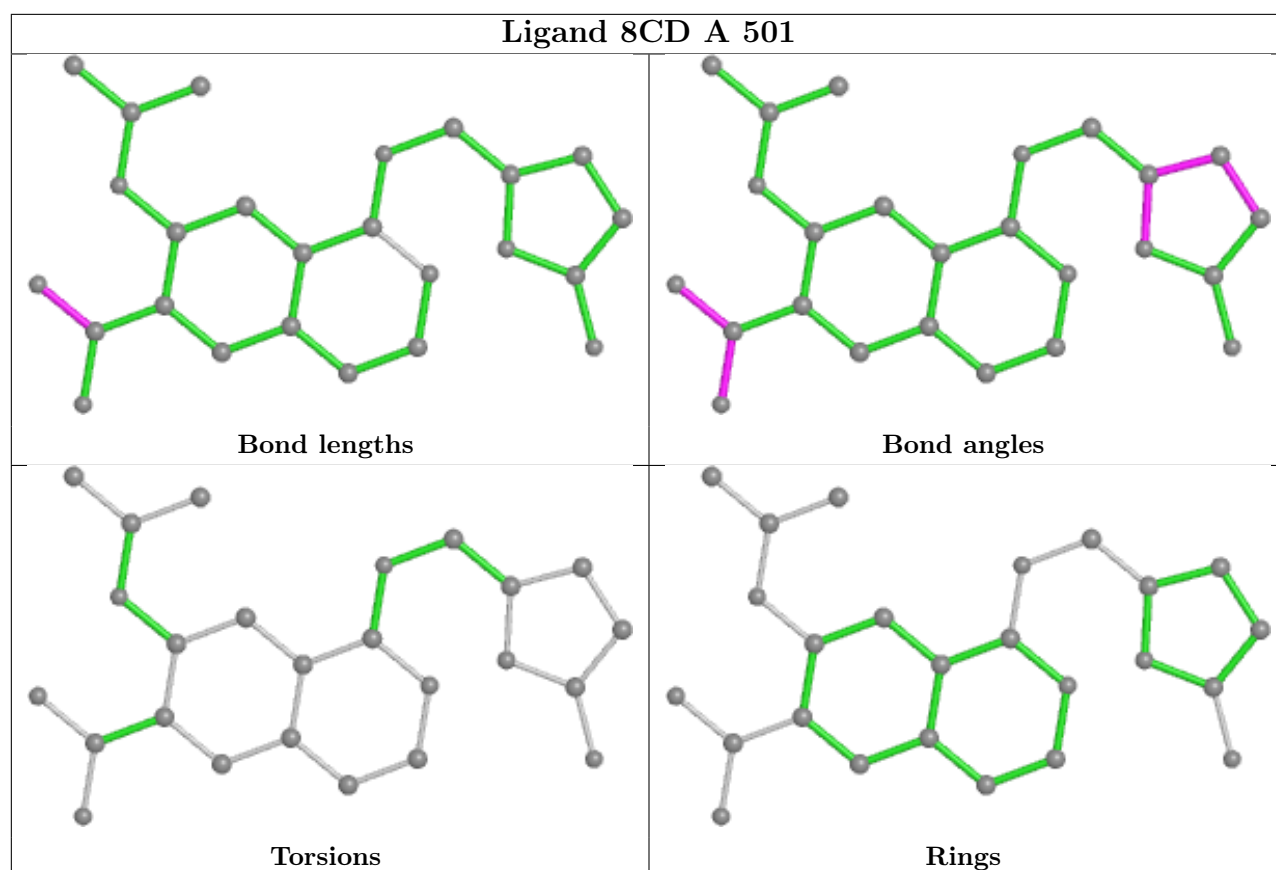
There are no ring outliers.

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

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	A	284/323 (87%)	0.16	14 (4%)	29 27	21, 39, 69, 91	17 (5%)
1	B	283/323 (87%)	0.35	13 (4%)	32 29	20, 37, 68, 98	17 (6%)
All	All	567/646 (87%)	0.26	27 (4%)	30 28	20, 38, 69, 98	34 (5%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	223	THR	6.1
1	A	197	PHE	5.0
1	A	343	VAL	4.4
1	B	256	ASP	4.1
1	A	335	ALA	3.7
1	B	255	GLY	3.3
1	A	226	LEU	3.2
1	A	336	SER	3.2
1	A	225	GLU	2.9
1	B	407	GLU	2.8
1	B	197	PHE	2.8
1	B	171	TYR	2.8
1	A	223	THR	2.8
1	A	222	THR	2.7
1	B	226	LEU	2.5
1	A	342	THR	2.4
1	A	349	VAL	2.4
1	A	395	LEU	2.3
1	B	224	GLU	2.3
1	B	404	GLU	2.3
1	A	206	ASN	2.3
1	A	393	PRO	2.2
1	B	225	GLU	2.2
1	B	390	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	342	THR	2.1
1	B	204	TYR	2.0
1	A	364	ILE	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	B	346	10/11	0.81	0.28	62,70,80,82	0
1	SEP	A	346	10/11	0.91	0.20	72,81,92,94	0
1	TPO	B	345	11/12	0.92	0.15	51,57,63,63	0
1	TPO	A	345	11/12	0.96	0.09	65,68,73,74	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

