



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:24 PM UTC

PDB ID : 2BVH / pdb_00002bvh
Title : Crystal structure of 6-hydroxy-D-nicotine oxidase from *Arthrobacter nicotinovorans*. Crystal Form 2 (P21)
Authors : Koetter, J.W.A.; Schulz, G.E.
Deposited on : 2005-06-28
Resolution : 2.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

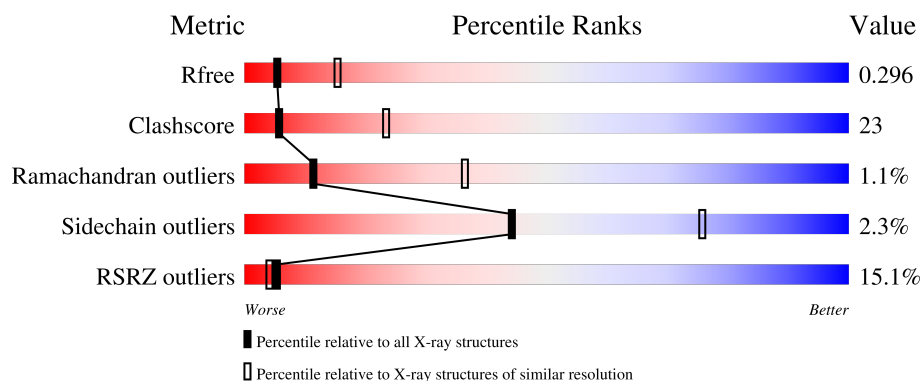
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	459	12% 61% 35% ..
1	B	459	13% 61% 35% ..
1	C	459	18% 61% 35% ..
1	D	459	16% 60% 36% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13808 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 6-HYDROXY-D-NICOTINE OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	0	0
			3399	2133	596	656	14			
1	B	453	Total	C	N	O	S	0	0	0
			3399	2133	596	656	14			
1	C	453	Total	C	N	O	S	0	0	0
			3399	2133	596	656	14			
1	D	453	Total	C	N	O	S	0	0	0
			3399	2133	596	656	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	433	SER	CYS	engineered mutation	UNP Q8GAG1
B	433	SER	CYS	engineered mutation	UNP Q8GAG1
C	433	SER	CYS	engineered mutation	UNP Q8GAG1
D	433	SER	CYS	engineered mutation	UNP Q8GAG1

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

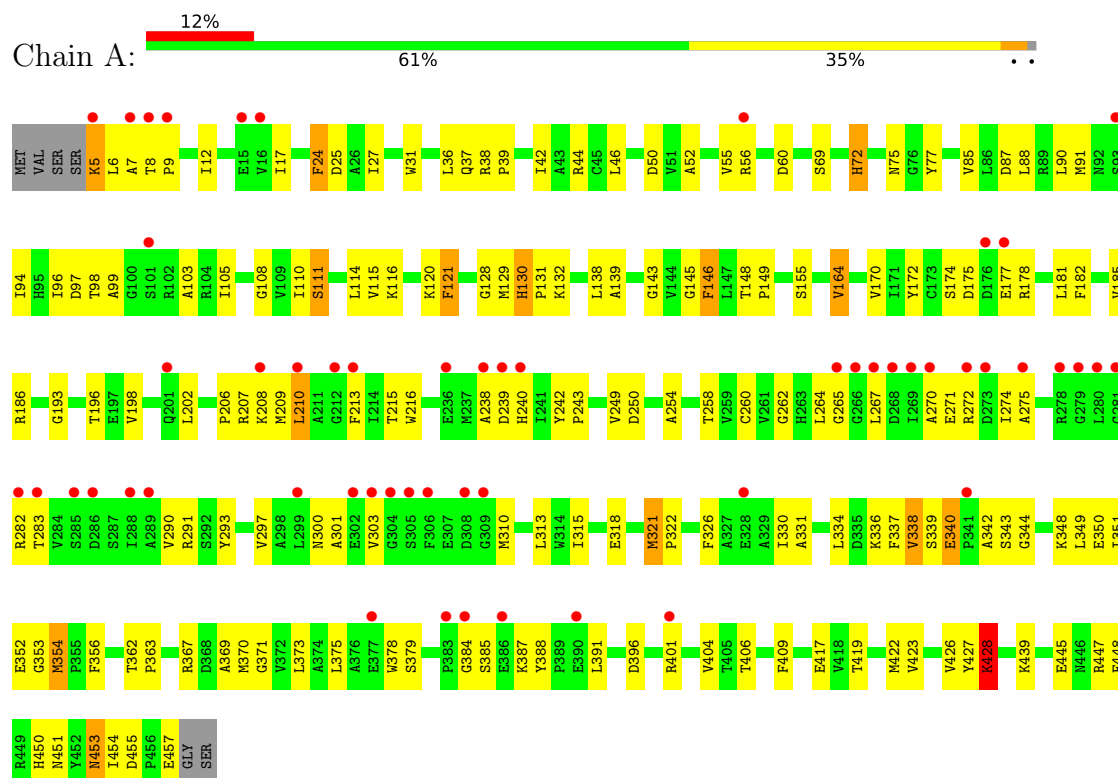


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
2	D	1	Total 53	C 27	N 9	O 15	P 2	0	0

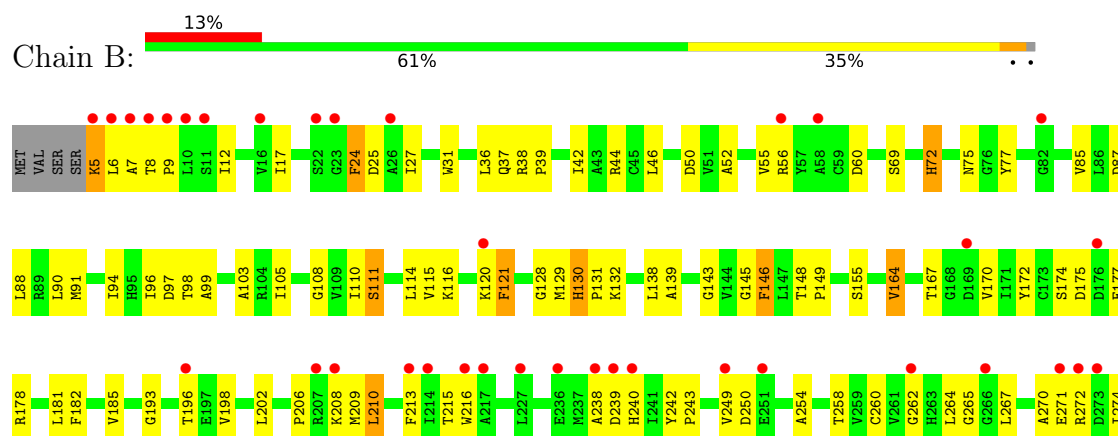
3 Residue-property plots

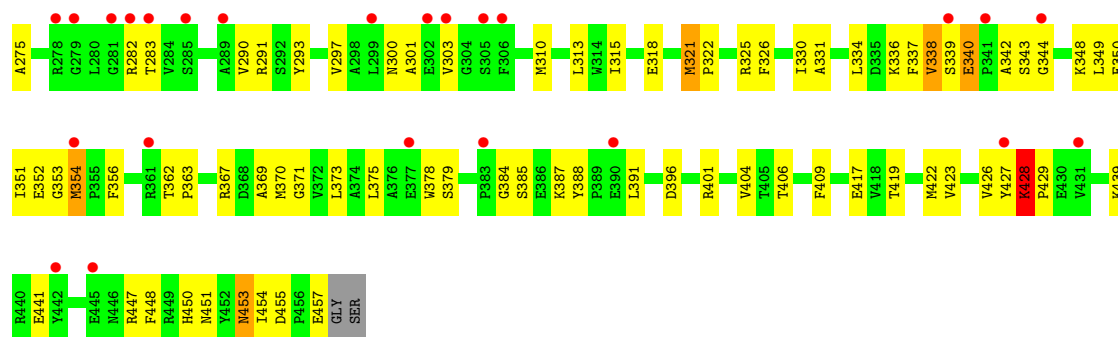
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 6-HYDROXY-D-NICOTINE OXIDASE

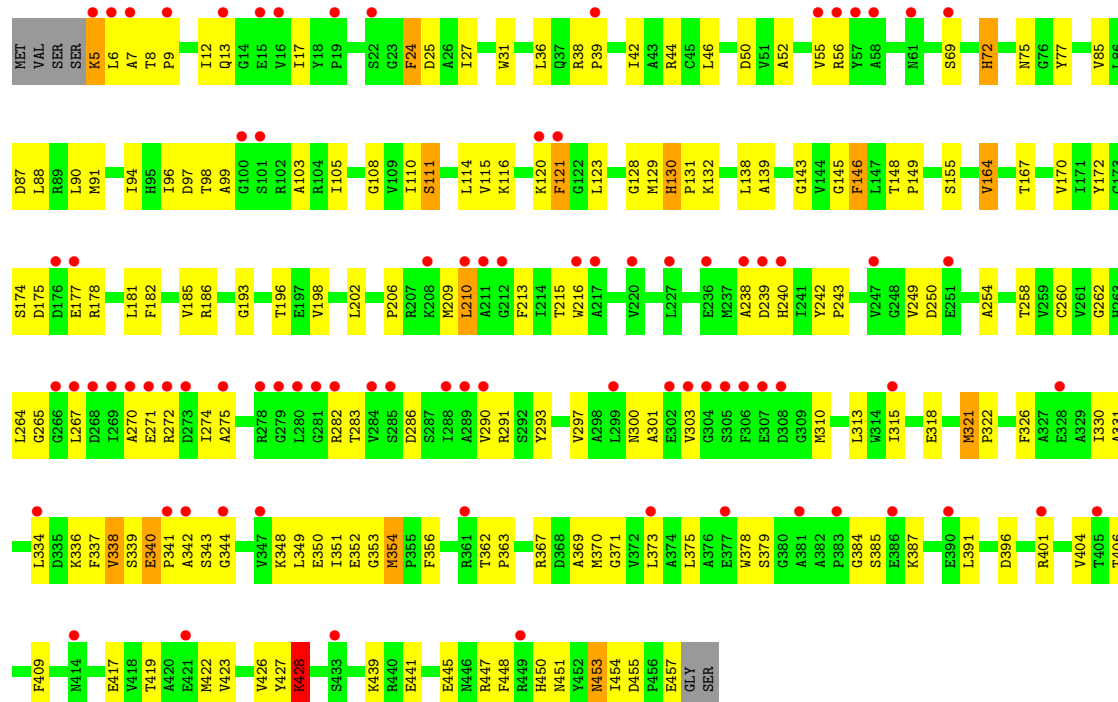


• Molecule 1: 6-HYDROXY-D-NICOTINE OXIDASE

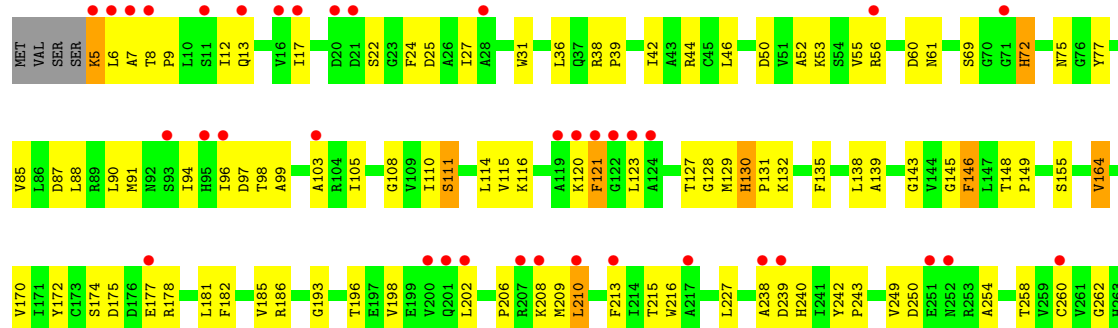


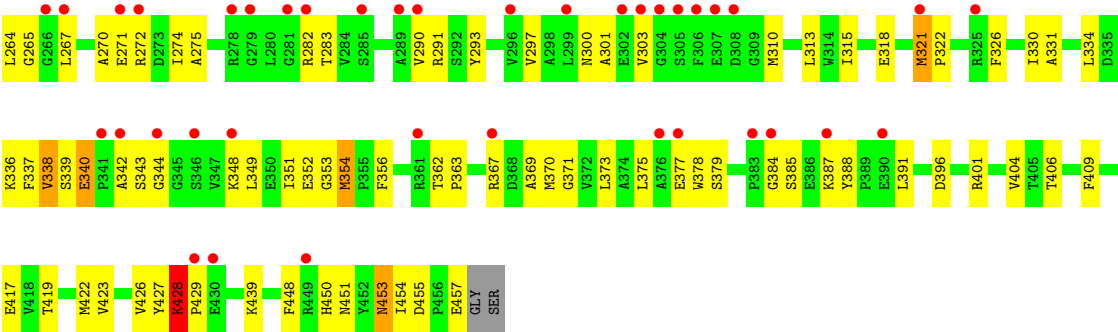


● Molecule 1: 6-HYDROXY-D-NICOTINE OXIDASE



● Molecule 1: 6-HYDROXY-D-NICOTINE OXIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.32Å 90.94Å 104.44Å 90.00° 100.31° 90.00°	Depositor
Resolution (Å)	44.30 – 2.90 44.30 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (44.30-2.90) 99.6 (44.30-2.90)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.16 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.274 , 0.297 0.274 , 0.296	Depositor DCC
R_{free} test set	2134 reflections (4.11%)	wwPDB-VP
Wilson B-factor (Å ²)	42.2	Xtriage
Anisotropy	0.385	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 40.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	13808	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.05% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.54	0/3465	1.06	19/4706 (0.4%)
1	B	0.54	0/3465	1.06	19/4706 (0.4%)
1	C	0.54	0/3465	1.06	19/4706 (0.4%)
1	D	0.54	0/3465	1.06	19/4706 (0.4%)
All	All	0.54	0/13860	1.06	76/18824 (0.4%)

There are no bond length outliers.

