



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:10 PM UTC

PDB ID : 8GDS / pdb_00008gds
Title : CRYSTAL STRUCTURE OF RHO-ASSOCIATED PROTEIN KINASE 2 (ROCK2) IN COMPLEX WITH 4-(4-(2-(2,3-DIHYDRO-1H-INDOL-1-YL)-2-OXOETHYL)PHENYL)-1(2H)-PHTHALAZINONE
Authors : Muckelbauer, J.K.
Deposited on : 2023-03-06
Resolution : 2.71 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

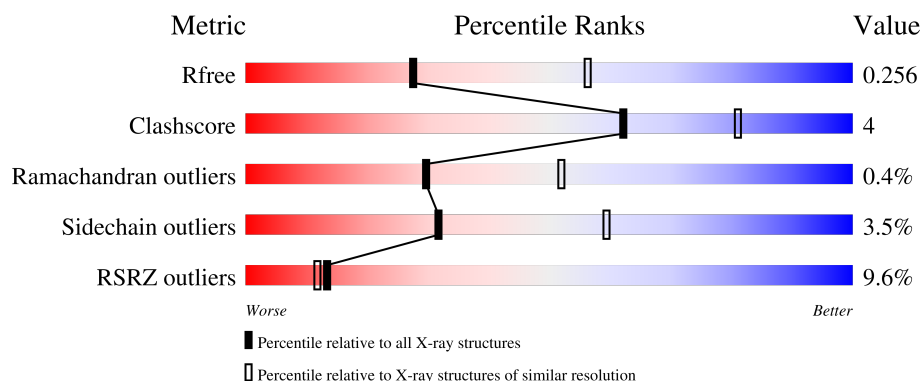
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	A	396	7% 86% 10% ..
1	B	396	11% 84% 12% ..
1	C	396	10% 83% 12% ..
1	D	396	10% 81% 14% ..

2 Entry composition [i](#)

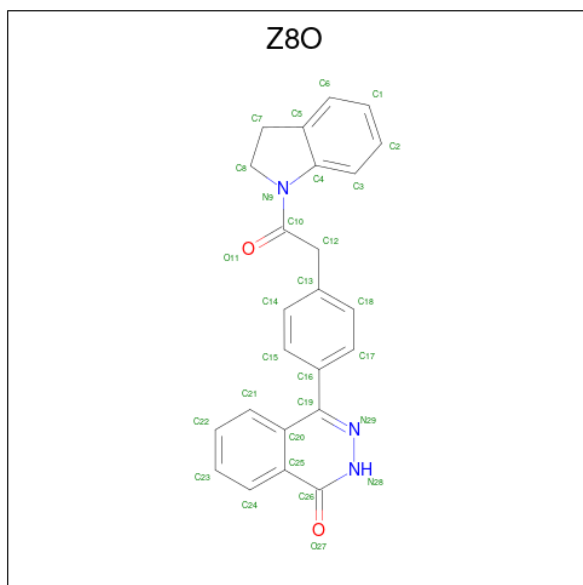
There are 4 unique types of molecules in this entry. The entry contains 12153 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	S	0	0	0
			2919	1881	477	543	18			
1	B	384	Total	C	N	O	S	0	0	0
			3004	1930	499	556	19			
1	C	385	Total	C	N	O	S	0	0	0
			3008	1938	497	554	19			
1	D	379	Total	C	N	O	S	0	0	0
			2978	1923	490	546	19			

- Molecule 2 is 4-{4-[2-(2,3-dihydro-1H-indol-1-yl)-2-oxoethyl]phenyl}phthalazin-1(2H)-one (CCD ID: Z8O) (formula: C₂₄H₁₉N₃O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			29	24	3	2		
2	B	1	Total	C	N	O	0	0
			29	24	3	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			29	24	3	2		
2	D	1	Total	C	N	O	0	0
			29	24	3	2		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

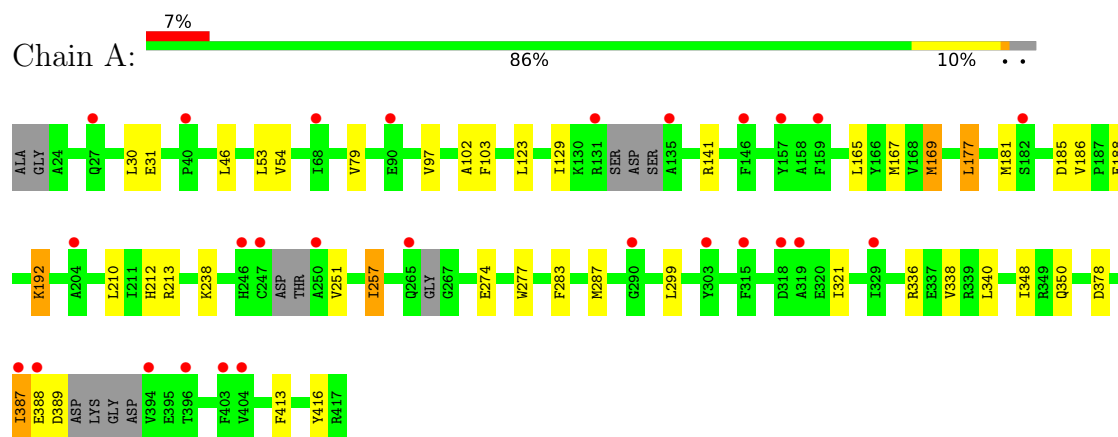
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	12	Total O 12 12	0	0
4	B	12	Total O 12 12	0	0
4	C	10	Total O 10 10	0	0
4	D	9	Total O 9 9	0	0

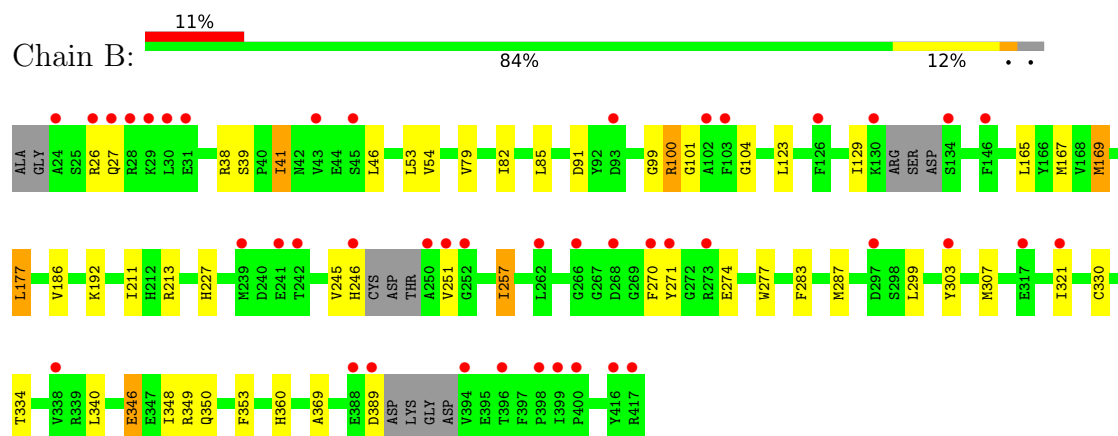
3 Residue-property plots [i](#)

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.

