



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2025 – 01:37 pm BST

PDB ID : 9HW6 / pdb_00009hw6
Title : Toxoplasma gondii GSK3b bound to LY2090314 and disulphide bonded through the C223 residue
Authors : Swale, C.; Diaz-Martin, S.; Bowler, M.W.
Deposited on : 2025-01-03
Resolution : 2.90 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	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

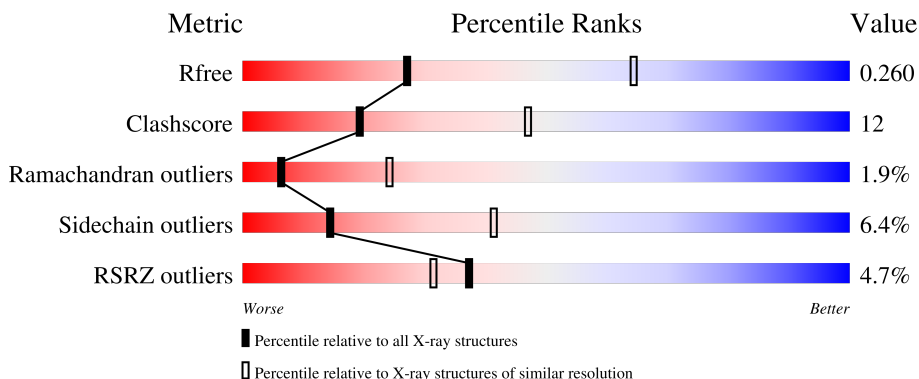
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	164625	2335 (2.90-2.90)
Clashscore	180529	2564 (2.90-2.90)
Ramachandran outliers	177936	2514 (2.90-2.90)
Sidechain outliers	177891	2516 (2.90-2.90)
RSRZ outliers	164620	2337 (2.90-2.90)

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	373	<div> <div>4%</div> <div>62%</div> <div>23%</div> <div>•</div> <div>11%</div> </div>
1	D	373	<div> <div>3%</div> <div>61%</div> <div>24%</div> <div>•</div> <div>12%</div> </div>
2	B	373	<div> <div>4%</div> <div>60%</div> <div>25%</div> <div>• •</div> <div>11%</div> </div>
2	F	373	<div> <div>6%</div> <div>63%</div> <div>21%</div> <div>•</div> <div>13%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10736 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 Putative cell-cycle-associated protein kinase GSK.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	332	Total	C	N	O	P	S	0	0	0
			2677	1711	458	491	2	15			
1	D	327	Total	C	N	O	P	S	0	0	0
			2627	1678	452	480	1	16			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP A0A125YY75
A	367	GLY	-	expression tag	UNP A0A125YY75
A	368	HIS	-	expression tag	UNP A0A125YY75
A	369	HIS	-	expression tag	UNP A0A125YY75
A	370	HIS	-	expression tag	UNP A0A125YY75
A	371	HIS	-	expression tag	UNP A0A125YY75
A	372	HIS	-	expression tag	UNP A0A125YY75
A	373	HIS	-	expression tag	UNP A0A125YY75
D	1	MET	-	initiating methionine	UNP A0A125YY75
D	367	GLY	-	expression tag	UNP A0A125YY75
D	368	HIS	-	expression tag	UNP A0A125YY75
D	369	HIS	-	expression tag	UNP A0A125YY75
D	370	HIS	-	expression tag	UNP A0A125YY75
D	371	HIS	-	expression tag	UNP A0A125YY75
D	372	HIS	-	expression tag	UNP A0A125YY75
D	373	HIS	-	expression tag	UNP A0A125YY75

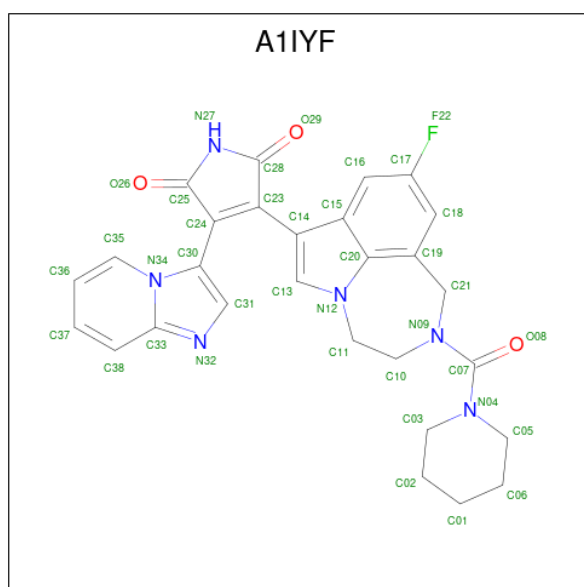
- Molecule 2 is a protein called Putative cell-cycle-associated protein kinase GSK.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	332	Total	C	N	O	S		0	0	0
			2659	1701	460	482	16				
2	F	325	Total	C	N	O	P	S	0	0	0
			2611	1675	446	473	1	16			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1	MET	-	initiating methionine	UNP A0A125YY75
B	367	GLY	-	expression tag	UNP A0A125YY75
B	368	HIS	-	expression tag	UNP A0A125YY75
B	369	HIS	-	expression tag	UNP A0A125YY75
B	370	HIS	-	expression tag	UNP A0A125YY75
B	371	HIS	-	expression tag	UNP A0A125YY75
B	372	HIS	-	expression tag	UNP A0A125YY75
B	373	HIS	-	expression tag	UNP A0A125YY75
F	1	MET	-	initiating methionine	UNP A0A125YY75
F	367	GLY	-	expression tag	UNP A0A125YY75
F	368	HIS	-	expression tag	UNP A0A125YY75
F	369	HIS	-	expression tag	UNP A0A125YY75
F	370	HIS	-	expression tag	UNP A0A125YY75
F	371	HIS	-	expression tag	UNP A0A125YY75
F	372	HIS	-	expression tag	UNP A0A125YY75
F	373	HIS	-	expression tag	UNP A0A125YY75

- Molecule 3 is 3-(6-fluoranyl-10-piperidin-1-ylcarbonyl-1,10-diazatricyclo[6.4.1.0^{4,13}]]trideca-2,4,6,8(13)-tetraen-3-yl)-4-imidazo[1,2-a]pyridin-3-yl-pyrrole-2,5-dione (CCD ID: A1IYF) (formula: C₂₈H₂₅FN₆O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			38	28	1	6	3		
3	B	1	Total	C	F	N	O	0	0
			38	28	1	6	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	D	1	Total	C	F	N	O	0	0
			38	28	1	6	3		
3	F	1	Total	C	F	N	O	0	0
			38	28	1	6	3		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

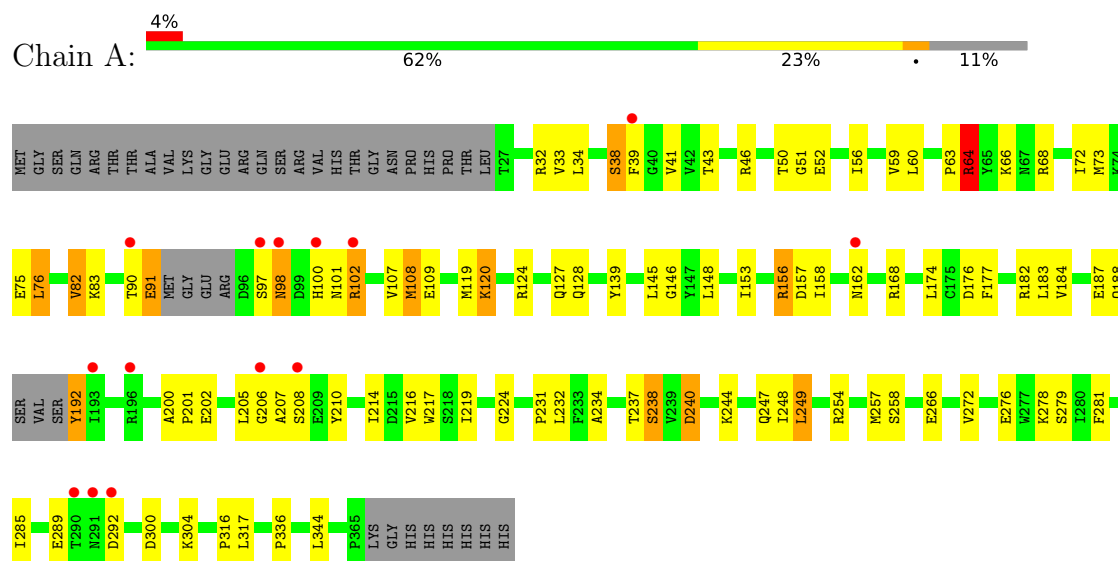


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		

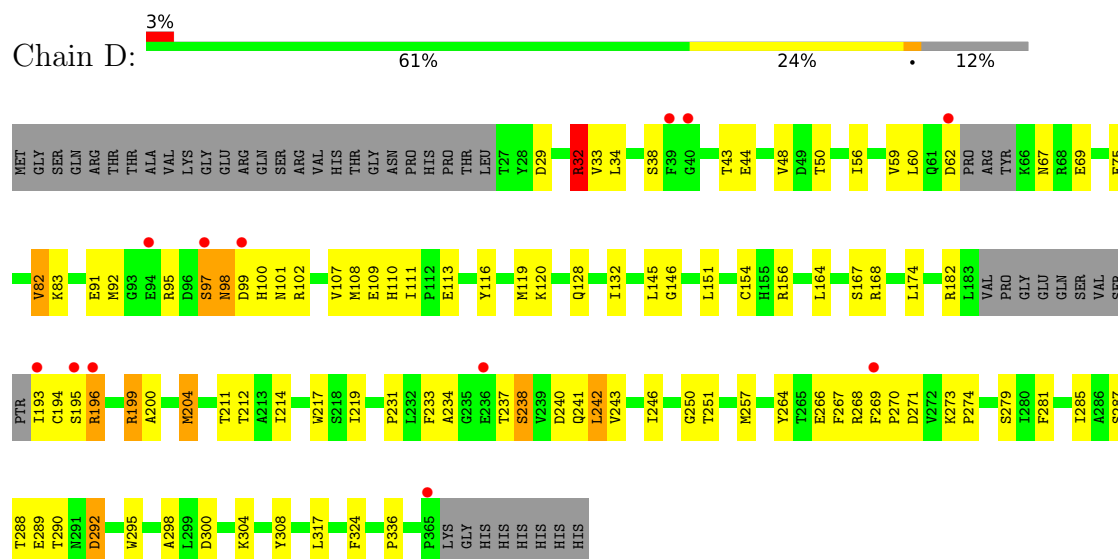
3 Residue-property plots [i](#)

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.

