



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2025 – 03:25 PM EDT

PDB ID : 3CEH  
Title : Human liver glycogen phosphorylase (tense state) in complex with the allosteric inhibitor AVE5688  
Authors : Wendt, K.U.; Dreyer, M.K.; Anderka, O.; Klabunde, T.; Loenze, P.; Defossa, E.; Schmoll, D.  
Deposited on : 2008-02-29  
Resolution : 2.80 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](mailto: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>.

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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

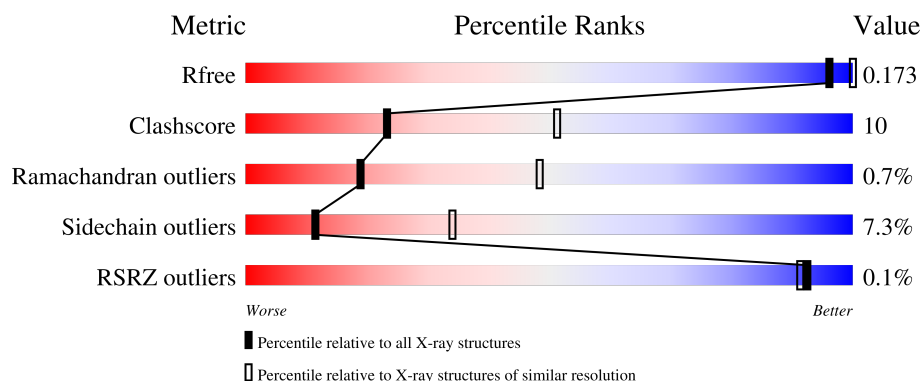
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 2.80 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	3657 (2.80-2.80)
Clashscore	180529	4123 (2.80-2.80)
Ramachandran outliers	177936	4071 (2.80-2.80)
Sidechain outliers	177891	4073 (2.80-2.80)
RSRZ outliers	164620	3659 (2.80-2.80)

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  $\geq 3$ , 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	 71% 24% ..
1	B	809	 75% 21% ..

## 2 Entry composition [i](#)

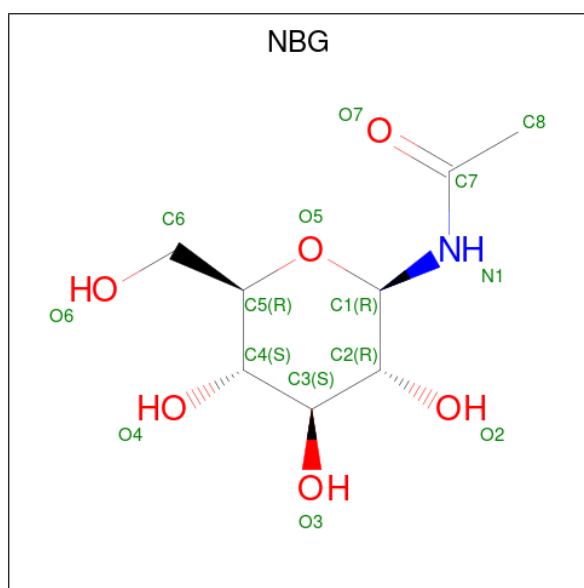
There are 7 unique types of molecules in this entry. The entry contains 13588 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	794	Total	C	N	O	S	0	2	0
			6471	4156	1101	1185	29			
1	B	794	Total	C	N	O	S	0	2	0
			6467	4154	1097	1187	29			

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



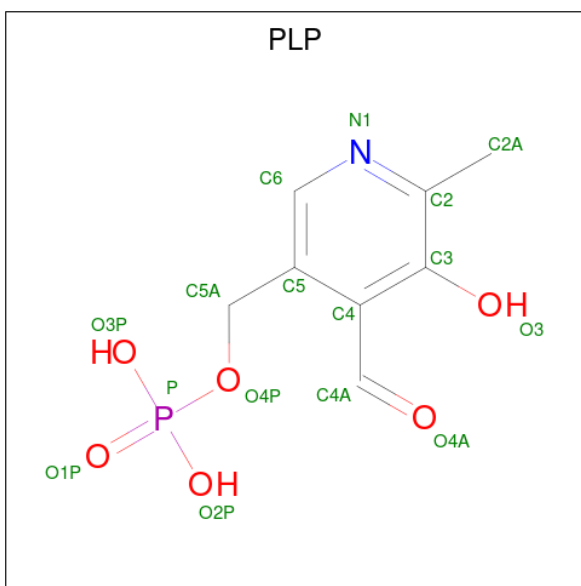
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula:  $O_4P$ ).



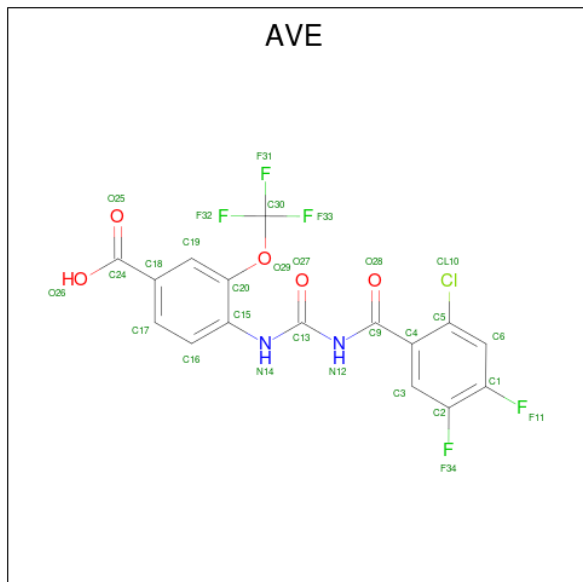
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	O	P		0	0
			5	4	1			
3	B	1	Total	O	P		0	0
			5	4	1			

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula:  $C_8H_{10}NO_6P$ ).



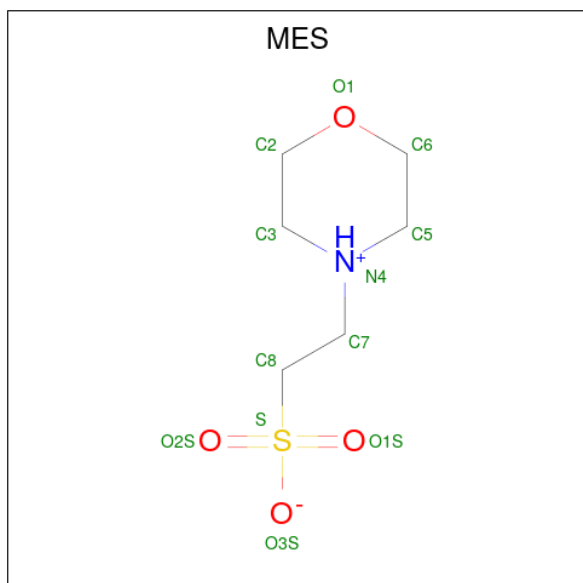
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0
			16	8	1	6	1	
4	B	1	Total	C	N	O	P	0
			16	8	1	6	1	

- Molecule 5 is 4-[3-(2-Chloro-4,5-difluoro-benzoyl)ureido]-3-trifluoromethoxybenzoic acid (three-letter code: AVE) (formula:  $C_{16}H_8ClF_5N_2O_5$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	Cl	F	N	O	0	0
			29	16	1	5	2	5		
5	B	1	Total	C	Cl	F	N	O	0	0
			29	16	1	5	2	5		

