



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:42 PM UTC

PDB ID : 4W7P / pdb_00004w7p
Title : Crystal Structure of ROCK 1 bound to YB-15-QD37
Authors : Sprague, E.R.
Deposited on : 2014-08-22
Resolution : 2.80 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

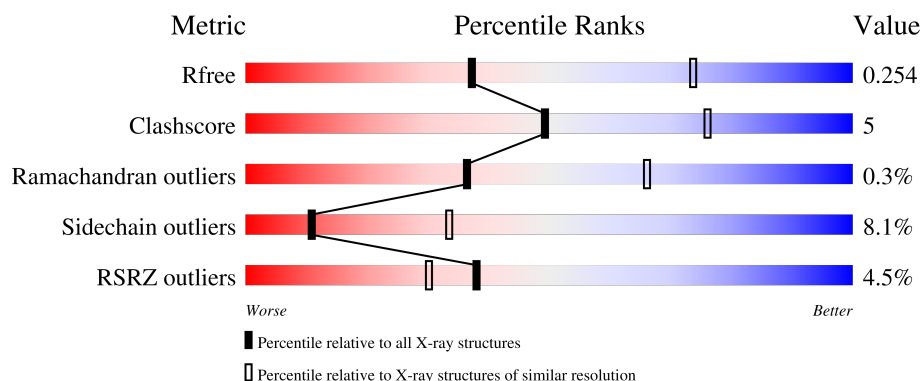
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	411	5% 71% 20% • 6%
1	B	411	5% 73% 18% • 6%
1	C	411	4% 69% 21% • 7%
1	D	411	2% 74% 18% • 6%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12769 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.

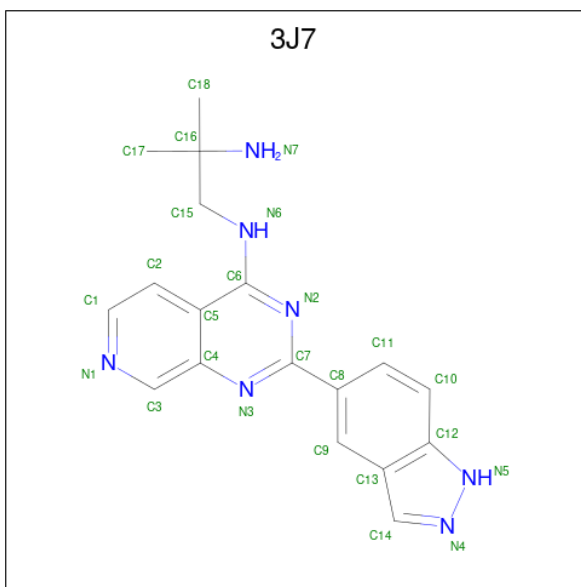
- Molecule 1 is a protein called Rho-associated protein kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			3178	2037	528	592	21			
1	B	387	Total	C	N	O	S	0	0	0
			3163	2027	520	595	21			
1	C	383	Total	C	N	O	S	0	0	0
			3128	2008	516	583	21			
1	D	387	Total	C	N	O	S	0	0	0
			3164	2027	524	592	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP Q13464
A	1	ALA	-	expression tag	UNP Q13464
B	0	GLY	-	expression tag	UNP Q13464
B	1	ALA	-	expression tag	UNP Q13464
C	0	GLY	-	expression tag	UNP Q13464
C	1	ALA	-	expression tag	UNP Q13464
D	0	GLY	-	expression tag	UNP Q13464
D	1	ALA	-	expression tag	UNP Q13464

- Molecule 2 is N 1 -[2-(1H-indazol-5-yl)pyrido[3,4-d]pyrimidin-4-yl]-2-methylpropane-1,2-diamine (CCD ID: 3J7) (formula: C₁₈H₁₉N₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	N	0	0
			25	18	7		
2	B	1	Total	C	N	0	0
			25	18	7		
2	C	1	Total	C	N	0	0
			25	18	7		
2	D	1	Total	C	N	0	0
			25	18	7		

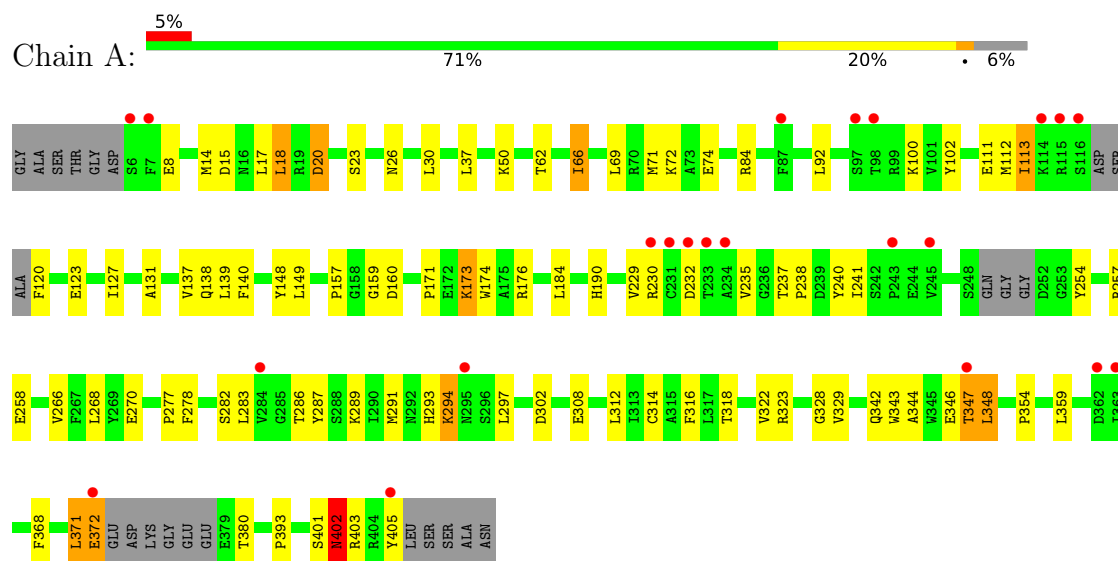
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		
3	B	8	Total	O	0	0
			8	8		
3	C	11	Total	O	0	0
			11	11		
3	D	12	Total	O	0	0
			12	12		

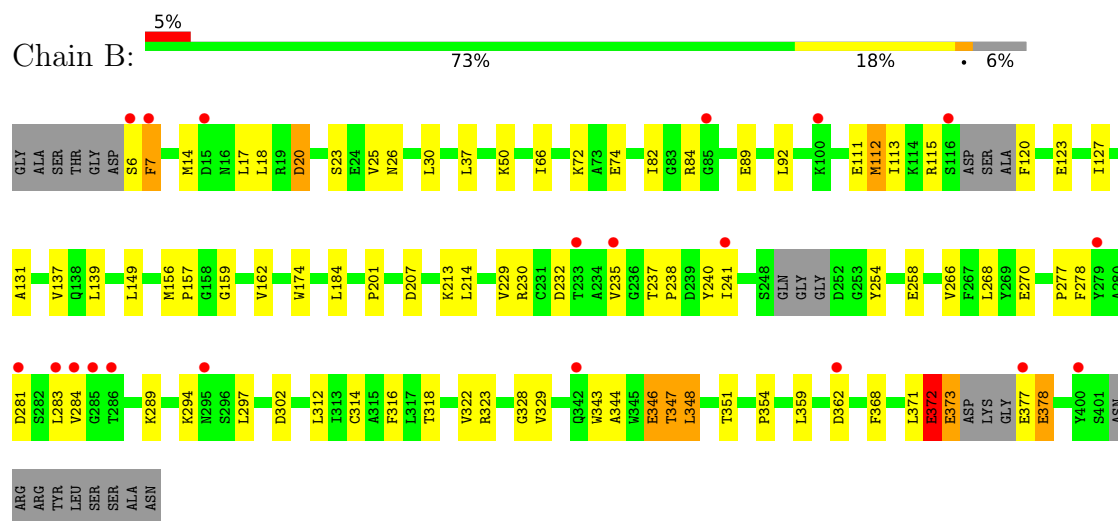
3 Residue-property plots

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: Rho-associated protein kinase 1

