



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:15 PM UTC

PDB ID : 3W4J / pdb_00003w4j
Title : Crystal Structure of human DAAO in complex with compound 12
Authors : Hondo, T.; Warizaya, M.; Niimi, T.; Namatame, I.; Yamaguchi, T.; Nakanishi, K.; Hamajima, T.; Harada, K.; Sakashita, H.; Matsumoto, Y.; Orita, M.; Watanabe, T.; Takeuchi, M.
Deposited on : 2013-01-09
Resolution : 2.74 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

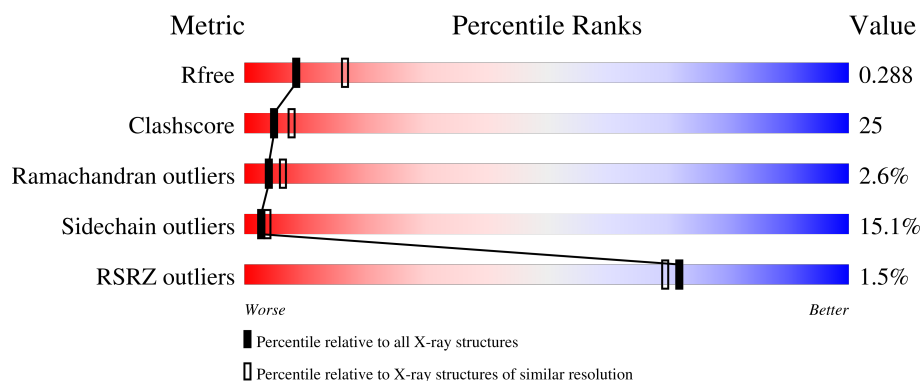
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.74 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	347	0% 51% 36% 10% ..
1	B	347	49% 39% 9% ..
1	C	347	2% 47% 38% 12% ..
1	D	347	3% 48% 37% 11% ..

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	2LD	D	402	-	-	X	-

2 Entry composition [i](#)

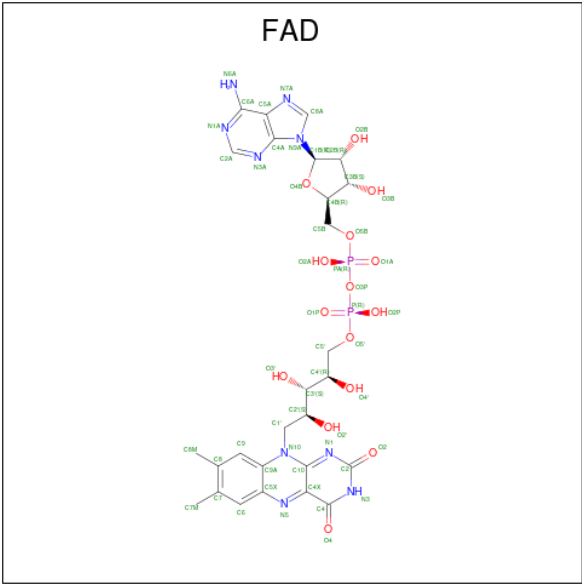
There are 3 unique types of molecules in this entry. The entry contains 11208 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 D-amino-acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2733	1751	479	494	9			
1	B	340	Total	C	N	O	S	0	0	0
			2733	1751	479	494	9			
1	C	340	Total	C	N	O	S	0	0	0
			2733	1751	479	494	9			
1	D	340	Total	C	N	O	S	0	0	0
			2733	1751	479	494	9			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



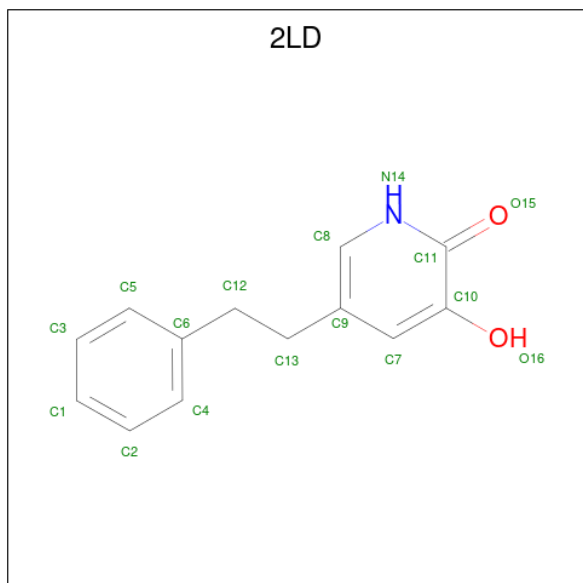
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is 3-hydroxy-5-(2-phenylethyl)pyridin-2(1H)-one (CCD ID: 2LD) (formula: $C_{13}H_{13}NO_2$).

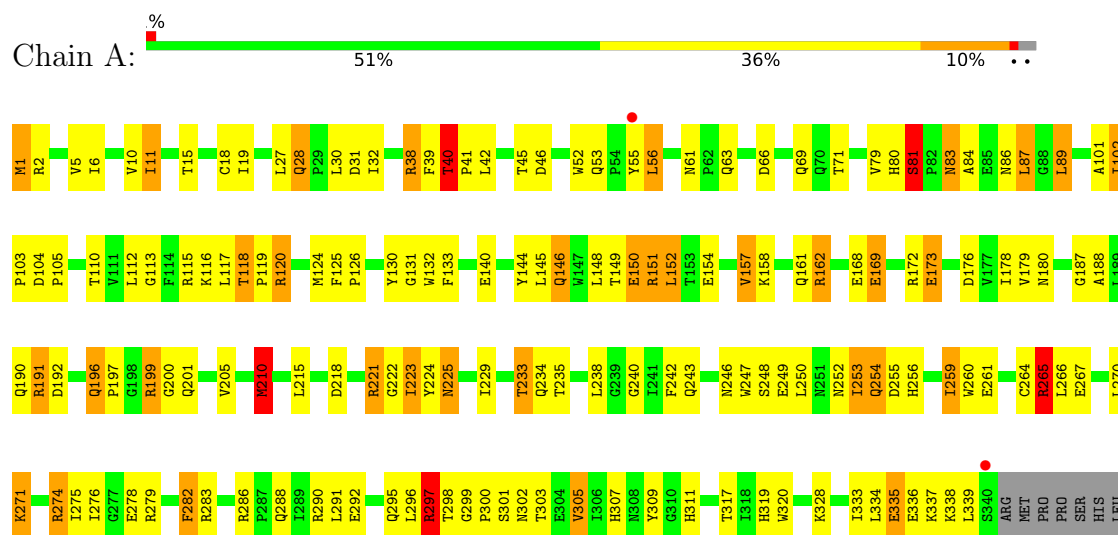


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O		0	0
			16	13	1	2			
3	B	1	Total	C	N	O		0	0
			16	13	1	2			
3	C	1	Total	C	N	O		0	0
			16	13	1	2			
3	D	1	Total	C	N	O		0	0
			16	13	1	2			

