



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:26 AM UTC

PDB ID : 4Y73 / pdb_00004y73
Title : Crystal structure of IRAK4 kinase domain with inhibitor
Authors : Lesburg, C.A.
Deposited on : 2015-02-13
Resolution : 2.14 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

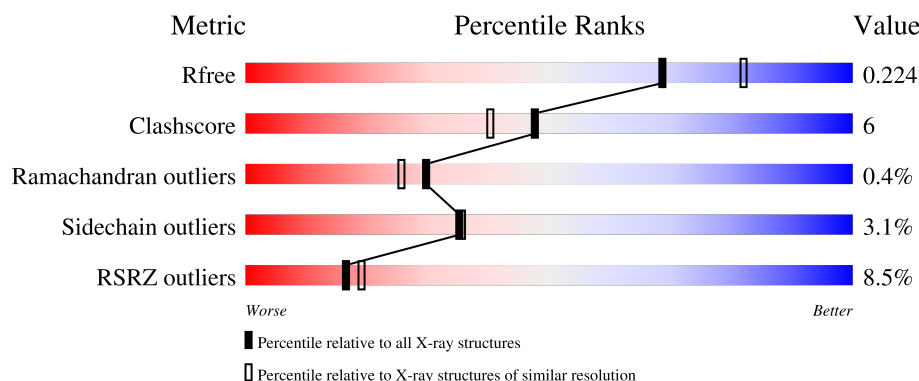
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.14 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	3689 (2.16-2.12)
Clashscore	190562	3812 (2.16-2.12)
Ramachandran outliers	187476	3773 (2.16-2.12)
Sidechain outliers	187428	3772 (2.16-2.12)
RSRZ outliers	180081	3691 (2.16-2.12)

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	302	5% 85% 10% ..
1	B	302	7% 84% 12% ..
1	C	302	11% 82% 14% ..
1	D	302	10% 84% 11% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9744 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.

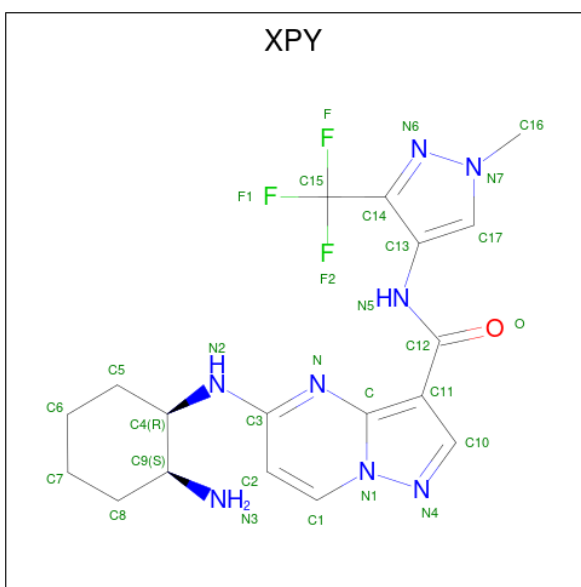
- Molecule 1 is a protein called Interleukin-1 receptor-associated kinase 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	P	S	0	1	0
			2310	1446	387	458	3	16			
1	B	292	Total	C	N	O	P	S	0	0	0
			2305	1442	386	459	3	15			
1	C	293	Total	C	N	O	P	S	0	0	0
			2310	1445	387	460	3	15			
1	D	291	Total	C	N	O	P	S	0	1	0
			2304	1442	386	458	3	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	159	GLY	-	expression tag	UNP Q9NWZ3
B	159	GLY	-	expression tag	UNP Q9NWZ3
C	159	GLY	-	expression tag	UNP Q9NWZ3
D	159	GLY	-	expression tag	UNP Q9NWZ3

- Molecule 2 is 5-([(1R,2S)-2-aminocyclohexyl]amino)-N-[1-methyl-3-(trifluoromethyl)-1H-pyrazol-4-yl]pyrazolo[1,5-a]pyrimidine-3-carboxamide (CCD ID: XPY) (formula: C₁₈H₂₁F₃N₈O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			30	18	3	8	1		
2	B	1	Total	C	F	N	O	0	0
			30	18	3	8	1		
2	C	1	Total	C	F	N	O	0	0
			30	18	3	8	1		
2	D	1	Total	C	F	N	O	0	0
			30	18	3	8	1		

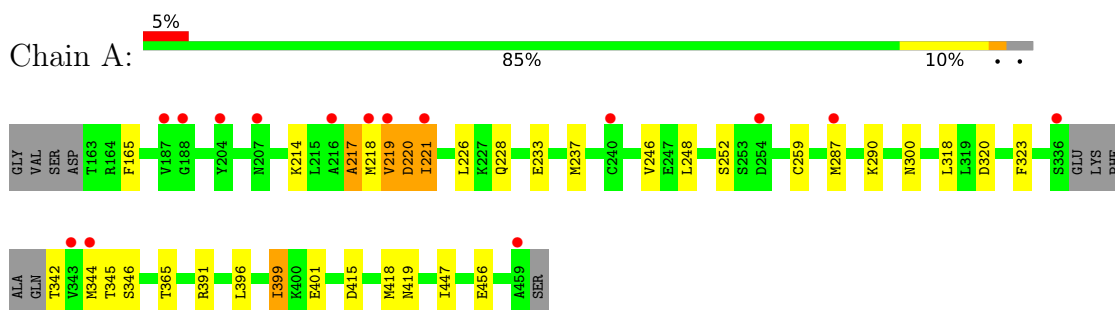
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	98	Total	O	0	0
			98	98		
3	B	86	Total	O	0	0
			86	86		
3	C	105	Total	O	0	0
			105	105		
3	D	106	Total	O	0	0
			106	106		

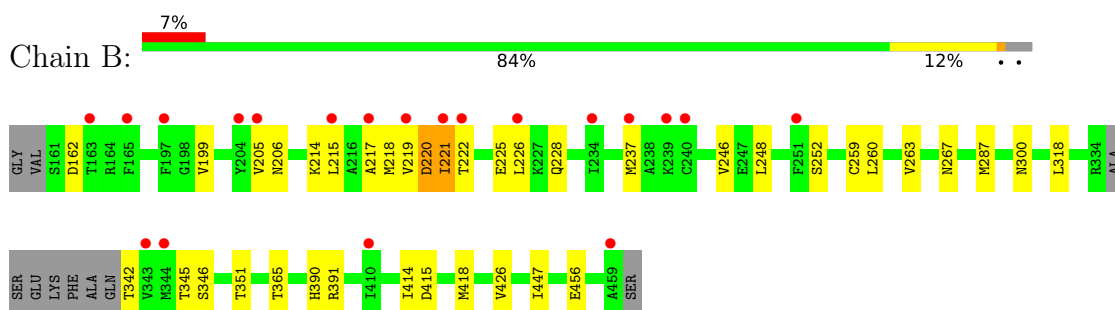
3 Residue-property plots [i](#)

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.

