



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:04 PM UTC

PDB ID : 5N22 / pdb_00005n22
Title : Structure of xEco2 acetyltransferase domain bound to K106-CoA conjugate
Authors : Chao, W.C.H.; Wade, B.O.; Singleton, M.R.
Deposited on : 2017-02-07
Resolution : 1.99 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

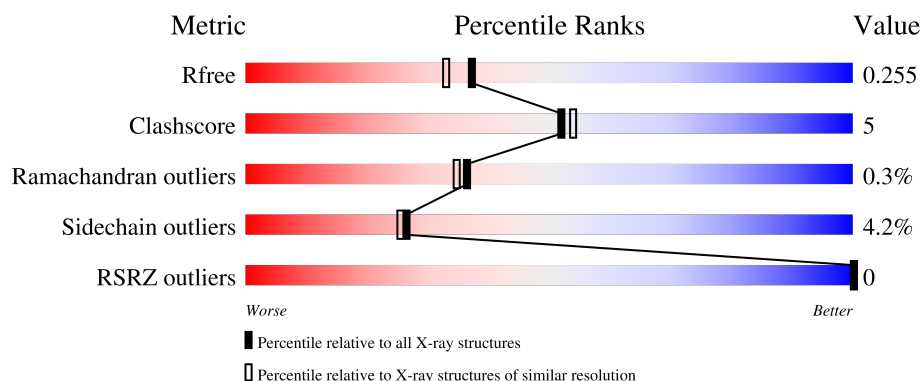
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	183	
1	B	183	
1	C	183	
1	D	183	
2	E	13	

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Mol	Chain	Length	Quality of chain
2	G	13	 69%31%
2	J	13	 8%92%
2	L	13	 8%92%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11698 atoms, of which 5693 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 XEco2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	168	Total	C	H	N	O	S	0	0	0
			2691	861	1348	225	247	10			
1	B	168	Total	C	H	N	O	S	0	0	0
			2688	861	1346	224	247	10			
1	C	168	Total	C	H	N	O	S	0	0	0
			2696	863	1352	225	246	10			
1	D	167	Total	C	H	N	O	S	0	0	0
			2677	858	1341	223	245	10			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	520	GLY	-	expression tag	UNP A8QZK6
A	521	SER	-	expression tag	UNP A8QZK6
A	522	MET	-	expression tag	UNP A8QZK6
B	520	GLY	-	expression tag	UNP A8QZK6
B	521	SER	-	expression tag	UNP A8QZK6
B	522	MET	-	expression tag	UNP A8QZK6
C	520	GLY	-	expression tag	UNP A8QZK6
C	521	SER	-	expression tag	UNP A8QZK6
C	522	MET	-	expression tag	UNP A8QZK6
D	520	GLY	-	expression tag	UNP A8QZK6
D	521	SER	-	expression tag	UNP A8QZK6
D	522	MET	-	expression tag	UNP A8QZK6

- Molecule 2 is a protein called GLY-ALA-LYS-LYX-ASP-GLN-TYR-PHE-LEU.

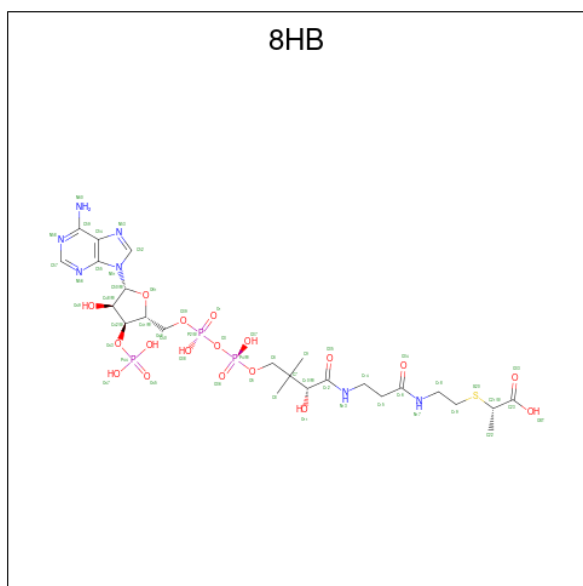
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	9	Total	C	H	N	O	0	0	0
			147	50	72	12	13			
2	G	9	Total	C	H	N	O	0	0	0
			147	50	72	12	13			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	1	Total	C	H	N	O	0	0	0
			20	6	11	2	1			
2	L	1	Total	C	H	N	O	0	0	0
			20	6	11	2	1			

- Molecule 3 is (2 {S})-2-[2-[3-[(2 {R})-4-[[[(2 {R}),3 {S}),4 {R}),5 {R}]]-5-(6-aminopurin-9-yl)-4-oxidanyl-3-phosphonooxy-oxolan-2-yl]methoxy-oxidanyl-phosphoryl]oxy-oxidanyl-phosphoryl]oxy-3,3-dimethyl-2-oxidanyl-butanoyl]amino]propanoylamino]ethylsulfanyl]propanoic acid (CCD ID: 8HB) (formula: C₂₄H₄₀N₇O₁₈P₃S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	E	1	Total	C	H	N	O	P	S	0	0
			87	24	35	7	17	3	1		
3	G	1	Total	C	H	N	O	P	S	0	0
			87	24	35	7	17	3	1		
3	J	1	Total	C	H	N	O	P	S	0	0
			87	24	35	7	17	3	1		
3	L	1	Total	C	H	N	O	P	S	0	0
			87	24	35	7	17	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	54	Total O	0	0
			54 54		
4	B	66	Total O	0	0
			66 66		

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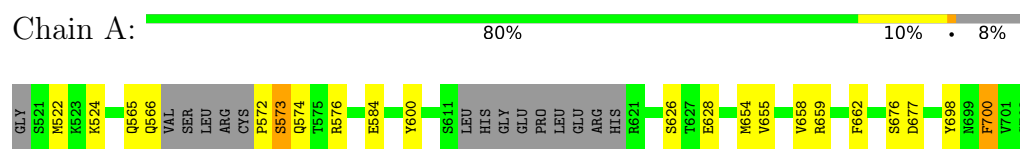
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	51	Total 51	O 51	0	0
4	D	62	Total 62	O 62	0	0
4	E	9	Total 9	O 9	0	0
4	G	8	Total 8	O 8	0	0
4	J	6	Total 6	O 6	0	0
4	L	8	Total 8	O 8	0	0

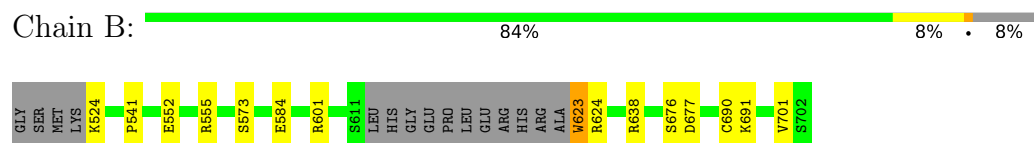
3 Residue-property plots

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.

