



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:06 PM UTC

PDB ID : 6ZYF / pdb_00006zyf
Title : Notum_Ghrelin complex
Authors : Zhao, Y.; Jones, E.Y.
Deposited on : 2020-07-31
Resolution : 2.19 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

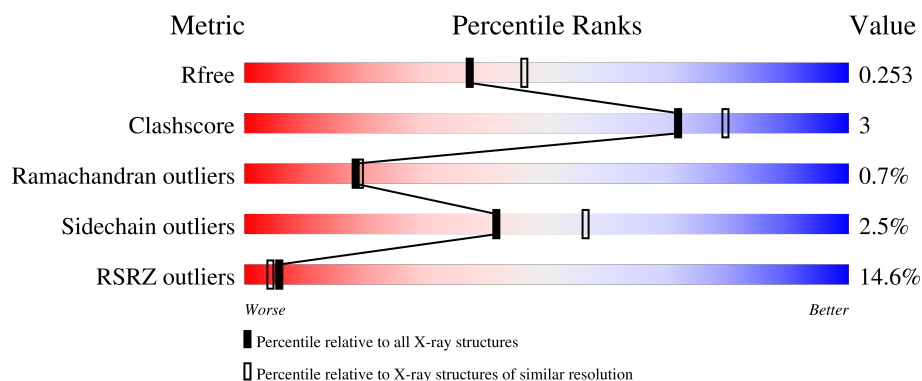
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	383	13% 84% 8% 8%
1	B	383	14% 82% 8% 9%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5730 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 Palmitoleoyl-protein carboxylesterase NOTUM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	0	0	0
			2817	1781	505	513	18			
1	B	349	Total	C	N	O	S	0	0	0
			2796	1768	503	507	18			

There are 28 discrepancies between the modelled and reference sequences:

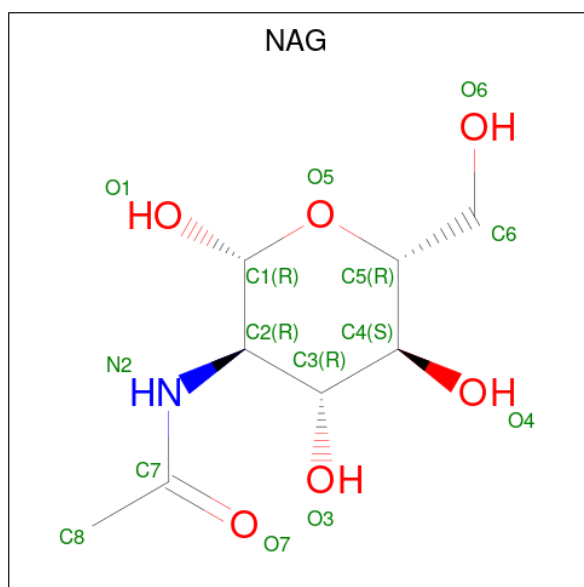
Chain	Residue	Modelled	Actual	Comment	Reference
A	78	GLU	-	expression tag	UNP Q6P988
A	79	THR	-	expression tag	UNP Q6P988
A	80	GLY	-	expression tag	UNP Q6P988
A	232	ALA	SER	conflict	UNP Q6P988
A	330	SER	CYS	conflict	UNP Q6P988
A	452	GLY	-	expression tag	UNP Q6P988
A	453	THR	-	expression tag	UNP Q6P988
A	454	LYS	-	expression tag	UNP Q6P988
A	455	HIS	-	expression tag	UNP Q6P988
A	456	HIS	-	expression tag	UNP Q6P988
A	457	HIS	-	expression tag	UNP Q6P988
A	458	HIS	-	expression tag	UNP Q6P988
A	459	HIS	-	expression tag	UNP Q6P988
A	460	HIS	-	expression tag	UNP Q6P988
B	78	GLU	-	expression tag	UNP Q6P988
B	79	THR	-	expression tag	UNP Q6P988
B	80	GLY	-	expression tag	UNP Q6P988
B	232	ALA	SER	conflict	UNP Q6P988
B	330	SER	CYS	conflict	UNP Q6P988
B	452	GLY	-	expression tag	UNP Q6P988
B	453	THR	-	expression tag	UNP Q6P988
B	454	LYS	-	expression tag	UNP Q6P988
B	455	HIS	-	expression tag	UNP Q6P988
B	456	HIS	-	expression tag	UNP Q6P988
B	457	HIS	-	expression tag	UNP Q6P988

