



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2025 – 03:15 PM EDT

PDB ID : 3CEJ
Title : Human glycogen phosphorylase (tense state) in complex with the allosteric inhibitor AVE2865
Authors : Wendt, K.U.; Dreyer, M.K.; Anderka, O.; Klabunde, T.; Loenze, P.; Defossa, E.; Schmoll, D.
Deposited on : 2008-02-29
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.4

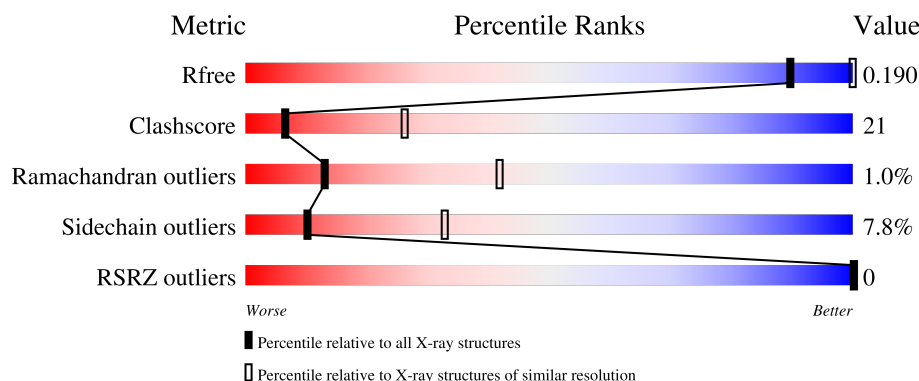
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



The reported resolution of this entry is 3.30 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}	164625	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)

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	809	
1	B	809	

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
3	PLP	A	832	-	-	X	-

2 Entry composition [i](#)

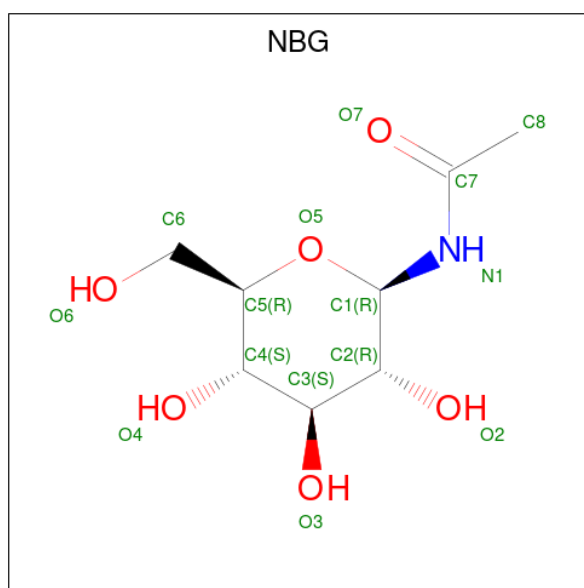
There are 5 unique types of molecules in this entry. The entry contains 13095 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycogen phosphorylase, liver form.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	790	Total	C	N	O	S	0	0	0
			6415	4123	1088	1175	29			
1	B	790	Total	C	N	O	S	0	0	0
			6415	4123	1088	1175	29			

- Molecule 2 is N-acetyl-beta-D-glucopyranosylamine (three-letter code: NBG) (formula: $C_8H_{15}NO_6$).