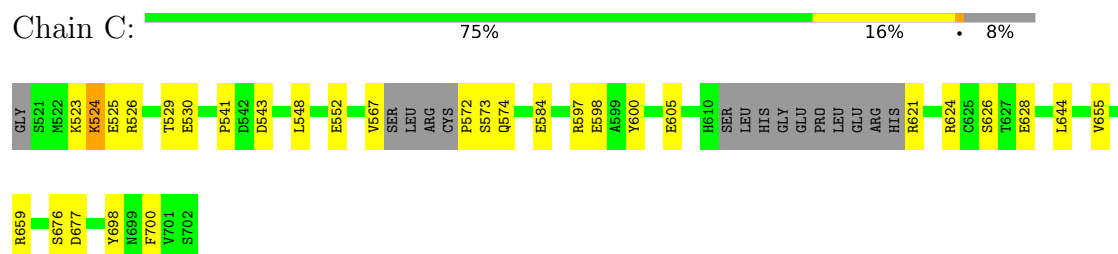
• Molecule 1: XEco2



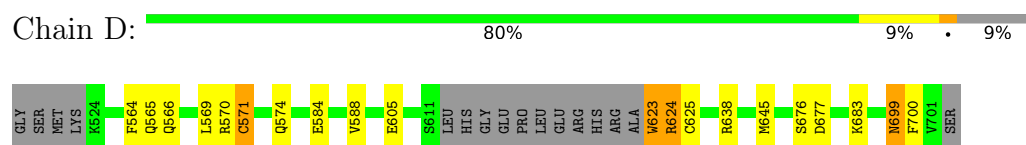
• Molecule 1: XEco2



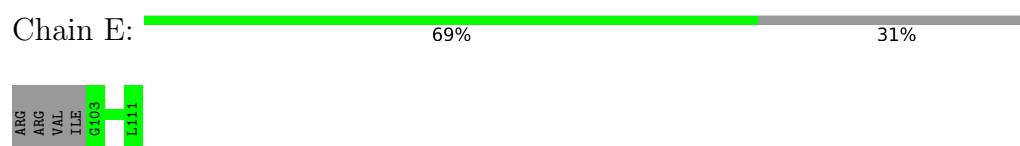
• Molecule 1: XEco2



• Molecule 1: XEco2



• Molecule 2: GLY-ALA-LYS-LYX-ASP-GLN-TYR-PHE-LEU



• Molecule 2: GLY-ALA-LYS-LYX-ASP-GLN-TYR-PHE-LEU



● Molecule 2: GLY-ALA-LYS-LYX-ASP-GLN-TYR-PHE-LEU



● Molecule 2: GLY-ALA-LYS-LYX-ASP-GLN-TYR-PHE-LEU



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	107.24Å 57.77Å 70.95Å 90.00° 89.97° 90.00°	Depositor
Resolution (Å)	59.16 – 1.99 59.16 – 1.99	Depositor EDS
% Data completeness (in resolution range)	98.5 (59.16-1.99) 98.4 (59.16-1.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.72 (at 1.98Å)	Xtriage
Refinement program	PHENIX (dev_2664: ???)	Depositor
R, R_{free}	0.211 , 0.253 0.212 , 0.255	Depositor DCC
R_{free} test set	2864 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.263	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.477 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11698	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.17% 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: 8HB

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	0.56	0/1373	0.68	0/1853
1	B	0.56	0/1373	0.69	0/1858
1	C	0.57	0/1374	0.66	0/1855
1	D	0.60	1/1367 (0.1%)	0.70	0/1850
2	E	0.63	0/76	0.76	0/99
2	G	0.71	0/76	0.77	0/99
2	J	1.11	0/8	1.26	0/8
2	L	1.51	0/8	1.69	0/8
All	All	0.58	1/5655 (0.0%)	0.69	0/7630

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	571	CYS	CB-SG	-5.75	1.62	1.81

There are no bond angle outliers.

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	1343	1348	1348	12	0
1	B	1342	1346	1346	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1344	1352	1352	16	0
1	D	1336	1341	1341	19	0
2	E	75	72	72	0	0
2	G	75	72	72	0	0
2	J	9	11	10	2	0
2	L	9	11	10	2	0
3	E	52	35	0	0	0
3	G	52	35	0	0	0
3	J	52	35	0	0	0
3	L	52	35	0	0	0
4	A	54	0	0	0	0
4	B	66	0	0	2	0
4	C	51	0	0	0	1
4	D	62	0	0	4	0
4	E	9	0	0	0	0
4	G	8	0	0	0	0
4	J	6	0	0	2	0
4	L	8	0	0	1	0
All	All	6005	5693	5551	57	1