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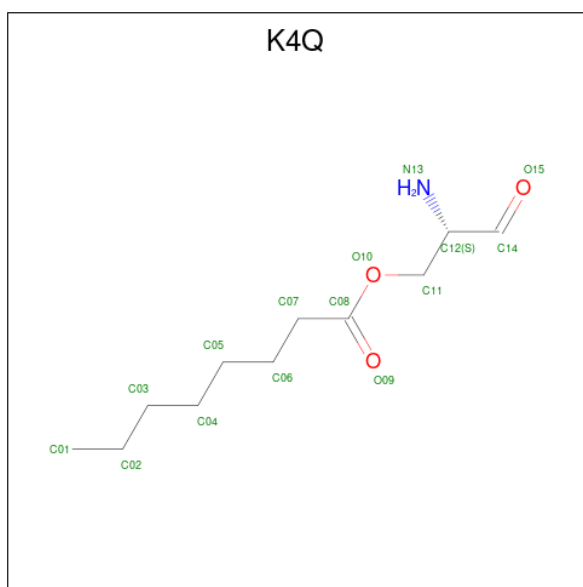
Chain	Residue	Modelled	Actual	Comment	Reference
B	458	HIS	-	expression tag	UNP Q6P988
B	459	HIS	-	expression tag	UNP Q6P988
B	460	HIS	-	expression tag	UNP Q6P988

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



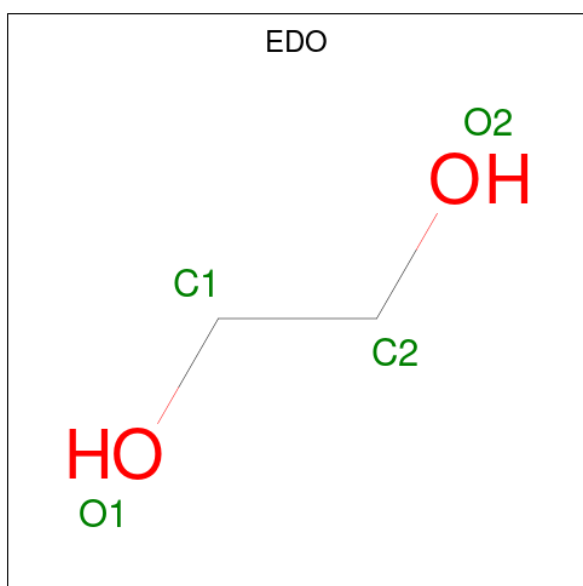
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is [(2 {S})-2-azanyl-3-oxidanylidene-propyl] octanoate (CCD ID: K4Q) (formula: $C_{11}H_{21}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	11	1	3		
3	B	1	Total	C	O	0	0	
			10	8	2			