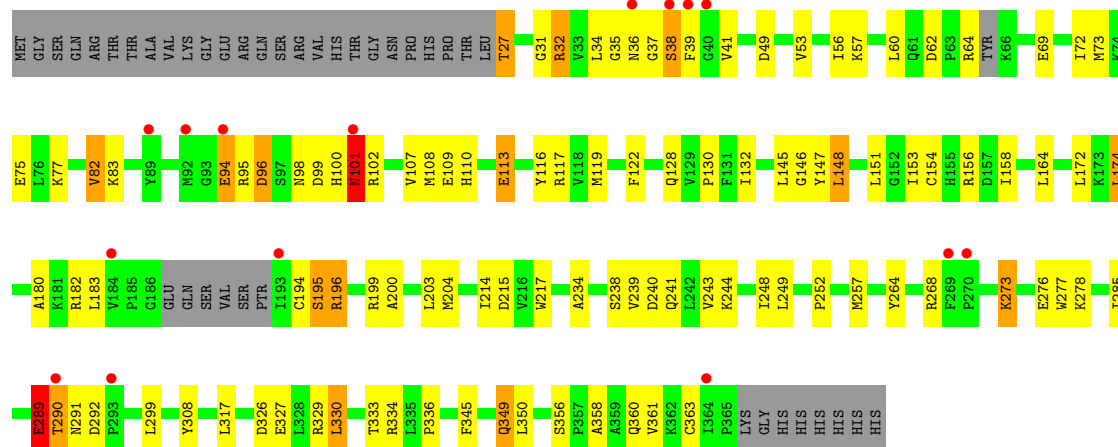
- Molecule 1: Putative cell-cycle-associated protein kinase GSK



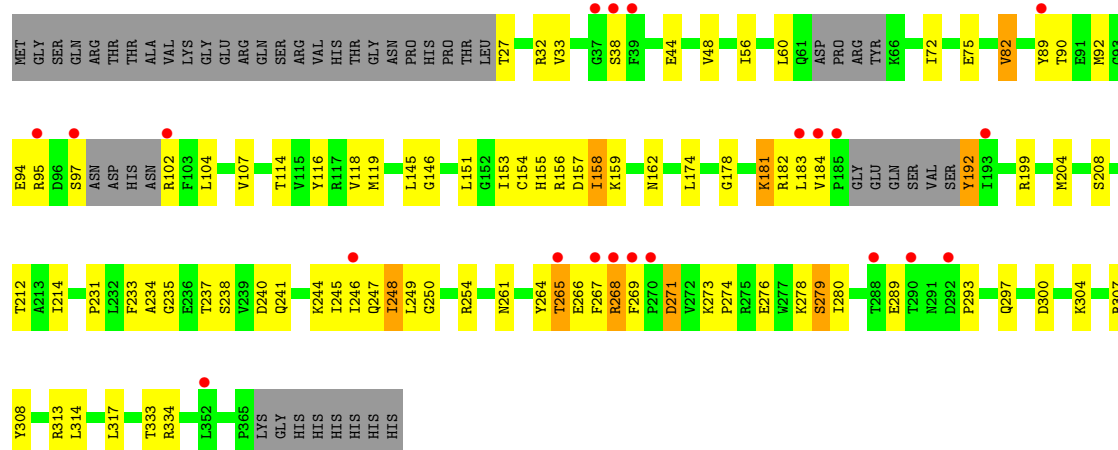
- Molecule 1: Putative cell-cycle-associated protein kinase GSK



- Molecule 2: Putative cell-cycle-associated protein kinase GSK



- Molecule 2: Putative cell-cycle-associated protein kinase GSK



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.91Å 161.73Å 83.28Å 90.00° 92.21° 90.00°	Depositor
Resolution (Å)	45.48 – 2.90 45.48 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.48-2.90) 92.4 (45.48-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.204 , 0.260 0.204 , 0.260	Depositor DCC
R_{free} test set	1998 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	54.4	Xtriage
Anisotropy	0.575	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.050 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10736	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.94% 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: A1IYF, PO4, SEP, 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	0.46	0/2710	0.68	0/3671
1	D	0.50	0/2673	0.75	0/3617
2	B	0.44	0/2718	0.67	0/3681
2	F	0.37	0/2651	0.63	0/3588
All	All	0.45	0/10752	0.68	0/14557

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	D	0	2
All	All	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	102	ARG	Sidechain
1	A	64	ARG	Sidechain
1	D	199	ARG	Sidechain
1	D	32	ARG	Sidechain

