



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2022 – 06:22 PM JST

PDB ID : 7FHS
Title : Crystal structure of DYRK1A in complex with RD0392
Authors : Kikuchi, M.; Sumida, T.; Hosoya, T.; Kii, I.; Umehara, T.
Deposited on : 2021-07-30
Resolution : 2.42 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 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 : 2.27
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) : 2.27

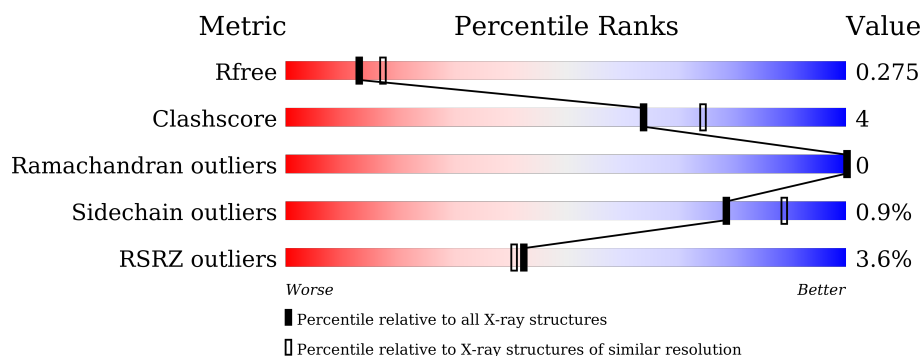
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.42 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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (2.44-2.40)

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	361	<div> <div>2%</div> <div>84%</div> <div>11%</div> <div>5%</div> </div>
1	B	361	<div> <div>3%</div> <div>86%</div> <div>9%</div> <div>5%</div> </div>
1	C	361	<div> <div>2%</div> <div>84%</div> <div>10%</div> <div>6%</div> </div>
1	D	361	<div> <div>6%</div> <div>79%</div> <div>15%</div> <div>5%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11546 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.

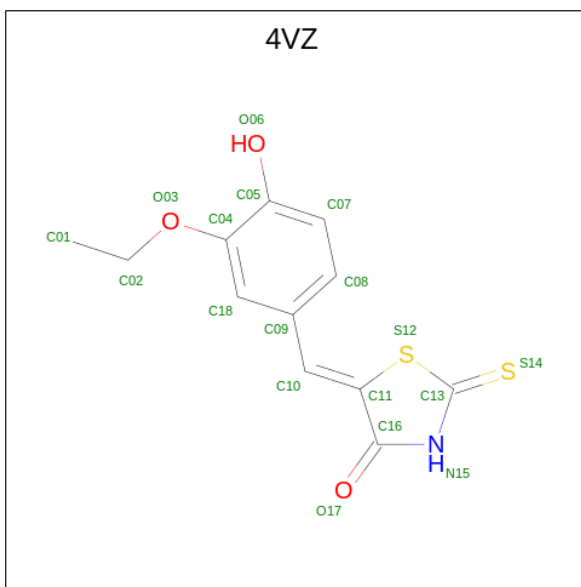
- Molecule 1 is a protein called Dual specificity tyrosine-phosphorylation-regulated kinase 1A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	343	Total	C	N	O	P	S	0	2	0
			2816	1813	481	504	1	17			
1	B	342	Total	C	N	O	P	S	0	0	0
			2800	1803	479	500	1	17			
1	C	341	Total	C	N	O	P	S	0	0	0
			2781	1792	474	497	1	17			
1	D	342	Total	C	N	O	P	S	0	0	0
			2795	1798	478	501	1	17			

There are 8 discrepancies between the modelled and reference sequences:

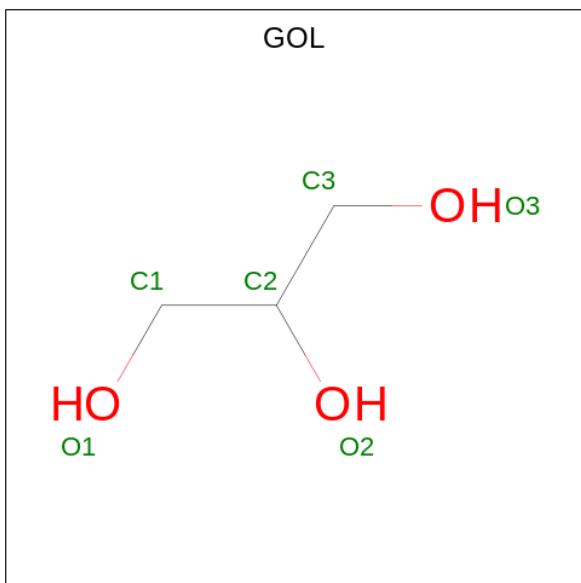
Chain	Residue	Modelled	Actual	Comment	Reference
A	125	GLY	-	expression tag	UNP Q13627
A	126	SER	-	expression tag	UNP Q13627
B	125	GLY	-	expression tag	UNP Q13627
B	126	SER	-	expression tag	UNP Q13627
C	125	GLY	-	expression tag	UNP Q13627
C	126	SER	-	expression tag	UNP Q13627
D	125	GLY	-	expression tag	UNP Q13627
D	126	SER	-	expression tag	UNP Q13627

- Molecule 2 is (5 {Z})-5-[(3-ethoxy-4-oxidanyl-phenyl)methylidene]-2-sulfanylidene-1,3-thiazolidin-4-one (three-letter code: 4VZ) (formula: C₁₂H₁₁NO₃S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			18	12	1	3	2		
2	B	1	Total	C	N	O	S	0	0
			18	12	1	3	2		
2	C	1	Total	C	N	O	S	0	0
			18	12	1	3	2		
2	D	1	Total	C	N	O	S	0	0
			18	12	1	3	2		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

