



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 01:28 am BST

PDB ID : 2BXS
Title : Human Monoamine Oxidase A in complex with Clorgyline, Crystal Form B
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Deposited on : 2005-07-27
Resolution : 3.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

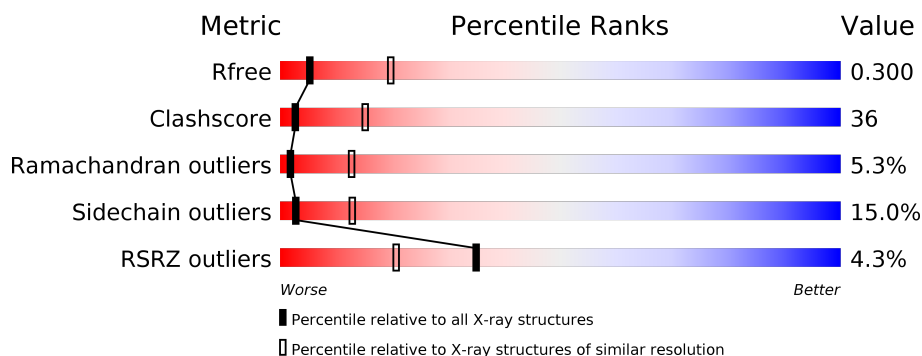
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)

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 on 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	527	
1	B	527	

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	MLG	A	601	X	-	-	-
3	MLG	B	601	X	-	-	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7900 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 AMINE OXIDASE [FLAVIN-CONTAINING] A.

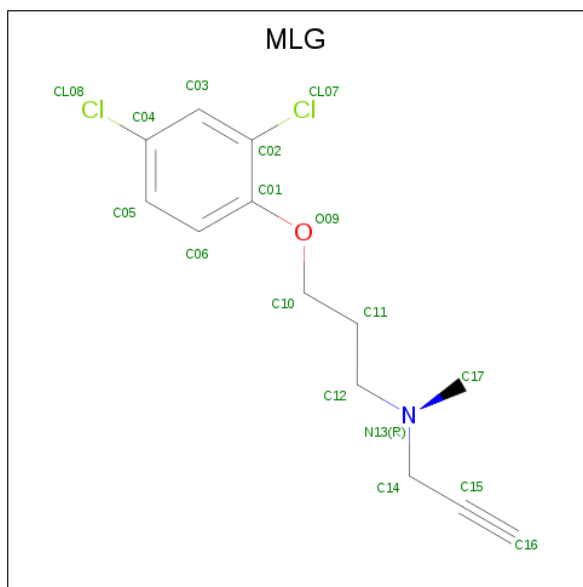
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	490	Total	C	N	O	S	0	0	0
			3880	2482	660	717	21			
1	B	490	Total	C	N	O	S	0	0	0
			3880	2482	660	717	21			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is N-[3-(2,4-DICHLOROPHENOXY)PROPYL]-N-METHYL-N-PROP-2-YNYL AMINE (three-letter code: MLG) (formula: C₁₃H₁₅Cl₂NO).

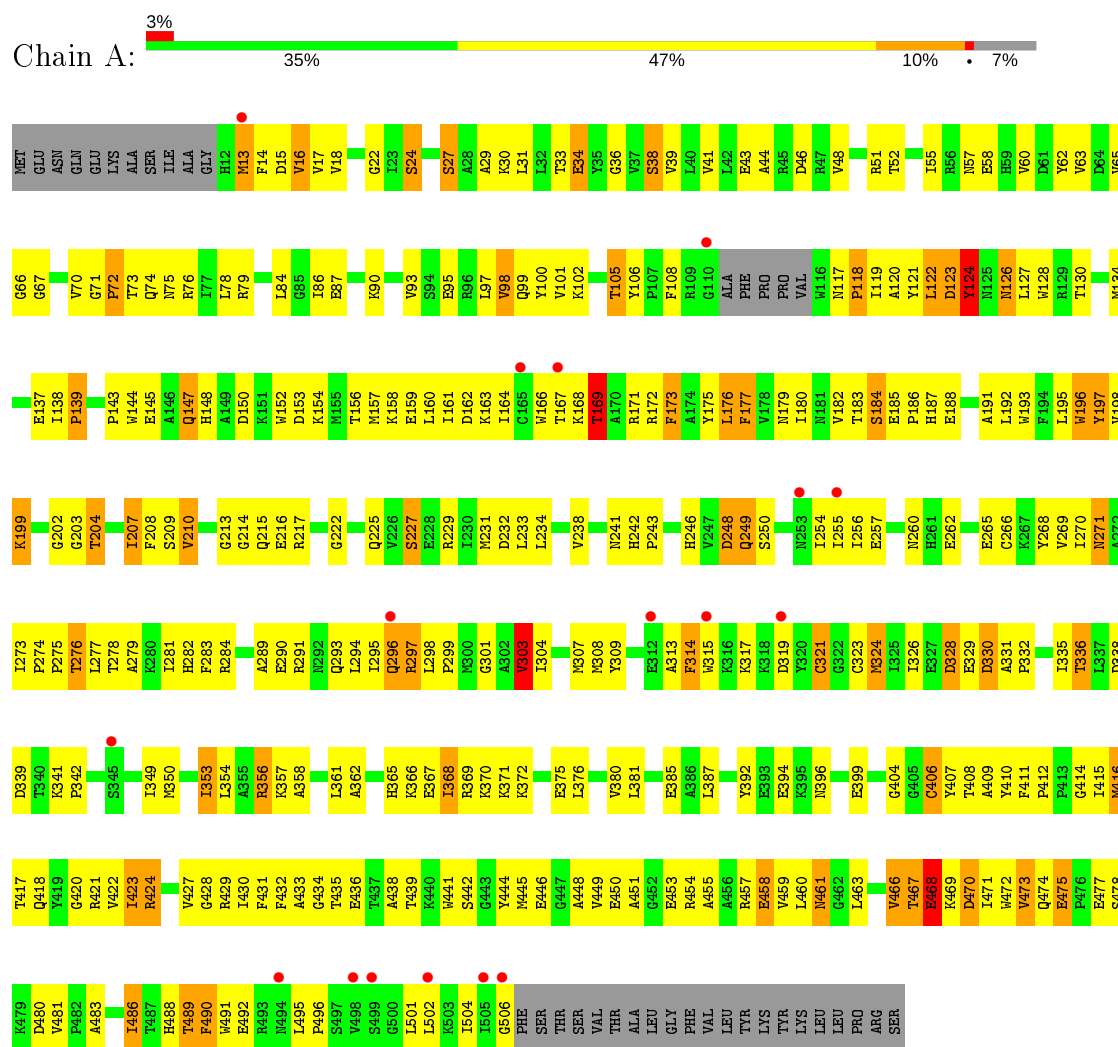


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			17	13	2	1	1		
3	B	1	Total	C	Cl	N	O	0	0
			17	13	2	1	1		

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: AMINE OXIDASE [FLAVIN-CONTAINING] A



I504	V70	E137	P275	I349	V427	I504
I505	G71	I138	T276	I350	G428	I505
PHE	P72	P139	T277	M350	R429	G506
SER	T73		T278		I430	
THR	Q74	P143	A279	I353	F431	SER
SER	N75	L354	K280	L354	F432	THR
VAL	R76	E145	I281	A355	A433	SER
THR	I77	A146	H282	R356	G434	VAL
		Q147	F283	K357	T435	THR
LEU	L84	H148	R284	A358	E436	THR
GLY	G85					LEU
PHE	I86	W152	R291	A362	W441	LEU
VAL	E87	D153	N292		S442	GLY
	T88	K154	Q293	H365	G443	PHE
	Y89	M155	L294	K366	Y444	VAL
K90		T156	I295	E367	M445	LEU
	V91	M157	Q296	I368	E446	TYR
N92		K158	R297	R369	G447	LYS
V93		E159	L298	K370	A448	LYS
S94		L160	P299	K371		LEU
E95		I161	M300	K372	A451	LEU
R96		D162	G301	I373	G452	LEU
L97		K163	A302	C374	E453	PRO
V98		I164	V303	E375	R454	ARG
	Q99	G165	I304	L376	A455	SER
Y100		W166	M307	L381	A456	
Y101		T167	M308	G382	R457	
K102		K168	Y309	S383	E458	
		T169		Q384	V459	
T105		A170	E312	E385	L460	
Y106		R171	A313	A386	M461	
P107		R172	F314	L387		
F108		F173	W315	E394	V466	
R109		A174	K316	K395	T467	
G110		Y175	K317	N396	K468	
ALA		L176	K318	K397	D470	
PHE		V177	D319	C398	I471	
PRO		W178	T320	E399	W472	
PRO		N179	C321	E400	V473	
VAL		I180	G322		Q474	
W116		N181	C323	T408	E475	
N117		W182	M324	A409		
P118		T183	I325	Y410	A483	
I119		S184	I326	F411		
A120		E185	E327	P412	T486	
Y121		R186	D328	P413	T487	
L122		H187	E329	G414	H488	
D123		E188	D330	I415	T489	
Y124		W189	A331	M416	F490	
M125		S190	P332	T417	W491	
N126		A191		Q418	E492	
L127		L192	I335	Y419	L495	
		W193	T336	G420	P496	
T130		F194	D339	R421		
I131		L195	T340	V422	G500	
D132		W196	K341	I423	L501	
M133		Y197	P342	R424	L502	
M134		V198	D343		K503	
G135		K199				
K136		Q200				

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	158.37Å 152.08Å 82.20Å 90.00° 104.52° 90.00°	Depositor
Resolution (Å)	15.00 – 3.15 59.26 – 3.15	Depositor EDS
% Data completeness (in resolution range)	90.5 (15.00-3.15) 90.4 (59.26-3.15)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.268 , 0.330 0.253 , 0.300	Depositor DCC
R_{free} test set	1502 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	68.1	Xtriage
Anisotropy	0.073	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 106.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.84	EDS
Total number of atoms	7900	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.51% 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: MLG, FAD

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	0.84	0/3973	0.84	1/5389 (0.0%)
1	B	0.81	1/3973 (0.0%)	0.82	2/5389 (0.0%)
All	All	0.82	1/7946 (0.0%)	0.83	3/10778 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	441	TRP	CB-CG	-5.02	1.41	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	353	ILE	CB-CA-C	5.56	122.73	111.60
1	B	353	ILE	N-CA-C	-5.09	97.26	111.00
1	A	303	VAL	CB-CA-C	-5.07	101.77	111.40

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	3880	0	3828	285	0
1	B	3880	0	3828	275	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	53	0	29	0	0
2	B	53	0	29	2	0
3	A	17	0	15	6	0
3	B	17	0	15	4	0
All	All	7900	0	7744	563	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 36.

