



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 04:02 AM UTC

PDB ID : 8QEL / pdb_00008qel
Title : PKR kinase domain- eIF2alpha in complex with compound
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Deposited on : 2023-08-31
Resolution : 2.45 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

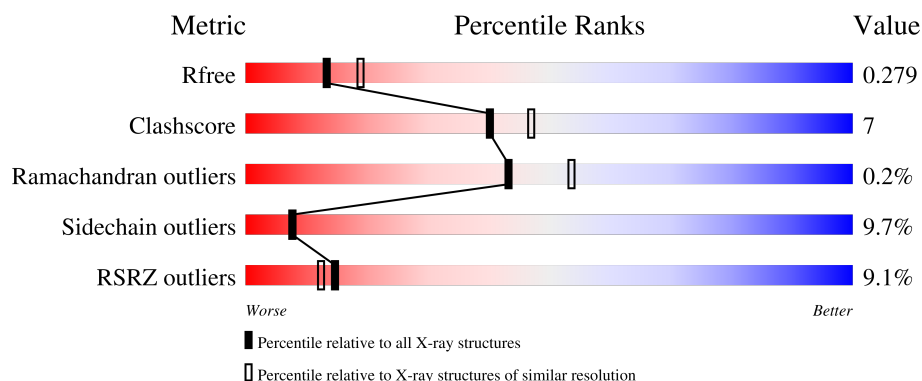
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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	173	10% 77% 13% • 7%
2	B	273	8% 75% 19% • •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3498 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 Eukaryotic translation initiation factor 2 subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	0	0	0
			1314	845	216	248	5			

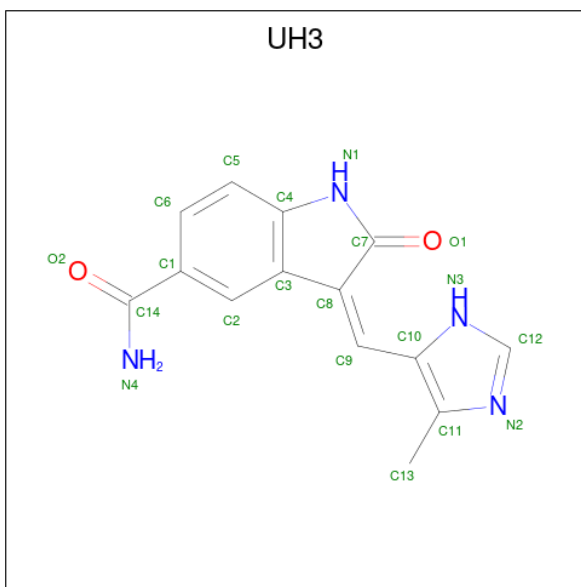
- Molecule 2 is a protein called Interferon-induced, double-stranded RNA-activated protein kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	267	Total	C	N	O	P	S	0	0
			2164	1380	370	406	1	7		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	256	ALA	-	expression tag	UNP P19525
B	257	HIS	-	expression tag	UNP P19525
B	351	SER	-	linker	UNP P19525
B	352	LYS	-	linker	UNP P19525
B	353	ASN	-	linker	UNP P19525
B	354	SER	-	linker	UNP P19525
B	355	SER	-	linker	UNP P19525
B	356	ARG	-	linker	UNP P19525
B	412	ASN	HIS	conflict	UNP P19525

- Molecule 3 is (3 {Z})-3-[(4-methyl-1 {H}-imidazol-5-yl)methylidene]-2-oxidanylidene-1 {H}-indole-5-carboxamide (CCD ID: UH3) (formula: C₁₄H₁₂N₄O₂) (labeled as "Ligand of Interest" by depositor).

