



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 11:47 PM UTC

PDB ID : 7ZZR / pdb_00007zzr
Title : HDAC2 in complex with inhibitory ligand
Authors : Cleasby, A.; Tisi, D.
Deposited on : 2022-05-26
Resolution : 2.17 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

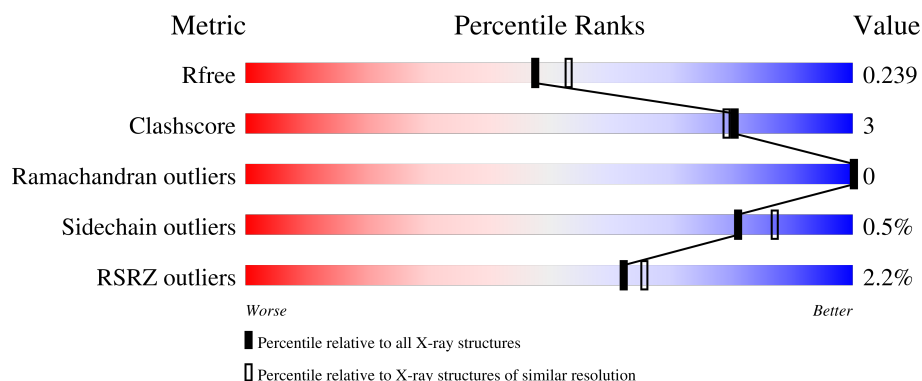
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	498	70% 26%
1	B	498	68% 6% 27%
1	C	498	69% 26%

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
5	EDO	A	607	-	-	X	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 10052 atoms, of which 57 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 Histone deacetylase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	3	0
			2986	1907	506	548	25			
1	B	366	Total	C	N	O	S	0	4	0
			2972	1897	500	548	27			
1	C	367	Total	C	N	O	S	0	3	0
			2974	1900	501	547	26			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	493	GLY	-	expression tag	UNP Q92769
A	494	SER	-	expression tag	UNP Q92769
A	495	SER	-	expression tag	UNP Q92769
A	496	GLY	-	expression tag	UNP Q92769
A	497	HIS	-	expression tag	UNP Q92769
A	498	HIS	-	expression tag	UNP Q92769
A	499	HIS	-	expression tag	UNP Q92769
A	500	HIS	-	expression tag	UNP Q92769
A	501	HIS	-	expression tag	UNP Q92769
A	502	HIS	-	expression tag	UNP Q92769
B	493	GLY	-	expression tag	UNP Q92769
B	494	SER	-	expression tag	UNP Q92769
B	495	SER	-	expression tag	UNP Q92769
B	496	GLY	-	expression tag	UNP Q92769
B	497	HIS	-	expression tag	UNP Q92769
B	498	HIS	-	expression tag	UNP Q92769
B	499	HIS	-	expression tag	UNP Q92769
B	500	HIS	-	expression tag	UNP Q92769
B	501	HIS	-	expression tag	UNP Q92769
B	502	HIS	-	expression tag	UNP Q92769
C	493	GLY	-	expression tag	UNP Q92769
C	494	SER	-	expression tag	UNP Q92769
C	495	SER	-	expression tag	UNP Q92769

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Chain	Residue	Modelled	Actual	Comment	Reference
C	496	GLY	-	expression tag	UNP Q92769
C	497	HIS	-	expression tag	UNP Q92769
C	498	HIS	-	expression tag	UNP Q92769
C	499	HIS	-	expression tag	UNP Q92769
C	500	HIS	-	expression tag	UNP Q92769
C	501	HIS	-	expression tag	UNP Q92769
C	502	HIS	-	expression tag	UNP Q92769

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		

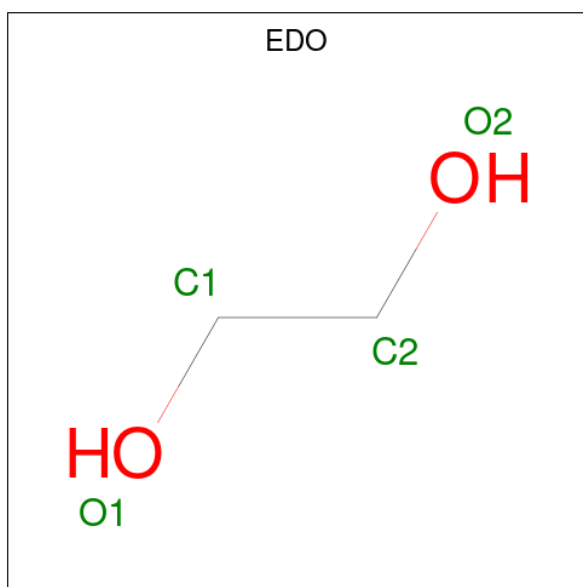
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