All (563) 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:408:THR:HG23	1:B:409:ALA:O	1.50	1.11
1:A:304:ILE:HB	1:A:353:ILE:CG2	1.90	1.02
1:A:304:ILE:HB	1:A:353:ILE:HG23	1.39	1.02
1:A:408:THR:HG23	1:A:409:ALA:O	1.59	1.01
1:B:422:VAL:O	1:B:424:ARG:N	1.96	0.99
1:A:210:VAL:HG22	1:A:214:GLY:HA3	1.47	0.96
1:A:422:VAL:O	1:A:424:ARG:N	1.99	0.96
1:B:210:VAL:HG22	1:B:214:GLY:HA3	1.49	0.94
1:A:120:ALA:HA	1:A:167:THR:HG21	1.52	0.92
1:B:130:THR:O	1:B:134:MET:HB2	1.70	0.91
1:A:130:THR:O	1:A:134:MET:HB2	1.71	0.89
1:B:304:ILE:HB	1:B:353:ILE:CG2	2.03	0.88
1:B:120:ALA:HA	1:B:167:THR:HG21	1.54	0.86
1:A:176:LEU:O	1:A:180:ILE:N	2.08	0.86
1:A:210:VAL:HG22	1:A:214:GLY:CA	2.06	0.84
1:B:304:ILE:HB	1:B:353:ILE:HG23	1.56	0.84
1:B:210:VAL:HG22	1:B:214:GLY:CA	2.07	0.84
1:B:323:CYS:HA	1:B:336:THR:HG22	1.61	0.82
1:A:210:VAL:HG13	1:A:213:GLY:C	1.99	0.82
1:A:471:ILE:O	1:A:471:ILE:HG22	1.79	0.81
1:A:299:PRO:HG2	1:A:410:TYR:CZ	2.16	0.81
1:A:396:ASN:ND2	1:A:399:GLU:HG2	1.95	0.80
1:A:416:MET:O	1:A:420:GLY:HA3	1.80	0.80
1:A:501:LEU:HA	1:A:504:ILE:HD12	1.64	0.80
1:A:210:VAL:HG13	1:A:213:GLY:CA	2.12	0.79
1:A:299:PRO:HB2	1:A:410:TYR:CE2	2.16	0.79
1:B:330:ASP:N	1:B:330:ASP:OD2	2.15	0.79
1:A:438:ALA:HB3	1:A:442:SER:HB2	1.61	0.79
1:A:330:ASP:OD2	1:A:330:ASP:N	2.16	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:GLY:O	1:A:225:GLN:HG3	1.84	0.78
1:B:210:VAL:HG13	1:B:213:GLY:CA	2.13	0.78
1:B:197:TYR:HE2	1:B:207:ILE:HD11	1.49	0.78
1:A:323:CYS:HA	1:A:336:THR:HG22	1.66	0.78
1:B:210:VAL:HG13	1:B:213:GLY:C	2.05	0.77
1:A:157:MET:O	1:A:161:ILE:HG13	1.85	0.75
1:B:216:GLU:OE2	3:B:601:MLG:H102	1.86	0.75
1:A:324:MET:HG3	1:A:326:ILE:HD11	1.68	0.75
1:B:454:ARG:HD2	1:B:472:TRP:CZ2	2.22	0.75
1:B:197:TYR:HH	1:B:444:TYR:HE1	1.34	0.75
1:B:34:GLU:OE1	1:B:34:GLU:HA	1.86	0.74
1:B:299:PRO:HG2	1:B:410:TYR:CZ	2.22	0.74
1:B:193:TRP:CG	1:B:411:PHE:HB2	2.23	0.73
1:B:324:MET:HG3	1:B:326:ILE:HD11	1.69	0.73
1:A:34:GLU:OE1	1:A:34:GLU:HA	1.86	0.73
1:B:52:THR:HG22	1:B:67:GLY:HA3	1.70	0.72
1:B:84:LEU:HD22	1:B:229:ARG:HB2	1.71	0.72
1:B:332:PRO:HD2	1:B:376:LEU:HD22	1.72	0.72
1:B:95:GLU:O	1:B:321:CYS:HB3	1.89	0.72
1:B:501:LEU:HA	1:B:504:ILE:HD12	1.71	0.71
1:B:416:MET:O	1:B:420:GLY:HA3	1.90	0.71
1:B:97:LEU:O	1:B:108:PHE:N	2.24	0.71
1:B:468:GLU:HG3	1:B:469:LYS:H	1.56	0.71
1:B:299:PRO:HD2	1:B:410:TYR:O	1.90	0.71
1:B:408:THR:CG2	1:B:409:ALA:O	2.33	0.71
1:A:299:PRO:HB2	1:A:410:TYR:HE2	1.56	0.71
1:A:176:LEU:HA	1:A:179:ASN:HB2	1.72	0.70
1:B:87:GLU:OE1	1:B:87:GLU:HA	1.90	0.70
1:B:18:VAL:HB	1:B:41:VAL:HG22	1.74	0.70
1:B:192:LEU:HD23	1:B:416:MET:HG2	1.73	0.70
1:A:273:ILE:HD11	1:A:278:THR:HA	1.74	0.69
1:A:18:VAL:HB	1:A:41:VAL:HG22	1.73	0.69
1:B:254:ILE:HD13	1:B:269:VAL:HG23	1.75	0.69
1:B:273:ILE:HD11	1:B:278:THR:HA	1.75	0.69
1:A:97:LEU:O	1:A:108:PHE:N	2.26	0.69
1:A:76:ARG:HH21	1:A:475:GLU:HG2	1.57	0.69
1:B:99:GLN:N	1:B:106:TYR:O	2.22	0.68
1:A:87:GLU:OE1	1:A:87:GLU:HA	1.93	0.67
1:A:467:THR:HB	1:A:470:ASP:HB2	1.74	0.67
3:B:601:MLG:H172	3:B:601:MLG:CL07	2.32	0.67
1:A:197:TYR:HE2	1:A:207:ILE:HD11	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:THR:HG22	1:A:67:GLY:HA3	1.75	0.67
1:A:438:ALA:HB3	1:A:442:SER:CB	2.25	0.67
1:A:185:GLU:OE2	1:A:356:ARG:HB3	1.95	0.66
1:B:467:THR:HB	1:B:470:ASP:HB2	1.78	0.66
1:B:41:VAL:HB	1:B:238:VAL:HG22	1.76	0.66
1:A:48:VAL:HG23	1:A:227:SER:HB3	1.76	0.66
1:A:147:GLN:HB3	1:A:148:HIS:HD2	1.61	0.66
1:B:135:GLY:O	1:B:199:LYS:NZ	2.29	0.66
1:B:176:LEU:O	1:B:180:ILE:N	2.16	0.65
1:A:254:ILE:HD13	1:A:269:VAL:HG23	1.78	0.65
1:A:299:PRO:HD2	1:A:410:TYR:O	1.97	0.65
1:B:279:ALA:HA	1:B:295:ILE:HD12	1.77	0.64
1:A:193:TRP:CG	1:A:411:PHE:HB2	2.31	0.64
1:B:156:THR:HG23	1:B:159:GLU:H	1.62	0.64
1:B:291:ARG:HH21	1:B:422:VAL:HG12	1.60	0.64
1:A:31:LEU:O	1:A:34:GLU:HB2	1.97	0.64
1:B:269:VAL:HG12	1:B:270:ILE:N	2.13	0.64
1:A:246:HIS:CD2	1:A:282:HIS:HB2	2.33	0.64
1:A:172:ARG:HA	1:A:175:TYR:CD2	2.33	0.64
1:B:222:GLY:O	1:B:225:GLN:HG3	1.97	0.64
1:B:197:TYR:OH	1:B:444:TYR:HE1	1.81	0.64
1:B:172:ARG:HA	1:B:175:TYR:CD2	2.31	0.63
1:B:299:PRO:CD	1:B:410:TYR:O	2.46	0.63
1:B:396:ASN:ND2	1:B:399:GLU:HG2	2.13	0.63
1:B:157:MET:O	1:B:161:ILE:HG13	1.98	0.63
1:A:467:THR:CB	1:A:470:ASP:HB2	2.28	0.63
1:A:95:GLU:O	1:A:321:CYS:HB3	1.98	0.63
1:A:454:ARG:HD2	1:A:472:TRP:CZ2	2.34	0.63
1:A:191:ALA:O	1:A:195:LEU:HD12	1.99	0.62
1:B:31:LEU:O	1:B:34:GLU:HB2	1.99	0.62
1:A:281:ILE:HB	1:A:283:PHE:CE1	2.35	0.62
1:B:225:GLN:O	1:B:229:ARG:HG2	1.99	0.62
1:A:156:THR:HG23	1:A:159:GLU:H	1.63	0.62
1:B:210:VAL:HG13	1:B:213:GLY:HA2	1.81	0.62
1:B:291:ARG:NH2	1:B:422:VAL:HG12	2.15	0.62
1:A:76:ARG:NH2	1:A:475:GLU:HG2	2.14	0.62
1:A:332:PRO:HD2	1:A:376:LEU:HD22	1.81	0.62
1:A:299:PRO:HG2	1:A:410:TYR:CE2	2.34	0.62
1:A:197:TYR:HH	1:A:444:TYR:HE1	1.47	0.62
1:A:152:TRP:O	1:A:191:ALA:HB3	2.00	0.61
1:B:118:PRO:O	1:B:121:TYR:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:23:ILE:HD12	1:B:445:MET:HG2	1.81	0.61
1:A:279:ALA:HA	1:A:295:ILE:HD12	1.82	0.61
1:A:99:GLN:N	1:A:106:TYR:O	2.33	0.61
1:B:153:ASP:OD2	1:B:417:THR:OG1	2.16	0.61
1:B:315:TRP:HB3	1:B:381:LEU:HD13	1.82	0.61
1:A:183:THR:HG1	1:A:301:GLY:HA3	1.64	0.61
1:A:354:LEU:HA	1:A:358:ALA:HB2	1.83	0.61
1:A:409:ALA:HB3	1:A:436:GLU:HG3	1.81	0.61
1:B:489:THR:O	1:B:492:GLU:HB2	2.01	0.61
1:A:439:THR:OG1	1:A:450:GLU:OE2	2.18	0.61
1:A:99:GLN:HE21	1:A:100:TYR:N	1.99	0.61
1:B:299:PRO:HG2	1:B:410:TYR:CE2	2.36	0.61
1:A:293:GLN:O	1:A:296:GLN:N	2.33	0.61
1:A:276:THR:O	1:A:279:ALA:HB3	2.01	0.60
1:B:143:PRO:HD2	1:B:144:TRP:CE3	2.36	0.60
1:A:471:ILE:O	1:A:471:ILE:CG2	2.48	0.60
1:B:168:LYS:O	1:B:171:ARG:N	2.34	0.60
1:A:134:MET:HG2	1:A:152:TRP:CH2	2.36	0.60
1:A:246:HIS:HA	1:A:282:HIS:O	2.01	0.60
1:B:183:THR:OG1	1:B:301:GLY:HA3	2.01	0.60
1:B:62:TYR:O	1:B:341:LYS:HE3	2.00	0.60
1:B:143:PRO:HG2	1:B:416:MET:SD	2.42	0.60
1:A:210:VAL:HG13	1:A:213:GLY:HA2	1.83	0.60
1:B:90:LYS:NZ	1:B:215:GLN:NE2	2.50	0.60
1:B:471:ILE:O	1:B:471:ILE:HG22	2.01	0.59
1:B:182:VAL:O	1:B:184:SER:HB2	2.02	0.59
1:A:158:LYS:HE3	1:A:162:ASP:OD2	2.01	0.59
1:B:84:LEU:HD22	1:B:229:ARG:CB	2.32	0.59
1:B:176:LEU:HA	1:B:179:ASN:HB2	1.83	0.59
1:B:246:HIS:CD2	1:B:282:HIS:HB2	2.37	0.59
1:A:143:PRO:HB3	1:A:196:TRP:CD1	2.37	0.59
1:A:255:ILE:HG12	1:A:265:GLU:HG2	1.83	0.59
1:B:197:TYR:CE2	1:B:207:ILE:HD11	2.34	0.59
1:B:341:LYS:HB3	1:B:342:PRO:HD2	1.85	0.59
1:A:168:LYS:O	1:A:169:THR:C	2.42	0.58
1:B:158:LYS:HE3	1:B:162:ASP:OD2	2.04	0.58
1:A:46:ASP:HA	1:A:241:ASN:HD21	1.69	0.58
1:A:144:TRP:CH2	1:A:421:ARG:HA	2.39	0.57
1:B:369:ARG:NH1	1:B:394:GLU:OE1	2.38	0.57
1:A:269:VAL:HG12	1:A:270:ILE:N	2.18	0.57
1:B:99:GLN:HE21	1:B:100:TYR:N	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:TRP:HB3	1:A:381:LEU:HD13	1.85	0.57
1:A:177:PHE:C	1:A:177:PHE:CD2	2.78	0.57
1:A:183:THR:OG1	1:A:301:GLY:HA3	2.03	0.57
1:B:297:ARG:HD3	1:B:415:ILE:HD11	1.87	0.57
1:A:246:HIS:HD2	1:A:282:HIS:HB2	1.68	0.57
1:A:396:ASN:HD22	1:A:399:GLU:HG2	1.68	0.57
1:B:176:LEU:HD23	1:B:177:PHE:N	2.21	0.56
1:A:62:TYR:O	1:A:341:LYS:CE	2.54	0.56
1:B:177:PHE:CD2	1:B:177:PHE:C	2.79	0.56
1:A:297:ARG:HD3	1:A:415:ILE:HD11	1.86	0.56
1:A:299:PRO:CB	1:A:410:TYR:CE2	2.89	0.56
1:A:315:TRP:CE3	1:A:349:ILE:HD11	2.40	0.56
1:A:51:ARG:O	1:A:66:GLY:HA3	2.06	0.56
1:B:29:ALA:HA	1:B:39:VAL:HG11	1.87	0.56
1:B:90:LYS:HZ3	1:B:215:GLN:NE2	2.04	0.56
1:A:307:MET:SD	1:A:350:MET:HG2	2.46	0.56
1:A:365:HIS:HD2	1:A:367:GLU:H	1.54	0.56
1:A:468:GLU:HG3	1:A:469:LYS:H	1.70	0.56
1:B:48:VAL:HG23	1:B:227:SER:HB3	1.88	0.56
1:B:454:ARG:HD2	1:B:472:TRP:CH2	2.39	0.56
1:B:76:ARG:HH21	1:B:475:GLU:HG2	1.69	0.56
1:B:76:ARG:NH2	1:B:475:GLU:HG2	2.20	0.56
1:B:168:LYS:O	1:B:169:THR:C	2.44	0.56
1:A:328:ASP:C	1:A:328:ASP:OD2	2.43	0.56
1:A:33:THR:O	1:A:36:GLY:N	2.37	0.56
1:B:315:TRP:CE3	1:B:349:ILE:HD11	2.41	0.56
1:B:72:PRO:HB3	1:B:483:ALA:HA	1.88	0.56
1:A:29:ALA:HA	1:A:39:VAL:HG11	1.88	0.55
1:A:407:TYR:OH	3:A:601:MLG:H173	2.07	0.55
1:A:156:THR:HG22	1:A:159:GLU:CD	2.27	0.55
1:A:192:LEU:HD23	1:A:416:MET:HG2	1.88	0.55
1:A:197:TYR:CD2	1:A:197:TYR:C	2.80	0.55
1:B:467:THR:CB	1:B:470:ASP:HB2	2.36	0.55
1:A:143:PRO:HD2	1:A:144:TRP:CE3	2.42	0.55
1:B:186:PRO:O	1:B:188:GLU:N	2.40	0.55
1:B:281:ILE:HB	1:B:283:PHE:CE1	2.41	0.55
1:B:293:GLN:O	1:B:296:GLN:N	2.40	0.55
1:A:274:PRO:HD2	1:A:277:LEU:HD12	1.89	0.55
1:A:118:PRO:O	1:A:121:TYR:N	2.40	0.55
1:A:157:MET:HG3	1:A:161:ILE:HD11	1.89	0.55
1:A:369:ARG:NH1	1:A:394:GLU:OE1	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:TYR:CD2	1:B:197:TYR:C	2.80	0.55
1:A:314:PHE:O	1:A:317:LYS:HB3	2.07	0.55
1:A:147:GLN:HB3	1:A:148:HIS:CD2	2.42	0.54
1:B:143:PRO:HD2	1:B:144:TRP:CZ3	2.43	0.54
1:B:185:GLU:O	1:B:188:GLU:HB2	2.07	0.54
1:B:86:ILE:HD13	1:B:225:GLN:HB2	1.89	0.54
1:B:260:ASN:HD21	1:B:262:GLU:HB2	1.72	0.54
1:B:431:PHE:CE2	1:B:458:GLU:HB3	2.42	0.54
1:A:153:ASP:OD2	1:A:417:THR:OG1	2.21	0.54
1:A:73:THR:HG23	1:A:483:ALA:CB	2.38	0.54
1:B:182:VAL:O	1:B:183:THR:C	2.45	0.54
1:B:369:ARG:NH1	1:B:394:GLU:OE2	2.40	0.54
1:B:185:GLU:OE2	1:B:356:ARG:HB3	2.08	0.54
1:B:365:HIS:HD2	1:B:367:GLU:H	1.55	0.54
1:B:147:GLN:HB3	1:B:148:HIS:HD2	1.72	0.54
1:B:246:HIS:HD2	1:B:282:HIS:HB2	1.72	0.54
1:A:90:LYS:NZ	1:A:215:GLN:NE2	2.56	0.54
1:A:62:TYR:O	1:A:341:LYS:HE3	2.07	0.54
1:B:152:TRP:O	1:B:191:ALA:HB3	2.07	0.54
1:B:52:THR:HA	1:B:67:GLY:H	1.72	0.54
1:B:433:ALA:HB1	1:B:451:ALA:HB1	1.90	0.54
1:A:371:LYS:O	1:A:375:GLU:HG2	2.08	0.54
1:B:299:PRO:HB2	1:B:410:TYR:CE2	2.43	0.54
1:B:354:LEU:HA	1:B:358:ALA:HB2	1.90	0.53
1:B:304:ILE:HD11	1:B:362:ALA:HB2	1.90	0.53
1:A:99:GLN:HB3	1:A:106:TYR:HB2	1.90	0.53
1:B:275:PRO:CD	1:B:436:GLU:HG2	2.38	0.53
1:A:44:ALA:HB1	1:A:243:PRO:HG3	1.91	0.53
1:A:431:PHE:CE2	1:A:458:GLU:HB3	2.44	0.53
1:A:291:ARG:HH21	1:A:422:VAL:HG12	1.72	0.53
1:B:468:GLU:CG	1:B:469:LYS:H	2.20	0.53
1:A:445:MET:O	1:A:446:GLU:C	2.47	0.53
1:B:491:TRP:HB3	1:B:495:LEU:HG	1.90	0.53
1:A:160:LEU:HG	1:A:164:ILE:HD11	1.91	0.53
1:B:46:ASP:HA	1:B:241:ASN:HD21	1.74	0.53
1:B:328:ASP:C	1:B:328:ASP:OD2	2.47	0.53
1:A:335:ILE:HG12	3:A:601:MLG:H03	1.91	0.53
1:B:133:ASN:HA	1:B:136:LYS:HD2	1.91	0.53
1:B:62:TYR:O	1:B:341:LYS:CE	2.57	0.53
1:A:225:GLN:O	1:A:229:ARG:HG2	2.09	0.52
1:B:490:PHE:HD2	1:B:491:TRP:N	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:ILE:HD11	1:A:362:ALA:HB2	1.91	0.52
1:B:490:PHE:CD2	1:B:490:PHE:C	2.81	0.52
1:B:502:LEU:O	1:B:506:GLY:N	2.33	0.52
1:A:331:ALA:O	1:A:357:LYS:NZ	2.37	0.52
1:A:291:ARG:NH2	1:A:422:VAL:HG12	2.25	0.52
1:B:256:ILE:N	1:B:256:ILE:HD12	2.24	0.52
1:B:488:HIS:HA	1:B:492:GLU:OE1	2.09	0.52
1:A:46:ASP:HA	1:A:241:ASN:ND2	2.24	0.52
1:A:502:LEU:O	1:A:506:GLY:N	2.36	0.52
1:A:335:ILE:HG21	3:A:601:MLG:CL07	2.46	0.52
1:B:134:MET:HG2	1:B:152:TRP:CH2	2.44	0.52
1:A:489:THR:O	1:A:492:GLU:HB2	2.09	0.52
1:B:246:HIS:HA	1:B:282:HIS:O	2.09	0.52
1:B:293:GLN:O	1:B:295:ILE:N	2.43	0.52
1:A:84:LEU:HD22	1:A:229:ARG:HB2	1.91	0.52
1:B:414:GLY:O	1:B:418:GLN:HB2	2.10	0.51
1:B:123:ASP:CG	1:B:166:TRP:H	2.13	0.51
1:B:124:TYR:OH	1:B:173:PHE:CD1	2.54	0.51
1:B:335:ILE:HG12	3:B:601:MLG:H03	1.92	0.51
1:A:414:GLY:O	1:A:418:GLN:HB2	2.10	0.51
1:B:444:TYR:HB3	2:B:600:FAD:O2	2.09	0.51
1:B:156:THR:HG22	1:B:159:GLU:CD	2.31	0.51
1:A:186:PRO:O	1:A:188:GLU:N	2.44	0.51
1:B:293:GLN:O	1:B:294:LEU:C	2.49	0.51
1:B:193:TRP:NE1	1:B:411:PHE:CD1	2.79	0.51
1:B:98:VAL:HB	1:B:324:MET:HB3	1.93	0.51
1:A:143:PRO:HG2	1:A:416:MET:SD	2.50	0.51
1:B:95:GLU:OE1	1:B:321:CYS:HA	2.09	0.51
1:A:41:VAL:HB	1:A:238:VAL:HG22	1.93	0.51
1:A:15:ASP:HB2	1:A:38:SER:O	2.11	0.51
1:A:491:TRP:HB3	1:A:495:LEU:HG	1.92	0.51
1:B:271:ASN:HB3	1:B:432:PHE:HD2	1.76	0.51
1:B:30:LYS:O	1:B:34:GLU:HG2	2.11	0.51
1:A:369:ARG:NH1	1:A:394:GLU:OE2	2.44	0.51
1:B:143:PRO:HB3	1:B:196:TRP:CD1	2.46	0.51
1:B:331:ALA:O	1:B:357:LYS:NZ	2.34	0.51
1:A:182:VAL:O	1:A:183:THR:C	2.49	0.51
1:B:248:ASP:HA	1:B:284:ARG:O	2.10	0.51
1:A:182:VAL:O	1:A:184:SER:HB2	2.11	0.50
1:A:168:LYS:O	1:A:171:ARG:N	2.44	0.50
1:A:303:VAL:HG13	1:A:354:LEU:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:ASP:OD1	1:A:339:ASP:N	2.44	0.50
1:A:72:PRO:HD3	1:A:481:VAL:CG1	2.41	0.50
1:B:321:CYS:SG	1:B:323:CYS:HB3	2.51	0.50
1:A:490:PHE:HD2	1:A:491:TRP:N	2.10	0.50
1:B:16:VAL:HA	1:B:268:TYR:O	2.11	0.50
1:A:275:PRO:CD	1:A:436:GLU:HG2	2.42	0.50
1:B:99:GLN:HB3	1:B:106:TYR:HB2	1.94	0.50