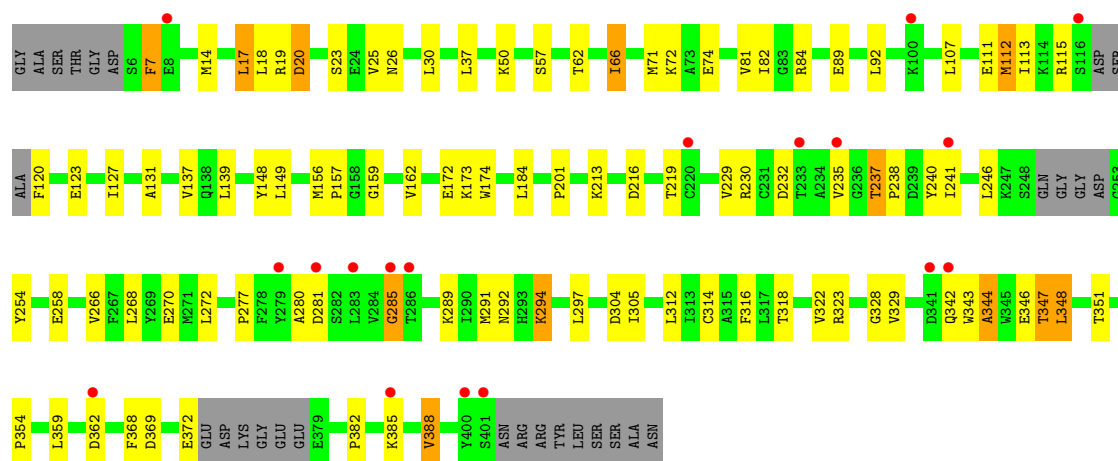


• Molecule 1: Rho-associated protein kinase 1

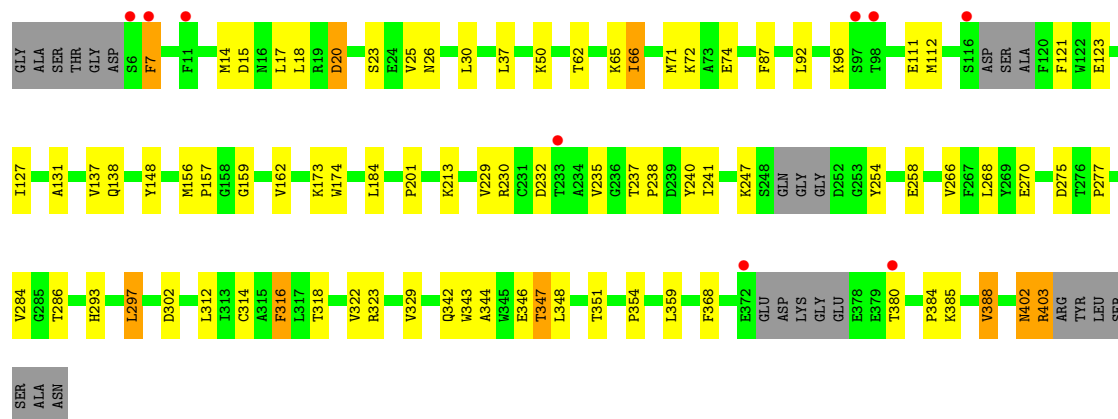
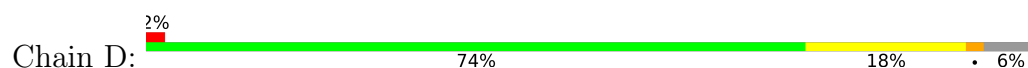


• Molecule 1: Rho-associated protein kinase 1





• Molecule 1: Rho-associated protein kinase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.55Å 179.66Å 89.27Å 90.00° 104.59° 90.00°	Depositor
Resolution (Å)	86.39 – 2.80 86.39 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (86.39-2.80) 99.6 (86.39-2.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.82Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.11.2, BUSTER 2.11.2	Depositor
R, R_{free}	0.206 , 0.246 0.212 , 0.254	Depositor DCC
R_{free} test set	2294 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 65.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12769	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.63% 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: 3J7

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	0.86	0/3253	1.37	19/4391 (0.4%)
1	B	0.86	1/3237 (0.0%)	1.38	16/4370 (0.4%)
1	C	0.86	1/3202 (0.0%)	1.38	23/4323 (0.5%)
1	D	0.84	0/3238	1.35	10/4371 (0.2%)
All	All	0.86	2/12930 (0.0%)	1.37	68/17455 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	112	MET	SD-CE	-5.98	1.64	1.79
1	B	112	MET	SD-CE	-5.79	1.65	1.79

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	286	THR	N-CA-C	-9.96	99.97	111.03
1	D	286	THR	N-CA-C	-8.10	102.40	111.14
1	C	7	PHE	CA-CB-CG	7.90	121.70	113.80
1	C	388	VAL	CB-CA-C	7.82	118.31	110.65
1	B	378	GLU	N-CA-C	7.70	121.10	110.24
1	B	7	PHE	N-CA-C	7.36	120.00	111.02
1	A	20	ASP	CA-CB-CG	6.84	119.44	112.60
1	B	348	LEU	N-CA-C	6.46	117.98	111.07
1	D	7	PHE	N-CA-C	6.21	118.60	111.02
1	D	20	ASP	CA-CB-CG	6.07	118.67	112.60
1	C	304	ASP	N-CA-C	-6.04	105.17	112.54
1	B	157	PRO	N-CA-C	5.93	121.27	113.86
1	D	157	PRO	N-CA-C	5.83	121.41	113.84
1	D	380	THR	N-CA-C	5.80	118.22	109.41
1	C	348	LEU	N-CA-C	5.79	117.26	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	157	PRO	N-CA-C	5.69	121.31	113.98
1	A	157	PRO	N-CA-C	5.68	120.97	113.86
1	B	237	THR	CB-CA-C	5.68	117.55	109.08
1	A	348	LEU	N-CA-C	5.67	117.13	111.07
1	A	371	LEU	CA-C-N	5.66	131.88	121.70
1	A	371	LEU	C-N-CA	5.66	131.88	121.70
1	B	377	GLU	CA-C-N	5.60	128.80	120.90
1	B	377	GLU	C-N-CA	5.60	128.80	120.90
1	D	385	LYS	N-CA-C	-5.58	106.51	113.38
1	C	369	ASP	CA-CB-CG	5.53	118.13	112.60
1	A	328	GLY	CA-C-N	5.49	128.27	120.53
1	A	328	GLY	C-N-CA	5.49	128.27	120.53
1	C	237	THR	CB-CA-C	5.48	117.24	109.08
1	D	302	ASP	CA-CB-CG	5.48	118.08	112.60
1	D	237	THR	CB-CA-C	5.44	117.18	109.08
1	A	302	ASP	CA-CB-CG	5.43	118.03	112.60
1	A	402	ASN	CA-CB-CG	5.31	117.91	112.60
1	B	207	ASP	CA-CB-CG	5.30	117.90	112.60
1	C	385	LYS	N-CA-C	-5.28	106.89	113.38
1	B	6	SER	CA-C-N	5.27	128.11	120.79
1	B	6	SER	C-N-CA	5.27	128.11	120.79
1	C	20	ASP	CA-CB-CG	5.26	117.86	112.60
1	A	160	ASP	CA-CB-CG	5.25	117.85	112.60
1	B	149	LEU	N-CA-C	-5.24	101.17	109.76
1	C	285	GLY	CA-C-N	5.23	127.75	120.63
1	C	285	GLY	C-N-CA	5.23	127.75	120.63
1	A	237	THR	CB-CA-C	5.23	116.87	109.08
1	C	362	ASP	CA-CB-CG	5.20	117.80	112.60
1	C	344	ALA	N-CA-C	-5.19	102.10	110.14
1	B	20	ASP	CA-CB-CG	5.18	117.78	112.60
1	B	302	ASP	N-CA-C	5.17	116.06	107.73
1	B	362	ASP	CA-CB-CG	5.15	117.75	112.60
1	A	149	LEU	N-CA-C	-5.15	101.31	109.76
1	C	328	GLY	CA-C-N	5.15	127.79	120.53
1	C	328	GLY	C-N-CA	5.15	127.79	120.53
1	C	57	SER	CA-C-N	5.15	127.17	120.28
1	C	57	SER	C-N-CA	5.15	127.17	120.28
1	A	148	TYR	N-CA-C	5.13	117.96	109.85
1	A	293	HIS	CA-C-N	5.13	127.16	120.28
1	A	293	HIS	C-N-CA	5.13	127.16	120.28
1	A	282	SER	CA-C-N	5.12	127.14	120.28
1	A	282	SER	C-N-CA	5.12	127.14	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	308	GLU	CB-CG-CD	5.11	121.29	112.60
1	C	292	ASN	CA-CB-CG	5.09	117.69	112.60
1	C	149	LEU	N-CA-C	-5.07	101.44	109.76
1	C	304	ASP	CA-C-N	5.07	128.18	120.77
1	C	304	ASP	C-N-CA	5.07	128.18	120.77
1	B	328	GLY	CA-C-N	5.04	127.64	120.53
1	B	328	GLY	C-N-CA	5.04	127.64	120.53
1	D	148	TYR	N-CA-C	5.03	117.06	109.41
1	C	148	TYR	N-CA-C	5.03	117.31	109.52
1	C	81	VAL	N-CA-CB	5.02	116.72	111.00
1	D	316	PHE	CA-CB-CG	5.01	118.81	113.80