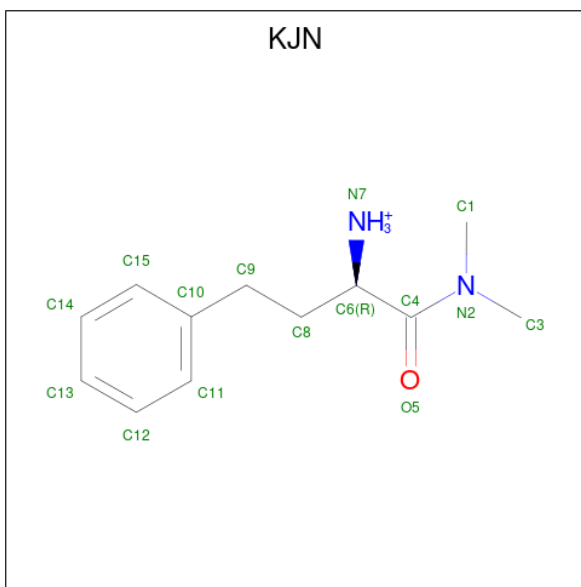
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



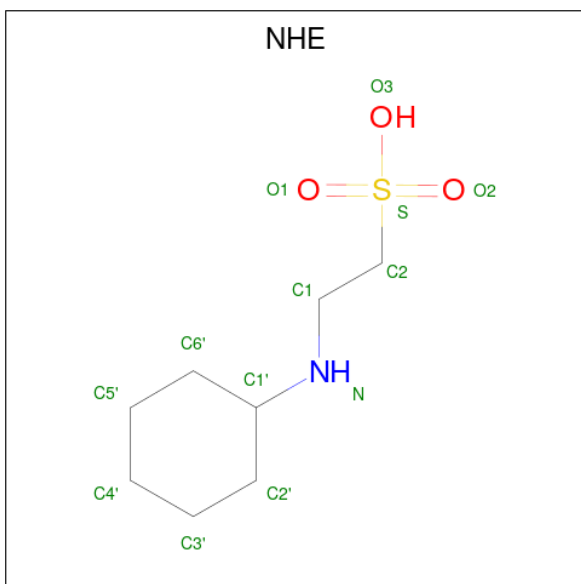
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	A	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total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

- Molecule 6 is [(2 {R})-1-(dimethylamino)-1-oxidanylidene-4-phenyl-butan-2-yl]azanium (CCD ID: KJN) (formula: C₁₂H₁₉N₂O) (labeled as "Ligand of Interest" by depositor).



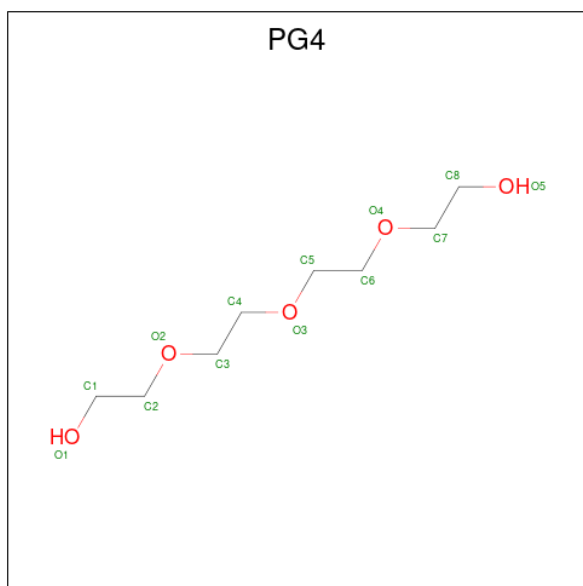
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	H	N	O	0	0
			34	12	19	2	1		
6	B	1	Total	C	H	N	O	0	0
			34	12	19	2	1		
6	C	1	Total	C	H	N	O	0	0
			34	12	19	2	1		

- Molecule 7 is 2-[N-CYCLOHEXYLAMINO]ETHANE SULFONIC ACID (CCD ID: NHE) (formula: C₈H₁₇NO₃S).



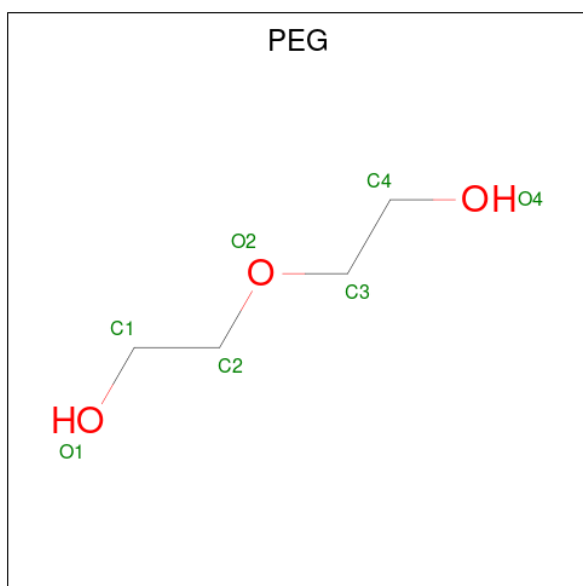
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	B	1	Total	C	N	O	S	0	0
			13	8	1	3	1		

