



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2025 – 03:15 PM EDT

PDB ID : 3CEJ  
Title : Human glycogen phosphorylase (tense state) in complex with the allosteric inhibitor AVE2865  
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Deposited on : 2008-02-29  
Resolution : 3.30 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

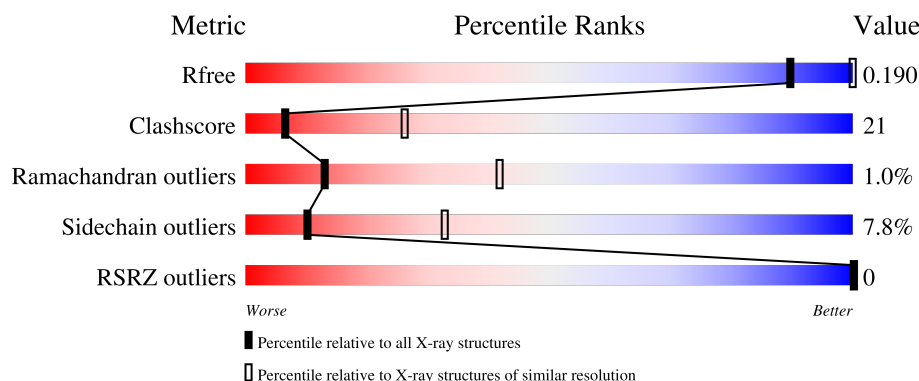
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 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  $\geq 3$ , 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	
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](#)

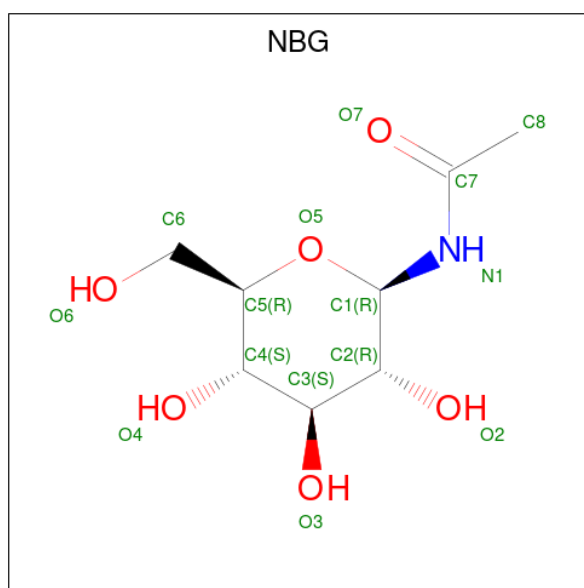
There are 5 unique types of molecules in this entry. The entry contains 13095 atoms, of which 0 are hydrogens and 0 are deuteriums.

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:  $C_8H_{15}NO_6$ ).



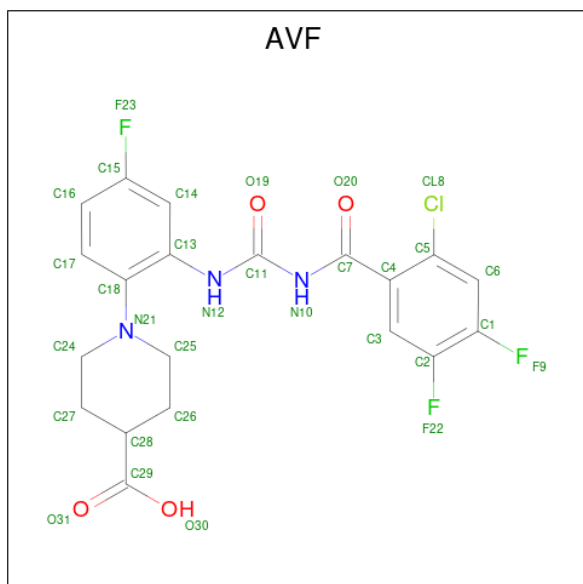
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	8	1	6		
2	B	1	Total	C	N	O	0	0
			15	8	1	6		

- 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		

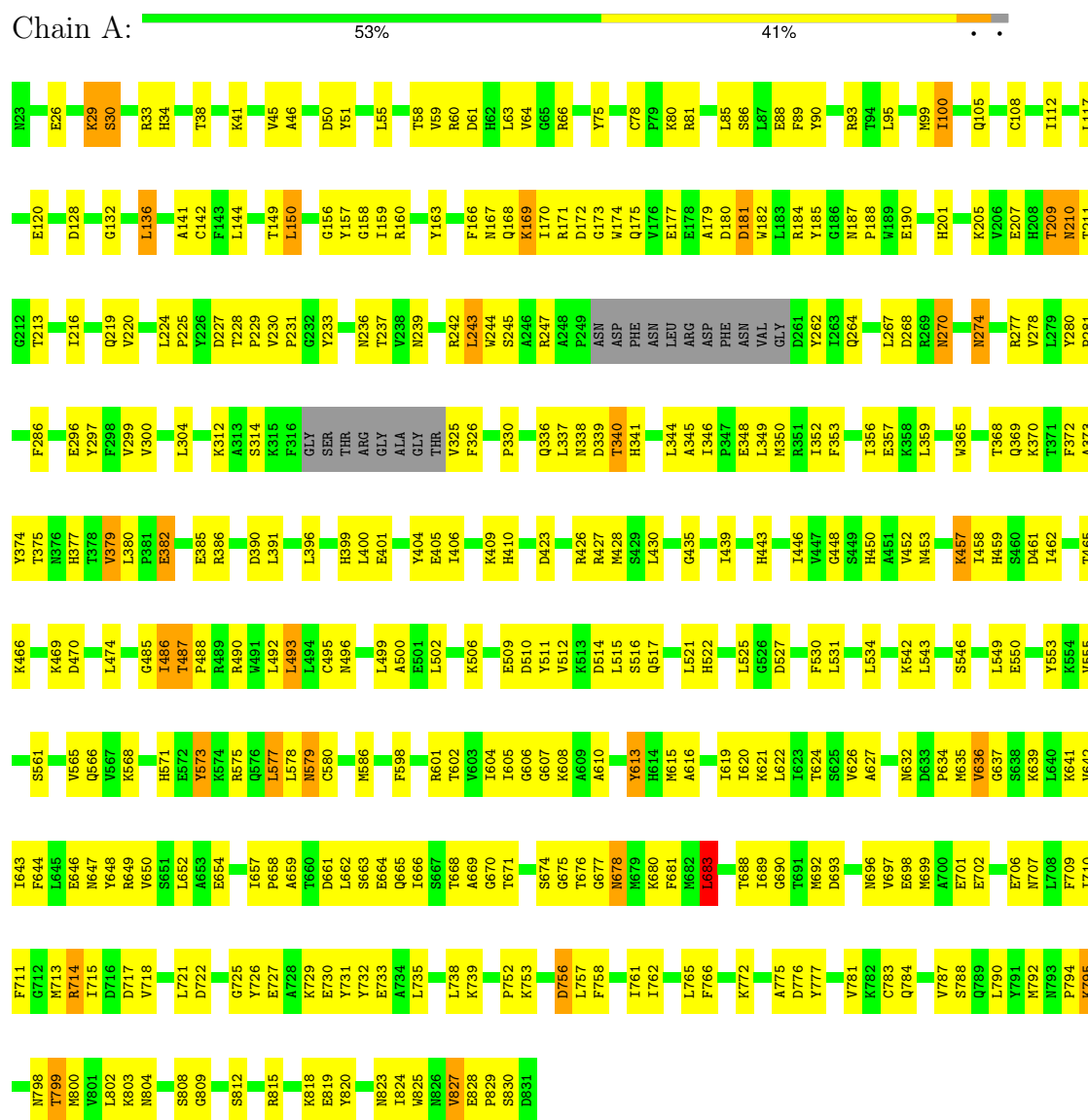
- Molecule 5 is water.

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	E532	G454	Q369	Q295	D217		L35
K803	K714	W636	E533	V455	K370	V299	T218	I125	H36
N804	K715	G637	L534	A456		V300	Q219	E126	F37
	D717	S638	A535	K457	Y374		V220	E127	T38
L805	V718	G639	K538	I458	T378	T303	V221	D128	L39
A806	A719			H459		L304	L222		V40
	A720	L645	K542	S460	E382	Q305	A223	L131	K41
S813	L721	E646	L543	D461		D306	L224	G132	D42
D814	D722	N647	V463	I462	E385	I307	P225	G133	R43
R815	K723	Y648	K464	V463	E386	I308	P229	G137	N44
T816	K724	R649	T465	T465	W387	R309	V230	R138	V45
I817		W650	K554		V392	R310	P231		A46
	E727	S651	S560	F468			Q232	F143	R49
I824	A728	L652		K469		S314		L144	D50
	K729	A653	F563	D470	L395	K315	N235	D145	F53
E828	E730	E654	D564	E473	R398	GLY	V238	S146	A54
P829	Y731		V565		I402	SER	N239	M147	L55
S830	Y732	I657	Q566	P476		THR		T149	A56
D831	E733	A659	V567	D477	E405	ARG	L243	L150	H57
		T660	K568	K478	I406	GLY	W244	G151	
	K739	D681	R569		N407	ALA	S245		L63
	I742	L662		K492	Q408	THR	A246	Y157	
	D743	S663	Y573	T487	K409	V325	E247	G158	W67
		E664	K574	P488	H410	F326	A248	I159	
	S751	Q665	R575	R489	D411	D327	P249	R160	Q71
	P752	I666	Q576	R490	L412	A328	ASN	Y161	Q72
	K753	S667	L577	W491	R413	F329	ASP	H73	H73
	Q754	T668	L578	L492		P330	PHE	Y74	Y74
	L757	A669	M579	L493	A416	D331	ASN	Y75	Y75
			C580	L494	L417	Q332	LEU	Q168	D76
		S674	L581	C495	F418		ARG	K169	K77
	T761	N678	H582	N496		L337	ASP	I170	C78
	T762	M679		P497	D421		PHE	W174	P79
	N763	K680	M586	G498		T340	ASN	Q175	K80
	F766	F681	Y587	L499	R426		VAL		R81
		M682	K591	A500	R427	A343	D261	D181	L85
	F771	L683	K592	E501	M428	L344	Y262		S86
	K772	N684	D593	L502	S429	A345	I263	R184	L87
		G685	I503	T503	L430	I346	Q264	E88	F89
	A775	A686	K596			P347	A265	Y90	M91
	D776	L687	L597	K506	S436	E348	V266	N187	G92
	Y777	T688	F598	I507	K437	L349		W189	M91
		I689	V599		R438		R269	R193	G92
	Y780	Q690	P600	Y511	N440	I352		P194	T94
	V781	T691	R601	V512	M441	V354	N274		L95
	K782	M692	T602	L515	A442	D355	I275	M197	Q96
	C783	D693	I604		H443		S276		
	Q784		T605	L518	L444	K388	R277	F202	M99
		N696	I606	H522	C445	L359			
		W697	G606		I446	P360	Y280		I100