- Molecule 6 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

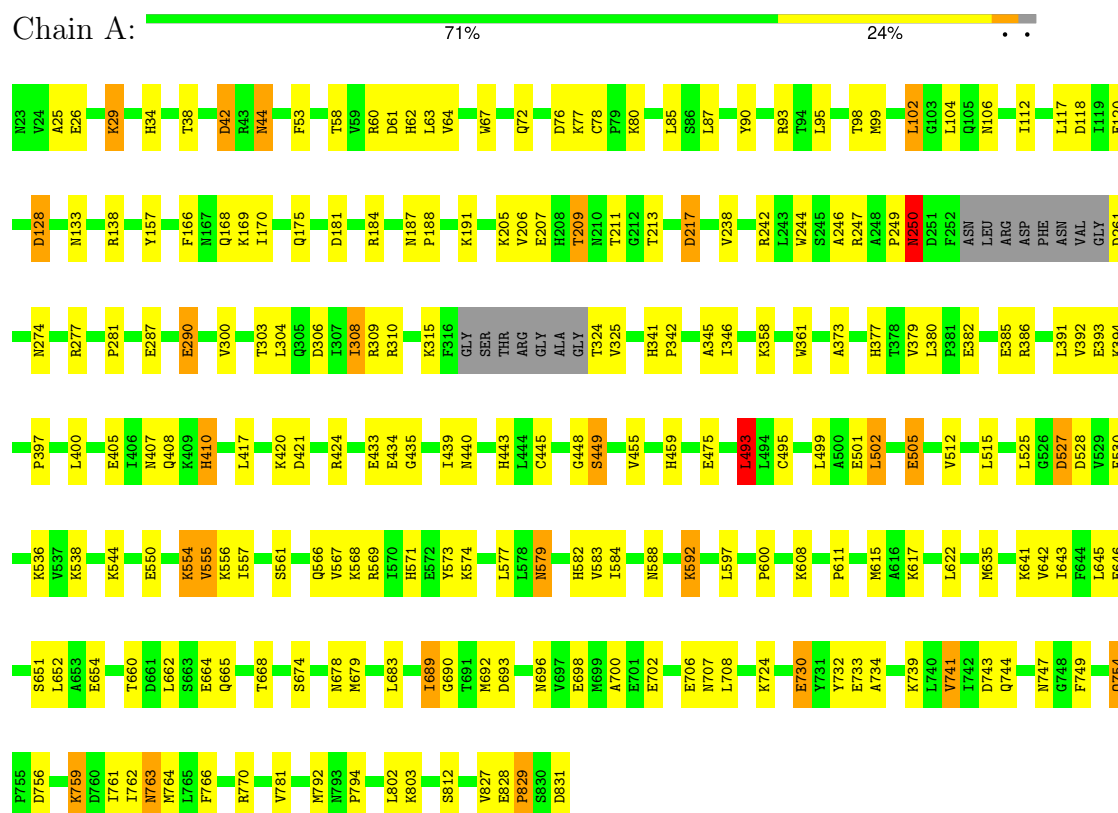
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	234	Total	O	0	0
			234	234		
7	B	274	Total	O	0	0
			274	274		

### 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



R438	L578	L740	R442	N579	V741	H443	I584	G748	F749	F750	S751	P752	K753	Q754	P755	D756	L757	L765	R770	F771	K772	A775	D776	Y777	Y780	V781	S788	Q789	L802	V827	E828	D831	F494	V495	I458	H459	I462	K466	K469	E473	Q480	R489	L492	L493	L494	C495	L502	K520	L525	F530	E540	K544	Q547	N558	V565	Q566	V567	K568	H571	E572	Y573	K574	R575	Q576	L577																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
I604	G607	P611	G612	Y613	H614	M615	A616	K617	I618	I619	I620	K621	V629	L645	E646	N647	I657	P658	E664	Q665	I666	E672	A673	G677	K680	L683	I689	M713	R714	D717	L721	D722	K723	K724	Y731	Y732	E733	K739																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																		</



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	124.11Å 124.11Å 122.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	43.60 – 2.80 43.60 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.2 (43.60-2.80) 99.2 (43.60-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.165 , 0.247 0.172 , 0.173	Depositor DCC
$R_{free}$ test set	2551 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.6	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 61.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l 0.069 for h,-h-k,-l 0.037 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13588	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: AVE, PO4, NBG, MES, PLP

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	0.70	1/6616 (0.0%)	0.77	5/8945 (0.1%)
1	B	0.72	0/6613	0.79	3/8943 (0.0%)
All	All	0.71	1/13229 (0.0%)	0.78	8/17888 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	CYS	CB-SG	-5.25	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	LEU	CA-CB-CG	7.62	132.84	115.30
1	A	770	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	493	LEU	CA-CB-CG	5.41	127.74	115.30
1	A	770	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	B	310	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	A	72	GLN	CB-CA-C	-5.14	100.12	110.40
1	A	138	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	42	ASP	CB-CA-C	5.03	120.45	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	249	PRO	Peptide

## 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	6471	0	6459	142	0
1	B	6467	0	6444	119	0
2	A	15	0	15	1	0
2	B	15	0	15	0	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
4	A	16	0	6	0	0
4	B	16	0	7	2	0
5	A	29	0	7	3	0
5	B	29	0	7	3	0
6	B	12	0	12	1	0
7	A	234	0	0	16	0
7	B	274	0	0	18	0
All	All	13588	0	12972	264	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 10.