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	2677	0	2681	65	1
1	D	2627	0	2640	77	1
2	B	2659	0	2680	69	0
2	F	2611	0	2639	53	0
3	A	38	0	0	0	0
3	B	38	0	0	2	0
3	D	38	0	0	1	0
3	F	38	0	0	0	0
4	B	5	0	0	0	0
4	D	5	0	0	0	0
All	All	10736	0	10640	246	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (246) 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:196:ARG:CA	1:D:199:ARG:HE	1.62	1.12
1:D:196:ARG:N	1:D:199:ARG:HE	1.46	1.12
1:D:196:ARG:HA	1:D:199:ARG:NE	1.65	1.09
1:D:196:ARG:HA	1:D:199:ARG:CZ	1.90	1.01
2:B:196:ARG:HB2	2:B:241:GLN:HE22	1.23	1.00
1:D:196:ARG:HA	1:D:199:ARG:NH2	1.79	0.97
2:F:181:LYS:HD2	2:F:183:LEU:H	1.28	0.96
1:D:196:ARG:CB	1:D:199:ARG:HH21	1.78	0.95
1:D:270:PRO:HD3	2:F:268:ARG:HG2	1.47	0.94
1:D:196:ARG:HB2	1:D:199:ARG:HH21	1.30	0.93
1:D:196:ARG:CA	1:D:199:ARG:NE	2.29	0.91
1:D:196:ARG:CA	1:D:199:ARG:HH21	1.84	0.90
1:D:196:ARG:H	1:D:199:ARG:HE	1.15	0.89
2:B:64:ARG:HD3	2:F:102:ARG:HD3	1.52	0.88
1:D:196:ARG:HB2	1:D:199:ARG:NH2	1.90	0.86
1:D:196:ARG:H	1:D:199:ARG:NE	1.76	0.84
1:D:196:ARG:N	1:D:199:ARG:NE	2.26	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:ARG:HA	1:D:199:ARG:HH21	1.41	0.80
1:A:63:PRO:HG3	1:A:102:ARG:HD2	1.66	0.78
1:D:251:THR:HG21	1:D:268:ARG:HH22	1.49	0.76
1:D:204:MET:HE1	1:D:241:GLN:HB3	1.67	0.76
1:A:32:ARG:HH21	2:F:97:SER:HB2	1.50	0.76
1:D:101:ASN:HD21	2:F:33:VAL:H	1.33	0.75
2:F:181:LYS:NZ	2:F:192:PTR:O3P	2.21	0.73
2:B:145:LEU:HD11	2:B:158:ILE:HG13	1.71	0.72
1:A:73:MET:HA	1:A:76:LEU:HD22	1.72	0.71
2:B:56:ILE:HG12	2:B:107:VAL:HG22	1.73	0.70
1:A:91:GLU:OE1	1:A:91:GLU:C	2.35	0.69
1:D:97:SER:OG	1:D:98:ASN:N	2.23	0.69
1:A:157:ASP:O	1:A:162:ASN:ND2	2.26	0.68
1:A:156:ARG:HG2	1:A:214:ILE:HD11	1.76	0.67
2:F:271:ASP:N	2:F:271:ASP:OD1	2.27	0.67
1:D:146:GLY:HA3	1:D:317:LEU:HG	1.76	0.67
1:A:63:PRO:HG3	1:A:102:ARG:CD	2.24	0.66
1:A:247:GLN:HA	1:A:272:VAL:HG11	1.78	0.66
1:D:196:ARG:CA	1:D:199:ARG:NH2	2.49	0.65
2:F:157:ASP:O	2:F:162:ASN:ND2	2.31	0.64
2:F:231:PRO:HB2	2:F:234:ALA:HB2	1.78	0.64
1:A:60:LEU:HD11	1:A:101:ASN:HB3	1.80	0.62
1:A:46:ARG:NH2	1:D:113:GLU:OE2	2.27	0.62
1:A:124:ARG:NH1	1:D:29:ASP:OD1	2.33	0.62
1:A:237:THR:HG23	1:A:240:ASP:H	1.65	0.62
1:A:336:PRO:HB2	1:D:50:THR:HA	1.81	0.61
1:D:56:ILE:HG12	1:D:107:VAL:HG22	1.81	0.61
2:F:89:TYR:CE1	2:F:104:LEU:HD13	2.35	0.61
2:F:155:HIS:HB3	2:F:158:ILE:HD11	1.83	0.61
2:B:73:MET:CE	2:B:108:MET:HE3	2.32	0.60
1:A:50:THR:HA	1:D:336:PRO:HB2	1.83	0.60
1:D:250:GLY:HA3	1:D:274:PRO:HG3	1.83	0.60
1:A:145:LEU:HD11	1:A:158:ILE:HG13	1.85	0.59
1:A:231:PRO:HB2	1:A:234:ALA:HB2	1.84	0.58
2:F:156:ARG:HG2	2:F:214:ILE:HD11	1.85	0.58
1:A:238:SEP:HB3	2:B:238:SER:HB2	1.83	0.58
1:D:242:LEU:O	1:D:246:ILE:HG12	2.03	0.58
2:F:56:ILE:HG12	2:F:107:VAL:HG22	1.84	0.58
2:F:276:GLU:O	2:F:279:SER:OG	2.21	0.58
2:B:327:GLU:HA	2:B:330:LEU:HD22	1.86	0.58
2:F:151:LEU:O	2:F:182:ARG:NH1	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:ARG:H	1:D:199:ARG:CD	2.16	0.57
2:F:233:PHE:HA	2:F:244:LYS:HG2	1.86	0.57
2:B:273:LYS:HE2	2:B:273:LYS:H	1.69	0.57
2:B:72:ILE:HG23	2:B:153:ILE:HD13	1.87	0.57
1:A:146:GLY:HA3	1:A:317:LEU:HG	1.87	0.56
2:B:32:ARG:NH1	2:B:34:LEU:HD23	2.21	0.56
1:A:205:LEU:O	1:A:207:ALA:N	2.37	0.56
2:B:148:LEU:HD22	2:B:153:ILE:HB	1.88	0.56
2:F:82:VAL:HG22	2:F:174:LEU:O	2.06	0.56
2:B:239:VAL:O	2:B:243:VAL:HG23	2.06	0.55
2:B:73:MET:HE1	2:B:108:MET:HE3	1.89	0.55
2:F:146:GLY:HA3	2:F:317:LEU:HG	1.88	0.55
2:B:37:GLY:O	2:B:39:PHE:N	2.39	0.55
1:D:75:GLU:OE1	1:D:182:ARG:NH2	2.39	0.55
2:F:181:LYS:HD2	2:F:183:LEU:N	2.11	0.55
2:F:248:ILE:HG22	2:F:249:LEU:HD12	1.89	0.55
2:B:326:ASP:HA	2:B:329:ARG:NH1	2.22	0.54
1:A:82:VAL:HG22	1:A:174:LEU:O	2.07	0.54
1:D:91:GLU:OE2	1:D:102:ARG:NH1	2.40	0.54
1:A:120:LYS:HD2	1:A:120:LYS:N	2.21	0.53
2:B:82:VAL:HG22	2:B:174:LEU:O	2.08	0.53
2:F:116:TYR:HA	2:F:119:MET:HE2	1.91	0.53
1:A:202:GLU:O	1:A:207:ALA:HB2	2.09	0.53
2:B:333:THR:O	2:B:334:ARG:NH1	2.36	0.53
2:B:146:GLY:HA3	2:B:317:LEU:HG	1.90	0.53
2:B:32:ARG:NH1	2:B:34:LEU:CD2	2.72	0.53
2:B:132:ILE:HG21	2:B:336:PRO:HG3	1.90	0.53
2:B:326:ASP:HA	2:B:329:ARG:HH12	1.74	0.53
2:B:108:MET:HE2	3:B:402:A1IYF:O26	2.09	0.52
1:A:168:ARG:HH22	1:D:168:ARG:NH2	2.06	0.52
2:B:285:ILE:O	2:B:289:GLU:HB2	2.09	0.52
2:B:329:ARG:HG2	2:B:345:PHE:CE1	2.45	0.52
1:D:33:VAL:HA	1:D:43:THR:HG22	1.92	0.52
1:D:240:ASP:O	1:D:243:VAL:HG22	2.10	0.52
1:D:151:LEU:O	1:D:182:ARG:NH1	2.43	0.51
2:B:196:ARG:CB	2:B:241:GLN:HE22	2.09	0.51
1:A:75:GLU:OE2	1:A:182:ARG:NH2	2.44	0.51
2:B:75:GLU:OE2	2:B:182:ARG:NH2	2.44	0.51
2:F:204:MET:HE1	2:F:245:ILE:HD12	1.93	0.51
1:A:33:VAL:HG22	1:A:43:THR:HG22	1.92	0.51
2:B:154:CYS:O	2:B:180:ALA:HA	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLU:C	1:A:91:GLU:CD	2.78	0.51
1:A:187:GLU:HG2	1:A:188:GLN:H	1.76	0.50
1:D:110:HIS:HA	3:D:402:A1IYF:O29	2.11	0.50
2:F:114:THR:O	2:F:118:VAL:HG23	2.11	0.50
1:A:240:ASP:O	1:A:244:LYS:HG2	2.12	0.50
1:A:248:ILE:HG22	1:A:249:LEU:HD23	1.92	0.50
2:F:247:GLN:O	2:F:248:ILE:HD13	2.11	0.50
1:A:63:PRO:HD2	1:A:100:HIS:O	2.11	0.50
2:B:99:ASP:C	2:B:101:ASN:H	2.20	0.50
2:F:32:ARG:HG2	2:F:44:GLU:HB2	1.94	0.50
2:B:290:THR:O	2:B:291:ASN:HB2	2.11	0.49
1:D:300:ASP:O	1:D:304:LYS:HG3	2.11	0.49
1:A:63:PRO:CG	1:A:102:ARG:HD2	2.39	0.49
1:A:83:LYS:HG3	1:A:109:GLU:OE1	2.12	0.49
2:F:72:ILE:HG23	2:F:153:ILE:HD13	1.93	0.49
1:D:298:ALA:HB2	1:D:324:PHE:CE1	2.48	0.49
1:D:237:THR:OG1	1:D:238:SEP:N	2.46	0.49
1:D:34:LEU:HD21	1:D:44:GLU:HG3	1.94	0.49
2:B:60:LEU:HD12	2:B:102:ARG:O	2.13	0.48
1:A:188:GLN:O	1:A:192:PTR:HE1	2.13	0.48
2:F:333:THR:O	2:F:334:ARG:NH1	2.46	0.48
1:D:237:THR:HG23	1:D:240:ASP:H	1.78	0.48
1:D:290:THR:HG22	1:D:292:ASP:HB2	1.94	0.48
2:F:249:LEU:HB3	2:F:308:TYR:CE2	2.49	0.48
1:A:156:ARG:NH1	1:A:210:TYR:OH	2.45	0.48
1:D:82:VAL:HG22	1:D:174:LEU:O	2.14	0.48
2:B:96:ASP:HB3	2:B:98:ASN:OD1	2.14	0.47
1:A:127:GLN:HG3	1:D:48:VAL:HG11	1.96	0.47
1:D:83:LYS:HG3	1:D:109:GLU:OE1	2.14	0.47
1:A:72:ILE:HG23	1:A:153:ILE:HD13	1.96	0.47
1:A:237:THR:HG22	1:A:240:ASP:HB2	1.96	0.47
2:B:145:LEU:HD13	2:B:215:ASP:HB3	1.95	0.47
2:F:38:SER:HB2	2:F:178:GLY:HA3	1.95	0.47
2:B:73:MET:HE2	2:B:108:MET:HE3	1.97	0.47
2:F:155:HIS:HB3	2:F:158:ILE:CD1	2.44	0.47
1:A:73:MET:HE2	1:A:177:PHE:HD1	1.80	0.47
1:D:231:PRO:HB2	1:D:234:ALA:HB2	1.95	0.47
2:F:60:LEU:HD12	2:F:102:ARG:O	2.14	0.47
2:B:32:ARG:HH12	2:B:34:LEU:CD2	2.28	0.47
1:A:139:TYR:CD1	1:A:344:LEU:HD22	2.50	0.47
2:B:122:PHE:CE2	2:B:130:PRO:HD3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:GLY:O	2:B:32:ARG:HB3	2.15	0.46
2:F:267:PHE:O	2:F:268:ARG:HB2	2.14	0.46
2:B:27:THR:HG22	2:B:49:ASP:OD1	2.15	0.46
2:B:164:LEU:O	2:B:172:LEU:HA	2.16	0.46
1:A:46:ARG:NH1	1:A:51:GLY:O	2.48	0.46
1:D:211:THR:OG1	1:D:212:THR:N	2.48	0.46
1:A:281:PHE:O	1:A:285:ILE:HG13	2.16	0.46
2:B:196:ARG:HB3	2:B:199:ARG:HH21	1.80	0.46
1:A:224:GLY:HA3	1:A:232:LEU:HD11	1.98	0.46
2:B:194:CYS:O	2:B:195:SER:C	2.58	0.46
1:A:300:ASP:OD2	1:A:304:LYS:NZ	2.48	0.46
2:B:116:TYR:HA	2:B:119:MET:HE2	1.98	0.46
2:B:147:TYR:CZ	2:B:151:LEU:HD11	2.50	0.46
1:D:67:ASN:OD1	1:D:69:GLU:HB3	2.15	0.46
2:B:110:HIS:HA	3:B:402:A1IYF:O29	2.16	0.46
2:F:278:LYS:HE2	2:F:278:LYS:H	1.81	0.46
2:B:356:SER:O	2:B:360:GLN:HG3	2.16	0.45
2:B:248:ILE:HG22	2:B:249:LEU:HD12	1.98	0.45
2:F:235:GLY:O	2:F:241:GLN:NE2	2.49	0.45
1:D:60:LEU:HG	1:D:62:ASP:HB2	1.99	0.45
1:A:73:MET:HE2	1:A:177:PHE:CD1	2.51	0.45
2:B:113:GLU:CG	2:B:117:ARG:HD2	2.46	0.45
2:B:156:ARG:HG2	2:B:214:ILE:HD11	1.99	0.45
1:D:128:GLN:OE1	1:D:288:THR:HG21	2.16	0.45
1:A:200:ALA:HA	1:A:217:TRP:CD1	2.52	0.45
1:D:99:ASP:OD2	2:F:32:ARG:NH2	2.49	0.45
2:F:248:ILE:CD1	2:F:280:ILE:HD11	2.46	0.45
2:F:261:ASN:HD22	2:F:264:TYR:HE2	1.65	0.45
1:A:63:PRO:HG3	1:A:102:ARG:NE	2.32	0.45
2:B:249:LEU:HB3	2:B:308:TYR:CE2	2.52	0.45
1:D:196:ARG:HE	1:D:196:ARG:HB3	1.61	0.44
2:F:244:LYS:HE2	2:F:244:LYS:HB2	1.75	0.44
1:D:281:PHE:O	1:D:285:ILE:HG13	2.17	0.44
2:B:83:LYS:HG3	2:B:109:GLU:OE1	2.18	0.44
1:A:97:SER:O	1:A:98:ASN:ND2	2.42	0.44
1:D:98:ASN:OD1	2:F:32:ARG:HD2	2.17	0.44
1:A:124:ARG:NH2	1:D:29:ASP:OD2	2.51	0.44
2:B:196:ARG:HB2	2:B:241:GLN:NE2	2.08	0.44
1:A:201:PRO:HD3	1:A:217:TRP:CD2	2.53	0.44
2:F:265:THR:HG23	2:F:266:GLU:OE1	2.18	0.44
2:B:38:SER:HB2	2:B:57:LYS:HZ3	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:145:LEU:HD12	1:D:219:ILE:HD11	1.98	0.44
2:B:203:LEU:HD11	2:B:214:ILE:HD12	2.00	0.43
1:D:145:LEU:HA	1:D:145:LEU:HD23	1.81	0.43
2:B:252:PRO:HG2	2:B:257:MET:HE1	2.00	0.43
2:B:257:MET:HG2	2:B:264:TYR:O	2.18	0.43
2:B:358:ALA:O	2:B:361:VAL:HG22	2.19	0.43
1:D:317:LEU:HA	1:D:317:LEU:HD23	1.77	0.43
1:A:39:PHE:CZ	2:B:36:ASN:ND2	2.87	0.43
1:A:38:SER:OG	1:A:176:ASP:OD1	2.30	0.43
1:A:145:LEU:HD12	1:A:219:ILE:HD11	2.00	0.43
2:B:200:ALA:HA	2:B:217:TRP:CD1	2.54	0.43
2:F:237:THR:HG23	2:F:240:ASP:H	1.83	0.43
2:B:113:GLU:HG3	2:B:117:ARG:HD2	2.01	0.43
2:B:277:TRP:HB3	2:B:299:LEU:HD22	2.00	0.43
1:D:32:ARG:HD3	2:F:95:ARG:HH22	1.84	0.43
1:D:246:ILE:HD13	1:D:308:TYR:OH	2.18	0.43
1:A:276:GLU:O	1:A:279:SER:HB3	2.19	0.43
1:D:116:TYR:HA	1:D:119:MET:HE2	2.00	0.43
2:F:250:GLY:HA3	2:F:274:PRO:HG3	2.01	0.43
1:A:145:LEU:HA	1:A:145:LEU:HD23	1.69	0.42
1:D:154:CYS:SG	1:D:156:ARG:HG3	2.59	0.42
2:F:307:ARG:HB2	2:F:313:ARG:HG2	2.00	0.42
1:A:188:GLN:HG3	1:A:208:SER:HB2	2.01	0.42
1:A:216:VAL:HG22	1:A:316:PRO:HG3	2.01	0.42
2:B:234:ALA:O	2:B:244:LYS:HD2	2.19	0.42
2:F:300:ASP:O	2:F:304:LYS:HG3	2.19	0.42
1:A:52:GLU:HA	1:D:167:SER:HB3	2.02	0.42
1:A:56:ILE:HG12	1:A:107:VAL:HG22	2.01	0.42
1:A:108:MET:HB2	1:A:108:MET:HE3	1.70	0.42
1:A:254:ARG:NE	1:A:266:GLU:OE2	2.44	0.42
1:D:111:ILE:HB	1:D:164:LEU:HB3	2.02	0.42
1:D:132:ILE:HD12	1:D:132:ILE:HA	1.90	0.42
2:F:254:ARG:HD2	2:F:266:GLU:OE2	2.19	0.42
2:F:145:LEU:HD23	2:F:145:LEU:HA	1.78	0.42
2:F:159:LYS:HG2	2:F:162:ASN:ND2	2.35	0.42
1:D:156:ARG:HG2	1:D:214:ILE:HD11	2.01	0.42
1:A:90:THR:CG2	1:A:91:GLU:N	2.81	0.42
1:D:92:MET:HE3	1:D:92:MET:HB3	1.84	0.42
1:D:98:ASN:HB3	1:D:99:ASP:H	1.60	0.42
2:B:57:LYS:NZ	2:B:69:GLU:OE1	2.53	0.42
2:B:60:LEU:HD11	2:B:101:ASN:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:278:LYS:H	2:F:278:LYS:CE	2.33	0.41
1:D:120:LYS:HA	1:D:120:LYS:HD3	1.88	0.41
2:B:199:ARG:O	2:B:204:MET:HE3	2.20	0.41
2:F:199:ARG:NH2	2:F:238:SER:OG	2.53	0.41
2:B:119:MET:HE2	2:B:119:MET:HB2	1.89	0.41
2:B:329:ARG:HE	2:B:363:CYS:HA	1.85	0.41
1:D:233:PHE:O	1:D:241:GLN:NE2	2.53	0.41
1:A:98:ASN:O	2:B:32:ARG:NE	2.37	0.41
1:D:200:ALA:HA	1:D:217:TRP:CD1	2.56	0.41
1:D:288:THR:OG1	1:D:295:TRP:NE1	2.41	0.41
1:A:278:LYS:HE2	1:A:278:LYS:HB2	1.89	0.41
1:A:39:PHE:HD2	1:A:59:VAL:HG23	1.85	0.40
2:B:349:GLN:HG3	2:B:350:LEU:N	2.36	0.40
1:D:257:MET:HG2	1:D:264:TYR:O	2.21	0.40
1:D:268:ARG:NH2	1:D:271:ASP:OD1	2.47	0.40
2:B:151:LEU:O	2:B:182:ARG:NH1	2.53	0.40
2:B:196:ARG:HB3	2:B:199:ARG:NH2	2.36	0.40
1:D:267:PHE:C	1:D:267:PHE:HD1	2.30	0.40
2:F:293:PRO:HB2	2:F:297:GLN:NE2	2.36	0.40
2:F:154:CYS:SG	2:F:212:THR:HA	2.61	0.40
1:D:269:PHE:HB3	1:D:270:PRO:HD2	2.04	0.40
1:A:34:LEU:HD23	1:A:34:LEU:HA	1.92	0.40
1:D:290:THR:CG2	1:D:292:ASP:HB2	2.51	0.40
2:F:75:GLU:OE1	2:F:182:ARG:NH2	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ARG:NH1	1:D:62:ASP:OD1[1_655]	1.74	0.46