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	130	HIS	CA-C-N	7.24	126.87	119.56
1	C	130	HIS	C-N-CA	7.24	126.87	119.56
1	A	130	HIS	CA-C-N	7.24	126.87	119.56
1	A	130	HIS	C-N-CA	7.24	126.87	119.56
1	B	130	HIS	CA-C-N	7.24	126.87	119.56
1	B	130	HIS	C-N-CA	7.24	126.87	119.56
1	D	130	HIS	CA-C-N	7.22	126.86	119.56
1	D	130	HIS	C-N-CA	7.22	126.86	119.56
1	D	352	GLU	N-CA-C	6.87	119.61	109.24
1	B	352	GLU	N-CA-C	6.85	119.58	109.24
1	A	352	GLU	N-CA-C	6.85	119.58	109.24
1	C	352	GLU	N-CA-C	6.84	119.56	109.24
1	D	146	PHE	N-CA-C	6.66	118.54	111.28
1	B	146	PHE	N-CA-C	6.64	118.52	111.28
1	A	146	PHE	N-CA-C	6.64	118.52	111.28
1	B	8	THR	CA-C-N	6.62	128.12	119.84
1	B	8	THR	C-N-CA	6.62	128.12	119.84
1	D	8	THR	CA-C-N	6.62	128.12	119.84
1	D	8	THR	C-N-CA	6.62	128.12	119.84
1	C	146	PHE	N-CA-C	6.61	118.49	111.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	THR	CA-C-N	6.61	128.10	119.84
1	A	8	THR	C-N-CA	6.61	128.10	119.84
1	C	8	THR	CA-C-N	6.61	128.10	119.84
1	C	8	THR	C-N-CA	6.61	128.10	119.84
1	B	453	ASN	N-CA-C	6.21	119.23	110.23
1	A	164	VAL	N-CA-C	-6.20	98.82	107.80
1	B	164	VAL	N-CA-C	-6.19	98.83	107.80
1	D	164	VAL	N-CA-C	-6.18	98.83	107.80
1	A	453	ASN	N-CA-C	6.18	119.19	110.23
1	C	164	VAL	N-CA-C	-6.18	98.84	107.80
1	C	453	ASN	N-CA-C	6.17	119.18	110.23
1	D	453	ASN	N-CA-C	6.15	119.15	110.23
1	C	210	LEU	N-CA-C	-6.06	99.32	108.96
1	D	428	LYS	CA-C-N	6.05	127.40	119.84
1	D	428	LYS	C-N-CA	6.05	127.40	119.84
1	B	428	LYS	CA-C-N	6.04	127.39	119.84
1	B	428	LYS	C-N-CA	6.04	127.39	119.84
1	C	428	LYS	CA-C-N	6.03	127.38	119.84
1	C	428	LYS	C-N-CA	6.03	127.38	119.84
1	A	428	LYS	CA-C-N	6.03	127.38	119.84
1	A	428	LYS	C-N-CA	6.03	127.38	119.84
1	D	75	ASN	N-CA-C	-5.89	106.09	113.28
1	A	75	ASN	N-CA-C	-5.87	106.12	113.28
1	C	75	ASN	N-CA-C	-5.87	106.12	113.28
1	B	75	ASN	N-CA-C	-5.86	106.14	113.28
1	D	210	LEU	N-CA-C	-5.63	99.34	108.41
1	A	210	LEU	N-CA-C	-5.63	99.35	108.41
1	B	210	LEU	N-CA-C	-5.63	99.35	108.41
1	D	56	ARG	N-CA-C	-5.51	105.19	111.14
1	B	56	ARG	N-CA-C	-5.49	105.21	111.14
1	A	56	ARG	N-CA-C	-5.48	105.22	111.14
1	C	56	ARG	N-CA-C	-5.47	105.23	111.14
1	C	262	GLY	N-CA-C	-5.44	100.29	113.18
1	A	262	GLY	N-CA-C	-5.43	100.31	113.18
1	B	262	GLY	N-CA-C	-5.43	100.32	113.18
1	D	262	GLY	N-CA-C	-5.42	100.32	113.18
1	D	340	GLU	CA-C-N	5.36	125.00	119.05
1	D	340	GLU	C-N-CA	5.36	125.00	119.05
1	B	265	GLY	N-CA-C	5.36	120.71	112.51
1	C	340	GLU	CA-C-N	5.35	124.99	119.05
1	C	340	GLU	C-N-CA	5.35	124.99	119.05
1	D	265	GLY	N-CA-C	5.35	120.70	112.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	265	GLY	N-CA-C	5.34	120.69	112.51
1	A	265	GLY	N-CA-C	5.34	120.68	112.51
1	A	340	GLU	CA-C-N	5.33	124.97	119.05
1	A	340	GLU	C-N-CA	5.33	124.97	119.05
1	B	242	TYR	N-CA-C	-5.30	98.11	109.81
1	C	242	TYR	N-CA-C	-5.29	98.12	109.81
1	B	340	GLU	CA-C-N	5.29	124.92	119.05
1	B	340	GLU	C-N-CA	5.29	124.92	119.05
1	A	242	TYR	N-CA-C	-5.28	98.13	109.81
1	D	242	TYR	N-CA-C	-5.27	98.17	109.81
1	C	31	TRP	N-CA-C	5.23	119.99	111.37
1	A	31	TRP	N-CA-C	5.21	119.97	111.37
1	D	31	TRP	N-CA-C	5.21	119.97	111.37
1	B	31	TRP	N-CA-C	5.21	119.96	111.37

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3399	0	3344	176	2
1	B	3399	0	3344	160	0
1	C	3399	0	3344	159	2
1	D	3399	0	3344	172	1
2	A	53	0	30	7	0
2	B	53	0	30	6	0
2	C	53	0	30	7	0
2	D	53	0	30	7	0
All	All	13808	0	13496	636	3

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 23.