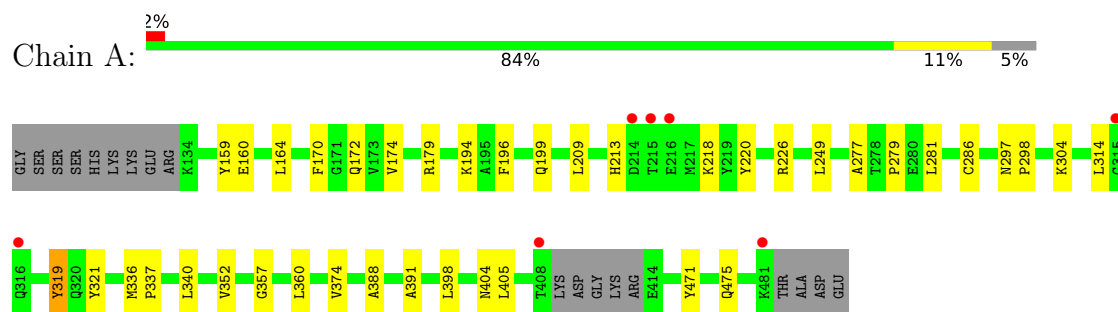
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	97	Total	O	0	0
			97	97		
4	B	52	Total	O	0	0
			52	52		
4	C	60	Total	O	0	0
			60	60		
4	D	43	Total	O	0	0
			43	43		

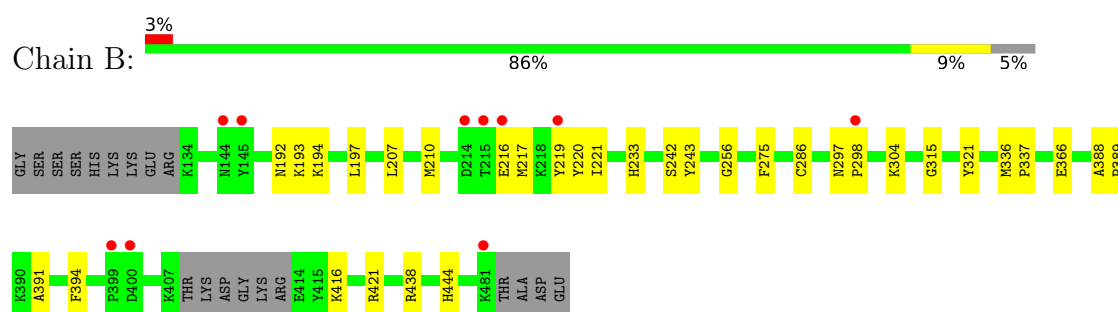
3 Residue-property plots [i](#)

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.

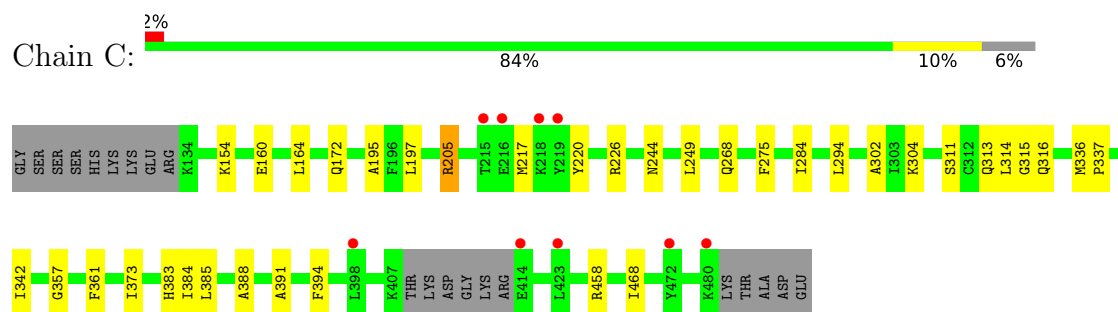
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



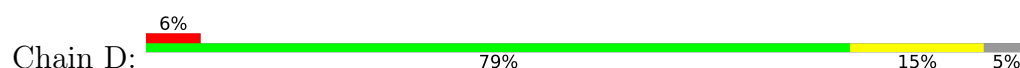
- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A

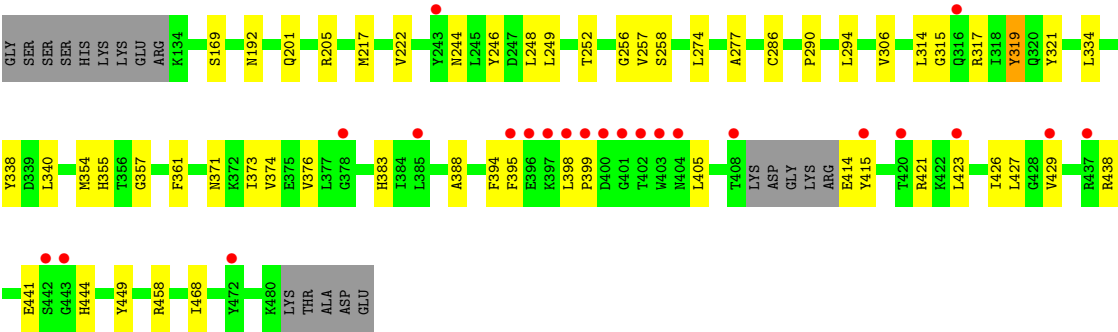


- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A



- Molecule 1: Dual specificity tyrosine-phosphorylation-regulated kinase 1A





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	87.63Å 88.18Å 228.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.00 – 2.42 48.12 – 2.42	Depositor EDS
% Data completeness (in resolution range)	99.3 (45.00-2.42) 99.3 (48.12-2.42)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.232 , 0.275 0.232 , 0.275	Depositor DCC
R_{free} test set	3319 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.453	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11546	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 2.64% 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: GOL, 4VZ, PTR

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	0.24	0/2864	0.51	0/3861
1	B	0.24	0/2848	0.50	0/3838
1	C	0.24	0/2829	0.50	0/3815
1	D	0.24	0/2843	0.51	0/3833
All	All	0.24	0/11384	0.50	0/15347