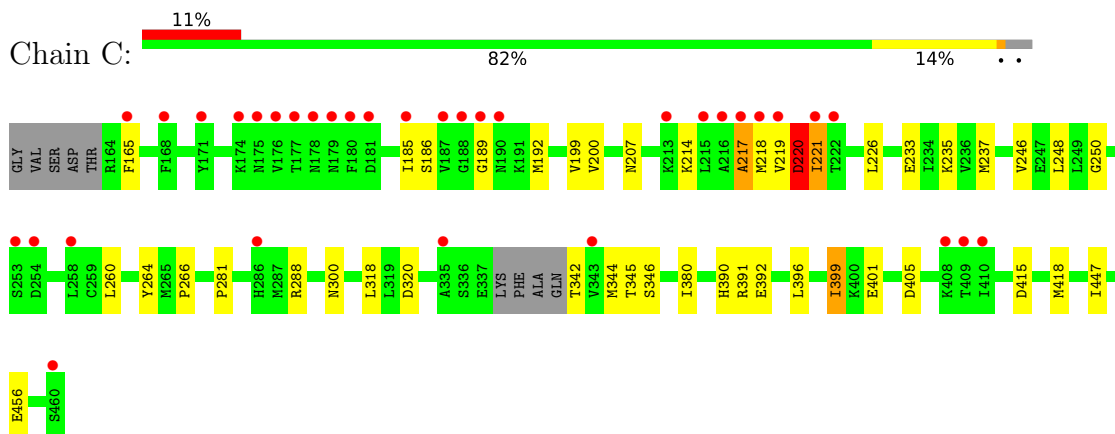
- Molecule 1: Interleukin-1 receptor-associated kinase 4



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



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



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



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	142.86Å 138.75Å 88.02Å 90.00° 124.59° 90.00°	Depositor
Resolution (Å)	74.24 – 2.14 74.24 – 2.14	Depositor EDS
% Data completeness (in resolution range)	99.2 (74.24-2.14) 99.3 (74.24-2.14)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.14Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.195 , 0.217 0.201 , 0.224	Depositor DCC
R_{free} test set	3869 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.504	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9744	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.93% 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: TPO, XPY, SEP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.83	0/2315	1.30	9/3120 (0.3%)
1	B	0.85	0/2310	1.31	8/3114 (0.3%)
1	C	0.85	0/2315	1.33	9/3120 (0.3%)
1	D	0.84	0/2309	1.30	8/3112 (0.3%)
All	All	0.84	0/9249	1.31	34/12466 (0.3%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	220	ASP	CA-C-N	7.12	134.51	121.70
1	B	220	ASP	C-N-CA	7.12	134.51	121.70
1	A	220	ASP	CA-C-N	7.00	134.30	121.70
1	A	220	ASP	C-N-CA	7.00	134.30	121.70
1	C	220	ASP	CA-CB-CG	6.92	119.52	112.60
1	C	217	ALA	CA-C-N	6.90	134.13	121.70
1	C	217	ALA	C-N-CA	6.90	134.13	121.70
1	D	220	ASP	CA-C-N	6.46	133.34	121.70
1	D	220	ASP	C-N-CA	6.46	133.34	121.70
1	A	456	GLU	CA-C-N	6.07	128.70	120.38
1	A	456	GLU	C-N-CA	6.07	128.70	120.38
1	D	320	ASP	CA-CB-CG	5.83	118.43	112.60
1	C	220	ASP	CA-C-N	5.74	132.04	121.70
1	C	220	ASP	C-N-CA	5.74	132.04	121.70
1	D	405	ASP	CA-C-N	5.63	130.35	122.08
1	D	405	ASP	C-N-CA	5.63	130.35	122.08
1	B	456	GLU	CA-C-N	5.57	128.31	120.28
1	B	456	GLU	C-N-CA	5.57	128.31	120.28
1	C	405	ASP	CA-C-N	5.49	130.15	122.08
1	C	405	ASP	C-N-CA	5.49	130.15	122.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	263	VAL	N-CA-C	-5.47	102.47	109.30
1	C	456	GLU	CA-C-N	5.44	128.12	120.28
1	C	456	GLU	C-N-CA	5.44	128.12	120.28
1	B	267	ASN	CA-CB-CG	-5.40	107.20	112.60
1	A	320	ASP	CA-CB-CG	5.29	117.89	112.60
1	D	220	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	165	PHE	CA-C-N	5.22	128.28	120.87
1	A	165	PHE	C-N-CA	5.22	128.28	120.87
1	D	456	GLU	CA-C-N	5.18	127.22	120.28
1	D	456	GLU	C-N-CA	5.18	127.22	120.28
1	A	217	ALA	CA-C-N	5.14	130.95	121.70
1	A	217	ALA	C-N-CA	5.14	130.95	121.70
1	B	351	THR	CA-C-N	5.04	128.38	120.82
1	B	351	THR	C-N-CA	5.04	128.38	120.82

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	2310	0	2274	21	0
1	B	2305	0	2265	30	0
1	C	2310	0	2270	30	0
1	D	2304	0	2264	31	0
2	A	30	0	21	0	0
2	B	30	0	21	0	0
2	C	30	0	21	0	0
2	D	30	0	21	0	0
3	A	98	0	0	1	0
3	B	86	0	0	1	0
3	C	105	0	0	0	0
3	D	106	0	0	0	0
All	All	9744	0	9157	103	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 6.