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	325/373 (87%)	303 (93%)	17 (5%)	5 (2%)	8	29
1	D	320/373 (86%)	296 (92%)	18 (6%)	6 (2%)	6	24
2	B	326/373 (87%)	292 (90%)	26 (8%)	8 (2%)	4	18
2	F	317/373 (85%)	293 (92%)	19 (6%)	5 (2%)	8	28
All	All	1288/1492 (86%)	1184 (92%)	80 (6%)	24 (2%)	6	24

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	101	ASN
2	B	195	SER
1	D	95	ARG
1	D	98	ASN
1	D	100	HIS
1	A	206	GLY
2	B	35	GLY
2	B	38	SER
2	B	94	GLU
1	D	97	SER
2	F	208	SER
1	A	183	LEU
1	A	258	SER
2	B	289	GLU
2	F	268	ARG
1	A	292	ASP
2	B	183	LEU
1	D	38	SER
2	F	269	PHE
2	F	289	GLU
1	A	38	SER
2	B	32	ARG
1	D	266	GLU
2	F	92	MET

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	295/330 (89%)	276 (94%)	19 (6%)	14	41
1	D	291/330 (88%)	276 (95%)	15 (5%)	19	50
2	B	296/331 (89%)	270 (91%)	26 (9%)	8	26
2	F	289/331 (87%)	274 (95%)	15 (5%)	19	50
All	All	1171/1322 (89%)	1096 (94%)	75 (6%)	14	41

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	VAL
1	A	64	ARG
1	A	66	LYS
1	A	68	ARG
1	A	76	LEU
1	A	82	VAL
1	A	91	GLU
1	A	98	ASN
1	A	108	MET
1	A	119	MET
1	A	120	LYS
1	A	128	GLN
1	A	148	LEU
1	A	156	ARG
1	A	184	VAL
1	A	240	ASP
1	A	249	LEU
1	A	257	MET
1	A	289	GLU
2	B	27	THR
2	B	41	VAL
2	B	53	VAL
2	B	62	ASP
2	B	77	LYS
2	B	82	VAL
2	B	94	GLU
2	B	95	ARG
2	B	96	ASP
2	B	100	HIS
2	B	101	ASN

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Mol	Chain	Res	Type
2	B	113	GLU
2	B	128	GLN
2	B	148	LEU
2	B	174	LEU
2	B	196	ARG
2	B	240	ASP
2	B	268	ARG
2	B	273	LYS
2	B	276	GLU
2	B	278	LYS
2	B	289	GLU
2	B	290	THR
2	B	292	ASP
2	B	330	LEU
2	B	349	GLN
1	D	32	ARG
1	D	59	VAL
1	D	82	VAL
1	D	108	MET
1	D	193	ILE
1	D	194	CYS
1	D	195	SER
1	D	196	ARG
1	D	204	MET
1	D	242	LEU
1	D	273	LYS
1	D	279	SER
1	D	287	SER
1	D	289	GLU
1	D	292	ASP
2	F	27	THR
2	F	48	VAL
2	F	82	VAL
2	F	90	THR
2	F	94	GLU
2	F	158	ILE
2	F	181	LYS
2	F	184	VAL
2	F	246	ILE
2	F	248	ILE
2	F	265	THR
2	F	271	ASP