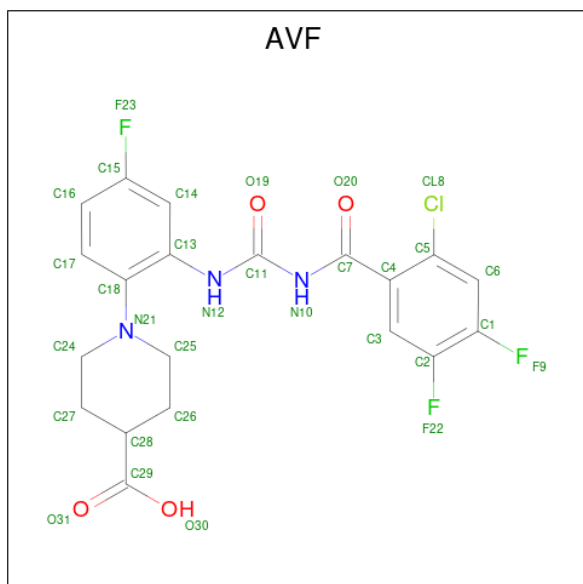
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
3	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 4 is 1-{2-[3-(2-Chloro-4,5-difluoro-benzoyl)-ureido]-4-fluoro-phenyl}-piperidine-4-carboxylic acid (three-letter code: AVF) (formula: $C_{20}H_{17}ClF_3N_3O_4$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	Cl	F	N	O	0	0
			31	20	1	3	3	4		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total	C	Cl	F	N	O	0	0
			31	20	1	3	3	4		

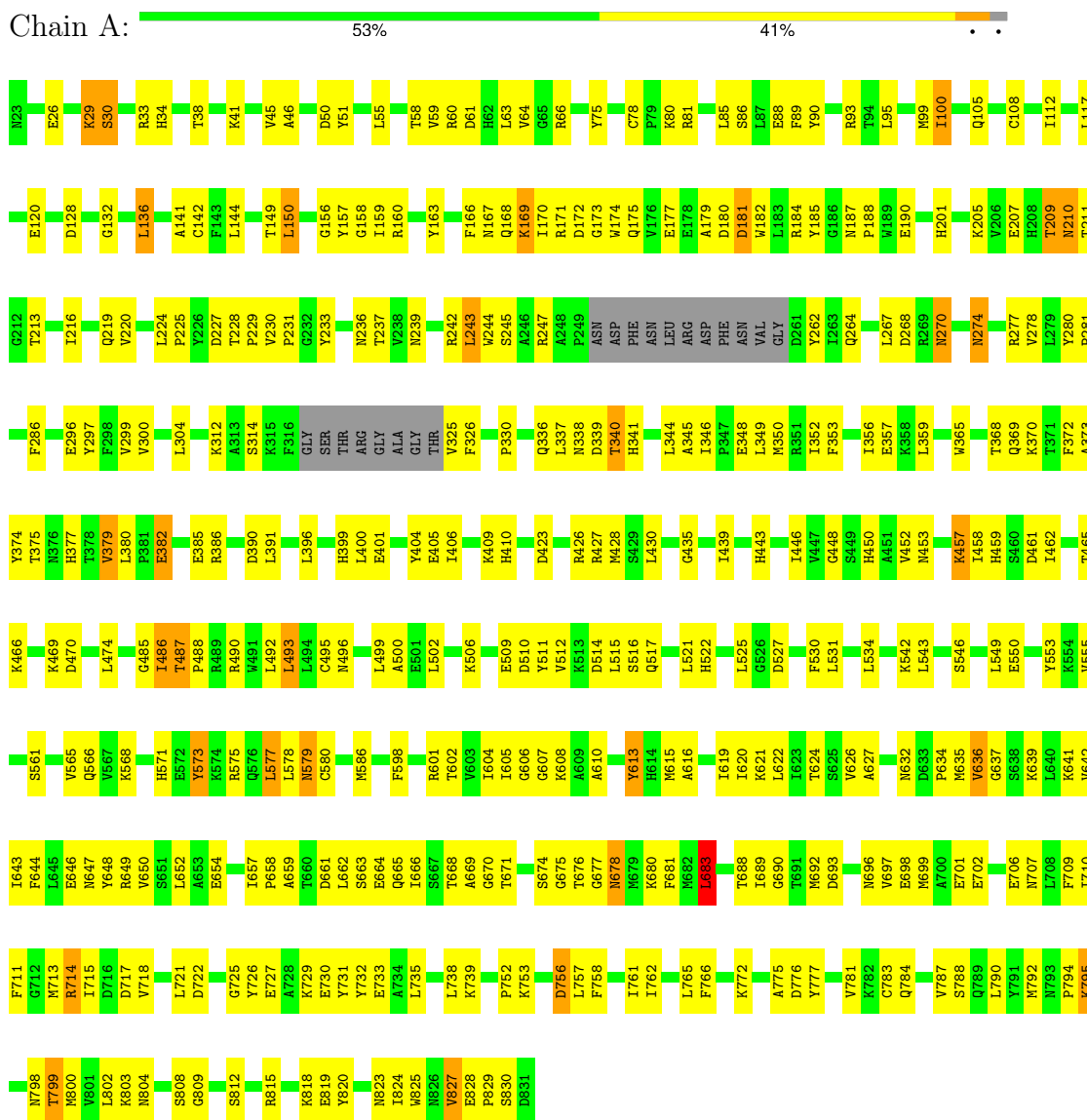
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	63	Total	O	0	0
			63	63		
5	B	78	Total	O	0	0
			78	78		