All (103) 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:B:221:ILE:HG21	1:B:226:LEU:HD11	1.34	1.08
1:D:217:ALA:HA	1:D:218:MET:HB3	1.33	1.06
1:B:222:THR:HB	1:B:225:GLU:HG3	1.44	0.95
1:B:217:ALA:HA	1:B:218:MET:CB	1.95	0.95
1:C:217:ALA:HA	1:C:218:MET:HB2	1.49	0.95
1:A:217:ALA:HA	1:A:218:MET:CB	1.98	0.93
1:C:220:ASP:HB3	1:C:221:ILE:HA	1.50	0.93
1:D:266:PRO:HG2	1:D:321[A]:GLU:HG3	1.55	0.89
1:B:221:ILE:HG21	1:B:226:LEU:CD1	2.02	0.89
1:A:287[B]:MET:HE1	1:A:290:LYS:HD3	1.59	0.84
1:B:221:ILE:CG2	1:B:226:LEU:CD1	2.56	0.83
1:B:217:ALA:HA	1:B:218:MET:HB3	1.61	0.82
1:D:180:PHE:CD2	1:D:214:LYS:HD2	2.15	0.80
1:A:217:ALA:HA	1:A:218:MET:HB3	1.63	0.80
1:B:221:ILE:CG2	1:B:226:LEU:HD11	2.12	0.80
1:B:237:MET:HE1	1:B:246:VAL:HG23	1.67	0.75
1:D:237:MET:HE1	1:D:246:VAL:HG23	1.73	0.70
1:D:287:MET:HE3	1:D:287:MET:HA	1.72	0.70
1:B:217:ALA:HA	1:B:218:MET:HB2	1.75	0.69
1:C:237:MET:HE1	1:C:246:VAL:HG23	1.75	0.67
1:B:390:HIS:O	1:C:391:ARG:HA	1.94	0.67
1:D:217:ALA:HA	1:D:218:MET:CB	2.15	0.66
1:B:287:MET:HG3	3:B:1116:HOH:O	1.96	0.65
1:A:217:ALA:HA	1:A:218:MET:HB2	1.76	0.65
1:C:220:ASP:HB2	1:C:221:ILE:HG13	1.79	0.65
1:B:391:ARG:HA	1:C:390:HIS:O	1.98	0.64
1:A:217:ALA:HB3	1:A:221:ILE:CG2	2.28	0.62
1:D:174:LYS:HG2	1:D:180:PHE:HE1	1.63	0.62
1:B:217:ALA:HB3	1:B:221:ILE:HG21	1.82	0.61
1:A:220:ASP:HB2	1:A:221:ILE:HG13	1.81	0.61
1:D:217:ALA:HB3	1:D:221:ILE:HG21	1.81	0.60
1:C:217:ALA:HA	1:C:218:MET:CB	2.30	0.60
1:B:246:VAL:HG11	1:B:318:LEU:HD12	1.84	0.60
1:B:217:ALA:HB3	1:B:221:ILE:CG2	2.33	0.59
1:A:217:ALA:HB3	1:A:221:ILE:HG21	1.84	0.58
1:C:233:GLU:HG2	1:C:260:LEU:HD13	1.85	0.58
1:C:217:ALA:HB3	1:C:221:ILE:HG21	1.85	0.58
1:C:220:ASP:CB	1:C:221:ILE:HA	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:ILE:HG23	1:B:226:LEU:CD1	2.35	0.56
1:B:237:MET:HE3	1:B:248:LEU:HB2	1.86	0.56
1:B:220:ASP:HB2	1:B:221:ILE:HG13	1.88	0.56
1:C:281:PRO:HD3	1:D:321[B]:GLU:HG2	1.88	0.56
1:B:220:ASP:HB2	1:B:221:ILE:HA	1.89	0.55
1:D:220:ASP:OD2	1:D:225:GLU:OE2	2.24	0.55
1:A:419:ASN:HB2	1:D:186:SER:CB	2.36	0.55
1:C:207:ASN:HA	1:D:187:VAL:HG23	1.90	0.54
1:C:220:ASP:HB3	1:C:221:ILE:CA	2.32	0.53
1:C:237:MET:HE3	1:C:248:LEU:HB2	1.91	0.52
1:C:396:LEU:HD12	1:C:399:ILE:HD13	1.91	0.52
1:D:246:VAL:HG11	1:D:318:LEU:HD12	1.92	0.52
1:A:396:LEU:HD12	1:A:399:ILE:HD13	1.92	0.52
1:A:220:ASP:HB2	1:A:221:ILE:HA	1.92	0.51
1:D:173:LEU:HA	1:D:176:VAL:HG22	1.92	0.51
1:B:221:ILE:CG2	1:B:226:LEU:HD13	2.40	0.51
1:A:419:ASN:HB2	1:D:186:SER:HB3	1.92	0.50
1:D:217:ALA:HB3	1:D:221:ILE:CG2	2.41	0.49
1:B:221:ILE:HG23	1:B:226:LEU:HD13	1.94	0.48
1:D:174:LYS:HG2	1:D:180:PHE:CE1	2.46	0.48
1:B:225:GLU:O	1:B:228:GLN:HB3	2.14	0.48
1:C:217:ALA:HB3	1:C:221:ILE:CG2	2.43	0.48
1:D:237:MET:HE3	1:D:248:LEU:HB2	1.94	0.48
1:A:246:VAL:HG11	1:A:318:LEU:HD12	1.96	0.48
1:D:183:ARG:HB2	1:D:189:GLY:HA3	1.95	0.48
1:A:237:MET:HG2	1:A:248:LEU:CB	2.44	0.47
1:A:391:ARG:HD3	3:A:1162:HOH:O	2.14	0.47
1:C:220:ASP:CB	1:C:221:ILE:HG13	2.44	0.47
1:D:227:LYS:HG2	1:D:258:LEU:HD11	1.97	0.47
1:D:217:ALA:CA	1:D:218:MET:HB3	2.24	0.46
1:B:215:LEU:HD11	1:B:260:LEU:HD12	1.97	0.46
1:D:321[A]:GLU:H	1:D:321[A]:GLU:CD	2.25	0.45
1:B:300:ASN:HA	1:B:447:ILE:HG21	1.99	0.44
1:C:415:ASP:HB3	1:C:418:MET:HE2	1.99	0.44
1:D:183:ARG:HB3	1:D:187:VAL:CG1	2.48	0.44
1:A:287[B]:MET:HE2	1:A:323:PHE:CB	2.48	0.44
1:A:287[B]:MET:HE2	1:A:323:PHE:HB3	2.00	0.44
1:A:300:ASN:HA	1:A:447:ILE:HG21	1.99	0.44
1:B:390:HIS:HB3	1:C:392:GLU:H	1.83	0.44
1:C:185:ILE:HD13	1:C:189:GLY:O	2.17	0.43
1:B:415:ASP:HB3	1:B:418:MET:HE2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:287:MET:HA	1:D:287:MET:CE	2.46	0.43
1:A:237:MET:HG2	1:A:248:LEU:HB2	2.00	0.43
1:D:217:ALA:HB1	1:D:219:VAL:H	1.83	0.43
1:D:237:MET:CE	1:D:246:VAL:HG23	2.47	0.43
1:C:192:MET:SD	1:C:264:TYR:HE1	2.41	0.42
1:C:281:PRO:CD	1:D:321[B]:GLU:HG2	2.49	0.42
1:C:300:ASN:HA	1:C:447:ILE:HG21	2.01	0.42
1:B:217:ALA:CA	1:B:218:MET:CB	2.82	0.42
1:B:414:ILE:HG12	1:B:426:VAL:HG11	2.01	0.42
1:C:246:VAL:HG11	1:C:318:LEU:HD12	2.02	0.42
1:A:252:SER:HB3	1:A:259:CYS:HB2	2.02	0.42
1:C:192:MET:HE3	1:C:200:VAL:HG12	2.02	0.42
1:D:191:LYS:HA	1:D:201:TYR:HD1	1.85	0.42
1:C:165:PHE:HB3	1:C:250:GLY:HA2	2.02	0.42
1:B:252:SER:HB3	1:B:259:CYS:HB2	2.00	0.41
1:C:221:ILE:HG21	1:C:226:LEU:HD13	2.02	0.41
1:C:281:PRO:HD3	1:D:321[B]:GLU:CG	2.49	0.41
1:D:220:ASP:CG	1:D:221:ILE:HA	2.46	0.41
1:D:300:ASN:HA	1:D:447:ILE:HG21	2.01	0.41
1:A:415:ASP:HB3	1:A:418:MET:HE2	2.03	0.41
1:B:205:VAL:HG23	1:B:206:ASN:H	1.86	0.41
1:C:266:PRO:HD2	1:C:320:ASP:HA	2.04	0.41
1:C:288:ARG:HB3	1:C:380:ILE:HG23	2.03	0.40
1:A:221:ILE:HG21	1:A:226:LEU:HD13	2.03	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	287/302 (95%)	277 (96%)	9 (3%)	1 (0%)	36 33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	286/302 (95%)	272 (95%)	13 (4%)	1 (0%)	36	33
1	C	287/302 (95%)	275 (96%)	10 (4%)	2 (1%)	18	13
1	D	286/302 (95%)	272 (95%)	13 (4%)	1 (0%)	36	33
All	All	1146/1208 (95%)	1096 (96%)	45 (4%)	5 (0%)	30	26