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Mol	Chain	Res	Type
2	F	273	LYS
2	F	279	SER
2	F	314	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	100	HIS
2	B	36	ASN
2	B	80	ASN
2	B	241	GLN
2	B	349	GLN
1	D	61	GLN
1	D	67	ASN
1	D	101	ASN
2	F	105	ASN
2	F	162	ASN
2	F	291	ASN
2	F	354	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
1	SEP	A	238	1	8,9,10	2.03	2 (25%)	8,12,14	3.30	4 (50%)
2	PTR	F	192	2	15,16,17	1.28	2 (13%)	19,22,24	0.53	0
1	SEP	D	238	1	8,9,10	1.71	1 (12%)	8,12,14	1.60	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	PTR	A	192	1	15,16,17	1.22	2 (13%)	19,22,24	0.77	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	SEP	A	238	1	-	1/5/8/10	-
2	PTR	F	192	2	-	2/10/11/13	0/1/1/1
1	SEP	D	238	1	-	4/5/8/10	-
1	PTR	A	192	1	-	2/10/11/13	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	192	PTR	OH-CZ	-4.18	1.31	1.40
1	A	238	SEP	P-O1P	3.88	1.63	1.50
1	D	238	SEP	P-O1P	3.57	1.62	1.50
1	A	192	PTR	OH-CZ	-3.55	1.32	1.40
1	A	238	SEP	P-OG	2.70	1.68	1.60
1	A	192	PTR	P-OH	2.70	1.63	1.59
2	F	192	PTR	P-OH	2.20	1.62	1.59

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	238	SEP	OG-CB-CA	5.95	113.94	108.14
1	A	238	SEP	P-OG-CB	4.44	130.53	118.30
1	A	238	SEP	O3P-P-OG	4.09	117.63	106.73
1	D	238	SEP	OG-CB-CA	3.78	111.82	108.14
1	A	238	SEP	OG-P-O1P	3.04	115.00	106.47
1	A	192	PTR	O3P-P-OH	2.48	113.01	105.24

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	192	PTR	C-CA-CB-CG
1	D	238	SEP	N-CA-CB-OG

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Mol	Chain	Res	Type	Atoms
1	D	238	SEP	CB-OG-P-O1P
1	D	238	SEP	CB-OG-P-O2P
1	D	238	SEP	CB-OG-P-O3P
2	F	192	PTR	N-CA-CB-CG
2	F	192	PTR	C-CA-CB-CG
1	A	192	PTR	N-CA-CB-CG
1	A	238	SEP	CA-CB-OG-P

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	238	SEP	1	0
2	F	192	PTR	1	0
1	D	238	SEP	1	0
1	A	192	PTR	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	$\# Z > 2$
4	PO4	B	401	-	4,4,4	0.87	0	6,6,6	0.47	0
3	A1IYF	D	402	-	41,44,44	3.34	12 (29%)	39,66,66	2.51	13 (33%)
3	A1IYF	F	401	-	41,44,44	2.57	15 (36%)	39,66,66	2.55	10 (25%)
3	A1IYF	A	401	-	41,44,44	2.68	15 (36%)	39,66,66	2.43	11 (28%)
3	A1IYF	B	402	-	41,44,44	2.97	19 (46%)	39,66,66	2.56	15 (38%)
4	PO4	D	401	-	4,4,4	0.96	0	6,6,6	0.33	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
3	A1IYF	B	402	-	-	0/6/49/49	0/6/7/7
3	A1IYF	F	401	-	-	1/6/49/49	0/6/7/7
3	A1IYF	D	402	-	-	1/6/49/49	0/6/7/7
3	A1IYF	A	401	-	-	1/6/49/49	0/6/7/7

All (61) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	A1IYF	C21-C19	-12.50	1.33	1.51
3	B	402	A1IYF	C21-C19	-9.19	1.37	1.51
3	D	402	A1IYF	C14-C15	8.53	1.49	1.42
3	A	401	A1IYF	C21-C19	-8.21	1.39	1.51
3	F	401	A1IYF	C21-C19	-7.68	1.40	1.51
3	D	402	A1IYF	C33-N32	6.86	1.39	1.33
3	B	402	A1IYF	C33-N32	6.39	1.39	1.33
3	B	402	A1IYF	C19-C20	-6.16	1.33	1.42
3	F	401	A1IYF	C05-N04	-5.89	1.36	1.47
3	D	402	A1IYF	C05-N04	-5.83	1.36	1.47
3	B	402	A1IYF	C14-C15	5.82	1.47	1.42
3	F	401	A1IYF	C11-N12	5.69	1.57	1.49
3	F	401	A1IYF	C14-C15	5.62	1.47	1.42
3	B	402	A1IYF	C38-C33	5.42	1.48	1.40
3	B	402	A1IYF	C07-N04	5.39	1.48	1.36
3	A	401	A1IYF	C07-N09	5.27	1.48	1.36
3	A	401	A1IYF	C05-N04	-5.15	1.37	1.47
3	A	401	A1IYF	C19-C20	-5.12	1.34	1.42
3	A	401	A1IYF	C14-C15	5.10	1.46	1.42
3	D	402	A1IYF	C13-N12	4.87	1.45	1.38
3	D	402	A1IYF	C19-C20	-4.72	1.35	1.42
3	D	402	A1IYF	C07-N04	4.55	1.46	1.36
3	D	402	A1IYF	C07-N09	4.43	1.46	1.36
3	A	401	A1IYF	C33-N32	4.41	1.37	1.33
3	A	401	A1IYF	C25-N27	3.94	1.46	1.38
3	F	401	A1IYF	C19-C20	-3.80	1.36	1.42
3	B	402	A1IYF	C03-N04	3.60	1.53	1.47
3	F	401	A1IYF	C33-N32	3.24	1.36	1.33
3	F	401	A1IYF	C13-N12	3.22	1.42	1.38
3	F	401	A1IYF	C38-C33	3.18	1.45	1.40
3	A	401	A1IYF	C28-N27	3.17	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	A1IYF	C38-C33	3.08	1.45	1.40
3	D	402	A1IYF	C28-N27	3.06	1.44	1.38
3	A	401	A1IYF	C21-N09	-3.05	1.41	1.46
3	A	401	A1IYF	C03-N04	3.02	1.52	1.47
3	B	402	A1IYF	C11-N12	2.98	1.54	1.49
3	F	401	A1IYF	C14-C23	-2.96	1.43	1.50
3	D	402	A1IYF	C03-N04	2.90	1.52	1.47
3	B	402	A1IYF	C35-N34	2.89	1.42	1.38
3	A	401	A1IYF	C07-N04	2.77	1.42	1.36
3	B	402	A1IYF	C14-C23	-2.71	1.44	1.50
3	F	401	A1IYF	C07-N09	2.64	1.42	1.36
3	A	401	A1IYF	C10-N09	-2.58	1.41	1.47
3	A	401	A1IYF	C11-N12	2.58	1.53	1.49
3	F	401	A1IYF	C25-N27	2.56	1.43	1.38
3	D	402	A1IYF	C11-N12	2.55	1.53	1.49
3	F	401	A1IYF	C10-C11	2.54	1.58	1.51
3	F	401	A1IYF	C28-N27	2.54	1.43	1.38
3	B	402	A1IYF	C37-C36	2.43	1.44	1.38
3	B	402	A1IYF	C13-N12	2.42	1.41	1.38
3	B	402	A1IYF	C10-C11	2.36	1.57	1.51
3	D	402	A1IYF	C30-C24	-2.26	1.45	1.49
3	F	401	A1IYF	C03-N04	2.23	1.51	1.47
3	F	401	A1IYF	C16-C17	2.17	1.39	1.36
3	B	402	A1IYF	C16-C15	-2.16	1.37	1.42
3	B	402	A1IYF	C05-N04	-2.12	1.43	1.47
3	B	402	A1IYF	C31-N32	2.12	1.41	1.36
3	B	402	A1IYF	C31-C30	2.12	1.41	1.37
3	B	402	A1IYF	C21-N09	-2.11	1.43	1.46
3	B	402	A1IYF	C07-N09	2.10	1.40	1.36
3	A	401	A1IYF	C31-N32	2.06	1.40	1.36