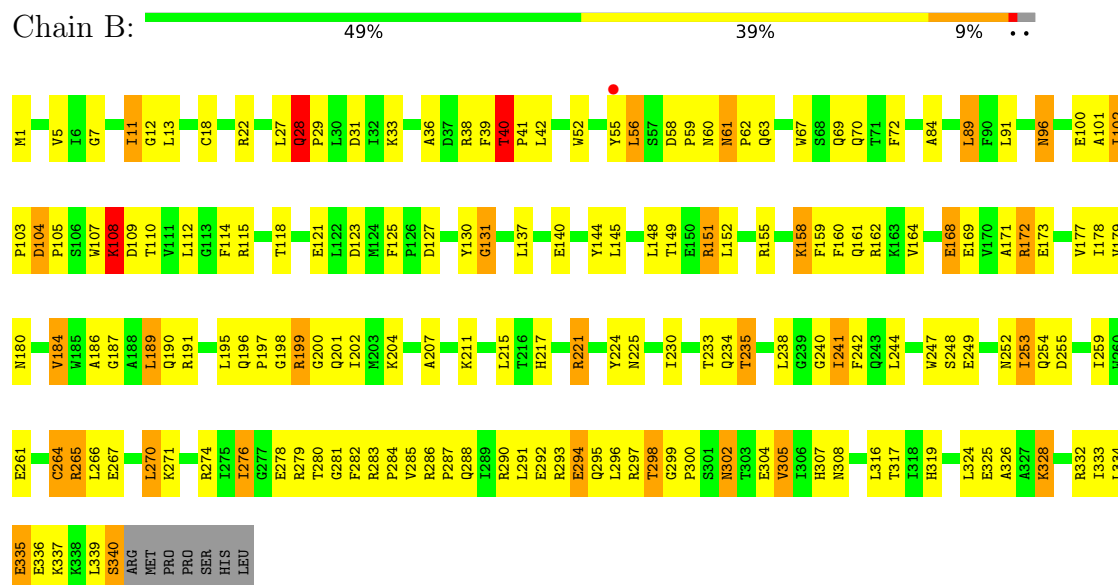
3 Residue-property plots

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.

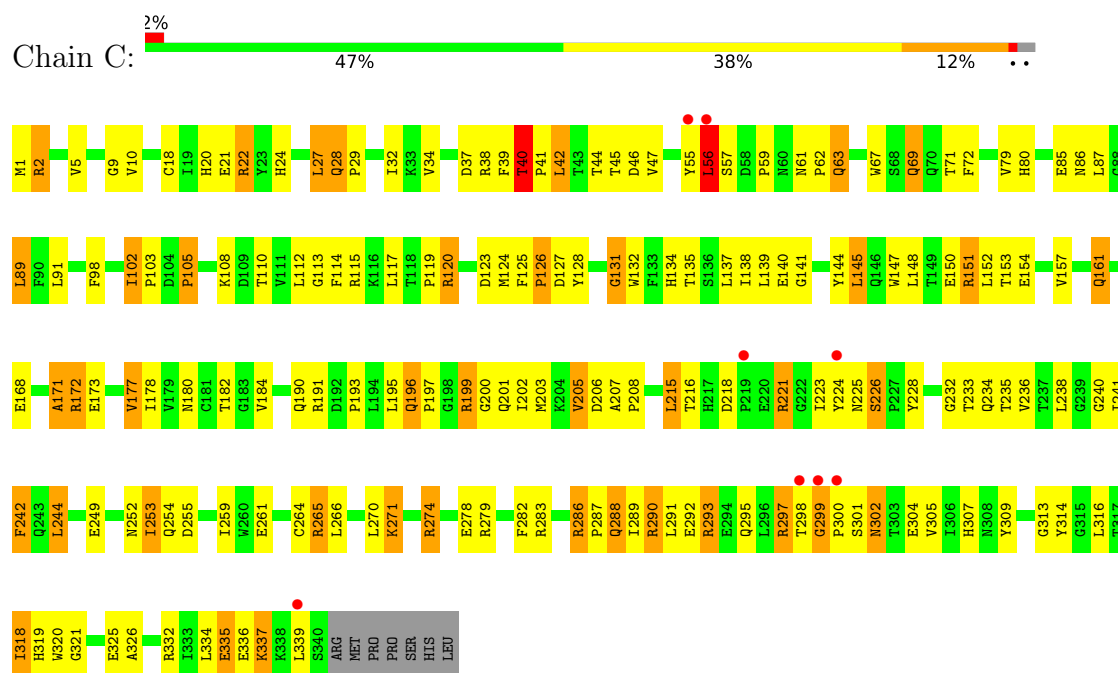
• Molecule 1: D-amino-acid oxidase



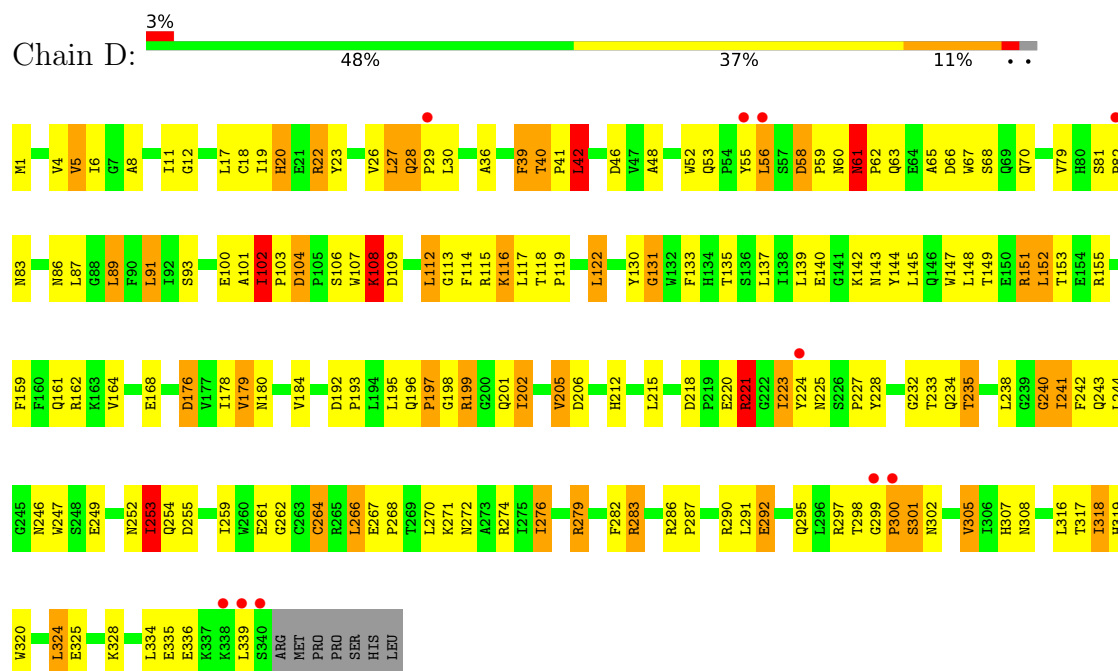
• Molecule 1: D-amino-acid oxidase



• Molecule 1: D-amino-acid oxidase



• Molecule 1: D-amino-acid oxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	149.25Å 182.32Å 50.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.74 50.00 – 2.74	Depositor EDS
% Data completeness (in resolution range)	97.5 (50.00-2.74) 97.6 (50.00-2.74)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.73Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.210 , 0.290 0.211 , 0.288	Depositor DCC
R_{free} test set	1826 reflections (4.88%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11208	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 28.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.7704e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 2LD, 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	1.33	8/2810 (0.3%)	1.51	38/3824 (1.0%)
1	B	1.34	11/2810 (0.4%)	1.41	24/3824 (0.6%)
1	C	1.21	4/2810 (0.1%)	1.34	27/3824 (0.7%)
1	D	1.19	5/2810 (0.2%)	1.38	31/3824 (0.8%)
All	All	1.27	28/11240 (0.2%)	1.41	120/15296 (0.8%)