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 <sup>2</sup> )	65.4	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 37.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	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 <sup>2</sup> )	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.*

<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 [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.

All (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
1:B:184:ARG:HG3	1:B:184:ARG:HH11	1.32	0.95
1:A:120:GLU:HG2	5:A:886:HOH:O	1.69	0.93
1:B:168:GLN:HG3	1:B:175:GLN:HG3	1.50	0.92
1:A:675:GLY:HA3	1:A:678:ASN:HD21	1.32	0.91
1:A:680:LYS:HZ2	3:A:832:PLP:H4A	1.09	0.90
1:B:160:ARG:HB2	1:B:243:LEU:HB3	1.50	0.90
1:B:274:ASN:HD22	1:B:277:ARG:HE	1.14	0.90
1:B:34:HIS:CE1	1:B:57:HIS:HB3	2.07	0.90
1:B:410:HIS:HE1	1:B:428:MET:O	1.55	0.90
1:A:575:ARG:NH2	1:A:776:ASP:HB2	1.88	0.89
1:B:455:VAL:H	1:B:459:HIS:HD2	1.20	0.88
1:A:100:ILE:HG13	1:A:105:GLN:OE1	1.75	0.87
1:A:181:ASP:OD2	1:A:184:ARG:HB2	1.74	0.87
1:A:649:ARG:HG2	1:A:649:ARG:HH11	1.40	0.87
1:A:680:LYS:HZ3	3:A:832:PLP:H4A	1.35	0.86
1:B:507:ILE:HG12	1:B:507:ILE:O	1.77	0.84
1:B:599:VAL:HB	5:B:884:HOH:O	1.77	0.83
1:A:274:ASN:ND2	1:A:277:ARG:HE	1.75	0.83
1:B:274:ASN:ND2	1:B:277:ARG:HE	1.74	0.83
1:A:714:ARG:HH11	1:A:714:ARG:CG	1.90	0.83
1:A:550:GLU:HA	5:A:863:HOH:O	1.82	0.79
1:A:713:MET:HB2	1:A:717:ASP:CB	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:575:ARG:HH22	1:A:776:ASP:HB2	1.48	0.78
1:B:714:ARG:N	1:B:714:ARG:HD2	1.97	0.78
1:B:680:LYS:O	1:B:682:MET:N	2.18	0.77
1:A:777:TYR:O	1:A:781:VAL:HG23	1.84	0.77
1:B:308:ILE:HD13	1:B:352:ILE:HG21	1.66	0.76
1:A:665:GLN:HB2	1:A:696:ASN:HD21	1.50	0.76
1:A:29:LYS:HB3	1:A:33:ARG:HH12	1.52	0.75
1:B:535:ALA:HB2	1:B:798:ASN:HD21	1.52	0.74
1:A:75:TYR:HA	1:A:81:ARG:HH22	1.53	0.74
1:A:756:ASP:O	1:A:758:PHE:N	2.21	0.74
1:B:329:PHE:HB3	1:B:330:PRO:HD3	1.69	0.74
1:B:78:CYS:SG	1:B:314:SER:HB2	2.27	0.74
1:B:55:LEU:HD22	1:B:122:LEU:HD12	1.69	0.73
1:A:30:SER:HB3	1:A:58:THR:HG23	1.69	0.73
1:A:729:LYS:O	1:A:733:GLU:HG2	1.89	0.73
1:B:184:ARG:HG3	1:B:184:ARG:NH1	2.03	0.73
1:B:455:VAL:H	1:B:459:HIS:CD2	2.06	0.73
1:A:515:LEU:C	1:A:517:GLN:H	1.92	0.73
1:B:93:ARG:HB3	1:B:126:GLU:OE1	1.89	0.73
1:A:168:GLN:HB3	1:A:647:ASN:HA	1.69	0.73
1:B:39:LEU:HD12	1:B:50:ASP:OD1	1.89	0.73
1:B:665:GLN:HB2	1:B:696:ASN:HD21	1.54	0.72
1:A:325:VAL:HB	5:A:853:HOH:O	1.91	0.71
1:B:665:GLN:CB	1:B:696:ASN:HD21	2.03	0.71
4:A:833:AVF:O19	4:A:833:AVF:H14	1.89	0.71
1:A:575:ARG:HB3	1:A:578:LEU:HB3	1.73	0.70
1:B:29:LYS:O	1:B:33:ARG:HB2	1.91	0.70
1:A:493:LEU:HD11	1:A:512:VAL:HG11	1.74	0.70
1:B:649:ARG:HG2	1:B:649:ARG:HH11	1.56	0.70
1:B:410:HIS:CE1	1:B:428:MET:O	2.43	0.70
1:A:649:ARG:HG2	1:A:649:ARG:NH1	2.07	0.69
1:A:495:CYS:HB2	1:A:654:GLU:O	1.92	0.69
1:B:657:ILE:HB	1:B:658:PRO:HD3	1.74	0.69
1:B:213:THR:HG21	1:B:398:ARG:NH2	2.08	0.69
1:A:622:LEU:HD23	1:A:626:VAL:HG23	1.75	0.69
1:B:777:TYR:O	1:B:781:VAL:HG23	1.93	0.68
1:B:713:MET:HB2	1:B:717:ASP:HB2	1.74	0.68
1:B:197:MET:HE2	1:B:222:LEU:HB3	1.75	0.68
1:B:554:LYS:O	1:B:554:LYS:HG3	1.94	0.68
1:A:515:LEU:O	1:A:517:GLN:N	2.27	0.67
1:A:675:GLY:HA3	1:A:678:ASN:ND2	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:714:ARG:HH11	1:A:714:ARG:HG3	1.60	0.67
1:B:174:TRP:CE2	1:B:621:LYS:HG3	2.30	0.67
1:A:692:MET:HE2	1:A:710:ILE:HG21	1.77	0.66
1:A:515:LEU:HB3	5:A:842:HOH:O	1.93	0.66
1:B:606:GLY:HA3	1:B:645:LEU:HB2	1.77	0.66
1:B:193:ARG:HB2	1:B:225:PRO:HG2	1.78	0.66
1:B:89:PHE:HD1	5:B:900:HOH:O	1.76	0.66
1:A:613:TYR:HE1	1:A:615:MET:HB3	1.61	0.66
1:B:405:GLU:OE1	1:B:405:GLU:HA	1.93	0.66
1:A:457:LYS:NZ	1:A:701:GLU:OE2	2.27	0.66
1:A:88:GLU:HG2	1:A:132:GLY:HA2	1.77	0.65
1:A:149:THR:HG23	1:A:233:TYR:HB3	1.77	0.65
1:A:330:PRO:HB3	1:A:370:LYS:HB3	1.78	0.65
1:A:732:TYR:CE1	1:A:739:LYS:HG3	2.31	0.65
1:A:230:VAL:HB	1:A:239:ASN:HB2	1.79	0.64
1:B:566:GLN:HE22	1:B:579:ASN:HB2	1.62	0.64
1:B:577:LEU:O	1:B:581:LEU:HG	1.97	0.64
1:A:714:ARG:HH11	1:A:714:ARG:HG2	1.62	0.64
1:B:85:LEU:HD21	1:B:300:VAL:HG22	1.78	0.64
1:B:680:LYS:O	1:B:683:LEU:N	2.29	0.64
1:B:149:THR:HA	1:B:235:ASN:ND2	2.12	0.64
1:A:553:TYR:OH	1:A:646:GLU:HG3	1.98	0.64
1:B:455:VAL:N	1:B:459:HIS:HD2	1.93	0.64
1:B:72:GLN:HG3	4:B:833:AVF:C16	2.29	0.63
1:B:428:MET:SD	1:B:470:ASP:HB3	2.37	0.63
1:B:754:GLN:HB3	1:B:757:LEU:HB2	1.79	0.63
1:A:225:PRO:HB3	1:A:244:TRP:CZ3	2.33	0.63
1:A:262:TYR:OH	1:B:166:PHE:HB3	1.98	0.63
1:A:726:TYR:HE1	1:A:775:ALA:HB2	1.64	0.63
1:B:224:LEU:HD12	1:B:225:PRO:HD2	1.81	0.63
1:A:149:THR:CG2	1:A:233:TYR:HB3	2.28	0.63
1:B:457:LYS:O	1:B:461:ASP:HB2	1.99	0.63
1:A:326:PHE:CE1	1:A:357:GLU:HG3	2.34	0.62
1:A:573:TYR:CD1	1:A:671:THR:HB	2.35	0.62
1:A:142:CYS:SG	1:A:487:THR:HG22	2.40	0.62
1:A:209:THR:OG1	1:A:210:ASN:N	2.27	0.62
1:A:60:ARG:HD3	1:A:188:PRO:O	2.00	0.61
1:B:615:MET:HE3	1:B:615:MET:HA	1.80	0.61
1:B:751:SER:HB2	1:B:754:GLN:O	2.00	0.61
1:B:482:LYS:HE2	1:B:824:ILE:HD12	1.80	0.61
1:B:543:LEU:O	1:B:547:GLN:HG3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:525:LEU:HD21	1:B:803:LYS:HG2	1.81	0.61
1:B:593:ASP:HB3	5:B:894:HOH:O	2.00	0.61
1:A:336:GLN:OE1	1:A:373:ALA:HB3	2.01	0.61
3:B:832:PLP:O4A	3:B:832:PLP:H5A1	2.01	0.61
1:A:515:LEU:HD22	1:A:812:SER:HB2	1.83	0.61
1:B:665:GLN:NE2	1:B:678:ASN:HA	2.15	0.61
1:A:169:LYS:HB3	1:A:171:ARG:HD3	1.83	0.61
1:A:446:ILE:HG12	1:A:452:VAL:HG21	1.82	0.61
1:A:136:LEU:HD12	1:A:377:HIS:CG	2.36	0.61
1:A:174:TRP:CZ2	1:A:621:LYS:HG3	2.36	0.61
1:A:650:VAL:HA	3:A:832:PLP:H2A1	1.83	0.60
1:B:449:SER:O	1:B:478:LYS:HE2	2.01	0.60
1:A:168:GLN:HB3	1:A:647:ASN:CA	2.31	0.60
1:B:496:ASN:HD22	1:B:658:PRO:HB3	1.66	0.60
1:A:278:VAL:HB	1:B:266:VAL:HG11	1.83	0.60
1:A:608:LYS:HE3	1:A:648:TYR:O	2.02	0.60
1:B:410:HIS:HD2	5:B:889:HOH:O	1.83	0.60
1:A:29:LYS:CB	1:A:33:ARG:HH12	2.14	0.60
1:A:274:ASN:HD22	1:A:277:ARG:HE	1.46	0.60
1:A:677:GLY:HA2	1:A:680:LYS:HD2	1.83	0.60
1:A:184:ARG:HD2	1:A:185:TYR:CZ	2.36	0.60
1:A:304:LEU:HD22	1:A:349:LEU:HD13	1.83	0.60
1:A:647:ASN:O	1:A:649:ARG:NH1	2.35	0.60
1:A:136:LEU:HD12	1:A:377:HIS:CD2	2.36	0.60