- Molecule 8 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 9 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	B	1	Total	C	O	0	0
			7	4	3		
9	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	307	Total	O	0	0
			307	307		
10	B	348	Total	O	0	0
			348	348		
10	C	253	Total	O	0	0
			253	253		

- Molecule 1: Histone deacetylase 2



GLY GLU GLY GLY ARG ARG ASN VAL ALA ASP HIS HIS LYS LYS GLY ALA LYS LYS ALA ARG ARG THR GLU ASP LYS LYS GLU THR GLU ASP LYS LYS THR ASP VAL LYS GLU GLU ASP LYS LYS ASP ASN SER GLY GLU LYS THR ASP THR LYS GLY THR LYS SER GLU GLN LEU SER ASN

PRO GLY SER GLY HIS HIS HIS HIS HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.99Å 97.70Å 138.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.69 – 2.17 76.69 – 2.17	Depositor EDS
% Data completeness (in resolution range)	90.0 (76.69-2.17) 90.0 (76.69-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.16Å)	Xtrriage
Refinement program	BUSTER 2.11.8 (20-APR-2021)	Depositor
R, R_{free}	0.188 , 0.247 0.190 , 0.239	Depositor DCC
R_{free} test set	2923 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtrriage
Anisotropy	0.325	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 59.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10052	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.17% 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: PG4, EDO, ZN, NHE, PEG, CA, NA, KJN

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	1.00	3/3070 (0.1%)	1.05	2/4143 (0.0%)
1	B	1.02	3/3056 (0.1%)	1.06	1/4126 (0.0%)
1	C	0.94	3/3057 (0.1%)	1.06	3/4126 (0.1%)
All	All	0.99	9/9183 (0.1%)	1.05	6/12395 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	363	TYR	C-N	6.95	1.42	1.33
1	A	199	MET	SD-CE	-6.54	1.63	1.79
1	C	199	MET	SD-CE	-6.41	1.63	1.79
1	B	69	MET	SD-CE	-6.33	1.63	1.79
1	B	103	GLU	CA-C	6.24	1.55	1.52
1	B	89	MET	SD-CE	-5.86	1.64	1.79
1	A	233	MET	SD-CE	-5.69	1.65	1.79
1	A	364	MET	SD-CE	-5.68	1.65	1.79
1	C	365	GLU	C-N	5.16	1.40	1.33

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	155	PHE	CA-CB-CG	5.97	119.77	113.80
1	A	155	PHE	CA-CB-CG	5.96	119.76	113.80
1	C	155	PHE	CA-CB-CG	5.46	119.27	113.80
1	C	363	TYR	CA-C-O	-5.12	115.62	121.00
1	A	108	PHE	CA-CB-CG	5.07	118.87	113.80
1	C	108	PHE	CA-CB-CG	5.01	118.81	113.80

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	2986	0	2898	18	0
1	B	2972	0	2872	18	0
1	C	2974	0	2886	9	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
5	A	16	0	23	9	0
5	B	12	0	18	3	0
5	C	12	0	18	0	0
6	A	15	19	0	1	0
6	B	15	19	0	1	0
6	C	15	19	0	1	0
7	B	13	0	16	0	0
8	B	13	0	18	0	0
9	B	28	0	40	3	0
9	C	7	0	10	1	0
10	A	307	0	0	1	0
10	B	348	0	0	1	0
10	C	253	0	0	2	0
All	All	9995	57	8799	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 3.