All (636) 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:C:441:GLU:HG3	1:D:7:ALA:HB1	1.31	1.09
1:C:441:GLU:HG3	1:D:7:ALA:CB	1.84	1.07
1:A:7:ALA:CB	1:B:441:GLU:HA	1.98	0.93
1:A:282:ARG:HE	1:A:283:THR:N	1.67	0.92
1:C:282:ARG:HE	1:C:283:THR:N	1.67	0.91
1:A:120:LYS:CA	1:D:53:LYS:HE2	2.01	0.91
1:D:282:ARG:HE	1:D:283:THR:N	1.67	0.91
1:B:282:ARG:HE	1:B:283:THR:N	1.67	0.90
1:A:120:LYS:HB3	1:D:53:LYS:HE2	1.59	0.83
1:D:310:MET:HE1	1:D:379:SER:HB2	1.62	0.81
1:A:120:LYS:CB	1:D:53:LYS:HE2	2.10	0.81
1:B:310:MET:HE1	1:B:379:SER:HB2	1.62	0.81
1:A:310:MET:HE1	1:A:379:SER:HB2	1.62	0.81
1:C:310:MET:HE1	1:C:379:SER:HB2	1.62	0.81
1:A:207:ARG:NH1	1:D:13:GLN:HG2	1.97	0.79
1:C:167:THR:HG22	1:D:60:ASP:HB3	1.65	0.79
1:A:120:LYS:HB3	1:D:53:LYS:CE	2.14	0.78
1:D:210:LEU:HD12	1:D:270:ALA:HB1	1.67	0.76
1:B:210:LEU:HD12	1:B:270:ALA:HB1	1.67	0.76
1:C:210:LEU:HD12	1:C:270:ALA:HB1	1.67	0.76
1:B:282:ARG:HA	1:B:282:ARG:NE	2.01	0.75
1:C:282:ARG:HA	1:C:282:ARG:NE	2.01	0.75
1:A:282:ARG:HA	1:A:282:ARG:NE	2.01	0.75
1:A:7:ALA:HB1	1:B:441:GLU:HA	1.69	0.74
1:C:441:GLU:HG3	1:D:7:ALA:HB2	1.70	0.74
1:A:427:TYR:O	1:A:428:LYS:HB2	1.88	0.74
1:D:282:ARG:NE	1:D:282:ARG:HA	2.01	0.74
1:A:210:LEU:HD12	1:A:270:ALA:HB1	1.67	0.73
1:B:271:GLU:HA	1:B:271:GLU:OE1	1.88	0.73
1:A:373:LEU:HG	1:A:375:LEU:CD1	2.18	0.73
1:B:373:LEU:HG	1:B:375:LEU:CD1	2.18	0.73
1:C:373:LEU:HG	1:C:375:LEU:CD1	2.18	0.73
1:C:427:TYR:O	1:C:428:LYS:HB2	1.88	0.73
1:D:427:TYR:O	1:D:428:LYS:HB2	1.88	0.72
1:C:282:ARG:HE	1:C:282:ARG:C	1.97	0.72
1:B:427:TYR:O	1:B:428:LYS:HB2	1.88	0.72
1:C:98:THR:HG23	1:C:121:PHE:HD1	1.55	0.72
1:D:373:LEU:HG	1:D:375:LEU:CD1	2.19	0.72
1:A:98:THR:HG23	1:A:121:PHE:HD1	1.55	0.72
1:C:271:GLU:OE1	1:C:271:GLU:HA	1.88	0.72
1:A:282:ARG:HE	1:A:282:ARG:C	1.97	0.72
1:A:271:GLU:OE1	1:A:271:GLU:HA	1.88	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:ASP:OD2	1:C:254:ALA:HB3	1.90	0.71
1:D:422:MET:O	1:D:426:VAL:HG23	1.91	0.71
1:B:98:THR:HG23	1:B:121:PHE:HD1	1.55	0.71
1:B:250:ASP:OD2	1:B:254:ALA:HB3	1.90	0.71
1:B:282:ARG:HE	1:B:282:ARG:C	1.97	0.71
1:A:422:MET:O	1:A:426:VAL:HG23	1.91	0.71
1:C:422:MET:O	1:C:426:VAL:HG23	1.91	0.71
1:D:271:GLU:OE1	1:D:271:GLU:HA	1.88	0.71
1:D:282:ARG:HE	1:D:282:ARG:C	1.97	0.71
1:D:131:PRO:CG	1:D:301:ALA:HB2	2.21	0.70
1:D:250:ASP:OD2	1:D:254:ALA:HB3	1.90	0.70
1:A:250:ASP:OD2	1:A:254:ALA:HB3	1.90	0.70
1:D:129:MET:HG3	1:D:145:GLY:HA2	1.73	0.70
1:A:129:MET:HG3	1:A:145:GLY:HA2	1.73	0.70
1:B:422:MET:O	1:B:426:VAL:HG23	1.91	0.70
1:B:129:MET:HG3	1:B:145:GLY:HA2	1.73	0.70
1:B:131:PRO:CG	1:B:301:ALA:HB2	2.21	0.70
1:A:131:PRO:CG	1:A:301:ALA:HB2	2.21	0.69
1:C:131:PRO:CG	1:C:301:ALA:HB2	2.21	0.69
1:D:98:THR:HG23	1:D:121:PHE:HD1	1.55	0.69
1:C:129:MET:HG3	1:C:145:GLY:HA2	1.74	0.69
1:D:331:ALA:HA	1:D:334:LEU:HD21	1.75	0.69
1:B:209:MET:HE3	1:B:264:LEU:HD23	1.75	0.69
1:C:209:MET:HE3	1:C:264:LEU:HD23	1.75	0.69
1:B:331:ALA:HA	1:B:334:LEU:HD21	1.75	0.69
1:A:103:ALA:HB2	1:A:202:LEU:HD11	1.76	0.68
1:A:209:MET:HE3	1:A:264:LEU:HD23	1.75	0.68
1:C:103:ALA:HB2	1:C:202:LEU:HD11	1.76	0.68
1:D:209:MET:HE3	1:D:264:LEU:HD23	1.75	0.68
1:A:120:LYS:HA	1:D:53:LYS:HE2	1.76	0.68
1:D:131:PRO:HG3	1:D:301:ALA:HB2	1.76	0.68
1:B:131:PRO:HG3	1:B:301:ALA:HB2	1.76	0.67
1:B:282:ARG:HE	1:B:282:ARG:CA	2.08	0.67
1:B:103:ALA:HB2	1:B:202:LEU:HD11	1.76	0.67
1:A:331:ALA:HA	1:A:334:LEU:HD21	1.75	0.67
1:A:131:PRO:HG3	1:A:301:ALA:HB2	1.76	0.67
1:C:331:ALA:HA	1:C:334:LEU:HD21	1.74	0.67
1:D:103:ALA:HB2	1:D:202:LEU:HD11	1.76	0.67
1:D:282:ARG:HE	1:D:283:THR:H	1.43	0.67
1:A:105:ILE:CD1	1:A:114:LEU:HD22	2.25	0.67
1:A:282:ARG:HE	1:A:282:ARG:CA	2.08	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:ILE:CD1	1:C:114:LEU:HD22	2.25	0.67
1:C:131:PRO:HG3	1:C:301:ALA:HB2	1.76	0.67
1:C:282:ARG:HE	1:C:283:THR:H	1.43	0.67
1:A:282:ARG:HH21	1:A:283:THR:H	1.43	0.66
1:C:282:ARG:HE	1:C:282:ARG:CA	2.08	0.66
1:B:282:ARG:HH21	1:B:283:THR:H	1.44	0.66
1:D:282:ARG:HE	1:D:282:ARG:CA	2.08	0.66
1:A:282:ARG:HE	1:A:283:THR:H	1.43	0.66
1:C:441:GLU:O	1:D:7:ALA:HB3	1.95	0.66
1:D:282:ARG:HH21	1:D:283:THR:H	1.44	0.66
1:B:282:ARG:HE	1:B:283:THR:H	1.43	0.66
1:C:105:ILE:HD13	1:C:114:LEU:HD22	1.78	0.66
1:D:105:ILE:CD1	1:D:114:LEU:HD22	2.25	0.66
1:D:105:ILE:HD13	1:D:114:LEU:HD22	1.78	0.65
1:C:282:ARG:HH21	1:C:283:THR:H	1.44	0.65
1:B:105:ILE:CD1	1:B:114:LEU:HD22	2.25	0.65
1:A:207:ARG:HH11	1:D:13:GLN:HG2	1.61	0.65
1:B:105:ILE:HD13	1:B:114:LEU:HD22	1.78	0.64
1:A:105:ILE:HD13	1:A:114:LEU:HD22	1.78	0.64
1:C:441:GLU:CG	1:D:7:ALA:HB1	2.19	0.64
1:D:373:LEU:HG	1:D:375:LEU:HD11	1.80	0.64
1:A:282:ARG:NE	1:A:282:ARG:CA	2.61	0.64
1:B:282:ARG:NE	1:B:282:ARG:CA	2.61	0.64
1:C:282:ARG:NE	1:C:282:ARG:CA	2.61	0.64
1:B:373:LEU:HG	1:B:375:LEU:HD11	1.80	0.63
1:A:120:LYS:CB	1:D:53:LYS:CE	2.74	0.63
1:A:373:LEU:HG	1:A:375:LEU:HD11	1.80	0.63
1:D:282:ARG:NE	1:D:282:ARG:CA	2.61	0.63
1:A:120:LYS:O	1:D:53:LYS:HE2	1.98	0.63
1:A:138:LEU:C	1:A:138:LEU:HD23	2.24	0.63
1:B:267:LEU:HA	1:B:270:ALA:HB3	1.81	0.62
1:C:138:LEU:C	1:C:138:LEU:HD23	2.24	0.62
1:C:373:LEU:HG	1:C:375:LEU:HD11	1.80	0.62
1:D:138:LEU:HD23	1:D:138:LEU:C	2.24	0.62
1:B:138:LEU:C	1:B:138:LEU:HD23	2.24	0.61
1:C:267:LEU:HA	1:C:270:ALA:HB3	1.81	0.61
1:B:310:MET:HE2	1:B:310:MET:HA	1.82	0.61
1:D:44:ARG:NH1	1:D:87:ASP:OD2	2.34	0.61
1:C:44:ARG:NH1	1:C:87:ASP:OD2	2.34	0.61
1:C:310:MET:HA	1:C:310:MET:HE2	1.82	0.61
1:D:321:MET:HE2	1:D:321:MET:HA	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ARG:NH1	1:A:87:ASP:OD2	2.34	0.61
1:A:310:MET:HA	1:A:310:MET:HE2	1.82	0.61
1:A:321:MET:HE2	1:A:321:MET:HA	1.83	0.61
1:A:351:ILE:HG22	1:A:370:MET:HE2	1.83	0.61
1:D:310:MET:HE2	1:D:310:MET:HA	1.82	0.61
1:C:351:ILE:HG22	1:C:370:MET:HE2	1.83	0.61
1:C:373:LEU:HG	1:C:375:LEU:HD12	1.83	0.61
1:D:267:LEU:HA	1:D:270:ALA:HB3	1.81	0.60
1:C:321:MET:HE2	1:C:321:MET:HA	1.83	0.60
1:D:351:ILE:HG22	1:D:370:MET:HE2	1.83	0.60
1:B:44:ARG:NH1	1:B:87:ASP:OD2	2.34	0.60
1:A:90:LEU:HD22	1:C:13:GLN:OE1	2.01	0.60
1:A:267:LEU:HA	1:A:270:ALA:HB3	1.81	0.60
1:C:441:GLU:O	1:D:7:ALA:CB	2.49	0.60
1:A:120:LYS:C	1:D:53:LYS:HE2	2.27	0.60
1:B:351:ILE:HG22	1:B:370:MET:HE2	1.83	0.60
1:A:340:GLU:HG3	1:A:343:SER:HB2	1.84	0.59
1:A:367:ARG:HG2	1:A:367:ARG:HH11	1.67	0.59
1:A:373:LEU:HG	1:A:375:LEU:HD12	1.83	0.59
1:B:373:LEU:HG	1:B:375:LEU:HD12	1.83	0.59
1:C:72:HIS:CE1	2:C:600:FAD:C7M	2.86	0.59
1:B:367:ARG:HG2	1:B:367:ARG:HH11	1.67	0.59
1:D:373:LEU:HG	1:D:375:LEU:HD12	1.83	0.59
1:C:340:GLU:HG3	1:C:343:SER:HB2	1.84	0.59
1:B:321:MET:HE2	1:B:321:MET:HA	1.83	0.59
1:B:72:HIS:CE1	2:B:600:FAD:C7M	2.86	0.59
1:A:72:HIS:CE1	2:A:600:FAD:C7M	2.86	0.59
1:A:46:LEU:HD21	1:C:13:GLN:OE1	2.03	0.59
1:D:72:HIS:CE1	2:D:600:FAD:C7M	2.86	0.58
1:A:120:LYS:HA	1:D:53:LYS:CE	2.33	0.58
1:D:367:ARG:HH11	1:D:367:ARG:HG2	1.67	0.58
1:C:121:PHE:HD2	1:C:121:PHE:N	2.02	0.58
1:B:409:PHE:CD1	1:B:422:MET:HE2	2.39	0.58
1:D:409:PHE:CD1	1:D:422:MET:HE2	2.39	0.58
1:B:120:LYS:C	1:B:121:PHE:HD2	2.12	0.58
1:C:367:ARG:HG2	1:C:367:ARG:HH11	1.67	0.58
1:C:409:PHE:CD1	1:C:422:MET:HE2	2.39	0.58
1:B:282:ARG:HE	1:B:282:ARG:HA	1.66	0.58
1:A:115:VAL:HG21	1:A:297:VAL:HG11	1.86	0.57
1:A:207:ARG:HD3	1:D:13:GLN:NE2	2.19	0.57
1:D:340:GLU:HG3	1:D:343:SER:HB2	1.84	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:PHE:HD2	1:A:121:PHE:N	2.02	0.57
1:C:342:ALA:C	1:C:344:GLY:H	2.12	0.57
1:A:342:ALA:C	1:A:344:GLY:H	2.12	0.57
1:B:115:VAL:HG21	1:B:297:VAL:HG11	1.86	0.57
1:D:120:LYS:C	1:D:121:PHE:HD2	2.12	0.57
1:A:120:LYS:C	1:A:121:PHE:HD2	2.12	0.57
1:B:340:GLU:HG3	1:B:343:SER:HB2	1.84	0.57
1:A:96:ILE:HB	1:A:121:PHE:CE1	2.39	0.57
1:B:96:ILE:HB	1:B:121:PHE:CE1	2.39	0.57
1:C:318:GLU:O	1:C:406:THR:HG23	2.05	0.57
1:B:121:PHE:N	1:B:121:PHE:CD2	2.73	0.57
1:B:272:ARG:O	1:B:275:ALA:HB3	2.05	0.57
1:D:272:ARG:O	1:D:275:ALA:HB3	2.05	0.57
1:A:409:PHE:CD1	1:A:422:MET:HE2	2.39	0.57
1:C:120:LYS:C	1:C:121:PHE:HD2	2.12	0.57
1:B:318:GLU:O	1:B:406:THR:HG23	2.05	0.57
1:D:115:VAL:HG21	1:D:297:VAL:HG11	1.87	0.57
1:A:318:GLU:O	1:A:406:THR:HG23	2.05	0.56
1:C:96:ILE:HB	1:C:121:PHE:CE1	2.39	0.56
1:C:272:ARG:O	1:C:275:ALA:HB3	2.05	0.56
1:A:60:ASP:CG	1:B:167:THR:HG22	2.30	0.56
1:C:121:PHE:N	1:C:121:PHE:CD2	2.73	0.56
1:A:121:PHE:N	1:A:121:PHE:CD2	2.73	0.56
1:D:96:ILE:HB	1:D:121:PHE:CE1	2.39	0.56
1:D:282:ARG:HE	1:D:282:ARG:HA	1.66	0.56
1:D:318:GLU:O	1:D:406:THR:HG23	2.05	0.56
1:B:121:PHE:HD2	1:B:121:PHE:N	2.02	0.56
1:C:115:VAL:HG21	1:C:297:VAL:HG11	1.86	0.56
1:D:210:LEU:HD13	1:D:274:ILE:HG13	1.88	0.56
1:D:121:PHE:HD2	1:D:121:PHE:N	2.02	0.56
1:D:249:VAL:HG22	1:D:337:PHE:HB3	1.87	0.56
1:B:210:LEU:HD13	1:B:274:ILE:HG13	1.88	0.56
1:B:342:ALA:C	1:B:344:GLY:H	2.12	0.56
1:A:272:ARG:O	1:A:275:ALA:HB3	2.05	0.56
1:D:342:ALA:C	1:D:344:GLY:H	2.12	0.56
1:A:210:LEU:HD13	1:A:274:ILE:HG13	1.88	0.56
1:C:249:VAL:HG22	1:C:337:PHE:HB3	1.87	0.56
1:B:455:ASP:OD1	1:B:457:GLU:N	2.39	0.55
1:A:216:TRP:NE1	1:A:283:THR:HG22	2.21	0.55
1:C:91:MET:HE1	1:C:196:THR:HB	1.89	0.55
1:A:354:MET:HE2	1:A:356:PHE:HD2	1.72	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:354:MET:HE2	1:D:356:PHE:HD2	1.72	0.55
1:B:249:VAL:HG22	1:B:337:PHE:HB3	1.88	0.55
1:C:210:LEU:HD13	1:C:274:ILE:HG13	1.88	0.55
1:D:121:PHE:N	1:D:121:PHE:CD2	2.73	0.55