1:A:299:PRO:CG	1:A:410:TYR:CE2	2.94	0.50
1:B:13:MET:C	1:B:14:PHE:CD2	2.85	0.50
1:B:256:ILE:HD11	1:B:266:CYS:SG	2.52	0.50
1:B:461:ASN:HB2	1:B:466:VAL:HG12	1.93	0.50
1:A:176:LEU:O	1:A:179:ASN:HB2	2.12	0.50
1:A:416:MET:O	1:A:420:GLY:CA	2.56	0.50
1:A:51:ARG:HG2	1:A:406:CYS:SG	2.52	0.50
1:B:225:GLN:HE21	1:B:229:ARG:NH2	2.10	0.50
1:B:51:ARG:O	1:B:66:GLY:HA3	2.12	0.50
1:A:468:GLU:CG	1:A:469:LYS:H	2.24	0.49
1:B:70:VAL:HA	1:B:74:GLN:OE1	2.12	0.49
1:A:197:TYR:CE2	1:A:207:ILE:HD11	2.45	0.49
1:A:409:ALA:CB	1:A:436:GLU:HG3	2.43	0.49
1:B:193:TRP:CD1	1:B:411:PHE:HB2	2.46	0.49
1:A:176:LEU:HD23	1:A:177:PHE:N	2.27	0.49
1:B:33:THR:O	1:B:36:GLY:N	2.41	0.49
1:A:143:PRO:HD2	1:A:144:TRP:CZ3	2.48	0.49
1:A:369:ARG:O	1:A:370:LYS:C	2.51	0.49
1:B:314:PHE:O	1:B:317:LYS:HB3	2.13	0.49
1:B:198:VAL:HG12	1:B:203:GLY:HA2	1.94	0.49
1:B:268:TYR:CG	1:B:459:VAL:HG13	2.47	0.49
1:A:203:GLY:O	1:A:204:THR:C	2.51	0.49
1:A:457:ARG:HA	1:A:460:LEU:HB2	1.95	0.49
1:B:126:ASN:ND2	1:B:126:ASN:C	2.66	0.49
1:A:144:TRP:CZ2	1:A:421:ARG:HA	2.48	0.49
1:A:365:HIS:CD2	1:A:367:GLU:H	2.31	0.48
1:A:117:ASN:HD22	1:A:120:ALA:HB2	1.78	0.48
1:B:276:THR:O	1:B:279:ALA:HB3	2.13	0.48
1:A:139:PRO:HG2	1:A:143:PRO:HA	1.95	0.48
1:A:199:LYS:O	1:A:202:GLY:N	2.39	0.48
1:A:271:ASN:HB3	1:A:432:PHE:HD2	1.78	0.48
1:A:160:LEU:O	1:A:164:ILE:HG13	2.14	0.48
1:A:24:SER:O	1:A:27:SER:N	2.47	0.48
1:A:73:THR:CG2	1:A:483:ALA:CB	2.91	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ILE:HA	1:A:139:PRO:HD2	1.39	0.48
1:A:365:HIS:HB3	1:A:368:ILE:HG13	1.96	0.48
1:B:196:TRP:CZ2	1:B:200:GLN:HG2	2.48	0.48
1:B:245:THR:OG1	1:B:246:HIS:ND1	2.47	0.48
1:A:13:MET:C	1:A:14:PHE:CD2	2.87	0.48
1:A:123:ASP:CG	1:A:166:TRP:H	2.16	0.48
1:A:293:GLN:O	1:A:294:LEU:C	2.52	0.48
1:B:160:LEU:HG	1:B:164:ILE:HD11	1.96	0.48
1:B:371:LYS:O	1:B:375:GLU:HG2	2.14	0.48
1:B:416:MET:HE2	1:B:420:GLY:HA3	1.96	0.48
1:A:256:ILE:HD12	1:A:256:ILE:N	2.29	0.47
1:B:471:ILE:O	1:B:471:ILE:CG2	2.62	0.47
1:A:335:ILE:CG2	3:A:601:MLG:CL07	2.99	0.47
1:B:365:HIS:CD2	1:B:367:GLU:H	2.31	0.47
1:A:176:LEU:CA	1:A:179:ASN:HB2	2.43	0.47
1:A:271:ASN:HB3	1:A:432:PHE:CD2	2.50	0.47
1:A:313:ALA:O	1:A:315:TRP:N	2.47	0.47
1:A:461:ASN:HB2	1:A:466:VAL:HG12	1.95	0.47
1:A:268:TYR:CG	1:A:459:VAL:HG13	2.50	0.47
1:A:433:ALA:HB1	1:A:451:ALA:HB1	1.97	0.47
1:A:90:LYS:HZ3	1:A:215:GLN:NE2	2.12	0.47
1:B:144:TRP:CH2	1:B:421:ARG:HA	2.49	0.47
1:B:196:TRP:CE2	1:B:200:GLN:HG2	2.50	0.47
1:B:255:ILE:HG12	1:B:265:GLU:HG2	1.97	0.47
1:B:409:ALA:HB3	1:B:436:GLU:HG3	1.95	0.47
1:A:185:GLU:O	1:A:188:GLU:HB2	2.14	0.47
1:A:197:TYR:OH	1:A:444:TYR:HE1	1.97	0.47
1:B:56:ARG:HH22	1:B:228:GLU:CD	2.18	0.47
1:A:299:PRO:CD	1:A:410:TYR:O	2.63	0.47
1:A:256:ILE:HD11	1:A:266:CYS:SG	2.55	0.47
1:A:93:VAL:HG12	1:A:93:VAL:O	2.15	0.47
1:B:123:ASP:OD2	1:B:166:TRP:N	2.41	0.47
1:B:130:THR:HG22	1:B:134:MET:HE2	1.97	0.47
1:B:177:PHE:CE2	1:B:181:ASN:ND2	2.83	0.47
1:B:177:PHE:HD2	1:B:177:PHE:C	2.18	0.47
1:B:269:VAL:HB	1:B:430:ILE:HG23	1.97	0.47
1:A:256:ILE:HD12	1:A:256:ILE:H	1.80	0.46
1:A:490:PHE:C	1:A:490:PHE:CD2	2.88	0.46
1:A:123:ASP:OD2	1:A:166:TRP:N	2.37	0.46
1:A:198:VAL:HG12	1:A:203:GLY:HA2	1.96	0.46
1:B:176:LEU:HG	1:B:180:ILE:CD1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:VAL:HG13	1:A:214:GLY:N	2.30	0.46
1:A:84:LEU:HD22	1:A:229:ARG:CB	2.45	0.46
1:A:458:GLU:O	1:A:459:VAL:C	2.53	0.46
1:A:86:ILE:HD13	1:A:225:GLN:HB2	1.97	0.46
1:B:147:GLN:HB3	1:B:148:HIS:CD2	2.50	0.46
1:B:197:TYR:C	1:B:197:TYR:HD2	2.19	0.46
1:B:292:ASN:O	1:B:296:GLN:NE2	2.49	0.46
1:B:466:VAL:HG13	1:B:470:ASP:HB3	1.96	0.46
3:B:601:MLG:C17	3:B:601:MLG:CL07	3.00	0.46
1:A:298:LEU:HA	1:A:299:PRO:HD3	1.70	0.46
1:B:249:GLN:HE22	1:B:428:GLY:HA3	1.81	0.46
1:B:117:ASN:OD1	1:B:118:PRO:HD2	2.15	0.46
1:B:46:ASP:HA	1:B:241:ASN:ND2	2.30	0.46
1:B:297:ARG:CD	1:B:415:ILE:HD11	2.46	0.46
1:B:445:MET:O	1:B:448:ALA:HB3	2.16	0.46
1:A:246:HIS:HB2	1:A:257:GLU:HB3	1.97	0.46
1:A:98:VAL:HB	1:A:324:MET:HB3	1.98	0.46
1:B:203:GLY:O	1:B:204:THR:C	2.53	0.46
1:B:457:ARG:HA	1:B:460:LEU:HB2	1.98	0.46
1:A:130:THR:HG22	1:A:134:MET:HE2	1.97	0.46
1:A:197:TYR:C	1:A:197:TYR:HD2	2.19	0.46
1:B:271:ASN:HB3	1:B:432:PHE:CD2	2.50	0.46
1:B:433:ALA:HB2	1:B:455:ALA:HB2	1.98	0.46
1:A:207:ILE:CG2	1:A:208:PHE:N	2.78	0.46
1:A:274:PRO:HB2	1:A:275:PRO:CD	2.45	0.46
1:B:246:HIS:HB2	1:B:257:GLU:HB3	1.97	0.46
1:B:271:ASN:OD1	1:B:278:THR:HG23	2.16	0.46
1:B:307:MET:SD	1:B:350:MET:HG2	2.55	0.46
1:A:279:ALA:HB2	1:A:295:ILE:HB	1.98	0.45
1:A:408:THR:OG1	1:A:436:GLU:OE1	2.27	0.45
1:B:303:VAL:HG13	1:B:354:LEU:HB3	1.98	0.45
1:B:490:PHE:CD2	1:B:491:TRP:N	2.83	0.45
1:A:307:MET:HB3	1:A:309:TYR:CE2	2.51	0.45
1:A:254:ILE:HG13	1:A:429:ARG:HH21	1.81	0.45
1:A:16:VAL:HA	1:A:268:TYR:O	2.17	0.45
1:B:57:ASN:O	1:B:60:VAL:HG22	2.16	0.45
1:B:186:PRO:C	1:B:188:GLU:H	2.20	0.45
1:B:245:THR:OG1	1:B:246:HIS:CE1	2.69	0.45
1:A:490:PHE:CD2	1:A:491:TRP:N	2.84	0.45
1:B:138:ILE:HA	1:B:139:PRO:HD2	1.49	0.45
1:B:183:THR:HG1	1:B:301:GLY:HA3	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:PRO:CG	1:B:436:GLU:HG2	2.47	0.45
1:B:445:MET:O	1:B:446:GLU:C	2.52	0.45
1:B:43:GLU:HG3	1:B:44:ALA:N	2.32	0.45
1:A:289:ALA:O	1:A:290:GLU:C	2.54	0.45
1:A:275:PRO:HD3	1:A:436:GLU:HG2	1.99	0.45
1:A:466:VAL:HG13	1:A:470:ASP:HB3	1.98	0.45
1:B:275:PRO:HD3	1:B:436:GLU:HG2	1.97	0.45
1:B:176:LEU:O	1:B:179:ASN:HB2	2.16	0.45
1:A:177:PHE:C	1:A:177:PHE:HD2	2.20	0.45
1:B:139:PRO:HG2	1:B:143:PRO:HA	1.99	0.44
1:B:408:THR:HG23	1:B:409:ALA:C	2.31	0.44
1:A:275:PRO:CG	1:A:436:GLU:HG2	2.47	0.44
1:A:198:VAL:O	1:A:203:GLY:HA2	2.18	0.44
1:A:22:GLY:O	1:A:24:SER:N	2.51	0.44
1:A:273:ILE:CD1	1:A:281:ILE:HD11	2.48	0.44
1:A:73:THR:HG23	1:A:483:ALA:HB2	1.98	0.44
1:B:256:ILE:HD12	1:B:256:ILE:H	1.82	0.44
1:B:291:ARG:O	1:B:294:LEU:N	2.50	0.44
1:B:339:ASP:HB2	1:B:350:MET:HB2	1.98	0.44
1:B:453:GLU:O	1:B:457:ARG:HG3	2.17	0.44
1:B:43:GLU:HG3	1:B:45:ARG:H	1.82	0.44
1:B:461:ASN:CB	1:B:471:ILE:HD11	2.48	0.44
1:A:332:PRO:HB3	1:A:361:LEU:CD1	2.47	0.44
1:A:416:MET:HE2	1:A:420:GLY:HA3	1.99	0.44
1:B:192:LEU:HA	1:B:195:LEU:HD12	2.00	0.44
1:B:232:ASP:O	1:B:234:LEU:N	2.51	0.44
1:B:307:MET:HB3	1:B:309:TYR:CE2	2.52	0.44
1:B:416:MET:CE	1:B:420:GLY:HA3	2.47	0.44
1:B:121:TYR:HA	1:B:124:TYR:HB2	1.99	0.44
1:A:154:LYS:HA	1:A:154:LYS:HD3	1.90	0.44
1:A:433:ALA:HB2	1:A:455:ALA:HB2	2.00	0.44
1:B:75:ASN:O	1:B:76:ARG:C	2.55	0.44
1:A:120:ALA:CA	1:A:167:THR:HG21	2.37	0.44
1:A:186:PRO:C	1:A:188:GLU:H	2.21	0.44
1:A:372:LYS:O	1:A:375:GLU:HG3	2.17	0.44
1:A:57:ASN:O	1:A:60:VAL:HG22	2.18	0.44
1:B:185:GLU:HA	1:B:185:GLU:OE1	2.17	0.44
1:A:338:ASP:OD1	1:A:338:ASP:C	2.56	0.44
1:A:341:LYS:HB3	1:A:342:PRO:HD2	1.99	0.44
1:A:445:MET:O	1:A:448:ALA:HB3	2.18	0.44
1:A:461:ASN:CB	1:A:471:ILE:HD11	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:CYS:HA	1:A:336:THR:O	2.18	0.43
1:A:30:LYS:O	1:A:34:GLU:HG2	2.18	0.43
1:A:78:LEU:O	1:A:79:ARG:C	2.56	0.43
1:B:299:PRO:CG	1:B:410:TYR:CE2	3.01	0.43
1:B:77:ILE:N	1:B:446:GLU:OE2	2.42	0.43
1:A:242:HIS:NE2	1:A:262:GLU:OE2	2.51	0.43
1:A:95:GLU:OE1	1:A:321:CYS:HA	2.18	0.43
1:A:185:GLU:HA	1:A:185:GLU:OE1	2.18	0.43
1:A:330:ASP:O	1:A:331:ALA:C	2.55	0.43
1:A:412:PRO:HG2	1:A:415:ILE:CG1	2.49	0.43
1:B:122:LEU:O	1:B:123:ASP:C	2.56	0.43
1:B:15:ASP:HB2	1:B:38:SER:O	2.18	0.43
1:B:155:MET:HB3	1:B:191:ALA:CB	2.49	0.43
1:B:192:LEU:O	1:B:195:LEU:HB2	2.18	0.43
1:A:254:ILE:HG13	1:A:429:ARG:NH2	2.34	0.43
1:A:416:MET:CE	1:A:420:GLY:HA3	2.48	0.43
1:B:246:HIS:NE2	1:B:282:HIS:HD2	2.16	0.43
1:A:124:TYR:OH	1:A:173:PHE:CD1	2.58	0.43
1:B:160:LEU:O	1:B:164:ILE:HG13	2.18	0.43
1:B:232:ASP:O	1:B:233:LEU:C	2.57	0.43
1:A:260:ASN:HD21	1:A:262:GLU:HB2	1.83	0.43
1:A:408:THR:CG2	1:A:409:ALA:O	2.49	0.43
1:B:190:SER:HB3	1:B:193:TRP:HB2	2.00	0.43
1:A:183:THR:O	1:A:183:THR:OG1	2.26	0.43
1:B:260:ASN:ND2	1:B:262:GLU:HB2	2.33	0.43
1:B:468:GLU:HG3	1:B:469:LYS:N	2.29	0.43
1:B:454:ARG:CD	1:B:472:TRP:CH2	3.00	0.43
1:A:271:ASN:C	1:A:271:ASN:ND2	2.72	0.43
1:A:291:ARG:O	1:A:294:LEU:N	2.52	0.43
1:A:293:GLN:O	1:A:295:ILE:N	2.51	0.43
1:A:445:MET:O	1:A:448:ALA:N	2.52	0.43
1:B:329:GLU:HA	1:B:329:GLU:OE1	2.18	0.43
1:B:18:VAL:HG11	1:B:25:GLY:O	2.19	0.43
1:B:193:TRP:CH2	1:B:410:TYR:HA	2.54	0.43
1:A:22:GLY:C	1:A:24:SER:N	2.72	0.43
1:A:339:ASP:HB2	1:A:350:MET:HB2	2.01	0.43
1:B:500:GLY:O	1:B:502:LEU:N	2.52	0.43
1:B:71:GLY:N	1:B:74:GLN:OE1	2.51	0.43
1:B:92:ASN:O	1:B:93:VAL:HG22	2.19	0.43
1:A:17:VAL:HG12	1:A:18:VAL:N	2.34	0.42
1:A:463:LEU:HA	1:A:463:LEU:HD23	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:HIS:HA	1:A:492:GLU:OE1	2.19	0.42
1:A:52:THR:HG21	1:A:445:MET:SD	2.59	0.42
1:A:52:THR:HG22	1:A:67:GLY:CA	2.46	0.42
1:B:273:ILE:CD1	1:B:281:ILE:HD11	2.49	0.42
1:A:191:ALA:C	1:A:195:LEU:HD12	2.39	0.42
1:A:144:TRP:CZ3	1:A:421:ARG:HA	2.54	0.42
1:A:453:GLU:O	1:A:457:ARG:HG3	2.19	0.42
1:B:186:PRO:C	1:B:188:GLU:N	2.73	0.42
1:A:124:TYR:HD2	1:A:128:TRP:CZ3	2.36	0.42
1:A:52:THR:HA	1:A:67:GLY:H	1.83	0.42
1:B:120:ALA:CA	1:B:167:THR:HG21	2.39	0.42
1:B:315:TRP:CD2	1:B:349:ILE:HD11	2.54	0.42
1:B:412:PRO:HG2	1:B:415:ILE:HG13	2.01	0.42
1:A:315:TRP:CD2	1:A:349:ILE:HD11	2.55	0.42
1:A:193:TRP:CD1	1:A:411:PHE:HB2	2.54	0.42
1:A:97:LEU:HD12	1:A:97:LEU:N	2.34	0.42
1:B:52:THR:HG22	1:B:67:GLY:CA	2.44	0.42
1:B:299:PRO:HD3	1:B:410:TYR:O	2.19	0.42
1:A:434:GLY:O	1:A:436:GLU:N	2.53	0.42
1:A:477:GLU:O	1:A:478:SER:C	2.57	0.42
3:A:601:MLG:H101	3:A:601:MLG:H06	1.69	0.42
1:A:70:VAL:HA	1:A:74:GLN:OE1	2.20	0.42
1:B:204:THR:OG1	1:B:205:THR:N	2.53	0.42
1:A:156:THR:HG22	1:A:159:GLU:OE2	2.19	0.42
1:A:232:ASP:O	1:A:234:LEU:N	2.53	0.42
1:A:254:ILE:HD11	1:A:429:ARG:HB2	2.01	0.42
1:A:329:GLU:HA	1:A:329:GLU:OE1	2.20	0.42
1:A:44:ALA:O	1:A:241:ASN:HA	2.20	0.42
1:B:298:LEU:HA	1:B:299:PRO:HD3	1.79	0.42
1:A:117:ASN:HA	1:A:118:PRO:HD2	1.92	0.41
1:A:126:ASN:ND2	1:A:126:ASN:C	2.72	0.41
1:A:269:VAL:HB	1:A:430:ILE:HG23	2.02	0.41
1:A:105:THR:HG21	1:A:380:VAL:O	2.20	0.41
1:A:415:ILE:HA	1:A:415:ILE:HD13	1.78	0.41
1:B:269:VAL:CG1	1:B:270:ILE:N	2.82	0.41
1:A:148:HIS:CD2	1:A:148:HIS:N	2.88	0.41
1:A:308:MET:CE	1:A:392:TYR:HD1	2.33	0.41
1:B:330:ASP:O	1:B:331:ALA:C	2.58	0.41
1:B:369:ARG:O	1:B:370:LYS:C	2.59	0.41
1:A:274:PRO:CB	1:A:275:PRO:CD	2.97	0.41
1:A:75:ASN:OD1	1:A:478:SER:N	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:ASN:C	1:B:271:ASN:ND2	2.73	0.41
1:B:408:THR:OG1	1:B:436:GLU:OE1	2.31	0.41
1:A:246:HIS:NE2	1:A:282:HIS:HD2	2.18	0.41
1:A:248:ASP:HA	1:A:284:ARG:O	2.20	0.41
1:B:155:MET:HB3	1:B:191:ALA:HB2	2.03	0.41
1:B:473:VAL:HG12	1:B:474:GLN:O	2.20	0.41
1:A:121:TYR:HA	1:A:124:TYR:HB2	2.03	0.41
1:B:196:TRP:CD2	1:B:196:TRP:C	2.93	0.41
1:A:216:GLU:OE2	3:A:601:MLG:H101	2.20	0.41
1:A:274:PRO:HB2	1:A:275:PRO:HD2	2.01	0.41
1:B:365:HIS:HB3	1:B:368:ILE:HG13	2.03	0.41
1:B:444:TYR:N	1:B:444:TYR:CD1	2.88	0.41
1:B:57:ASN:O	1:B:59:HIS:N	2.54	0.41
1:B:132:ASP:O	1:B:135:GLY:N	2.35	0.41
1:B:156:THR:CG2	1:B:159:GLU:H	2.32	0.41
1:B:172:ARG:HA	1:B:175:TYR:HD2	1.81	0.41
1:B:416:MET:O	1:B:420:GLY:CA	2.64	0.41
1:B:369:ARG:NH1	1:B:394:GLU:CD	2.74	0.41
1:B:192:LEU:CD2	1:B:416:MET:HG2	2.48	0.41
1:A:249:GLN:HE22	1:A:428:GLY:HA3	1.86	0.41
1:A:449:VAL:O	1:A:453:GLU:HG3	2.21	0.41
1:B:89:TYR:CE2	1:B:218:LYS:HB2	2.56	0.41
1:A:122:LEU:O	1:A:123:ASP:C	2.59	0.41
1:A:196:TRP:O	1:A:196:TRP:CG	2.71	0.41
1:A:444:TYR:CD1	1:A:444:TYR:N	2.88	0.41
1:B:304:ILE:HB	1:B:353:ILE:HG22	1.98	0.41
1:B:373:ILE:O	1:B:376:LEU:HB3	2.20	0.41
1:B:397:TRP:HA	1:B:400:GLU:HG2	2.01	0.41
1:B:468:GLU:C	1:B:470:ASP:N	2.74	0.41
1:A:473:VAL:HG12	1:A:474:GLN:O	2.21	0.41
1:B:292:ASN:HA	1:B:295:ILE:HD11	2.03	0.41
1:B:443:GLY:O	2:B:600:FAD:H1'2	2.20	0.41
1:A:117:ASN:OD1	1:A:118:PRO:HD2	2.21	0.40
1:B:193:TRP:CZ2	1:B:410:TYR:HA	2.56	0.40
1:B:245:THR:HG1	1:B:246:HIS:CE1	2.39	0.40
1:B:100:TYR:HD2	1:B:326:ILE:HG23	1.86	0.40
1:A:172:ARG:HA	1:A:175:TYR:HD2	1.83	0.40
1:A:454:ARG:HD2	1:A:472:TRP:CH2	2.56	0.40
1:A:71:GLY:O	1:A:74:GLN:HB2	2.21	0.40
1:B:144:TRP:CD1	1:B:144:TRP:C	2.94	0.40
1:B:415:ILE:HD13	1:B:415:ILE:HA	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:SER:HB3	1:B:193:TRP:CB	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	486/527 (92%)	386 (79%)	73 (15%)	27 (6%)	2	12
1	B	486/527 (92%)	389 (80%)	72 (15%)	25 (5%)	2	13
All	All	972/1054 (92%)	775 (80%)	145 (15%)	52 (5%)	2	13