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2816	0	2812	23	0
1	B	2800	0	2804	25	0
1	C	2781	0	2776	22	0
1	D	2795	0	2789	37	0
2	A	18	0	0	0	0
2	B	18	0	0	0	0
2	C	18	0	0	0	0
2	D	18	0	0	0	0
3	A	18	0	24	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	6	0	8	1	0
3	D	6	0	8	0	0
4	A	97	0	0	0	0
4	B	52	0	0	0	0
4	C	60	0	0	0	0
4	D	43	0	0	0	0
All	All	11546	0	11221	94	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 (94) 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:D:201:GLN:HB3	1:D:205:ARG:HH12	1.53	0.73
1:A:314:LEU:O	1:B:315:GLY:HA2	1.95	0.67
1:B:197:LEU:HD23	1:D:319:TYR:HD1	1.62	0.63
1:B:220:TYR:O	1:B:304:LYS:HA	1.98	0.63
1:A:164:LEU:HD11	1:A:172:GLN:HB3	1.80	0.63
1:C:314:LEU:O	1:D:315:GLY:HA2	2.00	0.61
1:C:315:GLY:HA2	1:D:314:LEU:O	2.01	0.60
1:B:336:MET:HB3	1:B:337:PRO:HD2	1.86	0.58
1:C:336:MET:HB3	1:C:337:PRO:HD2	1.86	0.58
1:B:297:ASN:OD1	1:B:298:PRO:HD2	2.05	0.57
1:C:220:TYR:O	1:C:304:LYS:HA	2.06	0.56
1:C:217:MET:CB	1:C:275:PHE:HB2	2.36	0.56
1:A:398:LEU:HD11	1:A:404:ASN:OD1	2.05	0.56
1:B:207:LEU:HD23	1:B:210:MET:HE3	1.89	0.55
1:A:164:LEU:HD12	1:A:174:VAL:HG12	1.87	0.55
1:D:371:ASN:HB3	1:D:415:TYR:CD2	2.43	0.54
1:A:213:HIS:O	1:A:218:LYS:HD3	2.09	0.52
1:C:217:MET:HB2	1:C:275:PHE:HB2	1.93	0.51
1:C:388:ALA:HB3	1:C:391:ALA:HB2	1.92	0.51
1:A:220:TYR:O	1:A:304:LYS:HA	2.10	0.51
1:C:244:ASN:HA	1:C:294:LEU:HA	1.93	0.51
1:D:361:PHE:CE1	1:D:373:ILE:HA	2.46	0.50
1:B:388:ALA:HB3	1:B:391:ALA:HB2	1.93	0.50
1:C:249:LEU:HD22	1:C:357:GLY:HA2	1.93	0.50
1:D:317:ARG:HG3	1:D:338:TYR:CE2	2.47	0.50
1:A:249:LEU:HD22	1:A:357:GLY:HA2	1.94	0.49
1:D:374:VAL:HG11	1:D:405:LEU:HD21	1.94	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:LYS:HE2	1:D:319:TYR:CZ	2.48	0.49
1:D:248:LEU:O	1:D:252:THR:HG23	2.12	0.48
1:D:256:GLY:HA3	1:D:355:HIS:O	2.14	0.48
1:B:197:LEU:HD23	1:D:319:TYR:CD1	2.46	0.47
1:B:256:GLY:O	1:B:438:ARG:NH2	2.47	0.47
1:C:458:ARG:HB3	1:C:468:ILE:HB	1.97	0.47
1:D:249:LEU:HD22	1:D:357:GLY:HA2	1.95	0.47
1:A:388:ALA:HB3	1:A:391:ALA:HB2	1.97	0.47
1:C:284:ILE:HG21	1:C:342:ILE:HD11	1.97	0.47
1:D:222:VAL:HB	1:D:306:VAL:HG12	1.97	0.47
1:B:192:ASN:OD1	1:D:321:PTR:HD1	2.14	0.47
1:A:194:LYS:NZ	1:C:311:SER:O	2.48	0.46
1:C:217:MET:HB3	1:C:275:PHE:HB2	1.96	0.46
1:A:374:VAL:HG11	1:A:405:LEU:HD11	1.98	0.46
1:A:170:PHE:HA	1:A:196:PHE:CD1	2.50	0.46
1:A:336:MET:HB3	1:A:337:PRO:HD2	1.98	0.46
1:B:217:MET:HB3	1:B:275:PHE:HB2	1.98	0.46
1:D:429:VAL:HG13	1:D:449:TYR:HB3	1.96	0.46
1:D:201:GLN:HB3	1:D:205:ARG:NH1	2.24	0.45
1:A:279:PRO:HG3	1:B:337:PRO:HB3	1.99	0.45
1:C:268:GLN:OE1	1:C:302:ALA:HA	2.17	0.45
1:A:209:LEU:HG	1:A:281:LEU:CD2	2.47	0.45
1:B:193:LYS:HE2	1:D:169:SER:OG	2.17	0.45
1:A:199[B]:GLN:OE1	1:C:195:ALA:HB2	2.16	0.45
1:C:385:LEU:HD23	1:C:385:LEU:HA	1.86	0.44
1:A:297:ASN:ND2	1:A:298:PRO:HD2	2.32	0.44
1:D:376:VAL:HA	1:D:421:ARG:O	2.16	0.44
1:D:249:LEU:HD21	1:D:354:MET:HA	1.99	0.44
1:D:258:SER:HA	1:D:438:ARG:HE	1.83	0.44
1:B:438:ARG:HD2	1:B:444:HIS:NE2	2.33	0.44
1:C:164:LEU:HD11	1:C:172:GLN:HB3	2.00	0.44
1:D:246:TYR:HB2	1:D:290:PRO:HB2	2.00	0.43
1:A:160:GLU:OE2	1:A:179:ARG:NE	2.49	0.43
1:A:471:TYR:O	1:A:475:GLN:HG2	2.18	0.43
1:B:210:MET:SD	1:B:221:ILE:HG21	2.59	0.43
1:D:244:ASN:HA	1:D:294:LEU:HA	2.00	0.43
1:D:398:LEU:HB3	1:D:399:PRO:HD2	2.01	0.43
1:A:159:TYR:OH	1:A:226:ARG:HD2	2.19	0.43
1:B:242:SER:OG	1:B:243:TYR:N	2.52	0.43
1:A:277:ALA:HA	1:A:340:LEU:CD2	2.48	0.43
1:D:277:ALA:HA	1:D:340:LEU:CD2	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:423:LEU:HA	1:D:426:ILE:HD12	2.00	0.43
1:C:361:PHE:CE1	1:C:373:ILE:HA	2.54	0.43
1:B:192:ASN:HB2	1:B:233:HIS:CE1	2.54	0.42
1:C:205:ARG:NH2	1:C:313:GLN:OE1	2.52	0.42
1:D:458:ARG:HB3	1:D:468:ILE:HB	2.02	0.42
1:B:219:TYR:O	1:B:304:LYS:CE	2.68	0.42
1:B:219:TYR:O	1:B:304:LYS:HE2	2.20	0.42
1:D:277:ALA:HA	1:D:340:LEU:HD22	2.00	0.42
1:A:209:LEU:HG	1:A:281:LEU:HD23	2.02	0.42
1:C:383:HIS:CE1	1:C:384:ILE:HG13	2.54	0.41
1:D:438:ARG:HD2	1:D:444:HIS:NE2	2.35	0.41
1:A:319:TYR:HD1	1:C:197:LEU:HD23	1.86	0.41
1:B:416:LYS:HD2	1:B:421:ARG:HB2	2.02	0.41
1:D:217:MET:HE1	1:D:274:LEU:HG	2.03	0.41
1:B:321:PTR:CE1	1:D:192:ASN:HD21	2.34	0.41
1:A:352:VAL:HG11	1:A:360:LEU:HD13	2.03	0.41
1:B:216:GLU:O	1:B:216:GLU:HG3	2.20	0.41
1:D:394:PHE:HB2	1:D:395:PHE:CD1	2.56	0.41
1:D:334:LEU:HB3	1:D:388:ALA:HB1	2.03	0.41
1:B:366:GLU:OE2	3:B:502:GOL:O1	2.39	0.40
1:D:257:VAL:O	1:D:355:HIS:ND1	2.54	0.40
1:C:154:LYS:HE3	1:C:160:GLU:HG2	2.04	0.40
1:B:388:ALA:HA	1:B:389:PRO:HD3	1.99	0.40
1:D:414:GLU:HG3	1:D:415:TYR:CD1	2.56	0.40
1:D:423:LEU:O	1:D:427:LEU:HG	2.21	0.40
1:D:438:ARG:HD3	1:D:441:GLU:OE1	2.22	0.40