1:A:249:VAL:HG22	1:A:337:PHE:HB3	1.87	0.55
1:A:282:ARG:HE	1:A:282:ARG:HA	1.66	0.55
1:B:91:MET:HE1	1:B:196:THR:HB	1.89	0.55
1:C:375:LEU:HD12	1:C:375:LEU:N	2.22	0.55
1:A:375:LEU:HD12	1:A:375:LEU:N	2.22	0.55
1:C:318:GLU:HB3	1:C:369:ALA:HB3	1.89	0.55
1:C:354:MET:HE2	1:C:356:PHE:HD2	1.72	0.55
1:D:455:ASP:OD1	1:D:457:GLU:N	2.39	0.55
1:A:318:GLU:HB3	1:A:369:ALA:HB3	1.89	0.55
1:B:216:TRP:NE1	1:B:283:THR:HG22	2.21	0.55
1:C:216:TRP:NE1	1:C:283:THR:HG22	2.21	0.55
1:D:91:MET:HE1	1:D:196:THR:HB	1.89	0.55
1:D:375:LEU:HD12	1:D:375:LEU:N	2.22	0.55
1:B:401:ARG:HG3	1:B:401:ARG:HH11	1.72	0.55
1:A:91:MET:HE1	1:A:196:THR:HB	1.89	0.54
1:A:401:ARG:HG3	1:A:401:ARG:HH11	1.72	0.54
1:B:375:LEU:HD12	1:B:375:LEU:N	2.22	0.54
1:D:216:TRP:NE1	1:D:283:THR:HG22	2.21	0.54
1:A:88:LEU:O	1:A:108:GLY:HA3	2.08	0.54
1:C:39:PRO:HB3	1:C:85:VAL:HG23	1.89	0.54
1:C:401:ARG:HG3	1:C:401:ARG:HH11	1.72	0.54
1:B:97:ASP:OD1	1:B:99:ALA:HB3	2.08	0.54
1:D:88:LEU:O	1:D:108:GLY:HA3	2.08	0.54
1:D:401:ARG:HG3	1:D:401:ARG:HH11	1.73	0.54
1:A:39:PRO:HB3	1:A:85:VAL:HG23	1.89	0.54
1:C:455:ASP:OD1	1:C:457:GLU:N	2.39	0.54
1:B:300:ASN:HA	1:B:303:VAL:HG22	1.90	0.54
1:D:300:ASN:HA	1:D:303:VAL:HG22	1.90	0.54
1:D:318:GLU:HB3	1:D:369:ALA:HB3	1.89	0.54
1:A:5:LYS:C	1:A:5:LYS:HD2	2.34	0.53
1:B:88:LEU:O	1:B:108:GLY:HA3	2.08	0.53
1:C:300:ASN:HA	1:C:303:VAL:HG22	1.90	0.53
1:A:60:ASP:CB	1:B:167:THR:HG22	2.38	0.53
1:B:210:LEU:HD12	1:B:270:ALA:CB	2.38	0.53
1:B:354:MET:HE2	1:B:356:PHE:HD2	1.72	0.53
1:C:5:LYS:HD2	1:C:5:LYS:C	2.33	0.53
1:D:97:ASP:OD1	1:D:99:ALA:HB3	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:ASP:OD1	1:A:99:ALA:HB3	2.08	0.53
1:B:5:LYS:HD2	1:B:5:LYS:C	2.33	0.53
1:A:46:LEU:HD11	1:C:13:GLN:HE22	1.74	0.53
1:C:97:ASP:OD1	1:C:99:ALA:HB3	2.08	0.53
1:A:5:LYS:HZ2	1:A:6:LEU:HB2	1.74	0.53
1:C:455:ASP:C	1:C:457:GLU:H	2.17	0.53
1:A:60:ASP:HB3	1:B:167:THR:HG22	1.91	0.53
1:A:300:ASN:HA	1:A:303:VAL:HG22	1.90	0.53
1:D:282:ARG:NE	1:D:283:THR:N	2.49	0.53
1:B:318:GLU:HB3	1:B:369:ALA:HB3	1.89	0.53
1:D:39:PRO:HB3	1:D:85:VAL:HG23	1.89	0.53
1:D:455:ASP:C	1:D:457:GLU:H	2.17	0.53
1:A:310:MET:HE1	1:A:379:SER:CB	2.37	0.53
1:B:39:PRO:HB3	1:B:85:VAL:HG23	1.89	0.53
1:C:88:LEU:O	1:C:108:GLY:HA3	2.08	0.53
1:A:455:ASP:OD1	1:A:457:GLU:N	2.39	0.52
1:D:5:LYS:C	1:D:5:LYS:HD2	2.34	0.52
1:A:455:ASP:C	1:A:457:GLU:H	2.17	0.52
1:B:455:ASP:C	1:B:457:GLU:H	2.17	0.52
1:A:210:LEU:HD12	1:A:270:ALA:CB	2.38	0.52
1:B:290:VAL:C	1:B:291:ARG:HG3	2.35	0.52
1:B:310:MET:HE1	1:B:379:SER:CB	2.37	0.52
1:D:290:VAL:C	1:D:291:ARG:HG3	2.35	0.52
1:B:215:THR:HG23	1:B:258:THR:OG1	2.10	0.51
1:C:282:ARG:HE	1:C:282:ARG:HA	1.66	0.51
2:C:600:FAD:O4'	2:C:600:FAD:H51A	2.10	0.51
1:D:310:MET:HE1	1:D:379:SER:CB	2.37	0.51
2:B:600:FAD:O4'	2:B:600:FAD:H51A	2.10	0.51
1:C:46:LEU:HD23	1:C:90:LEU:HB3	1.92	0.51
1:C:290:VAL:C	1:C:291:ARG:HG3	2.35	0.51
2:D:600:FAD:H51A	2:D:600:FAD:O4'	2.10	0.51
1:A:69:SER:HB2	2:A:600:FAD:O1P	2.10	0.51
1:A:215:THR:HG23	1:A:258:THR:OG1	2.10	0.51
1:A:282:ARG:NE	1:A:283:THR:N	2.49	0.51
1:A:282:ARG:NH2	1:A:283:THR:H	2.08	0.51
1:A:290:VAL:C	1:A:291:ARG:HG3	2.35	0.51
1:B:282:ARG:NH2	1:B:283:THR:H	2.08	0.51
1:B:116:LYS:O	1:B:120:LYS:HG3	2.11	0.51
1:C:282:ARG:NH2	1:C:283:THR:H	2.08	0.51
1:D:282:ARG:NE	1:D:283:THR:H	2.09	0.51
1:B:69:SER:HB2	2:B:600:FAD:O1P	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:SER:HB2	2:C:600:FAD:O1P	2.10	0.51
1:A:116:LYS:O	1:A:120:LYS:HG3	2.11	0.50
1:C:310:MET:HE1	1:C:379:SER:CB	2.37	0.50
1:D:282:ARG:NH2	1:D:283:THR:H	2.08	0.50
1:C:210:LEU:HD12	1:C:270:ALA:CB	2.38	0.50
1:D:116:LYS:O	1:D:120:LYS:HG3	2.11	0.50
1:D:215:THR:HG23	1:D:258:THR:OG1	2.10	0.50
1:A:98:THR:CG2	1:A:121:PHE:HD1	2.25	0.50
1:C:215:THR:HG23	1:C:258:THR:OG1	2.10	0.50
1:C:385:SER:C	1:C:387:LYS:H	2.19	0.50
1:D:69:SER:HB2	2:D:600:FAD:O1P	2.10	0.50
1:A:46:LEU:HD23	1:A:90:LEU:HB3	1.92	0.50
1:A:385:SER:C	1:A:387:LYS:H	2.19	0.50
1:B:385:SER:C	1:B:387:LYS:H	2.19	0.50
1:B:451:ASN:O	1:B:453:ASN:N	2.44	0.50
1:A:451:ASN:O	1:A:453:ASN:N	2.44	0.50
1:C:451:ASN:O	1:C:453:ASN:N	2.44	0.50
2:A:600:FAD:H51A	2:A:600:FAD:O4'	2.10	0.49
1:B:46:LEU:HD23	1:B:90:LEU:HB3	1.92	0.49
1:D:148:THR:N	1:D:149:PRO:CD	2.75	0.49
1:D:451:ASN:O	1:D:453:ASN:N	2.44	0.49
1:A:143:GLY:HA2	2:A:600:FAD:O2	2.12	0.49
1:A:148:THR:N	1:A:149:PRO:CD	2.75	0.49
1:B:97:ASP:O	1:B:97:ASP:CG	2.55	0.49
1:D:46:LEU:HD23	1:D:90:LEU:HB3	1.92	0.49
1:D:354:MET:HE2	1:D:356:PHE:CD2	2.47	0.49
1:A:354:MET:HE2	1:A:356:PHE:CD2	2.47	0.49
1:B:354:MET:HE2	1:B:356:PHE:CD2	2.47	0.49
1:C:143:GLY:HA2	2:C:600:FAD:O2	2.13	0.49
1:A:445:GLU:HG3	1:B:60:ASP:O	2.12	0.49
1:C:72:HIS:CE1	2:C:600:FAD:HM72	2.47	0.49
1:C:97:ASP:CG	1:C:97:ASP:O	2.55	0.49
1:D:210:LEU:HD12	1:D:270:ALA:CB	2.38	0.49
1:C:116:LYS:O	1:C:120:LYS:HG3	2.11	0.49
1:A:321:MET:HG3	1:A:404:VAL:HG12	1.94	0.49
1:B:326:PHE:O	1:B:330:ILE:HG12	2.13	0.49
1:D:72:HIS:CE1	2:D:600:FAD:HM72	2.47	0.49
1:D:326:PHE:O	1:D:330:ILE:HG12	2.13	0.49
1:A:213:PHE:CE1	1:A:260:CYS:HB2	2.48	0.49
1:B:72:HIS:CE1	2:B:600:FAD:HM72	2.47	0.49
1:A:120:LYS:CA	1:D:53:LYS:CE	2.81	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:MET:CG	1:B:404:VAL:HA	2.43	0.49
1:C:148:THR:N	1:C:149:PRO:CD	2.75	0.49
1:D:17:ILE:HD13	1:D:27:ILE:HG13	1.95	0.49
1:A:326:PHE:O	1:A:330:ILE:HG12	2.13	0.49
1:C:213:PHE:CE1	1:C:260:CYS:HB2	2.48	0.49
1:D:213:PHE:CE1	1:D:260:CYS:HB2	2.48	0.49
1:D:321:MET:CG	1:D:404:VAL:HA	2.43	0.49
1:D:337:PHE:O	1:D:338:VAL:HB	2.12	0.49
1:A:17:ILE:HD13	1:A:27:ILE:HG13	1.95	0.48
1:A:72:HIS:CE1	2:A:600:FAD:HM72	2.47	0.48
1:B:148:THR:N	1:B:149:PRO:CD	2.75	0.48
1:B:321:MET:HG3	1:B:404:VAL:HG12	1.94	0.48
1:D:143:GLY:HA2	2:D:600:FAD:O2	2.12	0.48
1:D:321:MET:HG3	1:D:404:VAL:HG12	1.94	0.48
1:A:336:LYS:HA	1:A:391:LEU:HD11	1.95	0.48
1:D:385:SER:C	1:D:387:LYS:H	2.19	0.48
1:B:143:GLY:HA2	2:B:600:FAD:O2	2.13	0.48
1:C:17:ILE:HD13	1:C:27:ILE:HG13	1.95	0.48
1:B:213:PHE:CE1	1:B:260:CYS:HB2	2.48	0.48
1:C:337:PHE:O	1:C:338:VAL:HB	2.12	0.48
1:C:321:MET:CG	1:C:404:VAL:HA	2.43	0.48
1:C:326:PHE:O	1:C:330:ILE:HG12	2.13	0.48
1:D:131:PRO:HG2	1:D:301:ALA:HB2	1.96	0.48
1:A:342:ALA:C	1:A:344:GLY:N	2.72	0.48
1:C:354:MET:HE2	1:C:356:PHE:CD2	2.47	0.48
1:A:282:ARG:NE	1:A:283:THR:H	2.09	0.48
1:C:321:MET:HG3	1:C:404:VAL:HG12	1.94	0.48
1:B:42:ILE:HG12	1:B:85:VAL:HB	1.96	0.48
1:B:282:ARG:NE	1:B:283:THR:H	2.10	0.48
1:B:336:LYS:HA	1:B:391:LEU:HD11	1.95	0.48
1:B:337:PHE:O	1:B:338:VAL:HB	2.12	0.48
1:D:342:ALA:C	1:D:344:GLY:N	2.72	0.48
1:A:321:MET:CG	1:A:404:VAL:HA	2.43	0.48
1:C:336:LYS:HA	1:C:391:LEU:HD11	1.95	0.48
1:D:42:ILE:HG12	1:D:85:VAL:HB	1.96	0.48
1:C:282:ARG:NE	1:C:283:THR:H	2.09	0.47
1:C:72:HIS:HB2	2:C:600:FAD:O2P	2.15	0.47
1:D:97:ASP:O	1:D:97:ASP:CG	2.55	0.47
1:A:337:PHE:O	1:A:338:VAL:HB	2.12	0.47
1:A:174:SER:HA	1:A:182:PHE:CD1	2.50	0.47
1:B:131:PRO:HG2	1:B:301:ALA:HB2	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:ASP:C	1:A:240:HIS:CD2	2.93	0.47
1:C:340:GLU:CG	1:C:343:SER:HB2	2.45	0.47
1:D:209:MET:O	1:D:290:VAL:HA	2.15	0.47
1:D:239:ASP:C	1:D:240:HIS:CD2	2.93	0.47
1:D:336:LYS:HA	1:D:391:LEU:HD11	1.95	0.47
1:D:340:GLU:CG	1:D:343:SER:HB2	2.45	0.47
1:A:97:ASP:CG	1:A:97:ASP:O	2.55	0.47
1:C:209:MET:O	1:C:290:VAL:HA	2.15	0.47
1:A:42:ILE:HG12	1:A:85:VAL:HB	1.96	0.47
1:B:72:HIS:HB2	2:B:600:FAD:O2P	2.14	0.47
1:B:174:SER:HA	1:B:182:PHE:CD1	2.50	0.47
1:B:209:MET:O	1:B:290:VAL:HA	2.15	0.47
1:B:239:ASP:C	1:B:240:HIS:CD2	2.93	0.47
1:B:340:GLU:CG	1:B:343:SER:HB2	2.45	0.47
1:B:342:ALA:C	1:B:344:GLY:N	2.72	0.47
1:C:174:SER:HA	1:C:182:PHE:CD1	2.50	0.47
1:C:239:ASP:C	1:C:240:HIS:CD2	2.93	0.47
1:D:12:ILE:HB	1:D:50:ASP:CG	2.40	0.47
1:D:401:ARG:HG3	1:D:401:ARG:NH1	2.30	0.47
1:A:209:MET:O	1:A:290:VAL:HA	2.15	0.47
1:B:17:ILE:HD13	1:B:27:ILE:HG13	1.95	0.47
1:C:110:ILE:O	1:C:111:SER:C	2.58	0.47
1:A:321:MET:HG3	1:A:404:VAL:HA	1.97	0.47
1:C:42:ILE:HG12	1:C:85:VAL:HB	1.96	0.47
1:C:172:TYR:O	1:C:178:ARG:HD2	2.15	0.47
1:A:12:ILE:HB	1:A:50:ASP:CG	2.40	0.47
1:D:72:HIS:HB2	2:D:600:FAD:O2P	2.15	0.47
1:D:172:TYR:O	1:D:178:ARG:HD2	2.15	0.47
1:D:174:SER:HA	1:D:182:PHE:CD1	2.50	0.47
1:C:164:VAL:HG22	1:C:170:VAL:HG22	1.97	0.46
1:C:401:ARG:HG3	1:C:401:ARG:NH1	2.30	0.46
1:B:98:THR:CG2	1:B:121:PHE:HD1	2.25	0.46
1:B:401:ARG:HG3	1:B:401:ARG:NH1	2.30	0.46
1:C:131:PRO:HG2	1:C:301:ALA:HB2	1.96	0.46
1:B:52:ALA:O	1:B:55:VAL:HG22	2.15	0.46
1:B:321:MET:HG3	1:B:404:VAL:HA	1.97	0.46
1:C:12:ILE:HB	1:C:50:ASP:CG	2.40	0.46
1:A:164:VAL:HG22	1:A:170:VAL:HG22	1.97	0.46
1:B:120:LYS:C	1:B:121:PHE:CD2	2.93	0.46
1:C:52:ALA:O	1:C:55:VAL:HG22	2.15	0.46
1:C:282:ARG:NE	1:C:283:THR:N	2.49	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:HIS:HB2	2:A:600:FAD:O2P	2.15	0.46
1:A:340:GLU:CG	1:A:343:SER:HB2	2.45	0.46
1:A:110:ILE:O	1:A:111:SER:C	2.58	0.46
1:A:419:THR:O	1:A:423:VAL:HG23	2.16	0.46
1:B:12:ILE:HB	1:B:50:ASP:CG	2.40	0.46
1:C:98:THR:CG2	1:C:121:PHE:HD1	2.25	0.46
1:D:164:VAL:HG22	1:D:170:VAL:HG22	1.97	0.46
1:A:131:PRO:HG2	1:A:301:ALA:HB2	1.96	0.46
1:A:313:LEU:HD13	1:A:417:GLU:OE2	2.16	0.46
1:B:111:SER:O	1:B:115:VAL:HG23	2.16	0.46
1:A:7:ALA:HB1	1:B:441:GLU:HG3	1.98	0.46
1:A:111:SER:O	1:A:115:VAL:HG23	2.16	0.46
1:A:172:TYR:O	1:A:178:ARG:HD2	2.15	0.46
1:B:419:THR:O	1:B:423:VAL:HG23	2.16	0.46
1:D:52:ALA:O	1:D:55:VAL:HG22	2.15	0.46