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	3178	0	3091	41	0
1	B	3163	0	3068	35	0
1	C	3128	0	3046	44	0
1	D	3164	0	3075	37	0
2	A	25	0	19	1	0
2	B	25	0	19	2	0
2	C	25	0	19	2	0
2	D	25	0	19	1	0
3	A	5	0	0	0	0
3	B	8	0	0	0	0
3	C	11	0	0	0	0
3	D	12	0	0	0	0
All	All	12769	0	12356	136	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 5.

All (136) 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:C:343:TRP:HB3	1:C:351:THR:HG21	1.55	0.88
1:C:344:ALA:H	1:C:347:THR:HG22	1.42	0.84
1:A:66:ILE:HD11	1:B:25:VAL:HG21	1.59	0.84
1:B:344:ALA:H	1:B:347:THR:HG22	1.49	0.77
1:C:37:LEU:HD13	1:D:37:LEU:HD13	1.67	0.75
1:C:25:VAL:HG21	1:D:66:ILE:HD11	1.69	0.74
1:D:402:ASN:H	1:D:402:ASN:HD22	1.36	0.73
1:B:346:GLU:HG3	1:D:247:LYS:HG2	1.70	0.73
1:C:240:TYR:OH	1:C:270:GLU:OE2	2.06	0.73
1:A:266:VAL:HG13	1:A:277:PRO:HD2	1.71	0.73
1:A:112:MET:HE1	1:A:120:PHE:HZ	1.54	0.73
1:A:137:VAL:HG11	2:A:501:3J7:H15	1.71	0.73
1:C:30:LEU:HB3	1:D:30:LEU:HB3	1.72	0.72
1:D:137:VAL:HG11	2:D:501:3J7:H15	1.72	0.71
1:C:266:VAL:HG13	1:C:277:PRO:HD2	1.73	0.70
1:B:316:PHE:O	1:B:323:ARG:HD2	1.91	0.70
1:D:266:VAL:HG13	1:D:277:PRO:HD2	1.74	0.70
1:A:316:PHE:O	1:A:323:ARG:HD2	1.91	0.69
1:C:137:VAL:HG11	2:C:501:3J7:H15	1.74	0.69
1:C:316:PHE:O	1:C:323:ARG:HD2	1.93	0.69
1:A:37:LEU:HD13	1:B:37:LEU:HD13	1.75	0.69
1:B:266:VAL:HG13	1:B:277:PRO:HD2	1.74	0.68
1:D:316:PHE:O	1:D:323:ARG:HD2	1.94	0.68
1:B:240:TYR:OH	1:B:270:GLU:OE2	2.08	0.68
1:D:240:TYR:OH	1:D:270:GLU:OE2	2.12	0.68
1:D:72:LYS:HG3	1:D:74:GLU:HG2	1.75	0.67
1:A:240:TYR:OH	1:A:270:GLU:OE2	2.12	0.65
1:D:138:GLN:HE22	1:D:403:ARG:HD3	1.59	0.65
1:B:343:TRP:HB3	1:B:351:THR:HG21	1.79	0.65
1:A:344:ALA:HB3	1:A:347:THR:HG22	1.79	0.64
1:B:72:LYS:HG3	1:B:74:GLU:HG2	1.80	0.64
1:C:72:LYS:HG3	1:C:74:GLU:HG2	1.81	0.62
1:A:72:LYS:HG3	1:A:74:GLU:HG2	1.81	0.61
1:D:343:TRP:HB3	1:D:351:THR:HG21	1.85	0.58
1:C:66:ILE:HD11	1:D:25:VAL:HG21	1.87	0.57
1:A:30:LEU:HB3	1:B:30:LEU:HB3	1.86	0.57
1:A:112:MET:HE1	1:A:120:PHE:CZ	2.38	0.57
1:C:230:ARG:HG2	1:C:254:TYR:HD1	1.71	0.56
1:D:230:ARG:HG2	1:D:254:TYR:HD1	1.71	0.56
1:B:230:ARG:HG2	1:B:254:TYR:HD1	1.70	0.55
1:B:351:THR:HA	1:D:284:VAL:HG11	1.88	0.55
1:B:112:MET:HE2	1:B:120:PHE:CZ	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:ARG:HG2	1:A:254:TYR:HD1	1.71	0.54
1:A:14:MET:HE1	1:B:66:ILE:HA	1.89	0.54
1:C:7:PHE:CE2	1:D:71:MET:HE2	2.45	0.52
1:C:280:ALA:HB2	1:C:289:LYS:HE3	1.90	0.52
1:C:230:ARG:HG2	1:C:254:TYR:CD1	2.45	0.52
1:B:314:CYS:O	1:B:318:THR:HG23	2.10	0.52
1:D:230:ARG:HG2	1:D:254:TYR:CD1	2.45	0.52
1:C:314:CYS:O	1:C:318:THR:HG23	2.10	0.51
1:D:293:HIS:O	1:D:297:LEU:HB2	2.11	0.51
1:A:230:ARG:HG2	1:A:254:TYR:CD1	2.45	0.51
1:B:230:ARG:HG2	1:B:254:TYR:CD1	2.45	0.51
1:A:287:TYR:O	1:A:291:MET:HG2	2.10	0.51
1:A:314:CYS:O	1:A:318:THR:HG23	2.11	0.50
1:B:84:ARG:HH21	1:B:371:LEU:HB3	1.76	0.50
1:C:172:GLU:OE1	1:C:305:ILE:HA	2.11	0.50
1:D:314:CYS:O	1:D:318:THR:HG23	2.12	0.50
1:A:138:GLN:HE22	1:A:403:ARG:HD3	1.77	0.50
1:A:84:ARG:HH22	1:A:372:GLU:HG3	1.77	0.49
1:A:66:ILE:HD12	1:B:14:MET:SD	2.53	0.49
1:C:172:GLU:HG2	1:C:272:LEU:HD22	1.94	0.49
1:B:162:VAL:HG23	1:B:201:PRO:HB2	1.94	0.49
1:D:174:TRP:CD1	1:D:354:PRO:HB3	2.48	0.49
1:C:20:ASP:HB3	1:C:23:SER:HB2	1.94	0.49
1:C:246:LEU:HD23	1:C:291:MET:SD	2.53	0.49
1:A:402:ASN:O	1:C:382:PRO:HB3	2.12	0.48
1:A:113:ILE:HD11	1:A:393:PRO:HG2	1.95	0.48
1:C:174:TRP:CD1	1:C:354:PRO:HB3	2.48	0.48
1:C:82:ILE:HD12	2:C:501:3J7:H9	1.94	0.48
1:B:372:GLU:O	1:B:373:GLU:HB2	2.13	0.48
1:A:127:ILE:O	1:A:131:ALA:HB2	2.14	0.48
1:A:20:ASP:HB3	1:A:23:SER:HB2	1.96	0.48
1:C:84:ARG:HG3	1:C:89:GLU:HG2	1.96	0.47
1:A:190:HIS:CE1	1:A:257:ARG:HB2	2.50	0.47