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

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

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	89	LEU	CA-C	-8.03	1.42	1.52
1	B	96	ASN	CA-C	7.70	1.62	1.52
1	B	244	LEU	N-CA	7.11	1.55	1.46
1	D	253	ILE	CA-C	6.67	1.61	1.52
1	C	207	ALA	CA-CB	-6.39	1.46	1.53
1	D	6	ILE	CA-CB	-6.22	1.46	1.54
1	A	253	ILE	CA-C	6.10	1.60	1.52
1	B	184	VAL	CA-CB	-5.99	1.46	1.54
1	D	48	ALA	CA-CB	-5.96	1.44	1.53
1	A	210	MET	CA-C	-5.88	1.45	1.52
1	C	265	ARG	CA-C	-5.81	1.45	1.52
1	A	11	ILE	CA-CB	-5.79	1.47	1.54
1	B	207	ALA	CA-CB	-5.75	1.45	1.53
1	A	267	GLU	N-CA	-5.63	1.41	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	THR	C-O	-5.54	1.17	1.24
1	D	61	ASN	CA-C	5.52	1.57	1.52
1	A	229	ILE	CA-CB	5.41	1.61	1.54
1	B	70	GLN	CA-C	-5.31	1.46	1.52
1	A	259	ILE	CA-CB	5.22	1.61	1.54
1	B	276	ILE	CA-C	-5.17	1.46	1.52
1	B	326	ALA	CA-CB	-5.16	1.45	1.53
1	C	56	LEU	CA-C	5.12	1.59	1.52
1	B	70	GLN	C-O	-5.08	1.18	1.24
1	D	102	ILE	CA-CB	5.07	1.60	1.54
1	B	11	ILE	CA-C	5.03	1.58	1.52
1	B	230	ILE	CA-CB	-5.01	1.47	1.54
1	A	225	ASN	CA-C	-5.01	1.46	1.52
1	C	57	SER	CA-C	5.01	1.58	1.52

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	THR	CA-C-N	-14.63	104.86	119.64
1	A	40	THR	C-N-CA	-14.63	104.86	119.64
1	B	28	GLN	CA-C-N	-9.55	108.37	120.79
1	B	28	GLN	C-N-CA	-9.55	108.37	120.79
1	A	28	GLN	CA-C-N	-9.14	108.41	119.84
1	A	28	GLN	C-N-CA	-9.14	108.41	119.84
1	C	40	THR	N-CA-C	8.68	129.00	109.81
1	B	40	THR	CA-C-N	-8.48	109.23	119.84
1	B	40	THR	C-N-CA	-8.48	109.23	119.84
1	D	118	THR	CA-C-N	-8.44	111.09	119.87
1	D	118	THR	C-N-CA	-8.44	111.09	119.87
1	B	40	THR	N-CA-C	8.39	128.36	109.81
1	D	131	GLY	N-CA-C	8.27	122.62	110.38
1	A	265	ARG	N-CA-C	-8.10	102.45	111.28
1	C	265	ARG	N-CA-C	-7.77	102.75	111.14
1	A	118	THR	CA-C-N	-7.69	111.72	119.56
1	A	118	THR	C-N-CA	-7.69	111.72	119.56
1	A	199	ARG	NE-CZ-NH1	-7.59	113.91	121.50
1	D	324	LEU	N-CA-C	-7.56	103.12	111.36
1	A	40	THR	N-CA-C	7.53	126.45	109.81
1	A	199	ARG	NE-CZ-NH2	7.51	125.96	119.20
1	A	131	GLY	N-CA-C	7.32	121.24	110.63
1	D	192	ASP	CA-C-N	-7.32	112.51	121.00
1	D	192	ASP	C-N-CA	-7.32	112.51	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	337	LYS	N-CA-C	-7.24	102.76	113.61
1	D	6	ILE	CB-CA-C	-7.05	101.32	110.98
1	A	267	GLU	CA-C-N	-7.04	112.45	119.56
1	A	267	GLU	C-N-CA	-7.04	112.45	119.56
1	D	28	GLN	CA-C-N	-6.87	111.25	119.84
1	D	28	GLN	C-N-CA	-6.87	111.25	119.84
1	D	40	THR	CA-C-N	-6.86	111.92	119.19
1	D	40	THR	C-N-CA	-6.86	111.92	119.19
1	D	4	VAL	N-CA-C	6.85	117.74	107.80
1	C	86	ASN	N-CA-C	6.84	118.82	111.36
1	C	102	ILE	CA-C-N	-6.76	113.34	120.03
1	C	102	ILE	C-N-CA	-6.76	113.34	120.03
1	A	148	LEU	N-CA-C	-6.68	104.00	111.28
1	C	286	ARG	CA-C-N	-6.57	113.38	119.82
1	C	286	ARG	C-N-CA	-6.57	113.38	119.82
1	D	58	ASP	CA-C-N	-6.56	113.01	119.90
1	D	58	ASP	C-N-CA	-6.56	113.01	119.90
1	D	104	ASP	CA-C-N	-6.47	113.97	120.31
1	D	104	ASP	C-N-CA	-6.47	113.97	120.31
1	B	40	THR	CB-CA-C	-6.45	97.47	110.17
1	B	241	ILE	N-CA-C	6.45	116.91	107.37
1	A	196	GLN	CA-C-N	6.34	126.67	119.83
1	A	196	GLN	C-N-CA	6.34	126.67	119.83
1	C	42	LEU	N-CA-C	6.33	120.79	111.87
1	C	24	HIS	N-CA-C	-6.32	105.57	113.28
1	A	157	VAL	N-CA-C	-6.30	100.58	108.89
1	B	89	LEU	CB-CA-C	-6.21	99.05	109.48
1	D	193	PRO	N-CA-C	-6.20	107.54	114.92
1	D	221	ARG	N-CA-C	6.14	119.87	112.38
1	C	232	GLY	N-CA-C	-6.05	104.46	112.81
1	B	199	ARG	NE-CZ-NH1	-6.01	115.48	121.50
1	B	58	ASP	N-CA-C	5.99	117.35	109.93
1	D	305	VAL	N-CA-C	5.99	116.70	107.78
1	B	328	LYS	N-CA-C	-5.96	103.75	111.02
1	C	271	LYS	N-CA-C	5.93	118.50	111.33
1	A	173	GLU	N-CA-C	5.92	120.11	113.01
1	C	40	THR	CB-CA-C	-5.88	98.59	110.17
1	D	42	LEU	CB-CA-C	-5.85	102.04	111.28
1	A	83	ASN	N-CA-C	-5.84	106.69	113.88
1	B	42	LEU	N-CA-C	5.82	119.94	112.26
1	C	40	THR	CA-C-N	-5.81	113.77	119.64
1	C	40	THR	C-N-CA	-5.81	113.77	119.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	272	ASN	CA-C-N	-5.81	112.17	122.74
1	D	272	ASN	C-N-CA	-5.81	112.17	122.74
1	A	66	ASP	N-CA-C	5.80	117.60	111.28
1	A	328	LYS	N-CA-C	-5.79	104.66	110.97
1	A	118	THR	N-CA-C	-5.77	102.84	110.40
1	A	18	CYS	N-CA-C	-5.77	105.74	112.89
1	A	283	ARG	CA-C-N	-5.75	112.65	119.84
1	A	283	ARG	C-N-CA	-5.75	112.65	119.84
1	B	230	ILE	CA-C-N	-5.69	114.07	119.76
1	B	230	ILE	C-N-CA	-5.69	114.07	119.76
1	B	305	VAL	N-CA-C	5.64	115.98	107.80
1	B	84	ALA	N-CA-C	5.63	118.15	111.33
1	C	9	GLY	N-CA-C	-5.63	103.96	112.41
1	C	131	GLY	N-CA-C	5.57	117.59	110.96
1	B	189	LEU	N-CA-C	-5.57	107.73	114.75
1	A	210	MET	N-CA-C	-5.54	99.49	108.41
1	A	200	GLY	N-CA-C	-5.52	102.46	110.90
1	C	318	ILE	N-CA-C	5.51	118.45	113.10
1	A	192	ASP	CA-C-N	-5.50	114.08	119.64
1	A	192	ASP	C-N-CA	-5.50	114.08	119.64
1	A	40	THR	CB-CA-C	-5.47	99.39	110.17
1	A	81	SER	CA-C-N	-5.42	113.06	119.84
1	A	81	SER	C-N-CA	-5.42	113.06	119.84
1	A	187	GLY	N-CA-C	5.41	119.19	112.64
1	C	69	GLN	N-CA-C	-5.40	105.39	111.28
1	A	282	PHE	N-CA-C	5.40	117.22	108.41
1	D	40	THR	N-CA-C	5.39	121.72	109.81
1	D	199	ARG	NE-CZ-NH1	-5.37	116.14	121.50
1	D	20	HIS	N-CA-C	5.36	117.81	111.33
1	D	197	PRO	N-CA-C	5.36	119.00	110.21
1	A	311	HIS	N-CA-C	-5.36	107.12	113.97
1	D	199	ARG	CG-CD-NE	-5.34	100.25	112.00
1	C	235	THR	CA-C-N	-5.33	116.58	123.19
1	C	235	THR	C-N-CA	-5.33	116.58	123.19
1	C	226	SER	N-CA-C	-5.32	101.95	110.10
1	B	61	ASN	CA-C-N	-5.27	115.46	120.83
1	B	61	ASN	C-N-CA	-5.27	115.46	120.83
1	D	30	LEU	N-CA-C	5.24	117.86	108.17
1	B	131	GLY	N-CA-C	5.21	118.19	110.42
1	B	72	PHE	N-CA-C	5.20	117.69	111.71
1	B	199	ARG	NE-CZ-NH2	5.18	123.86	119.20
1	C	2	ARG	N-CA-C	-5.18	100.07	108.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	288	GLN	N-CA-C	5.17	116.28	108.07
1	D	292	GLU	N-CA-C	5.14	116.10	108.60
1	B	162	ARG	N-CA-C	5.13	116.87	108.76
1	A	276	ILE	CB-CA-C	-5.12	106.57	111.44
1	C	177	VAL	N-CA-C	5.11	116.02	108.45
1	C	153	THR	N-CA-C	-5.10	105.37	111.03
1	B	253	ILE	N-CA-C	5.09	119.92	109.34
1	D	48	ALA	N-CA-C	5.07	117.70	110.24
1	D	205	VAL	CB-CA-C	5.06	118.19	110.90
1	A	53	GLN	CA-C-N	5.06	125.77	120.11
1	A	53	GLN	C-N-CA	5.06	125.77	120.11
1	C	199	ARG	NE-CZ-NH1	-5.01	116.49	121.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	39	PHE	Peptide