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:226:TYR:HA	5:A:607:EDO:H22	1.50	0.91
1:B:135:ASP:OD2	5:B:608:EDO:H22	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:ASN:HB3	5:A:607:EDO:H21	1.68	0.75
1:C:89:MET:HE3	1:C:96:MET:HE1	1.69	0.74
1:A:229:VAL:HG22	5:A:607:EDO:H11	1.70	0.72
1:A:226:TYR:CA	5:A:607:EDO:H22	2.17	0.72
1:B:205:LYS:HD3	1:B:278[B]:CYS:SG	2.33	0.69
1:A:205:LYS:HD2	1:A:278[B]:CYS:SG	2.36	0.65
1:B:241:SER:HB3	1:B:364[B]:MET:SD	2.40	0.61
1:C:245:ILE:HG21	1:C:364[A]:MET:HE3	1.86	0.58
1:A:226:TYR:C	5:A:607:EDO:H22	2.30	0.57
9:C:604:PEG:H11	10:C:866:HOH:O	2.03	0.57
1:C:199:MET:HE1	1:C:378:LEU:HD11	1.86	0.56
1:A:199:MET:HE1	1:A:378:LEU:HD11	1.86	0.56
1:B:245:ILE:HG21	1:B:364[A]:MET:HE3	1.90	0.55
1:B:360:THR:O	1:B:364[B]:MET:HG3	2.07	0.54
1:B:199:MET:HE1	1:B:378:LEU:HD11	1.87	0.54
1:B:112:PHE:O	1:B:116:GLN:HG3	2.09	0.53
1:B:35:MET:HE3	6:B:613:KJN:C12	2.38	0.53
1:A:14:LYS:HB2	1:A:136:MET:CE	2.40	0.51
1:B:181:ASP:HB2	1:B:265:GLN:OE1	2.12	0.50
1:C:234:ARG:NH2	1:C:363:TYR:CD2	2.80	0.50
1:A:205:LYS:CD	1:A:278[B]:CYS:SG	3.00	0.50
1:B:56:MET:HB3	1:B:325:LEU:HD21	1.94	0.50
1:C:241:SER:HB3	1:C:364[B]:MET:SD	2.52	0.50
1:B:104:ASP:HB2	10:B:929:HOH:O	2.13	0.48
1:A:181:ASP:HB2	1:A:265:GLN:OE1	2.14	0.48
1:C:181:ASP:HB2	1:C:265:GLN:OE1	2.14	0.47
1:B:350:ILE:HB	9:B:612:PEG:H32	1.97	0.47
1:B:47:LEU:HD23	1:B:52:LEU:HD12	1.97	0.47
1:B:135:ASP:HB3	5:B:609:EDO:H21	1.96	0.46
1:A:229:VAL:CG2	5:A:607:EDO:H11	2.41	0.46
1:B:27:TYR:CE2	9:B:606:PEG:H31	2.51	0.46
1:A:228:ALA:O	5:A:607:EDO:O2	2.33	0.45
1:B:135:ASP:OD2	5:B:608:EDO:C2	2.57	0.44
1:A:17:CYS:O	1:A:137:ALA:HA	2.17	0.44
1:C:104:ASP:HB2	10:C:847:HOH:O	2.17	0.43
1:A:229:VAL:HG22	5:A:607:EDO:C1	2.43	0.43
1:A:226:TYR:HA	5:A:607:EDO:C2	2.34	0.42
1:B:350:ILE:HA	9:B:612:PEG:H32	2.00	0.42
1:A:14:LYS:CB	1:A:136:MET:CE	2.98	0.42
1:B:368:LYS:HG2	1:B:372:PHE:CE2	2.56	0.41
1:A:368:LYS:NZ	10:A:720:HOH:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:CYS:SG	6:A:608:KJN:C15	3.09	0.40
1:C:35:MET:HE3	6:C:608:KJN:C12	2.51	0.40
1:C:216:LEU:HD11	1:C:370:ARG:HG2	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	370/498 (74%)	366 (99%)	4 (1%)	0	100	100
1	B	368/498 (74%)	365 (99%)	3 (1%)	0	100	100
1	C	368/498 (74%)	365 (99%)	3 (1%)	0	100	100
All	All	1106/1494 (74%)	1096 (99%)	10 (1%)	0	100	100

There are no Ramachandran outliers to report.

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	320/425 (75%)	319 (100%)	1 (0%)	86	91
1	B	320/425 (75%)	319 (100%)	1 (0%)	86	91
1	C	320/425 (75%)	317 (99%)	3 (1%)	70	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	960/1275 (75%)	955 (100%)	5 (0%)	81	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	SER
1	B	90	SER
1	C	13	LYS
1	C	90	SER
1	C	326	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	ASN
1	C	172	HIS
1	C	369	GLN

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](#)

Of 29 ligands modelled in this entry, 9 are monoatomic - leaving 20 for Mogul analysis.