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	219	VAL
1	B	219	VAL
1	C	219	VAL
1	C	220	ASP
1	D	218	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	252/259 (97%)	243 (96%)	9 (4%)	31	30
1	B	252/259 (97%)	247 (98%)	5 (2%)	48	53
1	C	252/259 (97%)	243 (96%)	9 (4%)	31	30
1	D	251/259 (97%)	242 (96%)	9 (4%)	31	30
All	All	1007/1036 (97%)	975 (97%)	32 (3%)	35	35

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	LYS
1	A	219	VAL
1	A	221	ILE
1	A	228	GLN
1	A	233	GLU
1	A	344	MET

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Mol	Chain	Res	Type
1	A	365	THR
1	A	399	ILE
1	A	401	GLU
1	B	162	ASP
1	B	199	VAL
1	B	214	LYS
1	B	221	ILE
1	B	365	THR
1	C	186	SER
1	C	199	VAL
1	C	214	LYS
1	C	220	ASP
1	C	221	ILE
1	C	235	LYS
1	C	344	MET
1	C	399	ILE
1	C	401	GLU
1	D	174	LYS
1	D	226	LEU
1	D	287	MET
1	D	321[A]	GLU
1	D	321[B]	GLU
1	D	365	THR
1	D	401	GLU
1	D	418	MET
1	D	439	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	229	GLN
1	A	451	GLN
1	B	166	HIS
1	B	244	ASN
1	B	451	GLN
1	C	175	ASN
1	C	207	ASN
1	C	228	GLN
1	C	286	HIS
1	C	307	HIS
1	C	451	GLN
1	D	229	GLN

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Mol	Chain	Res	Type
1	D	232	GLN
1	D	419	ASN
1	D	451	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

12 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	TPO	D	345	1	8,10,11	1.26	1 (12%)	10,14,16	1.53	1 (10%)
1	TPO	B	345	1	8,10,11	1.00	0	10,14,16	1.40	1 (10%)
1	SEP	A	346	1	8,9,10	0.72	0	7,12,14	1.24	1 (14%)
1	TPO	A	342	1	8,10,11	1.20	0	10,14,16	1.20	1 (10%)
1	TPO	C	345	1	8,10,11	1.31	2 (25%)	10,14,16	1.20	0
1	SEP	D	346	1	8,9,10	0.98	0	7,12,14	1.06	0
1	TPO	D	342	1	8,10,11	1.23	1 (12%)	10,14,16	1.09	1 (10%)
1	SEP	B	346	1	8,9,10	1.12	1 (12%)	7,12,14	1.03	0
1	TPO	A	345	1	8,10,11	1.20	1 (12%)	10,14,16	1.47	1 (10%)
1	TPO	B	342	1	8,10,11	1.09	0	10,14,16	1.24	1 (10%)
1	SEP	C	346	1	8,9,10	0.94	0	7,12,14	1.14	1 (14%)
1	TPO	C	342	1	8,10,11	1.18	1 (12%)	10,14,16	1.06	1 (10%)

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	TPO	D	345	1	-	3/9/11/13	-
1	TPO	B	345	1	-	3/9/11/13	-
1	SEP	A	346	1	-	0/6/8/10	-
1	TPO	A	342	1	-	1/9/11/13	-
1	TPO	C	345	1	-	3/9/11/13	-
1	SEP	D	346	1	-	0/6/8/10	-
1	TPO	D	342	1	-	1/9/11/13	-
1	SEP	B	346	1	-	0/6/8/10	-
1	TPO	A	345	1	-	5/9/11/13	-
1	TPO	B	342	1	-	1/9/11/13	-
1	SEP	C	346	1	-	0/6/8/10	-
1	TPO	C	342	1	-	1/9/11/13	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	342	TPO	P-OG1	-2.47	1.55	1.59
1	D	342	TPO	P-OG1	-2.41	1.55	1.59
1	C	345	TPO	CB-CA	2.36	1.58	1.53
1	B	346	SEP	P-O1P	2.22	1.57	1.50
1	A	345	TPO	CB-CA	2.10	1.58	1.53
1	D	345	TPO	P-OG1	-2.06	1.55	1.59
1	C	345	TPO	CG2-CB	2.04	1.56	1.51

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	345	TPO	O3P-P-OG1	3.39	119.07	105.85
1	A	345	TPO	P-OG1-CB	-2.40	116.81	123.33
1	A	342	TPO	P-OG1-CB	-2.34	116.97	123.33
1	B	345	TPO	O3P-P-OG1	2.30	114.81	105.85
1	D	342	TPO	P-OG1-CB	-2.29	117.10	123.33
1	B	342	TPO	P-OG1-CB	-2.22	117.30	123.33
1	C	346	SEP	OG-CB-CA	2.19	110.28	108.14
1	C	342	TPO	P-OG1-CB	-2.11	117.60	123.33
1	A	346	SEP	OG-CB-CA	2.07	110.16	108.14