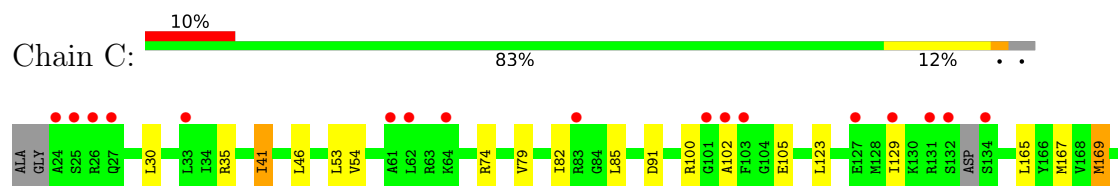
- Molecule 1: Rho-associated protein kinase 2

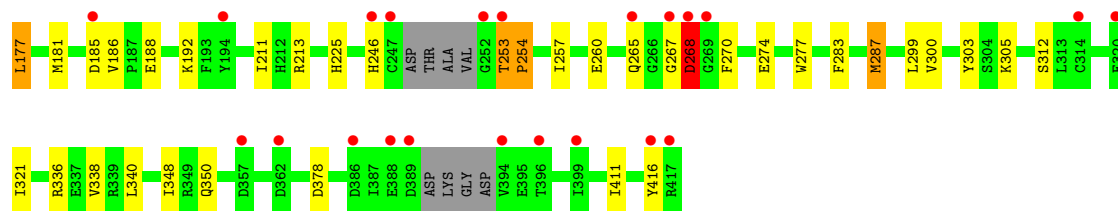


- Molecule 1: Rho-associated protein kinase 2

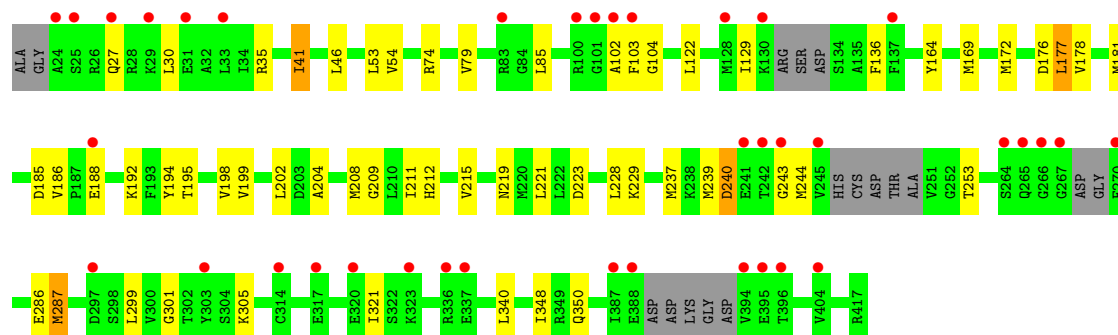
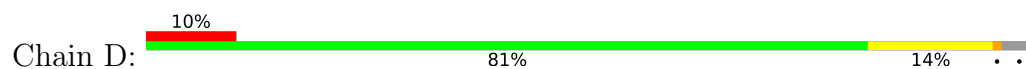


- Molecule 1: Rho-associated protein kinase 2





● Molecule 1: Rho-associated protein kinase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	143.08Å 143.33Å 134.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	98.03 – 2.71 98.03 – 2.71	Depositor EDS
% Data completeness (in resolution range)	69.1 (98.03-2.71) 69.2 (98.03-2.71)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.69Å)	Xtriage
Refinement program	BUSTER	Depositor
R, R_{free}	0.217 , 0.248 0.233 , 0.256	Depositor DCC
R_{free} test set	566 reflections (0.98%)	wwPDB-VP
Wilson B-factor (Å ²)	53.2	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 64.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.017 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12153	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 19.72% 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: Z8O, SO4

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	0.79	1/2991 (0.0%)	1.11	11/4077 (0.3%)
1	B	0.74	1/3079 (0.0%)	1.10	5/4181 (0.1%)
1	C	0.75	1/3084 (0.0%)	1.12	13/4190 (0.3%)
1	D	0.76	0/3052	1.12	11/4141 (0.3%)
All	All	0.76	3/12206 (0.0%)	1.11	40/16589 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	169	MET	SD-CE	-6.40	1.63	1.79
1	C	169	MET	SD-CE	-5.86	1.64	1.79
1	B	169	MET	SD-CE	-5.03	1.67	1.79