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	$\# Z > 2$
9	PEG	B	612	-	6,6,6	0.40	0	5,5,5	0.34	0
8	PG4	B	605	-	12,12,12	0.32	0	11,11,11	0.60	0
5	EDO	A	604	-	3,3,3	0.60	0	2,2,2	0.40	0
5	EDO	B	610	-	3,3,3	0.43	0	2,2,2	0.49	0
5	EDO	A	605	-	3,3,3	0.49	0	2,2,2	0.27	0
6	KJN	C	608	2	15,15,15	0.27	0	19,19,19	0.54	0
6	KJN	B	613	2	15,15,15	0.38	0	19,19,19	0.80	1 (5%)
5	EDO	A	607	-	3,3,3	0.67	0	2,2,2	0.46	0
9	PEG	B	606	-	6,6,6	0.33	0	5,5,5	0.26	0
5	EDO	C	606	-	3,3,3	0.65	0	2,2,2	0.20	0
9	PEG	B	607	-	6,6,6	0.21	0	5,5,5	0.17	0
5	EDO	C	605	-	3,3,3	1.04	0	2,2,2	0.19	0
5	EDO	B	608	-	3,3,3	0.58	0	2,2,2	0.29	0
7	NHE	B	604	-	13,13,13	0.55	0	16,17,17	0.69	0
5	EDO	B	609	-	3,3,3	0.69	0	2,2,2	0.45	0
5	EDO	C	607	-	3,3,3	0.60	0	2,2,2	0.18	0
9	PEG	C	604	-	6,6,6	0.61	0	5,5,5	0.47	0
5	EDO	A	606	-	3,3,3	0.76	0	2,2,2	0.25	0
9	PEG	B	611	-	6,6,6	0.10	0	5,5,5	0.11	0
6	KJN	A	608	2	15,15,15	0.39	0	19,19,19	0.78	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
9	PEG	B	612	-	-	2/4/4/4	-
8	PG4	B	605	-	-	3/10/10/10	-
5	EDO	A	604	-	-	0/1/1/1	-
5	EDO	B	610	-	-	1/1/1/1	-
5	EDO	A	605	-	-	1/1/1/1	-
6	KJN	C	608	2	-	0/13/13/13	0/1/1/1
6	KJN	B	613	2	-	0/13/13/13	0/1/1/1
5	EDO	A	607	-	-	0/1/1/1	-
9	PEG	B	606	-	-	1/4/4/4	-
5	EDO	C	606	-	-	1/1/1/1	-
9	PEG	B	607	-	-	2/4/4/4	-
5	EDO	C	605	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	EDO	B	608	-	-	1/1/1/1	-
7	NHE	B	604	-	-	3/7/15/15	0/1/1/1
5	EDO	B	609	-	-	1/1/1/1	-
5	EDO	C	607	-	-	1/1/1/1	-
9	PEG	C	604	-	-	2/4/4/4	-
5	EDO	A	606	-	-	1/1/1/1	-
9	PEG	B	611	-	-	2/4/4/4	-
6	KJN	A	608	2	-	0/13/13/13	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	613	KJN	C6-C4-N2	2.35	121.19	118.53

There are no chirality outliers.

All (22) torsion outliers are listed below:

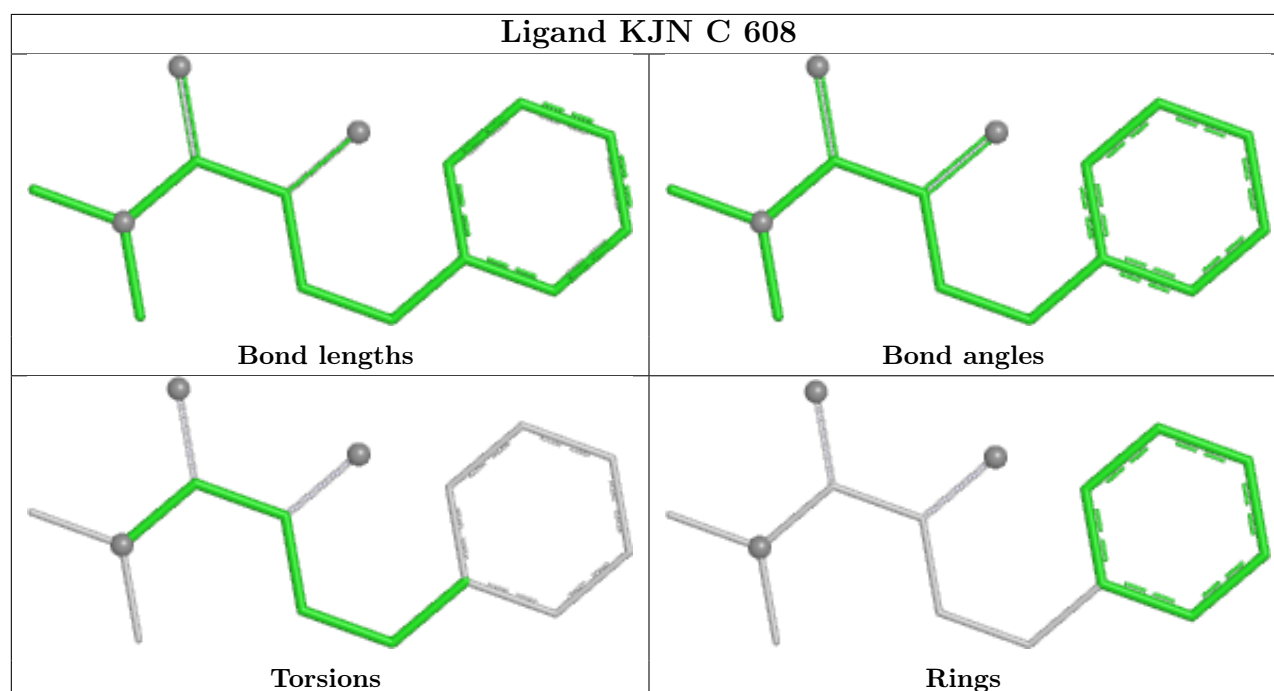
Mol	Chain	Res	Type	Atoms
8	B	605	PG4	O2-C3-C4-O3
9	B	611	PEG	O2-C3-C4-O4
9	B	606	PEG	O2-C3-C4-O4
9	C	604	PEG	O2-C3-C4-O4
5	A	605	EDO	O1-C1-C2-O2
5	A	606	EDO	O1-C1-C2-O2
5	C	607	EDO	O1-C1-C2-O2
9	B	612	PEG	O1-C1-C2-O2
7	B	604	NHE	C1-C2-S-O3
7	B	604	NHE	C1-C2-S-O1
7	B	604	NHE	C1-C2-S-O2
9	B	611	PEG	C4-C3-O2-C2
8	B	605	PG4	C6-C5-O3-C4
9	B	612	PEG	C1-C2-O2-C3
5	B	610	EDO	O1-C1-C2-O2
5	C	606	EDO	O1-C1-C2-O2
9	B	607	PEG	O1-C1-C2-O2
9	B	607	PEG	C1-C2-O2-C3
8	B	605	PG4	C8-C7-O4-C6
5	B	608	EDO	O1-C1-C2-O2
5	B	609	EDO	O1-C1-C2-O2
9	C	604	PEG	C4-C3-O2-C2