All (264) 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:B:274:ASN:ND2	1:B:277:ARG:HH11	1.40	1.20
1:A:274:ASN:ND2	1:A:277:ARG:HH11	1.38	1.18
1:B:413:ARG:HG2	1:B:413:ARG:HH11	1.14	1.13
1:B:217:ASP:HB3	7:B:1088:HOH:O	1.57	1.02
1:A:274:ASN:HD22	1:A:277:ARG:HH11	1.03	0.95
1:B:274:ASN:ND2	1:B:277:ARG:NH1	2.13	0.94
1:A:274:ASN:ND2	1:A:277:ARG:NH1	2.15	0.94
1:B:274:ASN:HD22	1:B:277:ARG:HH11	1.15	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:792:MET:HE1	7:A:1063:HOH:O	1.74	0.87
1:A:274:ASN:HD22	1:A:277:ARG:NH1	1.73	0.84
1:A:250:ASN:HA	7:A:1026:HOH:O	1.77	0.83
1:B:290:GLU:HG3	1:B:391:LEU:HD11	1.60	0.83
1:B:544:LYS:HD3	7:B:1036:HOH:O	1.80	0.81
1:A:554:LYS:O	1:A:555:VAL:HG23	1.81	0.80
1:B:413:ARG:HH11	1:B:413:ARG:CG	1.93	0.79
1:A:324:THR:N	7:A:995:HOH:O	2.17	0.77
1:A:44:ASN:H	1:A:44:ASN:HD22	1.31	0.76
1:A:615:MET:HA	1:A:615:MET:HE3	1.68	0.76
1:A:455:VAL:H	1:A:459:HIS:HD2	1.34	0.75
1:B:167:ASN:ND2	1:B:647:ASN:HD21	1.84	0.74
1:A:732:TYR:CE1	1:A:739:LYS:HG3	2.22	0.74
1:B:413:ARG:HG2	1:B:413:ARG:NH1	1.87	0.74
1:A:290:GLU:HG3	1:A:391:LEU:HD11	1.68	0.74
1:B:380:LEU:HD12	1:B:380:LEU:H	1.52	0.73
1:A:44:ASN:HD22	1:A:44:ASN:N	1.87	0.72
1:B:211:THR:HG22	1:B:211:THR:O	1.89	0.71
1:A:693:ASP:O	1:A:696:ASN:HB2	1.90	0.71
1:A:515:LEU:HD22	1:A:812:SER:HB2	1.72	0.71
1:A:207:GLU:HG2	1:A:209:THR:HG22	1.72	0.70
1:B:423:ASP:HB3	7:B:1098:HOH:O	1.91	0.70
1:B:168:GLN:HG3	1:B:175:GLN:HG3	1.72	0.70
1:A:34:HIS:HE1	1:A:61:ASP:OD2	1.75	0.70
1:B:458:ILE:O	1:B:462:ILE:HD13	1.93	0.69
1:A:475:GLU:HB3	7:A:1017:HOH:O	1.92	0.68
1:A:493:LEU:HD11	1:A:512:VAL:HG11	1.75	0.68
1:A:274:ASN:HD21	1:A:277:ARG:HH11	1.39	0.68
4:B:832:PLP:O4A	4:B:832:PLP:H5A1	1.96	0.66
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.79	0.66
1:B:455:VAL:H	1:B:459:HIS:HD2	1.43	0.65
1:A:26:GLU:HB3	7:A:936:HOH:O	1.97	0.64
1:A:128:ASP:OD2	1:A:651:SER:OG	2.12	0.64
1:B:274:ASN:HD22	1:B:277:ARG:NH1	1.86	0.63
1:B:286:PHE:CD1	1:B:385:GLU:HG2	2.34	0.63
1:A:341:HIS:HB2	1:A:342:PRO:HD3	1.81	0.63
1:B:584:ILE:HG22	1:B:741:VAL:HG22	1.79	0.62
1:A:662:LEU:HD11	1:A:689:ILE:HB	1.81	0.62
1:B:721:LEU:HD23	1:B:772:LYS:HD3	1.81	0.62
1:B:247:ARG:HD2	7:B:1064:HOH:O	2.00	0.62
1:B:713:MET:HB3	1:B:717:ASP:HB2	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:GLU:HA	1:B:357:GLU:OE2	1.98	0.62
1:B:174:TRP:CE2	1:B:621:LYS:HG3	2.35	0.61
1:B:575:ARG:HD3	1:B:666:ILE:O	2.00	0.61
1:A:678:ASN:OD1	1:A:679:MET:N	2.33	0.61
1:A:80:LYS:HB3	1:A:827:VAL:HG12	1.83	0.61
1:B:219:GLN:OE1	1:B:219:GLN:HA	2.00	0.61
1:B:170:ILE:HG12	1:B:646:GLU:HG2	1.83	0.61
1:A:455:VAL:H	1:A:459:HIS:CD2	2.17	0.61
1:B:405:GLU:HA	1:B:405:GLU:OE2	2.01	0.60
1:A:615:MET:HA	1:A:615:MET:CE	2.31	0.60
1:B:568:LYS:NZ	4:B:832:PLP:O3P	2.34	0.60
1:A:53:PHE:HE1	1:A:188:PRO:HD3	1.66	0.60
1:B:754:GLN:HB2	1:B:757:LEU:HB2	1.82	0.60
1:B:466:LYS:HB2	1:B:466:LYS:NZ	2.16	0.60
1:B:731:TYR:CE2	1:B:775:ALA:HA	2.37	0.60
1:A:304:LEU:O	1:A:308:ILE:HG13	2.02	0.59
1:A:300:VAL:HG13	1:A:345:ALA:HA	1.83	0.59
1:B:42:ASP:HB2	7:B:1027:HOH:O	2.02	0.59
1:B:274:ASN:HD21	1:B:277:ARG:HH11	1.42	0.59
1:A:106:ASN:HB2	7:A:926:HOH:O	2.03	0.58
1:A:64:VAL:HG13	1:B:40:VAL:HG13	1.85	0.58
1:A:98:THR:HG22	1:A:102:LEU:HD22	1.86	0.58
1:A:133:ASN:HB3	1:A:569:ARG:NH1	2.18	0.58
1:B:458:ILE:O	1:B:462:ILE:CD1	2.51	0.58
1:B:234:MET:HA	7:B:945:HOH:O	2.03	0.57
1:A:205:LYS:HE3	7:A:1057:HOH:O	2.03	0.57
1:A:118:ASP:HB2	7:A:1054:HOH:O	2.04	0.57
1:A:566:GLN:HB2	1:A:664:GLU:HB2	1.85	0.57
1:A:434:GLU:N	1:A:434:GLU:OE1	2.37	0.57
1:A:502:LEU:HA	1:A:505:GLU:HG3	1.86	0.57
1:B:308:ILE:HD13	1:B:352:ILE:HG21	1.86	0.56
1:B:747:ASN:HB2	7:B:1078:HOH:O	2.05	0.56
1:B:136:LEU:C	1:B:136:LEU:HD23	2.26	0.56
1:B:568:LYS:O	1:B:607:GLY:HA3	2.04	0.56
1:A:166:PHE:O	1:A:608:LYS:NZ	2.30	0.56
1:A:707:ASN:ND2	1:A:803:LYS:HD2	2.22	0.55
1:A:571:HIS:HB2	1:A:574:LYS:HD2	1.87	0.55
1:B:572:GLU:HG3	1:B:613:TYR:OH	2.06	0.55
1:B:283:ASP:O	1:B:571[B]:HIS:NE2	2.40	0.54
1:B:198:LEU:HD13	1:B:305:GLN:HB2	1.88	0.54
1:B:751:SER:N	1:B:752:PRO:HD3	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:GLN:O	1:A:690:GLY:CA	2.56	0.54
1:A:538:LYS:HE2	7:A:846:HOH:O	2.08	0.54
1:A:665:GLN:O	1:A:690:GLY:HA2	2.08	0.54
1:A:584:ILE:HG22	1:A:741:VAL:HG22	1.90	0.53
1:B:615:MET:O	1:B:619:ILE:HG13	2.08	0.53
1:A:44:ASN:H	1:A:44:ASN:ND2	2.03	0.53
1:A:579:ASN:C	1:A:579:ASN:HD22	2.13	0.53
1:A:181:ASP:OD2	1:A:184:ARG:HD3	2.08	0.52
1:A:25:ALA:O	1:A:29:LYS:HD2	2.10	0.52
1:A:455:VAL:HG23	1:A:674:SER:HB2	1.91	0.52
1:A:556:LYS:O	1:A:641:LYS:HE3	2.09	0.52
1:B:167:ASN:ND2	1:B:647:ASN:ND2	2.57	0.52
1:B:469:LYS:HG2	1:B:473:GLU:OE1	2.08	0.52
1:B:777:TYR:O	1:B:781:VAL:HG23	2.09	0.52
1:A:493:LEU:HD21	1:A:512:VAL:HG13	1.92	0.52
1:B:382:GLU:CD	1:B:770:ARG:HH22	2.12	0.52
1:A:170:ILE:HG12	1:A:646:GLU:HG2	1.92	0.52
1:A:407:ASN:O	1:A:410:HIS:HB3	2.10	0.52
1:A:763:ASN:C	1:A:763:ASN:HD22	2.13	0.52
1:A:582:HIS:HD2	1:A:781:VAL:HG22	1.74	0.51
1:A:93:ARG:HD2	7:A:954:HOH:O	2.10	0.51
1:B:566:GLN:HB2	1:B:664:GLU:HB2	1.92	0.51
1:A:763:ASN:C	1:A:763:ASN:ND2	2.64	0.51
1:A:707:ASN:HD21	1:A:803:LYS:HD2	1.75	0.51
1:A:759:LYS:HE3	1:A:759:LYS:O	2.10	0.51
1:A:550:GLU:HG2	1:A:555:VAL:O	2.10	0.51
1:B:442:ALA:O	1:B:446:ILE:HG13	2.11	0.51
1:B:566:GLN:HE22	1:B:576:GLN:HA	1.75	0.51
1:A:361:TRP:CH2	1:A:405:GLU:HG3	2.46	0.51
1:A:87:LEU:HD23	1:A:341:HIS:HB3	1.93	0.50
1:B:34:HIS:HE1	1:B:61:ASP:OD2	1.93	0.50
1:A:53:PHE:CE1	1:A:188:PRO:HD3	2.46	0.50
1:A:157:TYR:HD2	1:A:244:TRP:HE1	1.58	0.50
1:A:445:CYS:O	1:A:449:SER:OG	2.25	0.50
1:B:677:GLY:HA2	1:B:680:LYS:HD2	1.92	0.50
1:A:168:GLN:HG3	1:A:175:GLN:HG3	1.94	0.50
1:B:339:ASP:OD2	1:B:378:THR:HG23	2.12	0.50
1:A:385:GLU:O	1:A:386:ARG:HG3	2.12	0.50
1:B:340:THR:O	1:B:343:ALA:HB2	2.12	0.50
1:A:421:ASP:CG	1:A:424:ARG:HB2	2.32	0.50