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: Glycogen phosphorylase, liver form



- Molecule 1: Glycogen phosphorylase, liver form



S788	E702	Y613	S523	Y447	W361	P281	H208	N101	W23
N793	F709	H614	F524	G448	S362	E287	T209	Q105	K29
N794	F710	M615	L525	S449	K363		T210		S30
N798	F711		F530	Y452	L367	L293	T211	D118	R33
W801	F712	I619	L531	N453	T368	K294	T212	L122	H34
L802	K713	K621	R532	G454	Q369	Q295	D217		L35
K803	K714	V636	E553	V455	K370	V299	T218	I125	H36
N804	R715	G637	L594	A456	Y374	V300	Q219	E126	F37
1805	D717	S638	A535	I458			V220	E127	T38
A806	V718	K639	K538	K459	T378	T303	V221	D128	L39
	A719			S460	E382	L304	L222		V40
S813	A720	L645	K542	D461		Q305	A223	L131	K41
D814	L721	E646	L543	I462	E385	D306	L224	G132	D42
R815	D722	N647	V463	V463	E386	I307	P225	N133	R43
T816	K723	Y648	K464	K464	W387	I308	P229	G137	N44
T817	K724	R649	T465	T465	V392	R309	V230	R138	V45
1817		W650	K554	F468		R310	P231		A46
	E727	S651	S560	K469	V392		Q232	F143	R49
1824	A728	L652		D470	L395	S314		L144	D50
E828	K729	A653	F563	E473		K315	N235	D145	F53
P829	Y731	E654	D564	P476	I402	F316	V238	S146	A54
S830	Y732		V565	D477			N239	M147	L55
D831	E733	I657	Q566	K478	E405	GLY		T149	A56
		P658	V567		I406	ARG	L243	L150	H57
	K739	A659	K568		N407	ALA	S245	G151	
		T660	R569	K432	W407	GLY	A246	Y157	L63
	I742	D661			Q408	THR	E247	G158	W67
	D743	S663	Y573	T487	K409	V325	A248	R160	
		E664	K574	P488	H410	F326	P249	Y161	Q71
	S751	Q665	R575	R489	L411	D327	ASN	H73	H73
	P752	I666	Q576	R490	D412	A328	ASP	Y74	Y74
	K753	S667	L577	W491	R413	F329	PHE	Y75	Y75
	Q754	T668	L578	L492		P330	ASN	D76	D76
		A669	M579	L493	A416	D331	LEU	K77	K77
	L757		C580	L494	I417	Q332	ASP	C78	C78
		S674	L581	C495	F418		PHE	P79	P79
	T761	N678	H582	N496	D421	L337	ASN	K80	K80
	T762	M679	M586	P497		T340	VAL	R81	R81
	N763	K680	Y587	G498	R426	A343	D261	D181	L85
	F766	F681		L499	R427	L344	Y262		S86
	F771	M682	K591	A500	M428	A345	I263	R184	L87
	K772	L683	R592	E501	S429	I346	Q264	N187	E88
		G685	D593	I503	L430	P347	A265	P188	Y90
	A775	A686	K596	K506	S436	E348	V266	M189	M91
	D776	I687	L597	I507	K437	L349		R193	G92
	Y777	T688	F598	V599	R438		R269	P194	T94
		I689	P600	Y511	I439	I352		M197	L95
	Y780	Q690	R601	V512	M440	F353	N274	F202	
	V781	T691	M692		M441	V354	I275		
	K782	M693	T602	L515	A442	D355	S276		Q96
	C783	D693	I604		H443		R277		
	Q784		T605	L518	L444	K388			M99
		N696	F606	H522	I446	L359	Y280		I100
		V697							
		E698				P360			