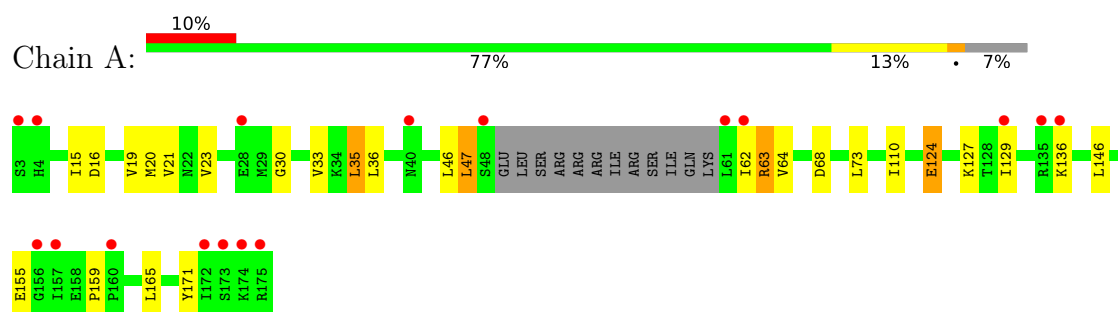


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			20	14	4	2		

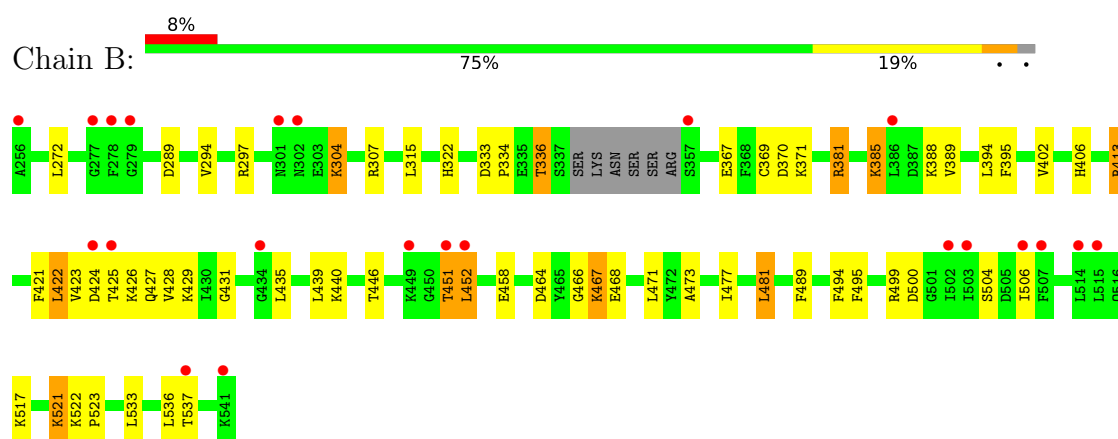
3 Residue-property plots [i](#)

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: Eukaryotic translation initiation factor 2 subunit alpha



- Molecule 2: Interferon-induced, double-stranded RNA-activated protein kinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	85.03Å 85.03Å 168.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	73.64 – 2.45 73.64 – 2.45	Depositor EDS
% Data completeness (in resolution range)	72.3 (73.64-2.45) 72.3 (73.64-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.45Å)	Xtriage
Refinement program	BUSTER 2.11.8 (8-JUN-2022)	Depositor
R, R_{free}	0.241 , 0.278 (Not available) , 0.279	Depositor DCC
R_{free} test set	942 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	76.7	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.032 for -h,-k,l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3498	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: UH3, TPO

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	0.68	0/1338	1.04	0/1802
2	B	0.67	0/2189	1.09	7/2933 (0.2%)
All	All	0.67	0/3527	1.07	7/4735 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	369	CYS	CA-C-N	6.74	129.61	120.38
2	B	369	CYS	C-N-CA	6.74	129.61	120.38
2	B	451	THR	CA-C-N	6.37	133.71	121.54
2	B	451	THR	C-N-CA	6.37	133.71	121.54
2	B	489	PHE	CA-CB-CG	6.11	119.91	113.80
2	B	289	ASP	CA-CB-CG	5.96	118.56	112.60
2	B	494	PHE	CA-CB-CG	5.27	119.07	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1314	0	1320	11	0
2	B	2164	0	2191	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	20	0	0	0	0
All	All	3498	0	3511	46	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 7.