1:A:698:GLU:O	1:A:702:GLU:HG2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:THR:HG23	1:B:355:ASP:OD2	2.11	0.50
1:B:339:ASP:O	1:B:342:PRO:HD2	2.12	0.50
1:A:550:GLU:OE2	1:A:557:ILE:N	2.42	0.49
1:B:170:ILE:CG1	1:B:646:GLU:HG2	2.41	0.49
1:A:678:ASN:OD1	1:A:679:MET:HG3	2.12	0.49
1:A:42:ASP:HB3	7:A:963:HOH:O	2.11	0.49
7:A:879:HOH:O	1:B:277:ARG:HD3	2.12	0.49
1:A:525:LEU:HD23	1:A:802:LEU:HD23	1.95	0.49
1:B:544:LYS:O	1:B:547:GLN:HB2	2.12	0.49
1:B:88:GLU:OE2	1:B:133:ASN:N	2.46	0.49
1:B:748:GLY:HA3	1:B:755:PRO:HA	1.95	0.49
1:A:392:VAL:HG21	1:A:439:ILE:HD12	1.94	0.49
1:A:58:THR:O	1:A:62:HIS:HD2	1.96	0.48
1:A:527:ASP:HB3	1:A:530:PHE:HB3	1.95	0.48
1:B:211:THR:O	1:B:211:THR:CG2	2.61	0.48
1:B:530:PHE:HE2	1:B:802:LEU:HD13	1.78	0.48
6:B:1:MES:H22	7:B:947:HOH:O	2.13	0.48
1:A:501:GLU:O	1:A:505:GLU:HG2	2.14	0.48
1:B:217:ASP:CB	7:B:1088:HOH:O	2.34	0.48
1:B:97:ASN:ND2	7:B:877:HOH:O	2.47	0.48
1:A:300:VAL:CG1	1:A:345:ALA:HA	2.44	0.47
1:A:561:SER:HB2	1:A:600:PRO:C	2.34	0.47
1:A:95:LEU:O	1:A:99:MET:HG3	2.14	0.47
1:B:525:LEU:HD23	1:B:802:LEU:HD23	1.96	0.47
1:B:192:SER:O	1:B:193:ARG:HD2	2.14	0.47
1:B:568:LYS:NZ	7:B:872:HOH:O	2.48	0.47
1:A:205:LYS:HE2	1:A:217:ASP:OD2	2.15	0.47
1:B:91:MET:HB2	1:B:129:ALA:HB3	1.96	0.47
1:A:309[A]:ARG:NH1	7:A:899:HOH:O	2.48	0.47
1:B:174:TRP:CZ2	1:B:621:LYS:HG3	2.49	0.47
1:B:565:VAL:HG22	1:B:604:ILE:HB	1.97	0.47
1:B:689:ILE:O	1:B:689:ILE:HG23	2.15	0.47
1:A:77:LYS:HA	1:A:77:LYS:HD3	1.72	0.47
1:A:583:VAL:HG11	1:A:642:VAL:HG21	1.97	0.47
1:B:324:THR:C	1:B:326:PHE:N	2.65	0.47
1:B:495:CYS:O	1:B:658:PRO:HG2	2.15	0.46
1:B:88:GLU:CD	1:B:133:ASN:HD22	2.19	0.46
1:A:67:TRP:HA	1:A:238:VAL:HB	1.97	0.46
1:B:432:GLU:HG2	7:B:990:HOH:O	2.16	0.46
1:A:206:VAL:HG13	1:A:213:THR:CG2	2.45	0.46
1:B:327:ASP:OD1	1:B:363:LYS:HE3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:PHE:HB3	1:B:330:PRO:HD3	1.96	0.46
1:A:310:ARG:NH2	3:A:3:PO4:O2	2.50	0.46
1:A:393:GLU:HB2	1:A:400:LEU:HD22	1.97	0.46
1:A:34:HIS:CD2	1:A:38:THR:OG1	2.64	0.45
1:B:331:ASP:HA	7:B:951:HOH:O	2.16	0.45
1:A:744:GLN:HB3	1:A:749:PHE:HB3	1.98	0.45
1:A:538:LYS:NZ	1:A:660:THR:O	2.29	0.45
1:B:453:ASN:HA	1:B:480:GLN:O	2.17	0.45
1:A:60:ARG:O	1:A:64:VAL:HG23	2.16	0.45
1:A:67:TRP:CZ2	5:A:833:AVE:H6	2.51	0.45
1:A:246:ALA:O	1:A:247:ARG:HD2	2.16	0.45
1:A:592:LYS:O	1:A:592:LYS:HG2	2.16	0.45
1:B:167:ASN:HD21	1:B:647:ASN:HD21	1.61	0.45
1:B:174:TRP:CD2	1:B:621:LYS:HG3	2.51	0.45
1:B:274:ASN:HD22	1:B:274:ASN:HA	1.59	0.45
1:B:80:LYS:HB3	1:B:827:VAL:HG12	1.99	0.45
1:A:373:ALA:HA	1:A:449:SER:HB3	1.98	0.45
1:A:455:VAL:N	1:A:459:HIS:HD2	2.09	0.45
1:B:492:LEU:HD22	1:B:683:LEU:HD11	1.99	0.45
1:A:206:VAL:HG23	1:A:397:PRO:HB2	1.99	0.45
1:A:493:LEU:HD21	1:A:512:VAL:CG1	2.47	0.45
1:A:579:ASN:O	1:A:583:VAL:HG23	2.17	0.44
1:B:158:GLY:HA2	1:B:299:VAL:HG21	1.99	0.44
1:B:443:HIS:CE1	7:B:956:HOH:O	2.70	0.44
1:A:700:ALA:HA	1:A:708:LEU:HD13	2.00	0.44
1:B:611:PRO:HA	1:B:617:LYS:HE3	1.98	0.44
1:A:617:LYS:HD3	7:A:859:HOH:O	2.16	0.44
1:A:828:GLU:HA	1:A:829:PRO:HD3	1.83	0.44
5:A:833:AVE:O25	1:B:44:ASN:ND2	2.51	0.44
1:B:193:ARG:HG3	1:B:242:ARG:HH21	1.83	0.44
1:A:615:MET:HE1	1:A:761:ILE:HG13	1.99	0.44
1:B:216:ILE:O	1:B:217:ASP:HB2	2.18	0.43
1:A:380:LEU:HB3	1:A:382:GLU:CD	2.39	0.43
5:B:833:AVE:O28	5:B:833:AVE:N14	2.42	0.43
1:A:763:ASN:HD22	1:A:764:MET:N	2.16	0.43
1:A:346:ILE:HD13	1:A:448:GLY:HA3	2.01	0.43
1:A:274:ASN:HD21	1:A:277:ARG:NH1	2.04	0.43
1:A:358:LYS:HA	1:A:358:LYS:HD3	1.77	0.43
1:B:577:LEU:HD13	1:B:765:LEU:HD21	2.01	0.43
1:A:440:ASN:ND2	1:A:443:HIS:CE1	2.87	0.43
1:B:23:ASN:OD1	1:B:23:ASN:C	2.57	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ASN:HA	1:A:188:PRO:HD2	1.79	0.42
1:A:250:ASN:ND2	1:A:250:ASN:H	2.17	0.42
1:A:98:THR:O	1:A:102:LEU:HB2	2.19	0.42
1:A:377:HIS:ND1	2:A:1:NBG:O6	2.48	0.42
1:A:754:GLN:C	1:A:756:ASP:H	2.23	0.42
1:B:87:LEU:HD23	1:B:341:HIS:HB2	2.01	0.42
1:B:566:GLN:NE2	1:B:576:GLN:HA	2.34	0.42
1:B:72:GLN:HE21	5:B:833:AVE:C24	2.32	0.42
1:B:657:ILE:HB	1:B:658:PRO:HD3	2.01	0.42
1:A:495:CYS:HB2	1:A:654:GLU:O	2.19	0.42
1:A:762:ILE:HG23	1:A:766:PHE:HE1	1.83	0.42
1:B:558:ASN:OD1	1:B:558:ASN:C	2.58	0.42
1:A:277:ARG:HD3	7:B:886:HOH:O	2.19	0.42
1:A:309[A]:ARG:NH2	7:A:904:HOH:O	2.53	0.42
1:B:584:ILE:CG2	1:B:741:VAL:HG22	2.49	0.42
1:A:34:HIS:CE1	1:A:61:ASP:OD2	2.65	0.42
1:A:730:GLU:O	1:A:734:ALA:CB	2.67	0.42
1:A:588:ASN:HD21	1:A:744:GLN:CD	2.23	0.42
1:B:341:HIS:CD2	1:B:341:HIS:N	2.88	0.42
1:A:67:TRP:CE2	5:A:833:AVE:H6	2.55	0.41
1:A:80:LYS:HD3	1:A:827:VAL:HG13	2.02	0.41
1:A:242:ARG:NH1	1:A:306:ASP:OD2	2.53	0.41
1:B:578:LEU:HD11	1:B:780:TYR:CD2	2.55	0.41
5:B:833:AVE:O27	5:B:833:AVE:H16	2.20	0.41
1:B:341:HIS:CD2	1:B:341:HIS:H	2.37	0.41
1:A:85:LEU:HD13	1:A:303:THR:HG21	2.01	0.41
1:A:112:ILE:HG23	1:A:117:LEU:HB2	2.02	0.41
1:A:325:VAL:HA	7:A:1002:HOH:O	2.21	0.41
1:A:261:ASP:OD2	1:A:261:ASP:C	2.59	0.41
1:B:34:HIS:HD2	1:B:38:THR:OG1	2.04	0.41
1:B:629:VAL:HG21	1:B:750:PHE:CD1	2.55	0.41
1:A:63:LEU:HB3	1:A:102:LEU:HD21	2.03	0.41
1:A:393:GLU:HB2	1:A:400:LEU:CD2	2.51	0.41
1:B:361:TRP:CD1	1:B:361:TRP:C	2.93	0.41
1:A:555:VAL:HG11	1:A:643:ILE:HD11	2.03	0.41
1:A:743:ASP:O	1:A:747:ASN:ND2	2.54	0.41
1:B:96:GLN:NE2	7:B:980:HOH:O	2.49	0.41
1:B:217:ASP:CG	7:B:1088:HOH:O	2.57	0.41
1:B:328:ALA:O	1:B:331:ASP:N	2.49	0.41
1:B:400:LEU:HD12	1:B:400:LEU:HA	1.86	0.41
1:B:672:GLU:O	1:B:673:ALA:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:436:SER:O	1:B:437:LYS:HB2	2.21	0.41
1:B:97:ASN:HA	1:B:494:LEU:HD12	2.03	0.40
1:B:666:ILE:HG13	7:B:862:HOH:O	2.21	0.40
1:A:515:LEU:CD2	1:A:812:SER:HB2	2.45	0.40
1:A:706:GLU:CD	1:A:706:GLU:H	2.24	0.40
1:B:262:TYR:CD2	1:B:263:ILE:HD13	2.56	0.40
1:A:102:LEU:HB3	1:A:104:LEU:HD12	2.03	0.40
1:B:280:TYR:HA	1:B:281:PRO:HD3	1.87	0.40
1:A:281:PRO:HG2	1:A:611:PRO:HD2	2.03	0.40
1:B:387:TRP:HA	1:B:388:PRO:HD3	1.98	0.40