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	240	ASP	CA-CB-CG	8.34	120.94	112.60
1	D	223	ASP	CA-CB-CG	7.67	120.27	112.60
1	A	102	ALA	CA-C-N	7.32	130.32	120.65
1	A	102	ALA	C-N-CA	7.32	130.32	120.65
1	C	102	ALA	CA-C-N	7.10	130.02	120.65
1	C	102	ALA	C-N-CA	7.10	130.02	120.65
1	D	102	ALA	CA-C-N	6.75	129.55	120.65
1	D	102	ALA	C-N-CA	6.75	129.55	120.65
1	C	254	PRO	N-CA-C	6.49	122.09	113.40
1	B	39	SER	N-CA-C	6.14	116.66	109.60
1	C	91	ASP	CA-CB-CG	5.96	118.56	112.60
1	D	253	THR	CB-CA-C	5.94	116.62	109.85
1	D	178	VAL	CA-C-N	5.71	128.40	120.29
1	D	178	VAL	C-N-CA	5.71	128.40	120.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	38	ARG	CA-C-N	5.54	128.54	120.51
1	B	38	ARG	C-N-CA	5.54	128.54	120.51
1	D	164	TYR	N-CA-C	5.42	118.10	109.81
1	A	185	ASP	N-CA-C	-5.32	99.85	108.41
1	D	103	PHE	CA-C-N	5.31	127.78	120.72
1	D	103	PHE	C-N-CA	5.31	127.78	120.72
1	B	346	GLU	CB-CG-CD	5.30	121.62	112.60
1	C	253	THR	CB-CA-C	5.26	117.94	109.41
1	D	185	ASP	N-CA-C	-5.26	99.94	108.41
1	A	103	PHE	CA-C-N	5.21	127.66	120.72
1	A	103	PHE	C-N-CA	5.21	127.66	120.72
1	C	338	VAL	N-CA-CB	-5.21	105.39	112.16
1	C	185	ASP	N-CA-C	-5.19	100.05	108.41
1	A	378	ASP	CA-CB-CG	5.11	117.71	112.60
1	C	336	ARG	CA-C-N	5.11	127.12	120.28
1	C	336	ARG	C-N-CA	5.11	127.12	120.28
1	A	338	VAL	N-CA-CB	-5.10	105.50	112.28
1	A	336	ARG	CA-C-N	5.07	127.08	120.28
1	A	336	ARG	C-N-CA	5.07	127.08	120.28
1	B	91	ASP	CA-CB-CG	5.05	117.65	112.60
1	C	268	ASP	CA-CB-CG	5.04	117.64	112.60
1	A	192	LYS	CA-C-N	5.04	127.48	120.63
1	A	192	LYS	C-N-CA	5.04	127.48	120.63
1	C	378	ASP	CA-CB-CG	5.03	117.63	112.60
1	C	267	GLY	CA-C-N	5.00	131.10	121.54
1	C	267	GLY	C-N-CA	5.00	131.10	121.54

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	2919	0	2668	19	0
1	B	3004	0	2801	30	0
1	C	3008	0	2812	29	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2978	0	2808	33	0
2	A	29	0	0	1	0
2	B	29	0	0	0	0
2	C	29	0	0	0	0
2	D	29	0	0	1	0
3	A	25	0	0	0	0
3	B	15	0	0	1	0
3	C	30	0	0	1	0
3	D	15	0	0	0	0
4	A	12	0	0	0	0
4	B	12	0	0	0	0
4	C	10	0	0	0	0
4	D	9	0	0	0	0
All	All	12153	0	11089	95	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 4.