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	123.27Å 123.27Å 121.88Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.47 – 3.30 19.47 – 3.30	Depositor EDS
% Data completeness (in resolution range)	81.2 (19.47-3.30) 81.2 (19.47-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 3.29Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.176 , 0.271 0.182 , 0.190	Depositor DCC
R_{free} test set	1243 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	65.4	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.074 for -h,-k,l 0.185 for h,-h-k,-l 0.078 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13095	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 3.98% 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: AVF, PLP, NBG

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	0.48	1/6559 (0.0%)	0.63	1/8869 (0.0%)
1	B	0.47	0/6559	0.63	0/8869
All	All	0.48	1/13118 (0.0%)	0.63	1/17738 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	108	CYS	CB-SG	-5.59	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	683	LEU	CA-CB-CG	5.03	126.87	115.30

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	6415	0	6411	276	0
1	B	6415	0	6409	274	0
2	A	15	0	15	0	0
2	B	15	0	15	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	16	0	8	8	0
3	B	16	0	6	2	0
4	A	31	0	16	3	0
4	B	31	0	16	6	0
5	A	63	0	0	8	0
5	B	78	0	0	11	0
All	All	13095	0	12896	551	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 21.

The worst 5 of 551 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:680:LYS:HZ1	3:A:832:PLP:C4A	1.30	1.42
1:A:680:LYS:NZ	3:A:832:PLP:H4A	0.91	1.23
1:A:64:VAL:HG13	1:B:40:VAL:HG13	1.35	1.08
1:A:713:MET:HB2	1:A:717:ASP:HB2	1.41	1.02
1:B:88:GLU:HG2	1:B:132:GLY:HA2	1.47	0.95

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	784/809 (97%)	659 (84%)	118 (15%)	7 (1%)	14	44
1	B	784/809 (97%)	693 (88%)	83 (11%)	8 (1%)	13	42
All	All	1568/1618 (97%)	1352 (86%)	201 (13%)	15 (1%)	13	42

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	757	LEU
1	A	181	ASP
1	A	435	GLY
1	A	516	SER
1	A	830	SER

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	692/706 (98%)	634 (92%)	58 (8%)	9	30
1	B	692/706 (98%)	642 (93%)	50 (7%)	12	36
All	All	1384/1412 (98%)	1276 (92%)	108 (8%)	10	33

5 of 108 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	827	VAL
1	B	245	SER
1	B	674	SER
1	B	63	LEU
1	B	184	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 36 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	459	HIS
1	B	798	ASN
1	B	481	ASN
1	B	547	GLN
1	A	459	HIS

5.3.3 RNA ⓘ

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$
4	AVF	A	833	-	33,33,33	1.33	5 (15%)	46,47,47	1.61	6 (13%)
3	PLP	B	832	1	16,16,16	2.22	5 (31%)	20,23,23	1.55	5 (25%)
4	AVF	B	833	-	33,33,33	1.29	4 (12%)	46,47,47	1.57	8 (17%)
2	NBG	A	1	-	15,15,15	0.49	0	21,21,21	0.76	0
3	PLP	A	832	1	16,16,16	1.23	1 (6%)	20,23,23	1.05	2 (10%)
2	NBG	B	2	-	15,15,15	0.69	0	21,21,21	1.46	4 (19%)