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 (57) 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:D:570:ARG:NH2	1:D:699:ASN:OD1	2.01	0.93
2:J:2:LYS:N	4:J:201:HOH:O	2.03	0.90
2:L:2:LYS:O	4:L:201:HOH:O	2.03	0.77
1:C:574:GLN:N	1:C:574:GLN:OE1	2.18	0.75
1:A:576:ARG:NH1	1:A:662:PHE:O	2.23	0.70
1:D:625:CYS:SG	1:D:700:PHE:CE2	2.84	0.70
1:D:605:GLU:HB3	1:D:623:TRP:CD1	2.32	0.63
1:D:584:GLU:OE1	1:D:584:GLU:N	2.34	0.60
1:D:566:GLN:NE2	4:D:802:HOH:O	2.35	0.59
1:C:526:ARG:NH2	1:C:543:ASP:OD2	2.36	0.58
1:A:572:PRO:HD2	1:A:574:GLN:CD	2.31	0.55
1:B:552:GLU:HG2	1:B:555:ARG:NH2	2.23	0.54
1:C:600:TYR:OH	1:D:571:CYS:HB2	2.09	0.53
1:D:625:CYS:SG	1:D:700:PHE:HE2	2.29	0.53
1:D:588:VAL:HG11	1:D:645:MET:HE2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:623:TRP:CE3	1:D:623:TRP:N	2.78	0.51
1:D:683:LYS:NZ	4:D:801:HOH:O	2.30	0.51
1:A:700:PHE:O	1:A:700:PHE:HD2	1.94	0.50
1:B:676:SER:O	1:B:677:ASP:C	2.53	0.50
1:D:624:ARG:HD2	4:D:805:HOH:O	2.11	0.50
2:J:2:LYS:CA	4:J:201:HOH:O	2.57	0.50
1:A:572:PRO:HD2	1:A:574:GLN:NE2	2.28	0.49
1:C:676:SER:HA	1:C:698:TYR:O	2.12	0.49
1:B:541:PRO:HB3	1:B:573:SER:O	2.13	0.49
1:A:676:SER:O	1:A:677:ASP:C	2.56	0.48
1:C:626:SER:OG	1:C:628:GLU:OE2	2.32	0.47
1:B:584:GLU:N	1:B:584:GLU:OE1	2.47	0.47
1:C:572:PRO:C	1:C:574:GLN:OE1	2.58	0.47
1:D:605:GLU:HB2	1:D:624:ARG:HG3	1.97	0.47
1:A:573:SER:O	1:A:573:SER:OG	2.32	0.46
1:A:626:SER:OG	1:A:628:GLU:OE1	2.33	0.46
1:D:564:PHE:HE1	1:D:566:GLN:HG2	1.82	0.44
1:A:676:SER:HA	1:A:698:TYR:O	2.17	0.44
1:C:676:SER:O	1:C:677:ASP:C	2.59	0.44
1:D:676:SER:O	1:D:677:ASP:C	2.60	0.44
1:D:570:ARG:CZ	1:D:699:ASN:OD1	2.65	0.43
1:D:677:ASP:O	2:L:2:LYS:HE2	2.18	0.43
1:A:655:VAL:O	1:A:659:ARG:HG3	2.17	0.43
1:B:690:CYS:O	1:B:691:LYS:HB2	2.18	0.43
1:B:701:VAL:HG22	4:B:803:HOH:O	2.19	0.43
1:C:524:LYS:HG2	1:C:525:GLU:O	2.19	0.43
1:C:605:GLU:OE2	1:C:624:ARG:NH2	2.50	0.43
1:A:654:MET:O	1:A:658:VAL:HG23	2.18	0.42
1:C:524:LYS:HG2	1:C:525:GLU:N	2.34	0.42
1:C:541:PRO:HB3	1:C:573:SER:HA	2.02	0.42
1:D:624:ARG:CD	4:D:805:HOH:O	2.67	0.42
1:B:601:ARG:NH2	4:B:808:HOH:O	2.53	0.41
1:C:655:VAL:O	1:C:659:ARG:HG3	2.21	0.41
1:C:548:LEU:O	1:C:552:GLU:HG3	2.20	0.41
1:C:572:PRO:N	1:C:574:GLN:OE1	2.53	0.41
1:A:584:GLU:OE1	1:A:584:GLU:N	2.54	0.41
1:A:600:TYR:CD1	1:A:600:TYR:N	2.89	0.40
1:B:623:TRP:CE3	1:B:623:TRP:HA	2.56	0.40
1:C:526:ARG:HH22	1:C:543:ASP:CG	2.29	0.40
1:C:529:THR:HG22	1:C:530:GLU:N	2.37	0.40
1:D:623:TRP:HZ3	1:D:683:LYS:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:588:VAL:HG11	1:D:645:MET:CE	2.51	0.40

All (1) 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)
4:C:838:HOH:O	4:C:842:HOH:O[2_745]	2.13	0.07

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	162/183 (88%)	157 (97%)	4 (2%)	1 (1%)	21	17
1	B	164/183 (90%)	160 (98%)	4 (2%)	0	100	100
1	C	162/183 (88%)	157 (97%)	5 (3%)	0	100	100
1	D	163/183 (89%)	159 (98%)	3 (2%)	1 (1%)	21	17
2	E	7/13 (54%)	7 (100%)	0	0	100	100
2	G	7/13 (54%)	7 (100%)	0	0	100	100
All	All	665/758 (88%)	647 (97%)	16 (2%)	2 (0%)	36	35

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	699	ASN
1	A	565	GLN

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	149/162 (92%)	144 (97%)	5 (3%)	32	33
1	B	150/162 (93%)	146 (97%)	4 (3%)	39	42
1	C	149/162 (92%)	140 (94%)	9 (6%)	17	14
1	D	149/162 (92%)	143 (96%)	6 (4%)	28	27
2	E	7/11 (64%)	7 (100%)	0	100	100
2	G	7/11 (64%)	7 (100%)	0	100	100
2	J	1/11 (9%)	0	1 (100%)	0	0
2	L	1/11 (9%)	0	1 (100%)	0	0
All	All	613/692 (89%)	587 (96%)	26 (4%)	26	25

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	522	MET
1	A	524	LYS
1	A	566	GLN
1	A	573	SER
1	A	700	PHE
1	B	524	LYS
1	B	623	TRP
1	B	624	ARG
1	B	638	ARG
1	C	523	LYS
1	C	524	LYS
1	C	567	VAL
1	C	584	GLU
1	C	597	ARG
1	C	598	GLU
1	C	621	ARG
1	C	644	LEU
1	C	700	PHE
1	D	565	GLN

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Mol	Chain	Res	Type
1	D	569	LEU
1	D	574	GLN
1	D	623	TRP
1	D	624	ARG
1	D	638	ARG
2	J	2	LYS
2	L	2	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	610	HIS

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](#)

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	$\# Z > 2$
3	8HB	E	201	2	50,54,55	2.74	16 (32%)	71,80,82	2.73	19 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	8HB	L	101	2	50,54,55	2.77	17 (34%)	71,80,82	2.48	16 (22%)
3	8HB	G	201	2	50,54,55	2.82	19 (38%)	71,80,82	2.86	22 (30%)
3	8HB	J	101	2	50,54,55	2.76	18 (36%)	71,80,82	2.60	20 (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
3	8HB	E	201	2	-	6/51/69/71	0/3/3/3
3	8HB	L	101	2	-	5/51/69/71	0/3/3/3
3	8HB	G	201	2	-	7/51/69/71	0/3/3/3
3	8HB	J	101	2	-	5/51/69/71	0/3/3/3