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	2733	0	2680	128	0
1	B	2733	0	2680	132	0
1	C	2733	0	2680	170	0
1	D	2733	0	2680	149	0
2	A	53	0	31	3	0
2	B	53	0	31	1	0
2	C	53	0	31	5	0
2	D	53	0	31	2	0
3	A	16	0	13	1	0
3	B	16	0	12	1	0
3	C	16	0	13	1	0
3	D	16	0	13	6	0
All	All	11208	0	10895	558	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 25.

All (558) 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:264:CYS:HB3	1:C:271:LYS:HZ2	1.08	1.19
1:B:221:ARG:CB	1:B:221:ARG:HH21	1.62	1.13
1:A:1:MET:CE	1:A:176:ASP:HB2	1.79	1.12
1:D:221:ARG:HB2	1:D:221:ARG:HH21	1.09	1.10
1:A:1:MET:HE1	1:A:176:ASP:HB2	1.27	1.09
1:D:22:ARG:HG3	1:D:22:ARG:HH21	1.04	1.08
1:D:221:ARG:HB2	1:D:221:ARG:NH2	1.69	1.08
1:C:264:CYS:HB3	1:C:271:LYS:NZ	1.68	1.07
1:D:264:CYS:SG	1:D:271:LYS:HD2	1.97	1.04
1:C:274:ARG:HE	1:C:274:ARG:HA	1.18	1.03
1:C:264:CYS:SG	1:C:271:LYS:HD3	1.99	1.03
1:A:290:ARG:HD2	1:A:292:GLU:OE2	1.61	1.01
1:A:221:ARG:HB2	1:A:221:ARG:CZ	1.92	0.98
1:D:297:ARG:HA	1:D:302:ASN:HB3	1.44	0.97
1:D:22:ARG:HH21	1:D:22:ARG:CG	1.78	0.97
1:D:283:ARG:HH21	1:D:283:ARG:HG3	1.29	0.97
1:A:180:ASN:HD22	1:A:307:HIS:HD2	1.06	0.95
1:B:264:CYS:SG	1:B:271:LYS:HG3	2.09	0.92
1:A:335:GLU:HG2	1:A:336:GLU:N	1.84	0.92
1:B:55:TYR:HE1	1:B:224:TYR:OH	1.50	0.92
1:D:283:ARG:NE	3:D:402:2LD:O15	2.01	0.92
1:B:290:ARG:HD2	1:B:292:GLU:OE2	1.70	0.92
1:B:180:ASN:HD22	1:B:307:HIS:HD2	1.00	0.91
1:A:55:TYR:HE1	1:A:224:TYR:HH	1.18	0.91
1:D:22:ARG:HG3	1:D:22:ARG:NH2	1.77	0.89
1:C:221:ARG:HB2	1:C:221:ARG:NH2	1.88	0.89
1:A:55:TYR:CE1	1:A:224:TYR:OH	2.23	0.89
1:D:55:TYR:HE1	1:D:224:TYR:OH	1.57	0.88
1:A:55:TYR:HE1	1:A:224:TYR:OH	1.53	0.88
1:B:221:ARG:HH21	1:B:221:ARG:HB3	1.37	0.88
1:B:221:ARG:HH21	1:B:221:ARG:HB2	1.37	0.87
1:A:180:ASN:HD22	1:A:307:HIS:CD2	1.92	0.87
1:B:264:CYS:HB3	1:B:271:LYS:HE3	1.54	0.86
1:C:2:ARG:HH21	1:C:2:ARG:HG2	1.38	0.86
1:A:1:MET:HE1	1:A:176:ASP:CB	2.06	0.85
1:C:40:THR:HG23	1:C:41:PRO:HD3	1.59	0.85
1:A:297:ARG:HA	1:A:302:ASN:HB3	1.57	0.84