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	THR
1	A	204	THR
1	A	209	SER
1	A	314	PHE
1	A	366	LYS
1	A	423	ILE
1	A	473	VAL
1	B	169	THR
1	B	204	THR
1	B	314	PHE
1	B	423	ILE
1	B	473	VAL
1	A	34	GLU
1	A	187	HIS
1	A	319	ASP
1	A	435	THR
1	A	441	TRP

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Mol	Chain	Res	Type
1	A	486	ILE
1	B	133	ASN
1	B	187	HIS
1	B	209	SER
1	B	319	ASP
1	B	366	LYS
1	B	486	ILE
1	A	118	PRO
1	A	127	LEU
1	B	34	GLU
1	B	118	PRO
1	B	183	THR
1	B	210	VAL
1	B	496	PRO
1	A	248	ASP
1	A	250	SER
1	A	468	GLU
1	A	496	PRO
1	B	122	LEU
1	B	127	LEU
1	B	468	GLU
1	A	102	LYS
1	A	122	LEU
1	A	210	VAL
1	A	490	PHE
1	B	58	GLU
1	B	102	LYS
1	B	435	THR
1	A	124	TYR
1	B	299	PRO
1	A	72	PRO
1	A	139	PRO
1	A	404	GLY
1	B	139	PRO
1	B	25	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	412/450 (92%)	346 (84%)	66 (16%)	2	10
1	B	412/450 (92%)	354 (86%)	58 (14%)	3	15
All	All	824/900 (92%)	700 (85%)	124 (15%)	3	13