1:B:20:ASP:HB3	1:B:23:SER:HB2	1.95	0.47
1:C:156:MET:SD	1:C:213:LYS:HD2	2.55	0.47
1:B:82:ILE:HD12	2:B:501:3J7:H13	1.97	0.46
1:C:14:MET:SD	1:D:66:ILE:HD12	2.55	0.46
1:B:174:TRP:CD1	1:B:354:PRO:HB3	2.50	0.46
1:A:84:ARG:HH21	1:A:371:LEU:HB3	1.81	0.46
1:A:174:TRP:CD1	1:A:354:PRO:HB3	2.50	0.46
1:B:137:VAL:HG11	2:B:501:3J7:H15	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ILE:O	1:B:131:ALA:HB2	2.16	0.45
1:A:18:LEU:HA	1:A:26:ASN:HA	1.98	0.45
1:C:107:LEU:HB3	1:C:112:MET:HE3	1.99	0.45
1:B:156:MET:SD	1:B:213:LYS:HD2	2.56	0.45
1:C:343:TRP:CD2	1:C:348:LEU:HD13	2.52	0.45
1:C:127:ILE:O	1:C:131:ALA:HB2	2.17	0.45
1:A:66:ILE:HA	1:B:14:MET:HE1	1.99	0.44
1:C:14:MET:HE1	1:D:66:ILE:HA	1.98	0.44
1:A:176:ARG:HG2	1:A:343:TRP:HZ2	1.82	0.44
1:C:18:LEU:HA	1:C:26:ASN:HA	1.99	0.44
1:C:84:ARG:NH2	1:C:372:GLU:HG3	2.32	0.44
1:B:184:LEU:HD12	1:B:348:LEU:HD23	2.00	0.44
1:C:112:MET:HE2	1:C:120:PHE:CE2	2.53	0.44
1:A:159:GLY:HA2	1:A:368:PHE:CZ	2.53	0.44
1:D:384:PRO:HB3	1:D:388:VAL:CG1	2.48	0.44
1:A:294:LYS:HD2	1:A:294:LYS:H	1.84	0.43
1:C:294:LYS:HD2	1:C:294:LYS:H	1.83	0.43
1:B:18:LEU:HA	1:B:26:ASN:HA	2.01	0.43
1:B:278:PHE:HB3	1:B:289:LYS:HB3	2.00	0.43
1:B:84:ARG:HG3	1:B:89:GLU:HG2	2.01	0.43
1:B:159:GLY:HA2	1:B:368:PHE:CZ	2.54	0.43
1:C:71:MET:HE2	1:D:7:PHE:HE1	1.84	0.43
1:D:18:LEU:HA	1:D:26:ASN:HA	2.01	0.43
1:D:238:PRO:O	1:D:241:ILE:HG22	2.18	0.43
1:A:278:PHE:HB3	1:A:289:LYS:HB3	2.01	0.42
1:C:17:LEU:HD21	1:D:65:LYS:HE3	2.01	0.42
1:C:172:GLU:HG2	1:C:272:LEU:CD2	2.48	0.42
1:A:69:LEU:HB2	1:B:14:MET:CE	2.50	0.42
1:A:171:PRO:HB2	1:A:173:LYS:HE3	2.01	0.42
1:C:159:GLY:HA2	1:C:368:PHE:CZ	2.53	0.42
1:D:20:ASP:HB3	1:D:23:SER:HB2	2.02	0.42
1:D:127:ILE:O	1:D:131:ALA:HB2	2.19	0.42
1:D:87:PHE:HD1	1:D:111:GLU:HB3	1.84	0.42
1:A:71:MET:HE2	1:B:7:PHE:HE1	1.83	0.42
1:C:107:LEU:HD13	1:C:112:MET:HE1	2.01	0.42
1:C:162:VAL:HG23	1:C:201:PRO:HB2	2.02	0.42
1:C:238:PRO:O	1:C:241:ILE:HG22	2.19	0.42
1:D:159:GLY:HA2	1:D:368:PHE:CZ	2.54	0.42
1:C:184:LEU:HD12	1:C:348:LEU:HD23	2.02	0.41
1:D:184:LEU:HD12	1:D:348:LEU:HD23	2.02	0.41
1:A:100:LYS:HD3	1:A:102:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:PHE:O	1:A:401:SER:HB2	2.21	0.41
1:C:66:ILE:HD12	1:D:14:MET:SD	2.60	0.41
1:D:156:MET:SD	1:D:213:LYS:HD2	2.61	0.41
1:A:184:LEU:HD12	1:A:348:LEU:HD23	2.02	0.41
1:A:403:ARG:HH21	1:A:405:TYR:HH	1.65	0.41
1:A:238:PRO:O	1:A:241:ILE:HG22	2.20	0.41
1:B:238:PRO:O	1:B:241:ILE:HG22	2.21	0.41
1:A:173:LYS:H	1:A:173:LYS:HG3	1.52	0.41
1:D:112:MET:HE2	1:D:121:PHE:HD2	1.86	0.40
1:D:162:VAL:HG23	1:D:201:PRO:HB2	2.03	0.40
1:C:237:THR:HA	1:C:238:PRO:HD2	1.95	0.40
1:D:344:ALA:HB3	1:D:347:THR:HG22	2.03	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	380/411 (92%)	364 (96%)	16 (4%)	0	100	100
1	B	379/411 (92%)	363 (96%)	14 (4%)	2 (0%)	24	55
1	C	375/411 (91%)	360 (96%)	13 (4%)	2 (0%)	24	55
1	D	379/411 (92%)	366 (97%)	12 (3%)	1 (0%)	36	66
All	All	1513/1644 (92%)	1453 (96%)	55 (4%)	5 (0%)	36	66

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	372	GLU
1	C	285	GLY
1	D	96	LYS

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Mol	Chain	Res	Type
1	B	115	ARG
1	C	216	ASP

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	348/363 (96%)	317 (91%)	31 (9%)	9	29
1	B	347/363 (96%)	320 (92%)	27 (8%)	11	35
1	C	343/363 (94%)	314 (92%)	29 (8%)	10	31
1	D	347/363 (96%)	322 (93%)	25 (7%)	13	39
All	All	1385/1452 (95%)	1273 (92%)	112 (8%)	11	33

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	GLU
1	A	15	ASP
1	A	17	LEU
1	A	18	LEU
1	A	50	LYS
1	A	62	THR
1	A	66	ILE
1	A	92	LEU
1	A	111	GLU
1	A	113	ILE
1	A	123	GLU
1	A	139	LEU
1	A	173	LYS
1	A	229	VAL
1	A	232	ASP
1	A	235	VAL
1	A	258	GLU
1	A	268	LEU
1	A	283	LEU

