



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 01:15 AM UTC

PDB ID : 6RFI / pdb_00006rfi
Title : IRAK4 IN COMPLEX WITH inhibitor
Authors : Xue, Y.; Degorce, S.L.; Robb, G.R.; Ferguson, A.D.
Deposited on : 2019-04-15
Resolution : 2.31 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

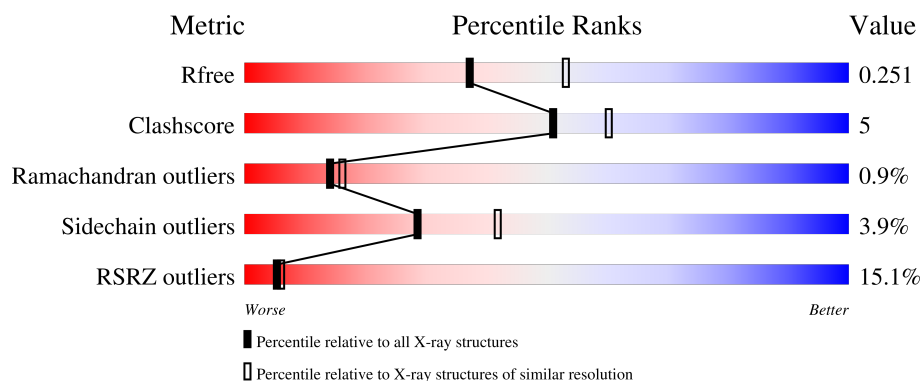
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	322	8% 72% 11% • 15%
1	B	322	17% 73% 12% • 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	501	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4604 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	275	Total	C	N	O	P	S	0	2	0
			2195	1378	369	431	2	15			
1	B	280	Total	C	N	O	P	S	0	0	0
			2218	1392	374	436	2	14			

There are 30 discrepancies between the modelled and reference sequences:

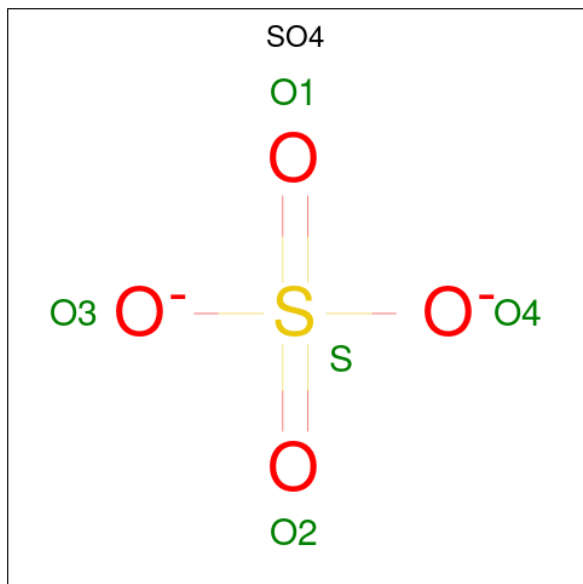
Chain	Residue	Modelled	Actual	Comment	Reference
A	139	MET	-	initiating methionine	UNP Q9NWZ3
A	140	HIS	-	expression tag	UNP Q9NWZ3
A	141	HIS	-	expression tag	UNP Q9NWZ3
A	142	HIS	-	expression tag	UNP Q9NWZ3
A	143	HIS	-	expression tag	UNP Q9NWZ3
A	144	HIS	-	expression tag	UNP Q9NWZ3
A	145	HIS	-	expression tag	UNP Q9NWZ3
A	146	HIS	-	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	139	MET	-	initiating methionine	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	HIS	-	expression tag	UNP Q9NWZ3
B	146	HIS	-	expression tag	UNP Q9NWZ3
B	147	GLU	-	expression tag	UNP Q9NWZ3
B	148	ASN	-	expression tag	UNP Q9NWZ3