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	MET
1	A	16	VAL
1	A	24	SER
1	A	27	SER
1	A	38	SER
1	A	43	GLU
1	A	55	ILE
1	A	58	GLU
1	A	63	VAL
1	A	65	VAL
1	A	98	VAL
1	A	101	VAL
1	A	105	THR
1	A	119	ILE
1	A	123	ASP
1	A	124	TYR
1	A	126	ASN
1	A	137	GLU
1	A	145	GLU
1	A	147	GLN
1	A	150	ASP
1	A	163	LYS
1	A	169	THR
1	A	173	PHE
1	A	176	LEU
1	A	177	PHE
1	A	184	SER
1	A	196	TRP
1	A	197	TYR
1	A	199	LYS
1	A	207	ILE
1	A	217	ARG
1	A	227	SER
1	A	231	MET

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Mol	Chain	Res	Type
1	A	233	LEU
1	A	249	GLN
1	A	271	ASN
1	A	276	THR
1	A	296	GLN
1	A	297	ARG
1	A	303	VAL
1	A	321	CYS
1	A	324	MET
1	A	328	ASP
1	A	330	ASP
1	A	336	THR
1	A	353	ILE
1	A	356	ARG
1	A	368	ILE
1	A	385	GLU
1	A	387	LEU
1	A	406	CYS
1	A	416	MET
1	A	423	ILE
1	A	424	ARG
1	A	427	VAL
1	A	458	GLU
1	A	461	ASN
1	A	466	VAL
1	A	467	THR
1	A	468	GLU
1	A	470	ASP
1	A	475	GLU
1	A	480	ASP
1	A	486	ILE
1	A	489	THR
1	B	16	VAL
1	B	24	SER
1	B	38	SER
1	B	43	GLU
1	B	55	ILE
1	B	65	VAL
1	B	98	VAL
1	B	101	VAL
1	B	105	THR
1	B	119	ILE

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Mol	Chain	Res	Type
1	B	123	ASP
1	B	124	TYR
1	B	126	ASN
1	B	137	GLU
1	B	145	GLU
1	B	147	GLN
1	B	169	THR
1	B	173	PHE
1	B	176	LEU
1	B	177	PHE
1	B	184	SER
1	B	197	TYR
1	B	199	LYS
1	B	207	ILE
1	B	227	SER
1	B	231	MET
1	B	233	LEU
1	B	245	THR
1	B	249	GLN
1	B	271	ASN
1	B	276	THR
1	B	296	GLN
1	B	297	ARG
1	B	303	VAL
1	B	321	CYS
1	B	323	CYS
1	B	324	MET
1	B	328	ASP
1	B	330	ASP
1	B	336	THR
1	B	353	ILE
1	B	356	ARG
1	B	385	GLU
1	B	387	LEU
1	B	416	MET
1	B	423	ILE
1	B	424	ARG
1	B	427	VAL
1	B	435	THR
1	B	458	GLU
1	B	461	ASN
1	B	466	VAL