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

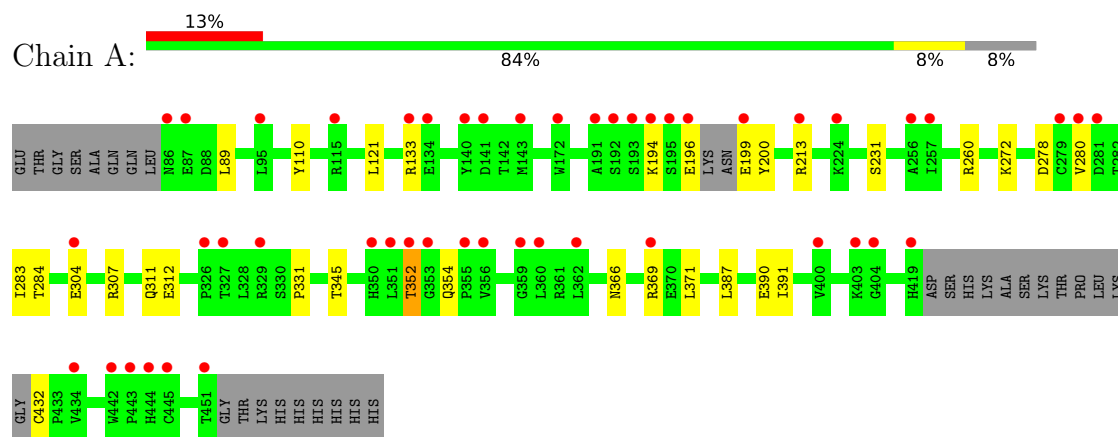
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	27	Total 27	O 27	0	0
5	B	29	Total 29	O 29	0	0

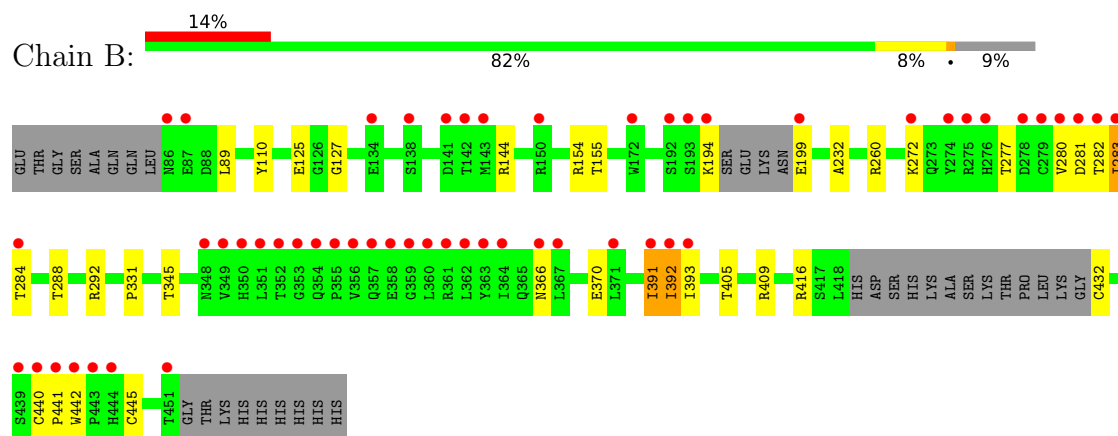
3 Residue-property plots [i](#)

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: Palmitoleoyl-protein carboxylesterase NOTUM



- Molecule 1: Palmitoleoyl-protein carboxylesterase NOTUM



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	75.42Å 184.07Å 61.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.04 – 2.19 92.04 – 2.19	Depositor EDS
% Data completeness (in resolution range)	98.7 (92.04-2.19) 98.8 (92.04-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.231 , 0.252 0.232 , 0.253	Depositor DCC
R_{free} test set	2289 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	38.0	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5730	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% 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: NAG, EDO, K4Q

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	0.12	0/2893	0.35	0/3935
1	B	0.11	0/2871	0.37	0/3905
All	All	0.11	0/5764	0.36	0/7840

There are no bond length outliers.

There are no bond angle outliers.

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	2817	0	2706	16	0
1	B	2796	0	2695	21	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
3	A	15	0	0	0	0
3	B	10	0	0	1	0
4	B	8	0	12	0	0
5	A	27	0	0	0	0
5	B	29	0	0	0	0
All	All	5730	0	5439	37	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 3.