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	401	A1IYF	C10-C11-N12	10.98	120.05	111.17
3	A	401	A1IYF	C10-C11-N12	9.70	119.02	111.17
3	D	402	A1IYF	C10-C11-N12	9.68	119.00	111.17
3	B	402	A1IYF	C10-C11-N12	9.59	118.93	111.17
3	D	402	A1IYF	O08-C07-N09	-5.02	112.77	123.80
3	B	402	A1IYF	O08-C07-N09	-4.94	112.94	123.80
3	F	401	A1IYF	O08-C07-N09	-4.56	113.79	123.80
3	A	401	A1IYF	O08-C07-N04	-4.10	114.78	123.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	A1IYF	C11-N12-C13	-4.02	118.86	124.91
3	A	401	A1IYF	O08-C07-N09	-3.95	115.11	123.80
3	D	402	A1IYF	C02-C03-N04	3.95	118.46	110.66
3	A	401	A1IYF	C11-N12-C13	-3.79	119.21	124.91
3	D	402	A1IYF	C05-N04-C03	-3.68	105.55	112.62
3	F	401	A1IYF	O08-C07-N04	-3.58	115.94	123.80
3	A	401	A1IYF	C28-N27-C25	-3.56	107.53	111.29
3	D	402	A1IYF	C11-N12-C13	-3.52	119.61	124.91
3	B	402	A1IYF	O08-C07-N04	-3.51	116.09	123.80
3	B	402	A1IYF	C24-C25-N27	3.48	108.73	106.62
3	F	401	A1IYF	C28-N27-C25	-3.44	107.66	111.29
3	B	402	A1IYF	C19-C18-C17	-3.32	115.25	119.13
3	A	401	A1IYF	C05-N04-C03	-3.28	106.31	112.62
3	A	401	A1IYF	C19-C21-N09	3.25	119.71	113.26
3	F	401	A1IYF	C11-N12-C13	-3.22	120.06	124.91
3	B	402	A1IYF	C19-C21-N09	3.19	119.60	113.26
3	B	402	A1IYF	C05-N04-C03	-3.14	106.58	112.62
3	F	401	A1IYF	C02-C03-N04	3.10	116.79	110.66
3	D	402	A1IYF	C28-N27-C25	-3.10	108.01	111.29
3	F	401	A1IYF	C05-N04-C03	-2.95	106.95	112.62
3	D	402	A1IYF	C19-C18-C17	-2.94	115.69	119.13
3	F	401	A1IYF	C23-C28-N27	2.91	108.38	106.62
3	D	402	A1IYF	O08-C07-N04	-2.87	117.50	123.80
3	F	401	A1IYF	C19-C21-N09	2.84	118.91	113.26
3	D	402	A1IYF	C06-C05-N04	-2.84	105.05	110.66
3	B	402	A1IYF	C28-N27-C25	-2.83	108.30	111.29
3	A	401	A1IYF	C02-C03-N04	2.83	116.25	110.66
3	B	402	A1IYF	C30-C31-N32	2.78	114.83	109.11
3	B	402	A1IYF	C16-C17-C18	2.67	126.20	124.09
3	A	401	A1IYF	C23-C28-N27	2.66	108.24	106.62
3	D	402	A1IYF	C16-C17-C18	2.65	126.19	124.09
3	D	402	A1IYF	C19-C21-N09	2.63	118.48	113.26
3	F	401	A1IYF	C19-C18-C17	-2.63	116.06	119.13
3	B	402	A1IYF	O29-C28-C23	2.53	131.60	128.17
3	B	402	A1IYF	F22-C17-C16	-2.46	115.47	119.17
3	A	401	A1IYF	C17-C16-C15	-2.42	116.90	118.80
3	A	401	A1IYF	C14-C13-N12	2.25	112.73	108.49
3	D	402	A1IYF	C30-C31-N32	2.20	113.63	109.11
3	B	402	A1IYF	C03-N04-C07	2.17	130.04	121.14
3	B	402	A1IYF	C02-C03-N04	2.08	114.77	110.66
3	D	402	A1IYF	C24-C25-N27	2.00	107.84	106.62

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	A1IYF	N09-C07-N04-C03
3	D	402	A1IYF	N09-C07-N04-C03
3	F	401	A1IYF	N09-C07-N04-C03

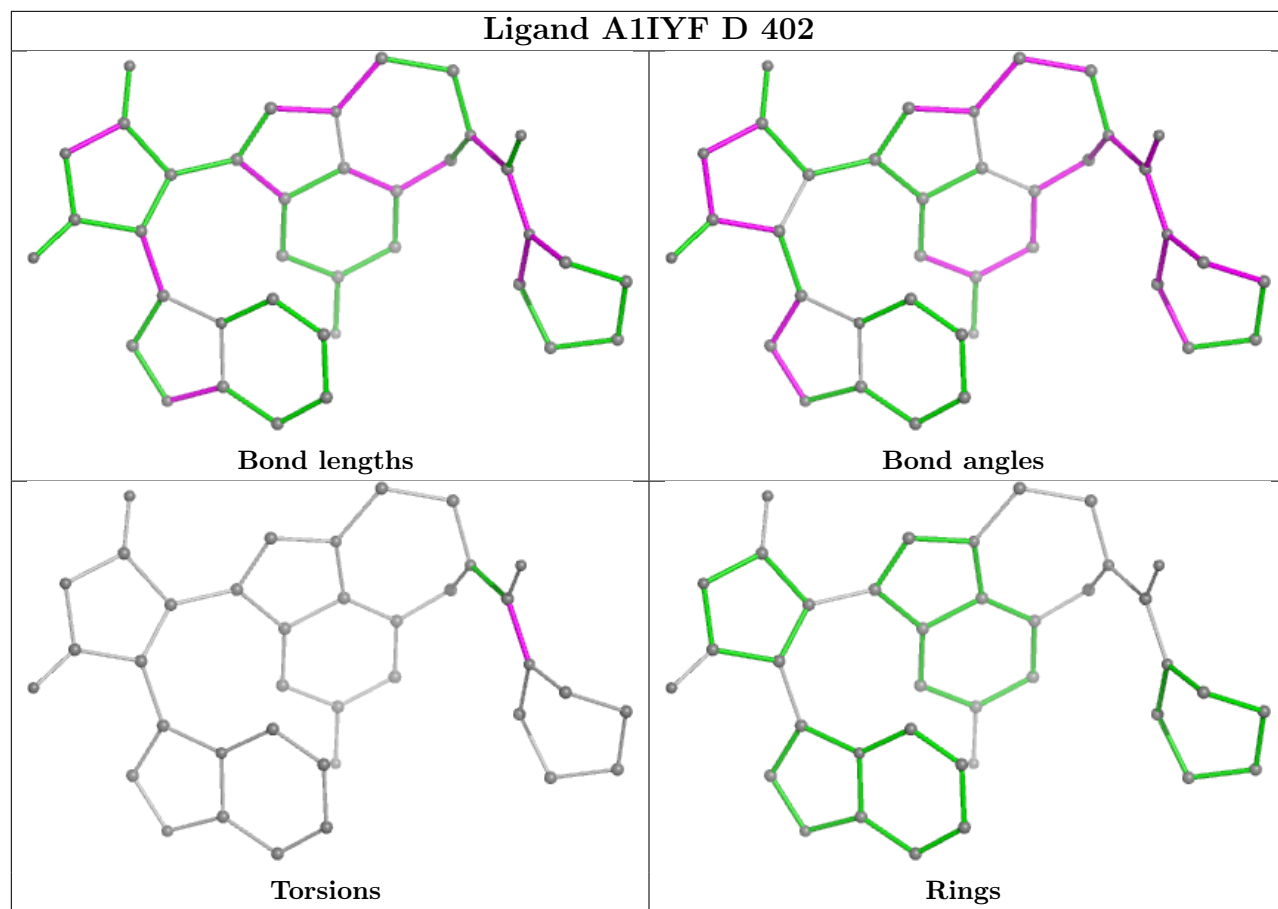
There are no ring outliers.

2 monomers are involved in 3 short contacts:

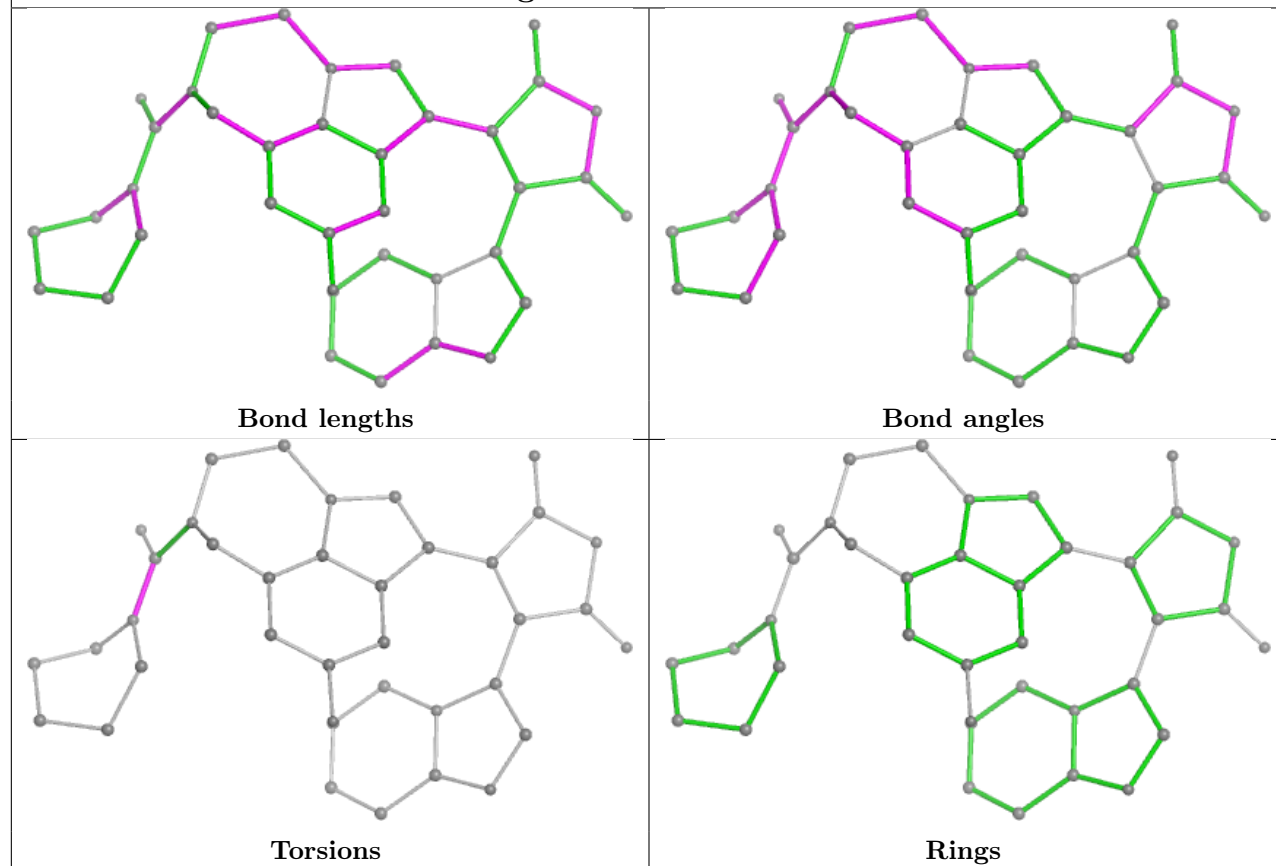
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	A1IYF	1	0
3	B	402	A1IYF	2	0

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.