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Mol	Chain	Res	Type
1	B	467	THR
1	B	468	GLU
1	B	470	ASP
1	B	475	GLU
1	B	486	ILE
1	B	489	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	99	GLN
1	A	133	ASN
1	A	147	GLN
1	A	148	HIS
1	A	187	HIS
1	A	215	GLN
1	A	237	GLN
1	A	241	ASN
1	A	263	HIS
1	A	282	HIS
1	A	296	GLN
1	A	365	HIS
1	A	396	ASN
1	A	401	GLN
1	A	494	ASN
1	B	99	GLN
1	B	133	ASN
1	B	147	GLN
1	B	148	HIS
1	B	212	ASN
1	B	215	GLN
1	B	237	GLN
1	B	241	ASN
1	B	263	HIS
1	B	282	HIS
1	B	296	GLN
1	B	365	HIS
1	B	401	GLN
1	B	494	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	FAD	A	600	1,3	51,58,58	1.36	9 (17%)	60,89,89	2.18	18 (30%)
3	MLG	A	601	2	16,17,17	2.79	4 (25%)	20,21,21	7.25	8 (40%)
2	FAD	B	600	1,3	51,58,58	1.61	7 (13%)	60,89,89	2.22	21 (35%)
3	MLG	B	601	2	16,17,17	2.49	2 (12%)	20,21,21	7.52	9 (45%)

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
2	FAD	A	600	1,3	-	6/30/50/50	0/6/6/6
3	MLG	A	601	2	1/1/1/1	5/9/10/10	0/1/1/1
3	MLG	B	601	2	1/1/1/1	4/9/10/10	0/1/1/1
2	FAD	B	600	1,3	-	5/30/50/50	0/6/6/6

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	MLG	C14-C15	-7.88	1.36	1.47
3	B	601	MLG	C14-C15	-6.96	1.38	1.47
3	B	601	MLG	C15-C16	6.35	1.37	1.18
3	A	601	MLG	C15-C16	6.20	1.36	1.18
2	B	600	FAD	C2A-N3A	5.33	1.40	1.32
2	B	600	FAD	C10-N1	3.96	1.38	1.33
3	A	601	MLG	C04-CL08	-3.69	1.66	1.74
2	B	600	FAD	C4X-N5	3.63	1.38	1.33
2	A	600	FAD	C10-N1	3.43	1.37	1.33
2	B	600	FAD	C4-N3	3.30	1.38	1.33
2	A	600	FAD	C2A-N3A	3.17	1.37	1.32
2	A	600	FAD	C2B-C1B	-2.92	1.49	1.53
2	B	600	FAD	C2B-C1B	-2.84	1.49	1.53
2	A	600	FAD	C4X-N5	2.74	1.37	1.33
2	B	600	FAD	C2A-N1A	2.67	1.38	1.33
2	A	600	FAD	C1'-N10	2.63	1.50	1.48
2	B	600	FAD	C9A-C5X	-2.57	1.37	1.42
2	A	600	FAD	C4-N3	2.54	1.37	1.33
2	A	600	FAD	C2A-N1A	2.26	1.38	1.33
2	A	600	FAD	O2'-C2'	-2.21	1.38	1.43
3	A	601	MLG	C02-CL07	-2.20	1.68	1.73
2	A	600	FAD	C9A-C5X	-2.20	1.38	1.42

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	MLG	C14-C15-C16	-31.22	125.30	177.67
3	B	601	MLG	C14-C15-C16	-31.13	125.45	177.67
3	B	601	MLG	C01-C02-CL07	-6.87	111.36	119.43
2	A	600	FAD	C1'-N10-C10	6.35	124.09	118.41
2	B	600	FAD	C9A-C5X-N5	-5.69	113.46	122.36
2	A	600	FAD	N3A-C2A-N1A	-5.57	119.97	128.68
2	A	600	FAD	C4-N3-C2	5.40	119.70	115.14
2	B	600	FAD	P-O3P-PA	-5.23	114.88	132.83
2	B	600	FAD	C4-N3-C2	5.22	119.55	115.14
2	B	600	FAD	C4X-N5-C5X	5.20	121.97	116.77
2	B	600	FAD	C1'-N10-C9A	5.17	122.36	118.29
2	A	600	FAD	P-O3P-PA	-4.86	116.14	132.83
2	A	600	FAD	C9A-C5X-N5	-4.84	114.80	122.36
3	B	601	MLG	C03-C04-CL08	4.57	124.86	119.15
3	B	601	MLG	C14-N13-C12	4.42	123.94	113.05
3	B	601	MLG	C03-C02-CL07	4.24	125.33	118.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	MLG	C14-N13-C12	4.12	123.18	113.05
3	B	601	MLG	C11-C12-N13	-4.03	101.88	113.79
2	B	600	FAD	C10-C4X-N5	-3.85	118.59	121.26
2	A	600	FAD	C9A-N10-C10	-3.74	117.01	121.91
2	B	600	FAD	C5A-C6A-N6A	-3.50	115.03	120.35
3	A	601	MLG	O09-C01-C02	3.40	120.60	116.40
2	A	600	FAD	O5'-C5'-C4'	-3.32	100.49	109.36
3	B	601	MLG	C15-C14-N13	3.30	120.73	113.45
2	A	600	FAD	C4X-N5-C5X	3.27	120.04	116.77
2	B	600	FAD	N6A-C6A-N1A	-3.23	111.87	118.57
2	A	600	FAD	O3'-C3'-C2'	-3.10	101.32	108.81
2	A	600	FAD	C6-C5X-N5	-3.03	115.71	119.05
2	B	600	FAD	C6-C5X-N5	-3.01	115.73	119.05
3	A	601	MLG	C03-C04-CL08	-3.01	115.39	119.15
2	A	600	FAD	C1B-N9A-C4A	-2.99	121.38	126.64
2	A	600	FAD	C4X-C4-N3	-2.95	119.39	123.43
2	B	600	FAD	O4'-C4'-C5'	-2.95	103.29	109.92
2	B	600	FAD	C4A-C5A-N7A	-2.92	106.36	109.40
3	B	601	MLG	C05-C04-CL08	-2.85	114.90	119.35
2	B	600	FAD	N3A-C2A-N1A	-2.83	124.26	128.68
2	B	600	FAD	O3'-C3'-C4'	-2.70	102.28	108.81
2	B	600	FAD	C4-C4X-N5	2.56	121.53	118.60
3	B	601	MLG	C06-C05-C04	2.56	121.94	119.24
2	A	600	FAD	C2B-C3B-C4B	2.48	107.46	102.64
2	B	600	FAD	O2'-C2'-C1'	-2.47	103.64	109.59
2	B	600	FAD	C4X-C4-N3	-2.41	120.14	123.43
2	B	600	FAD	O5'-C5'-C4'	-2.39	102.97	109.36
2	A	600	FAD	O3B-C3B-C4B	-2.35	104.26	111.05
3	A	601	MLG	C15-C14-N13	2.33	118.59	113.45
2	B	600	FAD	O2B-C2B-C1B	-2.23	102.61	110.85
3	A	601	MLG	C02-C03-C04	-2.21	116.24	118.71
2	B	600	FAD	C1B-N9A-C4A	-2.20	122.78	126.64
2	A	600	FAD	C4-C4X-C10	2.19	121.40	119.95
2	B	600	FAD	C9A-N10-C10	-2.19	119.04	121.91
2	A	600	FAD	C4A-C5A-N7A	-2.17	107.14	109.40
2	B	600	FAD	C4X-C10-N10	-2.16	118.08	120.30
2	A	600	FAD	C4X-C10-N10	-2.13	118.12	120.30
2	A	600	FAD	O2B-C2B-C1B	-2.09	103.14	110.85
3	A	601	MLG	C03-C02-CL07	-2.08	115.14	118.49
3	A	601	MLG	C01-C02-CL07	2.08	121.86	119.43

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	601	MLG	N13
3	B	601	MLG	N13

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C2'-C1'-N10-C10
2	A	600	FAD	O3'-C3'-C4'-O4'
2	A	600	FAD	O3'-C3'-C4'-C5'
3	A	601	MLG	C15-C14-N13-C17
3	B	601	MLG	C10-C11-C12-N13
3	B	601	MLG	C15-C14-N13-C17
3	A	601	MLG	O09-C10-C11-C12
2	A	600	FAD	C2'-C3'-C4'-O4'
2	A	600	FAD	C2'-C3'-C4'-C5'
2	B	600	FAD	C3B-C4B-C5B-O5B
3	A	601	MLG	C11-C12-N13-C17
3	B	601	MLG	C11-C12-N13-C17
2	B	600	FAD	O4B-C4B-C5B-O5B
3	A	601	MLG	C11-C10-O09-C01
2	B	600	FAD	C5B-O5B-PA-O3P
3	A	601	MLG	C15-C14-N13-C12
3	B	601	MLG	C15-C14-N13-C12
2	B	600	FAD	C5B-O5B-PA-O2A
2	B	600	FAD	O3'-C3'-C4'-C5'
2	A	600	FAD	O4B-C4B-C5B-O5B

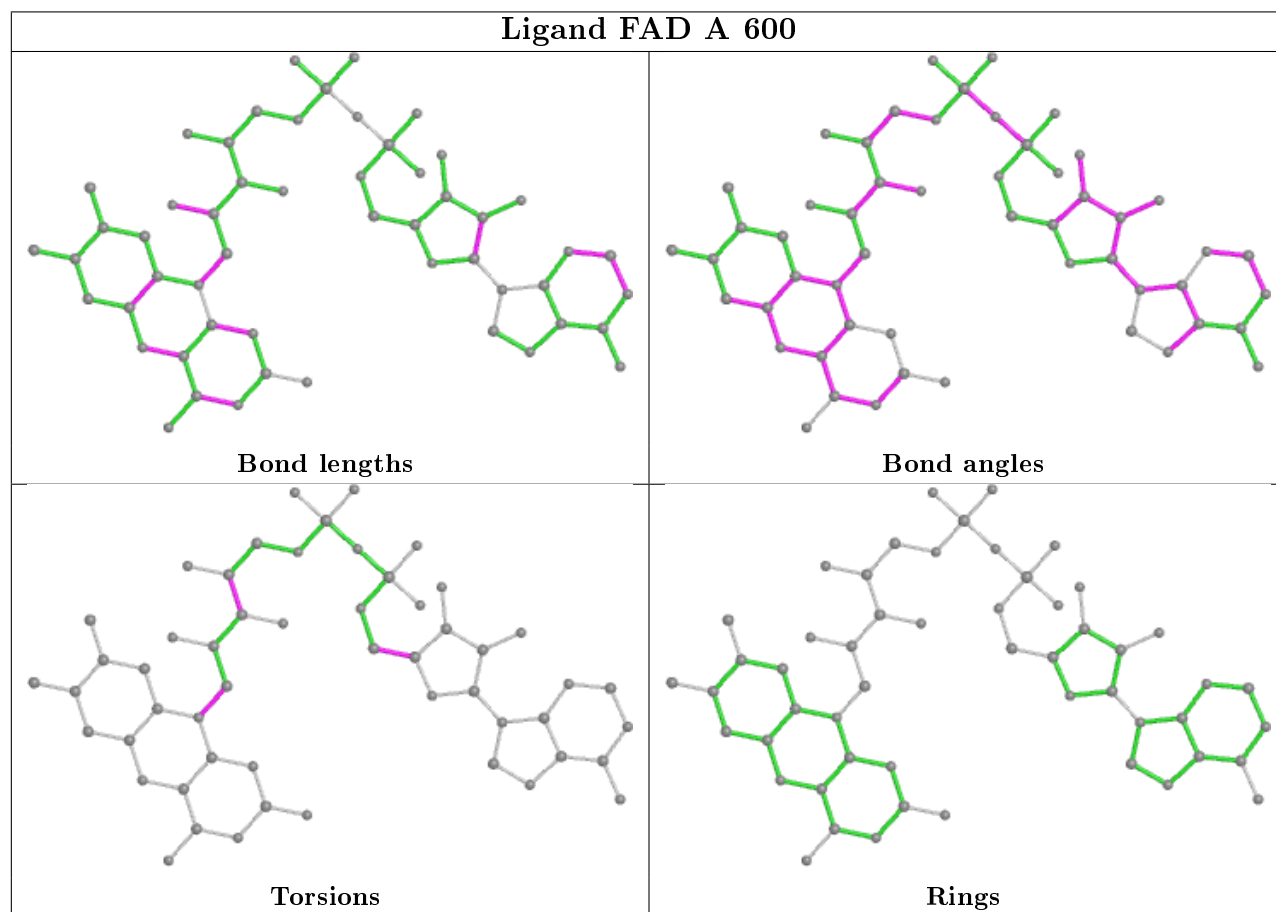
There are no ring outliers.