All (95) 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:35:ARG:NH1	1:D:35:ARG:HH12	1.59	1.01
1:C:35:ARG:HH12	1:D:35:ARG:NH1	1.63	0.95
1:A:251:VAL:HG13	1:A:257:ILE:HD13	1.53	0.88
1:C:35:ARG:HH12	1:D:35:ARG:HH12	0.81	0.75
1:A:167:MET:HB3	1:A:169:MET:HE2	1.69	0.75
1:B:167:MET:HB3	1:B:169:MET:HE2	1.69	0.74
1:C:167:MET:HB3	1:C:169:MET:HE2	1.70	0.73
1:B:330:CYS:O	1:B:334:THR:HG23	1.88	0.72
1:A:53:LEU:HD13	1:B:53:LEU:HD13	1.74	0.70
1:B:360:HIS:ND1	3:B:502:SO4:O3	2.27	0.68
1:C:411:ILE:O	1:D:74:ARG:NH2	2.28	0.67
1:D:212:HIS:HE1	1:D:219:ASN:HD22	1.46	0.63
1:C:53:LEU:HD13	1:D:53:LEU:HD13	1.80	0.62
1:C:246:HIS:ND1	1:C:270:PHE:HE1	1.98	0.61
1:B:246:HIS:HD1	1:B:270:PHE:HE1	1.49	0.61
1:B:246:HIS:ND1	1:B:270:PHE:HE1	1.99	0.59
1:C:186:VAL:HG21	1:C:287:MET:HE2	1.83	0.59
1:B:251:VAL:HG13	1:B:257:ILE:HD13	1.84	0.59
1:C:254:PRO:HB3	1:C:303:TYR:HE1	1.69	0.57
1:A:46:LEU:HB3	1:B:46:LEU:HB3	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:VAL:HG21	1:A:79:VAL:HG21	1.86	0.57
1:C:123:LEU:HB2	1:C:165:LEU:HB2	1.87	0.56
1:C:254:PRO:HA	1:C:257:ILE:HD12	1.87	0.56
1:D:195:THR:O	1:D:199:VAL:HG23	2.04	0.56
1:D:54:VAL:HG21	1:D:79:VAL:HG21	1.88	0.56
1:C:246:HIS:ND1	1:C:270:PHE:CE1	2.73	0.55
1:C:54:VAL:HG21	1:C:79:VAL:HG21	1.88	0.54
1:D:172:MET:HE1	1:D:229:LYS:HD2	1.89	0.54
1:B:123:LEU:HB2	1:B:165:LEU:HB2	1.91	0.53
1:B:100:ARG:HH22	1:B:389:ASP:HA	1.74	0.53
1:A:212:HIS:O	1:A:213:ARG:HB2	2.09	0.52
1:B:54:VAL:HG21	1:B:79:VAL:HG21	1.90	0.52
1:A:188:GLU:O	1:A:192:LYS:HB2	2.10	0.52
1:A:123:LEU:HB2	1:A:165:LEU:HB2	1.91	0.52
1:D:177:LEU:HD23	1:D:287:MET:HE1	1.91	0.51
1:B:346:GLU:H	1:B:346:GLU:CD	2.19	0.50
1:D:104:GLY:HA3	1:D:122:LEU:O	2.12	0.50
1:C:416:TYR:CZ	1:D:27:GLN:HG3	2.48	0.49
1:A:30:LEU:HD13	1:B:85:LEU:HB2	1.94	0.49
1:B:245:VAL:HG12	1:B:246:HIS:N	2.28	0.49
1:B:211:ILE:HG22	1:B:213:ARG:HG3	1.93	0.48
1:A:169:MET:HE3	2:A:501:Z8O:C12	2.43	0.48
1:C:30:LEU:HD13	1:D:85:LEU:HB2	1.94	0.48
1:D:176:ASP:HB3	1:D:221:LEU:HD23	1.95	0.48
1:A:274:GLU:HA	1:A:277:TRP:HD1	1.78	0.48
1:B:192:LYS:HD3	1:B:353:PHE:O	2.14	0.48
1:D:301:GLY:O	1:D:305:LYS:HG3	2.14	0.48
1:A:30:LEU:HD11	1:B:82:ILE:HG23	1.95	0.47
1:C:46:LEU:HB3	1:D:46:LEU:HB3	1.96	0.47
1:C:85:LEU:HB2	1:D:30:LEU:HD13	1.96	0.47
1:C:274:GLU:HA	1:C:277:TRP:HD1	1.77	0.47
1:D:172:MET:HE2	1:D:229:LYS:HB2	1.95	0.47
1:D:212:HIS:CE1	1:D:219:ASN:HD22	2.30	0.47
1:D:188:GLU:O	1:D:192:LYS:HB2	2.14	0.47
1:B:346:GLU:HG3	1:B:349:ARG:NH2	2.30	0.47
1:C:188:GLU:O	1:C:192:LYS:HB2	2.15	0.47
1:B:340:LEU:HG	1:B:348:ILE:HG12	1.97	0.47
1:A:141:ARG:NH1	1:A:413:PHE:CE1	2.83	0.47
1:B:274:GLU:HA	1:B:277:TRP:HD1	1.79	0.47
1:B:303:TYR:O	1:B:307:MET:HG2	2.15	0.47
1:D:172:MET:CE	1:D:229:LYS:HB2	2.44	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ARG:HD2	1:B:271:TYR:HE2	1.80	0.47
1:C:100:ARG:HG3	1:C:105:GLU:HB3	1.97	0.47
1:A:416:TYR:CZ	1:B:27:GLN:HG3	2.50	0.46
1:B:99:GLY:O	1:B:100:ARG:HB2	2.15	0.46
1:C:211:ILE:HG22	1:C:213:ARG:HG3	1.95	0.46
1:D:204:ALA:O	1:D:208:MET:HG3	2.16	0.46
1:C:74:ARG:HD3	1:D:136:PHE:HB2	1.97	0.45
1:D:340:LEU:HG	1:D:348:ILE:HG12	1.98	0.45
1:C:340:LEU:HG	1:C:348:ILE:HG12	1.98	0.45
1:A:97:VAL:CG1	1:A:387:ILE:HG12	2.46	0.45
1:C:41:ILE:HG13	1:C:41:ILE:O	2.17	0.45
1:D:209:GLY:HA2	1:D:239:MET:HE2	2.00	0.44
1:D:169:MET:HE2	2:D:501:Z8O:C14	2.48	0.44
1:C:177:LEU:HD22	1:C:283:PHE:CZ	2.53	0.43
1:B:186:VAL:HG21	1:B:287:MET:HE2	2.01	0.43
1:B:246:HIS:ND1	1:B:270:PHE:CE1	2.80	0.43
1:B:41:ILE:HG13	1:B:41:ILE:O	2.19	0.43
1:A:186:VAL:HG21	1:A:287:MET:HE2	2.00	0.43
1:D:186:VAL:HG21	1:D:287:MET:HE2	2.01	0.43
1:D:194:TYR:O	1:D:198:VAL:HG23	2.19	0.42
1:C:82:ILE:HG23	1:D:30:LEU:HD11	2.02	0.42
1:D:211:ILE:HD12	1:D:239:MET:HG2	2.00	0.42
1:C:253:THR:HA	1:C:254:PRO:HD3	1.86	0.42
1:D:239:MET:HB3	1:D:243:GLY:HA2	2.02	0.42
1:B:245:VAL:CG1	1:B:246:HIS:N	2.83	0.42
1:C:225:HIS:NE2	3:C:504:SO4:O3	2.35	0.42
1:A:210:LEU:HD23	1:A:238:LYS:HA	2.00	0.42
1:D:41:ILE:HG13	1:D:41:ILE:O	2.21	0.41
1:A:340:LEU:HG	1:A:348:ILE:HG12	2.02	0.41
1:C:305:LYS:O	1:C:312:SER:OG	2.34	0.41
1:A:177:LEU:HD22	1:A:283:PHE:CZ	2.57	0.41
1:B:177:LEU:HD22	1:B:283:PHE:CZ	2.56	0.40
1:B:227:HIS:CD2	1:B:369:ALA:HB2	2.56	0.40
1:D:202:LEU:HD21	1:D:215:VAL:HG21	2.02	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	374/396 (94%)	365 (98%)	8 (2%)	1 (0%)	36	59
1	B	376/396 (95%)	362 (96%)	11 (3%)	3 (1%)	16	35
1	C	377/396 (95%)	366 (97%)	9 (2%)	2 (0%)	24	46
1	D	369/396 (93%)	358 (97%)	11 (3%)	0	100	100
All	All	1496/1584 (94%)	1451 (97%)	39 (3%)	6 (0%)	30	52

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	100	ARG
1	B	104	GLY
1	C	268	ASP
1	A	388	GLU
1	C	265	GLN
1	B	101	GLY

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	290/346 (84%)	280 (97%)	10 (3%)	32	60
1	B	305/346 (88%)	297 (97%)	8 (3%)	40	69
1	C	307/346 (89%)	296 (96%)	11 (4%)	31	58
1	D	306/346 (88%)	293 (96%)	13 (4%)	26	53

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1208/1384 (87%)	1166 (96%)	42 (4%)	32 59

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	GLU
1	A	129	ILE
1	A	177	LEU
1	A	181	MET
1	A	257	ILE
1	A	299	LEU
1	A	321	ILE
1	A	350	GLN
1	A	387	ILE
1	A	389	ASP
1	B	26	ARG
1	B	41	ILE
1	B	129	ILE
1	B	177	LEU
1	B	257	ILE
1	B	299	LEU
1	B	321	ILE
1	B	350	GLN
1	C	41	ILE
1	C	129	ILE
1	C	177	LEU
1	C	181	MET
1	C	260	GLU
1	C	268	ASP
1	C	287	MET
1	C	299	LEU
1	C	300	VAL
1	C	321	ILE
1	C	350	GLN
1	D	41	ILE
1	D	129	ILE
1	D	177	LEU
1	D	181	MET
1	D	228	LEU
1	D	237	MET
1	D	240	ASP
1	D	244	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	286	GLU
1	D	287	MET
1	D	299	LEU
1	D	321	ILE
1	D	350	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	GLN
1	B	148	ASN
1	B	406	ASN
1	C	148	ASN
1	C	309	HIS
1	D	148	ASN
1	D	212	HIS