1:B:74:TYR:OH	1:B:239:ASN:ND2	2.33	0.60
1:B:174:TRP:CZ2	1:B:621:LYS:HG3	2.36	0.60
1:B:662:LEU:HD22	1:B:787:VAL:HG11	1.82	0.60
1:B:567:VAL:HA	1:B:606:GLY:O	2.01	0.59
1:A:731:TYR:O	1:A:735:LEU:HB2	2.02	0.59
1:B:41:LYS:HD2	1:B:46:ALA:HA	1.84	0.59
1:A:80:LYS:HB3	1:A:827:VAL:HG13	1.84	0.59
1:A:615:MET:O	1:A:619:ILE:HG13	2.03	0.59
1:B:499:LEU:HD22	1:B:503:ILE:HD11	1.83	0.59
1:A:243:LEU:HB2	5:A:834:HOH:O	2.01	0.58
1:B:680:LYS:O	1:B:681:PHE:C	2.42	0.58
1:B:138:ARG:HH22	1:B:490:ARG:HH11	1.52	0.58
1:B:714:ARG:HD2	1:B:714:ARG:H	1.69	0.58
1:B:410:HIS:CD2	5:B:889:HOH:O	2.55	0.58
1:B:713:MET:HB2	1:B:717:ASP:CB	2.33	0.58
1:B:542:LYS:HA	1:B:659:ALA:HB1	1.84	0.58
1:B:387:TRP:HD1	1:B:441:MET:HG3	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:506:LYS:HD2	1:B:524:PHE:CE2	2.39	0.58
1:B:668:THR:OG1	1:B:771:PHE:O	2.15	0.58
1:A:665:GLN:CB	1:A:696:ASN:HD21	2.17	0.58
1:A:514:ASP:O	1:A:517:GLN:HG2	2.03	0.57
1:A:29:LYS:HB3	1:A:33:ARG:NH1	2.18	0.57
1:A:500:ALA:O	1:A:511:TYR:OH	2.21	0.57
1:B:649:ARG:HG2	1:B:649:ARG:NH1	2.19	0.57
1:A:160:ARG:HB2	1:A:243:LEU:HB3	1.86	0.57
1:B:565:VAL:HA	1:B:604:ILE:O	2.04	0.57
1:A:493:LEU:HD21	1:A:512:VAL:HG13	1.87	0.57
1:B:729:LYS:O	1:B:733:GLU:HG2	2.04	0.57
1:B:732:TYR:CZ	1:B:739:LYS:HD2	2.40	0.57
1:A:493:LEU:HD21	1:A:512:VAL:CG1	2.35	0.57
1:A:575:ARG:HH22	1:A:776:ASP:CB	2.15	0.56
1:B:430:LEU:HD21	1:B:444:LEU:HA	1.87	0.56
1:B:327:ASP:OD1	1:B:363:LYS:HE2	2.05	0.56
1:B:221:VAL:HG21	1:B:275:ILE:HD12	1.87	0.56
1:A:613:TYR:CE1	1:A:615:MET:HB3	2.41	0.56
1:B:678:ASN:OD1	1:B:679:MET:N	2.39	0.56
1:B:698:GLU:O	1:B:702:GLU:HG2	2.05	0.56
1:B:500:ALA:HA	1:B:511:TYR:OH	2.05	0.56
1:A:401:GLU:O	1:A:405:GLU:HB2	2.05	0.56
1:A:568:LYS:O	1:A:607:GLY:HA3	2.06	0.55
1:B:564:ASP:HB3	1:B:603:VAL:HA	1.88	0.55
1:A:34:HIS:HE1	1:A:61:ASP:OD2	1.89	0.55
1:A:571:HIS:CD2	1:A:613:TYR:HE2	2.24	0.55
1:B:71:GLN:HG3	4:B:833:AVF:CL8	2.44	0.55
1:B:131:LEU:HD22	1:B:161:TYR:HB2	1.87	0.55
1:B:522:HIS:HD2	1:B:525:LEU:HD11	1.71	0.55
1:B:709:PHE:HE2	1:B:786:LYS:HB3	1.69	0.55
1:A:580:CYS:SG	1:A:622:LEU:HD22	2.46	0.55
1:A:605:ILE:O	1:A:644:PHE:HA	2.06	0.55
1:B:496:ASN:OD1	1:B:499:LEU:HB2	2.07	0.55
1:B:579:ASN:ND2	5:B:868:HOH:O	2.39	0.55
1:B:647:ASN:O	1:B:649:ARG:NH1	2.40	0.55
1:A:34:HIS:HD2	1:A:38:THR:OG1	1.89	0.55
1:A:93:ARG:O	1:A:490:ARG:NH2	2.39	0.55
1:B:158:GLY:O	1:B:243:LEU:HA	2.07	0.55
1:A:542:LYS:HA	1:A:659:ALA:HB1	1.88	0.54
1:B:538:LYS:HZ2	1:B:660:THR:H	1.53	0.54
1:A:41:LYS:HD3	1:A:45:VAL:HG23	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LEU:C	1:A:517:GLN:N	2.60	0.54
1:A:531:LEU:HD22	1:A:798:ASN:HB3	1.89	0.54
1:A:542:LYS:NZ	1:A:561:SER:O	2.36	0.54
1:A:336:GLN:HB2	1:A:825:TRP:HE1	1.73	0.54
1:A:669:ALA:HB3	1:A:718:VAL:HG21	1.90	0.54
1:A:515:LEU:CD2	1:A:812:SER:HB2	2.37	0.54
1:A:709:PHE:HZ	1:A:790:LEU:HD22	1.72	0.54
1:A:280:TYR:CE1	1:B:263:ILE:HG13	2.42	0.54
1:B:535:ALA:HB2	1:B:798:ASN:ND2	2.22	0.54
1:B:34:HIS:HD2	1:B:38:THR:OG1	1.90	0.54
1:B:597:LEU:HG	1:B:597:LEU:O	2.07	0.54
1:B:170:ILE:HG12	1:B:646:GLU:HG2	1.90	0.54
1:B:465:THR:O	1:B:469:LYS:HB2	2.08	0.54
1:A:300:VAL:HG13	1:A:345:ALA:HA	1.89	0.54
1:B:714:ARG:HH11	1:B:714:ARG:HG2	1.73	0.53
1:B:128:ASP:OD2	1:B:651:SER:HB3	2.09	0.53
1:A:485:GLY:O	1:A:486:ILE:HG23	2.08	0.53
1:A:465:THR:O	1:A:469:LYS:HB2	2.08	0.53
1:A:698:GLU:O	1:A:702:GLU:HG2	2.07	0.53
1:B:739:LYS:HG3	1:B:743:ASP:OD2	2.08	0.53
4:A:833:AVF:O19	4:A:833:AVF:C14	2.57	0.53
1:B:76:ASP:O	1:B:315:LYS:HE2	2.07	0.53
1:B:248:ALA:HB3	1:B:269:ARG:CZ	2.39	0.53
1:B:330:PRO:HB3	1:B:370:LYS:HB3	1.91	0.53
1:B:369:GLN:HA	1:B:448:GLY:O	2.09	0.53
1:B:709:PHE:CE2	1:B:786:LYS:HB3	2.44	0.53
1:B:354:VAL:O	1:B:358:LYS:HA	2.08	0.53
1:B:815:ARG:HD2	1:B:815:ARG:C	2.29	0.53
1:A:792:MET:O	1:A:794:PRO:HD3	2.09	0.53
1:B:507:ILE:O	1:B:507:ILE:CG1	2.54	0.53
1:B:184:ARG:HH11	1:B:184:ARG:CG	2.15	0.53
1:B:813:SER:O	1:B:817:ILE:HG12	2.09	0.52
1:A:339:ASP:CG	1:A:340:THR:H	2.12	0.52
1:B:615:MET:HE1	1:B:761:ILE:HG12	1.91	0.52
1:B:502:LEU:HD11	1:B:533:GLU:HB3	1.91	0.52
1:B:144:LEU:HD13	1:B:230:VAL:HG21	1.92	0.52
1:B:538:LYS:NZ	1:B:660:THR:H	2.08	0.52
1:A:172:ASP:O	1:A:174:TRP:CD1	2.62	0.52
1:A:627:ALA:HA	1:A:642:VAL:HB	1.92	0.52
1:B:89:PHE:HB3	1:B:91:MET:HG2	1.92	0.52
1:B:96:GLN:HE21	1:B:105:GLN:HE22	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ILE:HG13	1:B:299:VAL:HB	1.92	0.51
1:A:41:LYS:HD2	1:A:46:ALA:HA	1.91	0.51
1:A:297:TYR:HB2	1:A:396:LEU:HD11	1.92	0.51
1:A:346:ILE:HD13	1:A:448:GLY:HA3	1.92	0.51
1:A:527:ASP:OD1	1:A:530:PHE:HB2	2.10	0.51
1:A:159:ILE:HG13	1:A:299:VAL:HB	1.92	0.51
1:A:488:PRO:O	1:A:492:LEU:HB3	2.11	0.51
1:A:99:MET:HB3	1:A:105:GLN:HA	1.92	0.51
1:A:664:GLU:O	1:A:665:GLN:NE2	2.43	0.51
1:B:53:PHE:HE1	1:B:188:PRO:HD3	1.75	0.51
1:B:409:LYS:O	1:B:412:ASP:HB2	2.09	0.51
1:B:601:ARG:NH2	1:B:788:SER:OG	2.41	0.51
1:A:267:LEU:HD13	1:B:274:ASN:OD1	2.11	0.51
1:A:496:ASN:OD1	1:A:499:LEU:HB2	2.10	0.51
1:A:521:LEU:HB3	1:A:802:LEU:HD11	1.93	0.51
1:A:738:LEU:HB2	1:A:777:TYR:CE2	2.46	0.51
1:A:158:GLY:O	1:A:243:LEU:HA	2.11	0.50
1:A:577:LEU:HD13	1:A:765:LEU:HD21	1.93	0.50
1:A:809:GLY:HA3	5:A:840:HOH:O	2.11	0.50
1:A:459:HIS:HA	1:A:462:ILE:HD12	1.93	0.50
1:A:636:VAL:CG2	1:A:637:GLY:N	2.74	0.50
1:B:413:ARG:HA	1:B:413:ARG:NE	2.26	0.50
1:B:566:GLN:NE2	1:B:579:ASN:HB2	2.26	0.50
1:A:546:SER:HA	1:A:549:LEU:HD12	1.94	0.50
1:A:662:LEU:HD22	1:A:787:VAL:HG11	1.94	0.50
1:B:49:ARG:HA	1:B:125:ILE:HG21	1.93	0.50
1:A:46:ALA:HB3	1:A:51:TYR:CZ	2.47	0.50
1:B:374:TYR:CD2	1:B:452:VAL:HG13	2.46	0.50
1:B:593:ASP:CB	5:B:894:HOH:O	2.59	0.50
1:B:208:HIS:ND1	1:B:213:THR:HB	2.27	0.49
1:A:181:ASP:OD2	1:A:184:ARG:CB	2.55	0.49
1:A:721:LEU:O	1:A:725:GLY:N	2.45	0.49
1:B:67:TRP:CH2	1:B:229:PRO:HD3	2.47	0.49
1:A:669:ALA:HB1	1:A:715:ILE:HA	1.94	0.49
1:A:565:VAL:HG22	1:A:604:ILE:HB	1.94	0.49
1:B:95:LEU:O	1:B:99:MET:HG3	2.13	0.49
1:A:182:TRP:CZ3	1:A:187:ASN:ND2	2.81	0.49
1:B:149:THR:C	1:B:151:GLY:H	2.14	0.49
1:B:71:GLN:CG	4:B:833:AVF:CL8	2.98	0.49
1:B:525:LEU:HD23	1:B:802:LEU:HD23	1.95	0.49