There are no symmetry-related clashes.

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	340/361 (94%)	327 (96%)	13 (4%)	0	100	100
1	B	337/361 (93%)	325 (96%)	12 (4%)	0	100	100
1	C	336/361 (93%)	323 (96%)	13 (4%)	0	100	100
1	D	337/361 (93%)	327 (97%)	10 (3%)	0	100	100
All	All	1350/1444 (94%)	1302 (96%)	48 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	303/319 (95%)	301 (99%)	2 (1%)	84	92
1	B	302/319 (95%)	300 (99%)	2 (1%)	84	92
1	C	299/319 (94%)	295 (99%)	4 (1%)	69	83
1	D	301/319 (94%)	298 (99%)	3 (1%)	76	87
All	All	1205/1276 (94%)	1194 (99%)	11 (1%)	78	89

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	286	CYS
1	A	319	TYR
1	B	286	CYS
1	B	394	PHE
1	C	205	ARG
1	C	226	ARG
1	C	316	GLN
1	C	394	PHE
1	D	286	CYS
1	D	319	TYR
1	D	383	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are

no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	PTR	C	321	1	15,16,17	0.47	0	19,22,24	0.60	0
1	PTR	B	321	1	15,16,17	0.47	0	19,22,24	0.78	0
1	PTR	D	321	1	15,16,17	0.49	0	19,22,24	0.70	0
1	PTR	A	321	1	15,16,17	0.45	0	19,22,24	0.87	1 (5%)

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	PTR	C	321	1	-	1/10/11/13	0/1/1/1
1	PTR	B	321	1	-	1/10/11/13	0/1/1/1
1	PTR	D	321	1	-	3/10/11/13	0/1/1/1
1	PTR	A	321	1	-	0/10/11/13	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	321	PTR	CG-CB-CA	2.02	118.19	114.10

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	321	PTR	O-C-CA-CB
1	C	321	PTR	O-C-CA-CB
1	D	321	PTR	O-C-CA-CB
1	D	321	PTR	CA-CB-CG-CD1
1	D	321	PTR	CA-CB-CG-CD2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	321	PTR	1	0
1	D	321	PTR	1	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	4VZ	A	501	-	19,19,19	1.69	4 (21%)	26,26,26	4.79	13 (50%)
3	GOL	A	504	-	5,5,5	0.09	0	5,5,5	0.35	0
3	GOL	A	503	-	5,5,5	0.11	0	5,5,5	0.31	0
3	GOL	D	502	-	5,5,5	0.07	0	5,5,5	0.31	0
3	GOL	A	502	-	5,5,5	0.08	0	5,5,5	0.37	0
2	4VZ	C	501	-	19,19,19	1.88	5 (26%)	26,26,26	4.95	12 (46%)
2	4VZ	B	501	-	19,19,19	1.95	4 (21%)	26,26,26	5.09	11 (42%)
3	GOL	B	502	-	5,5,5	0.07	0	5,5,5	0.40	0
2	4VZ	D	501	-	19,19,19	1.96	5 (26%)	26,26,26	4.81	12 (46%)