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
4	AVF	A	833	-	-	0/20/30/30	0/3/3/3
3	PLP	B	832	1	-	4/8/8/8	0/1/1/1
4	AVF	B	833	-	-	0/20/30/30	0/3/3/3
2	NBG	A	1	-	-	0/6/26/26	0/1/1/1
3	PLP	A	832	1	-	2/8/8/8	0/1/1/1
2	NBG	B	2	-	-	1/6/26/26	0/1/1/1

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	832	PLP	C3-C2	-5.75	1.35	1.41
3	B	832	PLP	C4-C5	-3.55	1.37	1.42
4	A	833	AVF	C13-N12	-3.32	1.35	1.41
3	B	832	PLP	C4-C3	-3.20	1.35	1.41
4	A	833	AVF	C28-C29	3.16	1.57	1.51

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	833	AVF	C7-N10-C11	-5.46	122.95	128.13
4	B	833	AVF	C17-C18-N21	-5.43	113.91	122.42
4	B	833	AVF	C7-N10-C11	-4.65	123.72	128.13
4	A	833	AVF	C17-C18-N21	-4.45	115.45	122.42
2	B	2	NBG	C3-C2-C1	3.71	115.31	109.86

There are no chirality outliers.

5 of 7 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	832	PLP	C5A-O4P-P-O1P
3	B	832	PLP	C5A-O4P-P-O2P
3	B	832	PLP	C5A-O4P-P-O3P
3	A	832	PLP	C3-C4-C4A-O4A
3	B	832	PLP	C3-C4-C4A-O4A

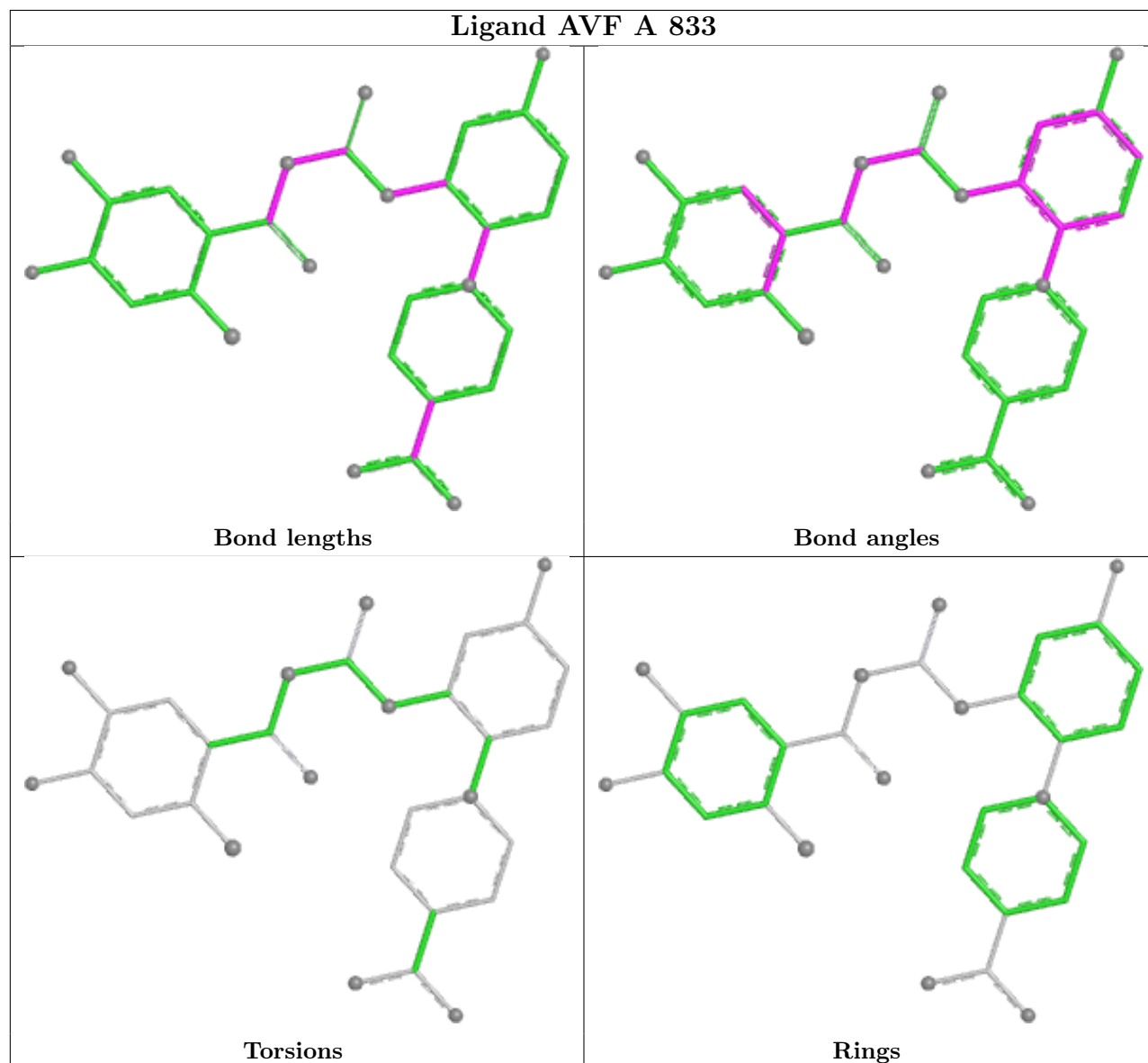
There are no ring outliers.