5.3.3 RNA [i](#)

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](#)

21 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
3	SO4	C	502	-	4,4,4	0.30	0	6,6,6	0.19	0
3	SO4	A	505	-	4,4,4	0.35	0	6,6,6	0.29	0
3	SO4	C	507	-	4,4,4	0.33	0	6,6,6	0.18	0
3	SO4	C	503	-	4,4,4	0.36	0	6,6,6	0.45	0
3	SO4	D	504	-	4,4,4	0.32	0	6,6,6	0.12	0
3	SO4	B	504	-	4,4,4	0.28	0	6,6,6	0.19	0
3	SO4	A	504	-	4,4,4	0.26	0	6,6,6	0.23	0
3	SO4	C	505	-	4,4,4	0.30	0	6,6,6	0.20	0
3	SO4	D	502	-	4,4,4	0.26	0	6,6,6	0.27	0
3	SO4	A	502	-	4,4,4	0.28	0	6,6,6	0.14	0
2	Z8O	C	501	-	33,33,33	0.32	0	45,47,47	0.62	0
3	SO4	D	503	-	4,4,4	0.33	0	6,6,6	0.40	0
2	Z8O	D	501	-	33,33,33	0.32	0	45,47,47	0.66	0
3	SO4	A	503	-	4,4,4	0.23	0	6,6,6	0.39	0
3	SO4	B	503	-	4,4,4	0.28	0	6,6,6	0.29	0
3	SO4	B	502	-	4,4,4	0.69	0	6,6,6	0.19	0
3	SO4	C	504	-	4,4,4	0.25	0	6,6,6	0.18	0
3	SO4	A	506	-	4,4,4	0.18	0	6,6,6	0.17	0
3	SO4	C	506	-	4,4,4	0.28	0	6,6,6	0.12	0
2	Z8O	B	501	-	33,33,33	0.27	0	45,47,47	0.60	0
2	Z8O	A	501	-	33,33,33	0.29	0	45,47,47	0.53	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	Z8O	D	501	-	-	4/12/21/21	0/5/5/5
2	Z8O	B	501	-	-	0/12/21/21	0/5/5/5
2	Z8O	C	501	-	-	0/12/21/21	0/5/5/5
2	Z8O	A	501	-	-	3/12/21/21	0/5/5/5

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	Z8O	C12-C10-N9-C8

Continued on next page...

Continued from previous page...