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:ASN:HD22	1:B:307:HIS:CD2	1.92	0.84
1:C:264:CYS:SG	1:C:271:LYS:CD	2.66	0.83
1:C:151:ARG:HH11	1:C:154:GLU:CD	1.88	0.82
1:B:40:THR:O	1:B:40:THR:OG1	1.88	0.81
1:C:39:PHE:O	1:C:41:PRO:HD2	1.79	0.81
1:C:252:ASN:HD22	1:C:255:ASP:H	1.27	0.81
1:D:91:LEU:HD23	1:D:137:LEU:HD23	1.62	0.81
1:C:120:ARG:HA	1:C:120:ARG:HE	1.44	0.81
1:B:221:ARG:CB	1:B:221:ARG:NH2	2.43	0.80
1:D:59:PRO:HG2	1:D:65:ALA:HB2	1.63	0.80
1:D:1:MET:HE1	1:D:176:ASP:HB2	1.63	0.80
1:D:252:ASN:HD21	1:D:254:GLN:HB2	1.45	0.80
1:D:55:TYR:HE1	1:D:224:TYR:HH	0.80	0.80
1:C:28:GLN:HB3	1:C:29:PRO:HD3	1.62	0.79
1:B:91:LEU:HD23	1:B:137:LEU:HD23	1.65	0.79
1:B:59:PRO:HG2	1:B:62:PRO:HA	1.63	0.79
1:B:252:ASN:HD22	1:B:255:ASP:H	1.31	0.79
1:C:38:ARG:NH2	2:C:401:FAD:H2B	1.98	0.79
1:C:61:ASN:HD21	1:C:63:GLN:HE21	1.28	0.78
1:C:199:ARG:HH12	1:C:201:GLN:HE21	1.32	0.77
1:D:255:ASP:O	1:D:259:ILE:HG13	1.85	0.77
1:A:1:MET:CE	1:A:176:ASP:CB	2.62	0.76
1:B:33:LYS:HG2	1:B:160:PHE:HE1	1.50	0.76
1:B:221:ARG:HB3	1:B:221:ARG:NH2	2.00	0.76
1:D:223:ILE:HG13	1:D:224:TYR:CD2	2.21	0.75
1:B:11:ILE:CG2	1:B:308:ASN:ND2	2.50	0.74
1:B:55:TYR:HE1	1:B:224:TYR:HH	0.75	0.74
1:D:102:ILE:HG12	1:D:103:PRO:HD2	1.69	0.74
1:C:289:ILE:HD11	1:C:314:TYR:HE2	1.53	0.73
1:A:69:GLN:NE2	1:A:110:THR:OG1	2.21	0.72
1:D:221:ARG:NH2	1:D:221:ARG:CB	2.50	0.72
1:D:283:ARG:HG3	1:D:283:ARG:NH2	2.03	0.72
1:B:161:GLN:HG3	1:D:249:GLU:O	1.90	0.72
1:B:335:GLU:HG3	1:B:336:GLU:H	1.54	0.72
1:C:150:GLU:O	1:C:154:GLU:HG2	1.89	0.72
1:C:199:ARG:HG3	1:C:282:PHE:CE1	2.24	0.72
1:B:264:CYS:CB	1:B:271:LYS:HE3	2.20	0.71
1:A:335:GLU:HG2	1:A:336:GLU:H	1.54	0.71
1:C:40:THR:CG2	1:C:41:PRO:HD3	2.20	0.71
1:C:264:CYS:CB	1:C:271:LYS:HZ2	1.97	0.71
1:C:274:ARG:HA	1:C:274:ARG:NE	2.01	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ASN:ND2	1:C:255:ASP:H	1.88	0.70
1:B:144:TYR:OH	1:B:319:HIS:HE1	1.73	0.70
1:C:105:PRO:HD2	1:C:108:LYS:HB3	1.74	0.70
1:A:221:ARG:HB2	1:A:221:ARG:NH2	2.07	0.69
1:A:199:ARG:HD2	1:A:248:SER:O	1.92	0.69
1:B:199:ARG:HG3	1:B:282:PHE:CE1	2.28	0.69
1:C:40:THR:O	1:C:40:THR:OG1	2.11	0.69
1:C:102:ILE:HG13	1:C:103:PRO:HD2	1.75	0.69
1:B:11:ILE:HG22	1:B:308:ASN:ND2	2.08	0.68
1:B:28:GLN:HB3	1:B:29:PRO:HD3	1.75	0.68
1:A:291:LEU:HA	1:A:307:HIS:O	1.93	0.68
1:B:298:THR:HG23	1:B:298:THR:O	1.92	0.68
1:A:274:ARG:HD2	1:D:274:ARG:HH12	1.58	0.68
1:B:286:ARG:HG2	1:B:288:GLN:O	1.94	0.68
1:C:38:ARG:HH22	2:C:401:FAD:H2B	1.56	0.68
1:C:140:GLU:OE1	1:C:233:THR:HB	1.94	0.68
1:A:5:VAL:HG22	1:A:179:VAL:HB	1.77	0.67
1:D:18:CYS:SG	1:D:324:LEU:HD23	2.34	0.67
1:D:55:TYR:HE1	1:D:224:TYR:CZ	2.12	0.67
1:B:293:ARG:HD3	1:B:333:ILE:HD11	1.76	0.67
1:D:27:LEU:HD21	1:D:339:LEU:HD23	1.77	0.66
1:B:91:LEU:HD23	1:B:137:LEU:CD2	2.25	0.66
1:B:180:ASN:ND2	1:B:307:HIS:HD2	1.84	0.66
1:C:199:ARG:HG3	1:C:282:PHE:HE1	1.61	0.66
1:C:79:VAL:HG13	1:C:80:HIS:CD2	2.31	0.66
1:C:172:ARG:HH12	1:C:299:GLY:HA3	1.61	0.66
1:A:264:CYS:HB3	1:A:271:LYS:NZ	2.11	0.65
1:B:249:GLU:H	1:D:161:GLN:HE21	1.42	0.65
1:A:252:ASN:HD22	1:A:255:ASP:H	1.45	0.65
1:C:2:ARG:HG2	1:C:2:ARG:NH2	2.11	0.65
1:D:102:ILE:CG1	1:D:103:PRO:HD2	2.27	0.65
1:D:283:ARG:HG2	2:D:401:FAD:HM82	1.79	0.65
1:B:39:PHE:O	1:B:41:PRO:HD2	1.95	0.65
1:A:15:THR:HG21	1:A:179:VAL:HG11	1.79	0.65
1:C:140:GLU:OE1	1:C:233:THR:CG2	2.45	0.65
1:C:91:LEU:HD23	1:C:137:LEU:CD2	2.28	0.64
1:A:252:ASN:HD21	1:A:254:GLN:HB2	1.61	0.64
1:D:201:GLN:HE22	1:D:252:ASN:H	1.44	0.64
1:A:264:CYS:CB	1:A:271:LYS:HZ2	2.11	0.64
1:D:91:LEU:HD23	1:D:137:LEU:CD2	2.26	0.64