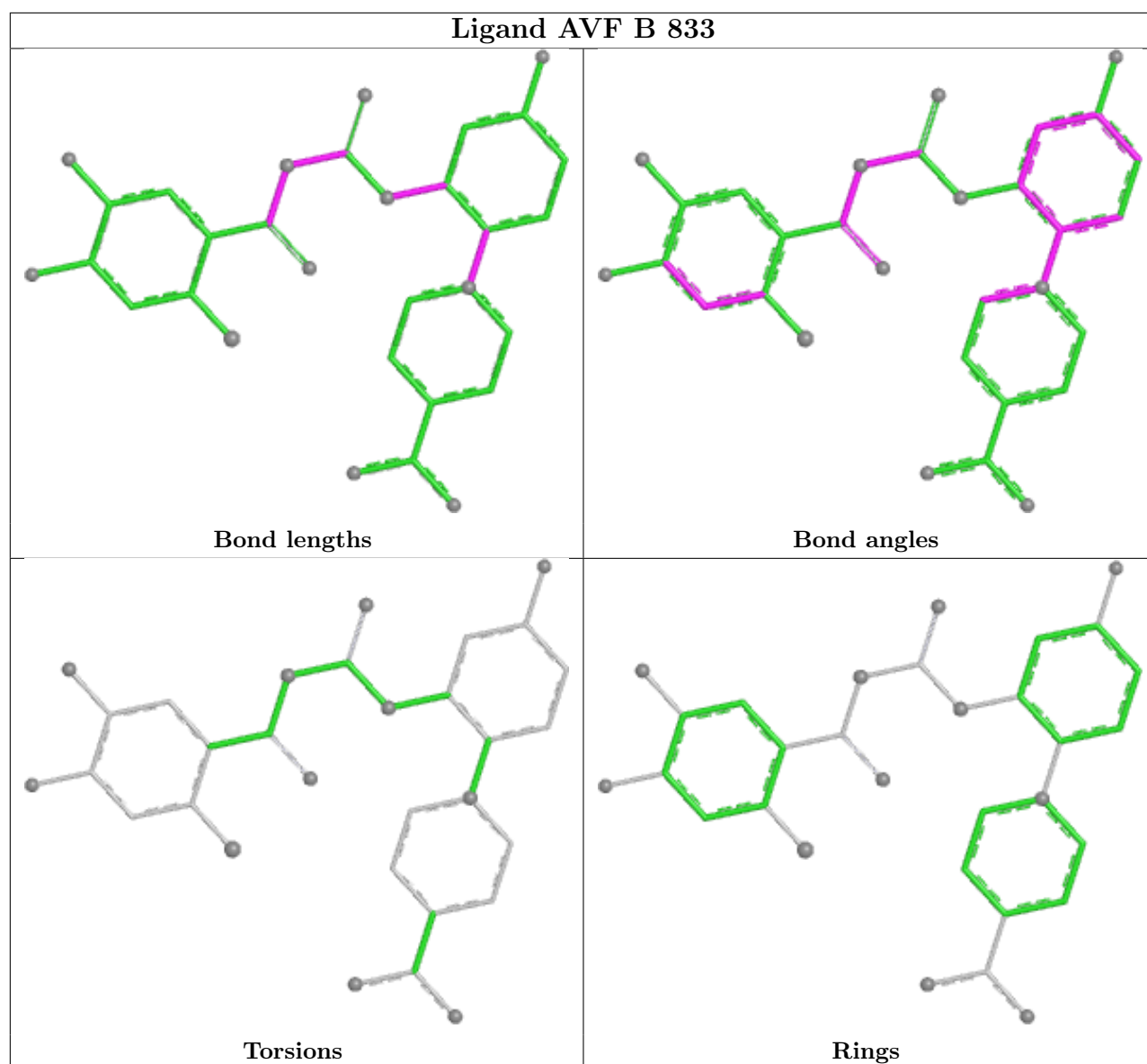
4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	833	AVF	3	0
3	B	832	PLP	2	0
4	B	833	AVF	6	0
3	A	832	PLP	8	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 [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	790/809 (97%)	-2.03	0 100 100	41, 56, 79, 86	0
1	B	790/809 (97%)	-2.03	0 100 100	38, 52, 68, 75	0
All	All	1580/1618 (97%)	-2.03	0 100 100	38, 54, 76, 86	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 monosaccharides in this entry.