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	O-C-CA-CB
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB
1	C	345	TPO	N-CA-CB-OG1
1	C	345	TPO	O-C-CA-CB
1	D	345	TPO	N-CA-CB-OG1
1	D	345	TPO	O-C-CA-CB
1	A	345	TPO	CB-OG1-P-O1P
1	B	345	TPO	CB-OG1-P-O1P
1	D	345	TPO	CB-OG1-P-O1P
1	A	345	TPO	CB-OG1-P-O2P
1	A	345	TPO	CB-OG1-P-O3P
1	C	345	TPO	CB-OG1-P-O2P
1	A	342	TPO	O-C-CA-CB
1	B	342	TPO	O-C-CA-CB
1	C	342	TPO	O-C-CA-CB
1	D	342	TPO	C-CA-CB-CG2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	XPY	A	1000	-	30,33,33	1.14	3 (10%)	37,49,49	1.40	7 (18%)
2	XPY	C	1000	-	30,33,33	1.16	4 (13%)	37,49,49	1.31	6 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	XPY	B	1000	-	30,33,33	1.32	6 (20%)	37,49,49	1.45	8 (21%)
2	XPY	D	1000	-	30,33,33	1.22	4 (13%)	37,49,49	1.41	8 (21%)

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	XPY	A	1000	-	-	0/18/29/29	0/4/4/4
2	XPY	C	1000	-	-	0/18/29/29	0/4/4/4
2	XPY	B	1000	-	-	0/18/29/29	0/4/4/4
2	XPY	D	1000	-	-	0/18/29/29	0/4/4/4

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	XPY	C17-C13	3.77	1.42	1.36
2	D	1000	XPY	C17-C13	3.22	1.41	1.36
2	C	1000	XPY	C17-C13	3.07	1.41	1.36
2	A	1000	XPY	C17-C13	3.06	1.41	1.36
2	C	1000	XPY	C4-N2	2.90	1.51	1.46
2	D	1000	XPY	C3-N	2.90	1.37	1.32
2	A	1000	XPY	C4-N2	2.86	1.51	1.46
2	D	1000	XPY	C4-N2	2.78	1.50	1.46
2	B	1000	XPY	C4-N2	2.74	1.50	1.46
2	C	1000	XPY	C3-N	2.69	1.37	1.32
2	B	1000	XPY	C3-N	2.44	1.36	1.32
2	A	1000	XPY	C3-N	2.36	1.36	1.32
2	B	1000	XPY	C1-N1	2.24	1.41	1.37
2	D	1000	XPY	N1-N4	-2.13	1.33	1.37
2	B	1000	XPY	C10-N4	2.12	1.36	1.32
2	B	1000	XPY	C2-C3	2.10	1.45	1.41
2	C	1000	XPY	N1-N4	-2.03	1.33	1.37

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1000	XPY	C2-C3-N2	-3.71	114.24	122.40
2	B	1000	XPY	C2-C3-N2	-3.69	114.29	122.40
2	D	1000	XPY	C15-C14-N6	3.54	122.69	118.50
2	A	1000	XPY	C15-C14-N6	3.53	122.69	118.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1000	XPY	C15-C14-N6	3.51	122.66	118.50
2	D	1000	XPY	C11-C-N	3.41	132.82	123.54
2	A	1000	XPY	C2-C3-N2	-3.35	115.03	122.40
2	C	1000	XPY	C2-C3-N2	-3.33	115.08	122.40
2	A	1000	XPY	C11-C-N	3.33	132.59	123.54
2	B	1000	XPY	C11-C-N	3.24	132.36	123.54
2	C	1000	XPY	C11-C-N	3.22	132.30	123.54
2	B	1000	XPY	C5-C4-N2	-2.79	106.18	110.69
2	C	1000	XPY	C5-C4-N2	-2.77	106.22	110.69
2	B	1000	XPY	C10-N4-N1	2.70	106.45	103.81
2	A	1000	XPY	C5-C4-N2	-2.66	106.40	110.69
2	C	1000	XPY	C15-C14-N6	2.57	121.55	118.50
2	B	1000	XPY	C2-C3-N	2.50	126.50	122.60
2	A	1000	XPY	C2-C3-N	2.43	126.39	122.60
2	C	1000	XPY	C10-N4-N1	2.41	106.16	103.81
2	C	1000	XPY	C2-C3-N	2.39	126.34	122.60
2	D	1000	XPY	C2-C3-N	2.38	126.32	122.60
2	D	1000	XPY	C10-N4-N1	2.30	106.06	103.81
2	B	1000	XPY	C15-C14-C13	-2.20	126.16	130.22
2	D	1000	XPY	C15-C14-C13	-2.14	126.27	130.22
2	D	1000	XPY	C10-C11-C12	-2.11	123.32	129.45
2	B	1000	XPY	C10-C11-C12	-2.08	123.41	129.45
2	A	1000	XPY	C9-C4-N2	2.07	113.90	109.94
2	D	1000	XPY	C3-N-C	-2.03	114.30	117.18
2	A	1000	XPY	C10-C11-C12	-2.01	123.62	129.45

There are no chirality outliers.