1:B:164:VAL:HG22	1:B:170:VAL:HG22	1.97	0.46
1:B:367:ARG:HG2	1:B:367:ARG:NH1	2.30	0.46
1:C:313:LEU:HD13	1:C:417:GLU:OE2	2.16	0.46
1:A:7:ALA:HB1	1:B:441:GLU:CA	2.40	0.46
1:D:114:LEU:HD12	1:D:114:LEU:O	2.16	0.46
1:B:313:LEU:HD13	1:B:417:GLU:OE2	2.16	0.45
1:C:111:SER:O	1:C:115:VAL:HG23	2.16	0.45
1:C:321:MET:HG3	1:C:404:VAL:HA	1.97	0.45
1:C:419:THR:O	1:C:423:VAL:HG23	2.16	0.45
1:A:52:ALA:O	1:A:55:VAL:HG22	2.16	0.45
1:A:114:LEU:O	1:A:114:LEU:HD12	2.16	0.45
1:D:98:THR:CG2	1:D:121:PHE:HD1	2.25	0.45
1:D:439:LYS:HE2	1:D:454:ILE:O	2.16	0.45
1:A:401:ARG:HG3	1:A:401:ARG:NH1	2.30	0.45
1:B:110:ILE:O	1:B:111:SER:C	2.58	0.45
1:D:111:SER:O	1:D:115:VAL:HG23	2.16	0.45
1:D:120:LYS:C	1:D:121:PHE:CD2	2.93	0.45
1:D:313:LEU:HD13	1:D:417:GLU:OE2	2.16	0.45
1:A:60:ASP:OD1	1:B:167:THR:HA	2.16	0.45
1:B:46:LEU:CD2	1:B:90:LEU:HB3	2.47	0.45
1:D:146:PHE:HB2	1:D:293:TYR:HE1	1.82	0.45
1:D:321:MET:HG3	1:D:404:VAL:HA	1.97	0.45
1:C:114:LEU:O	1:C:114:LEU:HD12	2.16	0.45
1:C:367:ARG:HG2	1:C:367:ARG:NH1	2.30	0.45
1:C:384:GLY:O	1:C:387:LYS:HB3	2.17	0.45
1:D:46:LEU:CD2	1:D:90:LEU:HB3	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:419:THR:O	1:D:423:VAL:HG23	2.16	0.45
1:A:146:PHE:HB2	1:A:293:TYR:HE1	1.82	0.45
1:A:367:ARG:HG2	1:A:367:ARG:NH1	2.30	0.45
1:B:238:ALA:HB1	1:B:354:MET:HG3	1.99	0.45
1:C:146:PHE:HB2	1:C:293:TYR:HE1	1.82	0.45
1:C:439:LYS:HE2	1:C:454:ILE:O	2.17	0.45
1:D:238:ALA:HB1	1:D:354:MET:HG3	1.99	0.45
1:B:130:HIS:CE1	1:B:132:LYS:HB2	2.52	0.45
1:B:146:PHE:HB2	1:B:293:TYR:HE1	1.82	0.45
1:B:172:TYR:O	1:B:178:ARG:HD2	2.15	0.45
1:C:46:LEU:CD2	1:C:90:LEU:HB3	2.47	0.45
1:D:5:LYS:HZ2	1:D:6:LEU:HB2	1.81	0.45
1:D:110:ILE:O	1:D:111:SER:C	2.58	0.45
1:A:384:GLY:O	1:A:387:LYS:HB3	2.17	0.45
1:B:114:LEU:HD12	1:B:114:LEU:O	2.16	0.45
1:B:351:ILE:HA	1:B:371:GLY:O	2.17	0.45
1:C:351:ILE:HA	1:C:371:GLY:O	2.17	0.45
1:D:384:GLY:O	1:D:387:LYS:HB3	2.17	0.45
1:A:439:LYS:HE2	1:A:454:ILE:O	2.16	0.45
1:A:120:LYS:HB3	1:D:53:LYS:HE3	1.96	0.45
1:A:46:LEU:CD2	1:A:90:LEU:HB3	2.47	0.44
1:A:130:HIS:CE1	1:A:132:LYS:HB2	2.52	0.44
1:C:130:HIS:CE1	1:C:132:LYS:HB2	2.52	0.44
1:B:175:ASP:OD1	1:B:175:ASP:N	2.48	0.44
1:C:5:LYS:HZ2	1:C:6:LEU:HB2	1.82	0.44
1:C:175:ASP:OD1	1:C:175:ASP:N	2.48	0.44
1:D:351:ILE:HA	1:D:371:GLY:O	2.17	0.44
1:A:175:ASP:OD1	1:A:175:ASP:N	2.48	0.44
1:B:439:LYS:HE2	1:B:454:ILE:O	2.16	0.44
1:A:238:ALA:HB1	1:A:354:MET:HG3	1.99	0.44
1:C:120:LYS:C	1:C:121:PHE:CD2	2.93	0.44
1:B:105:ILE:HG13	1:B:198:VAL:HG12	2.00	0.44
1:C:342:ALA:C	1:C:344:GLY:N	2.72	0.44
1:D:130:HIS:CE1	1:D:132:LYS:HB2	2.52	0.44
1:D:367:ARG:HG2	1:D:367:ARG:NH1	2.30	0.44
1:A:120:LYS:C	1:A:121:PHE:CD2	2.93	0.44
1:A:351:ILE:HA	1:A:371:GLY:O	2.17	0.44
1:A:447:ARG:HA	1:A:447:ARG:HD3	1.86	0.44
1:B:384:GLY:O	1:B:387:LYS:HB3	2.17	0.43
1:C:181:LEU:HD12	1:C:185:VAL:HG23	1.99	0.43
1:C:238:ALA:HB1	1:C:354:MET:HG3	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:338:VAL:HG22	1:D:339:SER:N	2.33	0.43
1:B:318:GLU:HA	1:B:370:MET:O	2.19	0.43
1:B:181:LEU:HD12	1:B:185:VAL:HG23	1.99	0.43
1:C:105:ILE:HG13	1:C:198:VAL:HG12	2.00	0.43
1:D:175:ASP:OD1	1:D:175:ASP:N	2.48	0.43
1:B:5:LYS:HZ2	1:B:6:LEU:HB2	1.84	0.43
1:B:5:LYS:NZ	1:B:6:LEU:HB2	2.34	0.43
1:B:282:ARG:NE	1:B:283:THR:N	2.49	0.43
1:A:181:LEU:HD12	1:A:185:VAL:HG23	1.99	0.43
1:A:338:VAL:HG22	1:A:339:SER:N	2.33	0.43
1:D:181:LEU:HD12	1:D:185:VAL:HG23	1.99	0.43
1:C:193:GLY:HA2	1:C:448:PHE:CE2	2.54	0.43
1:A:91:MET:HE1	1:A:196:THR:CB	2.49	0.43
1:C:213:PHE:CE1	1:C:260:CYS:SG	3.12	0.43
1:A:193:GLY:HA2	1:A:448:PHE:CE2	2.54	0.43
1:B:193:GLY:HA2	1:B:448:PHE:CE2	2.54	0.43
1:B:213:PHE:CE1	1:B:260:CYS:SG	3.12	0.43
1:D:5:LYS:NZ	1:D:6:LEU:HB2	2.34	0.43
1:A:378:TRP:CD1	1:A:378:TRP:C	2.97	0.42
1:C:378:TRP:CD1	1:C:378:TRP:C	2.97	0.42
1:D:105:ILE:HG13	1:D:198:VAL:HG12	2.00	0.42
1:D:378:TRP:CD1	1:D:378:TRP:C	2.97	0.42
1:A:213:PHE:CE1	1:A:260:CYS:SG	3.12	0.42
1:B:338:VAL:HG22	1:B:339:SER:N	2.33	0.42
1:B:378:TRP:CD1	1:B:378:TRP:C	2.97	0.42
1:C:315:ILE:HG21	1:C:396:ASP:CG	2.44	0.42
1:D:193:GLY:HA2	1:D:448:PHE:CE2	2.54	0.42
1:A:36:LEU:O	1:A:38:ARG:HG2	2.19	0.42
1:C:210:LEU:HD23	1:C:210:LEU:HA	1.89	0.42
1:C:249:VAL:O	1:C:249:VAL:HG23	2.19	0.42
1:D:334:LEU:HA	1:D:337:PHE:CD2	2.54	0.42
1:A:334:LEU:HA	1:A:337:PHE:CD2	2.54	0.42
1:B:36:LEU:O	1:B:38:ARG:HG2	2.20	0.42
1:D:315:ILE:HG21	1:D:396:ASP:CG	2.44	0.42
1:D:330:ILE:HD12	1:D:349:LEU:CD2	2.50	0.42
1:A:105:ILE:HG13	1:A:198:VAL:HG12	2.00	0.42
1:A:177:GLU:O	1:A:178:ARG:C	2.63	0.42
1:A:318:GLU:HA	1:A:370:MET:O	2.19	0.42
1:C:243:PRO:HD2	1:C:353:GLY:HA2	2.01	0.42
1:C:318:GLU:HA	1:C:370:MET:O	2.19	0.42
1:C:338:VAL:HG22	1:C:339:SER:N	2.33	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:LEU:O	1:D:38:ARG:HG2	2.19	0.42
1:A:330:ILE:HD12	1:A:349:LEU:CD2	2.50	0.42
1:B:243:PRO:HD2	1:B:353:GLY:HA2	2.01	0.42
1:C:91:MET:HE1	1:C:196:THR:CB	2.49	0.42
1:C:94:ILE:HA	1:C:105:ILE:HG22	2.02	0.42
1:C:340:GLU:HB2	1:C:343:SER:HB2	2.02	0.42
1:C:362:THR:HB	1:C:363:PRO:HD2	2.02	0.42
1:D:206:PRO:HD2	1:D:293:TYR:HB2	2.02	0.42
1:A:340:GLU:HB2	1:A:343:SER:HB2	2.02	0.42
1:C:5:LYS:NZ	1:C:6:LEU:HB2	2.34	0.42
1:C:334:LEU:HA	1:C:337:PHE:CD2	2.54	0.42
1:D:318:GLU:HA	1:D:370:MET:O	2.19	0.42
1:A:362:THR:HB	1:A:363:PRO:HD2	2.02	0.42
1:B:206:PRO:HD2	1:B:293:TYR:HB2	2.02	0.42
1:B:447:ARG:HA	1:B:447:ARG:HD3	1.86	0.42
1:D:177:GLU:O	1:D:178:ARG:C	2.63	0.42
1:A:139:ALA:O	1:A:155:SER:HB3	2.20	0.42
1:B:177:GLU:O	1:B:178:ARG:C	2.63	0.42
1:B:249:VAL:O	1:B:249:VAL:HG23	2.19	0.42
1:C:139:ALA:O	1:C:155:SER:HB3	2.20	0.42
1:C:445:GLU:HG3	1:D:61:ASN:C	2.45	0.42
1:D:340:GLU:HB2	1:D:343:SER:HB2	2.02	0.42
1:A:7:ALA:HB3	1:B:441:GLU:HA	1.92	0.42
1:B:334:LEU:HA	1:B:337:PHE:CD2	2.54	0.42
1:C:123:LEU:HD23	1:C:123:LEU:HA	1.75	0.42
1:C:330:ILE:HD12	1:C:349:LEU:CD2	2.50	0.42
1:D:77:TYR:HB3	1:D:450:HIS:O	2.20	0.42
1:D:91:MET:HE1	1:D:196:THR:CB	2.49	0.42
1:D:213:PHE:CE1	1:D:260:CYS:SG	3.12	0.42
1:D:243:PRO:HD2	1:D:353:GLY:HA2	2.01	0.42
1:D:362:THR:HB	1:D:363:PRO:HD2	2.02	0.42
1:B:6:LEU:HG	1:B:7:ALA:N	2.35	0.41
1:B:362:THR:HB	1:B:363:PRO:HD2	2.02	0.41
1:C:36:LEU:O	1:C:38:ARG:HG2	2.19	0.41
1:C:206:PRO:HD2	1:C:293:TYR:HB2	2.02	0.41
1:D:72:HIS:CE1	2:D:600:FAD:HM73	2.55	0.41
1:A:5:LYS:NZ	1:A:6:LEU:HB2	2.34	0.41
1:A:206:PRO:HD2	1:A:293:TYR:HB2	2.02	0.41
1:A:315:ILE:HG21	1:A:396:ASP:CG	2.44	0.41
1:B:94:ILE:HA	1:B:105:ILE:HG22	2.02	0.41
1:B:315:ILE:HG21	1:B:396:ASP:CG	2.44	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:330:ILE:HD12	1:B:349:LEU:CD2	2.50	0.41
1:B:340:GLU:HB2	1:B:343:SER:HB2	2.02	0.41
1:B:428:LYS:HA	1:B:429:PRO:HD3	1.93	0.41
1:B:455:ASP:C	1:B:457:GLU:N	2.79	0.41
1:D:6:LEU:HG	1:D:7:ALA:N	2.35	0.41
1:A:77:TYR:HB3	1:A:450:HIS:O	2.20	0.41
1:A:94:ILE:HA	1:A:105:ILE:HG22	2.02	0.41
1:B:375:LEU:CD1	1:B:375:LEU:N	2.84	0.41
1:C:177:GLU:O	1:C:178:ARG:C	2.63	0.41
1:D:94:ILE:HA	1:D:105:ILE:HG22	2.02	0.41
1:A:6:LEU:HG	1:A:7:ALA:N	2.35	0.41
1:A:72:HIS:CE1	2:A:600:FAD:HM73	2.55	0.41
1:A:385:SER:C	1:A:387:LYS:N	2.79	0.41
1:B:325:ARG:HA	1:B:325:ARG:HD2	1.91	0.41
1:C:6:LEU:HG	1:C:7:ALA:N	2.35	0.41
1:C:447:ARG:HA	1:C:447:ARG:HD3	1.86	0.41
1:B:385:SER:C	1:B:387:LYS:N	2.79	0.41
1:C:72:HIS:CE1	2:C:600:FAD:HM73	2.55	0.41
1:D:428:LYS:HA	1:D:429:PRO:HD3	1.93	0.41
1:D:455:ASP:C	1:D:457:GLU:N	2.79	0.41
1:A:243:PRO:HD2	1:A:353:GLY:HA2	2.01	0.41
1:A:249:VAL:O	1:A:249:VAL:HG23	2.19	0.41
1:B:24:PHE:O	1:B:27:ILE:N	2.54	0.41
1:B:91:MET:HE1	1:B:196:THR:CB	2.49	0.41
1:B:139:ALA:O	1:B:155:SER:HB3	2.20	0.41
1:C:24:PHE:O	1:C:27:ILE:N	2.54	0.41
1:C:77:TYR:HB3	1:C:450:HIS:O	2.20	0.41
1:D:139:ALA:O	1:D:155:SER:HB3	2.20	0.41
1:D:375:LEU:CD1	1:D:375:LEU:N	2.84	0.41
1:D:377:GLU:O	1:D:378:TRP:HB3	2.21	0.41
1:D:387:LYS:CG	1:D:388:TYR:N	2.84	0.41
1:A:24:PHE:O	1:A:27:ILE:N	2.54	0.41
1:A:128:GLY:HA3	1:A:138:LEU:HD11	2.02	0.41
1:B:77:TYR:HB3	1:B:450:HIS:O	2.20	0.41
1:B:387:LYS:CG	1:B:388:TYR:N	2.84	0.41
1:D:227:LEU:HD12	1:D:227:LEU:HA	1.92	0.41
1:D:249:VAL:O	1:D:249:VAL:HG23	2.19	0.41
1:A:330:ILE:HD12	1:A:349:LEU:HD22	2.03	0.41
1:A:375:LEU:CD1	1:A:375:LEU:N	2.84	0.41
1:B:37:GLN:OE1	1:B:37:GLN:N	2.50	0.41
1:C:385:SER:C	1:C:387:LYS:N	2.79	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:LYS:CG	1:A:388:TYR:N	2.84	0.40
1:C:340:GLU:HA	1:C:341:PRO:HD2	1.95	0.40
1:D:330:ILE:HD12	1:D:349:LEU:HD22	2.03	0.40
1:B:210:LEU:HD23	1:B:210:LEU:HA	1.89	0.40
1:C:186:ARG:O	1:C:363:PRO:HD2	2.22	0.40
1:D:208:LYS:O	1:D:267:LEU:HD21	2.21	0.40
1:A:37:GLN:OE1	1:A:37:GLN:N	2.50	0.40
1:A:208:LYS:O	1:A:267:LEU:HD21	2.21	0.40
1:D:186:ARG:O	1:D:363:PRO:HD2	2.22	0.40
1:A:186:ARG:O	1:A:363:PRO:HD2	2.22	0.40
1:A:350:GLU:OE2	1:A:375:LEU:HD21	2.22	0.40
1:B:208:LYS:O	1:B:267:LEU:HD21	2.21	0.40
1:B:350:GLU:OE2	1:B:375:LEU:HD21	2.22	0.40
1:D:127:THR:HG22	1:D:135:PHE:CD1	2.57	0.40
1:B:128:GLY:HA3	1:B:138:LEU:HD11	2.02	0.40
1:C:128:GLY:HA3	1:C:138:LEU:HD11	2.02	0.40
1:C:330:ILE:HD12	1:C:349:LEU:HD22	2.03	0.40
1:C:350:GLU:OE2	1:C:375:LEU:HD21	2.22	0.40
1:D:123:LEU:HD23	1:D:123:LEU:HA	1.75	0.40
1:D:128:GLY:HA3	1:D:138:LEU:HD11	2.02	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:SER:OG	1:D:428:LYS:NZ[2_656]	2.07	0.13
1:A:282:ARG:CD	1:C:286:ASP:OD2[1_455]	2.13	0.07
1:A:282:ARG:CD	1:C:286:ASP:CG[1_455]	2.15	0.05