1:B:600:PRO:HA	1:B:639:LYS:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:LYS:O	1:B:554:LYS:CG	2.60	0.49
1:B:511:TYR:O	1:B:515:LEU:HA	2.13	0.49
1:B:530:PHE:HE2	1:B:802:LEU:HD13	1.77	0.49
1:A:86:SER:HB3	1:A:89:PHE:CE1	2.47	0.49
1:A:150:LEU:HD21	1:A:818:LYS:HG3	1.93	0.49
1:A:624:THR:O	1:A:627:ALA:HB3	2.12	0.49
1:A:632:ASN:O	1:A:634:PRO:HD3	2.12	0.48
1:A:157:TYR:HE2	1:A:244:TRP:CZ2	2.32	0.48
1:A:423:ASP:O	1:A:427:ARG:HB2	2.13	0.48
1:A:680:LYS:HZ1	3:A:832:PLP:H4A	0.68	0.48
1:A:690:GLY:O	1:A:710:ILE:HA	2.13	0.48
1:A:689:ILE:HG12	1:A:711:PHE:CE2	2.49	0.48
1:A:396:LEU:HB3	1:A:399:HIS:ND1	2.29	0.48
1:B:146:SER:HB2	1:B:817:ILE:HG13	1.95	0.48
1:B:170:ILE:HA	1:B:174:TRP:O	2.14	0.48
1:B:231:PRO:HA	1:B:238:VAL:HG22	1.96	0.48
1:B:679:MET:O	1:B:680:LYS:O	2.31	0.48
1:B:87:LEU:HD22	1:B:299:VAL:HG11	1.95	0.48
1:B:721:LEU:HA	1:B:724:LYS:HB3	1.96	0.48
1:A:602:THR:HG23	1:A:641:LYS:HB2	1.96	0.48
1:B:346:ILE:CD1	1:B:445:CYS:HA	2.44	0.48
1:A:286:PHE:CD1	1:A:385:GLU:HA	2.49	0.48
1:A:225:PRO:HB3	1:A:244:TRP:CE3	2.49	0.48
1:B:75:TYR:HA	1:B:81:ARG:NH2	2.28	0.48
1:B:669:ALA:HB3	1:B:718:VAL:HG21	1.96	0.48
1:B:304:LEU:HD11	1:B:345:ALA:HB1	1.96	0.48
1:B:522:HIS:HB2	5:B:913:HOH:O	2.13	0.48
1:A:380:LEU:HB3	1:A:382:GLU:OE2	2.14	0.47
1:B:428:MET:CG	1:B:470:ASP:HB3	2.43	0.47
1:B:446:ILE:HD11	1:B:468:PHE:CE2	2.49	0.47
1:B:762:ILE:O	1:B:766:PHE:HD1	1.96	0.47
1:A:168:GLN:HG3	1:A:175:GLN:HG3	1.96	0.47
1:B:455:VAL:HG23	1:B:674:SER:HB3	1.97	0.47
1:B:181:ASP:OD2	1:B:184:ARG:NH1	2.48	0.47
1:A:190:GLU:HA	1:A:227:ASP:O	2.14	0.47
1:A:522:HIS:O	1:A:525:LEU:HG	2.13	0.47
1:A:799:THR:O	1:A:803:LYS:HG3	2.15	0.47
1:B:293:LEU:HB2	1:B:387:TRP:CZ3	2.49	0.47
1:B:538:LYS:NZ	1:B:658:PRO:O	2.47	0.47
1:A:174:TRP:CE2	1:A:621:LYS:HG3	2.49	0.47
1:A:692:MET:HG3	1:A:697:VAL:HG22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:212:GLY:HA3	1:B:358:LYS:HE2	1.96	0.47
1:B:573:TYR:HA	1:B:771:PHE:CG	2.49	0.47
1:B:30:SER:O	1:B:34:HIS:HB2	2.15	0.47
1:B:340:THR:O	1:B:343:ALA:N	2.48	0.47
1:B:463:VAL:HG13	1:B:468:PHE:HD1	1.80	0.47
1:B:575:ARG:NH2	1:B:776:ASP:HB2	2.30	0.47
4:B:833:AVF:H14	4:B:833:AVF:O19	2.13	0.47
1:B:88:GLU:CD	1:B:133:ASN:H	2.17	0.47
1:A:372:PHE:O	1:A:450:HIS:HD2	1.97	0.47
1:A:772:LYS:HB3	1:A:775:ALA:HB3	1.97	0.47
1:B:213:THR:HG23	1:B:355:ASP:OD2	2.15	0.47
1:B:443:HIS:HA	1:B:446:ILE:HD12	1.97	0.47
1:B:742:ILE:HG23	1:B:762:ILE:HD12	1.97	0.47
1:B:518:LEU:O	1:B:806:ALA:HA	2.14	0.47
1:B:665:GLN:HB3	1:B:696:ASN:HD21	1.77	0.47
1:A:180:ASP:O	1:A:182:TRP:N	2.42	0.46
1:A:296:GLU:HB2	1:A:344:LEU:HD12	1.98	0.46
1:A:542:LYS:NZ	1:A:661:ASP:OD2	2.41	0.46
1:A:800:MET:O	1:A:804:ASN:ND2	2.48	0.46
1:B:651:SER:O	1:B:654:GLU:HB2	2.16	0.46
3:B:832:PLP:O4A	3:B:832:PLP:C5A	2.63	0.46
1:A:555:VAL:HG13	1:A:641:LYS:HD2	1.97	0.46
1:B:586:MET:SD	1:B:601:ARG:HD2	2.55	0.46
1:A:410:HIS:HE1	1:A:428:MET:O	1.98	0.46
1:B:711:PHE:CE1	1:B:780:TYR:HB2	2.50	0.46
1:A:157:TYR:HD2	1:A:244:TRP:HE1	1.63	0.46
1:A:676:THR:OG1	3:A:832:PLP:O4A	2.31	0.46
1:B:42:ASP:OD2	1:B:44:ASN:HB2	2.15	0.46
4:B:833:AVF:HN12	4:B:833:AVF:H24A	1.80	0.46
1:A:229:PRO:O	1:A:231:PRO:HD3	2.15	0.46
1:A:341:HIS:HD2	1:A:385:GLU:OE1	1.98	0.46
1:B:781:VAL:O	1:B:784:GLN:HB2	2.16	0.46
1:A:173:GLY:O	1:A:621:LYS:HA	2.15	0.46
1:A:693:ASP:O	1:A:696:ASN:HB2	2.16	0.46
1:B:55:LEU:CD2	1:B:122:LEU:HD12	2.43	0.46
1:B:436:SER:O	1:B:438:ARG:HG3	2.15	0.46
1:A:66:ARG:HD2	1:A:236:ASN:HA	1.97	0.46
1:A:502:LEU:HD11	1:A:534:LEU:HA	1.96	0.46
1:B:161:TYR:HE1	1:B:295:GLN:NE2	2.14	0.46
1:B:308:ILE:CD1	1:B:352:ILE:HG21	2.41	0.46
1:B:578:LEU:O	1:B:579:ASN:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:645:LEU:HD23	1:B:645:LEU:HA	1.79	0.46
1:B:685:GLY:HA2	1:B:801:VAL:HG13	1.97	0.46
1:A:26:GLU:HA	1:A:29:LYS:HG3	1.96	0.46
1:A:201:HIS:HA	1:A:219:GLN:O	2.16	0.46
1:B:430:LEU:HD21	1:B:444:LEU:CA	2.45	0.46
1:A:714:ARG:HG2	1:A:714:ARG:NH1	2.31	0.46
1:B:280:TYR:HA	1:B:281:PRO:HD3	1.79	0.46
1:B:340:THR:OG1	1:B:385:GLU:HG3	2.16	0.46
1:A:78:CYS:SG	1:A:314:SER:HB2	2.56	0.45
1:A:555:VAL:HG11	1:A:643:ILE:HD11	1.98	0.45
1:B:587:TYR:O	1:B:591:LYS:HG2	2.16	0.45
1:A:170:ILE:HG12	1:A:646:GLU:HG2	1.98	0.45
1:A:795:LYS:O	1:A:799:THR:OG1	2.33	0.45
1:B:531:LEU:HD22	1:B:798:ASN:HB3	1.97	0.45
1:B:565:VAL:HG22	1:B:604:ILE:HB	1.98	0.45
1:A:264:GLN:NE2	1:A:268:ASP:OD1	2.49	0.45
1:A:586:MET:SD	1:A:601:ARG:HD2	2.56	0.45
1:A:820:TYR:CD1	1:A:824:ILE:HD12	2.51	0.45
1:A:663:SER:HB2	1:A:681:PHE:HB3	1.99	0.45
1:B:681:PHE:HB3	1:B:686:ALA:HB3	1.99	0.45
1:B:596:LYS:HG3	1:B:597:LEU:N	2.31	0.45
1:A:549:LEU:HD22	1:A:643:ILE:HG21	1.99	0.45
1:B:511:TYR:CD2	1:B:518:LEU:HD21	2.51	0.45
1:B:691:THR:C	1:B:693:ASP:H	2.20	0.45
1:A:177:GLU:OE1	1:A:177:GLU:N	2.50	0.45
1:A:156:GLY:O	1:A:242:ARG:N	2.46	0.45
1:A:566:GLN:HB2	1:A:664:GLU:HB2	1.98	0.45
1:A:157:TYR:HE2	1:A:244:TRP:HZ2	1.65	0.45
1:A:375:THR:HG23	1:A:453:ASN:HD21	1.82	0.44
1:A:663:SER:HB3	1:A:688:THR:HA	1.99	0.44
4:A:833:AVF:HN12	4:A:833:AVF:H24A	1.81	0.44
1:B:613:TYR:CE1	1:B:615:MET:HB3	2.52	0.44
1:A:458:ILE:HG23	1:A:459:HIS:H	1.81	0.44
1:A:410:HIS:CE1	1:A:428:MET:O	2.71	0.44
1:A:579:ASN:C	1:A:579:ASN:HD22	2.21	0.44
1:B:261:ASP:HB3	1:B:264:GLN:HB3	2.00	0.44
1:B:491:TRP:HA	1:B:495:CYS:SG	2.58	0.44
1:A:386:ARG:HA	1:A:439:ILE:O	2.17	0.44
1:A:575:ARG:HD3	1:A:666:ILE:O	2.18	0.44
1:B:325:VAL:HB	1:B:326:PHE:H	1.63	0.44
1:B:349:LEU:O	1:B:353:PHE:N	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:VAL:O	1:B:468:PHE:HB2	2.17	0.44
1:B:575:ARG:HD3	1:B:666:ILE:O	2.18	0.44
1:A:616:ALA:O	1:A:620:ILE:HG13	2.17	0.44
1:A:727:GLU:O	1:A:730:GLU:HG2	2.17	0.44
1:B:482:LYS:HE2	1:B:824:ILE:CD1	2.48	0.44
1:B:804:ASN:HD22	1:B:804:ASN:H	1.64	0.44
1:A:349:LEU:HG	1:A:353:PHE:CE1	2.53	0.44
1:A:325:VAL:HB	1:A:326:PHE:H	1.59	0.44
1:A:604:ILE:HA	1:A:643:ILE:O	2.17	0.44
1:B:407:ASN:HB2	1:B:430:LEU:HB2	2.00	0.44
1:B:464:LYS:NZ	1:B:476:PRO:O	2.50	0.44
1:B:772:LYS:HB3	1:B:775:ALA:HB3	2.00	0.44
1:A:400:LEU:HD12	1:A:400:LEU:HA	1.87	0.43
1:A:657:ILE:HB	1:A:658:PRO:HD3	1.99	0.43
1:A:669:ALA:HB3	1:A:718:VAL:CG2	2.47	0.43
1:A:699:MET:HB3	1:A:699:MET:HE2	1.63	0.43
1:B:34:HIS:CD2	1:B:38:THR:OG1	2.69	0.43