6.4 Ligands [i](#)

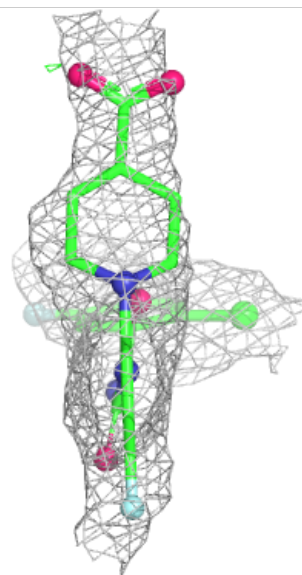
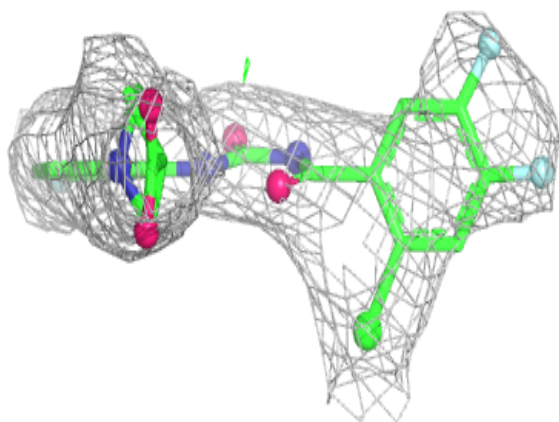
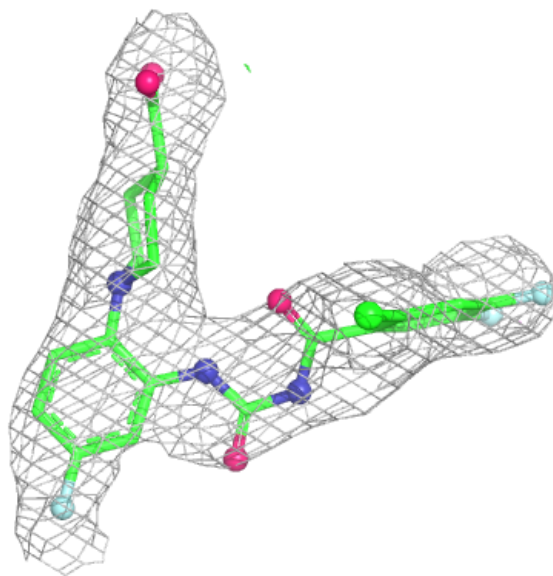
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NBG	A	1	15/15	1.00	0.03	52,53,55,56	0
2	NBG	B	2	15/15	1.00	0.03	57,58,60,61	0
3	PLP	A	832	16/16	1.00	0.02	43,46,49,49	0
3	PLP	B	832	16/16	1.00	0.03	42,45,47,47	0
4	AVF	A	833	31/31	1.00	0.02	52,55,56,58	0
4	AVF	B	833	31/31	1.00	0.02	51,53,56,56	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.