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	451/459 (98%)	404 (90%)	42 (9%)	5 (1%)	11	36
1	B	451/459 (98%)	404 (90%)	42 (9%)	5 (1%)	11	36
1	C	451/459 (98%)	404 (90%)	42 (9%)	5 (1%)	11	36
1	D	451/459 (98%)	404 (90%)	42 (9%)	5 (1%)	11	36
All	All	1804/1836 (98%)	1616 (90%)	168 (9%)	20 (1%)	11	36

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	24	PHE
1	A	338	VAL
1	B	24	PHE
1	B	338	VAL
1	C	24	PHE
1	C	338	VAL
1	D	24	PHE
1	D	338	VAL
1	A	25	ASP
1	B	25	ASP
1	C	25	ASP
1	D	25	ASP
1	A	428	LYS
1	B	428	LYS
1	C	428	LYS
1	D	428	LYS
1	A	9	PRO
1	B	9	PRO
1	C	9	PRO
1	D	9	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	353/358 (99%)	345 (98%)	8 (2%)	44	76

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	353/358 (99%)	345 (98%)	8 (2%)	44	76
1	C	353/358 (99%)	345 (98%)	8 (2%)	44	76
1	D	353/358 (99%)	345 (98%)	8 (2%)	44	76
All	All	1412/1432 (99%)	1380 (98%)	32 (2%)	44	76

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	72	HIS
1	A	111	SER
1	A	121	PHE
1	A	321	MET
1	A	322	PRO
1	A	348	LYS
1	A	354	MET
1	B	5	LYS
1	B	72	HIS
1	B	111	SER
1	B	121	PHE
1	B	321	MET
1	B	322	PRO
1	B	348	LYS
1	B	354	MET
1	C	5	LYS
1	C	72	HIS
1	C	111	SER
1	C	121	PHE
1	C	321	MET
1	C	322	PRO
1	C	348	LYS
1	C	354	MET
1	D	5	LYS
1	D	72	HIS
1	D	111	SER
1	D	121	PHE
1	D	321	MET
1	D	322	PRO
1	D	348	LYS
1	D	354	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	95	HIS
1	A	141	ASN
1	A	201	GLN
1	A	312	ASN
1	A	446	ASN
1	A	450	HIS
1	A	453	ASN
1	B	13	GLN
1	B	29	ASN
1	B	95	HIS
1	B	141	ASN
1	B	201	GLN
1	B	312	ASN
1	B	446	ASN
1	B	450	HIS
1	B	453	ASN
1	C	29	ASN
1	C	95	HIS
1	C	141	ASN
1	C	201	GLN
1	C	312	ASN
1	C	446	ASN
1	C	450	HIS
1	C	453	ASN
1	D	13	GLN
1	D	29	ASN
1	D	95	HIS
1	D	141	ASN
1	D	201	GLN
1	D	312	ASN
1	D	446	ASN
1	D	450	HIS
1	D	453	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	C	600	1	58,58,58	1.21	6 (10%)	85,89,89	1.77	19 (22%)
2	FAD	A	600	1	58,58,58	1.21	6 (10%)	85,89,89	1.77	19 (22%)
2	FAD	B	600	1	58,58,58	1.21	6 (10%)	85,89,89	1.77	18 (21%)
2	FAD	D	600	1	58,58,58	1.21	6 (10%)	85,89,89	1.78	19 (22%)

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	C	600	1	-	1/34/50/50	0/6/6/6
2	FAD	A	600	1	-	1/34/50/50	0/6/6/6
2	FAD	B	600	1	-	1/34/50/50	0/6/6/6
2	FAD	D	600	1	-	1/34/50/50	0/6/6/6

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	600	FAD	C10-N1	3.58	1.40	1.33
2	B	600	FAD	C10-N1	3.58	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	FAD	C10-N1	3.56	1.40	1.33
2	A	600	FAD	C10-N1	3.55	1.40	1.33
2	B	600	FAD	C5A-N7A	-3.20	1.33	1.39
2	C	600	FAD	C5A-N7A	-3.17	1.33	1.39
2	A	600	FAD	C5A-N7A	-3.17	1.33	1.39
2	D	600	FAD	C5A-N7A	-3.14	1.33	1.39
2	C	600	FAD	PA-O1A	3.05	1.61	1.50
2	A	600	FAD	PA-O1A	3.04	1.61	1.50
2	D	600	FAD	PA-O1A	3.02	1.61	1.50
2	B	600	FAD	PA-O1A	3.02	1.61	1.50
2	D	600	FAD	C5X-N5	-2.61	1.34	1.39
2	A	600	FAD	C5X-N5	-2.58	1.34	1.39
2	B	600	FAD	C5X-N5	-2.58	1.34	1.39
2	C	600	FAD	C5X-N5	-2.57	1.34	1.39
2	A	600	FAD	C8A-N9A	-2.29	1.33	1.37
2	B	600	FAD	C8A-N9A	-2.29	1.33	1.37
2	D	600	FAD	C8A-N9A	-2.27	1.33	1.37
2	C	600	FAD	C8A-N9A	-2.27	1.33	1.37
2	D	600	FAD	C4A-N9A	-2.07	1.33	1.37
2	C	600	FAD	C4A-N9A	-2.07	1.33	1.37
2	B	600	FAD	C4A-N9A	-2.05	1.33	1.37
2	A	600	FAD	C4A-N9A	-2.05	1.33	1.37

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	600	FAD	O2P-P-O3P	-6.20	90.52	107.27
2	A	600	FAD	O2P-P-O3P	-6.19	90.53	107.27
2	D	600	FAD	O2P-P-O3P	-6.19	90.55	107.27
2	B	600	FAD	O2P-P-O3P	-6.18	90.56	107.27
2	C	600	FAD	C5A-C4A-N3A	-5.26	119.48	126.72
2	D	600	FAD	C5A-C4A-N3A	-5.24	119.50	126.72
2	A	600	FAD	C5A-C4A-N3A	-5.24	119.50	126.72
2	B	600	FAD	C5A-C4A-N3A	-5.21	119.54	126.72
2	D	600	FAD	N3A-C2A-N1A	-4.79	121.33	128.58
2	B	600	FAD	N3A-C2A-N1A	-4.77	121.36	128.58
2	A	600	FAD	N3A-C2A-N1A	-4.76	121.37	128.58
2	C	600	FAD	N3A-C2A-N1A	-4.75	121.40	128.58
2	B	600	FAD	O3P-P-O1P	-4.06	98.50	110.70
2	D	600	FAD	O3P-P-O1P	-4.05	98.52	110.70
2	A	600	FAD	O3P-P-O1P	-4.04	98.54	110.70
2	C	600	FAD	O3P-P-O1P	-4.03	98.58	110.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	600	FAD	N3A-C4A-N9A	3.79	133.62	127.17
2	A	600	FAD	N3A-C4A-N9A	3.79	133.61	127.17
2	D	600	FAD	N3A-C4A-N9A	3.78	133.60	127.17
2	B	600	FAD	N3A-C4A-N9A	3.78	133.59	127.17
2	D	600	FAD	C2A-N3A-C4A	3.66	120.76	111.83
2	C	600	FAD	C2A-N3A-C4A	3.65	120.75	111.83
2	A	600	FAD	C2A-N3A-C4A	3.65	120.75	111.83
2	B	600	FAD	C2A-N3A-C4A	3.65	120.74	111.83
2	C	600	FAD	C4-N3-C2	-3.05	120.22	125.64
2	D	600	FAD	C4-N3-C2	-3.04	120.25	125.64
2	A	600	FAD	C4-N3-C2	-3.03	120.25	125.64
2	A	600	FAD	O5'-P-O1P	3.02	120.92	108.94
2	C	600	FAD	O5'-P-O1P	3.02	120.91	108.94
2	B	600	FAD	O5'-P-O1P	3.02	120.91	108.94
2	B	600	FAD	C4-N3-C2	-3.01	120.29	125.64
2	D	600	FAD	O5'-P-O1P	3.01	120.88	108.94
2	C	600	FAD	C4X-C4-N3	2.78	120.34	113.25
2	D	600	FAD	C4X-C4-N3	2.78	120.32	113.25
2	D	600	FAD	N9A-C8A-N7A	-2.77	110.00	113.94
2	A	600	FAD	C4X-C4-N3	2.77	120.31	113.25
2	B	600	FAD	N9A-C8A-N7A	-2.77	110.00	113.94
2	C	600	FAD	N9A-C8A-N7A	-2.77	110.00	113.94
2	A	600	FAD	N9A-C8A-N7A	-2.77	110.01	113.94
2	B	600	FAD	C4X-C4-N3	2.77	120.29	113.25
2	D	600	FAD	C5X-N5-C4X	2.67	122.41	118.09
2	B	600	FAD	C5X-N5-C4X	2.66	122.40	118.09
2	A	600	FAD	C5X-N5-C4X	2.65	122.37	118.09
2	C	600	FAD	C5X-N5-C4X	2.62	122.33	118.09
2	B	600	FAD	C5A-N7A-C8A	2.53	107.42	103.45
2	C	600	FAD	C5A-N7A-C8A	2.53	107.42	103.45
2	A	600	FAD	C5A-N7A-C8A	2.52	107.41	103.45
2	D	600	FAD	C5A-N7A-C8A	2.51	107.39	103.45
2	C	600	FAD	C4A-C5A-N7A	-2.45	107.78	110.58
2	A	600	FAD	C4A-C5A-N7A	-2.44	107.80	110.58
2	D	600	FAD	C4A-C5A-N7A	-2.44	107.80	110.58
2	B	600	FAD	C4A-C5A-N7A	-2.42	107.82	110.58
2	D	600	FAD	C10-C4X-N5	-2.41	119.88	124.81
2	D	600	FAD	O4-C4-C4X	-2.40	120.18	126.53
2	B	600	FAD	C10-C4X-N5	-2.40	119.91	124.81
2	A	600	FAD	C10-C4X-N5	-2.39	119.92	124.81
2	B	600	FAD	O4-C4-C4X	-2.39	120.22	126.53
2	C	600	FAD	O4-C4-C4X	-2.39	120.22	126.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	FAD	O4-C4-C4X	-2.39	120.23	126.53
2	C	600	FAD	C10-C4X-N5	-2.38	119.95	124.81
2	D	600	FAD	C4A-N9A-C8A	2.08	107.92	105.74
2	A	600	FAD	C4A-N9A-C8A	2.06	107.90	105.74
2	B	600	FAD	C4A-N9A-C8A	2.06	107.90	105.74
2	C	600	FAD	C4A-N9A-C8A	2.05	107.89	105.74
2	D	600	FAD	O2P-P-O1P	2.05	121.97	112.44
2	A	600	FAD	O2P-P-O1P	2.04	121.94	112.44
2	B	600	FAD	O2P-P-O1P	2.04	121.93	112.44
2	C	600	FAD	O2P-P-O1P	2.04	121.92	112.44
2	D	600	FAD	O3P-PA-O1A	-2.02	104.63	110.70
2	C	600	FAD	O3P-PA-O1A	-2.02	104.63	110.70
2	A	600	FAD	O3P-PA-O1A	-2.02	104.63	110.70
2	C	600	FAD	O2A-PA-O3P	2.02	112.73	107.27
2	B	600	FAD	O3P-PA-O1A	-2.01	104.64	110.70
2	D	600	FAD	O2A-PA-O3P	2.00	112.68	107.27
2	A	600	FAD	O2A-PA-O3P	2.00	112.68	107.27

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C5'-O5'-P-O2P
2	B	600	FAD	C5'-O5'-P-O2P
2	C	600	FAD	C5'-O5'-P-O2P
2	D	600	FAD	C5'-O5'-P-O2P

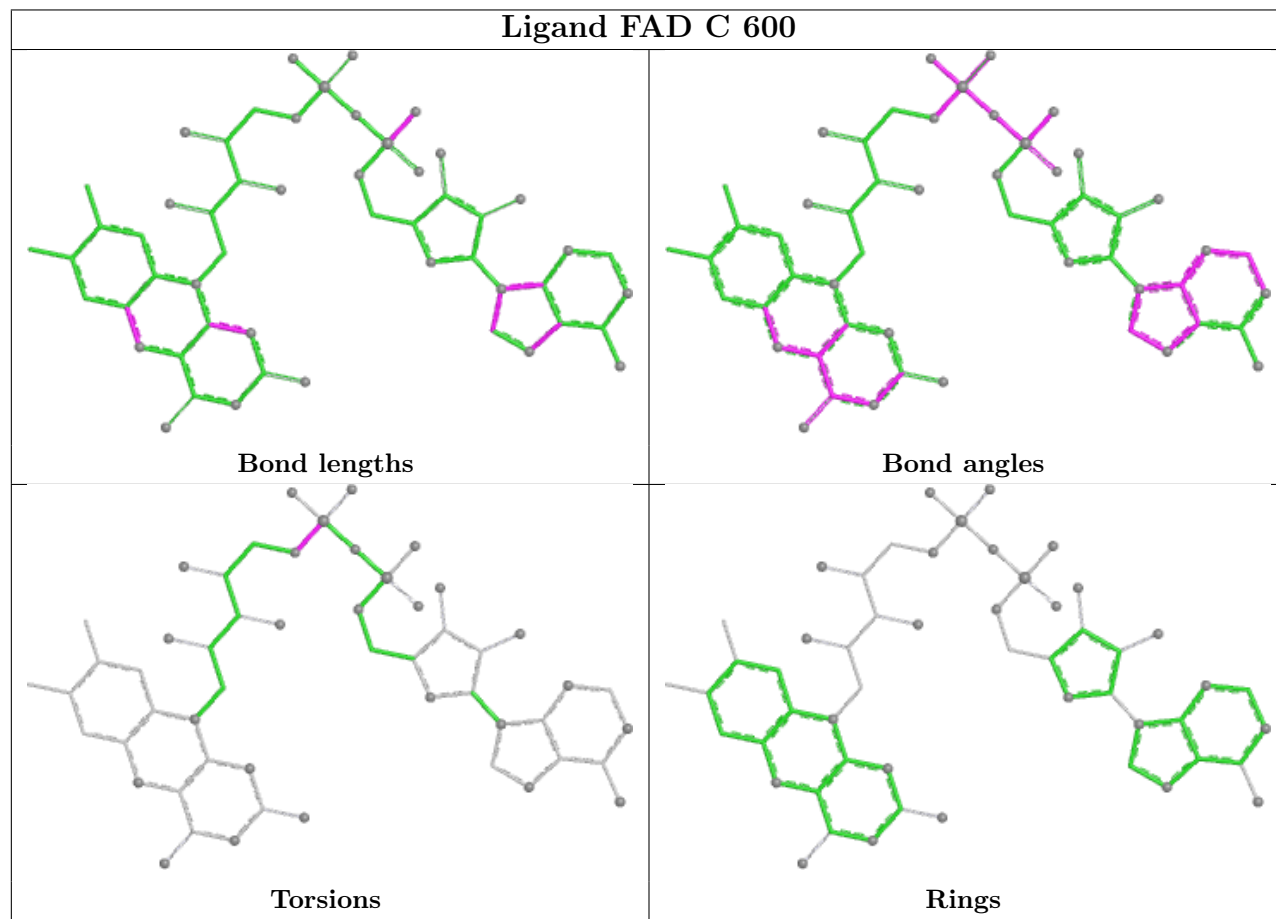
There are no ring outliers.