All (37) 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:194:LYS:NZ	1:A:196:GLU:O	2.13	0.78
1:B:282:THR:HG22	1:B:283:ILE:H	1.59	0.67
1:A:366:ASN:ND2	1:A:369:ARG:HH22	1.99	0.61
1:B:391:ILE:O	1:B:393:ILE:N	2.28	0.61
1:B:260:ARG:HG2	1:B:331:PRO:HG2	1.85	0.57
1:B:154:ARG:HG3	1:B:155:THR:HG23	1.88	0.54
1:A:366:ASN:HD22	1:A:369:ARG:HH22	1.54	0.52
1:B:391:ILE:HG13	1:B:392:ILE:H	1.76	0.50
1:A:133:ARG:CZ	1:A:199:GLU:HB3	2.41	0.50
1:B:391:ILE:C	1:B:393:ILE:H	2.19	0.48
1:B:282:THR:C	1:B:284:THR:H	2.22	0.47
1:B:391:ILE:HG23	1:B:392:ILE:HG23	1.98	0.46
1:A:89:LEU:HB3	1:A:110:TYR:HB3	1.98	0.46
1:A:283:ILE:HG13	1:A:284:THR:HG23	1.98	0.46
1:B:194:LYS:HE2	1:B:199:GLU:CD	2.41	0.45
1:A:194:LYS:HZ1	1:A:196:GLU:HB3	1.82	0.45
1:B:366:ASN:O	1:B:370:GLU:HG2	2.16	0.45
1:B:440:CYS:HA	1:B:441:PRO:HD3	1.80	0.45
1:A:194:LYS:HZ3	1:A:196:GLU:C	2.14	0.45
1:A:133:ARG:NH1	1:A:200:TYR:H	2.15	0.44
1:B:288:THR:O	1:B:292:ARG:HG3	2.18	0.44
1:B:282:THR:HG22	1:B:283:ILE:N	2.31	0.43
1:B:283:ILE:O	1:B:345:THR:HG22	2.18	0.43
1:B:440:CYS:HB2	1:B:442:TRP:NE1	2.33	0.43
1:B:232:ALA:HB1	3:B:502:K4Q:C08	2.49	0.43
1:A:278:ASP:O	1:A:280:VAL:HG22	2.19	0.42
1:A:311:GLN:HG2	1:A:312:GLU:N	2.34	0.42
1:B:409:ARG:HA	1:B:409:ARG:HD2	1.86	0.42
1:A:283:ILE:O	1:A:345:THR:HG22	2.20	0.42
1:A:231:SER:HB3	1:A:390:GLU:HG2	2.01	0.42
1:B:89:LEU:HB3	1:B:110:TYR:HB3	2.01	0.42
1:B:280:VAL:HG23	1:B:281:ASP:H	1.85	0.42
1:A:260:ARG:HG2	1:A:331:PRO:HG2	2.02	0.41
1:B:391:ILE:HG13	1:B:392:ILE:N	2.35	0.41
1:A:304:GLU:OE1	1:A:307:ARG:NH2	2.53	0.41
1:B:283:ILE:HG13	1:B:284:THR:HG23	2.03	0.40
1:A:352:THR:HB	1:A:354:GLN:HG3	2.04	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	346/383 (90%)	330 (95%)	15 (4%)	1 (0%)	36	42
1	B	343/383 (90%)	327 (95%)	12 (4%)	4 (1%)	10	8
All	All	689/766 (90%)	657 (95%)	27 (4%)	5 (1%)	18	19

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	283	ILE
1	B	391	ILE
1	B	392	ILE
1	A	391	ILE
1	B	127	GLY

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	305/332 (92%)	298 (98%)	7 (2%)	44	59
1	B	303/332 (91%)	295 (97%)	8 (3%)	40	55
All	All	608/664 (92%)	593 (98%)	15 (2%)	42	56

