



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:25 AM EDT

PDB ID : 5UIR / pdb_00005uir
Title : Crystal structure of IRAK4 in complex with compound 11
Authors : Han, S.; Chang, J.S.
Deposited on : 2017-01-14
Resolution : 2.64 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

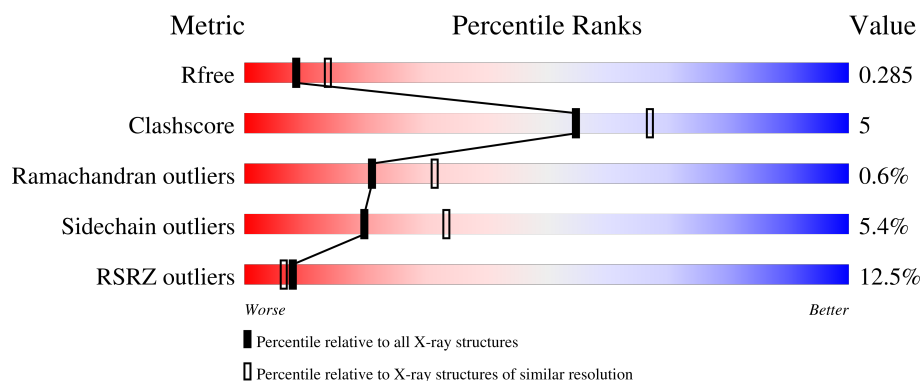
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.64 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	2053 (2.66-2.62)
Clashscore	190562	2097 (2.66-2.62)
Ramachandran outliers	187476	2066 (2.66-2.62)
Sidechain outliers	187428	2066 (2.66-2.62)
RSRZ outliers	180081	2052 (2.66-2.62)

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	323	11% 69% 14% • 16%
1	B	323	11% 68% 15% • 15%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4441 atoms, of which 36 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	272	Total	C	N	O	P	S	0	0	0
			2155	1357	361	421	2	14			
1	B	276	Total	C	N	O	P	S	0	1	0
			2168	1360	368	422	3	15			

There are 32 discrepancies between the modelled and reference sequences:

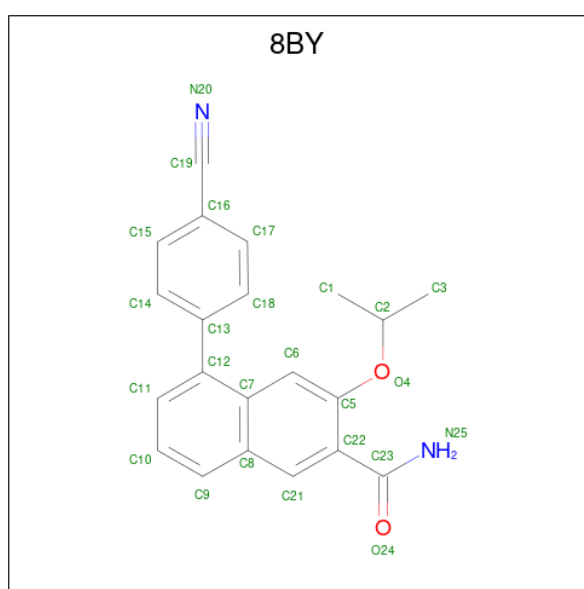
Chain	Residue	Modelled	Actual	Comment	Reference
A	138	MET	-	initiating methionine	UNP Q9NWZ3
A	139	HIS	-	expression tag	UNP Q9NWZ3
A	140	HIS	-	expression tag	UNP Q9NWZ3
A	141	HIS	-	expression tag	UNP Q9NWZ3
A	142	HIS	-	expression tag	UNP Q9NWZ3
A	143	HIS	-	expression tag	UNP Q9NWZ3
A	144	HIS	-	expression tag	UNP Q9NWZ3
A	145	GLY	-	expression tag	UNP Q9NWZ3
A	146	GLY	-	expression tag	UNP Q9NWZ3
A	147	GLU	-	expression tag	UNP Q9NWZ3
A	148	ASN	-	expression tag	UNP Q9NWZ3
A	149	LEU	-	expression tag	UNP Q9NWZ3
A	150	TYR	-	expression tag	UNP Q9NWZ3
A	151	PHE	-	expression tag	UNP Q9NWZ3
A	152	GLN	-	expression tag	UNP Q9NWZ3
A	153	GLY	-	expression tag	UNP Q9NWZ3
B	138	MET	-	initiating methionine	UNP Q9NWZ3
B	139	HIS	-	expression tag	UNP Q9NWZ3
B	140	HIS	-	expression tag	UNP Q9NWZ3
B	141	HIS	-	expression tag	UNP Q9NWZ3
B	142	HIS	-	expression tag	UNP Q9NWZ3
B	143	HIS	-	expression tag	UNP Q9NWZ3
B	144	HIS	-	expression tag	UNP Q9NWZ3
B	145	GLY	-	expression tag	UNP Q9NWZ3
B	146	GLY	-	expression tag	UNP Q9NWZ3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	147	GLU	-	expression tag	UNP Q9NWZ3
B	148	ASN	-	expression tag	UNP Q9NWZ3
B	149	LEU	-	expression tag	UNP Q9NWZ3
B	150	TYR	-	expression tag	UNP Q9NWZ3
B	151	PHE	-	expression tag	UNP Q9NWZ3
B	152	GLN	-	expression tag	UNP Q9NWZ3
B	153	GLY	-	expression tag	UNP Q9NWZ3