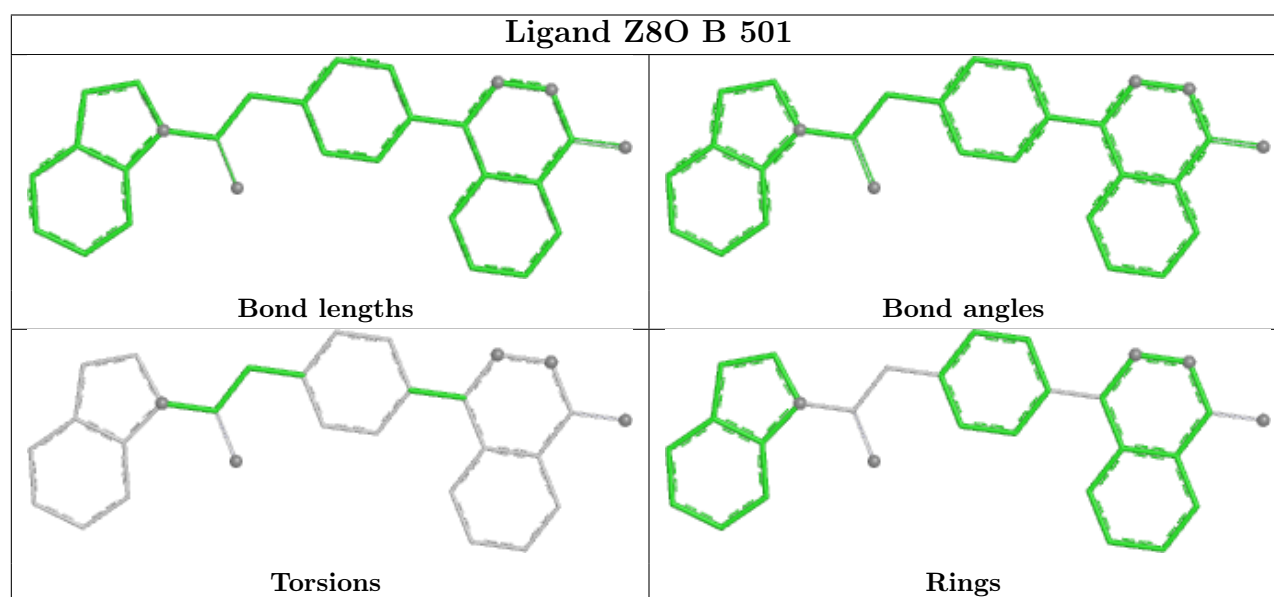
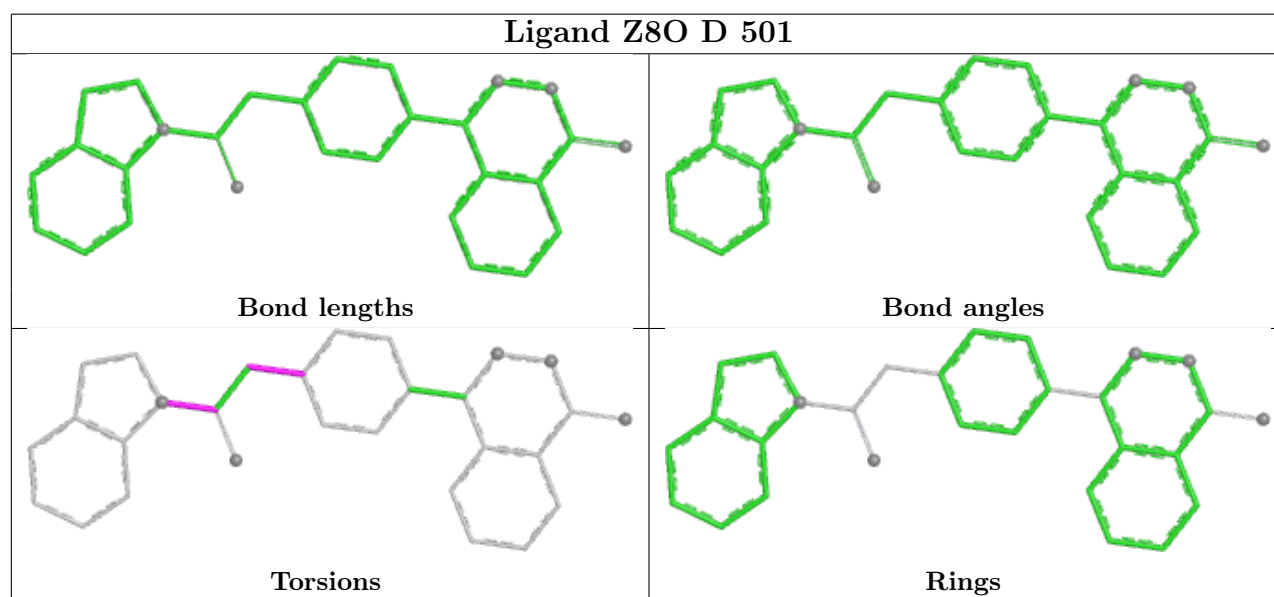
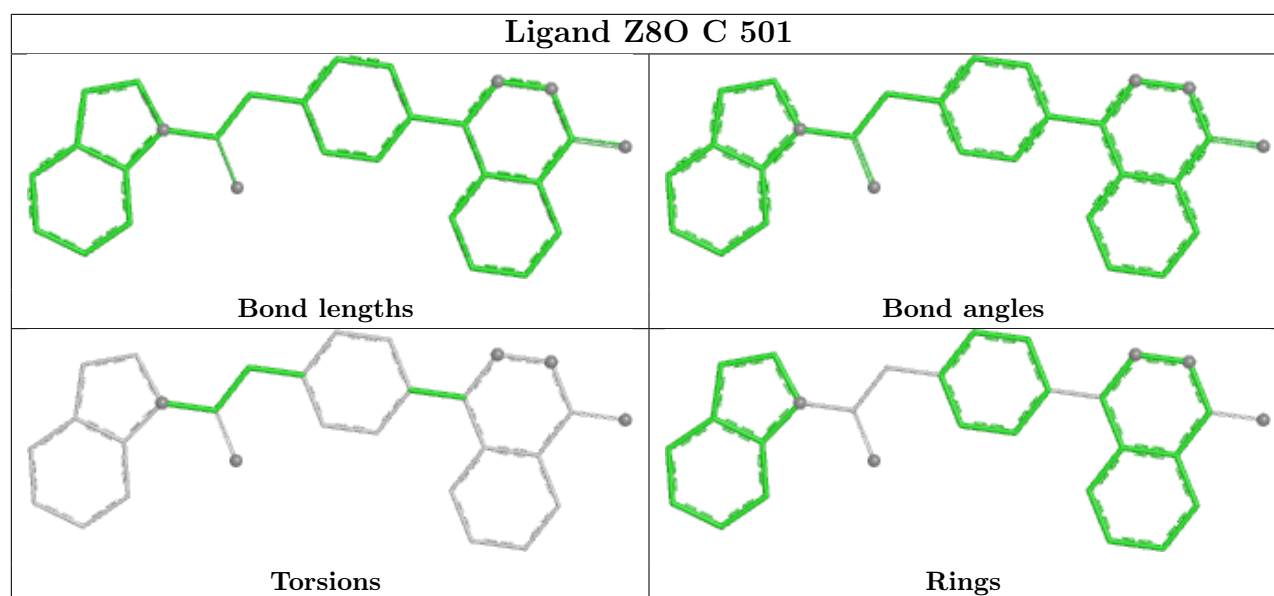
Mol	Chain	Res	Type	Atoms
2	D	501	Z8O	C12-C10-N9-C8
2	A	501	Z8O	O11-C10-N9-C8
2	D	501	Z8O	O11-C10-N9-C8
2	D	501	Z8O	C10-C12-C13-C14
2	D	501	Z8O	C10-C12-C13-C18
2	A	501	Z8O	O11-C10-N9-C4

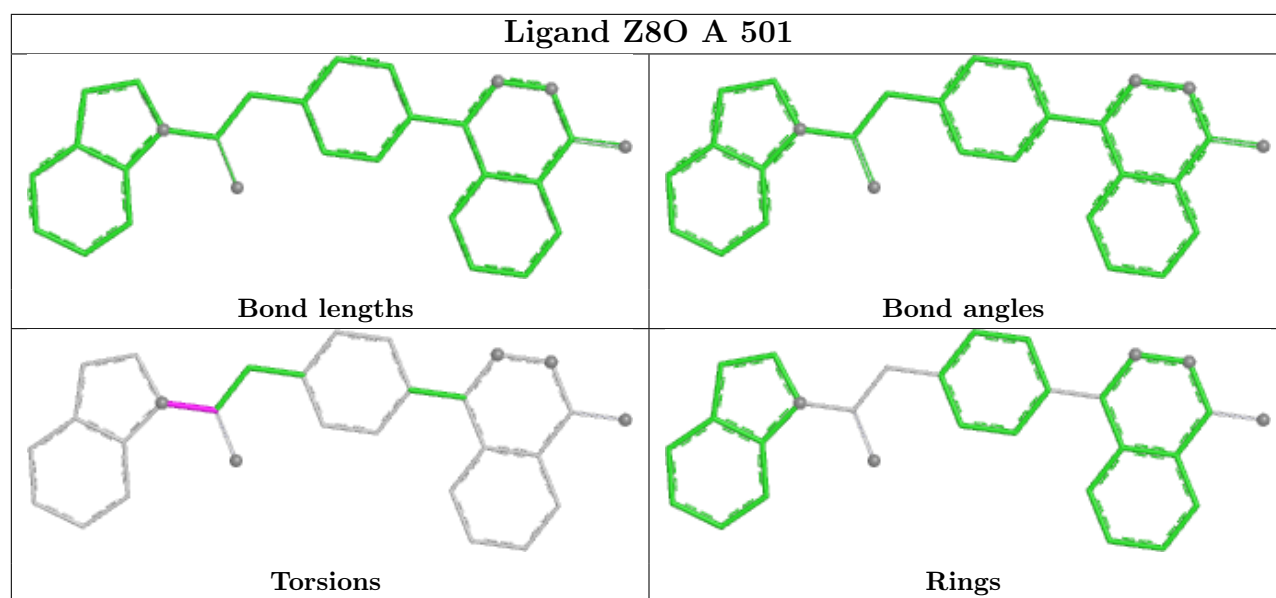
There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	501	Z8O	1	0
3	B	502	SO4	1	0
3	C	504	SO4	1	0
2	A	501	Z8O	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.