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	121	LEU

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Mol	Chain	Res	Type
1	A	213	ARG
1	A	272	LYS
1	A	352	THR
1	A	371	LEU
1	A	387	LEU
1	A	432	CYS
1	B	125	GLU
1	B	144	ARG
1	B	272	LYS
1	B	277	THR
1	B	405	THR
1	B	416	ARG
1	B	432	CYS
1	B	445	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	102	ASN
1	A	366	ASN
1	B	92	HIS
1	B	102	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAG	B	501	1	14,14,15	0.29	0	17,19,21	0.41	0
4	EDO	B	504	-	3,3,3	0.43	0	2,2,2	0.38	0
2	NAG	A	501	1	14,14,15	0.32	0	17,19,21	0.45	0
3	K4Q	A	502	-	13,14,14	1.04	2 (15%)	10,15,15	1.24	1 (10%)
3	K4Q	B	502	-	9,9,14	1.11	1 (11%)	9,9,15	0.95	0
4	EDO	B	503	-	3,3,3	0.43	0	2,2,2	0.37	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	NAG	B	501	1	-	2/6/23/26	0/1/1/1
4	EDO	B	504	-	-	0/1/1/1	-
2	NAG	A	501	1	-	2/6/23/26	0/1/1/1
3	K4Q	A	502	-	-	3/12/14/14	-
3	K4Q	B	502	-	-	0/7/7/14	-
4	EDO	B	503	-	-	0/1/1/1	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	502	K4Q	O10-C08	2.90	1.40	1.30
3	A	502	K4Q	O10-C08	2.45	1.40	1.33
3	A	502	K4Q	O10-C11	-2.10	1.40	1.45

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	502	K4Q	O10-C08-C07	3.00	120.97	111.83

There are no chirality outliers.

All (7) torsion outliers are listed below:

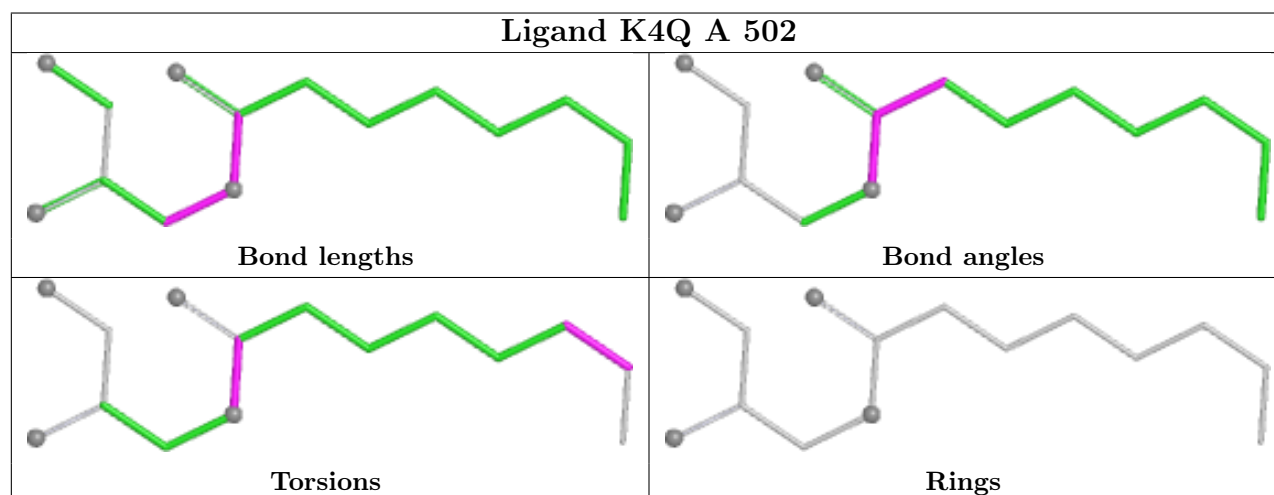
Mol	Chain	Res	Type	Atoms
2	A	501	NAG	C4-C5-C6-O6
2	A	501	NAG	O5-C5-C6-O6
3	A	502	K4Q	C01-C02-C03-C04
3	A	502	K4Q	O09-C08-O10-C11
2	B	501	NAG	C4-C5-C6-O6
3	A	502	K4Q	C07-C08-O10-C11
2	B	501	NAG	O5-C5-C6-O6