- Molecule 2 is 5-(4-cyanophenyl)-3-[(propan-2-yl)oxy]naphthalene-2-carboxamide (CCD ID: 8BY) (formula: C₂₁H₁₈N₂O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			43	21	18	2	2		
2	B	1	Total	C	H	N	O	0	0
			43	21	18	2	2		

- Molecule 3 is water.

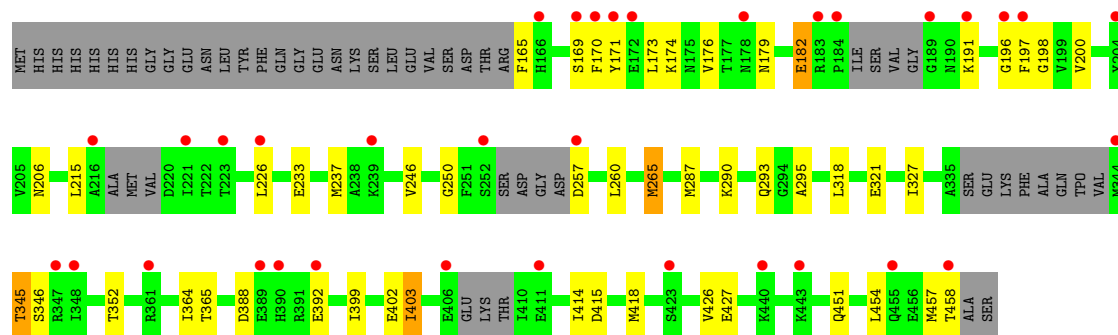
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total	O	0	0
			19	19		
3	B	13	Total	O	0	0
			13	13		

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.

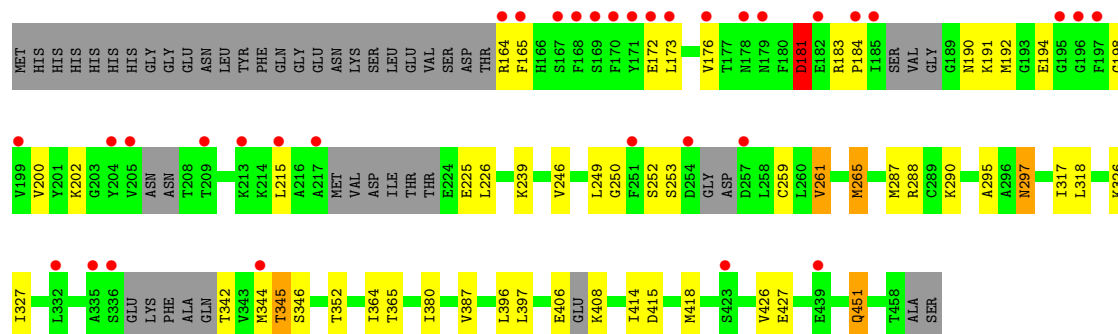
- Molecule 1: Interleukin-1 receptor-associated kinase 4