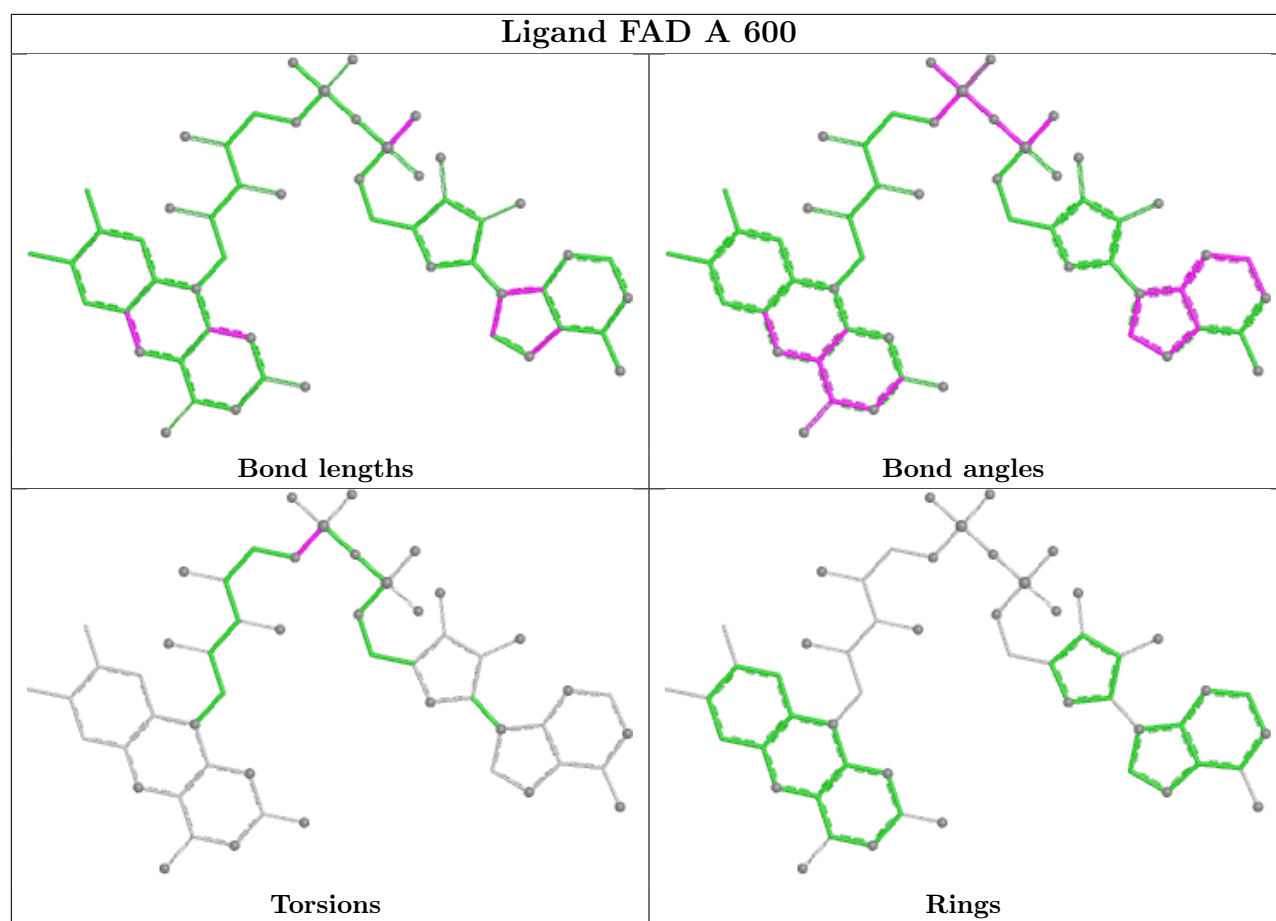
4 monomers are involved in 27 short contacts:

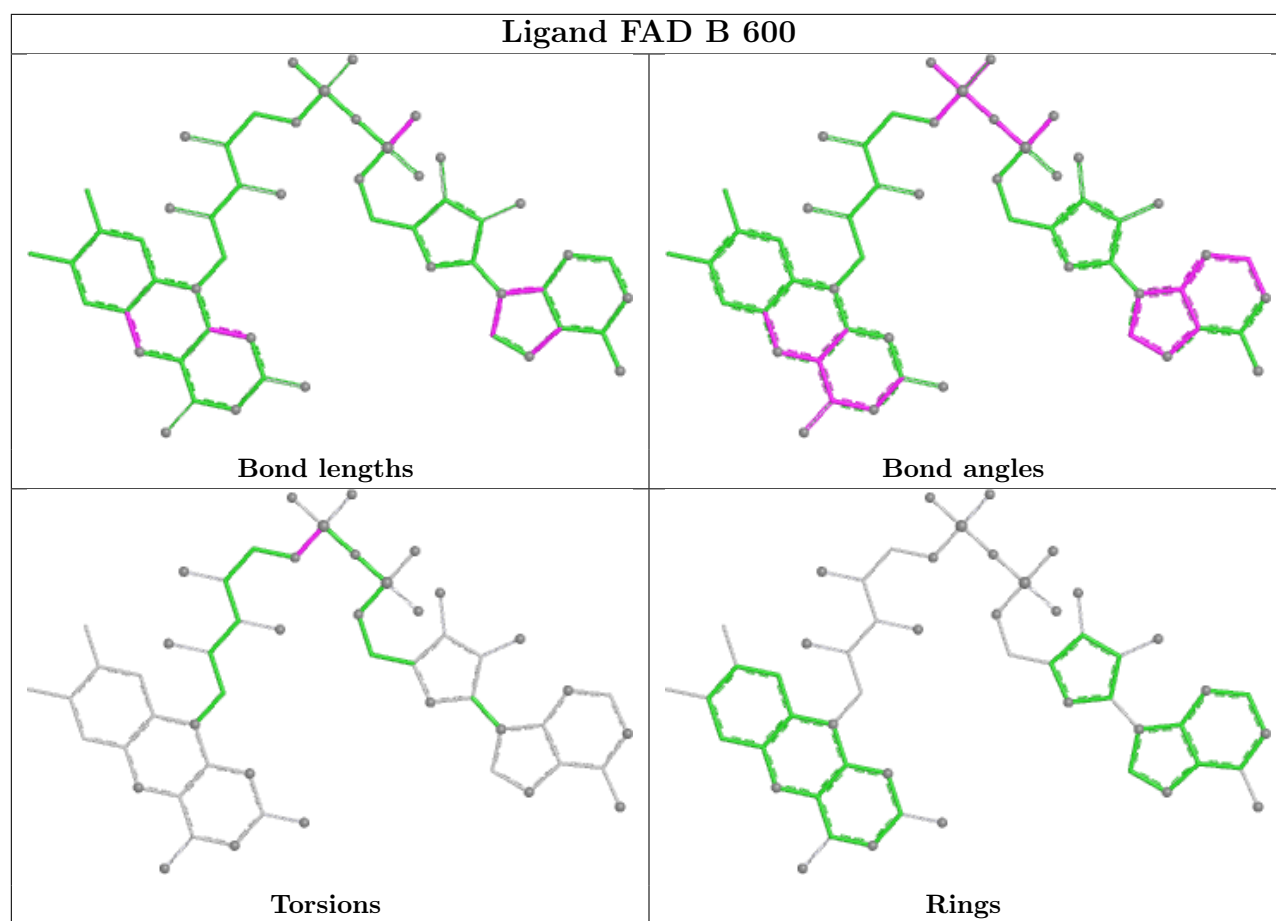
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	600	FAD	7	0
2	A	600	FAD	7	0
2	B	600	FAD	6	0
2	D	600	FAD	7	0

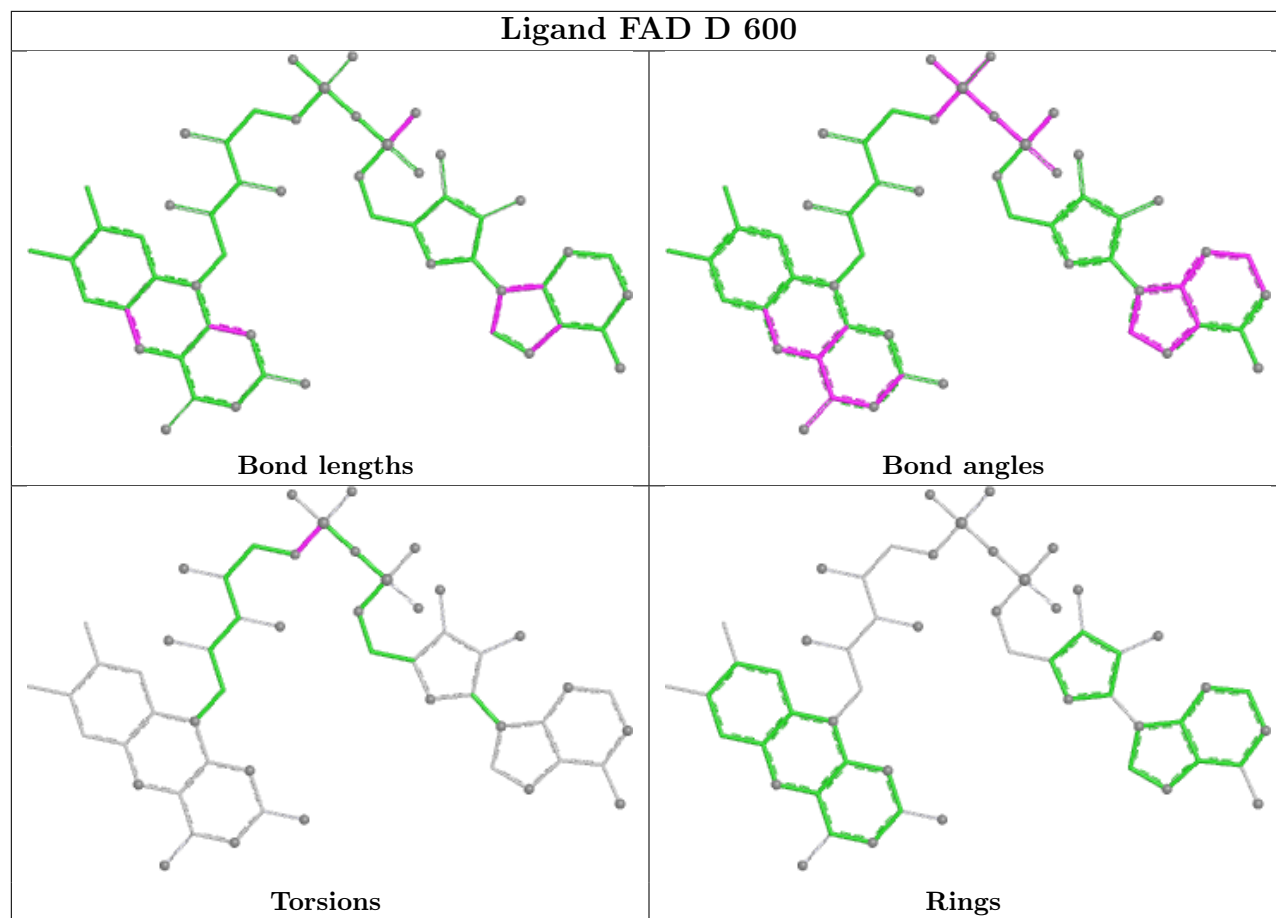
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	453/459 (98%)	0.74	55 (12%) 8 7	8, 32, 83, 154	0
1	B	453/459 (98%)	1.10	60 (13%) 7 6	22, 46, 97, 168	0
1	C	453/459 (98%)	1.16	83 (18%) 3 3	18, 42, 92, 164	0
1	D	453/459 (98%)	1.16	75 (16%) 4 3	23, 47, 98, 169	0
All	All	1812/1836 (98%)	1.04	273 (15%) 5 4	8, 42, 95, 169	0