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	101	8HB	C48-C42	-9.57	1.32	1.53
3	L	101	8HB	C48-C42	-9.37	1.32	1.53
3	E	201	8HB	C48-C42	-9.26	1.32	1.53
3	G	201	8HB	C48-C42	-9.10	1.33	1.53
3	L	101	8HB	O61-C41	-6.93	1.29	1.45
3	E	201	8HB	O61-C41	-6.59	1.30	1.45
3	J	101	8HB	O61-C41	-6.16	1.31	1.45
3	L	101	8HB	C12-N13	6.14	1.48	1.33
3	G	201	8HB	O61-C41	-6.13	1.31	1.45
3	G	201	8HB	C12-N13	6.09	1.47	1.33
3	E	201	8HB	C12-N13	5.74	1.47	1.33
3	E	201	8HB	C16-N17	5.73	1.47	1.33
3	G	201	8HB	C16-N17	5.70	1.46	1.33
3	J	101	8HB	C12-N13	5.68	1.46	1.33
3	E	201	8HB	O61-C50	5.55	1.54	1.42
3	L	101	8HB	C59-N60	5.28	1.47	1.34
3	G	201	8HB	O61-C50	5.23	1.54	1.42
3	L	101	8HB	C16-N17	5.19	1.45	1.33
3	J	101	8HB	C16-N17	4.93	1.45	1.33
3	L	101	8HB	C50-N51	-4.82	1.33	1.46
3	G	201	8HB	P2-O3	4.81	1.64	1.59
3	G	201	8HB	C59-N60	4.76	1.46	1.34
3	J	101	8HB	C59-N60	4.71	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	101	8HB	O61-C50	4.68	1.52	1.42
3	E	201	8HB	C59-N60	4.63	1.46	1.34
3	J	101	8HB	C50-N51	-4.52	1.33	1.46
3	G	201	8HB	C50-N51	-4.44	1.34	1.46
3	J	101	8HB	O61-C50	4.11	1.51	1.42
3	J	101	8HB	P44-O43	4.04	1.66	1.59
3	E	201	8HB	C50-N51	-3.91	1.35	1.46
3	E	201	8HB	P2-O3	3.81	1.63	1.59
3	J	101	8HB	P2-O3	3.72	1.63	1.59
3	G	201	8HB	C42-C41	3.51	1.62	1.52
3	E	201	8HB	C42-C41	3.45	1.61	1.52
3	L	101	8HB	C42-C41	3.43	1.61	1.52
3	G	201	8HB	P4-O3	3.39	1.63	1.59
3	J	101	8HB	C42-C41	3.36	1.61	1.52
3	L	101	8HB	P44-O43	3.32	1.65	1.59
3	G	201	8HB	O35-C12	-3.15	1.17	1.23
3	J	101	8HB	C54-N53	-3.11	1.33	1.39
3	J	101	8HB	C54-C55	-3.08	1.33	1.39
3	L	101	8HB	C54-N53	-3.02	1.33	1.39
3	J	101	8HB	O49-C48	2.99	1.50	1.43
3	E	201	8HB	P44-O43	2.98	1.64	1.59
3	L	101	8HB	O49-C48	2.97	1.50	1.43
3	G	201	8HB	C6-C7	2.94	1.57	1.52
3	E	201	8HB	O49-C48	2.93	1.50	1.43
3	L	101	8HB	C54-C55	-2.84	1.34	1.39
3	G	201	8HB	P44-O43	2.84	1.64	1.59
3	E	201	8HB	O35-C12	-2.81	1.18	1.23
3	E	201	8HB	C54-C55	-2.80	1.34	1.39
3	G	201	8HB	C54-N53	-2.68	1.34	1.39
3	G	201	8HB	O49-C48	2.64	1.49	1.43
3	J	101	8HB	C55-N51	-2.60	1.32	1.37
3	J	101	8HB	C52-N51	-2.52	1.33	1.37
3	L	101	8HB	C52-N51	-2.46	1.33	1.37
3	J	101	8HB	C52-N53	2.41	1.36	1.31
3	E	201	8HB	C54-N53	-2.35	1.34	1.39
3	G	201	8HB	C52-N53	2.30	1.36	1.31
3	G	201	8HB	C54-C55	-2.27	1.35	1.39
3	L	101	8HB	P2-O39	2.18	1.67	1.59
3	L	101	8HB	O35-C12	-2.17	1.19	1.23
3	L	101	8HB	C55-N51	-2.16	1.33	1.37
3	J	101	8HB	C19-S20	2.15	1.84	1.81
3	G	201	8HB	O34-C16	-2.12	1.19	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	201	8HB	C55-N51	-2.11	1.33	1.37
3	E	201	8HB	C52-N51	-2.10	1.34	1.37
3	L	101	8HB	C52-N53	2.06	1.35	1.31
3	J	101	8HB	P4-O3	2.05	1.61	1.59
3	G	201	8HB	C55-N51	-2.02	1.33	1.37