Chain A: 



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

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	87.69Å 110.86Å 140.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	68.78 – 2.64 68.78 – 2.64	Depositor EDS
% Data completeness (in resolution range)	97.9 (68.78-2.64) 98.0 (68.78-2.64)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.42 (at 2.65Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.219 , 0.277 0.227 , 0.285	Depositor DCC
R_{free} test set	1028 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å ²)	44.7	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4441	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.89 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0274e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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, SEP, 8BY

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	0.88	1/2167 (0.0%)	1.36	9/2915 (0.3%)
1	B	0.87	1/2171 (0.0%)	1.35	9/2916 (0.3%)
All	All	0.88	2/4338 (0.0%)	1.35	18/5831 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	265	MET	SD-CE	-6.58	1.63	1.79
1	A	265	MET	SD-CE	-5.83	1.65	1.79

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	PHE	CA-CB-CG	7.03	120.83	113.80
1	B	297	ASN	CA-CB-CG	6.91	119.51	112.60
1	A	198	GLY	N-CA-C	6.53	120.28	110.75
1	B	225	GLU	CA-C-N	6.38	130.00	120.31
1	B	225	GLU	C-N-CA	6.38	130.00	120.31
1	B	397	LEU	N-CA-CB	-5.95	100.43	110.49
1	A	451	GLN	CA-C-N	5.65	127.79	120.44
1	A	451	GLN	C-N-CA	5.65	127.79	120.44
1	B	451	GLN	CA-C-N	5.47	127.55	120.44
1	B	451	GLN	C-N-CA	5.47	127.55	120.44
1	A	196	GLY	N-CA-C	-5.30	105.50	112.82
1	A	388	ASP	CA-C-N	5.16	127.15	120.44
1	A	388	ASP	C-N-CA	5.16	127.15	120.44
1	B	198	GLY	N-CA-C	5.13	116.95	110.38
1	B	396	LEU	CA-C-N	5.10	131.28	121.54
1	B	396	LEU	C-N-CA	5.10	131.28	121.54
1	A	293	GLN	CA-C-N	5.02	125.51	119.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	GLN	C-N-CA	5.02	125.51	119.94

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	2155	0	2117	18	0
1	B	2168	0	2135	23	5
2	A	25	18	0	0	0
2	B	25	18	0	0	0
3	A	19	0	0	0	0
3	B	13	0	0	0	0
All	All	4405	36	4252	41	5