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)
2:B:521:LYS:HZ3	2:B:522:LYS:HE2	1.32	0.95
2:B:413:ARG:HG3	2:B:413:ARG:HH21	1.28	0.94
2:B:333:ASP:HB3	2:B:336:THR:HB	1.61	0.83
1:A:63:ARG:HH11	1:A:63:ARG:H	1.28	0.82
2:B:495:PHE:O	2:B:499:ARG:HG2	1.85	0.76
2:B:468:GLU:HG3	2:B:523:PRO:HB3	1.70	0.72
2:B:521:LYS:NZ	2:B:522:LYS:HE2	2.05	0.71
2:B:421:PHE:HE2	2:B:431:GLY:HA3	1.63	0.62
2:B:413:ARG:NH2	2:B:435:LEU:O	2.35	0.59
2:B:322:HIS:HB2	2:B:367:GLU:HB2	1.87	0.57
2:B:413:ARG:HH21	2:B:413:ARG:CG	2.09	0.57
2:B:371:LYS:HB2	2:B:422:LEU:HB2	1.87	0.56
1:A:21:VAL:HG12	1:A:35:LEU:HD22	1.89	0.55
1:A:30:GLY:HA2	1:A:47:LEU:HD13	1.90	0.54
2:B:477:ILE:O	2:B:481:LEU:HB2	2.08	0.53
2:B:477:ILE:HG22	2:B:481:LEU:HD22	1.90	0.53
2:B:413:ARG:HG3	2:B:413:ARG:NH2	2.08	0.53
2:B:473:ALA:O	2:B:477:ILE:HG12	2.09	0.52
2:B:521:LYS:HZ3	2:B:522:LYS:CE	2.14	0.52
2:B:424:ASP:HB3	2:B:427:GLN:HB2	1.93	0.51
1:A:124:GLU:HA	1:A:127:LYS:HE3	1.92	0.50
2:B:381:ARG:NH2	2:B:481:LEU:O	2.43	0.48
2:B:421:PHE:CE2	2:B:431:GLY:HA3	2.45	0.48
1:A:110:ILE:HG12	1:A:171:TYR:CE1	2.48	0.47
2:B:504:SER:HB3	2:B:506:ILE:HG12	1.97	0.47
2:B:402:VAL:HG12	2:B:406:HIS:CE1	2.50	0.47
2:B:521:LYS:NZ	2:B:522:LYS:CE	2.78	0.45
1:A:19:VAL:HG21	1:A:35:LEU:HD13	1.98	0.45
2:B:381:ARG:HG2	2:B:381:ARG:O	2.15	0.45
2:B:395:PHE:HB2	2:B:481:LEU:HD23	1.98	0.45
2:B:467:LYS:H	2:B:467:LYS:NZ	2.13	0.45
1:A:129:ILE:HD11	1:A:159:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:425:THR:O	2:B:426:LYS:HB2	2.17	0.44
2:B:297:ARG:HD3	2:B:334:PRO:HG3	2.00	0.44
1:A:23:VAL:HG12	1:A:33:VAL:HG12	1.99	0.43
2:B:466:GLY:HA3	2:B:467:LYS:HZ3	1.83	0.43
2:B:533:LEU:HA	2:B:536:LEU:HD12	1.99	0.43
2:B:385:LYS:HE2	2:B:385:LYS:HB2	1.90	0.42
1:A:15:ILE:O	1:A:16:ASP:HB2	2.20	0.42
2:B:423:VAL:HG21	2:B:429:LYS:HE3	2.02	0.42
2:B:402:VAL:CG1	2:B:406:HIS:CE1	3.03	0.41
1:A:20:MET:HG3	1:A:36:LEU:HD12	2.01	0.41
2:B:394:LEU:HD22	2:B:428:VAL:HG13	2.03	0.41
1:A:63:ARG:H	1:A:63:ARG:HD3	1.85	0.41
2:B:304:LYS:O	2:B:307:ARG:HD2	2.21	0.40
2:B:468:GLU:HA	2:B:471:LEU:HD12	2.02	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	157/173 (91%)	153 (98%)	4 (2%)	0	100	100
2	B	262/273 (96%)	249 (95%)	12 (5%)	1 (0%)	30	37
All	All	419/446 (94%)	402 (96%)	16 (4%)	1 (0%)	43	54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	452	LEU

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	145/160 (91%)	132 (91%)	13 (9%)	9	10
2	B	236/245 (96%)	212 (90%)	24 (10%)	7	6
All	All	381/405 (94%)	344 (90%)	37 (10%)	8	8

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	46	LEU
1	A	47	LEU
1	A	62	ILE
1	A	63	ARG
1	A	64	VAL
1	A	68	ASP
1	A	73	LEU
1	A	124	GLU
1	A	136	LYS
1	A	146	LEU
1	A	155	GLU
1	A	165	LEU
2	B	272	LEU
2	B	294	VAL
2	B	304	LYS
2	B	315	LEU
2	B	336	THR
2	B	370	ASP
2	B	381	ARG
2	B	385	LYS
2	B	388	LYS
2	B	389	VAL
2	B	413	ARG
2	B	422	LEU
2	B	439	LEU
2	B	440	LYS

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Mol	Chain	Res	Type
2	B	451	THR
2	B	452	LEU
2	B	458	GLU
2	B	464	ASP
2	B	467	LYS
2	B	481	LEU
2	B	500	ASP
2	B	517	LYS
2	B	521	LYS
2	B	537	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	24	GLN
1	A	170	ASN
2	B	324	ASN
2	B	406	HIS
2	B	459	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	TPO	B	446	2	8,10,11	1.27	1 (12%)	10,14,16	1.56	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
2	TPO	B	446	2	-	1/9/11/13	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	446	TPO	P-OG1	-2.50	1.55	1.59