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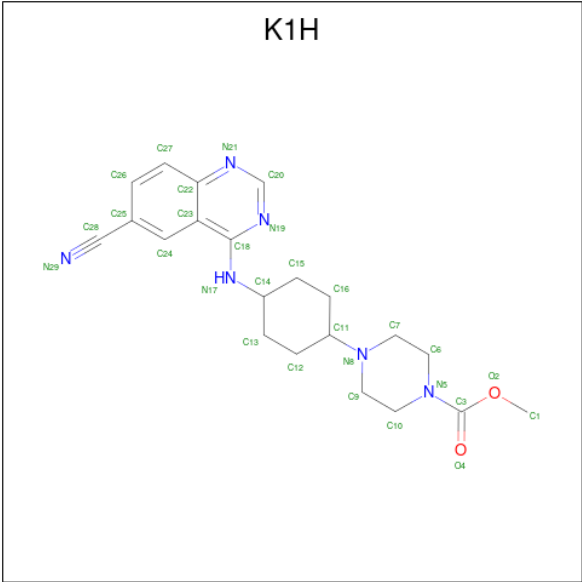
Chain	Residue	Modelled	Actual	Comment	Reference
B	149	LEU	-	expression tag	UNP Q9NWZ3
B	150	TYR	-	expression tag	UNP Q9NWZ3
B	151	PHE	-	expression tag	UNP Q9NWZ3
B	152	GLN	-	expression tag	UNP Q9NWZ3
B	153	GLY	-	expression tag	UNP Q9NWZ3

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is methyl 4-[4-[(6-cyanoquinazolin-4-yl)amino]cyclohexyl]piperazine-1-carboxylate (CCD ID: K1H) (formula: C₂₁H₂₆N₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			29	21	6	2		
3	B	1	Total	C	N	O	0	0
			29	21	6	2		

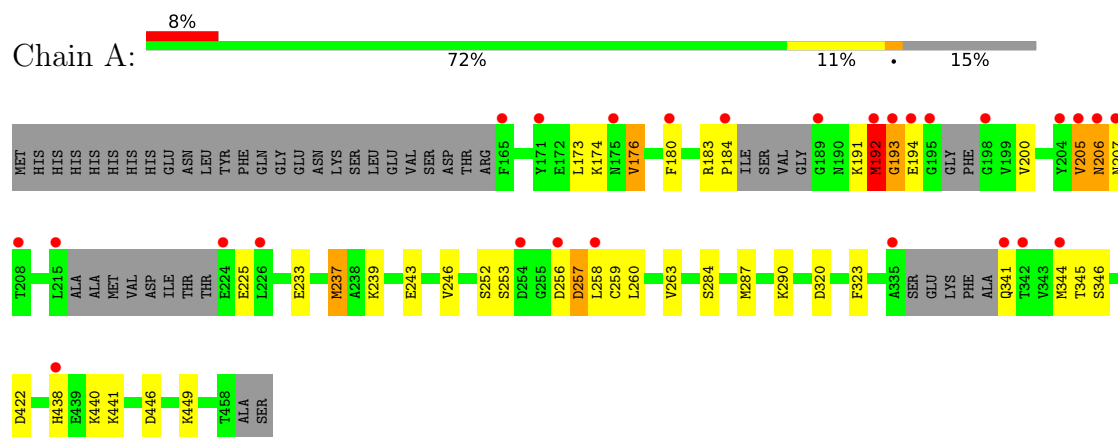
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	62	Total	O	0	0
			62	62		
4	B	61	Total	O	0	0
			61	61		

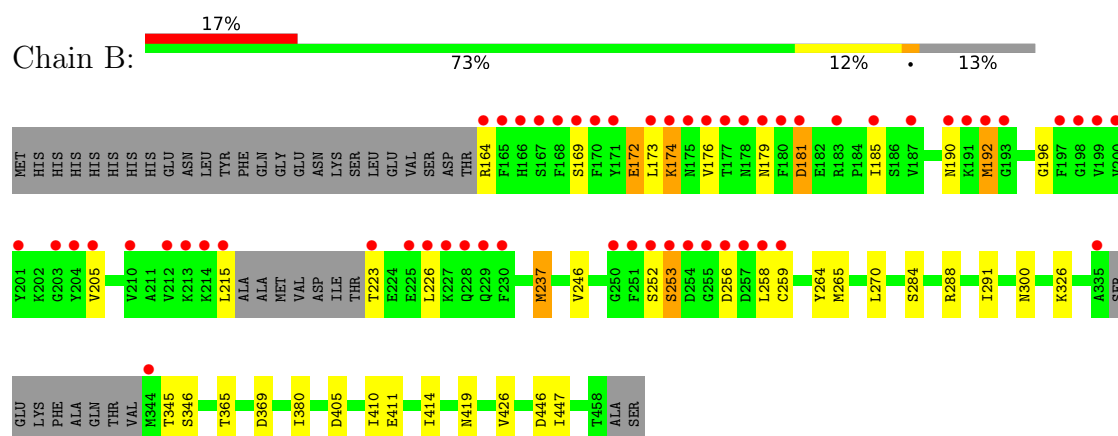
3 Residue-property plots

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



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	87.90Å 116.78Å 141.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	58.39 – 2.31 58.39 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.8 (58.39-2.31) 100.0 (58.39-2.31)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.32Å)	Xtriage
Refinement program	BUSTER 2.11.6 PACIOREK	Depositor
R, R_{free}	0.210 , 0.236 0.215 , 0.251	Depositor DCC
R_{free} test set	1621 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	44.2	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 58.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4604	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.09% 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: SO4, SEP, TPO, K1H