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (41) 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:A:237:MET:HA	1:A:237:MET:HE2	1.57	0.85
1:A:246:VAL:HG11	1:A:318:LEU:HD12	1.66	0.77
1:B:246:VAL:HG11	1:B:318:LEU:HD12	1.70	0.74
1:B:287[B]:MET:HE1	1:B:290:LYS:HD3	1.72	0.69
1:B:265:MET:HE1	1:B:326:LYS:HG3	1.75	0.66
1:B:192:MET:HE3	1:B:200:VAL:HG12	1.78	0.66
1:A:345:TPO:HB	1:A:364:ILE:HD11	1.79	0.65
1:B:297:ASN:HD22	1:B:451:GLN:HE21	1.45	0.63
1:B:181:ASP:HB2	1:B:190:ASN:HB2	1.84	0.60
1:B:415:ASP:HB3	1:B:418:MET:HE2	1.85	0.58
1:A:415:ASP:HB3	1:A:418:MET:HE2	1.84	0.57
1:A:233:GLU:HG2	1:A:260:LEU:HD13	1.87	0.57
1:A:399:ILE:O	1:A:403:ILE:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:ILE:HG12	1:B:426:VAL:HG11	1.86	0.56
1:B:252:SER:HB3	1:B:259:CYS:HB2	1.88	0.55
1:A:414:ILE:HG12	1:A:426:VAL:HG11	1.88	0.55
1:B:345:TPO:HB	1:B:364:ILE:HD11	1.89	0.55
1:A:237:MET:HA	1:A:237:MET:CE	2.35	0.54
1:B:165:PHE:HB3	1:B:250:GLY:HA2	1.89	0.54
1:B:265:MET:CE	1:B:326:LYS:HG3	2.38	0.53
1:A:174:LYS:HG2	1:A:179:ASN:HA	1.90	0.52
1:B:297:ASN:ND2	1:B:451:GLN:HE21	2.10	0.50
1:A:169:SER:C	1:A:171:TYR:H	2.20	0.49
1:A:454:LEU:O	1:A:457:MET:HB2	2.12	0.49
1:B:191:LYS:HE3	1:B:194:GLU:HB2	1.95	0.48
1:A:165:PHE:HB3	1:A:250:GLY:HA2	1.96	0.48
1:A:182:GLU:HA	1:A:191:LYS:HB2	1.96	0.48
1:B:288:ARG:HB3	1:B:380:ILE:HG23	1.97	0.47
1:B:181:ASP:CB	1:B:190:ASN:HB2	2.44	0.47
1:A:173:LEU:HA	1:A:176:VAL:HG22	1.97	0.46
1:B:215:LEU:HD22	1:B:226:LEU:HD22	1.99	0.45
1:A:215:LEU:HB3	1:A:226:LEU:HD22	1.98	0.44
1:B:249:LEU:HB2	1:B:261:VAL:HG13	2.01	0.43
1:B:181:ASP:C	1:B:183:ARG:H	2.27	0.43
1:A:287:MET:HE3	1:A:290:LYS:HB2	2.01	0.42
1:B:295:ALA:HA	1:B:327:ILE:HD11	2.01	0.42
1:A:295:ALA:HA	1:A:327:ILE:HD11	2.01	0.42
1:B:173:LEU:HA	1:B:176:VAL:HG22	2.01	0.41
1:B:265:MET:HG3	1:B:318:LEU:HB3	2.02	0.41
1:A:265:MET:HG3	1:A:318:LEU:HB3	2.02	0.41
1:B:317:ILE:HG12	1:B:327:ILE:HD13	2.03	0.41

All (5) 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:B:172:GLU:CD	1:B:172:GLU:OE2[4_565]	1.41	0.79
1:B:172:GLU:CD	1:B:172:GLU:CD[4_565]	1.49	0.71
1:B:172:GLU:CB	1:B:172:GLU:OE1[4_565]	1.82	0.38
1:B:172:GLU:CG	1:B:172:GLU:CD[4_565]	1.85	0.35
1:B:172:GLU:CG	1:B:172:GLU:OE1[4_565]	2.12	0.08

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	258/323 (80%)	248 (96%)	10 (4%)	0	100	100
1	B	261/323 (81%)	247 (95%)	11 (4%)	3 (1%)	11	16
All	All	519/646 (80%)	495 (95%)	21 (4%)	3 (1%)	21	31

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	184	PRO
1	B	181	ASP
1	B	202	LYS

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	235/278 (84%)	222 (94%)	13 (6%)	19	32
1	B	233/278 (84%)	221 (95%)	12 (5%)	21	34
All	All	468/556 (84%)	443 (95%)	25 (5%)	20	34

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	PHE
1	A	182	GLU
1	A	200	VAL