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	4VZ	A	501	-	-	0/7/19/19	0/2/2/2
3	GOL	A	504	-	-	0/4/4/4	-
3	GOL	A	503	-	-	2/4/4/4	-
3	GOL	D	502	-	-	2/4/4/4	-
3	GOL	A	502	-	-	0/4/4/4	-
2	4VZ	C	501	-	-	0/7/19/19	0/2/2/2
2	4VZ	B	501	-	-	0/7/19/19	0/2/2/2
3	GOL	B	502	-	-	2/4/4/4	-
2	4VZ	D	501	-	-	0/7/19/19	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	4VZ	C13-S14	-4.46	1.58	1.66
2	D	501	4VZ	C13-S14	-4.43	1.58	1.66
2	A	501	4VZ	C13-S14	-4.36	1.58	1.66
2	B	501	4VZ	C13-S14	-4.19	1.58	1.66
2	B	501	4VZ	C09-C10	3.86	1.54	1.46
2	C	501	4VZ	C09-C10	3.54	1.53	1.46
2	D	501	4VZ	C13-S12	3.41	1.79	1.74
2	C	501	4VZ	C13-S12	3.28	1.79	1.74
2	B	501	4VZ	C18-C04	3.01	1.44	1.38
2	D	501	4VZ	C09-C10	3.01	1.52	1.46
2	D	501	4VZ	C18-C04	2.88	1.44	1.38
2	B	501	4VZ	C16-N15	2.83	1.43	1.38
2	A	501	4VZ	C18-C04	2.76	1.43	1.38
2	C	501	4VZ	C18-C04	2.72	1.43	1.38
2	D	501	4VZ	C16-N15	2.52	1.43	1.38
2	A	501	4VZ	C09-C10	2.44	1.51	1.46
2	A	501	4VZ	C16-N15	2.18	1.42	1.38
2	C	501	4VZ	C16-N15	2.02	1.42	1.38

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	4VZ	C10-C11-C16	17.35	134.20	120.47
2	C	501	4VZ	C10-C11-C16	17.04	133.96	120.47
2	D	501	4VZ	C10-C11-C16	16.55	133.57	120.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	4VZ	C10-C11-C16	15.96	133.10	120.47
2	C	501	4VZ	C11-C16-N15	9.12	117.83	110.22
2	B	501	4VZ	C13-S12-C11	8.69	96.95	92.42
2	D	501	4VZ	C11-C16-N15	8.66	117.44	110.22
2	A	501	4VZ	C11-C16-N15	8.64	117.43	110.22
2	C	501	4VZ	C16-C11-S12	-8.15	103.75	109.84
2	B	501	4VZ	C11-C16-N15	8.06	116.94	110.22
2	B	501	4VZ	C16-C11-S12	-7.88	103.95	109.84
2	A	501	4VZ	C16-C11-S12	-7.85	103.98	109.84
2	D	501	4VZ	C16-C11-S12	-7.58	104.18	109.84
2	A	501	4VZ	C13-S12-C11	7.42	96.29	92.42
2	C	501	4VZ	C13-S12-C11	7.14	96.14	92.42
2	D	501	4VZ	C13-S12-C11	6.55	95.83	92.42
2	B	501	4VZ	S14-C13-N15	6.24	133.40	126.29
2	B	501	4VZ	C10-C11-S12	-5.76	121.85	129.22
2	A	501	4VZ	S14-C13-N15	5.74	132.84	126.29
2	D	501	4VZ	C10-C11-S12	-5.44	122.25	129.22
2	C	501	4VZ	C10-C11-S12	-5.41	122.29	129.22
2	D	501	4VZ	S14-C13-N15	5.20	132.22	126.29
2	A	501	4VZ	C10-C11-S12	-4.92	122.92	129.22
2	C	501	4VZ	S14-C13-N15	4.64	131.58	126.29
2	B	501	4VZ	C13-N15-C16	-4.49	112.88	117.77
2	D	501	4VZ	C13-N15-C16	-4.44	112.94	117.77
2	C	501	4VZ	C13-N15-C16	-4.40	112.98	117.77
2	A	501	4VZ	C13-N15-C16	-4.39	113.00	117.77
2	C	501	4VZ	O17-C16-N15	-4.13	115.48	125.08
2	D	501	4VZ	O17-C16-N15	-3.95	115.91	125.08
2	B	501	4VZ	S12-C13-S14	-3.91	117.31	124.39
2	B	501	4VZ	C08-C09-C18	-3.83	113.92	118.71
2	B	501	4VZ	O17-C16-N15	-3.82	116.21	125.08
2	C	501	4VZ	C08-C09-C18	-3.79	113.97	118.71
2	D	501	4VZ	C08-C09-C18	-3.65	114.16	118.71
2	A	501	4VZ	O17-C16-N15	-3.64	116.61	125.08
2	A	501	4VZ	S12-C13-S14	-3.61	117.85	124.39
2	A	501	4VZ	C08-C09-C18	-3.56	114.26	118.71
2	C	501	4VZ	C09-C18-C04	3.46	124.85	120.17
2	D	501	4VZ	S12-C13-S14	-3.44	118.17	124.39
2	B	501	4VZ	C09-C18-C04	3.39	124.75	120.17
2	D	501	4VZ	C09-C18-C04	3.34	124.68	120.17
2	A	501	4VZ	C09-C18-C04	3.13	124.40	120.17
2	C	501	4VZ	S12-C13-S14	-2.91	119.12	124.39
2	A	501	4VZ	C09-C10-C11	2.36	134.16	130.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	501	4VZ	O03-C04-C05	2.14	119.60	114.89
2	C	501	4VZ	O03-C04-C05	2.14	119.58	114.89
2	A	501	4VZ	O03-C04-C05	2.03	119.35	114.89

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	GOL	C1-C2-C3-O3
3	B	502	GOL	O1-C1-C2-C3
3	D	502	GOL	O1-C1-C2-O2
3	D	502	GOL	O1-C1-C2-C3
3	A	503	GOL	O2-C2-C3-O3
3	B	502	GOL	O1-C1-C2-O2