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	0.85	1/2214 (0.0%)	1.39	10/2978 (0.3%)
1	B	0.88	1/2233 (0.0%)	1.35	6/3006 (0.2%)
All	All	0.86	2/4447 (0.0%)	1.37	16/5984 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	237	MET	SD-CE	-6.02	1.64	1.79
1	A	237	MET	SD-CE	-5.67	1.65	1.79

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	320	ASP	CA-CB-CG	6.99	119.58	112.60
1	A	206	ASN	CA-C-N	6.46	131.31	122.07
1	A	206	ASN	C-N-CA	6.46	131.31	122.07
1	A	446	ASP	CA-CB-CG	6.42	119.02	112.60
1	A	257	ASP	CA-CB-CG	6.03	118.63	112.60
1	B	419	ASN	CA-CB-CG	5.91	118.51	112.60
1	B	446	ASP	CA-CB-CG	5.80	118.40	112.60
1	B	181	ASP	CA-CB-CG	5.69	118.29	112.60
1	B	172	GLU	CA-C-N	5.57	130.89	121.14
1	B	172	GLU	C-N-CA	5.57	130.89	121.14
1	B	369	ASP	CA-CB-CG	5.38	117.98	112.60
1	A	176	VAL	N-CA-C	-5.13	106.09	113.07
1	A	225	GLU	CA-C-N	5.12	127.56	120.29
1	A	225	GLU	C-N-CA	5.12	127.56	120.29
1	A	422	ASP	CA-C-N	5.08	127.40	120.54
1	A	422	ASP	C-N-CA	5.08	127.40	120.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2195	0	2159	20	0
1	B	2218	0	2181	26	0
2	A	5	0	0	0	8
2	B	5	0	0	0	0
3	A	29	0	0	0	0
3	B	29	0	0	0	0
4	A	62	0	0	0	0
4	B	61	0	0	0	0
All	All	4604	0	4340	46	8