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	446	TPO	P-OG1-CB	-3.54	113.72	123.33

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	446	TPO	O-C-CA-CB

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](#)

1 ligand is 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
3	UH3	B	4000	-	21,22,22	0.45	0	31,32,32	0.65	1 (3%)

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	UH3	B	4000	-	-	0/8/20/20	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(°)
3	B	4000	UH3	C10-C11-N2	2.11	110.37	107.97

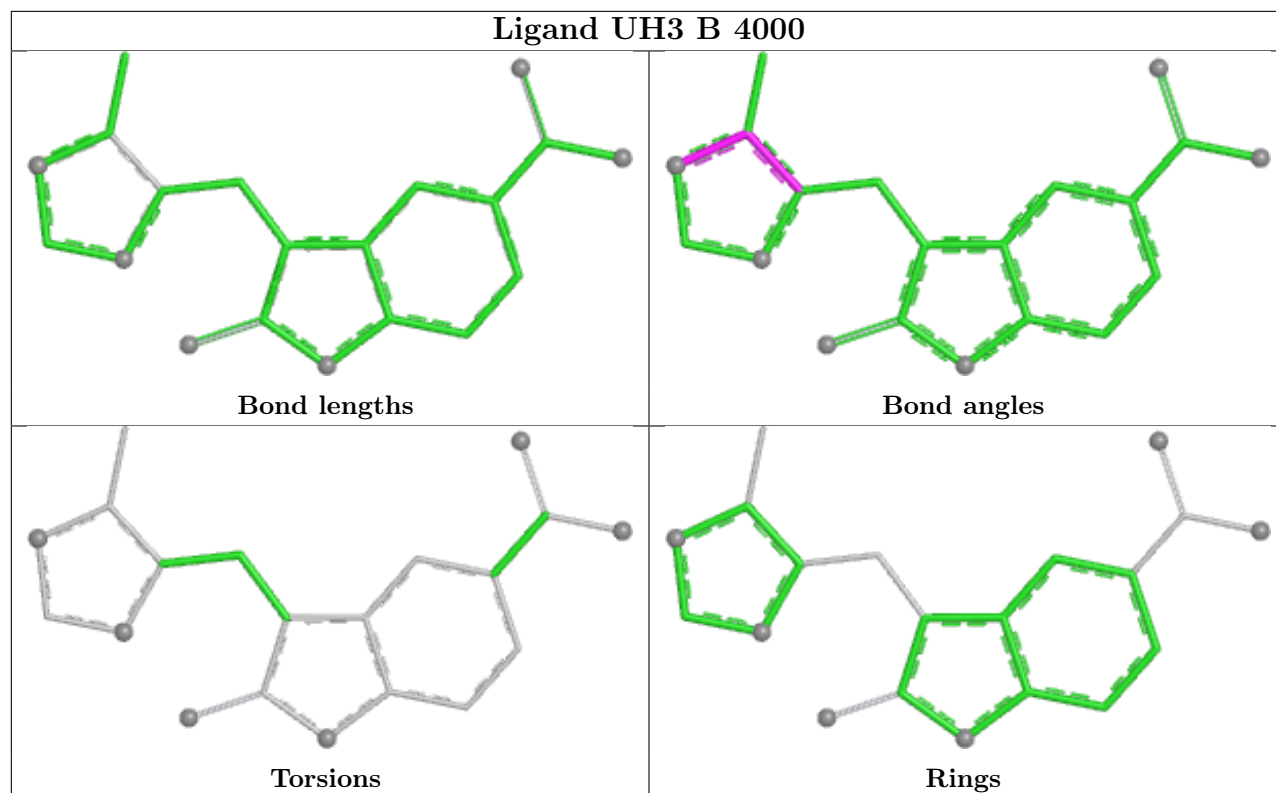
There are no chirality outliers.