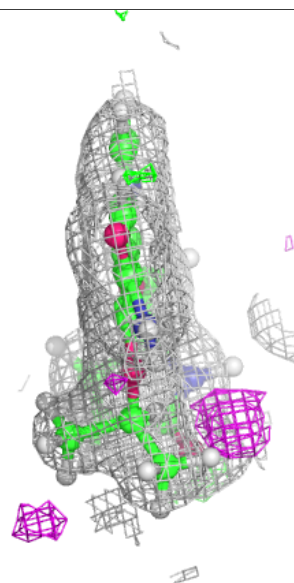
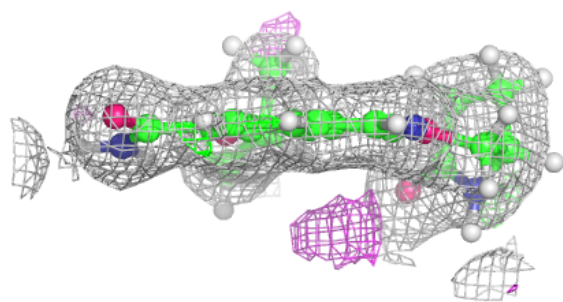
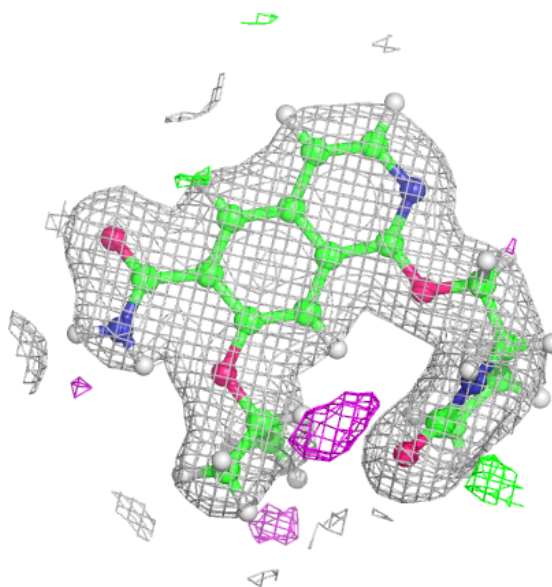
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	8CD	A	501	25/25	0.97	0.09	20,25,27,28	21
2	8CD	B	501	25/25	0.97	0.13	20,22,25,26	21

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.

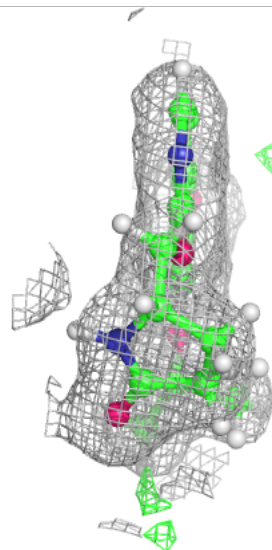
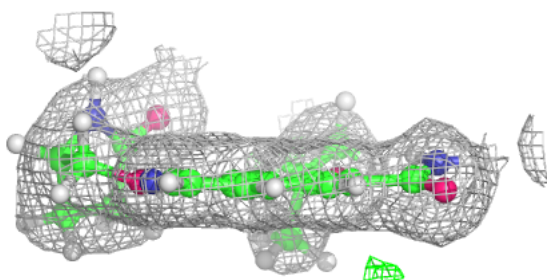
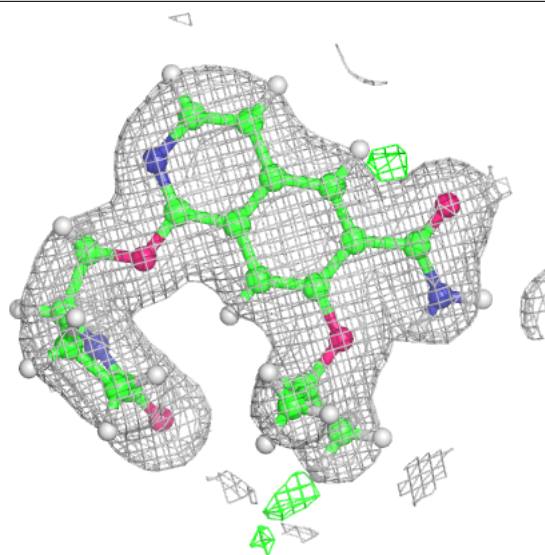
Electron density around 8CD A 501:

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



Electron density around 8CD B 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.