All (273) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	285	SER	6.3
1	C	279	GLY	6.0
1	A	279	GLY	5.9
1	A	5	LYS	5.5
1	D	121	PHE	5.5
1	A	383	PRO	5.5
1	C	282	ARG	5.2
1	B	5	LYS	5.2
1	A	266	GLY	5.2
1	A	212	GLY	5.0
1	A	56	ARG	5.0
1	C	266	GLY	4.9
1	B	6	LEU	4.8
1	C	289	ALA	4.8
1	D	5	LYS	4.8
1	B	279	GLY	4.6
1	D	303	VAL	4.6
1	A	278	ARG	4.6
1	C	272	ARG	4.6
1	A	306	PHE	4.5
1	B	7	ALA	4.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	7	ALA	4.3
1	B	23	GLY	4.3
1	A	289	ALA	4.3
1	C	386	GLU	4.3
1	A	236	GLU	4.3
1	B	303	VAL	4.2
1	A	303	VAL	4.2
1	C	303	VAL	4.2
1	D	344	GLY	4.1
1	B	306	PHE	4.1
1	D	306	PHE	4.1
1	C	278	ARG	4.1
1	A	9	PRO	4.1
1	A	305	SER	4.1
1	C	236	GLU	4.0
1	D	8	THR	3.9
1	C	5	LYS	3.9
1	D	304	GLY	3.9
1	A	275	ALA	3.8
1	C	177	GLU	3.8
1	A	386	GLU	3.7
1	D	302	GLU	3.7
1	C	239	ASP	3.7
1	C	305	SER	3.6
1	C	302	GLU	3.5
1	A	239	ASP	3.5
1	C	307	GLU	3.5
1	B	390	GLU	3.5
1	B	251	GLU	3.5
1	C	275	ALA	3.5
1	D	16	VAL	3.4
1	D	279	GLY	3.4
1	C	433	SER	3.4
1	C	306	PHE	3.4
1	A	265	GLY	3.4
1	C	100	GLY	3.4
1	D	325	ARG	3.4
1	D	122	GLY	3.4
1	D	251	GLU	3.4
1	B	169	ASP	3.4
1	A	210	LEU	3.3
1	B	239	ASP	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	302	GLU	3.3
1	B	207	ARG	3.3
1	A	308	ASP	3.3
1	C	383	PRO	3.3
1	C	238	ALA	3.3
1	D	96	ILE	3.3
1	B	10	LEU	3.3
1	D	6	LEU	3.3
1	B	278	ARG	3.3
1	D	383	PRO	3.3
1	B	240	HIS	3.3
1	D	296	VAL	3.3
1	A	272	ARG	3.2
1	C	212	GLY	3.2
1	C	373	LEU	3.2
1	D	7	ALA	3.2
1	D	119	ALA	3.2
1	B	305	SER	3.1
1	D	123	LEU	3.1
1	D	361	ARG	3.1
1	A	268	ASP	3.1
1	C	390	GLU	3.1
1	D	377	GLU	3.1
1	C	267	LEU	3.1
1	B	249	VAL	3.1
1	B	8	THR	3.1
1	C	299	LEU	3.1
1	C	121	PHE	3.1
1	D	252	ASN	3.1
1	C	414	ASN	3.0
1	D	217	ALA	3.0
1	A	280	LEU	3.0
1	A	176	ASP	3.0
1	A	299	LEU	3.0
1	C	6	LEU	3.0
1	C	268	ASP	3.0
1	A	8	THR	3.0
1	C	449	ARG	2.9
1	B	341	PRO	2.9
1	B	377	GLU	2.9
1	C	22	SER	2.9
1	C	271	GLU	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	95	HIS	2.9
1	C	269	ILE	2.9
1	A	304	GLY	2.9
1	D	266	GLY	2.9
1	A	213	PHE	2.9
1	D	213	PHE	2.9
1	B	262	GLY	2.9
1	B	271	GLU	2.9
1	C	377	GLU	2.9
1	A	269	ILE	2.9
1	B	9	PRO	2.8
1	C	284	VAL	2.8
1	A	283	THR	2.8
1	B	266	GLY	2.8
1	B	344	GLY	2.8
1	C	13	GLN	2.8
1	D	299	LEU	2.8
1	D	305	SER	2.8
1	C	304	GLY	2.8
1	C	344	GLY	2.8
1	C	16	VAL	2.8
1	C	288	ILE	2.8
1	A	240	HIS	2.8
1	C	240	HIS	2.8
1	C	285	SER	2.7
1	A	390	GLU	2.7
1	D	21	ASP	2.7
1	A	341	PRO	2.7
1	B	56	ARG	2.7
1	B	361	ARG	2.7
1	C	342	ALA	2.7
1	D	208	LYS	2.7
1	B	176	ASP	2.7
1	C	341	PRO	2.7
1	D	13	GLN	2.7
1	A	238	ALA	2.7
1	B	282	ARG	2.7
1	A	16	VAL	2.7
1	A	282	ARG	2.6
1	D	384	GLY	2.6
1	B	208	LYS	2.6
1	D	239	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	120	LYS	2.6
1	A	7	ALA	2.6
1	D	289	ALA	2.6
1	C	280	LEU	2.6
1	C	15	GLU	2.6
1	D	201	GLN	2.6
1	A	267	LEU	2.5
1	C	247	VAL	2.5
1	C	315	ILE	2.5
1	D	200	VAL	2.5
1	B	289	ALA	2.5
1	B	285	SER	2.5
1	D	124	ALA	2.5
1	D	71	GLY	2.5
1	A	270	ALA	2.5
1	B	238	ALA	2.5
1	C	308	ASP	2.4
1	D	210	LEU	2.4
1	C	19	PRO	2.4
1	D	93	SER	2.4
1	B	236	GLU	2.4
1	C	217	ALA	2.4
1	C	220	VAL	2.4
1	C	347	VAL	2.4
1	D	207	ARG	2.4
1	C	208	LYS	2.4
1	D	103	ALA	2.4
1	C	61	ASN	2.4
1	A	288	ILE	2.4
1	B	383	PRO	2.4
1	A	281	GLY	2.4
1	D	20	ASP	2.4
1	D	56	ARG	2.4
1	D	285	SER	2.4
1	D	390	GLU	2.4
1	B	26	ALA	2.4
1	C	211	ALA	2.4
1	D	321	MET	2.4
1	C	210	LEU	2.4
1	D	267	LEU	2.4
1	A	328	GLU	2.4
1	C	421	GLU	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	93	SER	2.4
1	B	283	THR	2.4
1	D	449	ARG	2.3
1	B	272	ARG	2.3
1	D	272	ARG	2.3
1	C	281	GLY	2.3
1	A	15	GLU	2.3
1	C	328	GLU	2.3
1	D	308	ASP	2.3
1	A	101	SER	2.3
1	B	22	SER	2.3
1	C	227	LEU	2.3
1	B	196	THR	2.3
1	B	427	TYR	2.3
1	A	309	GLY	2.3
1	B	82	GLY	2.3
1	D	238	ALA	2.3
1	D	430	GLU	2.3
1	C	273	ASP	2.3
1	D	120	LYS	2.3
1	B	431	VAL	2.3
1	C	9	PRO	2.3
1	B	58	ALA	2.3
1	B	217	ALA	2.3
1	D	342	ALA	2.3
1	C	120	LYS	2.3
1	C	56	ARG	2.3
1	B	354	MET	2.2
1	B	11	SER	2.2
1	C	381	ALA	2.2
1	D	376	ALA	2.2
1	D	387	LYS	2.2
1	A	201	GLN	2.2
1	C	101	SER	2.2
1	D	307	GLU	2.2
1	C	176	ASP	2.2
1	C	55	VAL	2.2
1	C	216	TRP	2.2
1	D	260	CYS	2.2
1	A	384	GLY	2.2
1	D	346	SER	2.2
1	C	251	GLU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	271	GLU	2.2
1	B	273	ASP	2.2
1	A	208	LYS	2.2
1	B	213	PHE	2.2
1	C	57	TYR	2.2
1	C	69	SER	2.2
1	C	334	LEU	2.2
1	B	445	GLU	2.2
1	C	58	ALA	2.2
1	A	273	ASP	2.1
1	B	281	GLY	2.1
1	B	227	LEU	2.1
1	B	299	LEU	2.1
1	D	429	PRO	2.1
1	A	286	ASP	2.1
1	A	401	ARG	2.1
1	D	28	ALA	2.1
1	B	214	ILE	2.1
1	C	39	PRO	2.1
1	D	17	ILE	2.1
1	D	290	VAL	2.1
1	D	341	PRO	2.1
1	C	361	ARG	2.1
1	C	401	ARG	2.1
1	D	278	ARG	2.1
1	B	216	TRP	2.1
1	D	177	GLU	2.1
1	D	11	SER	2.0
1	D	348	LYS	2.0
1	B	16	VAL	2.0
1	D	281	GLY	2.0
1	D	367	ARG	2.0
1	C	405	THR	2.0
1	C	270	ALA	2.0
1	A	177	GLU	2.0
1	A	377	GLU	2.0
1	B	339	SER	2.0
1	D	202	LEU	2.0
1	D	282	ARG	2.0
1	A	302	GLU	2.0
1	B	442	TYR	2.0
1	C	290	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

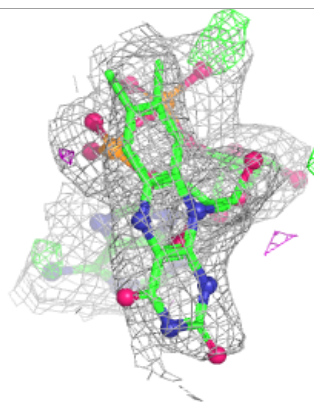
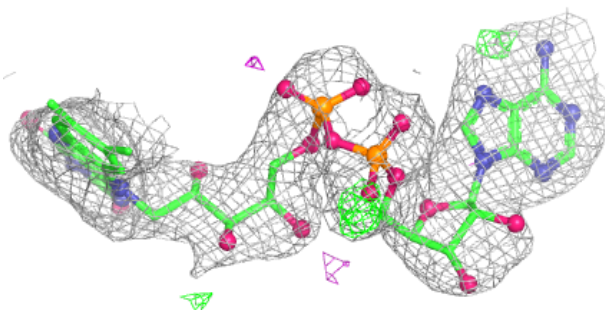
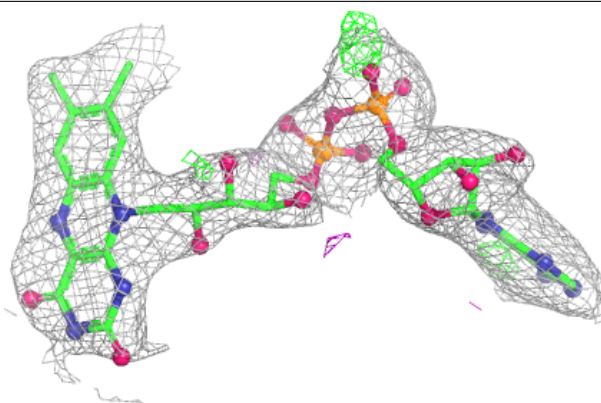
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	B	600	53/53	0.90	0.14	41,45,54,54	0
2	FAD	C	600	53/53	0.93	0.12	37,40,49,50	0
2	FAD	D	600	53/53	0.93	0.13	42,46,55,55	0
2	FAD	A	600	53/53	0.95	0.12	27,30,39,40	0

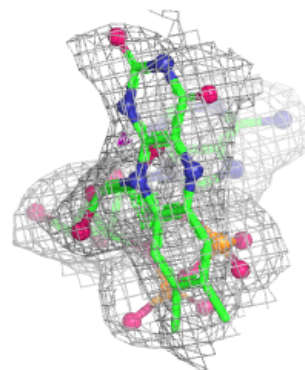
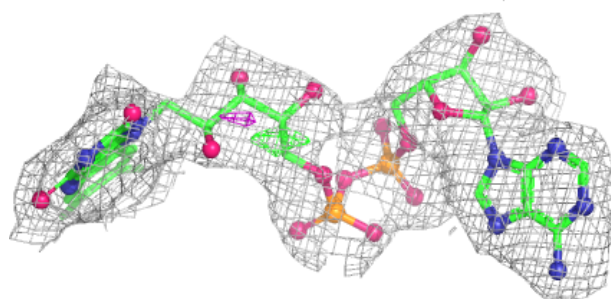
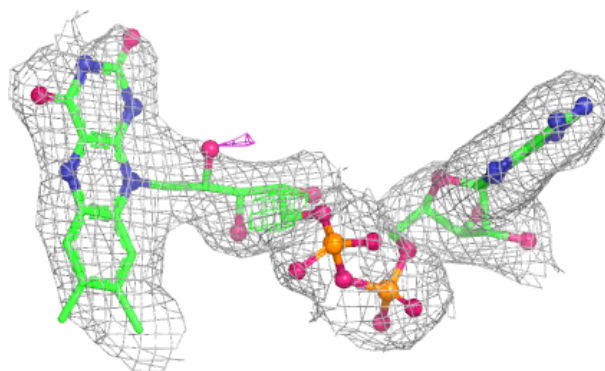
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 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)

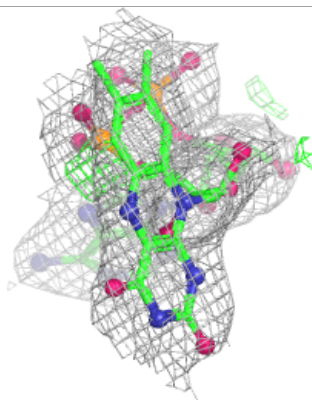
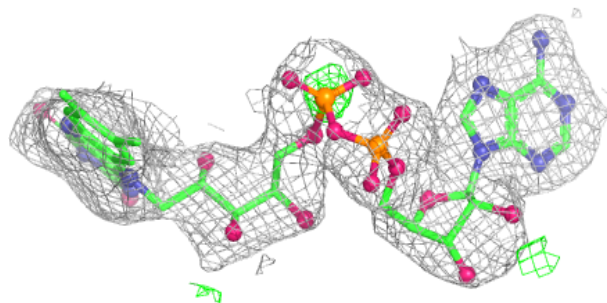
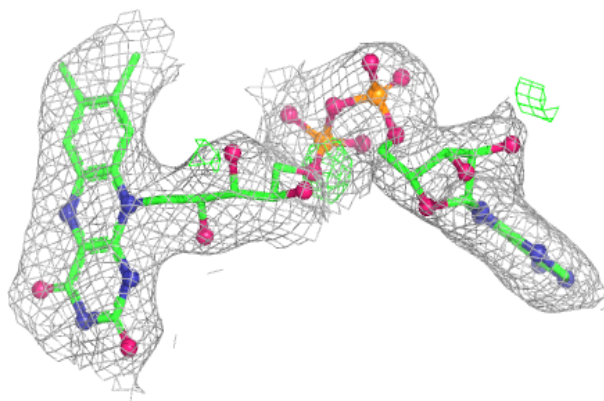
**Electron density around FAD C 600:**

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

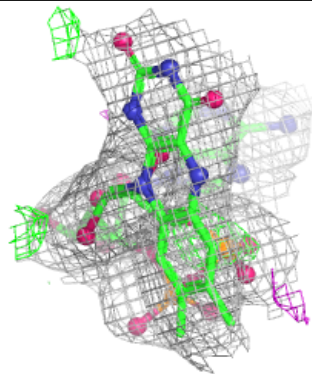
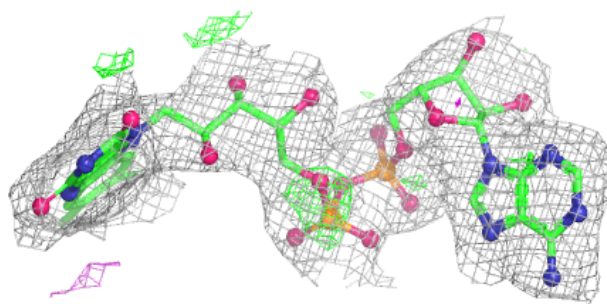
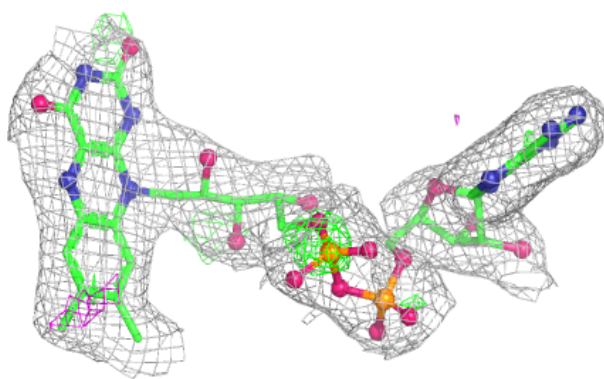


Electron density around FAD D 600:

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

**Electron density around FAD A 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.