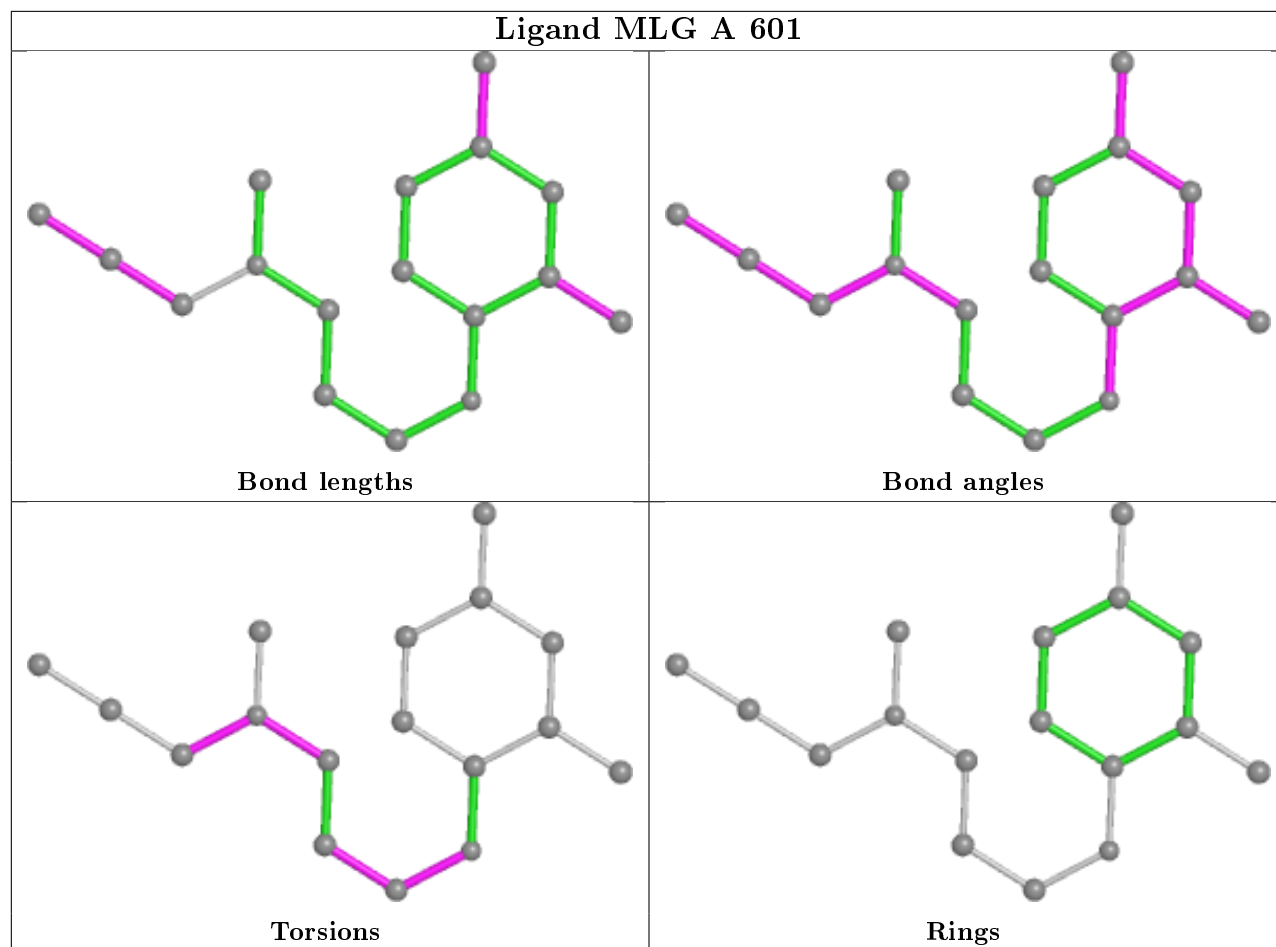
3 monomers are involved in 12 short contacts:

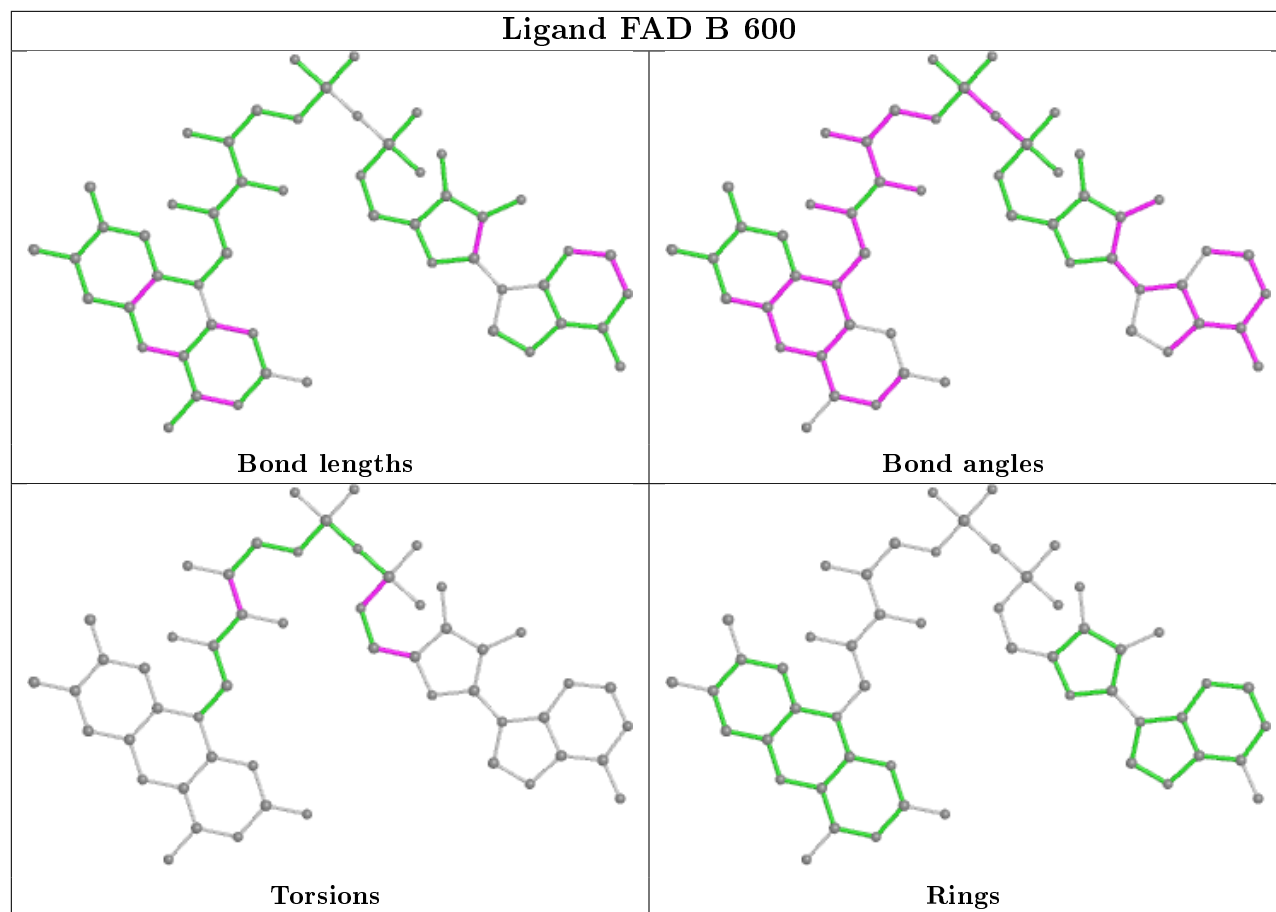
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	601	MLG	6	0
2	B	600	FAD	2	0
3	B	601	MLG	4	0

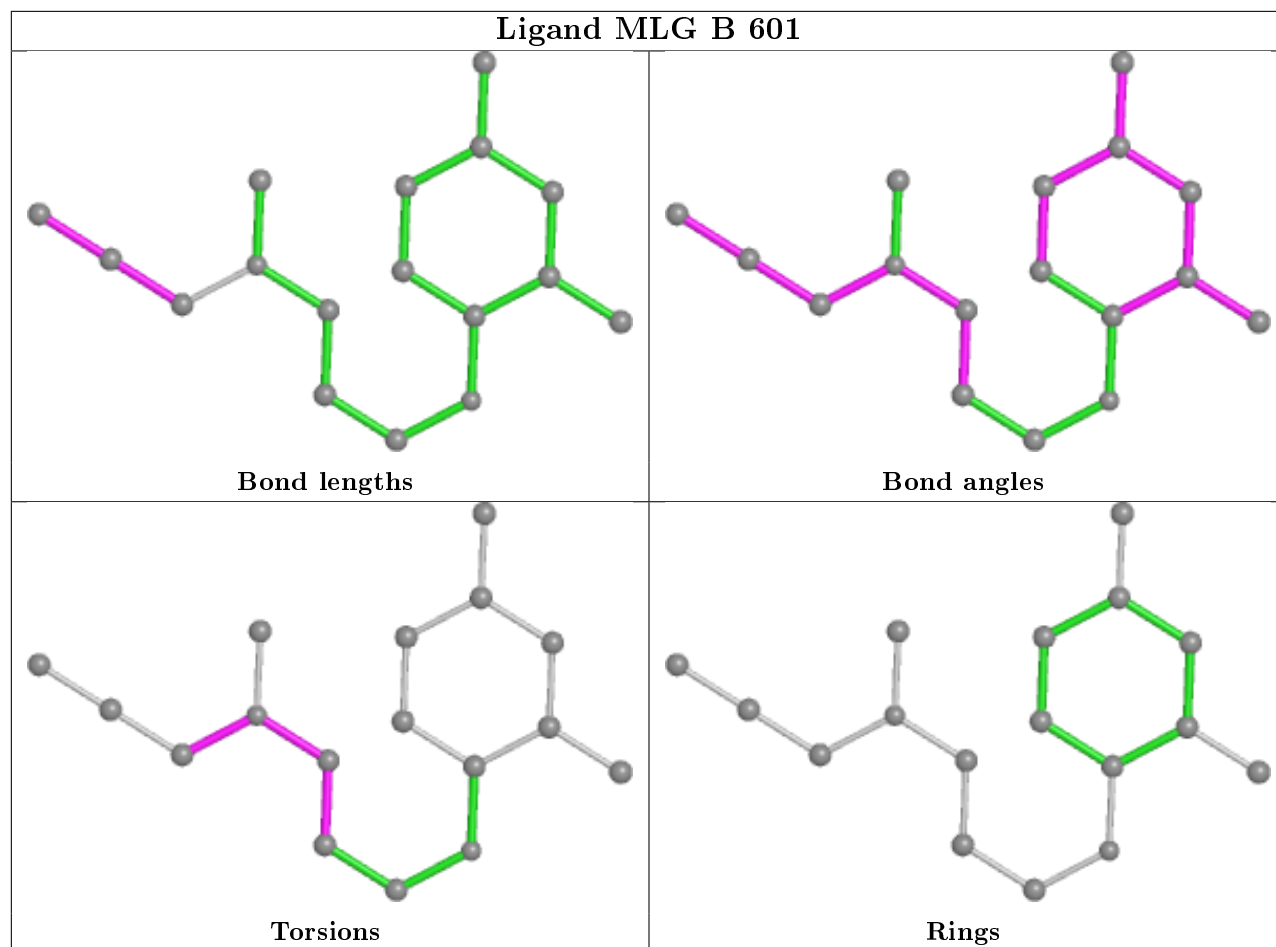
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	490/527 (92%)	0.09	17 (3%)	44 27	36, 38, 39, 41	0
1	B	490/527 (92%)	0.27	25 (5%)	28 15	36, 38, 39, 41	0
All	All	980/1054 (92%)	0.18	42 (4%)	35 21	36, 38, 39, 41	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	116	TRP	5.7
1	B	117	ASN	4.9
1	B	16	VAL	3.5
1	B	92	ASN	3.2
1	B	120	ALA	3.1
1	A	13	MET	3.1
1	A	312	GLU	3.1
1	B	383	SER	3.0
1	A	502	LEU	3.0
1	B	312	GLU	2.9
1	A	255	ILE	2.7
1	A	165	CYS	2.7
1	B	14	PHE	2.7
1	A	319	ASP	2.6
1	B	319	ASP	2.6
1	B	253	ASN	2.6
1	B	167	THR	2.6
1	B	308	MET	2.5
1	B	118	PRO	2.5
1	B	170	ALA	2.5
1	B	266	CYS	2.5
1	B	320	TYR	2.5
1	A	110	GLY	2.4
1	A	345	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	165	CYS	2.4
1	A	167	THR	2.4
1	B	502	LEU	2.4
1	B	13	MET	2.3
1	B	124	TYR	2.3
1	B	58	GLU	2.3
1	A	315	TRP	2.3
1	A	505	ILE	2.3
1	B	505	ILE	2.2
1	A	253	ASN	2.2
1	A	498	VAL	2.2
1	A	494	ASN	2.1
1	B	247	VAL	2.1
1	A	499	SER	2.1
1	A	506	GLY	2.0
1	A	296	GLN	2.0
1	B	59	HIS	2.0
1	B	343	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