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 (46) 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:284:SER:H	1:A:287[A]:MET:HE3	1.35	0.92
1:A:237:MET:HE1	1:A:246:VAL:HG23	1.63	0.81
1:A:193:GLY:HA3	1:A:200:VAL:H	1.44	0.79
1:B:237:MET:HE1	1:B:246:VAL:HG23	1.64	0.78
1:B:192:MET:HE1	1:B:264:TYR:HE1	1.47	0.77
1:A:183:ARG:HD3	1:A:184:PRO:HD2	1.72	0.72
1:B:173:LEU:HA	1:B:176:VAL:HG22	1.75	0.67
1:B:192:MET:HE1	1:B:264:TYR:CE1	2.31	0.65
1:A:205:VAL:HG23	1:A:206:ASN:H	1.60	0.65
1:A:438[B]:HIS:HD2	1:A:440:LYS:H	1.49	0.60
1:A:256:ASP:HA	1:A:257:ASP:HB3	1.84	0.59
1:B:181:ASP:HB3	1:B:190:ASN:HB2	1.88	0.56
1:B:169:SER:HB3	1:B:172:GLU:HG3	1.90	0.54
1:B:265:MET:CE	1:B:326:LYS:HD2	2.37	0.54
1:A:287[B]:MET:HE1	1:A:290:LYS:HD2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:MET:HE3	1:A:200:VAL:HG12	1.92	0.52
1:B:215:LEU:HD12	1:B:258:LEU:HB2	1.93	0.50
1:A:284:SER:N	1:A:287[A]:MET:HE3	2.16	0.50
1:A:233:GLU:HG2	1:A:260:LEU:HD13	1.95	0.49
1:B:300:ASN:HA	1:B:447:ILE:HG21	1.93	0.48
1:B:288:ARG:HB3	1:B:380:ILE:HG23	1.95	0.48
1:B:176:VAL:HG11	1:B:205:VAL:HG22	1.95	0.48
1:B:265:MET:HE2	1:B:326:LYS:HB2	1.97	0.47
1:B:174:LYS:O	1:B:179:ASN:HA	2.14	0.47
1:B:215:LEU:HB3	1:B:226:LEU:HD21	1.97	0.47
1:B:253:SER:HA	1:B:258:LEU:HD22	1.98	0.45
1:B:192:MET:HB2	1:B:192:MET:HE3	1.63	0.45
1:A:193:GLY:CA	1:A:200:VAL:H	2.22	0.44
1:B:284:SER:O	1:B:288:ARG:HG3	2.17	0.44
1:A:287[B]:MET:HE2	1:A:323:PHE:HB3	2.01	0.43
1:A:252:SER:HB3	1:A:259:CYS:HB2	2.01	0.43
1:B:237:MET:CE	1:B:246:VAL:HG23	2.42	0.43
1:A:341:GLN:HB3	1:A:441:LYS:HZ1	1.84	0.43
1:B:410:ILE:O	1:B:414:ILE:HG13	2.18	0.43
1:B:270:LEU:HD13	1:B:291:ILE:HG21	2.01	0.43
1:B:173:LEU:HA	1:B:176:VAL:CG2	2.46	0.42
1:A:173:LEU:HA	1:A:176:VAL:HG22	2.00	0.42
1:A:193:GLY:HA3	1:A:200:VAL:N	2.22	0.41
1:B:265:MET:HE1	1:B:326:LYS:HD2	2.02	0.41
1:A:174:LYS:HA	1:A:180:PHE:CE2	2.55	0.41
1:B:411:GLU:HA	1:B:414:ILE:HD12	2.01	0.41
1:B:252:SER:HB3	1:B:259:CYS:HB2	2.03	0.40
1:B:414:ILE:HG12	1:B:426:VAL:HG11	2.04	0.40
1:A:287[B]:MET:HE2	1:A:323:PHE:CB	2.51	0.40
1:A:438[B]:HIS:CD2	1:A:440:LYS:H	2.34	0.40
1:B:288:ARG:HB3	1:B:380:ILE:CG2	2.51	0.40

All (8) 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)
2:A:501:SO4:O1	2:A:501:SO4:O4[3_455]	0.13	2.07
2:A:501:SO4:S	2:A:501:SO4:S[3_455]	0.36	1.84
2:A:501:SO4:O2	2:A:501:SO4:O3[3_455]	0.71	1.49
2:A:501:SO4:S	2:A:501:SO4:O3[3_455]	1.24	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501:SO4:S	2:A:501:SO4:O4[3_455]	1.40	0.80
2:A:501:SO4:S	2:A:501:SO4:O1[3_455]	1.55	0.65
2:A:501:SO4:O3	2:A:501:SO4:O3[3_455]	1.78	0.42
2:A:501:SO4:S	2:A:501:SO4:O2[3_455]	1.79	0.41

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	265/322 (82%)	251 (95%)	10 (4%)	4 (2%)	8	7
1	B	272/322 (84%)	263 (97%)	8 (3%)	1 (0%)	30	37
All	All	537/644 (83%)	514 (96%)	18 (3%)	5 (1%)	14	16

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	MET
1	B	196	GLY
1	A	193	GLY
1	A	258	LEU
1	A	205	VAL

5.3.2 Protein sidechains [i](#)

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	242/280 (86%)	232 (96%)	10 (4%)	27	40
1	B	243/280 (87%)	234 (96%)	9 (4%)	30	44
All	All	485/560 (87%)	466 (96%)	19 (4%)	28	42

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	191	LYS
1	A	192	MET
1	A	194	GLU
1	A	207	ASN
1	A	239	LYS
1	A	243	GLU
1	A	253	SER
1	A	263	VAL
1	A	344	MET
1	A	449	LYS
1	B	164	ARG
1	B	174	LYS
1	B	185	ILE
1	B	192	MET
1	B	223	THR
1	B	253	SER
1	B	256	ASP
1	B	365	THR
1	B	405	ASP

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	175	ASN
1	A	179	ASN
1	A	206	ASN
1	A	232	GLN
1	A	286	HIS
1	A	435	GLN
1	A	442	ASN
1	B	179	ASN
1	B	206	ASN
1	B	297	ASN
1	B	394	GLN

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Mol	Chain	Res	Type
1	B	419	ASN
1	B	438	HIS
1	B	451	GLN
1	B	452	GLN