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	384/396 (96%)	0.73	27 (7%) 22 20	29, 46, 70, 83	0
1	B	384/396 (96%)	0.90	43 (11%) 10 9	27, 51, 79, 95	0
1	C	385/396 (97%)	0.82	39 (10%) 12 11	32, 52, 77, 89	0
1	D	379/396 (95%)	0.88	38 (10%) 12 11	35, 55, 80, 88	0
All	All	1532/1584 (96%)	0.83	147 (9%) 13 12	27, 51, 77, 95	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	250	ALA	6.9
1	C	132	SER	6.5
1	B	389	ASP	6.3
1	C	247	CYS	5.9
1	B	266	GLY	5.1
1	C	394	VAL	5.1
1	A	247	CYS	5.0
1	C	389	ASP	4.8
1	D	270	PHE	4.3
1	D	265	GLN	4.2
1	D	267	GLY	4.0
1	C	24	ALA	3.9
1	B	130	LYS	3.9
1	D	241	GLU	3.8
1	B	251	VAL	3.8
1	D	24	ALA	3.8
1	B	394	VAL	3.8
1	D	245	VAL	3.7
1	C	103	PHE	3.7
1	A	27	GLN	3.7
1	C	268	ASP	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	297	ASP	3.6
1	D	103	PHE	3.6
1	C	417	ARG	3.6
1	D	101	GLY	3.6
1	D	396	THR	3.5
1	B	146	PHE	3.5
1	A	396	THR	3.5
1	D	31	GLU	3.5
1	D	264	SER	3.4
1	D	387	ILE	3.4
1	A	388	GLU	3.4
1	D	102	ALA	3.4
1	A	394	VAL	3.4
1	B	396	THR	3.4
1	B	273	ARG	3.4
1	B	29	LYS	3.3
1	D	266	GLY	3.3
1	D	395	GLU	3.2
1	A	387	ILE	3.2
1	D	128	MET	3.2
1	C	396	THR	3.2
1	B	388	GLU	3.2
1	D	314	CYS	3.1
1	A	250	ALA	3.1
1	B	268	ASP	3.1
1	D	130	LYS	3.0
1	B	134	SER	3.0
1	C	33	LEU	3.0
1	D	394	VAL	3.0
1	A	318	ASP	3.0
1	C	265	GLN	2.9
1	B	400	PRO	2.8
1	A	131	ARG	2.8
1	B	27	GLN	2.8
1	D	303	TYR	2.8
1	D	388	GLU	2.8
1	C	102	ALA	2.8
1	A	246	HIS	2.8
1	C	320	GLU	2.7
1	C	267	GLY	2.7
1	B	242	THR	2.7
1	C	386	ASP	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	303	TYR	2.7
1	C	64	LYS	2.7
1	C	246	HIS	2.7
1	B	241	GLU	2.7
1	C	25	SER	2.7
1	C	185	ASP	2.7
1	C	194	TYR	2.6
1	D	100	ARG	2.6
1	C	253	THR	2.6
1	C	131	ARG	2.6
1	C	129	ILE	2.6
1	B	398	PRO	2.6
1	B	30	LEU	2.5
1	B	31	GLU	2.5
1	B	270	PHE	2.5
1	B	102	ALA	2.5
1	A	135	ALA	2.5
1	C	83	ARG	2.5
1	D	83	ARG	2.5
1	B	271	TYR	2.5
1	A	182	SER	2.4
1	C	314	CYS	2.4
1	C	362	ASP	2.4
1	D	317	GLU	2.4
1	B	24	ALA	2.4
1	C	61	ALA	2.4
1	B	317	GLU	2.4
1	B	239	MET	2.4
1	B	252	GLY	2.4
1	A	403	PHE	2.4
1	A	90	GLU	2.4
1	C	416	TYR	2.3
1	C	357	ASP	2.3
1	B	321	ILE	2.3
1	D	25	SER	2.3
1	D	137	PHE	2.3
1	A	319	ALA	2.3
1	C	134	SER	2.3
1	D	27	GLN	2.3
1	A	315	PHE	2.3
1	B	246	HIS	2.2
1	C	26	ARG	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	159	PHE	2.2
1	A	68	ILE	2.2
1	B	399	ILE	2.2
1	C	399	ILE	2.2
1	A	40	PRO	2.2
1	C	269	GLY	2.2
1	A	146	PHE	2.2
1	A	157	TYR	2.2
1	B	28	ARG	2.1
1	D	29	LYS	2.1
1	A	290	GLY	2.1
1	C	252	GLY	2.1
1	A	329	ILE	2.1
1	B	297	ASP	2.1
1	A	204	ALA	2.1
1	C	27	GLN	2.1
1	A	303	TYR	2.1
1	C	101	GLY	2.1
1	A	404	VAL	2.1
1	B	45	SER	2.1
1	B	126	PHE	2.1
1	D	188	GLU	2.1
1	D	320	GLU	2.1
1	A	265	GLN	2.1
1	B	43	VAL	2.1
1	B	338	VAL	2.1
1	B	103	PHE	2.1
1	C	127	GLU	2.1
1	C	388	GLU	2.1
1	B	262	LEU	2.1
1	B	416	TYR	2.1
1	B	93	ASP	2.0
1	D	337	GLU	2.0
1	D	323	LYS	2.0
1	D	242	THR	2.0
1	C	62	LEU	2.0
1	D	404	VAL	2.0
1	B	26	ARG	2.0
1	D	336	ARG	2.0
1	D	33	LEU	2.0
1	D	243	GLY	2.0
1	B	417	ARG	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](#)