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Mol	Chain	Res	Type
1	A	294	LYS
1	A	297	LEU
1	A	312	LEU
1	A	322	VAL
1	A	329	VAL
1	A	342	GLN
1	A	346	GLU
1	A	347	THR
1	A	359	LEU
1	A	372	GLU
1	A	380	THR
1	A	402	ASN
1	B	17	LEU
1	B	50	LYS
1	B	92	LEU
1	B	111	GLU
1	B	113	ILE
1	B	123	GLU
1	B	139	LEU
1	B	214	LEU
1	B	229	VAL
1	B	232	ASP
1	B	235	VAL
1	B	258	GLU
1	B	268	LEU
1	B	281	ASP
1	B	283	LEU
1	B	284	VAL
1	B	294	LYS
1	B	297	LEU
1	B	312	LEU
1	B	322	VAL
1	B	329	VAL
1	B	346	GLU
1	B	347	THR
1	B	359	LEU
1	B	372	GLU
1	B	373	GLU
1	B	378	GLU
1	C	17	LEU
1	C	19	ARG
1	C	50	LYS

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Mol	Chain	Res	Type
1	C	62	THR
1	C	66	ILE
1	C	92	LEU
1	C	111	GLU
1	C	113	ILE
1	C	115	ARG
1	C	123	GLU
1	C	139	LEU
1	C	173	LYS
1	C	219	THR
1	C	229	VAL
1	C	232	ASP
1	C	235	VAL
1	C	258	GLU
1	C	268	LEU
1	C	281	ASP
1	C	294	LYS
1	C	297	LEU
1	C	312	LEU
1	C	322	VAL
1	C	329	VAL
1	C	342	GLN
1	C	346	GLU
1	C	347	THR
1	C	359	LEU
1	C	388	VAL
1	D	15	ASP
1	D	17	LEU
1	D	50	LYS
1	D	62	THR
1	D	66	ILE
1	D	92	LEU
1	D	123	GLU
1	D	173	LYS
1	D	229	VAL
1	D	232	ASP
1	D	235	VAL
1	D	258	GLU
1	D	268	LEU
1	D	275	ASP
1	D	297	LEU
1	D	312	LEU

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Mol	Chain	Res	Type
1	D	322	VAL
1	D	329	VAL
1	D	342	GLN
1	D	346	GLU
1	D	347	THR
1	D	359	LEU
1	D	388	VAL
1	D	402	ASN
1	D	403	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	54	ASN
1	A	91	GLN
1	A	167	ASN
1	A	327	ASN
1	A	342	GLN
1	B	54	ASN
1	B	91	GLN
1	B	167	ASN
1	B	292	ASN
1	B	293	HIS
1	B	327	ASN
1	C	54	ASN
1	C	292	ASN
1	C	293	HIS
1	C	295	ASN
1	C	327	ASN
1	D	26	ASN
1	D	54	ASN
1	D	91	GLN
1	D	167	ASN
1	D	327	ASN
1	D	402	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

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	3J7	B	501	-	23,28,28	1.60	4 (17%)	30,41,41	1.62	5 (16%)
2	3J7	C	501	-	23,28,28	1.57	3 (13%)	30,41,41	1.79	6 (20%)
2	3J7	A	501	-	23,28,28	1.86	7 (30%)	30,41,41	1.48	5 (16%)
2	3J7	D	501	-	23,28,28	1.57	3 (13%)	30,41,41	1.63	7 (23%)

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	3J7	B	501	-	-	3/10/10/10	0/4/4/4
2	3J7	C	501	-	-	1/10/10/10	0/4/4/4
2	3J7	A	501	-	-	2/10/10/10	0/4/4/4
2	3J7	D	501	-	-	2/10/10/10	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	3J7	C6-N6	4.38	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	3J7	C6-N6	4.29	1.41	1.34
2	D	501	3J7	C6-N6	4.26	1.41	1.34
2	A	501	3J7	C6-N6	4.16	1.41	1.34
2	A	501	3J7	C2-C1	3.66	1.41	1.36
2	D	501	3J7	C2-C1	3.37	1.41	1.36
2	C	501	3J7	C2-C1	3.27	1.41	1.36
2	B	501	3J7	C2-C1	3.04	1.40	1.36
2	A	501	3J7	C9-C8	2.58	1.44	1.39
2	A	501	3J7	C3-N1	2.46	1.36	1.32
2	A	501	3J7	C10-C11	2.44	1.42	1.38
2	A	501	3J7	N5-N4	-2.34	1.34	1.36
2	B	501	3J7	C9-C8	2.33	1.43	1.39
2	A	501	3J7	C11-C8	2.33	1.44	1.39
2	D	501	3J7	C9-C8	2.30	1.43	1.39
2	B	501	3J7	C10-C11	2.22	1.42	1.38
2	C	501	3J7	C4-N3	-2.03	1.34	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	3J7	C12-N5-N4	5.88	114.40	111.52
2	C	501	3J7	C12-N5-N4	5.37	114.16	111.52
2	A	501	3J7	C12-N5-N4	4.40	113.68	111.52
2	D	501	3J7	C12-N5-N4	3.75	113.36	111.52
2	C	501	3J7	C1-C2-C5	-3.70	116.60	119.75
2	D	501	3J7	C9-C13-C12	-3.63	116.88	119.13
2	C	501	3J7	C9-C13-C12	-3.19	117.15	119.13
2	A	501	3J7	C17-C16-C15	3.18	115.06	109.87
2	B	501	3J7	C1-C2-C5	-3.05	117.15	119.75
2	D	501	3J7	C6-N2-C7	2.78	120.90	117.20
2	B	501	3J7	C9-C13-C12	-2.65	117.48	119.13
2	C	501	3J7	C18-C16-C15	2.56	114.06	109.87
2	D	501	3J7	C7-N3-C4	2.49	118.26	116.56
2	A	501	3J7	C6-N2-C7	2.41	120.40	117.20
2	D	501	3J7	N3-C7-N2	-2.39	123.31	126.49
2	D	501	3J7	C1-C2-C5	-2.34	117.76	119.75
2	A	501	3J7	C9-C13-C12	-2.13	117.81	119.13
2	A	501	3J7	C1-C2-C5	-2.12	117.95	119.75
2	D	501	3J7	C17-C16-C15	2.09	113.29	109.87
2	B	501	3J7	C6-N2-C7	2.09	119.98	117.20
2	C	501	3J7	C6-N2-C7	2.07	119.95	117.20
2	B	501	3J7	C17-C16-C15	2.02	113.17	109.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	3J7	C5-C6-N6	2.01	122.76	120.76

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	3J7	N6-C15-C16-N7
2	B	501	3J7	N6-C15-C16-C17
2	B	501	3J7	N6-C15-C16-C18
2	B	501	3J7	N6-C15-C16-N7
2	D	501	3J7	N6-C15-C16-N7
2	D	501	3J7	N6-C15-C16-C17
2	C	501	3J7	N2-C6-N6-C15
2	A	501	3J7	N6-C15-C16-C17