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Mol	Chain	Res	Type
1	A	206	ASN
1	A	257	ASP
1	A	321	GLU
1	A	352	THR
1	A	365	THR
1	A	392	GLU
1	A	402	GLU
1	A	403	ILE
1	A	427	GLU
1	A	458	THR
1	B	164	ARG
1	B	181	ASP
1	B	239	LYS
1	B	253	SER
1	B	261	VAL
1	B	344	MET
1	B	352	THR
1	B	365	THR
1	B	387	VAL
1	B	406	GLU
1	B	408	LYS
1	B	427	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	HIS
1	A	207	ASN
1	A	229	GLN
1	A	435	GLN
1	B	175	ASN
1	B	228	GLN
1	B	293	GLN
1	B	305	ASN
1	B	451	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

5 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	B	345	1	8,10,11	1.66	2 (25%)	10,14,16	1.32	1 (10%)
1	SEP	A	346	1	8,9,10	0.93	0	7,12,14	2.45	1 (14%)
1	TPO	A	345	1	8,10,11	1.26	1 (12%)	10,14,16	1.18	1 (10%)
1	TPO	B	342	1	8,10,11	1.44	1 (12%)	10,14,16	1.28	1 (10%)
1	SEP	B	346	1	8,9,10	0.82	0	7,12,14	2.23	2 (28%)

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	B	345	1	-	3/9/11/13	-
1	SEP	A	346	1	-	2/6/8/10	-
1	TPO	A	345	1	-	4/9/11/13	-
1	TPO	B	342	1	-	2/9/11/13	-
1	SEP	B	346	1	-	2/6/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	342	TPO	P-OG1	-3.02	1.54	1.59
1	B	345	TPO	P-OG1	-2.77	1.54	1.59
1	B	345	TPO	CB-CA	2.69	1.59	1.53
1	A	345	TPO	CB-CA	2.02	1.58	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	346	SEP	OG-CB-CA	5.67	113.67	108.14
1	B	346	SEP	OG-CB-CA	5.15	113.16	108.14
1	A	345	TPO	O2P-P-OG1	2.41	115.23	105.85
1	B	346	SEP	O3P-P-OG	2.16	112.30	106.67
1	B	345	TPO	CG2-CB-CA	2.15	117.45	113.26
1	B	342	TPO	P-OG1-CB	-2.15	117.49	123.33

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	345	TPO	N-CA-CB-OG1
1	A	345	TPO	CA-CB-OG1-P
1	A	346	SEP	N-CA-CB-OG
1	A	346	SEP	C-CA-CB-OG
1	B	345	TPO	N-CA-CB-OG1
1	B	345	TPO	O-C-CA-CB
1	B	346	SEP	N-CA-CB-OG
1	B	346	SEP	C-CA-CB-OG
1	B	342	TPO	CB-OG1-P-O2P
1	B	345	TPO	CA-CB-OG1-P
1	A	345	TPO	O-C-CA-CB
1	B	342	TPO	O-C-CA-CB
1	A	345	TPO	CB-OG1-P-O1P

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	345	TPO	1	0
1	A	345	TPO	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	8BY	A	800	-	27,27,27	0.27	0	38,38,38	0.59	1 (2%)
2	8BY	B	801	-	27,27,27	0.34	0	38,38,38	0.55	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	8BY	A	800	-	-	0/14/24/24	0/3/3/3
2	8BY	B	801	-	-	0/14/24/24	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	8BY	C5-O4-C2	2.24	123.66	119.53

There are no chirality outliers.