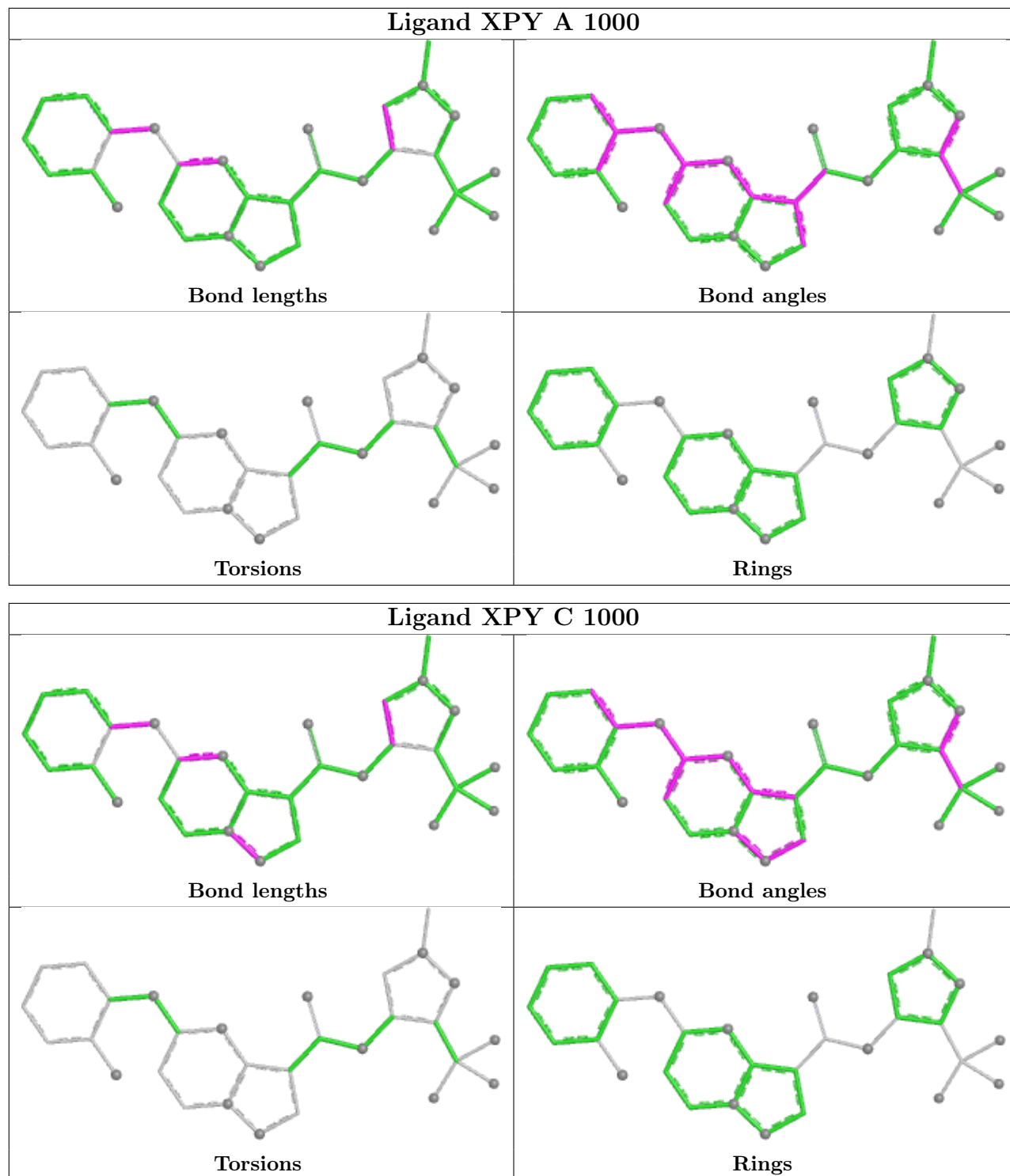
There are no torsion outliers.

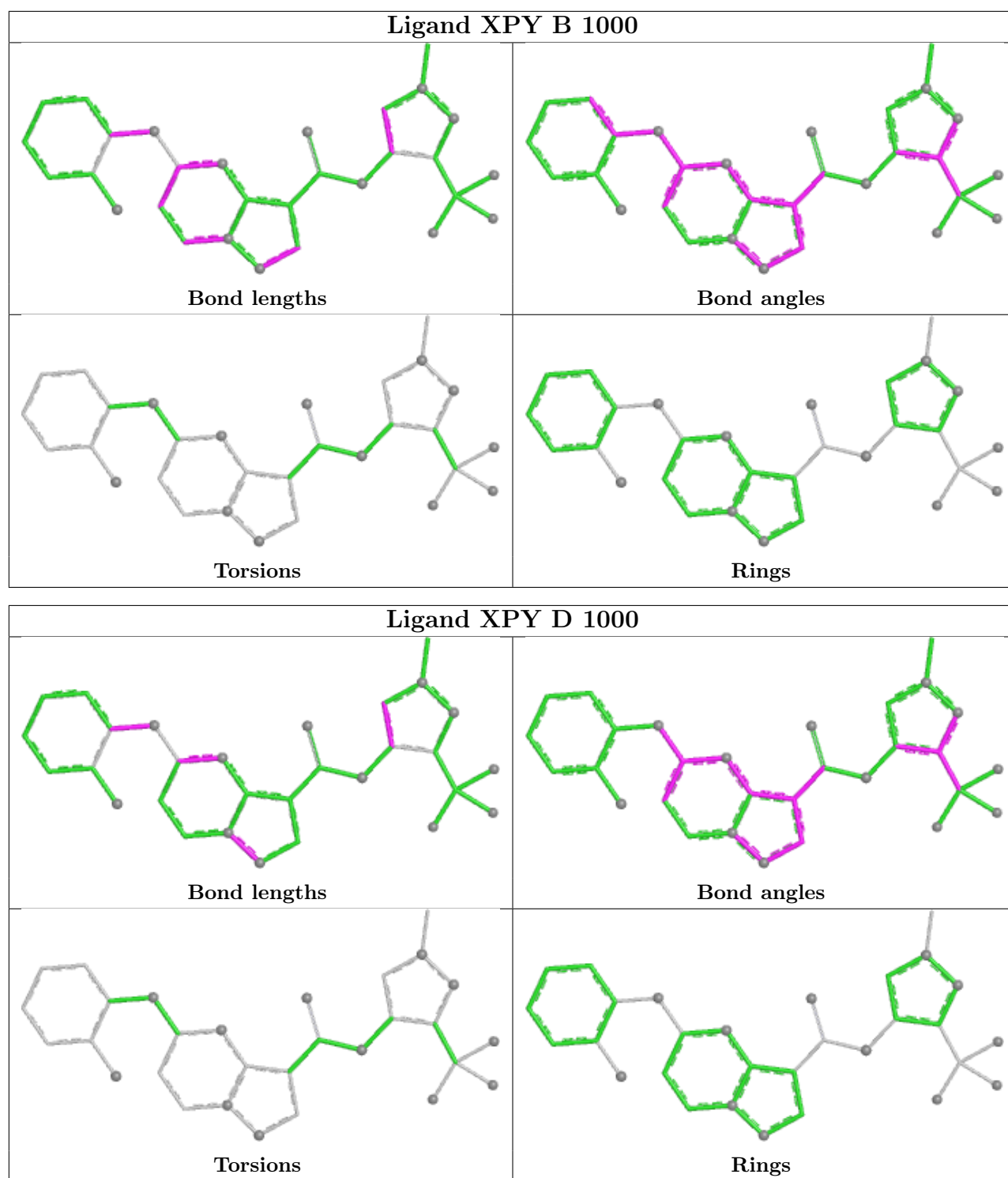
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	289/302 (95%)	0.51	15 (5%)	33 37	18, 52, 91, 108	1 (0%)
1	B	289/302 (95%)	0.52	20 (6%)	23 26	28, 51, 94, 120	0
1	C	290/302 (96%)	0.48	34 (11%)	9 11	27, 48, 95, 112	0
1	D	288/302 (95%)	0.55	29 (10%)	12 14	23, 50, 95, 121	1 (0%)
All	All	1156/1208 (95%)	0.52	98 (8%)	16 19	18, 50, 94, 121	2 (0%)