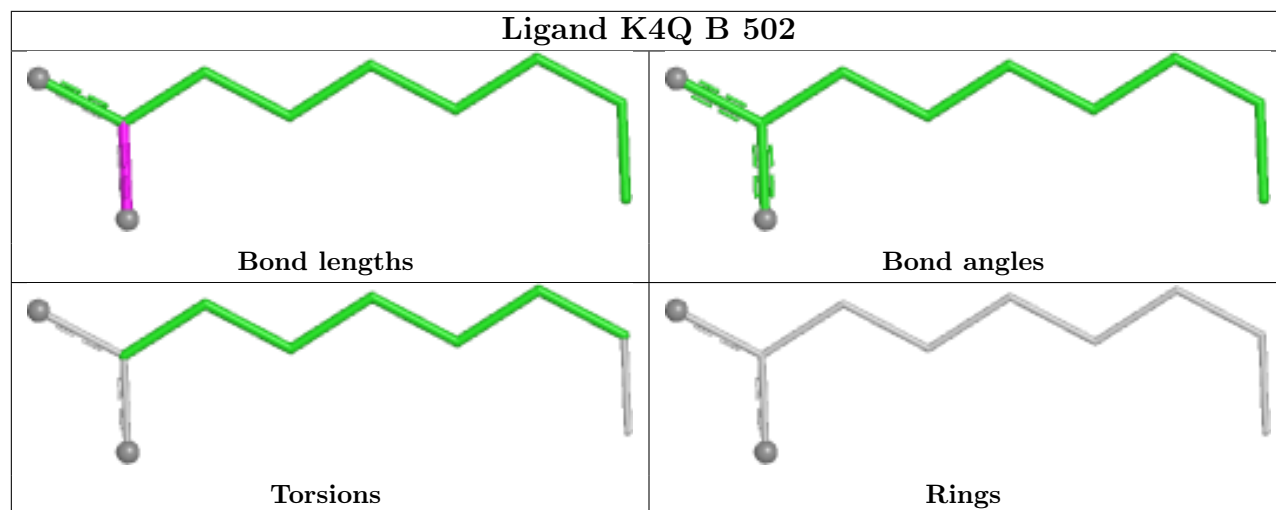
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	K4Q	1	0

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





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	352/383 (91%)	0.79	48 (13%) 7 5	31, 50, 88, 140	0
1	B	349/383 (91%)	0.91	54 (15%) 5 4	27, 48, 103, 165	0
All	All	701/766 (91%)	0.85	102 (14%) 6 4	27, 50, 101, 165	0