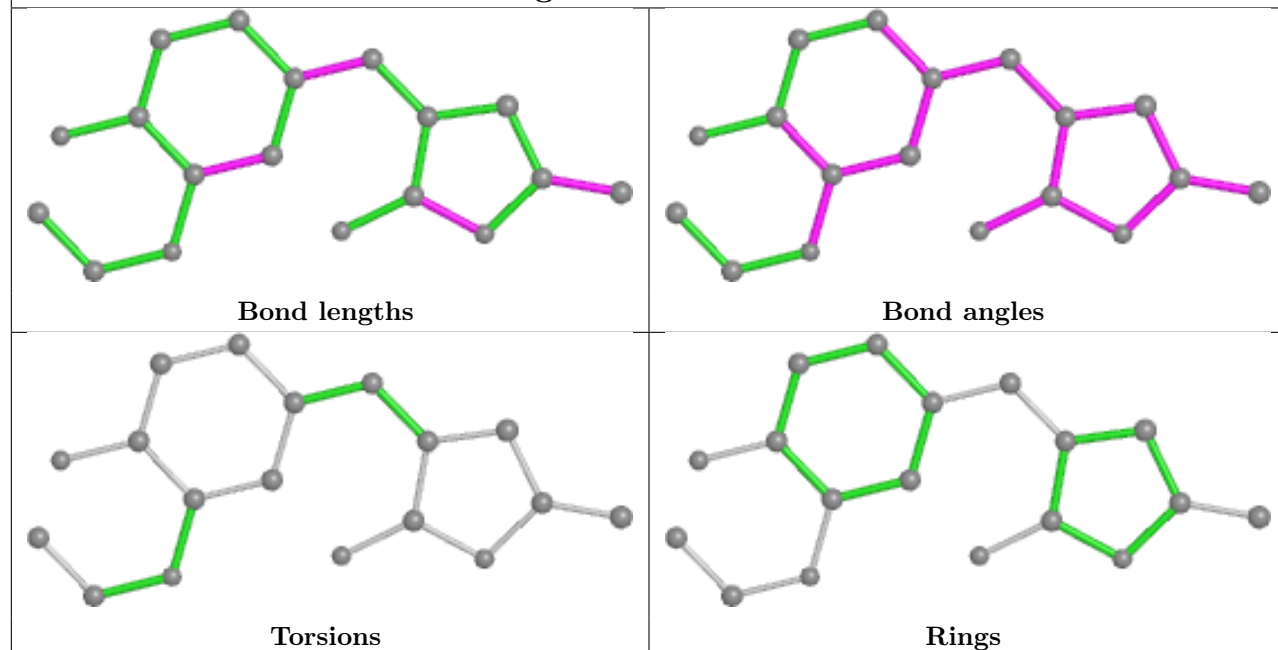
There are no ring outliers.

1 monomer is involved in 1 short contact:

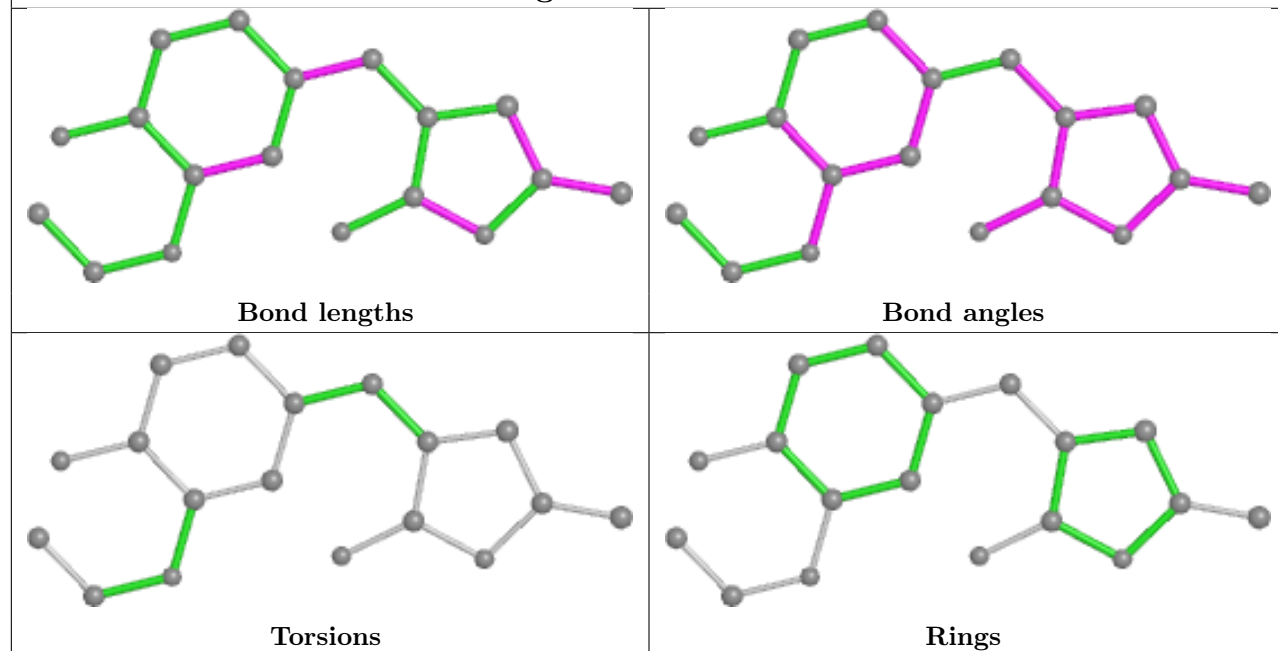
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	GOL	1	0