There are no symmetry-related clashes.

## 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	790/809 (98%)	718 (91%)	64 (8%)	8 (1%)	13	39
1	B	790/809 (98%)	737 (93%)	49 (6%)	4 (0%)	25	56
All	All	1580/1618 (98%)	1455 (92%)	113 (7%)	12 (1%)	19	44

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	250	ASN
1	B	315	LYS
1	A	435	GLY
1	A	410	HIS
1	A	568	LYS
1	B	76[A]	ASP
1	B	76[B]	ASP
1	B	520	LYS

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Mol	Chain	Res	Type
1	A	555	VAL
1	A	829	PRO
1	A	741	VAL
1	A	794	PRO

### 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	698/706 (99%)	643 (92%)	55 (8%)	10	30
1	B	698/706 (99%)	652 (93%)	46 (7%)	14	39
All	All	1396/1412 (99%)	1295 (93%)	101 (7%)	11	34

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	42	ASP
1	A	44	ASN
1	A	76	ASP
1	A	90	TYR
1	A	102	LEU
1	A	120	GLU
1	A	128	ASP
1	A	169	LYS
1	A	191	LYS
1	A	209	THR
1	A	211	THR
1	A	217	ASP
1	A	250	ASN
1	A	287	GLU
1	A	290	GLU
1	A	308	ILE
1	A	315	LYS
1	A	379	VAL