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	442	TRP	8.7
1	B	441	PRO	7.8
1	B	440	CYS	6.1
1	B	194	LYS	5.2
1	B	283	ILE	5.1
1	B	356	VAL	5.0
1	B	444	HIS	4.8
1	A	353	GLY	4.6
1	B	355	PRO	4.6
1	B	352	THR	4.2
1	A	87	GLU	4.2
1	A	451	THR	4.1
1	B	451	THR	4.1
1	A	86	ASN	4.0
1	B	280	VAL	3.9
1	B	199	GLU	3.9
1	A	196	GLU	3.9
1	A	444	HIS	3.9
1	B	359	GLY	3.8
1	A	195	SER	3.8
1	B	443	PRO	3.8
1	B	86	ASN	3.7
1	A	352	THR	3.7
1	B	353	GLY	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	359	GLY	3.6
1	B	391	ILE	3.6
1	B	439	SER	3.5
1	B	172	TRP	3.4
1	B	349	VAL	3.4
1	A	194	LYS	3.3
1	A	419	HIS	3.2
1	A	434	VAL	3.1
1	B	350	HIS	3.1
1	A	281	ASP	3.1
1	A	191	ALA	3.1
1	A	143	MET	3.0
1	A	362	LEU	3.0
1	B	364	ILE	3.0
1	B	393	ILE	2.9
1	B	284	THR	2.9
1	A	224	LYS	2.9
1	B	282	THR	2.8
1	A	256	ALA	2.8
1	B	134	GLU	2.8
1	A	355	PRO	2.8
1	A	280	VAL	2.8
1	A	257	ILE	2.8
1	A	115	ARG	2.7
1	B	371	LEU	2.7
1	B	357	GLN	2.7
1	B	143	MET	2.7
1	B	192	SER	2.7
1	B	193	SER	2.7
1	A	213	ARG	2.7
1	B	362	LEU	2.7
1	B	141	ASP	2.7
1	A	193	SER	2.6
1	A	304	GLU	2.6
1	B	366	ASN	2.6
1	A	356	VAL	2.6
1	A	351	LEU	2.5
1	B	351	LEU	2.5
1	A	172	TRP	2.5
1	B	360	LEU	2.5
1	A	442	TRP	2.5
1	A	199	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	329	ARG	2.5
1	A	141	ASP	2.4
1	B	138	SER	2.4
1	A	369	ARG	2.4
1	A	445	CYS	2.4
1	B	274	TYR	2.3
1	B	276	HIS	2.3
1	B	348	ASN	2.3
1	B	392	ILE	2.3
1	B	278	ASP	2.3
1	A	133	ARG	2.2
1	B	272	LYS	2.2
1	A	95	LEU	2.2
1	A	140	TYR	2.2
1	B	281	ASP	2.2
1	B	142	THR	2.2
1	B	358	GLU	2.1
1	A	360	LEU	2.1
1	A	192	SER	2.1
1	B	363	TYR	2.1
1	A	326	PRO	2.1
1	A	327	THR	2.1
1	B	150	ARG	2.1
1	A	400	VAL	2.1
1	B	279	CYS	2.1
1	B	354	GLN	2.1
1	B	87	GLU	2.0
1	B	367	LEU	2.0
1	B	361	ARG	2.0
1	A	443	PRO	2.0
1	A	403	LYS	2.0
1	A	134	GLU	2.0
1	B	275	ARG	2.0
1	A	279	CYS	2.0
1	A	350	HIS	2.0
1	A	404	GLY	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