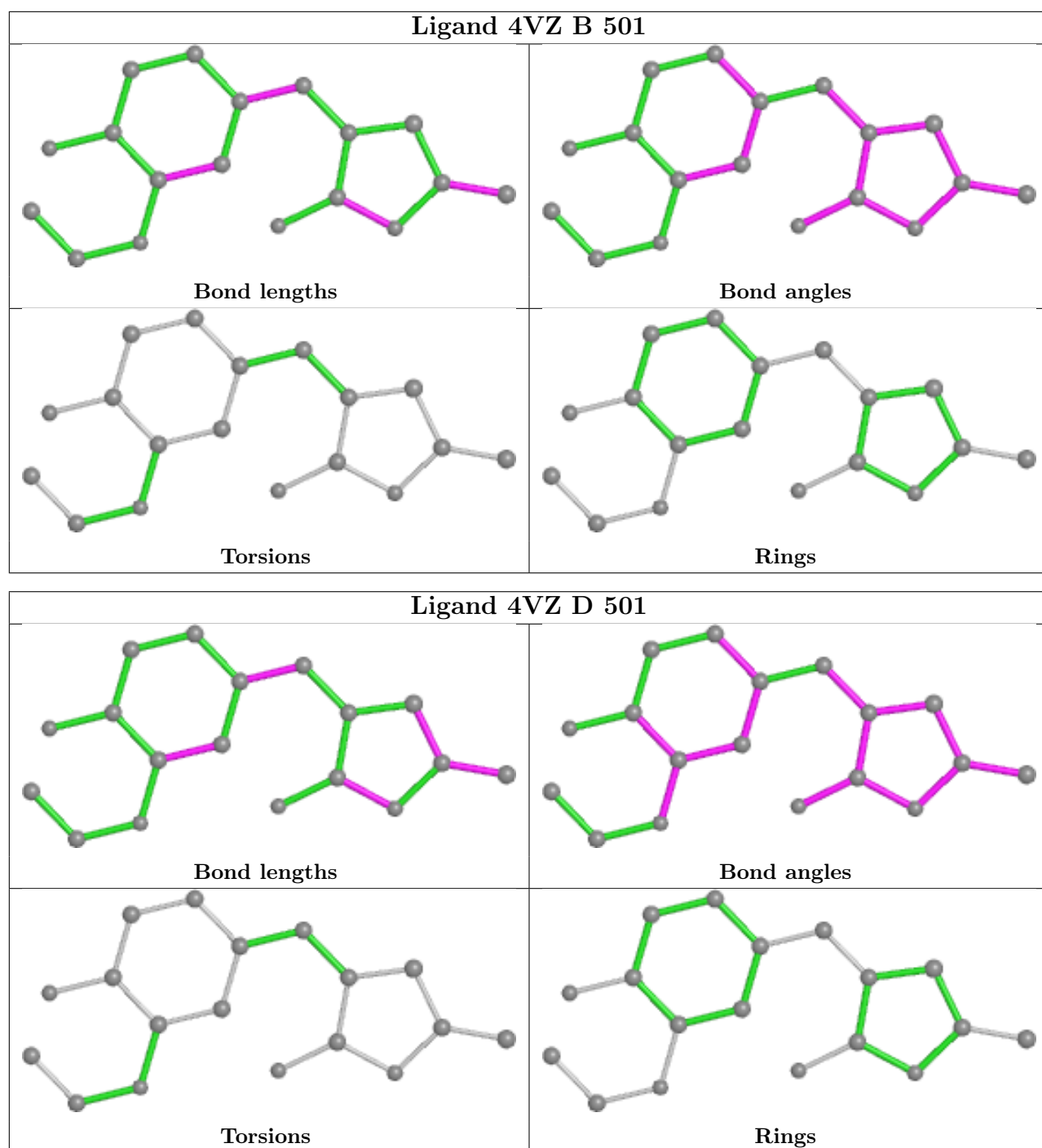
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 4VZ A 501



Ligand 4VZ C 501





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	342/361 (94%)	-0.04	7 (2%) 65 62	27, 39, 62, 95	0
1	B	341/361 (94%)	0.21	10 (2%) 51 49	31, 50, 83, 107	0
1	C	340/361 (94%)	0.17	9 (2%) 56 53	28, 51, 85, 113	0
1	D	341/361 (94%)	0.43	23 (6%) 17 15	29, 58, 93, 121	0
All	All	1364/1444 (94%)	0.19	49 (3%) 42 41	27, 49, 87, 121	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	219	TYR	5.9
1	C	398	LEU	5.3
1	D	399	PRO	4.8
1	C	216	GLU	4.6
1	C	215	THR	4.4
1	B	399	PRO	4.4
1	A	316	GLN	4.0
1	D	400	ASP	3.9
1	D	423	LEU	3.7
1	D	402	THR	3.6
1	D	420	THR	3.6
1	B	214	ASP	3.3
1	D	395	PHE	3.2
1	A	408	THR	3.1
1	B	481	LYS	3.1
1	D	404	ASN	3.1
1	D	472	TYR	2.9
1	D	401	GLY	2.9
1	C	218	LYS	2.9
1	D	398	LEU	2.9
1	D	378	GLY	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	472	TYR	2.9
1	B	215	THR	2.9
1	D	415	TYR	2.6
1	D	403	TRP	2.6
1	D	397	LYS	2.5
1	D	429	VAL	2.5
1	D	442	SER	2.5
1	B	144	ASN	2.5
1	A	315	GLY	2.5
1	D	408	THR	2.4
1	B	145	TYR	2.3
1	D	243	TYR	2.3
1	D	396	GLU	2.3
1	A	216	GLU	2.3
1	A	481	LYS	2.2
1	C	480	LYS	2.2
1	A	214	ASP	2.2
1	A	215	THR	2.2
1	B	400	ASP	2.2
1	C	423	LEU	2.2
1	C	219	TYR	2.1
1	D	316	GLN	2.1
1	D	443	GLY	2.1
1	D	385	LEU	2.1
1	B	216	GLU	2.1
1	B	298	PRO	2.0
1	D	437	ARG	2.0
1	C	414	GLU	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	PTR	D	321	16/17	0.92	0.15	55,60,60,60	0
1	PTR	C	321	16/17	0.97	0.13	45,48,49,52	0
1	PTR	B	321	16/17	0.97	0.13	34,36,39,39	0
1	PTR	A	321	16/17	0.98	0.13	32,33,38,42	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