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	101	8HB	N60-C59-N58	-9.59	97.02	118.38
3	L	101	8HB	C50-N51-C52	-9.45	106.13	127.09
3	G	201	8HB	C50-N51-C52	-9.39	106.26	127.09
3	E	201	8HB	N60-C59-N58	-9.35	97.56	118.38
3	G	201	8HB	N60-C59-N58	-9.13	98.05	118.38
3	E	201	8HB	C50-N51-C52	-8.75	107.69	127.09
3	L	101	8HB	C55-N51-C50	8.28	146.00	126.63
3	G	201	8HB	C55-N51-C50	8.24	145.90	126.63
3	J	101	8HB	C50-N51-C52	-8.11	109.09	127.09
3	L	101	8HB	N60-C59-N58	-8.09	100.37	118.38
3	J	101	8HB	C54-C59-N60	8.00	143.09	123.29
3	E	201	8HB	C55-N51-C50	7.65	144.51	126.63
3	E	201	8HB	C54-C59-N60	7.29	141.32	123.29
3	E	201	8HB	C22-C21-C23	-7.12	103.87	112.18
3	J	101	8HB	C55-N51-C50	7.12	143.27	126.63
3	G	201	8HB	C54-C59-N60	7.07	140.78	123.29
3	L	101	8HB	C54-C59-N60	6.93	140.43	123.29
3	G	201	8HB	C22-C21-C23	-6.48	104.62	112.18
3	J	101	8HB	N58-C57-N56	-5.46	120.32	128.58
3	L	101	8HB	N58-C57-N56	-5.30	120.56	128.58
3	G	201	8HB	N58-C57-N56	-5.19	120.73	128.58
3	E	201	8HB	N58-C57-N56	-5.08	120.90	128.58
3	E	201	8HB	O61-C50-N51	4.95	117.60	108.09
3	G	201	8HB	O37-P4-O3	4.95	120.64	107.27
3	J	101	8HB	C22-C21-C23	-4.74	106.65	112.18
3	G	201	8HB	O61-C50-N51	4.34	116.43	108.09
3	G	201	8HB	C54-C55-N56	-3.98	121.23	126.72
3	G	201	8HB	C19-C18-N17	-3.69	104.70	112.41
3	J	101	8HB	O5-C6-C7	-3.52	104.89	110.55
3	J	101	8HB	N51-C52-N53	-3.42	109.09	113.94
3	J	101	8HB	O61-C50-N51	3.42	114.65	108.09
3	E	201	8HB	C54-C55-N56	-3.41	122.03	126.72
3	L	101	8HB	C19-C18-N17	-3.38	105.35	112.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	201	8HB	O46-P44-O43	3.35	118.89	105.85
3	E	201	8HB	O5-C6-C7	-3.34	105.18	110.55
3	G	201	8HB	N51-C52-N53	-3.27	109.30	113.94
3	J	101	8HB	C14-C15-C16	-3.23	107.02	112.39
3	G	201	8HB	O5-C6-C7	-3.18	105.43	110.55
3	G	201	8HB	O49-C48-C50	-3.13	99.33	110.10
3	L	101	8HB	C54-C55-N56	-3.10	122.45	126.72
3	E	201	8HB	N51-C52-N53	-3.09	109.55	113.94
3	L	101	8HB	N51-C52-N53	-3.06	109.59	113.94
3	G	201	8HB	C18-N17-C16	-3.05	117.14	122.82
3	J	101	8HB	C19-C18-N17	-3.05	106.06	112.41
3	G	201	8HB	C57-N56-C55	3.01	119.18	111.83
3	L	101	8HB	O5-C6-C7	-2.98	105.75	110.55
3	J	101	8HB	O49-C48-C50	-2.92	100.05	110.10
3	L	101	8HB	C22-C21-C23	-2.84	108.87	112.18
3	J	101	8HB	C8-C7-C10	2.80	113.54	108.77
3	E	201	8HB	C9-C7-C10	2.79	113.52	108.77
3	J	101	8HB	C54-C55-N56	-2.69	123.01	126.72
3	E	201	8HB	O3-P4-O36	2.67	118.75	110.70
3	E	201	8HB	C57-N56-C55	2.66	118.33	111.83
3	G	201	8HB	C9-C7-C10	2.59	113.18	108.77
3	E	201	8HB	C48-C50-N51	-2.55	106.98	113.30
3	L	101	8HB	O61-C50-N51	2.48	112.84	108.09
3	E	201	8HB	C19-C18-N17	-2.45	107.31	112.41
3	G	201	8HB	C42-C48-C50	2.45	105.27	99.89
3	E	201	8HB	C8-C7-C10	2.42	112.89	108.77
3	J	101	8HB	C9-C7-C6	2.38	112.14	108.22
3	J	101	8HB	C42-C48-C50	2.35	105.06	99.89
3	G	201	8HB	N56-C55-N51	2.35	131.16	127.17
3	L	101	8HB	C57-N56-C55	2.34	117.56	111.83
3	J	101	8HB	C57-N56-C55	2.34	117.54	111.83
3	J	101	8HB	C54-C55-N51	2.33	108.35	105.81
3	L	101	8HB	C14-C15-C16	-2.33	108.51	112.39
3	G	201	8HB	C8-C7-C10	2.33	112.74	108.77
3	G	201	8HB	C48-C50-N51	-2.27	107.67	113.30
3	E	201	8HB	O49-C48-C50	-2.26	102.31	110.10
3	E	201	8HB	C42-C48-C50	2.24	104.83	99.89
3	E	201	8HB	P44-O43-C42	-2.24	117.44	123.43
3	J	101	8HB	P44-O43-C42	-2.20	117.55	123.43
3	L	101	8HB	C18-N17-C16	-2.17	118.78	122.82
3	J	101	8HB	O34-C16-N17	-2.04	119.03	123.03
3	G	201	8HB	C40-C41-C42	-2.03	107.60	114.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	101	8HB	O47-P44-O46	2.03	115.42	107.80
3	L	101	8HB	C48-C50-N51	-2.02	108.28	113.30

There are no chirality outliers.

All (23) torsion outliers are listed below:

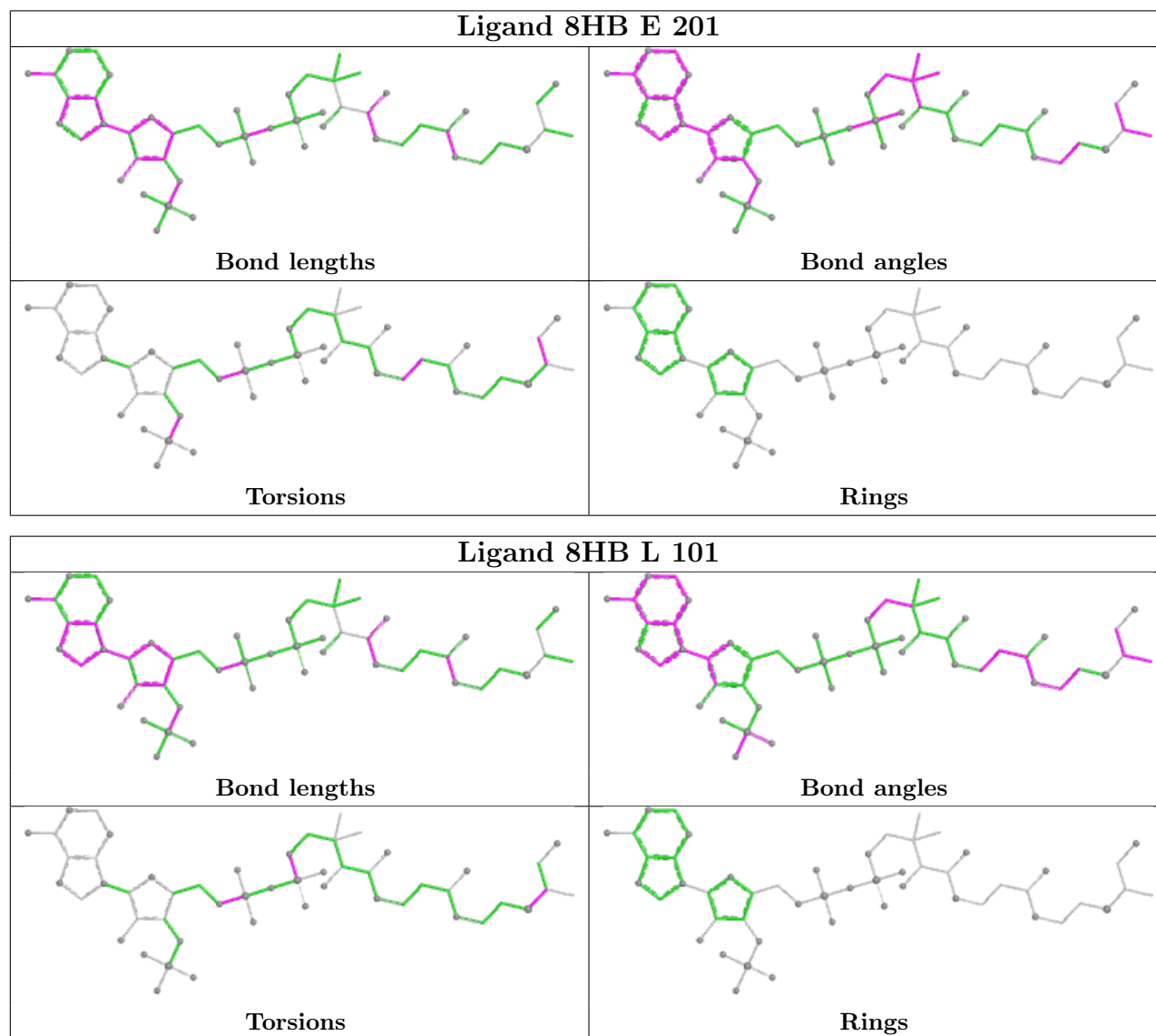
Mol	Chain	Res	Type	Atoms
3	E	201	8HB	C40-O39-P2-O3
3	E	201	8HB	C40-O39-P2-O38
3	E	201	8HB	C22-C21-C23-O33
3	G	201	8HB	C40-O39-P2-O3
3	G	201	8HB	C40-O39-P2-O38
3	G	201	8HB	C6-O5-P4-O36
3	G	201	8HB	C22-C21-C23-O33
3	J	101	8HB	C40-O39-P2-O3
3	J	101	8HB	C40-O39-P2-O38
3	J	101	8HB	C22-C21-S20-C19
3	L	101	8HB	C40-O39-P2-O3
3	L	101	8HB	C40-O39-P2-O38
3	L	101	8HB	C6-O5-P4-O36
3	G	201	8HB	N13-C14-C15-C16
3	L	101	8HB	C22-C21-S20-C19
3	E	201	8HB	C40-O39-P2-O1
3	G	201	8HB	C40-O39-P2-O1
3	J	101	8HB	C40-O39-P2-O1
3	L	101	8HB	C40-O39-P2-O1
3	G	201	8HB	C48-C42-O43-P44
3	E	201	8HB	C42-O43-P44-O47
3	J	101	8HB	C42-O43-P44-O47
3	E	201	8HB	N13-C14-C15-C16

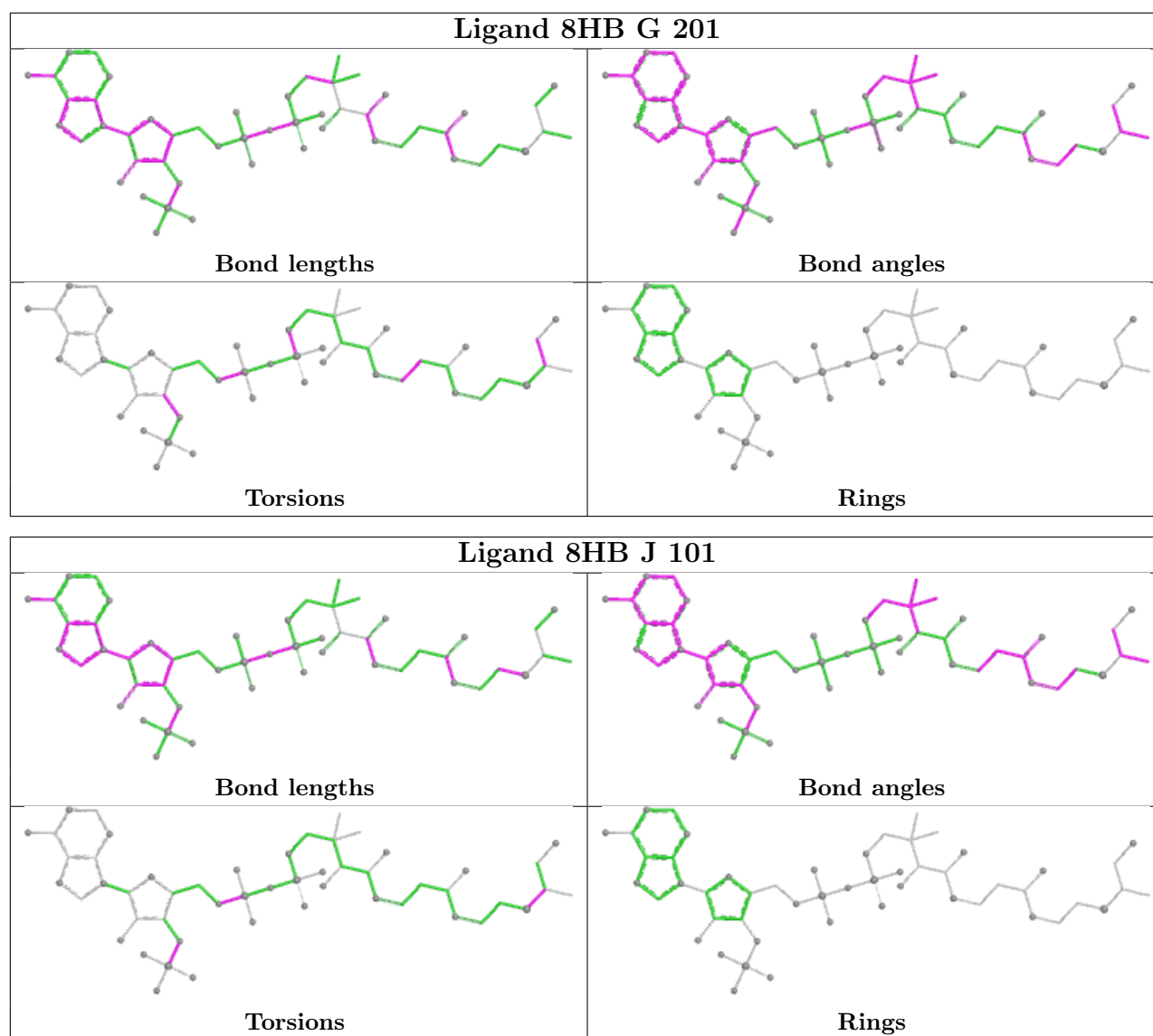
There are no ring outliers.