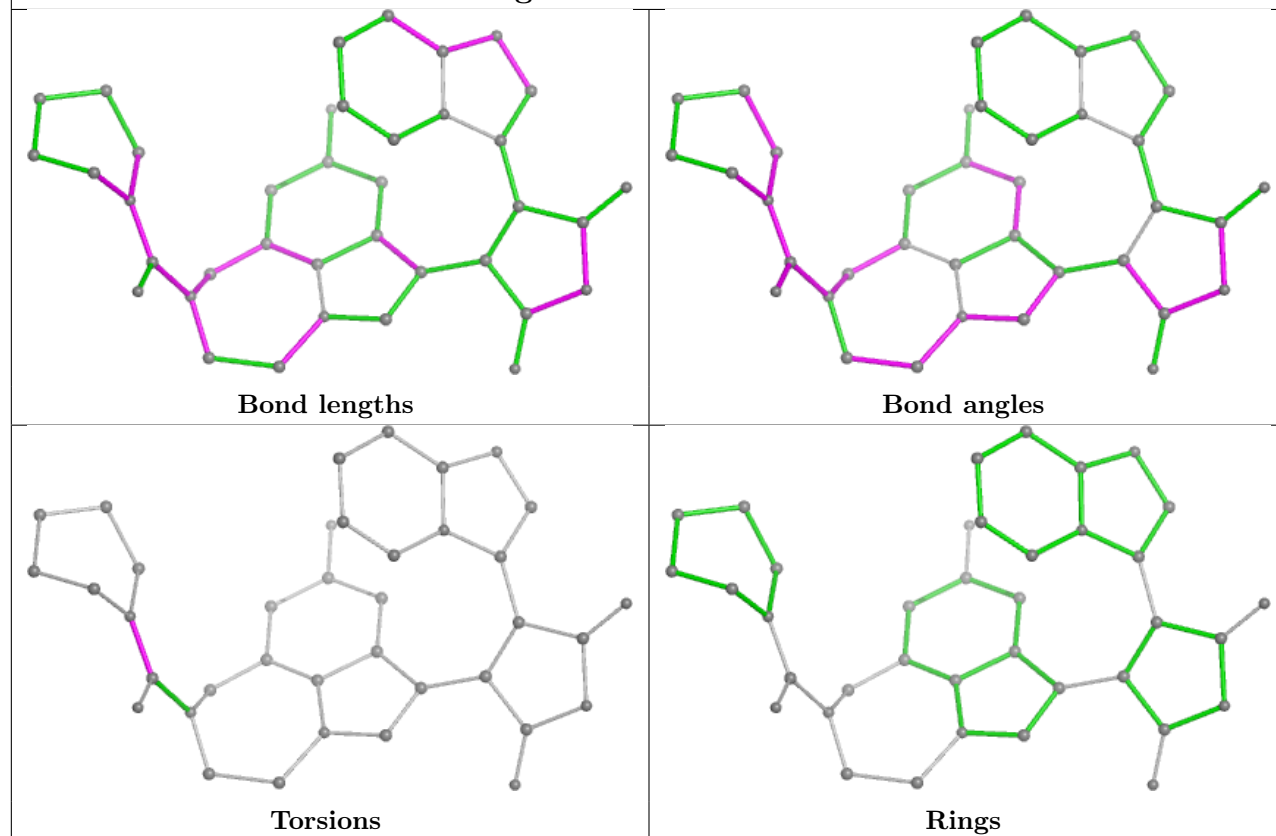
Ligand A1IYF D 402

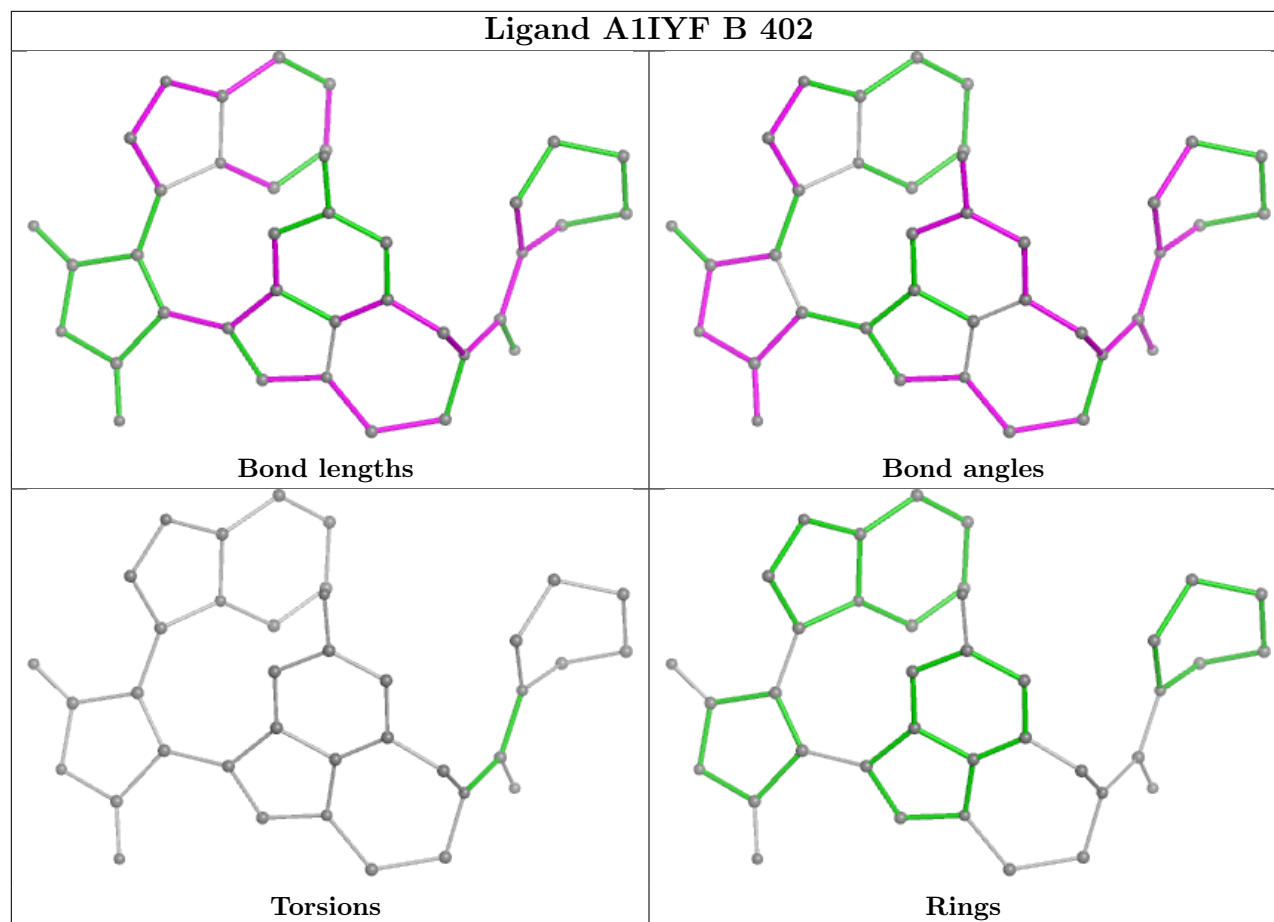


Ligand A1IYF F 401



Ligand A1IYF A 401





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	330/373 (88%)	0.04	14 (4%) 41 35	37, 52, 88, 115	0
1	D	326/373 (87%)	0.11	12 (3%) 45 39	35, 52, 86, 108	0
2	B	332/373 (89%)	0.19	15 (4%) 39 32	38, 55, 95, 118	0
2	F	324/373 (86%)	0.43	21 (6%) 26 22	42, 67, 99, 123	0
All	All	1312/1492 (87%)	0.19	62 (4%) 37 31	35, 56, 93, 123	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	39	PHE	4.6
1	D	99	ASP	4.2
2	F	270	PRO	4.0
1	D	196	ARG	3.7
2	F	290	THR	3.6
2	F	97	SER	3.5
1	D	39	PHE	3.5
1	D	62	ASP	3.4
1	A	291	ASN	3.2
1	D	365	PRO	3.1
2	F	246	ILE	3.1
2	F	89	TYR	3.1
1	A	162	ASN	3.1
2	F	265	THR	3.1
1	A	102	ARG	3.0
1	A	290	THR	3.0
2	F	269	PHE	2.9
2	F	183	LEU	2.8
2	F	267	PHE	2.8
1	A	193	ILE	2.8
2	F	37	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	39	PHE	2.7
1	A	292	ASP	2.7
1	A	98	ASN	2.7
1	D	193	ILE	2.7
1	A	196	ARG	2.6
1	A	206	GLY	2.6
2	B	270	PRO	2.6
2	F	38	SER	2.6
2	F	193	ILE	2.6
2	F	185	PRO	2.6
2	F	268	ARG	2.6
2	B	364	ILE	2.5
2	B	36	ASN	2.5
2	B	94	GLU	2.5
2	B	293	PRO	2.5
2	F	184	VAL	2.5
1	D	40	GLY	2.3
2	B	39	PHE	2.3
2	F	102	ARG	2.3
2	B	193	ILE	2.3
2	B	184	VAL	2.3
2	F	288	THR	2.3
1	A	90	THR	2.2
2	B	89	TYR	2.2
2	B	92	MET	2.2
1	D	195	SER	2.2
2	F	292	ASP	2.1
1	A	97	SER	2.1
1	A	208	SER	2.1
2	B	38	SER	2.1
2	B	290	THR	2.1
2	F	352	LEU	2.1
2	B	101	ASN	2.1
1	D	236	GLU	2.0
2	F	95	ARG	2.0
2	B	40	GLY	2.0
2	B	269	PHE	2.0
1	D	97	SER	2.0
1	D	94	GLU	2.0
1	D	269	PHE	2.0
1	A	100	HIS	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
2	PTR	F	192	16/17	0.68	0.15	105,112,115,115	0
1	PTR	A	192	16/17	0.73	0.17	87,96,104,105	0
1	SEP	A	238	10/11	0.81	0.14	50,59,71,80	0
1	SEP	D	238	10/11	0.83	0.12	66,76,89,92	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