1:B:582:HIS:CD2	1:B:784:GLN:HG3	2.52	0.43
1:B:679:MET:O	1:B:680:LYS:C	2.55	0.43
1:A:493:LEU:HD21	1:A:512:VAL:CG2	2.48	0.43
1:A:550:GLU:HG2	1:A:555:VAL:O	2.18	0.43
1:A:577:LEU:CD1	1:A:765:LEU:HD21	2.48	0.43
1:A:819:GLU:O	1:A:823:ASN:ND2	2.51	0.43
1:B:374:TYR:CG	1:B:445:CYS:HB3	2.53	0.43
1:B:492:LEU:HD12	1:B:492:LEU:HA	1.78	0.43
1:A:55:LEU:O	1:A:59:VAL:HG23	2.18	0.43
1:A:379:VAL:O	1:A:380:LEU:C	2.57	0.43
1:B:575:ARG:C	1:B:577:LEU:N	2.71	0.43
1:B:724:LYS:HE2	5:B:911:HOH:O	2.18	0.43
1:A:163:TYR:CD2	1:A:179:ALA:HB1	2.53	0.43
1:A:348:GLU:O	1:A:352:ILE:HG13	2.18	0.43
1:A:714:ARG:CG	1:A:714:ARG:NH1	2.61	0.43
1:B:80:LYS:HG3	1:B:332:GLN:C	2.39	0.43
1:B:487:THR:HG23	1:B:490:ARG:HB3	2.00	0.43
1:B:506:LYS:HG3	1:B:530:PHE:CD1	2.54	0.43
1:A:300:VAL:CG1	1:A:345:ALA:HA	2.48	0.43
1:A:369:GLN:O	1:A:450:HIS:HB3	2.19	0.43
1:A:711:PHE:HB3	1:A:783:CYS:SG	2.59	0.43
1:A:666:ILE:HG22	1:A:711:PHE:HZ	1.84	0.43
1:B:143:PHE:O	1:B:147:MET:HG3	2.19	0.43
1:B:187:ASN:HA	1:B:188:PRO:HD2	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:PHE:HB3	1:B:421:ASP:HB2	2.01	0.43
1:B:652:LEU:O	1:B:652:LEU:HD22	2.19	0.43
1:A:207:GLU:HB2	1:A:216:ILE:HG12	2.01	0.43
1:B:150:LEU:O	1:B:829:PRO:HB3	2.18	0.43
1:B:615:MET:O	1:B:619:ILE:HG13	2.19	0.43
1:A:714:ARG:NH1	5:A:891:HOH:O	2.51	0.43
1:B:363:LYS:O	1:B:367:LEU:HG	2.19	0.43
4:B:833:AVF:H24A	4:B:833:AVF:O20	2.19	0.43
1:B:80:LYS:HE3	1:B:330:PRO:O	2.19	0.43
1:B:428:MET:HG2	1:B:470:ASP:HB3	2.00	0.43
1:B:563:PHE:HD2	1:B:659:ALA:O	2.02	0.43
1:B:615:MET:CE	1:B:761:ILE:HG12	2.48	0.43
1:B:714:ARG:HH11	1:B:714:ARG:CG	2.32	0.43
1:A:141:ALA:O	1:A:144:LEU:HB2	2.19	0.42
1:A:312:LYS:HB3	1:A:312:LYS:HE2	1.84	0.42
1:B:575:ARG:HB3	1:B:578:LEU:CB	2.49	0.42
1:A:187:ASN:HB3	1:A:190:GLU:HG2	2.01	0.42
1:A:356:ILE:HG22	1:A:357:GLU:OE1	2.19	0.42
1:B:131:LEU:CD2	1:B:161:TYR:HB2	2.49	0.42
1:B:360:PRO:O	1:B:361:TRP:C	2.58	0.42
1:B:582:HIS:CE1	1:B:586:MET:SD	3.12	0.42
1:B:683:LEU:O	1:B:683:LEU:HD22	2.19	0.42
1:B:693:ASP:O	1:B:696:ASN:HB2	2.19	0.42
1:B:85:LEU:HD13	1:B:303:THR:HG21	2.02	0.42
1:A:85:LEU:HD21	1:A:300:VAL:HG22	2.01	0.42
1:A:400:LEU:HG	1:A:404:TYR:CE2	2.54	0.42
1:B:392:VAL:HG21	1:B:439:ILE:HD12	2.00	0.42
1:B:538:LYS:HG3	1:B:542:LYS:HD2	2.00	0.42
1:B:720:ALA:O	1:B:724:LYS:N	2.49	0.42
1:A:112:ILE:HG23	1:A:117:LEU:HB2	2.02	0.42
1:A:185:TYR:CD2	1:B:194:PRO:HB3	2.53	0.42
1:A:280:TYR:HA	1:A:281:PRO:HD3	1.77	0.42
1:A:427:ARG:NE	1:A:470:ASP:OD1	2.52	0.42
1:B:387:TRP:CD1	1:B:441:MET:HG3	2.52	0.42
1:B:202:PHE:CD1	1:B:395:LEU:HD11	2.54	0.42
1:B:567:VAL:HB	1:B:648:TYR:CE1	2.55	0.42
1:B:188:PRO:HG2	1:B:189:TRP:CD1	2.55	0.42
1:B:303:THR:O	1:B:307:ILE:HG13	2.20	0.42
1:A:374:TYR:O	1:A:452:VAL:HA	2.19	0.42
1:A:663:SER:HB2	1:A:681:PHE:CB	2.49	0.42
1:A:330:PRO:HG2	1:A:370:LYS:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:LYS:HG3	1:A:530:PHE:HE1	1.85	0.42
1:A:663:SER:OG	1:A:665:GLN:NE2	2.53	0.42
1:A:665:GLN:HG3	1:A:678:ASN:HB3	2.02	0.42
1:A:670:GLY:HA3	1:A:715:ILE:HD13	2.02	0.42
1:A:714:ARG:N	1:A:714:ARG:CD	2.82	0.42
1:A:368:THR:HG23	1:A:372:PHE:CD1	2.54	0.42
1:A:604:ILE:HG23	1:A:643:ILE:HB	2.01	0.42
1:A:683:LEU:HD22	1:A:683:LEU:O	2.19	0.42
1:A:706:GLU:HG2	1:A:707:ASN:N	2.35	0.42
1:B:246:ALA:N	1:B:276:SER:OG	2.53	0.42
1:A:64:VAL:HG11	1:B:36:HIS:O	2.20	0.41
1:A:170:ILE:CG1	1:A:646:GLU:HG2	2.50	0.41
1:A:668:THR:HB	1:A:671:THR:HG21	2.01	0.41
1:A:689:ILE:HD13	1:A:784:GLN:NE2	2.35	0.41
1:A:812:SER:HB3	5:A:842:HOH:O	2.20	0.41
1:B:582:HIS:HB2	1:B:780:TYR:HE2	1.85	0.41
1:A:405:GLU:OE2	1:A:409:LYS:HE3	2.19	0.41
1:A:598:PHE:HB3	1:A:639:LYS:HE3	2.03	0.41
1:A:732:TYR:CZ	1:A:739:LYS:HG3	2.55	0.41
1:A:270:ASN:O	1:A:274:ASN:ND2	2.53	0.41
1:B:167:ASN:HD22	1:B:167:ASN:HA	1.65	0.41
1:B:413:ARG:O	1:B:416:ALA:HB3	2.20	0.41
1:B:530:PHE:HE2	1:B:802:LEU:CD1	2.33	0.41
1:B:133:ASN:O	1:B:569:ARG:HD3	2.20	0.41
1:B:157:TYR:HH	1:B:310:ARG:HH22	1.65	0.41
1:B:213:THR:CG2	1:B:398:ARG:NH2	2.81	0.41
1:A:729:LYS:H	1:A:729:LYS:HG3	1.61	0.41
1:B:662:LEU:HD11	1:B:689:ILE:HB	2.03	0.41
1:A:168:GLN:HE21	1:A:175:GLN:HG3	1.86	0.41
1:A:666:ILE:HG22	1:A:711:PHE:CZ	2.55	0.41
1:A:762:ILE:HG23	1:A:766:PHE:CD1	2.55	0.41
1:A:828:GLU:HA	1:A:829:PRO:HD3	1.83	0.41
1:B:88:GLU:HB3	1:B:137:GLY:HA2	2.03	0.41
1:B:688:THR:N	5:B:849:HOH:O	2.53	0.41
1:B:729:LYS:C	1:B:731:TYR:H	2.23	0.41
1:A:493:LEU:HD21	1:A:512:VAL:HG22	2.03	0.41
1:B:361:TRP:CH2	1:B:402:ILE:HG23	2.56	0.41
1:B:525:LEU:CD2	1:B:803:LYS:HG2	2.50	0.41
1:B:733:GLU:HG2	1:B:733:GLU:H	1.69	0.41
1:A:224:LEU:HD12	1:A:225:PRO:HD2	2.02	0.41
1:A:649:ARG:HH11	1:A:649:ARG:CG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:815:ARG:C	1:A:815:ARG:HD2	2.41	0.41
1:B:664:GLU:OE1	1:B:780:TYR:OH	2.24	0.41
1:B:793:ASN:O	1:B:794:PRO:C	2.58	0.41
1:A:144:LEU:HD23	1:A:144:LEU:HA	1.87	0.41
1:A:338:ASN:OD1	1:A:377:HIS:NE2	2.54	0.41
1:A:357:GLU:CB	1:A:359:LEU:HG	2.51	0.41
1:A:365:TRP:CZ3	1:A:406:ILE:HG12	2.56	0.41
1:A:470:ASP:O	1:A:474:LEU:HD13	2.21	0.41
1:B:67:TRP:O	1:B:71:GLN:HG2	2.21	0.41
1:B:187:ASN:ND2	5:B:864:HOH:O	2.53	0.41
1:B:67:TRP:CZ3	1:B:229:PRO:HD3	2.56	0.41
1:B:329:PHE:HB3	1:B:330:PRO:CD	2.47	0.41
1:B:709:PHE:HB3	1:B:783:CYS:SG	2.60	0.41
1:A:346:ILE:HA	1:A:372:PHE:CE1	2.56	0.40
1:A:606:GLY:HA2	1:A:644:PHE:CE1	2.56	0.40
1:A:680:LYS:HZ3	3:A:832:PLP:C4A	2.07	0.40
1:A:350:MET:SD	1:A:365:TRP:HA	2.61	0.40
1:B:577:LEU:O	1:B:580:CYS:HB3	2.22	0.40
1:A:41:LYS:HE3	1:A:50:ASP:OD2	2.21	0.40
1:A:166:PHE:O	1:A:608:LYS:NZ	2.43	0.40
1:A:458:ILE:O	1:A:461:ASP:HB3	2.21	0.40
1:A:610:ALA:HB3	1:A:613:TYR:HB2	2.03	0.40
1:B:345:ALA:HA	1:B:348:GLU:HB3	2.02	0.40
1:A:368:THR:HG23	1:A:372:PHE:HD1	1.86	0.40
1:A:499:LEU:HD23	1:A:499:LEU:HA	1.88	0.40
1:B:493:LEU:HD21	1:B:512:VAL:CG2	2.51	0.40
1:B:692:MET:HB3	1:B:714:ARG:HG3	2.03	0.40
1:A:428:MET:CE	1:A:474:LEU:HD22	2.51	0.40
1:A:430:LEU:CD2	1:A:443:HIS:HB3	2.51	0.40
1:B:101:ASN:HB3	1:B:232:GLY:O	2.21	0.40
1:B:665:GLN:HB2	1:B:696:ASN:ND2	2.27	0.40
1:B:751:SER:O	1:B:752:PRO:C	2.59	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	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