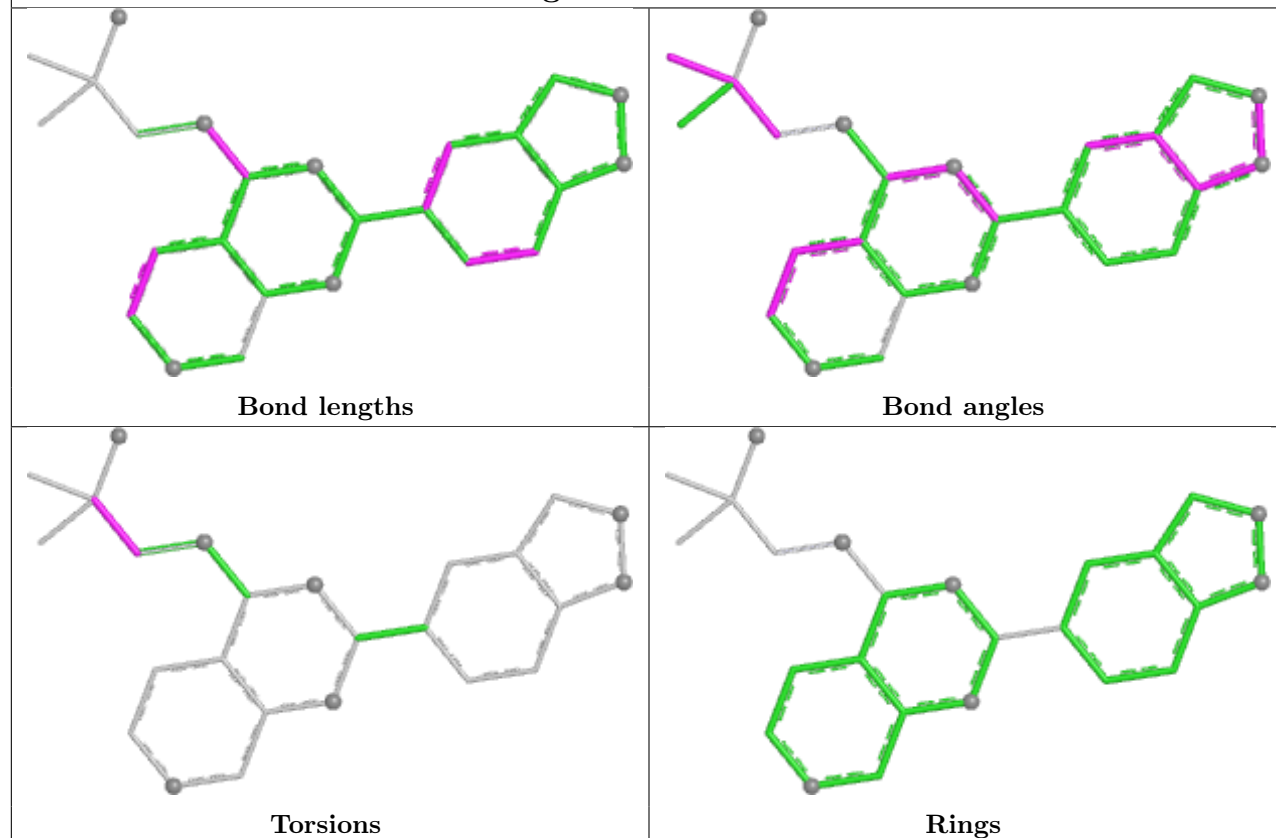
There are no ring outliers.

4 monomers are involved in 6 short contacts:

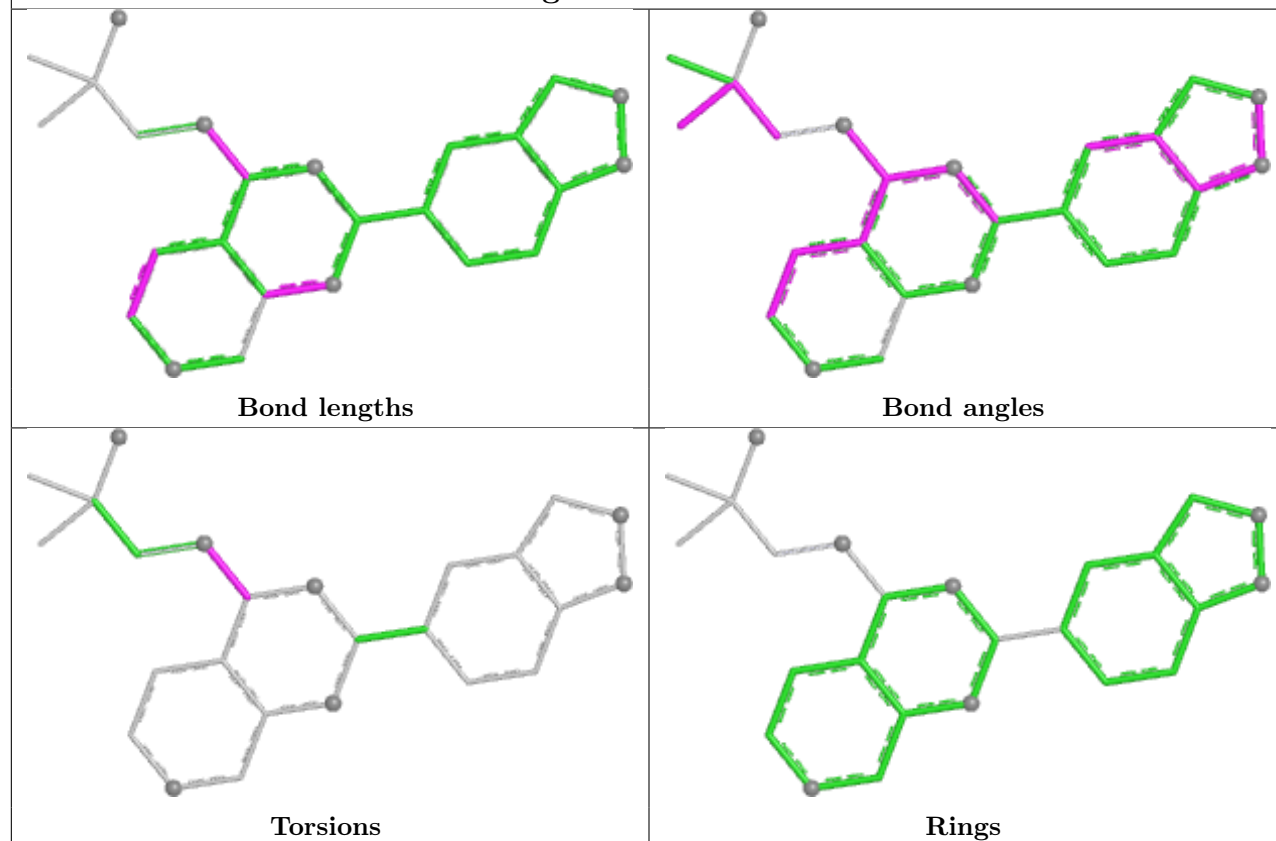
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	3J7	2	0
2	C	501	3J7	2	0
2	A	501	3J7	1	0
2	D	501	3J7	1	0

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.