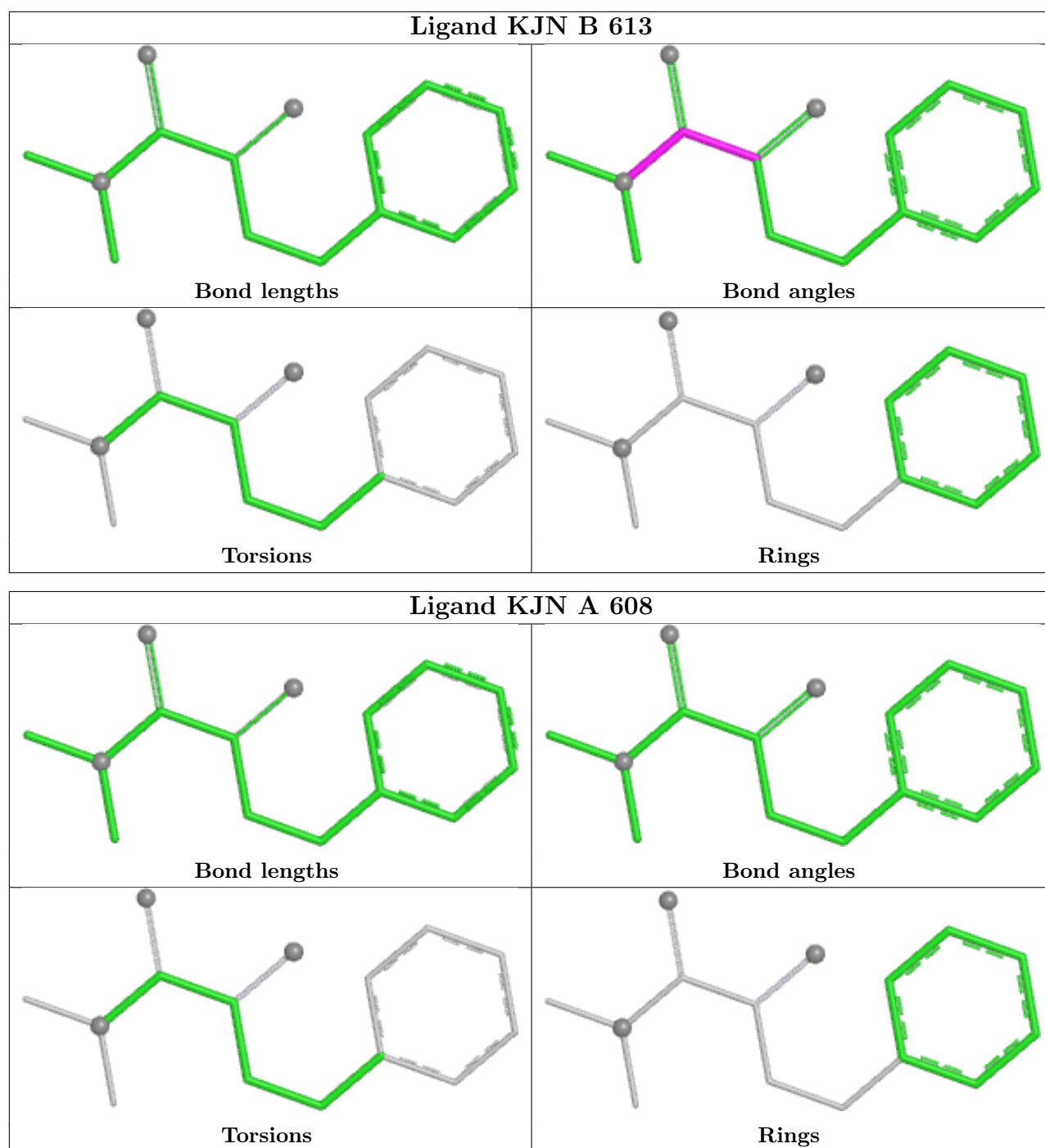
There are no ring outliers.