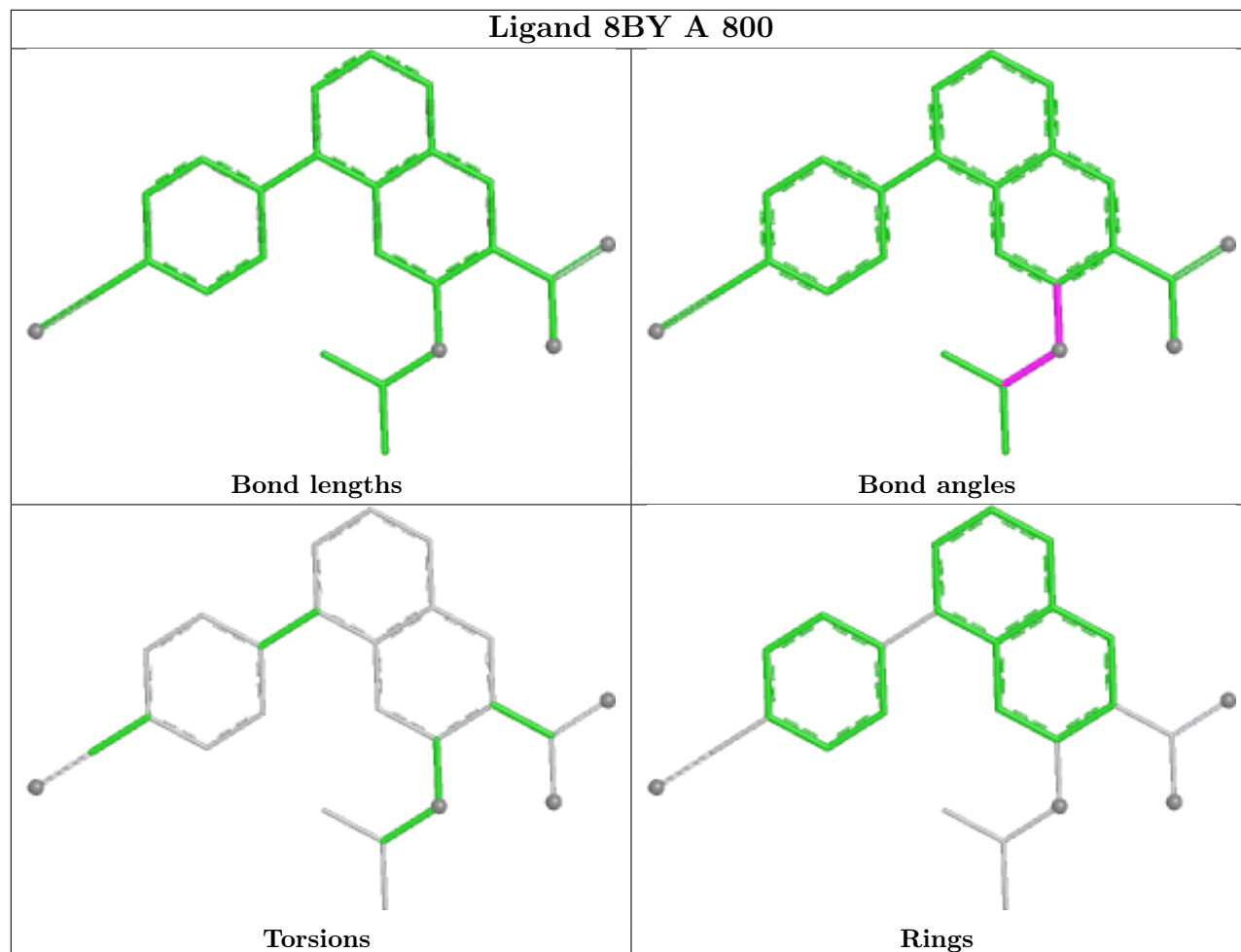
There are no torsion outliers.

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 [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	270/323 (83%)	0.75	34 (12%) 8 6	24, 52, 90, 112	17 (6%)
1	B	273/323 (84%)	0.71	34 (12%) 8 6	24, 55, 130, 163	1 (0%)
All	All	543/646 (84%)	0.73	68 (12%) 8 6	24, 53, 115, 163	18 (3%)