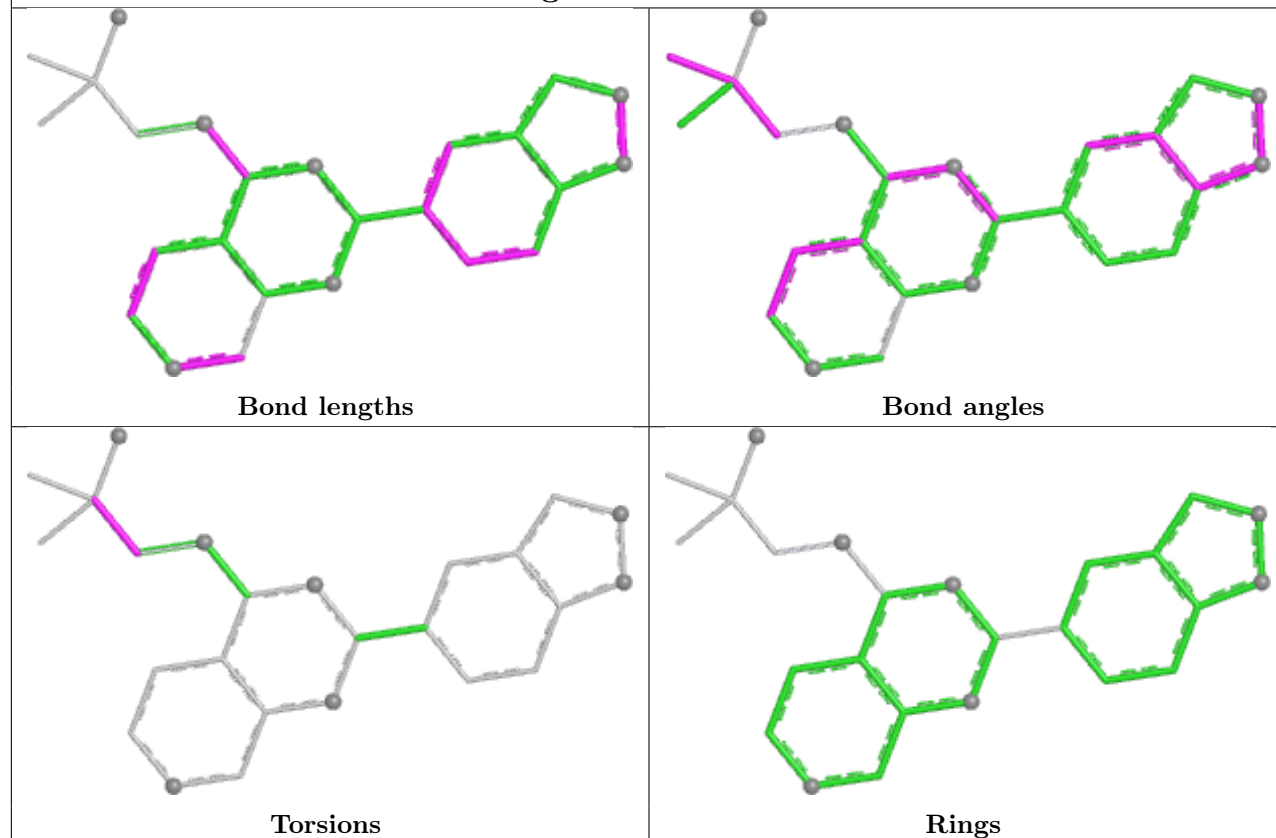
Ligand 3J7 B 501



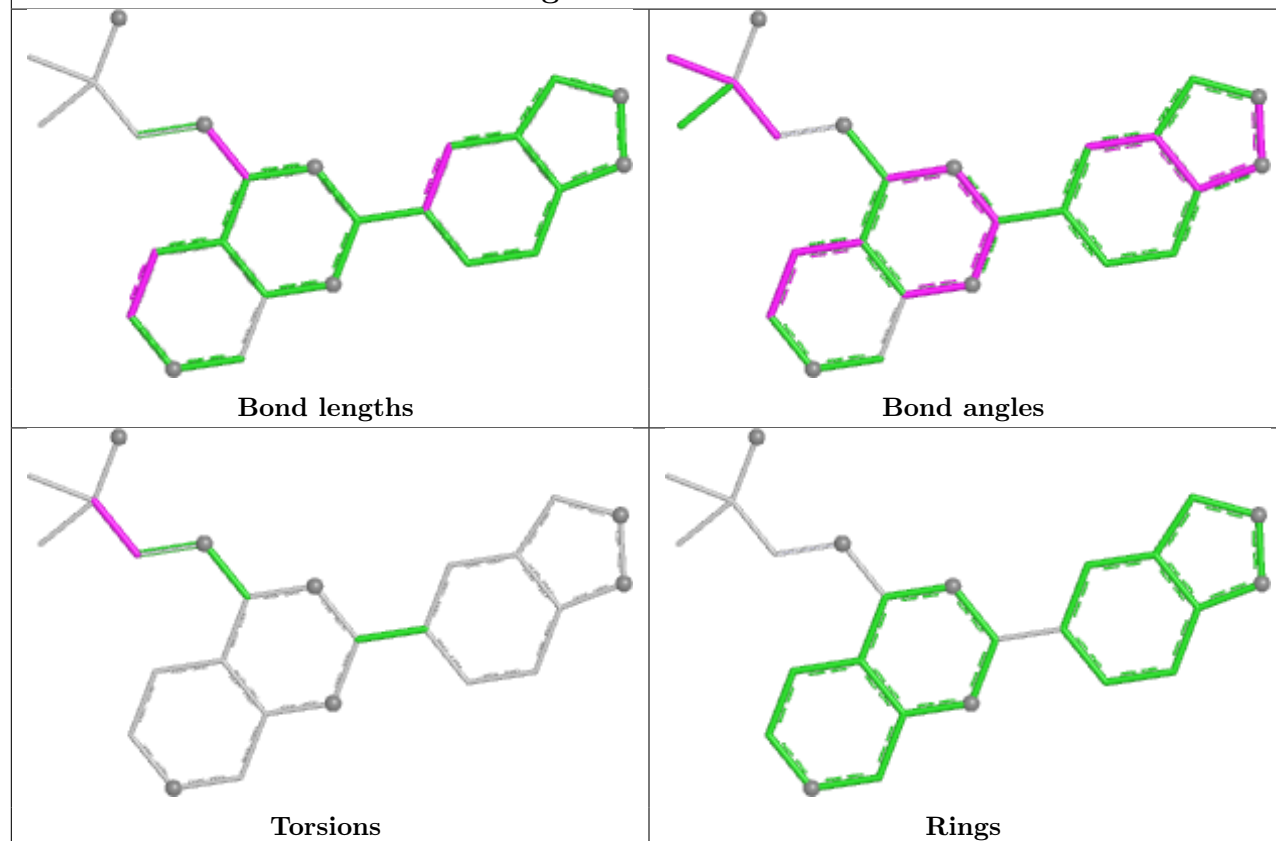
Ligand 3J7 C 501



Ligand 3J7 A 501



Ligand 3J7 D 501



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	388/411 (94%)	0.39	22 (5%)	29 22	25, 49, 81, 98	0
1	B	387/411 (94%)	0.53	20 (5%)	33 25	31, 52, 92, 114	0
1	C	383/411 (93%)	0.28	18 (4%)	36 29	24, 46, 77, 101	0
1	D	387/411 (94%)	0.30	9 (2%)	61 51	26, 46, 76, 104	0
All	All	1545/1644 (93%)	0.37	69 (4%)	38 30	24, 48, 85, 114	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	116	SER	5.1
1	B	7	PHE	4.6
1	D	7	PHE	4.5
1	A	363	ILE	4.3
1	B	100	LYS	3.7
1	C	342	GLN	3.7
1	C	283	LEU	3.4
1	A	7	PHE	3.3
1	B	283	LEU	3.3
1	B	235	VAL	3.1
1	B	279	TYR	3.1
1	C	116	SER	3.1
1	A	295	ASN	3.0
1	B	295	ASN	3.0
1	A	362	ASP	2.9
1	B	284	VAL	2.9
1	D	380	THR	2.9
1	B	285	GLY	2.8
1	C	235	VAL	2.8
1	A	233	THR	2.8
1	B	342	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	6	SER	2.7
1	A	97	SER	2.7
1	B	281	ASP	2.5
1	C	8	GLU	2.5
1	D	97	SER	2.5
1	B	85	GLY	2.5
1	C	285	GLY	2.4
1	C	362	ASP	2.4
1	B	400	TYR	2.4
1	A	232	ASP	2.4
1	B	362	ASP	2.4
1	C	341	ASP	2.4
1	A	98	THR	2.4
1	B	15	ASP	2.3
1	A	116	SER	2.3
1	A	347	THR	2.3
1	D	116	SER	2.3
1	A	234	ALA	2.3
1	B	6	SER	2.3
1	D	98	THR	2.3
1	D	233	THR	2.3
1	C	400	TYR	2.3
1	A	230	ARG	2.3
1	C	233	THR	2.3
1	B	241	ILE	2.2
1	C	100	LYS	2.2
1	C	281	ASP	2.2
1	C	220	CYS	2.2
1	C	286	THR	2.2
1	C	385	LYS	2.2
1	D	11	PHE	2.2
1	A	245	VAL	2.2
1	A	284	VAL	2.2
1	A	231	CYS	2.2
1	A	87	PHE	2.1
1	A	405	TYR	2.1
1	C	279	TYR	2.1
1	D	6	SER	2.1
1	C	241	ILE	2.1
1	B	233	THR	2.1
1	B	377	GLU	2.1
1	D	372	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	401	SER	2.1
1	A	243	PRO	2.1
1	A	115	ARG	2.0
1	A	372	GLU	2.0
1	B	286	THR	2.0
1	A	114	LYS	2.0

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](#)