1:A:218:ASP:OD2	1:A:221:ARG:NH1	2.30	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:PHE:CD1	1:B:242:PHE:C	2.76	0.63
1:B:177:VAL:HG22	1:B:304:GLU:HB2	1.79	0.63
1:C:199:ARG:HH12	1:C:201:GLN:NE2	1.95	0.63
1:B:27:LEU:HD21	1:B:334:LEU:HD21	1.80	0.63
1:A:105:PRO:HD3	1:A:132:TRP:CZ2	2.34	0.63
1:B:233:THR:HG23	1:B:234:GLN:HG2	1.79	0.63
1:C:221:ARG:HB2	1:C:221:ARG:HH21	1.63	0.63
1:D:318:ILE:O	1:D:319:HIS:C	2.41	0.63
1:A:140:GLU:OE1	1:A:233:THR:HB	1.98	0.63
1:C:10:VAL:HB	1:C:45:THR:HG21	1.81	0.62
1:A:286:ARG:HH21	1:A:286:ARG:HG2	1.65	0.62
1:C:274:ARG:HE	1:C:274:ARG:CA	2.04	0.62
1:B:264:CYS:SG	1:B:271:LYS:HE3	2.40	0.62
1:A:61:ASN:HD21	1:A:63:GLN:NE2	1.97	0.62
1:B:297:ARG:HA	1:B:302:ASN:HB3	1.81	0.62
1:A:10:VAL:HB	1:A:45:THR:HG21	1.82	0.62
1:D:39:PHE:O	1:D:41:PRO:HD2	1.99	0.61
1:A:1:MET:HG2	1:A:27:LEU:HD13	1.81	0.61
1:A:144:TYR:OH	1:A:319:HIS:HE1	1.83	0.61
1:D:252:ASN:ND2	1:D:254:GLN:HB2	2.13	0.61
1:A:260:TRP:CD1	1:A:260:TRP:C	2.77	0.61
1:B:225:ASN:HA	1:B:240:GLY:O	2.00	0.61
1:B:255:ASP:O	1:B:259:ILE:HG13	2.01	0.61
1:C:242:PHE:CD1	1:C:242:PHE:C	2.79	0.61
1:A:101:ALA:HA	1:A:130:TYR:CD2	2.35	0.61
1:A:178:ILE:HB	1:A:305:VAL:HG22	1.83	0.60
1:B:204:LYS:HD2	1:B:235:THR:HG21	1.82	0.60
1:A:201:GLN:HE22	1:A:252:ASN:H	1.47	0.60
1:B:107:TRP:O	1:B:109:ASP:N	2.35	0.60
1:C:91:LEU:HD23	1:C:137:LEU:HD23	1.81	0.60
1:A:56:LEU:HD22	1:A:56:LEU:H	1.66	0.60
1:D:117:LEU:HD12	1:D:131:GLY:HA3	1.82	0.60
1:A:40:THR:O	1:A:40:THR:OG1	2.18	0.60
1:B:144:TYR:OH	1:B:319:HIS:CE1	2.55	0.60
1:A:264:CYS:SG	1:A:271:LYS:HD3	2.42	0.60
1:C:40:THR:HG23	1:C:41:PRO:CD	2.31	0.59
1:C:144:TYR:OH	1:C:319:HIS:HE1	1.85	0.59
1:C:286:ARG:HD3	1:C:288:GLN:O	2.02	0.59
1:A:52:TRP:HE3	1:A:52:TRP:O	1.85	0.59
1:C:293:ARG:NH1	1:C:336:GLU:OE1	2.36	0.59
1:A:286:ARG:HG2	1:A:288:GLN:O	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:GLU:O	1:B:279:ARG:HG2	2.03	0.59
1:C:20:His:C	1:C:22:ARG:H	2.11	0.59
1:C:283:ARG:HG3	2:C:401:FAD:HM82	1.85	0.59
1:D:197:PRO:HG3	1:D:247:TRP:CE2	2.38	0.59
1:A:221:ARG:CZ	1:A:221:ARG:CB	2.73	0.58
1:D:297:ARG:H	1:D:297:ARG:HD3	1.67	0.58
1:A:61:ASN:HB2	1:A:288:GLN:OE1	2.03	0.58
1:A:161:GLN:HG3	1:C:249:GLU:O	2.02	0.58
1:C:180:ASN:HB3	1:C:307:HIS:HD2	1.68	0.58
1:B:5:VAL:HG22	1:B:179:VAL:HB	1.84	0.58
1:C:171:ALA:O	1:C:172:ARG:C	2.47	0.58
1:C:221:ARG:HB2	1:C:221:ARG:CZ	2.32	0.58
1:D:41:PRO:HB2	1:D:42:LEU:HD23	1.84	0.58
1:A:140:GLU:OE1	1:A:233:THR:CG2	2.52	0.58
1:C:141:GLY:O	1:C:145:LEU:HB2	2.04	0.58
1:D:268:PRO:C	1:D:270:LEU:H	2.12	0.58
1:C:178:ILE:HB	1:C:305:VAL:HG22	1.86	0.57
1:A:113:GLY:HA3	1:B:115:ARG:NH1	2.19	0.57
1:B:151:ARG:O	1:B:155:ARG:HG3	2.04	0.57
1:B:168:GLU:O	1:B:172:ARG:HD3	2.04	0.57
1:B:202:ILE:O	1:B:278:GLU:HG3	2.03	0.57
1:C:114:PHE:HZ	1:C:132:TRP:CD1	2.22	0.57
1:B:28:GLN:HB3	1:B:29:PRO:CD	2.35	0.57
1:D:5:VAL:HG13	1:D:179:VAL:HB	1.86	0.57
1:D:23:TYR:HA	1:D:26:VAL:HG22	1.86	0.57
1:B:61:ASN:HD21	1:B:63:GLN:HE21	1.53	0.56
1:C:114:PHE:CZ	1:C:132:TRP:CD1	2.93	0.56
1:D:252:ASN:HD22	1:D:255:ASP:H	1.53	0.56
1:D:58:ASP:OD1	1:D:106:SER:HB3	2.06	0.56
1:B:242:PHE:C	1:B:242:PHE:HD1	2.13	0.56
1:A:1:MET:HG2	1:A:27:LEU:CD1	2.35	0.56
1:C:79:VAL:HG21	1:C:91:LEU:HG	1.87	0.56
1:C:242:PHE:C	1:C:242:PHE:HD1	2.14	0.56
1:D:102:ILE:CD1	1:D:103:PRO:HD2	2.35	0.56
1:B:199:ARG:HG3	1:B:282:PHE:HE1	1.70	0.56
1:C:120:ARG:HB3	1:D:112:LEU:CD1	2.36	0.56
1:C:177:VAL:HG22	1:C:304:GLU:HB2	1.88	0.56
1:D:107:TRP:O	1:D:109:ASP:N	2.39	0.56
1:C:224:TYR:HB2	1:C:242:PHE:HD2	1.70	0.55
1:D:201:GLN:NE2	1:D:252:ASN:H	2.04	0.55
1:B:55:TYR:CE1	1:B:224:TYR:OH	2.38	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:CYS:HB3	1:C:271:LYS:HZ3	1.67	0.55