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	TPO	A	345	1	8,10,11	1.16	1 (12%)	10,14,16	1.17	1 (10%)
1	SEP	B	346	1	8,9,10	0.87	0	7,12,14	2.40	2 (28%)
1	SEP	A	346	1	8,9,10	1.00	0	7,12,14	2.01	3 (42%)
1	TPO	B	345	1	8,10,11	1.46	1 (12%)	10,14,16	1.31	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	A	345	1	-	4/9/11/13	-
1	SEP	B	346	1	-	5/6/8/10	-
1	SEP	A	346	1	-	0/6/8/10	-
1	TPO	B	345	1	-	3/9/11/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	345	TPO	CB-CA	3.15	1.60	1.53
1	A	345	TPO	CB-CA	2.34	1.58	1.53

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	346	SEP	OG-CB-CA	4.97	112.98	108.14
1	B	346	SEP	OG-P-O1P	3.18	115.03	106.44
1	A	346	SEP	OG-CB-CA	2.85	110.92	108.14
1	A	346	SEP	O3P-P-OG	2.77	113.89	106.67
1	A	346	SEP	OG-P-O1P	2.63	113.54	106.44
1	B	345	TPO	O2P-P-OG1	2.58	115.90	105.85
1	A	345	TPO	O2P-P-OG1	2.55	115.78	105.85

There are no chirality outliers.

All (12) 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	346	SEP	N-CA-CB-OG
1	B	346	SEP	C-CA-CB-OG
1	B	346	SEP	CB-OG-P-O1P
1	B	346	SEP	CB-OG-P-O2P
1	B	346	SEP	CB-OG-P-O3P
1	B	345	TPO	CA-CB-OG1-P
1	A	345	TPO	CB-OG1-P-O3P
1	B	345	TPO	O-C-CA-CB
1	A	345	TPO	CG2-CB-OG1-P

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	SO4	B	501	-	4,4,4	0.32	0	6,6,6	0.17	0
3	K1H	B	502	-	31,32,32	0.33	0	43,44,44	0.56	0
2	SO4	A	501	-	4,4,4	0.25	0	6,6,6	0.09	0
3	K1H	A	502	-	31,32,32	0.37	0	43,44,44	0.50	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	K1H	A	502	-	-	1/16/36/36	0/4/4/4
3	K1H	B	502	-	-	2/16/36/36	0/4/4/4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	K1H	O4-C3-N5-C6
3	B	502	K1H	O2-C3-N5-C6
3	A	502	K1H	C16-C11-N8-C9