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Mol	Chain	Res	Type
1	A	394	LYS
1	A	408	GLN
1	A	417	LEU
1	A	420	LYS
1	A	433	GLU
1	A	449	SER
1	A	493	LEU
1	A	499	LEU
1	A	502	LEU
1	A	505	GLU
1	A	527	ASP
1	A	528	ASP
1	A	536	LYS
1	A	544	LYS
1	A	554	LYS
1	A	567	VAL
1	A	573	TYR
1	A	577	LEU
1	A	579	ASN
1	A	592	LYS
1	A	597	LEU
1	A	622	LEU
1	A	635	MET
1	A	645	LEU
1	A	652	LEU
1	A	668	THR
1	A	683	LEU
1	A	689	ILE
1	A	692	MET
1	A	724	LYS
1	A	730	GLU
1	A	733	GLU
1	A	754	GLN
1	A	759	LYS
1	A	763	ASN
1	A	831	ASP
1	B	90	TYR
1	B	102	LEU
1	B	109	ASP
1	B	121	GLU
1	B	150	LEU
1	B	209	THR

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Mol	Chain	Res	Type
1	B	213	THR
1	B	216	ILE
1	B	245	SER
1	B	251	ASP
1	B	312	LYS
1	B	337	LEU
1	B	380	LEU
1	B	382	GLU
1	B	384	LEU
1	B	386	ARG
1	B	390	ASP
1	B	394	LYS
1	B	413	ARG
1	B	433	GLU
1	B	438	ARG
1	B	447	VAL
1	B	453	ASN
1	B	466	LYS
1	B	480	GLN
1	B	489	ARG
1	B	502	LEU
1	B	540	GLU
1	B	544	LYS
1	B	547	GLN
1	B	568	LYS
1	B	573	TYR
1	B	577	LEU
1	B	579	ASN
1	B	645	LEU
1	B	666	ILE
1	B	714	ARG
1	B	723	LYS
1	B	724	LYS
1	B	733	GLU
1	B	739	LYS
1	B	751	SER
1	B	788	SER
1	B	789	GLN
1	B	828	GLU
1	B	831	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	34	HIS
1	A	44	ASN
1	A	62	HIS
1	A	97	ASN
1	A	106	ASN
1	A	167	ASN
1	A	239	ASN
1	A	250	ASN
1	A	270	ASN
1	A	274	ASN
1	A	284	ASN
1	A	369	GLN
1	A	459	HIS
1	A	481	ASN
1	A	541	ASN
1	A	566	GLN
1	A	579	ASN
1	A	582	HIS
1	A	747	ASN
1	A	763	ASN
1	A	789	GLN
1	B	32	ASN
1	B	34	HIS
1	B	72	GLN
1	B	96	GLN
1	B	105	GLN
1	B	167	ASN
1	B	208	HIS
1	B	239	ASN
1	B	264	GLN
1	B	270	ASN
1	B	274	ASN
1	B	305	GLN
1	B	410	HIS
1	B	459	HIS
1	B	481	ASN
1	B	541	ASN
1	B	566	GLN
1	B	579	ASN
1	B	614	HIS
1	B	789	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](#)

9 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	PO4	A	3	-	4,4,4	1.21	0	6,6,6	1.06	0
6	MES	B	1	-	12,12,12	1.98	1 (8%)	15,16,16	2.46	8 (53%)
5	AVE	B	833	-	30,30,30	1.23	3 (10%)	43,44,44	1.77	7 (16%)
3	PO4	B	4	-	4,4,4	0.96	0	6,6,6	1.22	0
4	PLP	B	832	1	16,16,16	1.44	3 (18%)	20,23,23	1.73	4 (20%)
4	PLP	A	832	1	16,16,16	1.27	3 (18%)	20,23,23	1.73	5 (25%)
5	AVE	A	833	-	30,30,30	1.43	4 (13%)	43,44,44	1.24	3 (6%)
2	NBG	A	1	-	15,15,15	1.62	3 (20%)	21,21,21	1.51	1 (4%)
2	NBG	B	2	-	15,15,15	0.49	0	21,21,21	0.56	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
6	MES	B	1	-	-	2/6/14/14	0/1/1/1
5	AVE	B	833	-	-	3/21/21/21	0/2/2/2
4	PLP	B	832	1	-	3/8/8/8	0/1/1/1
4	PLP	A	832	1	-	4/8/8/8	0/1/1/1
5	AVE	A	833	-	-	0/21/21/21	0/2/2/2
2	NBG	A	1	-	-	0/6/26/26	0/1/1/1
2	NBG	B	2	-	-	0/6/26/26	0/1/1/1

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1	MES	C8-S	-6.42	1.68	1.77
5	A	833	AVE	C18-C24	3.99	1.58	1.49
5	B	833	AVE	C15-N14	-3.54	1.34	1.41
5	A	833	AVE	C15-N14	-3.45	1.35	1.41
2	A	1	NBG	O5-C1	-3.39	1.38	1.43
4	B	832	PLP	C2-N1	3.02	1.39	1.33
2	A	1	NBG	C2-C1	-2.95	1.49	1.53
5	A	833	AVE	C4-C9	2.75	1.55	1.50
4	B	832	PLP	C6-N1	2.72	1.40	1.34
4	A	832	PLP	C2-N1	2.60	1.38	1.33
5	B	833	AVE	C4-C9	2.47	1.55	1.50
5	A	833	AVE	C13-N12	-2.32	1.34	1.39
4	B	832	PLP	C4-C5	-2.30	1.38	1.42
4	A	832	PLP	C4-C5	-2.24	1.38	1.42
4	A	832	PLP	C3-C2	-2.13	1.38	1.41
2	A	1	NBG	O5-C5	-2.10	1.39	1.44
5	B	833	AVE	C19-C18	-2.02	1.36	1.39

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	833	AVE	C9-N12-C13	-6.35	122.11	128.13
6	B	1	MES	C5-N4-C3	5.45	120.58	108.84
4	B	832	PLP	C3-C4-C5	4.44	121.84	118.28
2	A	1	NBG	O5-C1-C2	-4.33	104.86	109.72
4	A	832	PLP	C3-C4-C5	4.00	121.49	118.28
5	B	833	AVE	O29-C20-C19	-3.81	112.92	122.77
6	B	1	MES	C7-N4-C5	3.49	120.53	111.24
4	B	832	PLP	C4-C3-C2	-3.43	118.21	120.14
5	B	833	AVE	C30-O29-C20	-3.42	109.34	118.42
5	A	833	AVE	C9-N12-C13	-3.13	125.16	128.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	832	PLP	C5-C6-N1	-3.06	118.86	123.83
6	B	1	MES	O3S-S-C8	3.04	111.95	106.00
4	A	832	PLP	O4A-C4A-C4	-2.99	117.72	124.80
6	B	1	MES	C6-C5-N4	-2.95	105.64	110.12
6	B	1	MES	C7-N4-C3	2.87	118.88	111.24
5	B	833	AVE	C19-C18-C24	-2.76	115.01	119.96
4	A	832	PLP	C4-C3-C2	-2.75	118.60	120.14
5	A	833	AVE	C17-C18-C24	2.74	125.80	120.37
5	B	833	AVE	C5-C6-C1	2.61	120.39	118.42
5	A	833	AVE	N14-C13-N12	2.58	119.82	114.22
4	B	832	PLP	O2P-P-O4P	2.57	113.37	106.67
6	B	1	MES	C6-O1-C2	2.35	117.49	109.88
4	B	832	PLP	C5-C6-N1	-2.30	120.09	123.83
5	B	833	AVE	F33-C30-O29	-2.26	101.95	111.74
6	B	1	MES	C2-C3-N4	-2.20	106.78	110.12
4	A	832	PLP	O2P-P-O4P	2.09	112.13	106.67
6	B	1	MES	O2S-S-C8	2.05	109.83	106.73
5	B	833	AVE	C6-C5-C4	-2.04	119.92	121.59

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	832	PLP	C5A-O4P-P-O1P
6	B	1	MES	C8-C7-N4-C5
5	B	833	AVE	F33-C30-O29-C20
5	B	833	AVE	F32-C30-O29-C20
4	B	832	PLP	C3-C4-C4A-O4A
5	B	833	AVE	F31-C30-O29-C20
6	B	1	MES	C8-C7-N4-C3
4	A	832	PLP	C3-C4-C4A-O4A
4	B	832	PLP	C6-C5-C5A-O4P
4	B	832	PLP	C5A-O4P-P-O1P
4	A	832	PLP	C5-C4-C4A-O4A
4	A	832	PLP	C5A-O4P-P-O3P

There are no ring outliers.