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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	168/183 (91%)	-0.91	0 100 100	22, 43, 90, 103	0
1	B	168/183 (91%)	-0.90	0 100 100	24, 44, 81, 113	0
1	C	168/183 (91%)	-0.91	0 100 100	24, 43, 83, 116	0
1	D	167/183 (91%)	-0.90	0 100 100	24, 44, 78, 106	0
2	E	9/13 (69%)	-0.65	0 100 100	44, 58, 63, 74	0
2	G	9/13 (69%)	-0.76	0 100 100	40, 59, 65, 65	0
2	J	1/13 (7%)	-0.71	0 100 100	56, 56, 56, 56	0
2	L	1/13 (7%)	-0.35	0 100 100	58, 58, 58, 58	0
All	All	691/784 (88%)	-0.90	0 100 100	22, 44, 84, 116	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

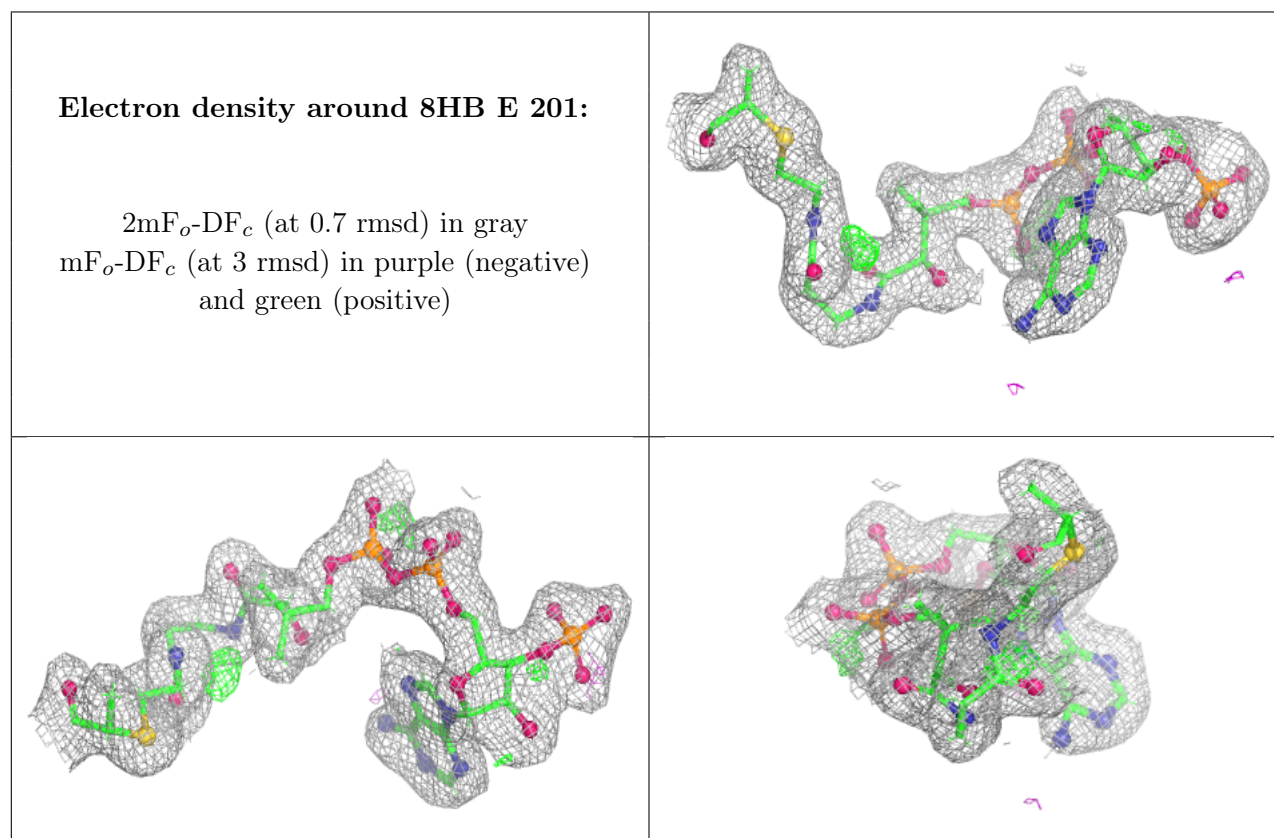
There are no oligosaccharides in this entry.

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.

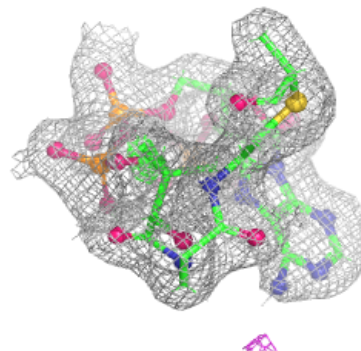
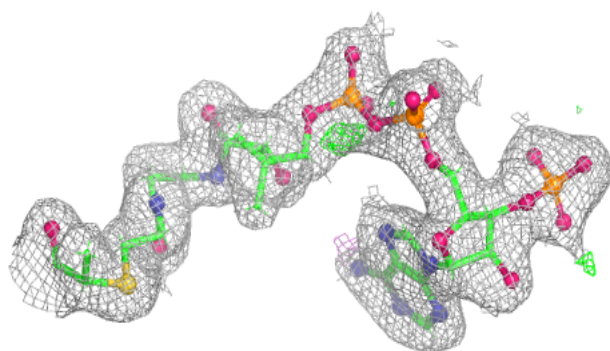
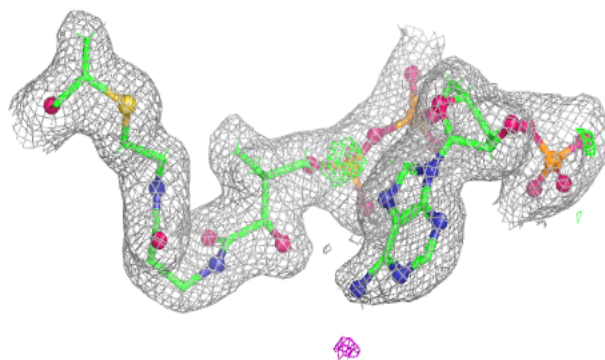
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	8HB	E	201	52/53	0.99	0.03	21,30,45,53	0
3	8HB	J	101	52/53	0.99	0.03	22,32,43,51	0
3	8HB	L	101	52/53	0.99	0.03	22,33,44,52	0
3	8HB	G	201	52/53	1.00	0.03	21,32,51,52	0