All (98) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	163	THR	5.4
1	B	240	CYS	4.6
1	A	240	CYS	4.4
1	B	221	ILE	4.4
1	C	410	ILE	4.0
1	D	170	PHE	4.0
1	D	253	SER	3.9
1	D	336	SER	3.9
1	D	258	LEU	3.8
1	B	205	VAL	3.7
1	A	221	ILE	3.7
1	C	187	VAL	3.7
1	A	219	VAL	3.6
1	B	217	ALA	3.6
1	D	252	SER	3.5
1	C	343	VAL	3.4
1	D	459	ALA	3.4
1	B	237	MET	3.4
1	B	343	VAL	3.3
1	D	410	ILE	3.3
1	B	219	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	215	LEU	3.1
1	A	459	ALA	3.1
1	C	180	PHE	3.1
1	A	218	MET	3.1
1	D	221	ILE	3.1
1	A	336	SER	3.1
1	C	176	VAL	3.0
1	C	221	ILE	3.0
1	A	187	VAL	2.9
1	C	219	VAL	2.9
1	C	181	ASP	2.9
1	A	344	MET	2.9
1	D	321[A]	GLU	2.9
1	C	222	THR	2.8
1	A	343	VAL	2.8
1	A	254	ASP	2.8
1	D	217	ALA	2.8
1	C	213	LYS	2.8
1	D	168	PHE	2.8
1	B	459	ALA	2.8
1	D	219	VAL	2.7
1	D	409	THR	2.7
1	C	168	PHE	2.7
1	C	175	ASN	2.7
1	C	253	SER	2.7
1	C	185	ILE	2.6
1	D	197	PHE	2.6
1	D	171	TYR	2.6
1	D	230	PHE	2.5
1	D	218	MET	2.5
1	D	167	SER	2.5
1	C	258	LEU	2.5
1	B	204	TYR	2.5
1	A	204	TYR	2.4
1	D	201	TYR	2.4
1	B	222	THR	2.4
1	B	344	MET	2.4
1	C	165	PHE	2.4
1	C	177	THR	2.4
1	D	166	HIS	2.4
1	D	226	LEU	2.3
1	C	216	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	408	LYS	2.3
1	C	335	ALA	2.3
1	B	226	LEU	2.3
1	B	197	PHE	2.3
1	C	171	TYR	2.3
1	C	460	SER	2.2
1	D	165	PHE	2.2
1	C	174	LYS	2.2
1	C	190	ASN	2.2
1	D	254	ASP	2.2
1	B	215	LEU	2.2
1	C	178	ASN	2.2
1	B	410	ILE	2.2
1	D	199	VAL	2.2
1	C	188	GLY	2.2
1	A	216	ALA	2.1
1	A	207	ASN	2.1
1	A	287[A]	MET	2.1
1	C	179	ASN	2.1
1	C	218	MET	2.1
1	C	254	ASP	2.1
1	B	234	ILE	2.1
1	D	349	VAL	2.1
1	A	188	GLY	2.1
1	D	205	VAL	2.1
1	C	408	LYS	2.1
1	C	217	ALA	2.1
1	D	259	CYS	2.1
1	D	439	GLU	2.1
1	C	409	THR	2.1
1	B	165	PHE	2.1
1	B	239	LYS	2.0
1	B	251	PHE	2.0
1	C	286	HIS	2.0
1	C	189	GLY	2.0

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

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
1	SEP	D	346	10/11	0.70	0.13	73,80,88,89	0
1	SEP	A	346	10/11	0.71	0.13	83,87,93,93	0
1	SEP	B	346	10/11	0.72	0.12	79,83,90,90	0
1	TPO	A	342	11/12	0.72	0.15	95,96,101,101	0
1	TPO	D	342	11/12	0.73	0.15	76,77,84,85	0
1	TPO	C	342	11/12	0.79	0.14	79,85,94,95	0
1	TPO	B	342	11/12	0.80	0.14	88,89,92,92	0
1	SEP	C	346	10/11	0.81	0.10	66,75,84,85	0
1	TPO	B	345	11/12	0.89	0.12	75,77,81,82	0
1	TPO	A	345	11/12	0.91	0.10	80,82,85,86	0
1	TPO	D	345	11/12	0.94	0.09	67,69,71,73	0
1	TPO	C	345	11/12	0.94	0.09	57,60,63,65	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

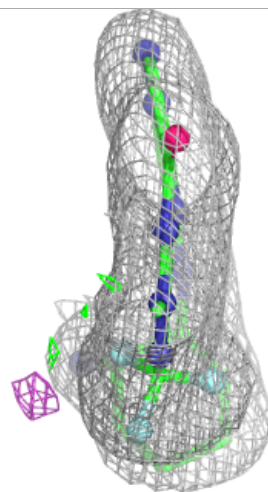
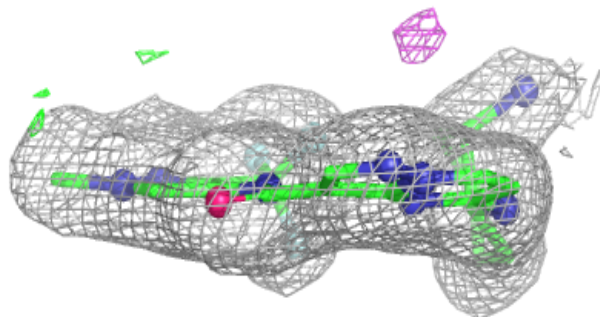
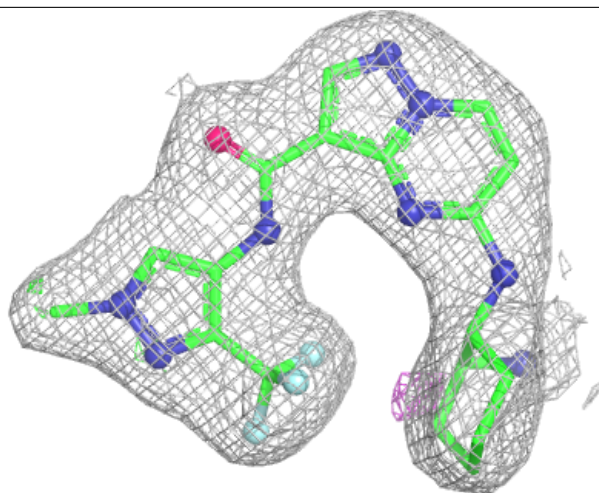
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	XPY	A	1000	30/30	0.95	0.07	29,40,48,50	0
2	XPY	D	1000	30/30	0.95	0.07	26,39,44,49	0
2	XPY	C	1000	30/30	0.96	0.07	27,35,42,42	0
2	XPY	B	1000	30/30	0.96	0.06	25,33,39,42	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.