6 monomers are involved in 11 short contacts:

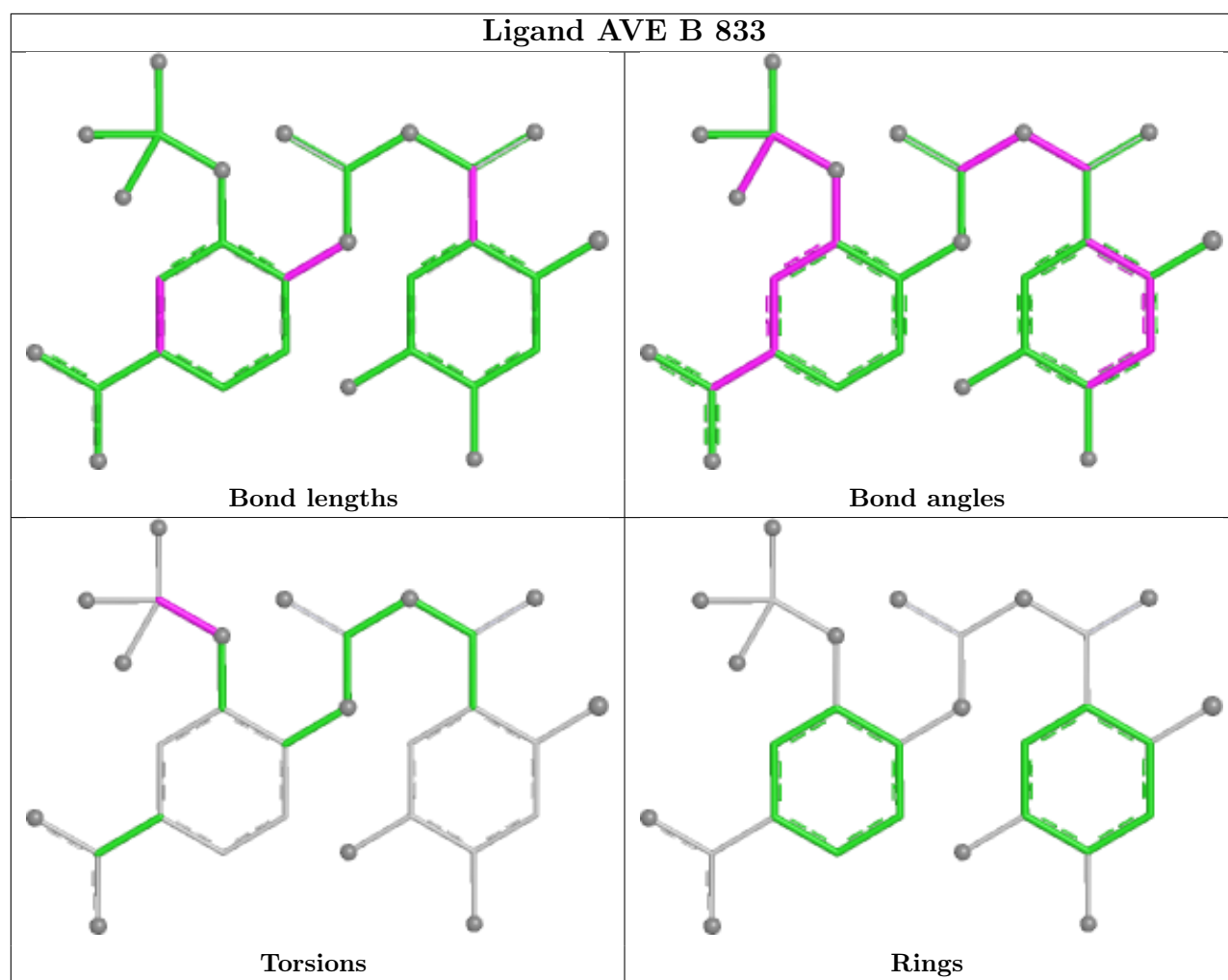
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3	PO4	1	0

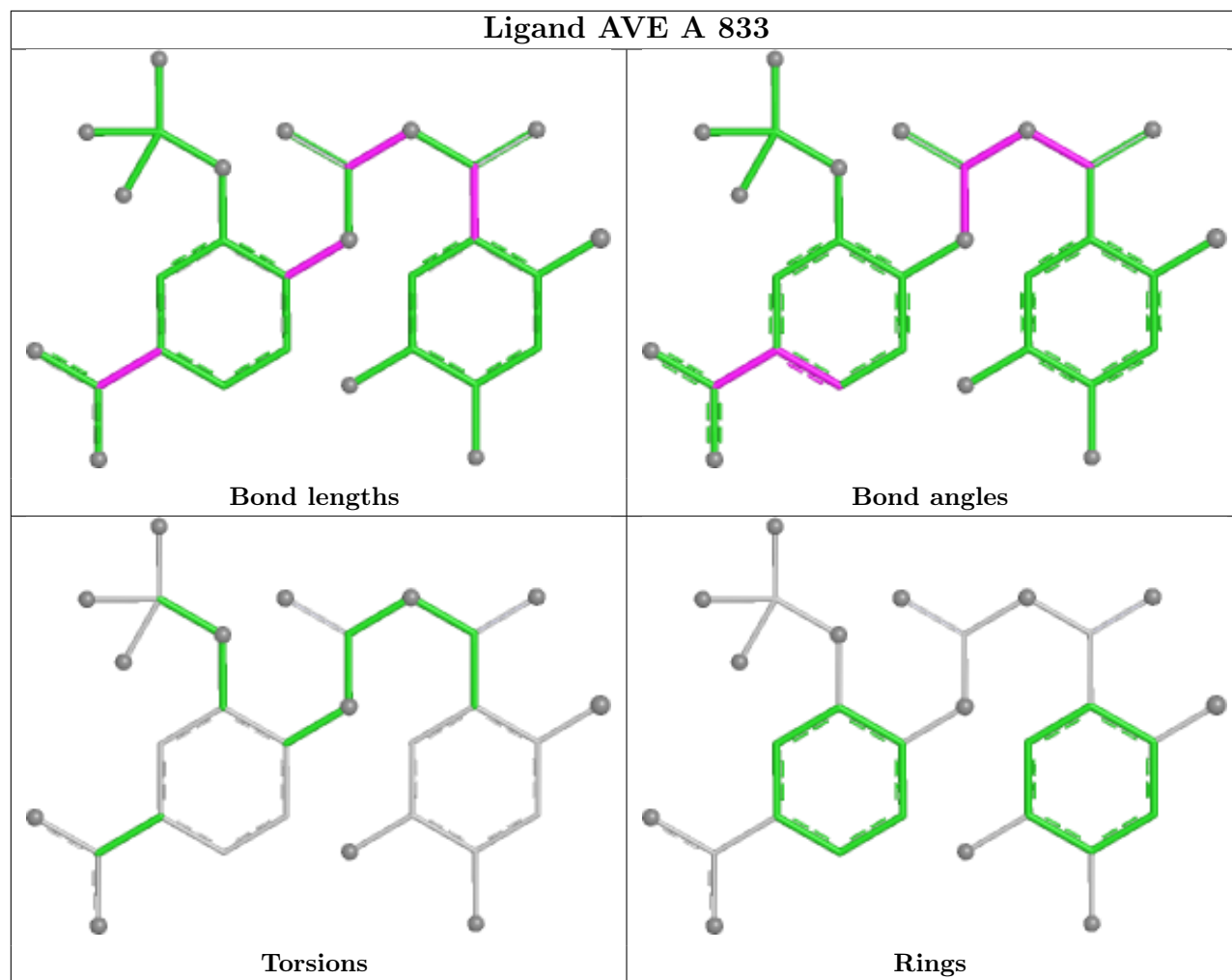
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	1	MES	1	0
5	B	833	AVE	3	0
4	B	832	PLP	2	0
5	A	833	AVE	3	0
2	A	1	NBG	1	0