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.

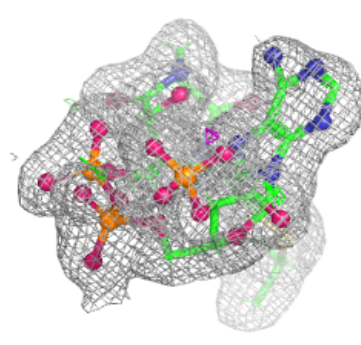
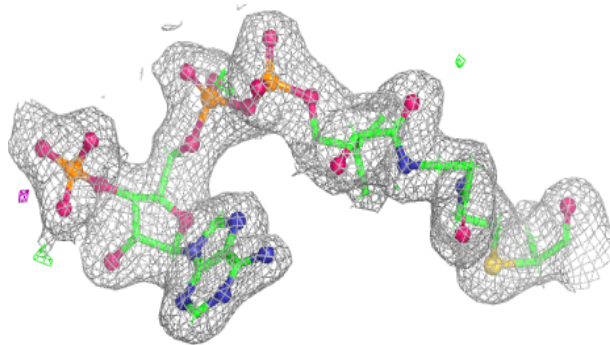
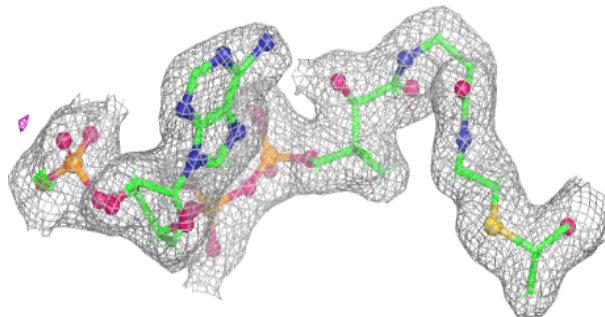


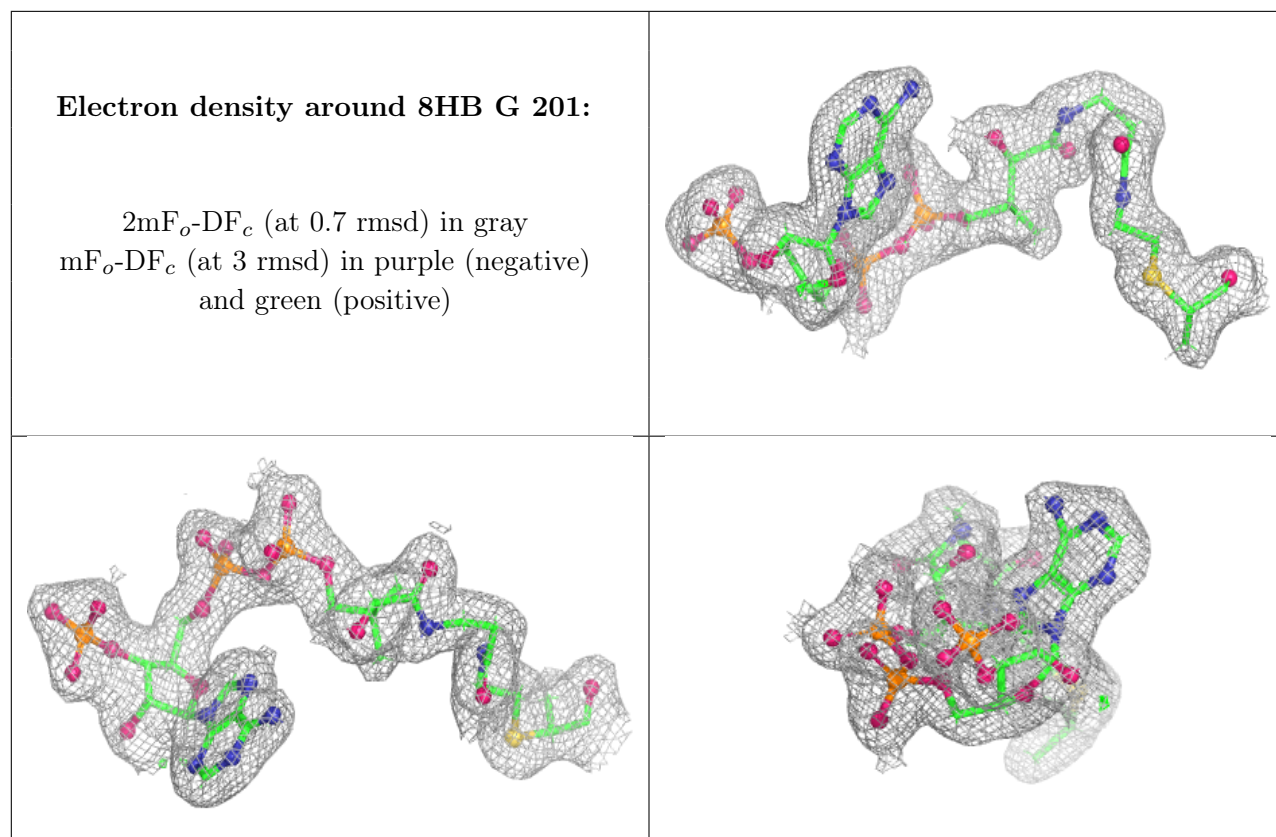
Electron density around 8HB J 101:

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

**Electron density around 8HB L 101:**

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





6.5 Other polymers [i](#)

There are no such residues in this entry.