All (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
1	B	76	ASP
1	B	681	PHE
1	B	730	GLU
1	A	674	SER
1	B	314	SER
1	B	680	LYS
1	A	752	PRO
1	B	568	LYS
1	B	593	ASP
1	B	498	GLY

### 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

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LYS
1	A	30	SER
1	A	63	LEU
1	A	90	TYR
1	A	95	LEU
1	A	100	ILE
1	A	128	ASP
1	A	136	LEU
1	A	150	LEU
1	A	167	ASN
1	A	169	LYS
1	A	205	LYS
1	A	209	THR
1	A	210	ASN
1	A	211	THR
1	A	213	THR
1	A	220	VAL
1	A	228	THR
1	A	237	THR
1	A	243	LEU
1	A	245	SER
1	A	247	ARG
1	A	270	ASN
1	A	274	ASN
1	A	337	LEU
1	A	340	THR
1	A	379	VAL
1	A	382	GLU
1	A	390	ASP
1	A	391	LEU
1	A	426	ARG
1	A	457	LYS
1	A	466	LYS
1	A	486	ILE
1	A	487	THR
1	A	493	LEU
1	A	509	GLU
1	A	510	ASP
1	A	543	LEU
1	A	573	TYR
1	A	577	LEU
1	A	579	ASN