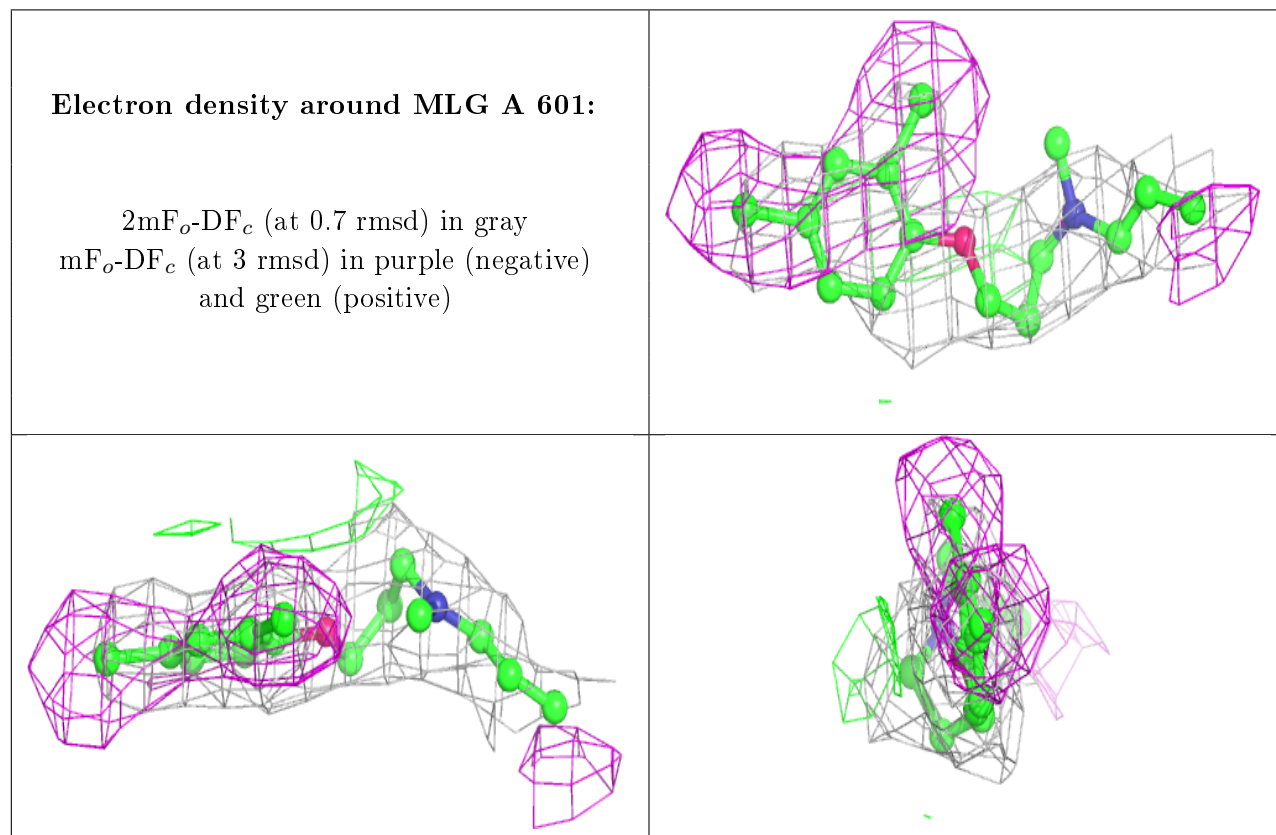
There are no carbohydrates in this entry.

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.

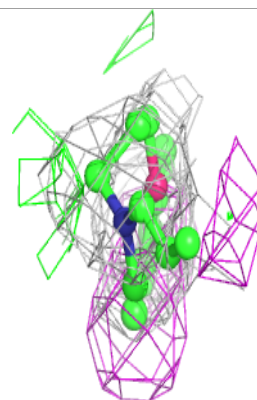
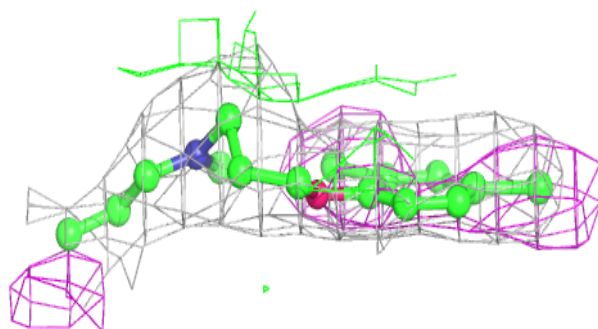
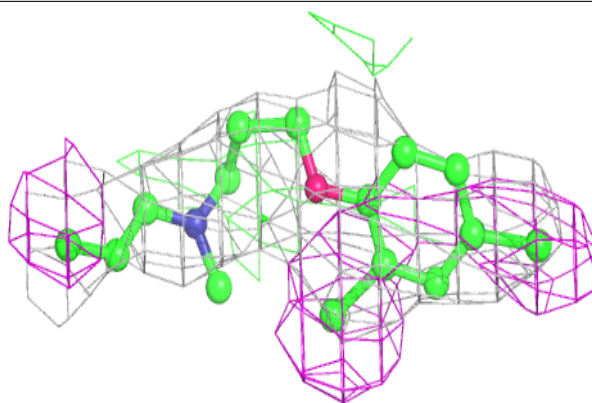
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MLG	A	601	17/17	0.82	0.36	44,54,62,65	0
3	MLG	B	601	17/17	0.83	0.40	46,56,63,64	0
2	FAD	B	600	53/53	0.96	0.17	25,32,40,43	0
2	FAD	A	600	53/53	0.97	0.14	26,32,37,43	0

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.

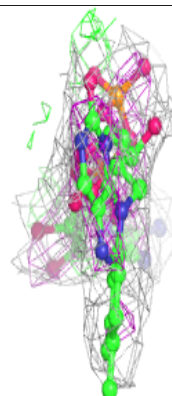
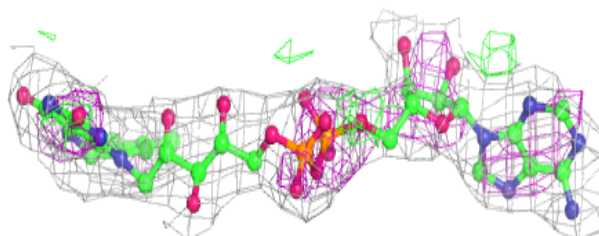
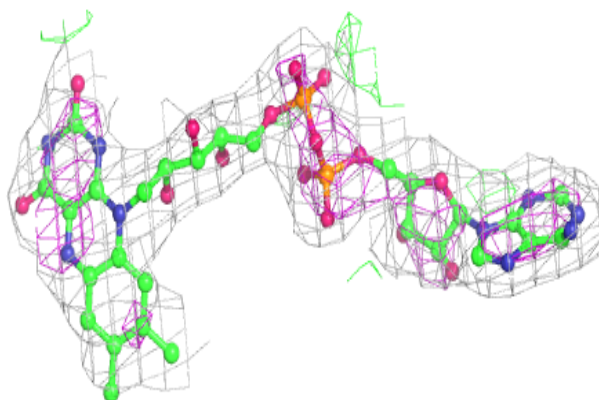


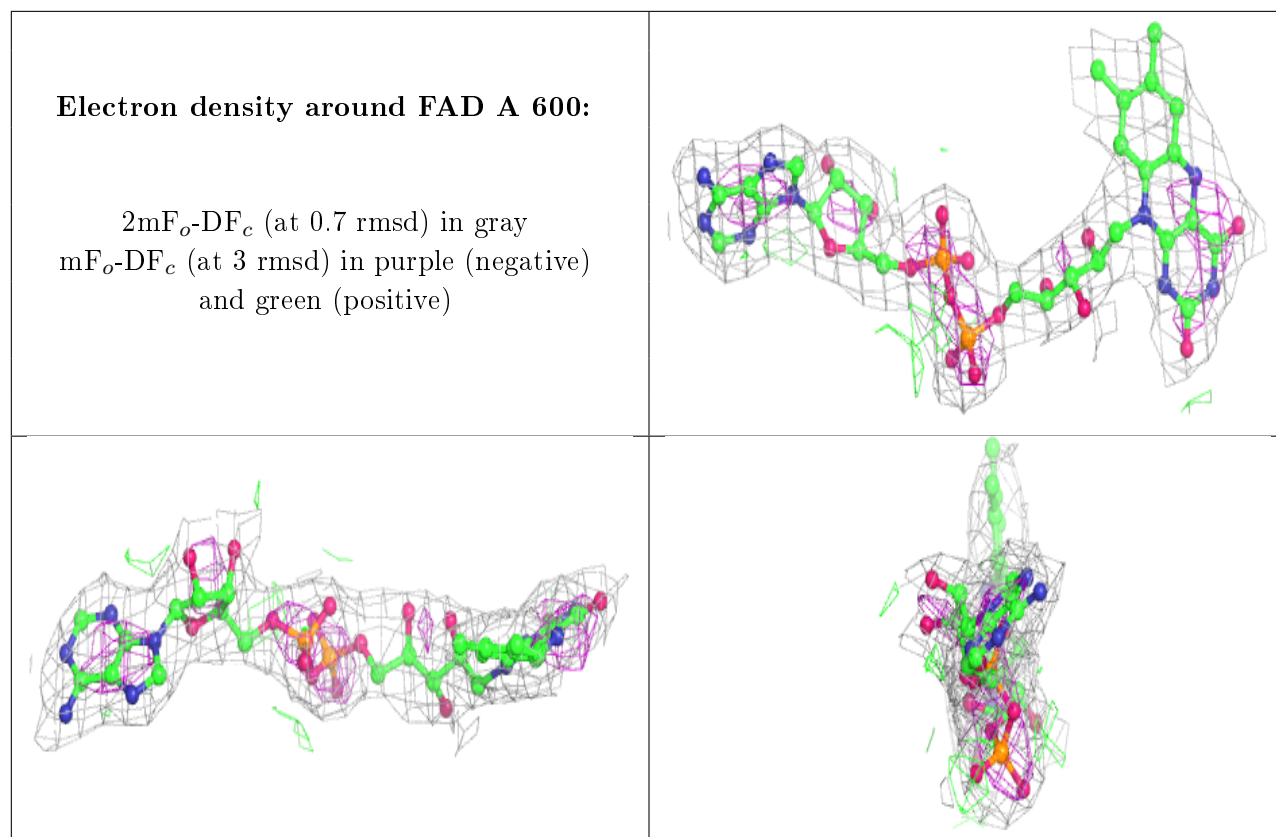
Electron density around MLG B 601:

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

**Electron density around FAD B 600:**

$2mF_o-DF_c$ (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.