9 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	612	PEG	2	0
6	C	608	KJN	1	0
6	B	613	KJN	1	0
5	A	607	EDO	9	0
9	B	606	PEG	1	0
5	B	608	EDO	2	0
5	B	609	EDO	1	0
9	C	604	PEG	1	0
6	A	608	KJN	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	369/498 (74%)	-0.10	3 (0%) 82 84	9, 18, 36, 54	3 (0%)
1	B	366/498 (73%)	-0.15	5 (1%) 73 77	7, 17, 35, 50	4 (1%)
1	C	367/498 (73%)	0.57	16 (4%) 39 44	15, 29, 47, 59	3 (0%)
All	All	1102/1494 (73%)	0.10	24 (2%) 62 66	7, 21, 43, 59	10 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	341	TYR	3.7
1	A	11	GLY	3.6
1	C	365	GLU	3.6
1	C	13	LYS	3.3
1	C	62	HIS	3.0
1	B	103	GLU	2.8
1	C	369	GLN	2.7
1	C	54	ARG	2.7
1	C	288	LYS	2.5
1	C	379	PRO	2.5
1	A	379	PRO	2.5
1	C	60	ARG	2.4
1	B	372	PHE	2.2
1	B	379	PRO	2.2
1	C	372	PHE	2.2
1	B	378	LEU	2.1
1	C	244	GLN	2.1
1	B	82	ARG	2.1
1	C	253	VAL	2.1
1	C	91	GLU	2.1
1	C	344	PRO	2.1
1	A	102	GLY	2.0
1	C	340	GLU	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	59	TYR	2.0

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(Å ²)	Q<0.9
9	PEG	B	612	7/7	0.76	0.31	41,42,42,42	0
5	EDO	C	606	4/4	0.77	0.16	45,46,47,47	0
9	PEG	B	611	7/7	0.78	0.20	55,55,56,56	0
5	EDO	B	608	4/4	0.84	0.17	55,55,55,55	0
5	EDO	C	605	4/4	0.86	0.14	28,29,30,30	0
9	PEG	C	604	7/7	0.88	0.13	30,30,32,32	0
5	EDO	C	607	4/4	0.89	0.12	37,38,39,40	0
6	KJN	C	608	15/15	0.89	0.12	14,16,22,22	34
9	PEG	B	606	7/7	0.89	0.10	31,31,33,33	0
5	EDO	B	610	4/4	0.89	0.12	38,38,38,39	0
5	EDO	A	607	4/4	0.89	0.17	25,25,26,27	0
5	EDO	A	604	4/4	0.89	0.11	39,40,40,41	0
9	PEG	B	607	7/7	0.90	0.11	37,38,41,42	0
7	NHE	B	604	13/13	0.90	0.13	19,20,25,25	13
6	KJN	A	608	15/15	0.91	0.13	10,13,17,17	34
5	EDO	A	606	4/4	0.92	0.10	31,31,31,31	0
6	KJN	B	613	15/15	0.92	0.12	10,15,19,20	34
5	EDO	B	609	4/4	0.92	0.13	29,29,30,30	0
5	EDO	A	605	4/4	0.92	0.11	30,31,31,31	0
8	PG4	B	605	13/13	0.92	0.09	28,29,30,31	0
4	NA	C	603	1/1	0.94	0.07	30,30,30,30	0
4	NA	A	603	1/1	0.98	0.04	21,21,21,21	0