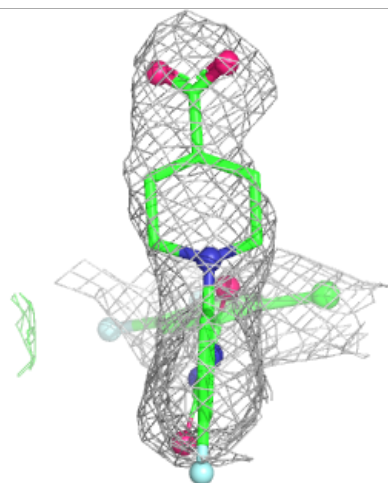
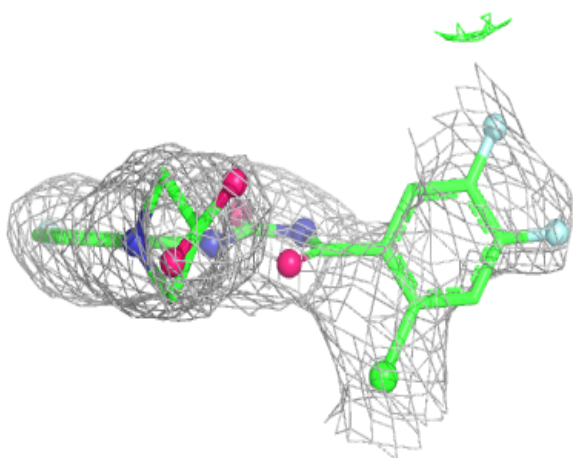
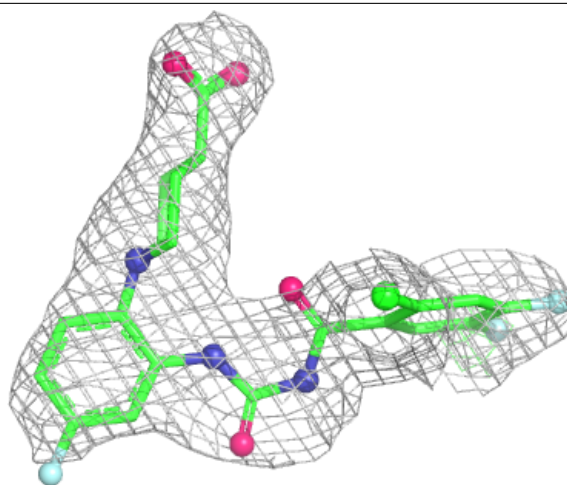
Electron density around AVF A 833:

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



Electron density around AVF B 833:

$2mF_o-DF_c$ (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.