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Mol	Chain	Res	Type
1	A	613	TYR
1	A	635	MET
1	A	636	VAL
1	A	652	LEU
1	A	678	ASN
1	A	683	LEU
1	A	714	ARG
1	A	722	ASP
1	A	753	LYS
1	A	756	ASP
1	A	761	ILE
1	A	788	SER
1	A	795	LYS
1	A	799	THR
1	A	808	SER
1	A	827	VAL
1	B	34	HIS
1	B	63	LEU
1	B	90	TYR
1	B	100	ILE
1	B	118	ASP
1	B	128	ASP
1	B	169	LYS
1	B	184	ARG
1	B	210	ASN
1	B	211	THR
1	B	213	THR
1	B	217	ASP
1	B	219	GLN
1	B	245	SER
1	B	274	ASN
1	B	287	GLU
1	B	300	VAL
1	B	305	GLN
1	B	337	LEU
1	B	353	PHE
1	B	363	LYS
1	B	378	THR
1	B	382	GLU
1	B	386	ARG
1	B	405	GLU
1	B	426	ARG

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Mol	Chain	Res	Type
1	B	453	ASN
1	B	473	GLU
1	B	489	ARG
1	B	502	LEU
1	B	507	ILE
1	B	560	SER
1	B	568	LYS
1	B	573	TYR
1	B	577	LEU
1	B	579	ASN
1	B	597	LEU
1	B	613	TYR
1	B	636	VAL
1	B	638	SER
1	B	652	LEU
1	B	674	SER
1	B	683	LEU
1	B	714	ARG
1	B	722	ASP
1	B	727	GLU
1	B	733	GLU
1	B	751	SER
1	B	763	ASN
1	B	828	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	34	HIS
1	A	62	HIS
1	A	167	ASN
1	A	270	ASN
1	A	274	ASN
1	A	284	ASN
1	A	369	GLN
1	A	376	ASN
1	A	410	HIS
1	A	450	HIS
1	A	453	ASN
1	A	459	HIS
1	A	481	ASN

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Mol	Chain	Res	Type
1	A	566	GLN
1	A	579	ASN
1	A	696	ASN
1	A	822	GLN
1	B	34	HIS
1	B	96	GLN
1	B	167	ASN
1	B	239	ASN
1	B	270	ASN
1	B	274	ASN
1	B	305	GLN
1	B	332	GLN
1	B	341	HIS
1	B	410	HIS
1	B	459	HIS
1	B	481	ASN
1	B	522	HIS
1	B	541	ASN
1	B	547	GLN
1	B	566	GLN
1	B	579	ASN
1	B	798	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
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

All (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
4	B	833	AVF	C11-N10	-3.05	1.32	1.39
4	B	833	AVF	C13-N12	-2.86	1.36	1.41
4	B	833	AVF	C18-N21	-2.83	1.35	1.41
4	B	833	AVF	C7-N10	-2.71	1.33	1.37
3	A	832	PLP	C2-N1	2.58	1.38	1.33
4	A	833	AVF	C7-N10	-2.50	1.33	1.37
3	B	832	PLP	P-O3P	-2.46	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	833	AVF	C11-N10	-2.38	1.34	1.39
4	A	833	AVF	C18-N21	-2.28	1.36	1.41
3	B	832	PLP	P-O2P	-2.28	1.46	1.54

All (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
3	B	832	PLP	O4A-C4A-C4	-3.22	117.17	124.80
4	A	833	AVF	C16-C15-C14	-3.19	119.03	123.23
2	B	2	NBG	C4-C3-C2	3.17	116.39	110.83
3	B	832	PLP	C2A-C2-C3	-2.82	117.50	120.80
4	B	833	AVF	C5-C6-C1	2.68	120.44	118.42
3	B	832	PLP	C2A-C2-N1	2.67	122.66	117.64
4	A	833	AVF	C13-C14-C15	2.66	122.20	117.62
3	B	832	PLP	O4P-P-O1P	2.61	113.48	106.44
2	B	2	NBG	O5-C5-C6	2.59	112.86	106.44
4	B	833	AVF	C25-N21-C18	-2.38	110.52	116.19
3	A	832	PLP	C5-C6-N1	-2.31	120.07	123.83
4	A	833	AVF	C18-C13-N12	2.26	122.78	118.61
2	B	2	NBG	O5-C1-C2	2.23	112.24	109.72
4	A	833	AVF	C3-C4-C5	2.19	120.26	117.84
4	B	833	AVF	C13-C14-C15	2.18	121.37	117.62
4	B	833	AVF	C16-C15-C14	-2.08	120.49	123.23
3	B	832	PLP	C5-C6-N1	-2.04	120.51	123.83
4	B	833	AVF	O20-C7-N10	2.03	125.24	122.27
4	B	833	AVF	C14-C13-C18	-2.03	117.58	119.80
3	A	832	PLP	O4A-C4A-C4	-2.02	120.00	124.80

There are no chirality outliers.

All (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

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Mol	Chain	Res	Type	Atoms
2	B	2	NBG	O5-C5-C6-O6
3	A	832	PLP	C5-C4-C4A-O4A

There are no ring outliers.

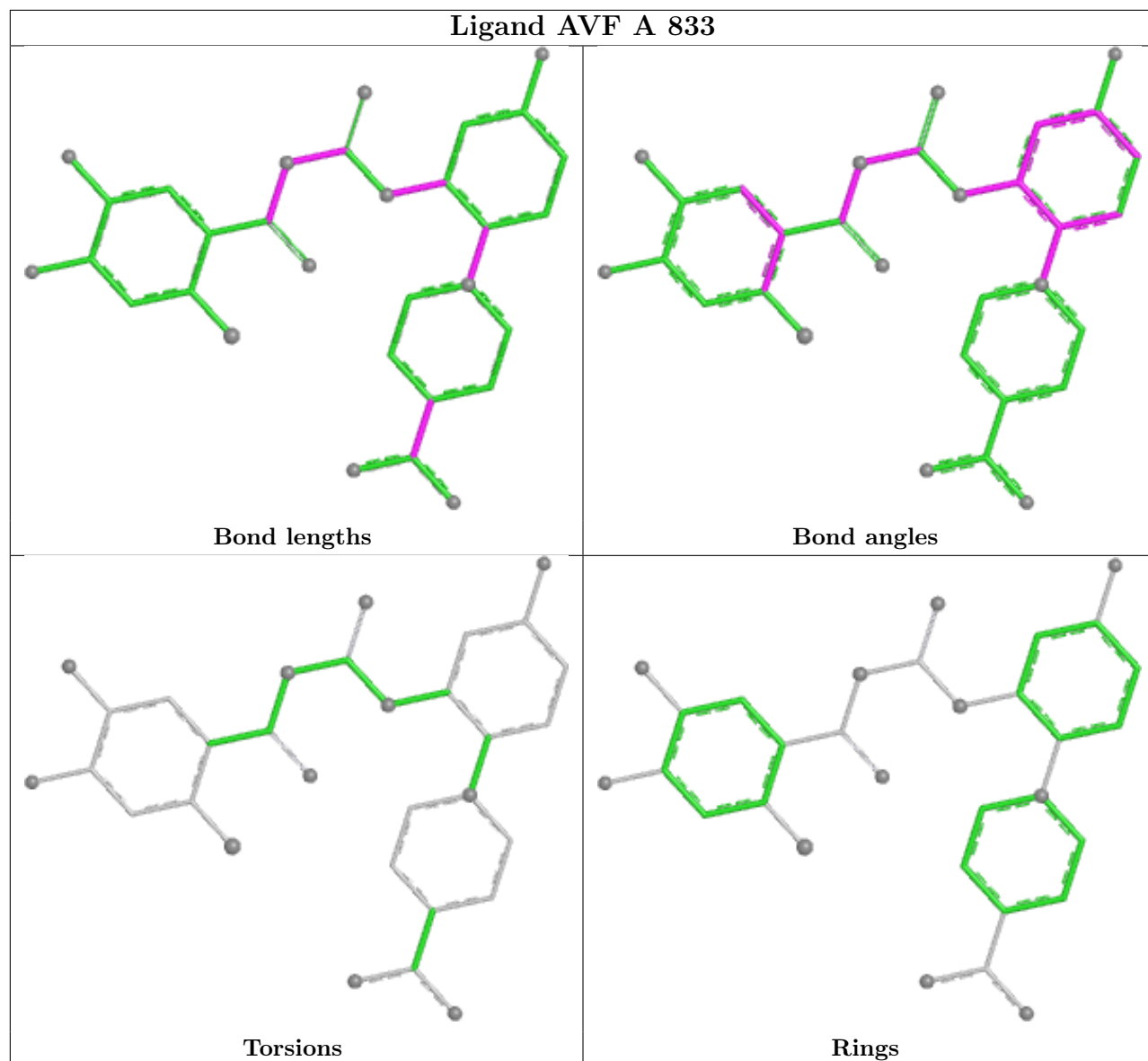
4 monomers are involved in 19 short contacts:

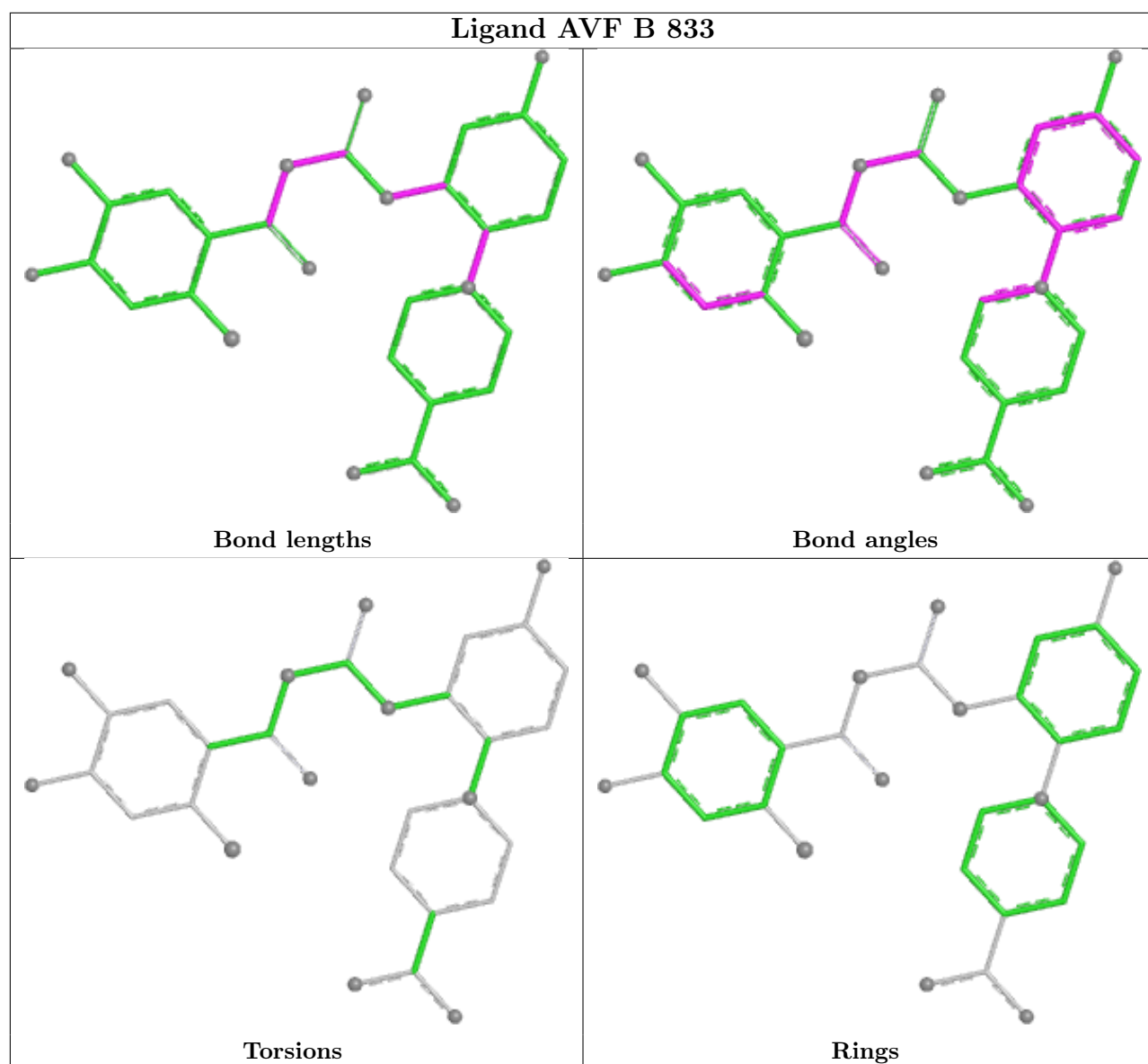
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	833	AVF	3	0
3	B	832	PLP	2	0
4	B	833	AVF	6	0
3	A	832	PLP	8	0

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.



## Ligand AVF A 833





## 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	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](#)

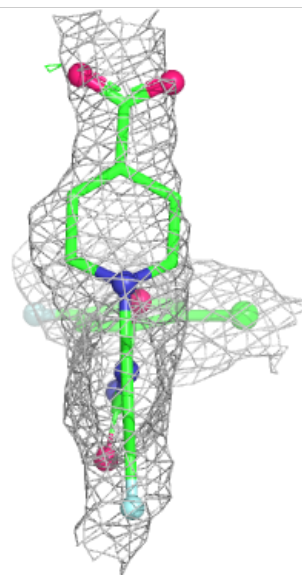
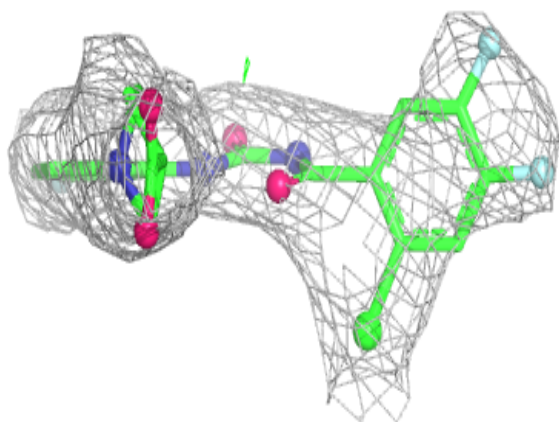
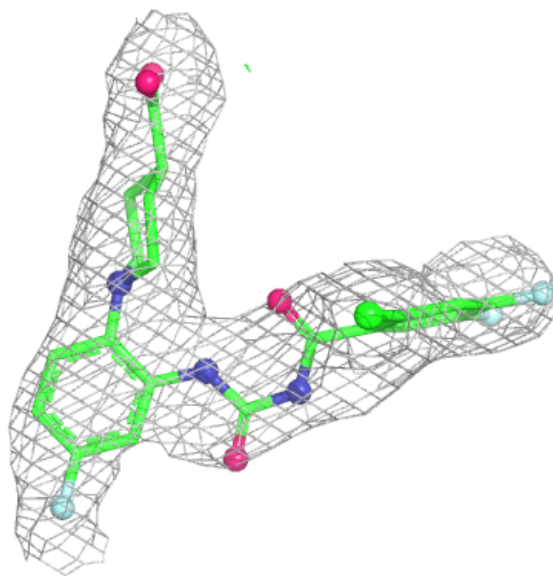
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 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
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.

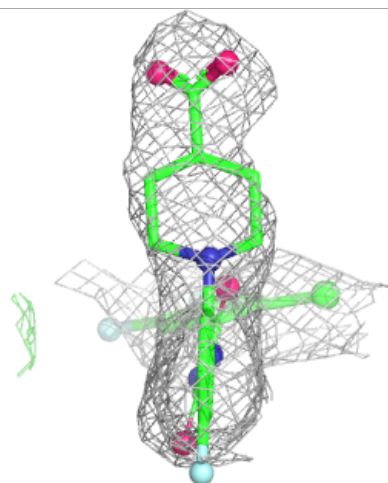
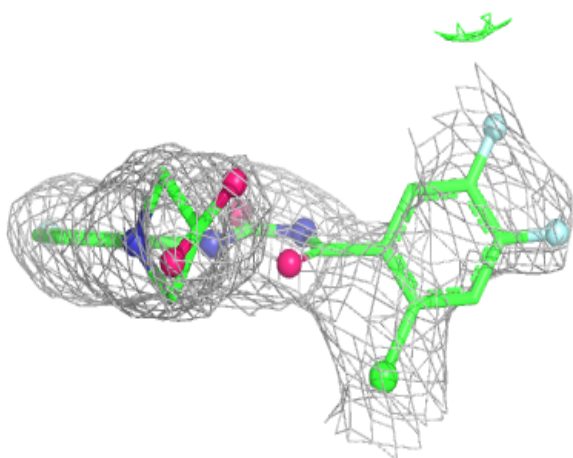
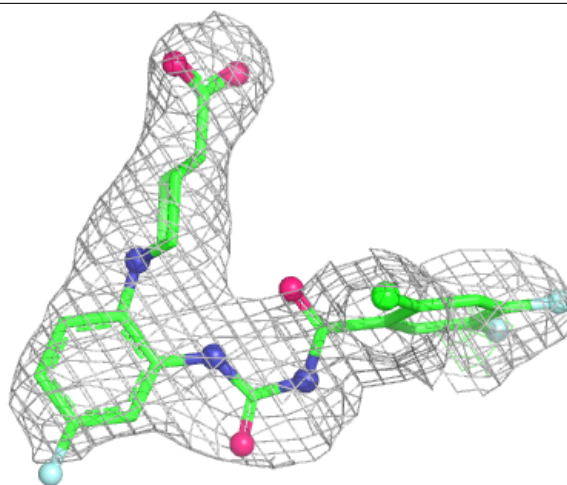
**Electron density around AVF A 833:**

$2mF_o-DF_c$  (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.