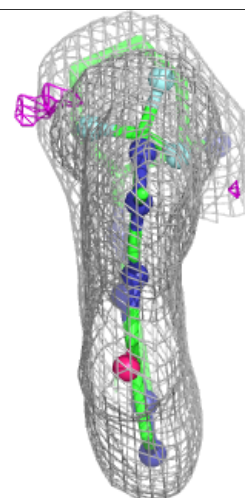
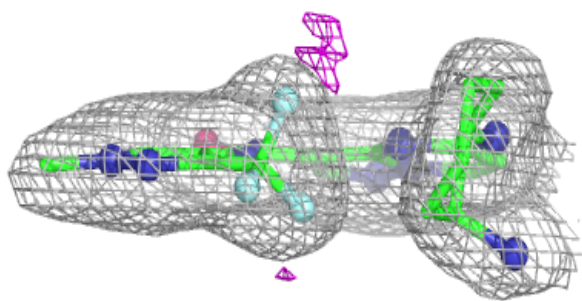
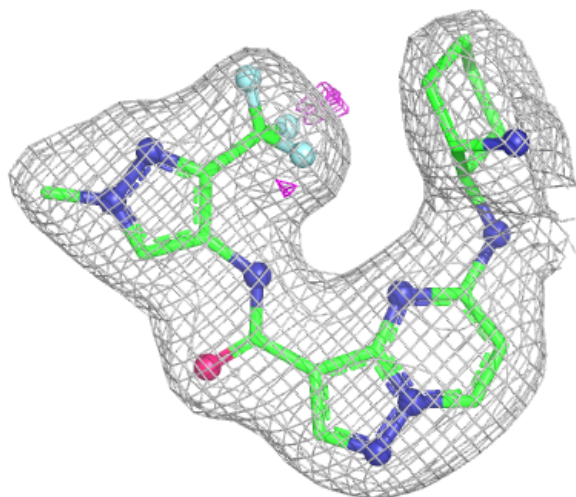
Electron density around XPY A 1000:

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



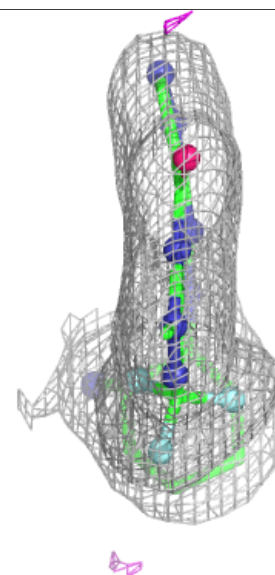
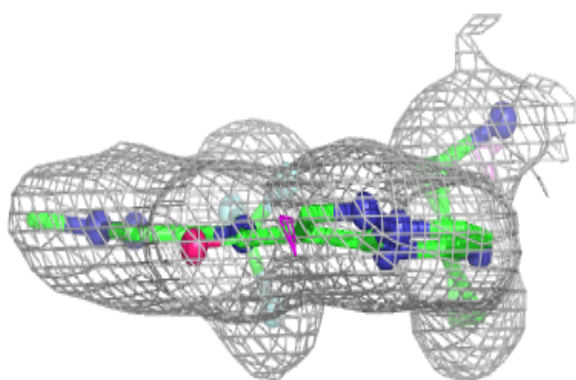
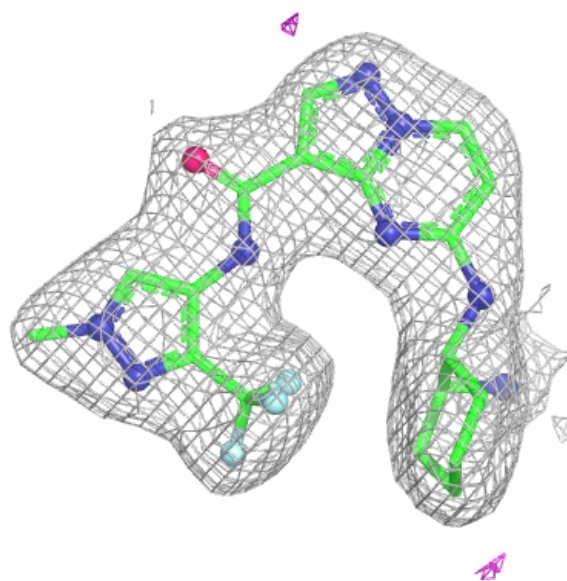
Electron density around XPY D 1000:

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



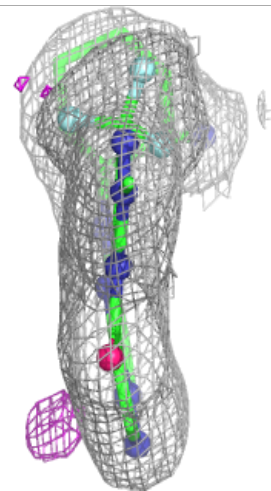
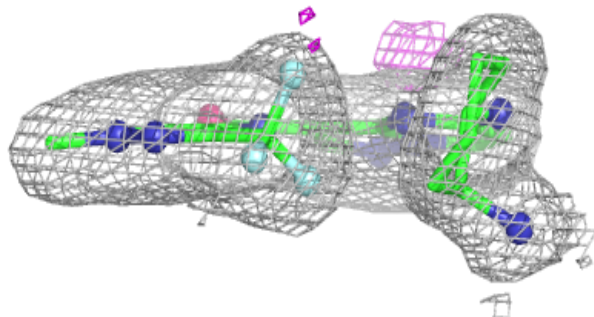
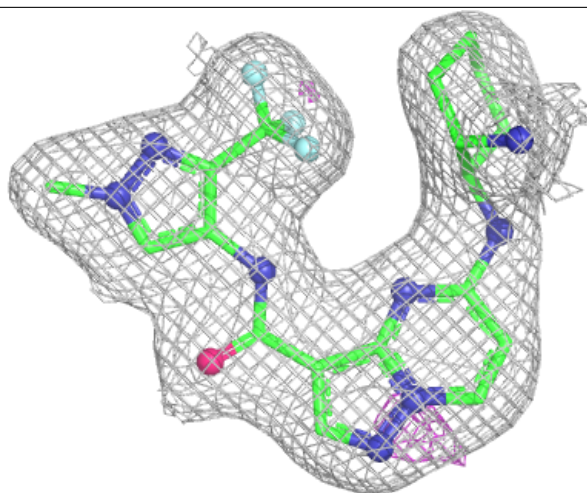
Electron density around XPY C 1000:

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



Electron density around XPY B 1000:

$2mF_o-DF_c$ (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.