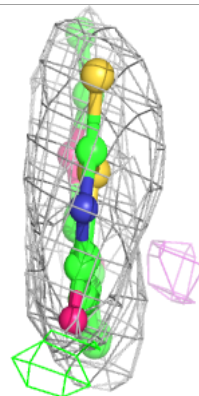
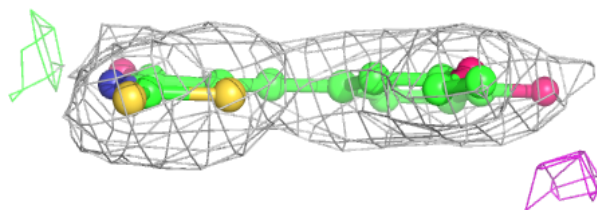
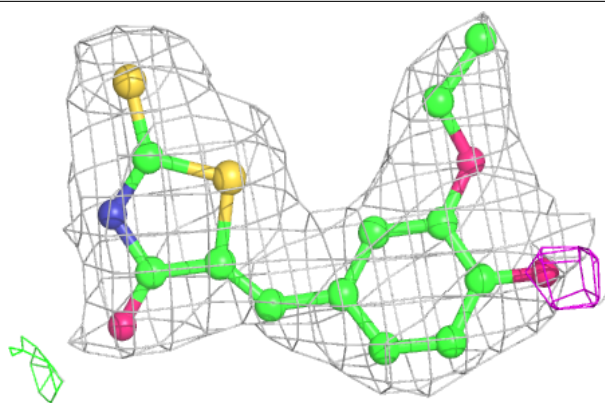
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	GOL	A	504	6/6	0.74	0.15	80,83,83,83	0
3	GOL	A	503	6/6	0.76	0.29	60,64,67,68	0
3	GOL	D	502	6/6	0.80	0.28	64,70,74,78	0
3	GOL	A	502	6/6	0.88	0.26	70,72,74,77	0
3	GOL	B	502	6/6	0.92	0.21	52,56,58,60	0
2	4VZ	B	501	18/18	0.94	0.12	44,48,56,60	0
2	4VZ	D	501	18/18	0.96	0.11	44,45,47,50	0
2	4VZ	A	501	18/18	0.96	0.15	34,35,40,44	0
2	4VZ	C	501	18/18	0.96	0.15	36,37,42,45	0

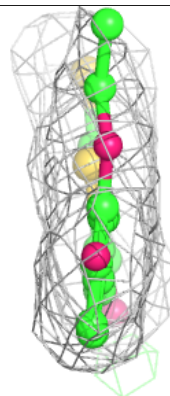
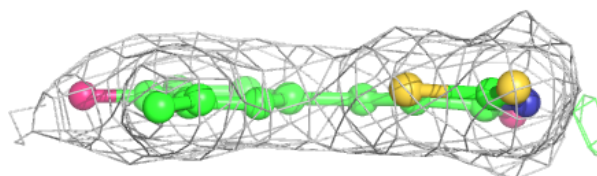
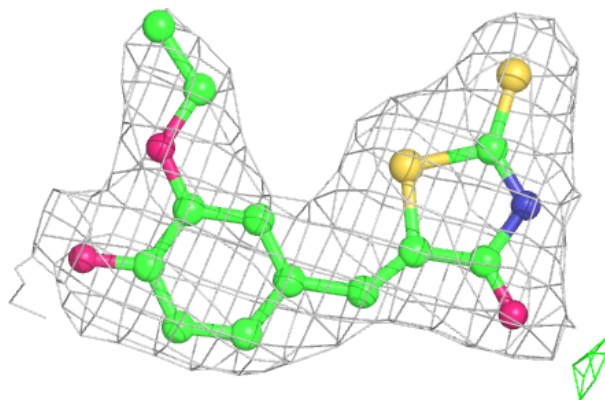
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 4VZ 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)

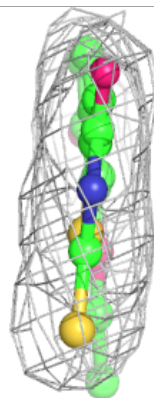
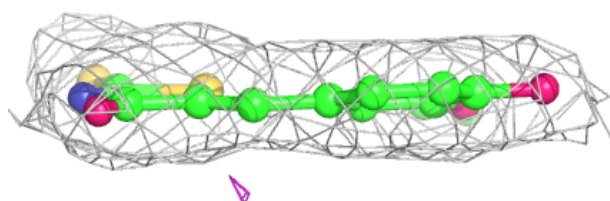
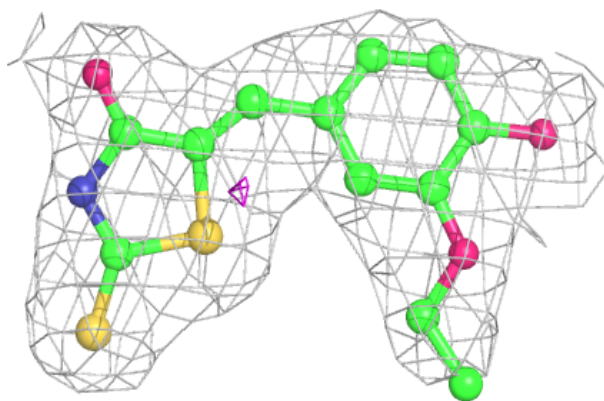
**Electron density around 4VZ D 501:**

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

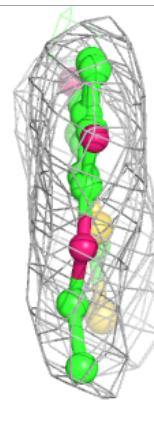
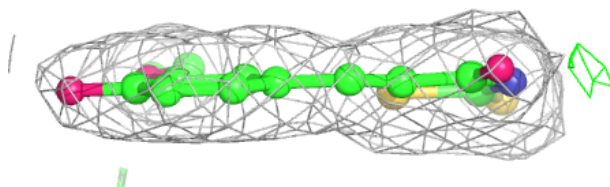
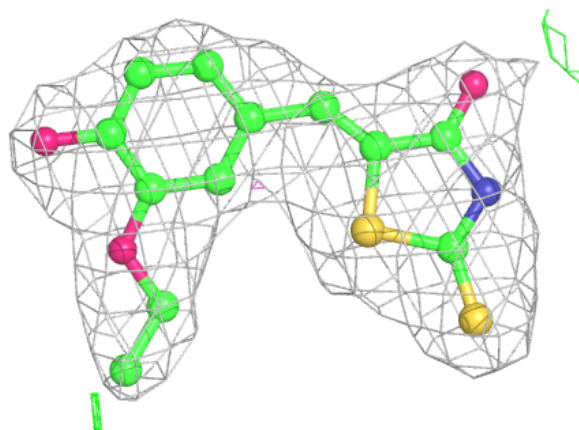


Electron density around 4VZ A 501:

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

**Electron density around 4VZ 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 [i](#)

There are no such residues in this entry.