1:D:232:GLY:N	1:D:235:THR:O	2.35	0.55
1:C:39:PHE:O	1:C:41:PRO:CD	2.53	0.55
1:C:150:GLU:HG3	1:C:151:ARG:NH2	2.22	0.55
1:C:224:TYR:HD2	1:C:242:PHE:CD2	2.24	0.55
1:D:283:ARG:NH2	1:D:283:ARG:CG	2.67	0.55
1:B:18:CYS:SG	1:B:324:LEU:HD23	2.47	0.55
1:C:69:GLN:NE2	1:C:110:THR:OG1	2.40	0.55
1:D:198:GLY:O	1:D:283:ARG:HG3	2.07	0.55
1:D:223:ILE:O	1:D:224:TYR:HB2	2.06	0.55
1:A:210:MET:HE3	1:A:210:MET:HA	1.89	0.54
1:A:256:HIS:C	1:A:256:HIS:CD2	2.85	0.54
1:C:233:THR:HG23	1:C:234:GLN:N	2.22	0.54
1:C:289:ILE:HD11	1:C:314:TYR:CE2	2.38	0.54
1:D:40:THR:O	1:D:46:ASP:OD2	2.25	0.54
1:A:27:LEU:HD12	1:A:30:LEU:HD13	1.88	0.54
1:C:55:TYR:HE1	1:C:224:TYR:HH	1.54	0.54
1:B:27:LEU:HD11	1:B:334:LEU:HD11	1.89	0.54
1:C:287:PRO:O	1:C:288:GLN:HB3	2.07	0.54
1:D:36:ALA:HB3	1:D:39:PHE:CZ	2.43	0.54
1:C:27:LEU:HD11	1:C:334:LEU:HD21	1.89	0.54
1:C:201:GLN:HE22	1:C:252:ASN:H	1.56	0.54
1:D:104:ASP:OD2	1:D:108:LYS:NZ	2.41	0.54
1:C:184:VAL:HG21	1:C:197:PRO:HB3	1.89	0.54
1:C:225:ASN:ND2	1:C:242:PHE:H	2.06	0.54
1:A:197:PRO:HG3	1:A:247:TRP:CE2	2.44	0.53
1:C:120:ARG:HB3	1:D:112:LEU:HD13	1.90	0.53
1:C:264:CYS:CB	1:C:271:LYS:NZ	2.58	0.53
1:A:199:ARG:NH2	1:A:250:LEU:O	2.41	0.53
1:A:255:ASP:O	1:A:259:ILE:HG12	2.08	0.53
1:C:32:ILE:HB	1:C:157:VAL:HG22	1.91	0.53
1:A:233:THR:HG23	1:A:234:GLN:HG2	1.91	0.53
1:D:151:ARG:O	1:D:155:ARG:HD2	2.09	0.53
1:C:297:ARG:HA	1:C:302:ASN:HD22	1.74	0.52
1:D:178:ILE:HB	1:D:305:VAL:HG22	1.91	0.52
1:B:140:GLU:OE1	1:B:233:THR:CG2	2.57	0.52
1:B:337:LYS:HB3	1:B:339:LEU:HD13	1.90	0.52
1:C:89:LEU:HA	1:C:138:ILE:O	2.10	0.52
1:C:201:GLN:NE2	1:C:252:ASN:H	2.07	0.52
1:D:112:LEU:CD2	1:D:112:LEU:N	2.73	0.52
1:A:61:ASN:OD1	1:A:63:GLN:HB2	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:GLU:HG3	1:A:151:ARG:NH2	2.24	0.52
1:B:299:GLY:O	1:B:300:PRO:C	2.53	0.52
1:C:39:PHE:C	1:C:41:PRO:HD2	2.34	0.52
1:C:278:GLU:O	1:C:279:ARG:HG2	2.08	0.52
1:D:297:ARG:HG3	1:D:302:ASN:HD22	1.75	0.52
1:A:297:ARG:HB2	1:A:297:ARG:CZ	2.40	0.52
1:D:112:LEU:N	1:D:112:LEU:HD22	2.24	0.52
1:C:27:LEU:HD11	1:C:334:LEU:CD2	2.40	0.52
1:C:144:TYR:OH	1:C:319:HIS:CE1	2.63	0.52
1:A:274:ARG:HD2	1:D:274:ARG:NH1	2.23	0.52
1:A:296:LEU:O	1:A:302:ASN:HB2	2.10	0.52
1:D:233:THR:HG23	1:D:234:GLN:HG2	1.92	0.52
1:A:120:ARG:HE	1:A:120:ARG:HA	1.75	0.52
1:B:199:ARG:HH12	1:B:201:GLN:NE2	2.08	0.52
1:B:161:GLN:HE21	1:D:249:GLU:H	1.58	0.51
1:C:221:ARG:CZ	1:C:221:ARG:CB	2.88	0.51
1:D:264:CYS:SG	1:D:271:LYS:CD	2.86	0.51
1:D:267:GLU:O	1:D:270:LEU:HB2	2.11	0.51
1:A:199:ARG:NH1	1:A:255:ASP:OD2	2.42	0.51
1:A:146:GLN:O	1:A:149:THR:HB	2.10	0.51
1:C:172:ARG:HH12	1:C:299:GLY:CA	2.23	0.51
1:B:335:GLU:HG3	1:B:336:GLU:N	2.24	0.51
1:D:41:PRO:CB	1:D:42:LEU:HD23	2.41	0.51
1:A:38:ARG:HH21	2:A:401:FAD:H2B	1.75	0.51
1:A:190:GLN:O	1:A:191:ARG:C	2.54	0.51
1:B:202:ILE:HD12	1:B:202:ILE:C	2.36	0.51
1:D:228:TYR:HH	3:D:402:2LD:H13	1.59	0.51
1:C:218:ASP:C	1:C:218:ASP:OD1	2.54	0.51
1:D:42:LEU:HD23	1:D:42:LEU:N	2.26	0.51
1:D:283:ARG:CD	3:D:402:2LD:O15	2.58	0.51
1:A:115:ARG:HG3	1:A:116:LYS:N	2.25	0.51
1:C:37:ASP:HB3	1:C:38:ARG:NH1	2.26	0.51
1:D:196:GLN:HB2	1:D:197:PRO:HD2	1.93	0.51
1:A:125:PHE:O	1:A:126:PRO:C	2.54	0.50
1:B:96:ASN:O	1:B:131:GLY:HA3	2.11	0.50
1:B:316:LEU:O	1:B:319:HIS:HD2	1.94	0.50
1:C:190:GLN:O	1:C:191:ARG:C	2.53	0.50
1:B:335:GLU:HA	1:B:340:SER:HB3	1.93	0.50
1:C:20:HIS:O	1:C:22:ARG:N	2.40	0.50
1:C:40:THR:O	1:C:46:ASP:OD2	2.29	0.50
1:C:140:GLU:OE1	1:C:233:THR:CB	2.59	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:290:ARG:HD2	1:C:292:GLU:OE2	2.11	0.50
1:D:22:ARG:CG	1:D:22:ARG:NH2	2.49	0.50