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 [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	794/809 (98%)	-0.73	0	100   100	12, 35, 61, 74	2 (0%)
1	B	794/809 (98%)	-0.87	1 (0%)	92   91	13, 31, 52, 70	2 (0%)
All	All	1588/1618 (98%)	-0.80	1 (0%)	92   91	12, 33, 58, 74	4 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	252	PHE	3.1

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	PLP	B	832	16/16	0.92	0.10	18,19,22,24	0
2	NBG	A	1	15/15	0.93	0.09	25,28,32,32	0
2	NBG	B	2	15/15	0.96	0.07	23,28,30,32	0
6	MES	B	1	12/12	0.96	0.09	48,51,58,58	0

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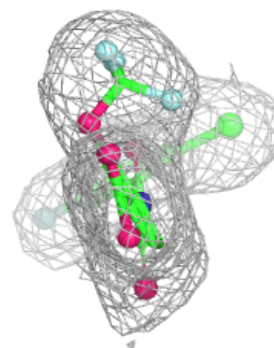
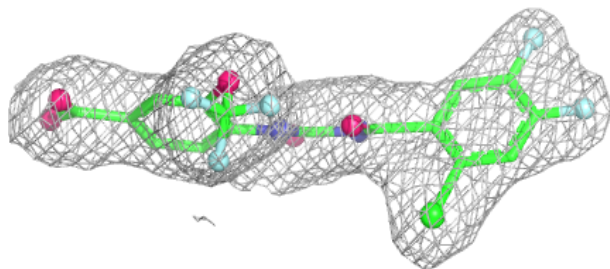
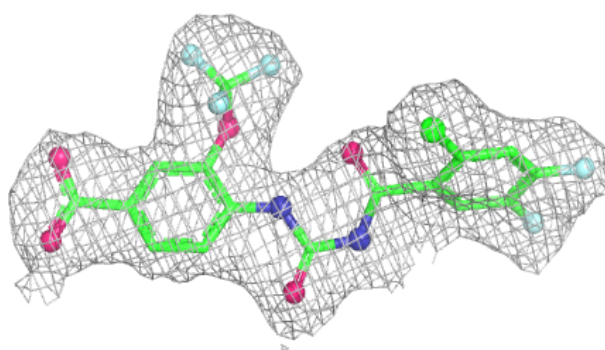
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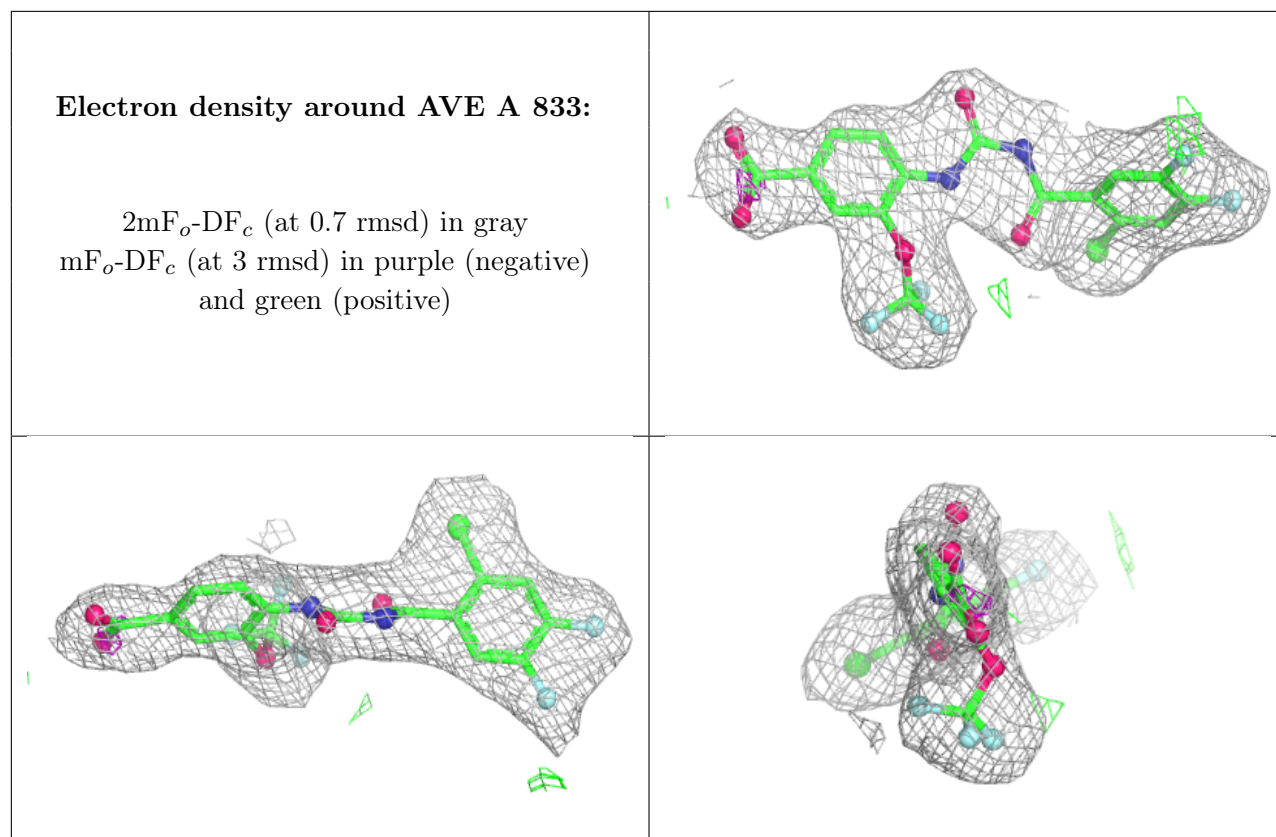
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	AVE	B	833	29/29	0.97	0.06	27,31,34,35	0
4	PLP	A	832	16/16	0.97	0.07	25,30,34,34	0
5	AVE	A	833	29/29	0.98	0.06	21,26,34,39	0
3	PO4	A	3	5/5	0.98	0.06	28,28,29,32	0
3	PO4	B	4	5/5	0.98	0.06	32,32,34,38	0

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 AVE B 833:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.