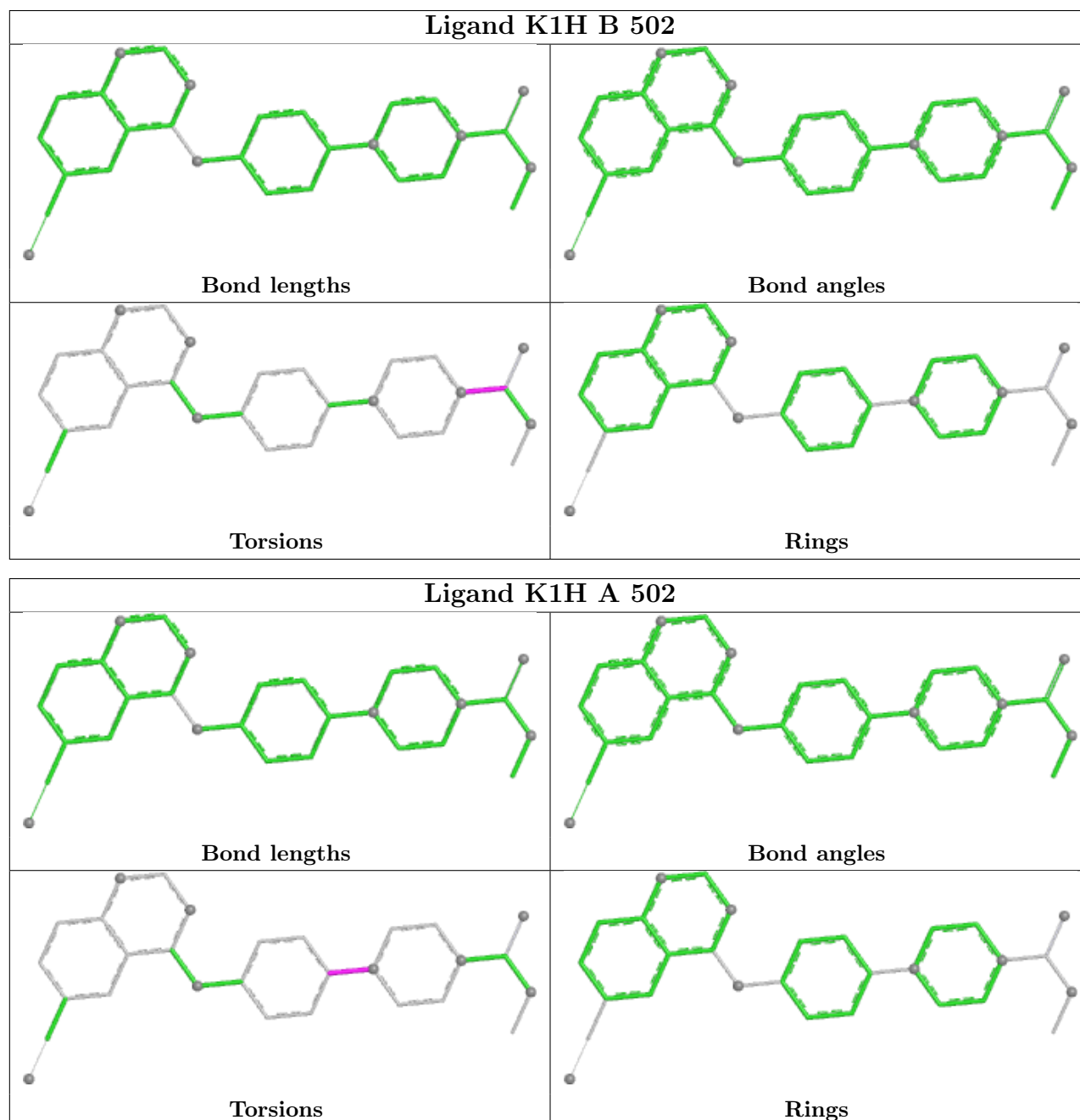
There are no ring outliers.

1 monomer is involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	SO4	0	8

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	273/322 (84%)	0.52	27 (9%) 13 14	22, 53, 103, 123	2 (0%)
1	B	278/322 (86%)	0.78	56 (20%) 3 3	32, 56, 92, 123	0
All	All	551/644 (85%)	0.65	83 (15%) 5 6	22, 54, 101, 123	2 (0%)

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	195	GLY	8.8
1	B	168	PHE	5.5
1	B	252	SER	5.3
1	B	226	LEU	5.0
1	B	171	TYR	4.9
1	B	223	THR	4.9
1	B	258	LEU	4.7
1	B	205	VAL	4.6
1	B	259	CYS	4.6
1	B	251	PHE	4.5
1	A	205	VAL	4.4
1	B	177	THR	4.3
1	A	204	TYR	4.3
1	B	170	PHE	4.2
1	A	184	PRO	4.2
1	B	197	PHE	4.2
1	B	335	ALA	4.1
1	B	230	PHE	4.0
1	B	178	ASN	4.0
1	A	342	THR	3.7
1	B	173	LEU	3.7
1	B	180	PHE	3.5
1	B	253	SER	3.4
1	A	189	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	185	ILE	3.2
1	B	212	VAL	3.2
1	A	175	ASN	3.1
1	B	179	ASN	3.1
1	B	229	GLN	3.1
1	B	250	GLY	3.1
1	B	200	VAL	3.1
1	B	215	LEU	3.1
1	B	192	MET	3.1
1	B	176	VAL	3.0
1	B	210	VAL	3.0
1	A	341	GLN	3.0
1	B	255	GLY	3.0
1	B	198	GLY	2.9
1	B	256	ASP	2.9
1	A	171	TYR	2.9
1	A	226	LEU	2.8
1	B	203	GLY	2.8
1	B	175	ASN	2.8
1	A	206	ASN	2.8
1	A	194	GLU	2.7
1	B	204	TYR	2.7
1	B	199	VAL	2.7
1	B	187	VAL	2.6
1	A	208	THR	2.6
1	A	215	LEU	2.6
1	B	169	SER	2.6
1	B	181	ASP	2.6
1	A	335	ALA	2.5
1	A	165	PHE	2.5
1	A	180	PHE	2.5
1	B	214	LYS	2.5
1	B	201	TYR	2.5
1	A	224	GLU	2.5
1	B	213	LYS	2.5
1	B	254	ASP	2.5
1	B	183	ARG	2.4
1	B	257	ASP	2.4
1	B	227	LYS	2.4
1	A	254	ASP	2.4
1	A	193	GLY	2.4
1	B	190	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	438[A]	HIS	2.3
1	B	166	HIS	2.3
1	B	167	SER	2.3
1	A	344	MET	2.2
1	A	192	MET	2.2
1	B	191	LYS	2.2
1	A	207	ASN	2.2
1	B	165	PHE	2.2
1	B	225	GLU	2.2
1	B	344	MET	2.1
1	B	174	LYS	2.1
1	A	258	LEU	2.1
1	B	228	GLN	2.1
1	A	198	GLY	2.1
1	B	193	GLY	2.1
1	A	256	ASP	2.0
1	B	164	ARG	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	0.74	0.15	84,92,102,103	0
1	SEP	A	346	10/11	0.75	0.13	88,96,104,105	0
1	TPO	B	345	11/12	0.93	0.10	71,76,82,83	0
1	TPO	A	345	11/12	0.93	0.09	83,87,90,93	0