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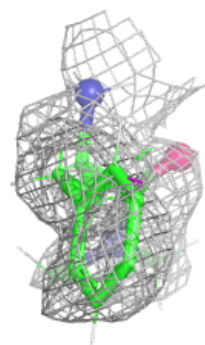
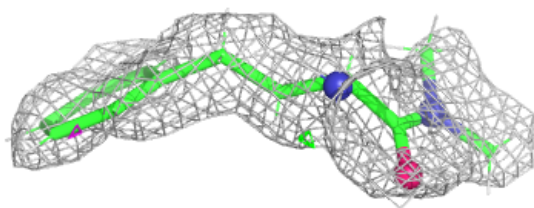
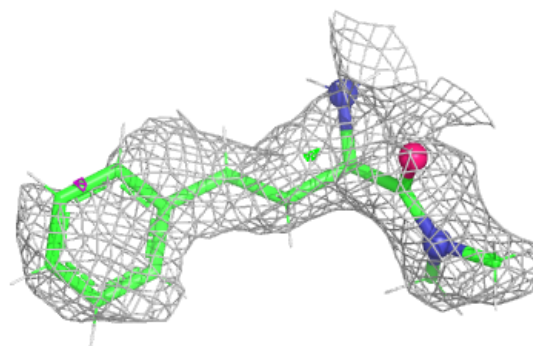
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	C	602	1/1	0.98	0.08	35,35,35,35	0
3	CA	A	602	1/1	0.99	0.10	25,25,25,25	0
3	CA	B	602	1/1	0.99	0.09	27,27,27,27	0
4	NA	B	603	1/1	0.99	0.04	15,15,15,15	0
2	ZN	C	601	1/1	1.00	0.01	25,25,25,25	0
2	ZN	A	601	1/1	1.00	0.04	15,15,15,15	0
2	ZN	B	601	1/1	1.00	0.05	16,16,16,16	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.

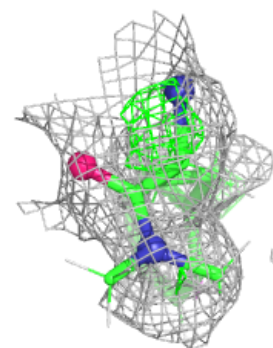
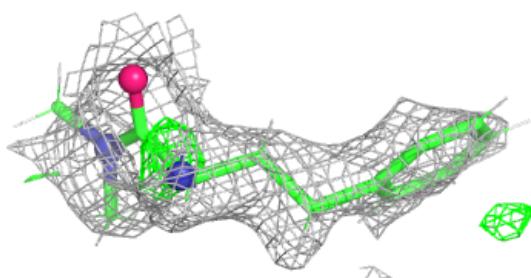
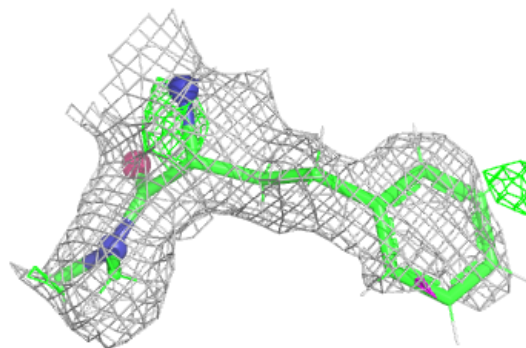
Electron density around KJN C 608:

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

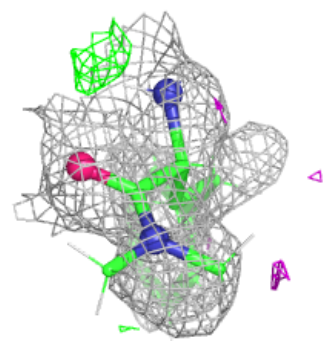
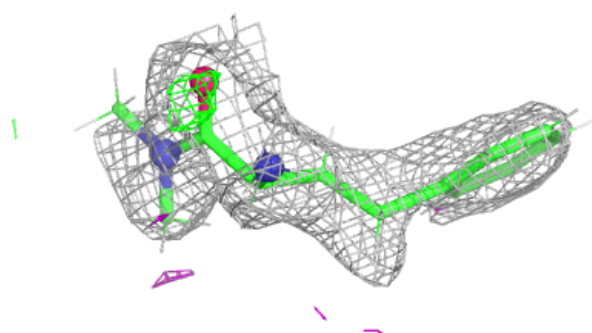
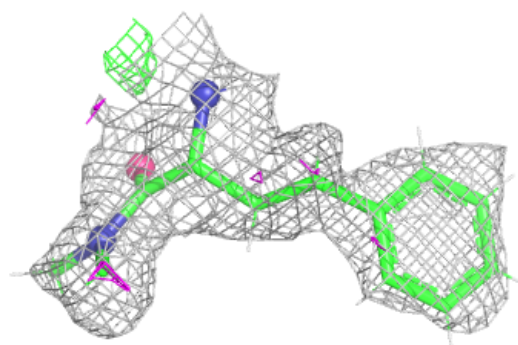


Electron density around KJN A 608:

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

**Electron density around KJN B 613:**

$2mF_o-DF_c$ (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.