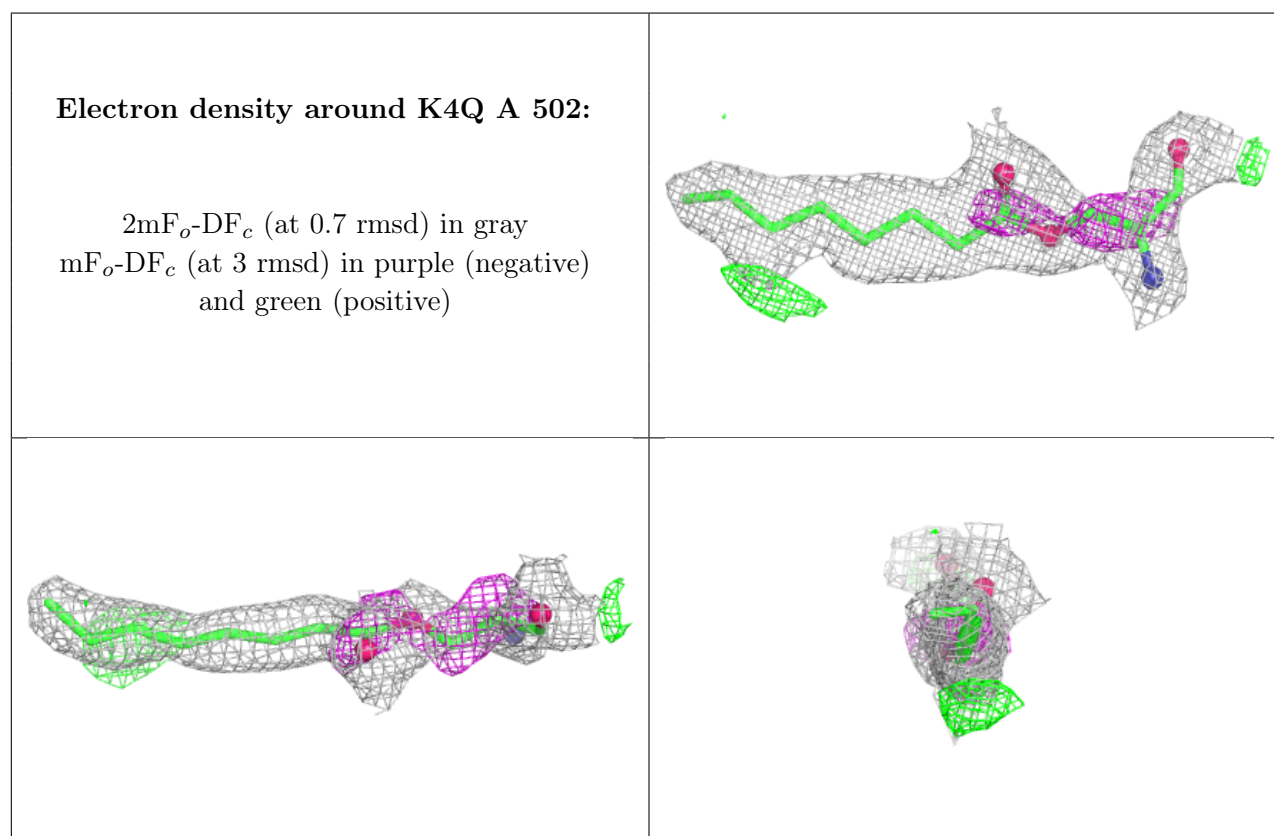
There are no oligosaccharides in this entry.

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.

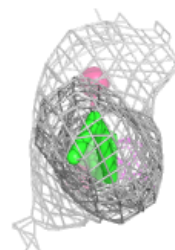
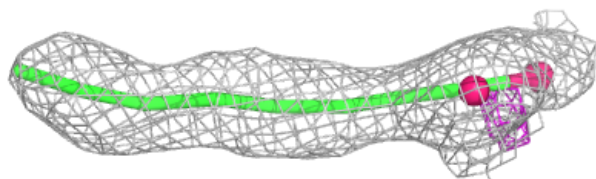
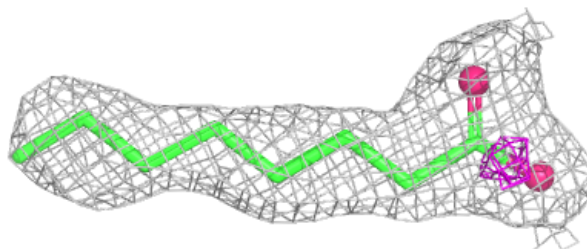
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	A	501	14/15	0.73	0.15	77,81,84,85	0
3	K4Q	A	502	15/15	0.77	0.17	42,47,56,57	0
2	NAG	B	501	14/15	0.78	0.14	73,77,82,83	0
3	K4Q	B	502	10/15	0.88	0.14	46,51,53,55	0
4	EDO	B	504	4/4	0.90	0.15	41,48,50,52	0
4	EDO	B	503	4/4	0.96	0.07	33,39,39,40	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 K4Q B 502:

$2mF_o-DF_c$ (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.