6.3 Carbohydrates [i](#)

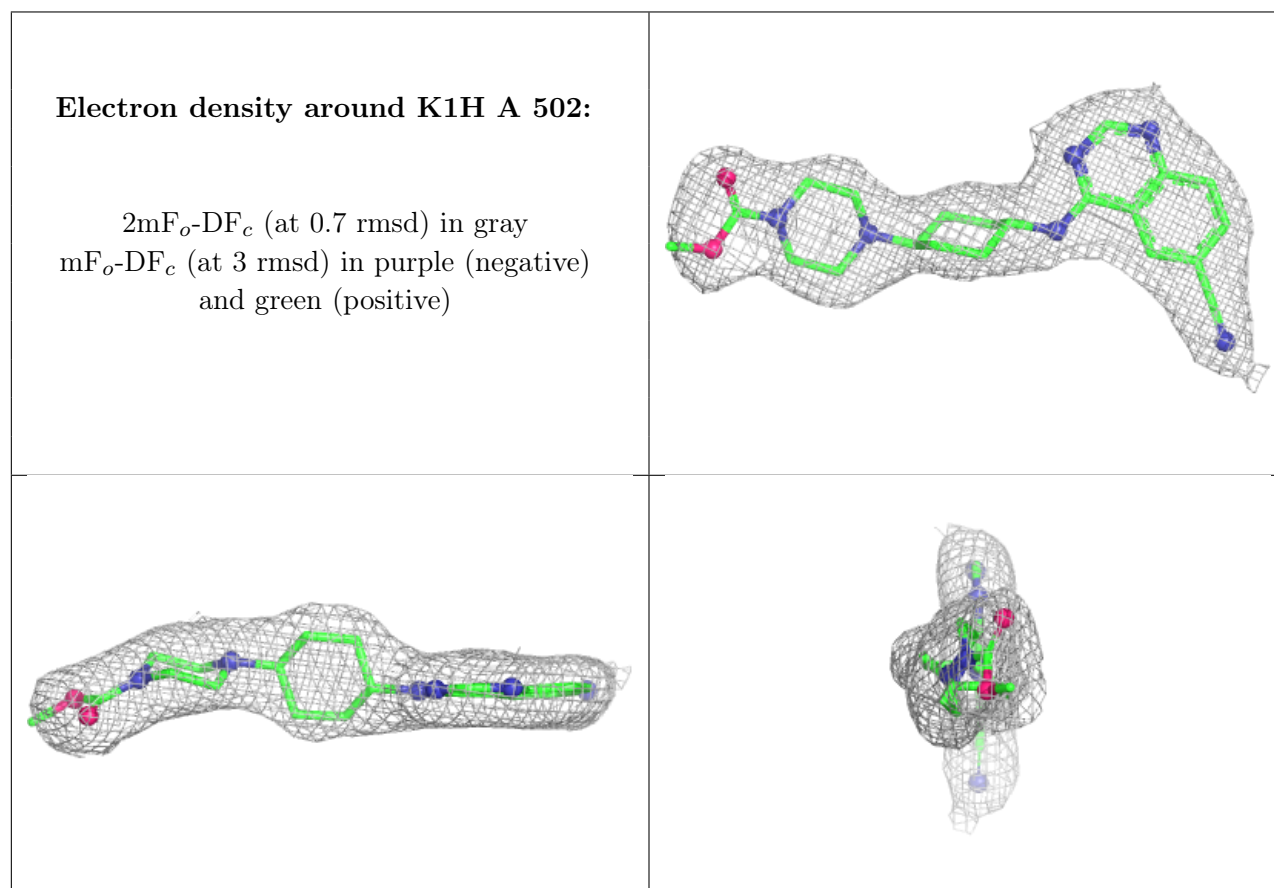
There are no oligosaccharides in this entry.