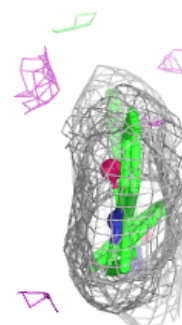
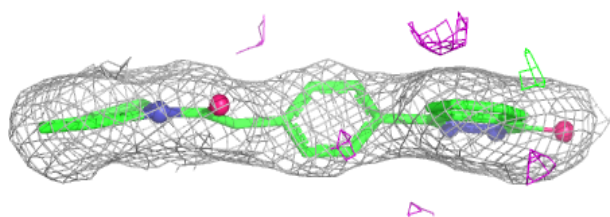
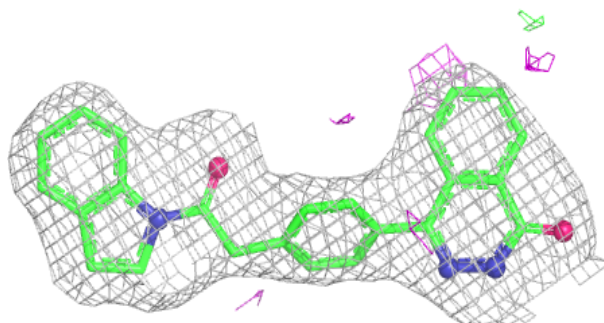
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	SO4	A	505	5/5	0.56	0.14	106,107,107,107	0
3	SO4	C	505	5/5	0.57	0.15	103,103,103,103	0
3	SO4	C	502	5/5	0.70	0.12	125,125,125,125	0
3	SO4	C	506	5/5	0.72	0.14	150,150,151,151	0
3	SO4	A	502	5/5	0.73	0.13	123,123,123,123	0
3	SO4	D	504	5/5	0.81	0.12	106,106,106,106	0
3	SO4	B	504	5/5	0.82	0.16	97,97,97,97	0
3	SO4	C	507	5/5	0.83	0.12	97,97,97,97	0
3	SO4	A	506	5/5	0.85	0.12	107,107,107,107	0
3	SO4	C	503	5/5	0.89	0.17	81,81,81,81	0
3	SO4	D	503	5/5	0.91	0.12	65,65,66,66	0
3	SO4	D	502	5/5	0.92	0.11	90,91,91,91	0
3	SO4	B	502	5/5	0.93	0.19	28,37,46,58	0
3	SO4	A	503	5/5	0.93	0.12	70,70,70,71	0
3	SO4	C	504	5/5	0.93	0.09	79,80,80,80	0
2	Z8O	A	501	29/29	0.94	0.11	36,39,42,42	0
3	SO4	B	503	5/5	0.94	0.08	66,66,66,66	0
2	Z8O	C	501	29/29	0.94	0.10	33,35,36,37	0
2	Z8O	B	501	29/29	0.95	0.10	32,33,34,35	0
3	SO4	A	504	5/5	0.95	0.08	60,60,60,60	0
2	Z8O	D	501	29/29	0.96	0.08	29,36,41,42	0

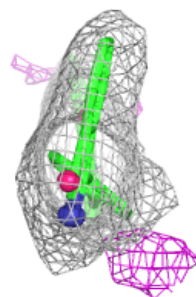
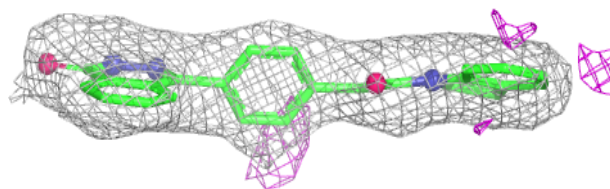
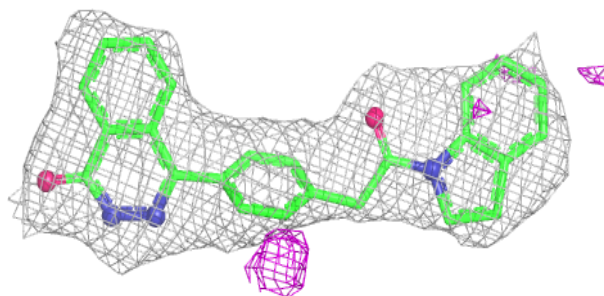
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Z8O 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)

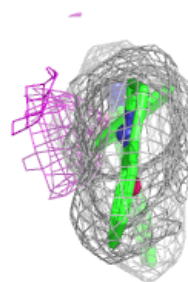
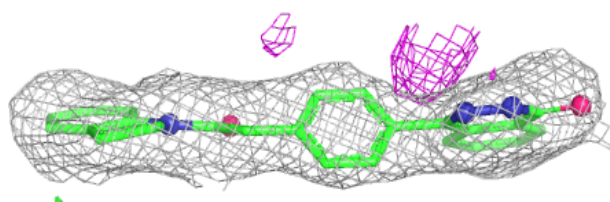
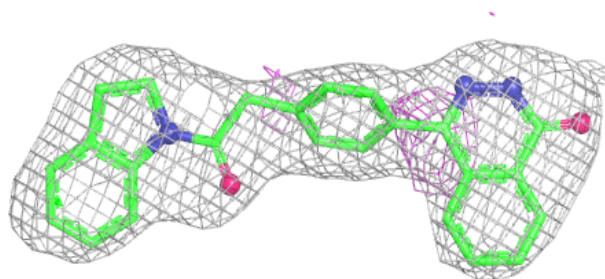
**Electron density around Z8O C 501:**

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

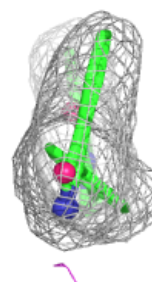
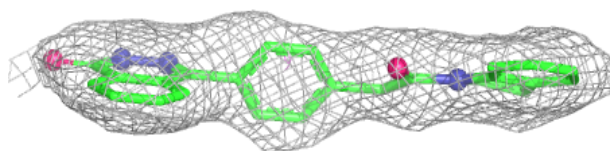
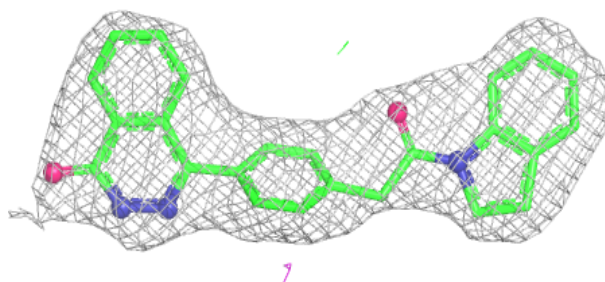


Electron density around Z8O B 501:

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

**Electron density around Z8O 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.