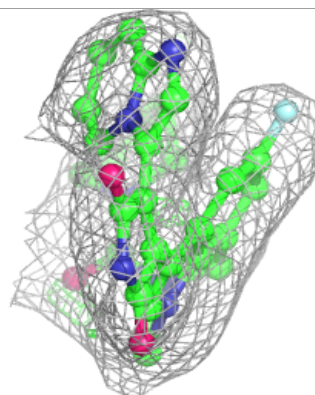
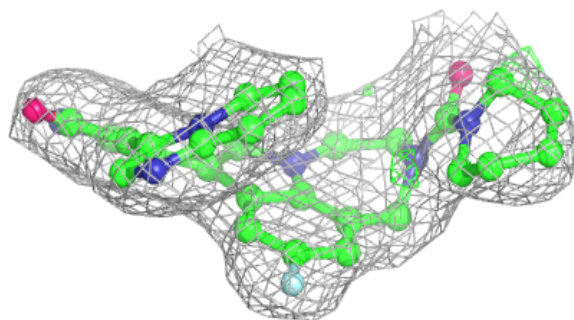
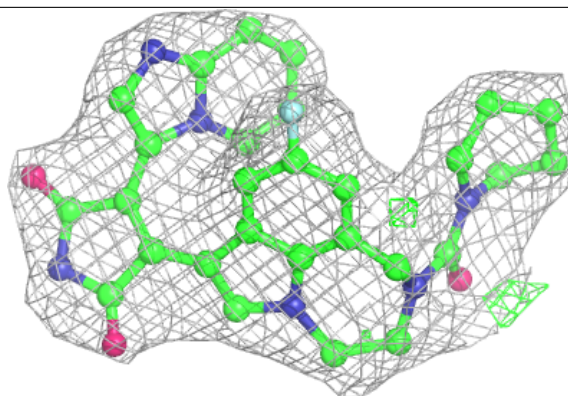
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	PO4	D	401	5/5	0.76	0.10	75,78,94,97	0
4	PO4	B	401	5/5	0.90	0.08	76,77,86,94	0
3	A1IYF	F	401	38/38	0.94	0.10	40,47,53,55	0
3	A1IYF	D	402	38/38	0.95	0.09	31,39,43,47	0
3	A1IYF	B	402	38/38	0.95	0.08	35,42,49,50	0
3	A1IYF	A	401	38/38	0.96	0.09	34,41,46,50	0

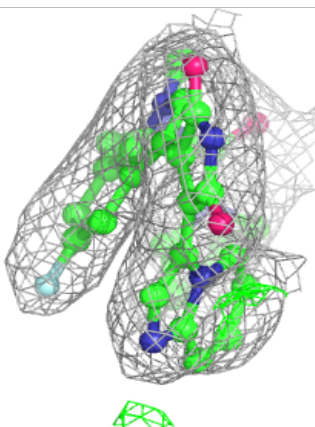
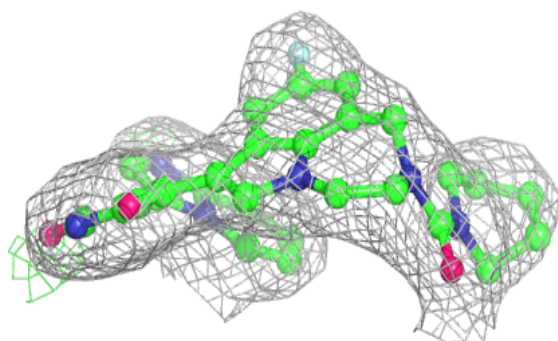
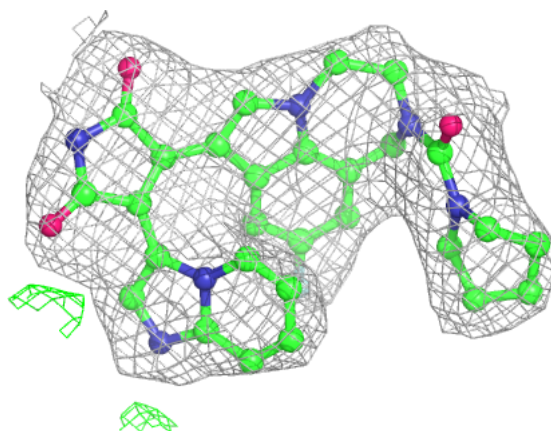
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1IYF F 401:

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

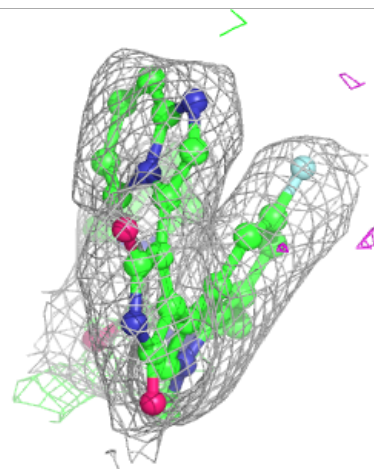
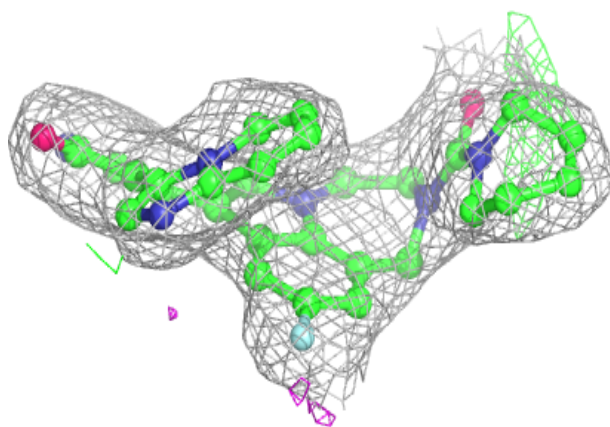
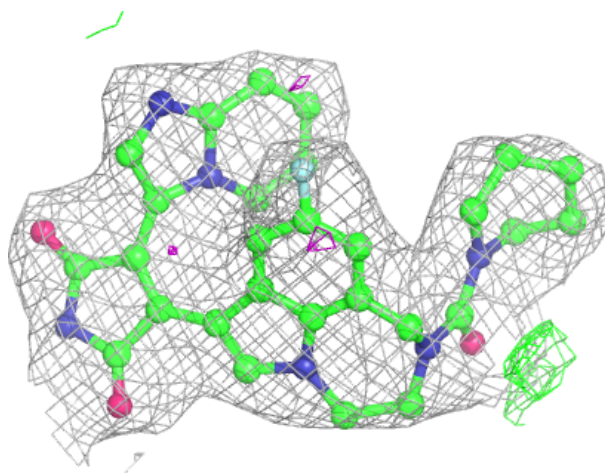
**Electron density around A1IYF D 402:**

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



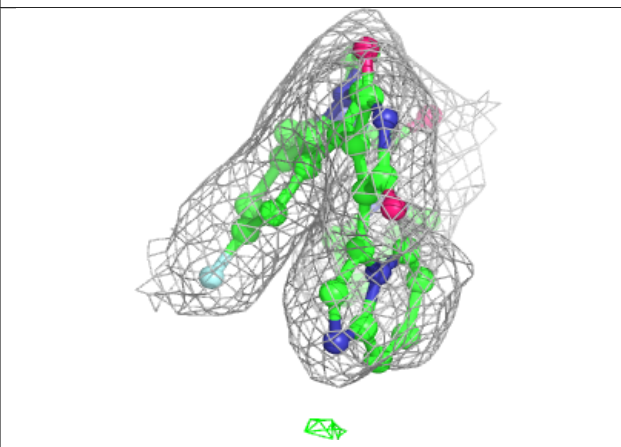
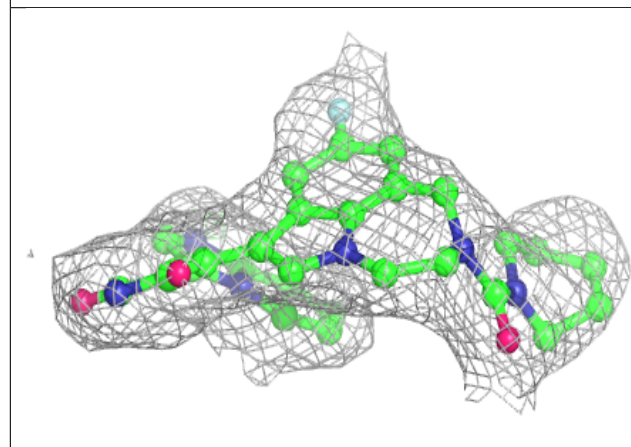
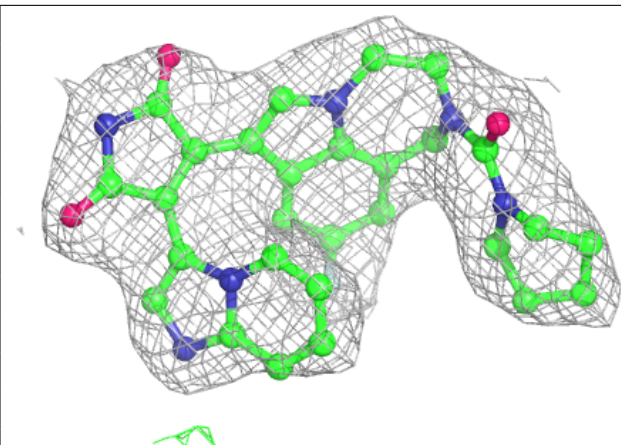
Electron density around A1IYF B 402:

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



Electron density around A1IYF A 401:

$2mF_o - DF_c$ (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.