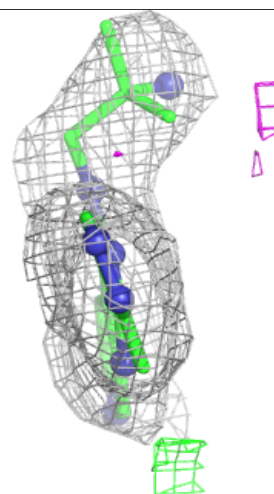
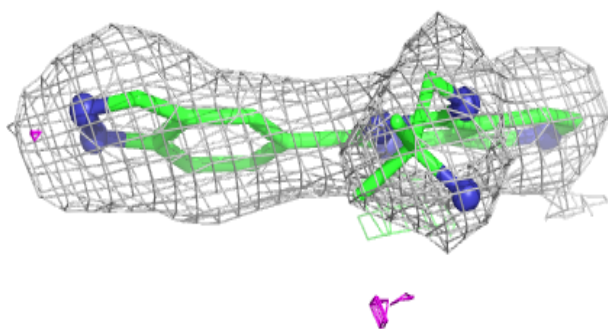
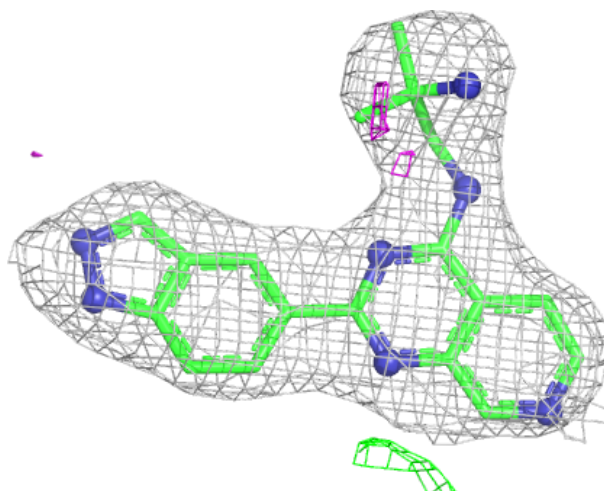
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	3J7	A	501	25/25	0.94	0.09	38,44,46,47	0
2	3J7	B	501	25/25	0.95	0.10	35,50,54,54	0
2	3J7	D	501	25/25	0.95	0.09	38,44,50,50	0
2	3J7	C	501	25/25	0.96	0.08	32,38,42,43	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.

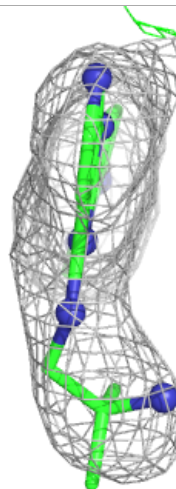
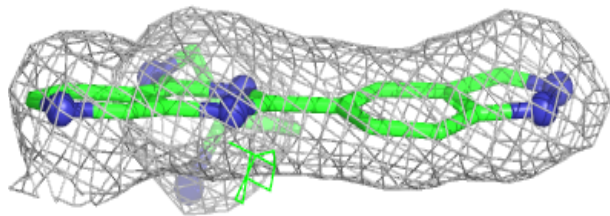
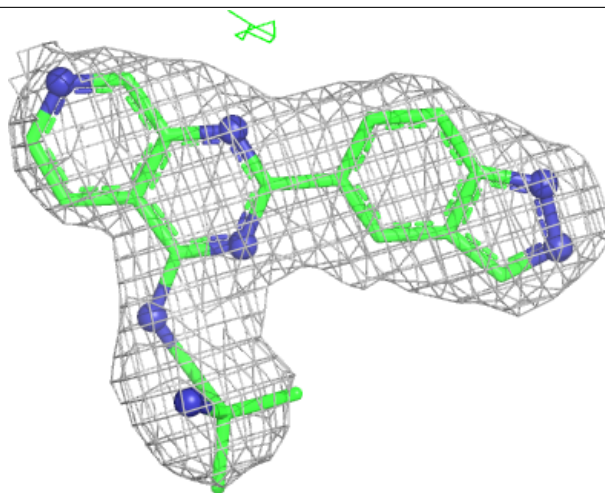
Electron density around 3J7 A 501:

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



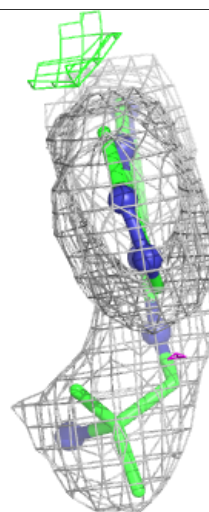
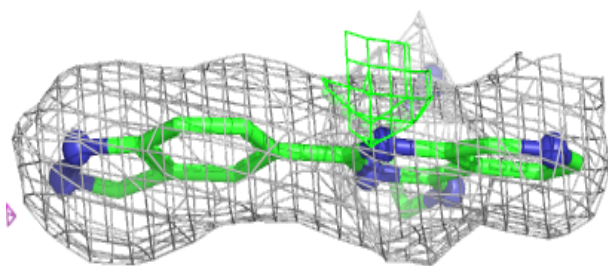
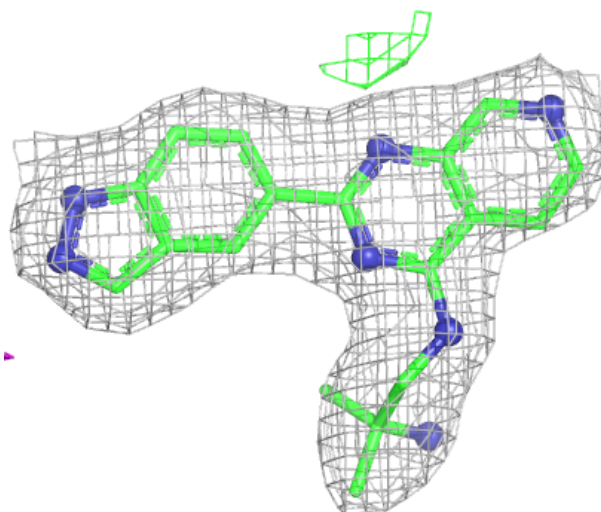
Electron density around 3J7 B 501:

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



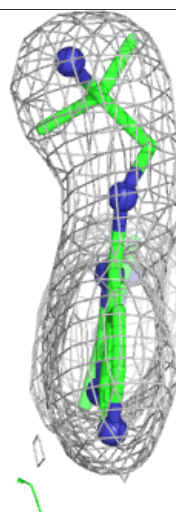
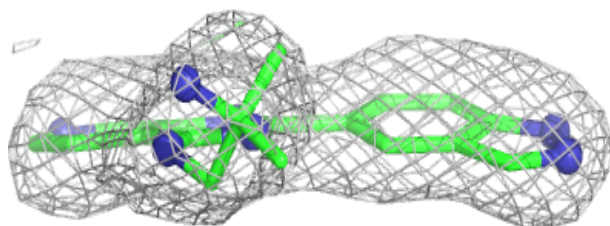
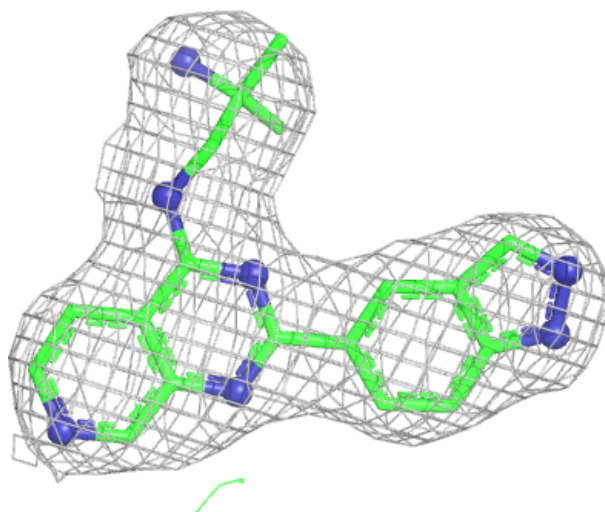
Electron density around 3J7 D 501:

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



Electron density around 3J7 C 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 ⓘ

There are no such residues in this entry.