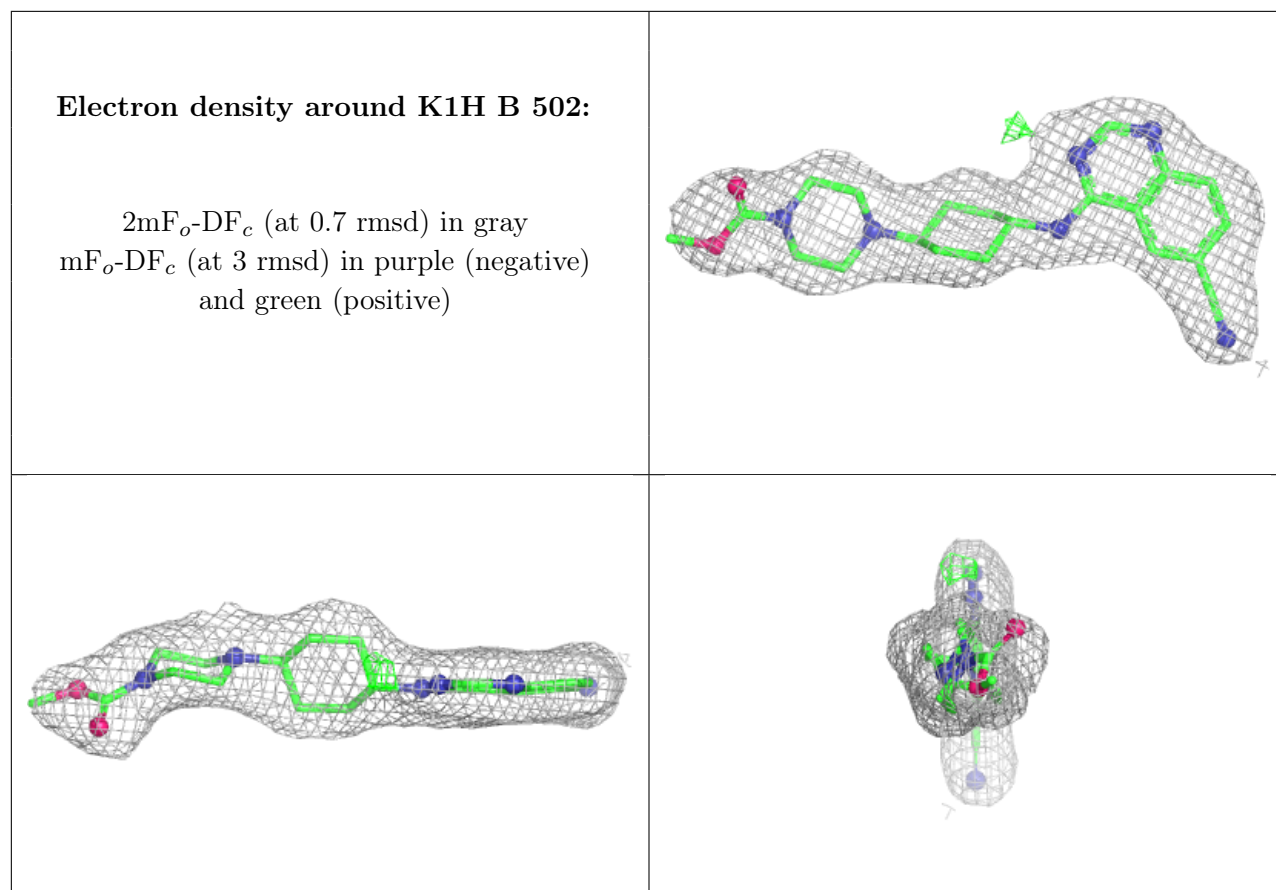
6.4 Ligands [i](#)

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	SO4	A	501	5/5	0.71	0.14	196,196,196,196	0
2	SO4	B	501	5/5	0.78	0.14	86,87,87,88	0
3	K1H	A	502	29/29	0.95	0.07	35,40,59,65	0
3	K1H	B	502	29/29	0.95	0.08	31,39,64,65	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.