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	204	TYR	5.4
1	B	185	ILE	4.9
1	B	171	TYR	4.9
1	B	205	VAL	4.9
1	A	196	GLY	4.8
1	A	347	ARG	4.5
1	A	184	PRO	4.4
1	B	254	ASP	4.3
1	A	348	ILE	4.1
1	A	440	LYS	3.9
1	A	344	MET	3.8
1	B	165	PHE	3.7
1	A	392	GLU	3.7
1	B	335	ALA	3.5
1	A	226	LEU	3.4
1	B	167	SER	3.4
1	A	389	GLU	3.3
1	B	251	PHE	3.2
1	B	178	ASN	3.2
1	A	390	HIS	3.2
1	A	443	LYS	3.2
1	B	257	ASP	3.1
1	A	170	PHE	3.1
1	A	252	SER	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	204	TYR	3.0
1	B	344	MET	2.9
1	B	179	ASN	2.9
1	A	189	GLY	2.8
1	A	361	ARG	2.8
1	B	176	VAL	2.8
1	B	336	SER	2.8
1	A	171	TYR	2.8
1	B	173	LEU	2.7
1	A	197	PHE	2.7
1	B	169	SER	2.7
1	B	199	VAL	2.7
1	B	195	GLY	2.6
1	B	197	PHE	2.6
1	B	170	PHE	2.6
1	B	172	GLU	2.6
1	A	169	SER	2.5
1	A	423	SER	2.5
1	A	257	ASP	2.5
1	B	439	GLU	2.5
1	B	196	GLY	2.5
1	B	164	ARG	2.3
1	A	239	LYS	2.3
1	A	183	ARG	2.3
1	A	458	THR	2.3
1	B	213	LYS	2.3
1	A	411	GLU	2.3
1	B	217	ALA	2.2
1	A	223	THR	2.2
1	A	455	GLN	2.2
1	B	423	SER	2.2
1	A	178	ASN	2.2
1	A	406	GLU	2.1
1	B	215	LEU	2.1
1	A	216	ALA	2.1
1	A	172	GLU	2.1
1	B	184	PRO	2.1
1	B	182	GLU	2.1
1	B	209	THR	2.1
1	B	332	LEU	2.1
1	A	166	HIS	2.1
1	A	221	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	168	PHE	2.1
1	A	191	LYS	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	SEP	B	346	10/11	0.75	0.14	101,107,117,118	0
1	TPO	B	342	11/12	0.76	0.15	96,100,104,106	0
1	SEP	A	346	10/11	0.80	0.11	85,93,105,106	0
1	TPO	B	345	11/12	0.87	0.14	88,95,99,101	0
1	TPO	A	345	11/12	0.93	0.11	74,79,85,86	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

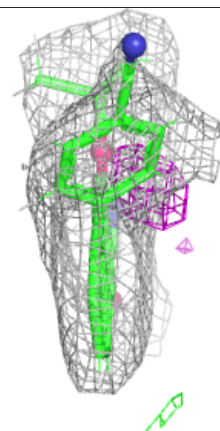
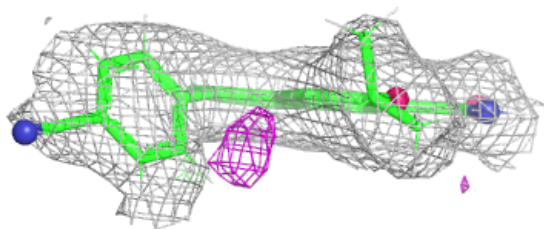
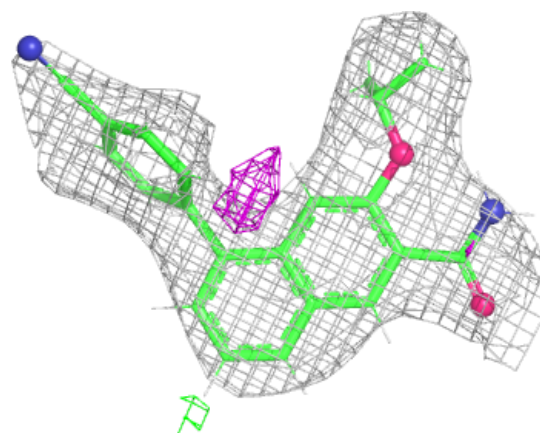
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	8BY	B	801	25/25	0.85	0.13	41,49,53,58	0
2	8BY	A	800	25/25	0.90	0.11	37,42,48,58	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 8BY A 800:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.