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	161/173 (93%)	0.87	17 (10%) 11 9	62, 78, 105, 111	1 (0%)
2	B	266/273 (97%)	0.76	22 (8%) 17 15	56, 78, 103, 112	0
All	All	427/446 (95%)	0.81	39 (9%) 15 12	56, 78, 105, 112	1 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	278	PHE	5.8
1	A	135	ARG	4.5
1	A	61	LEU	4.0
2	B	507	PHE	3.9
1	A	173	SER	3.7
2	B	502	ILE	3.6
1	A	175	ARG	3.4
1	A	3	SER	3.2
2	B	541	LYS	3.1
2	B	301	ASN	3.1
2	B	515	LEU	3.1
2	B	277	GLY	3.0
2	B	279	GLY	3.0
1	A	157	ILE	2.9
2	B	452	LEU	2.9
1	A	174	LYS	2.7
2	B	425	THR	2.7
2	B	451	THR	2.7
1	A	136	LYS	2.6
2	B	302	ASN	2.6
1	A	4	HIS	2.5
2	B	434	GLY	2.5
1	A	48	SER	2.5
1	A	28	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	160	PRO	2.3
1	A	172	ILE	2.3
2	B	256	ALA	2.2
1	A	156	GLY	2.2
2	B	514	LEU	2.2
2	B	506	ILE	2.2
1	A	40	ASN	2.1
2	B	357	SER	2.1
1	A	62	ILE	2.1
2	B	503	ILE	2.1
2	B	386	LEU	2.1
2	B	537	THR	2.1
2	B	449	LYS	2.1
1	A	129	ILE	2.0
2	B	424	ASP	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	TPO	B	446	11/12	0.94	0.09	75,86,92,92	0

6.3 Carbohydrates [i](#)

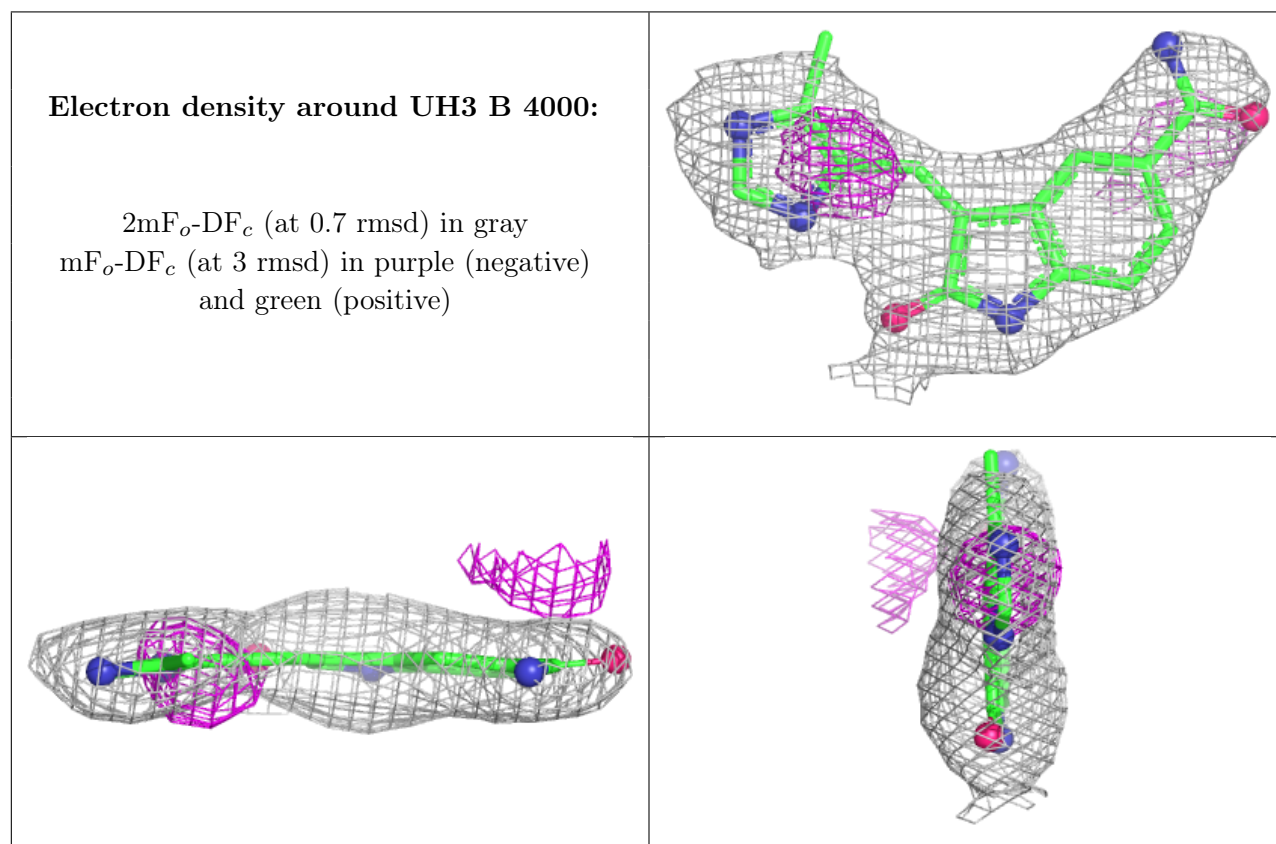
There are no oligosaccharides in this entry.

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
3	UH3	B	4000	20/20	0.91	0.12	70,71,74,74	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.