1:A:38:ARG:HH21	2:A:401:FAD:C2B	2.24	0.50
1:C:112:LEU:HB2	1:C:135:THR:HB	1.93	0.50
1:C:332:ARG:O	1:C:335:GLU:HG3	2.12	0.50
1:B:204:LYS:HD2	1:B:235:THR:CG2	2.41	0.50
1:B:274:ARG:NH1	1:C:274:ARG:HD2	2.26	0.50
1:A:1:MET:HE3	1:A:176:ASP:OD1	2.11	0.50
1:C:105:PRO:HD2	1:C:105:PRO:O	2.11	0.50
1:D:87:LEU:HD12	1:D:87:LEU:N	2.27	0.50
1:A:243:GLN:NE2	1:A:246:ASN:HD22	2.09	0.50
1:B:36:ALA:HB3	1:B:39:PHE:CZ	2.47	0.50
1:A:242:PHE:C	1:A:243:GLN:HG3	2.37	0.49
1:C:196:GLN:CD	1:C:244:LEU:HD21	2.37	0.49
1:B:123:ASP:C	1:B:125:PHE:H	2.19	0.49
1:C:201:GLN:HE22	1:C:252:ASN:HB3	1.77	0.49
1:D:52:TRP:CD1	1:D:317:THR:HG23	2.47	0.49
1:A:42:LEU:HD21	1:C:279:ARG:NH2	2.27	0.49
1:B:33:LYS:HG2	1:B:160:PHE:CE1	2.40	0.49
1:B:178:ILE:HB	1:B:305:VAL:HG22	1.95	0.49
1:A:144:TYR:OH	1:A:319:HIS:CE1	2.65	0.49
1:A:117:LEU:HD21	1:A:133:PHE:HB2	1.93	0.49
1:C:2:ARG:NH2	1:C:2:ARG:CG	2.75	0.49
1:A:52:TRP:O	1:A:52:TRP:CE3	2.65	0.49
1:C:184:VAL:HA	1:C:195:LEU:HD11	1.94	0.49
1:C:1:MET:HB3	1:C:29:PRO:O	2.12	0.49
1:C:105:PRO:O	1:C:105:PRO:CD	2.61	0.49
1:B:56:LEU:HD11	1:B:217:HIS:CE1	2.48	0.49
1:B:283:ARG:HG2	2:B:401:FAD:HM82	1.95	0.49
1:B:298:THR:O	1:B:298:THR:CG2	2.60	0.49
1:D:318:ILE:O	1:D:320:TRP:N	2.46	0.49
1:A:249:GLU:H	1:C:161:GLN:NE2	2.11	0.49
1:B:115:ARG:NH2	1:B:121:GLU:OE2	2.35	0.49
1:B:199:ARG:HD2	1:B:248:SER:O	2.12	0.49
1:C:119:PRO:O	1:C:120:ARG:C	2.55	0.49
1:B:291:LEU:HA	1:B:307:HIS:O	2.12	0.48
1:A:61:ASN:HD21	1:A:63:GLN:HE21	1.60	0.48
1:B:161:GLN:HG3	1:D:249:GLU:C	2.39	0.48
1:B:171:ALA:O	1:B:172:ARG:C	2.56	0.48
1:D:83:ASN:O	1:D:86:ASN:N	2.46	0.48
1:A:71:THR:HA	1:A:320:TRP:HB3	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:THR:HG23	1:B:159:PHE:HE1	1.77	0.48
1:B:158:LYS:HE2	1:B:158:LYS:HA	1.95	0.48
1:B:325:GLU:OE1	1:B:325:GLU:HA	2.13	0.48
1:C:69:GLN:CD	1:C:110:THR:HG23	2.39	0.48
1:C:115:ARG:NH1	1:D:113:GLY:HA3	2.29	0.48
1:C:120:ARG:HA	1:C:120:ARG:NE	2.21	0.48
1:D:116:LYS:HD2	1:D:130:TYR:OH	2.12	0.48
1:B:69:GLN:OE1	1:B:110:THR:HG23	2.14	0.48
1:A:40:THR:CG2	1:A:41:PRO:HD3	2.44	0.48
1:A:169:GLU:O	1:A:173:GLU:HG2	2.14	0.48
1:A:249:GLU:H	1:C:161:GLN:HE21	1.62	0.48
1:C:140:GLU:OE1	1:C:233:THR:HG21	2.14	0.48
1:C:233:THR:HG23	1:C:234:GLN:HG2	1.95	0.48
1:A:79:VAL:HA	1:A:89:LEU:HD13	1.96	0.47
1:D:55:TYR:HE1	1:D:224:TYR:CE2	2.31	0.47
1:C:98:PHE:HZ	1:C:132:TRP:CZ3	2.32	0.47
1:D:241:ILE:HD13	1:D:241:ILE:HA	1.62	0.47
1:A:124:MET:HE1	1:B:91:LEU:HD11	1.96	0.47
1:B:101:ALA:HA	1:B:130:TYR:CD2	2.49	0.47
1:B:149:THR:HG23	1:B:159:PHE:CE1	2.49	0.47
1:B:184:VAL:N	1:B:284:PRO:HB3	2.29	0.47
1:B:286:ARG:HD3	1:B:288:GLN:O	2.13	0.47
1:A:162:ARG:HG3	1:A:162:ARG:O	2.14	0.47
1:A:278:GLU:O	1:A:279:ARG:HG2	2.15	0.47
1:C:28:GLN:HB3	1:C:29:PRO:CD	2.37	0.47
1:D:266:LEU:HD22	1:D:266:LEU:O	2.14	0.47
1:A:83:ASN:O	1:A:84:ALA:C	2.57	0.47
1:D:206:ASP:HB2	1:D:276:ILE:HD11	1.97	0.47
1:A:117:LEU:CD2	1:A:133:PHE:HB2	2.45	0.47
1:C:91:LEU:HD23	1:C:137:LEU:HD21	1.97	0.47
1:D:268:PRO:C	1:D:270:LEU:N	2.71	0.47
1:C:180:ASN:CB	1:C:307:HIS:HD2	2.27	0.47
1:D:264:CYS:HB3	1:D:271:LYS:NZ	2.30	0.47
1:A:104:ASP:OD1	1:A:116:LYS:HE2	2.14	0.47
1:A:83:ASN:O	1:A:86:ASN:N	2.48	0.47
1:A:140:GLU:OE1	1:A:233:THR:CB	2.62	0.47
1:A:309:TYR:CD1	1:A:309:TYR:C	2.92	0.47
1:C:38:ARG:NH2	2:C:401:FAD:C2B	2.74	0.47
1:C:241:ILE:HD13	1:C:255:ASP:HB3	1.97	0.47
1:D:17:LEU:HB2	1:D:152:LEU:HD11	1.96	0.47
1:D:59:PRO:HG2	1:D:65:ALA:CB	2.41	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:61:ASN:CG	1:D:63:GLN:HE21	2.22	0.47
1:D:81:SER:HB2	1:D:82:PRO:HD2	1.96	0.47
1:C:223:ILE:O	1:C:224:TYR:HB2	2.15	0.46
1:D:119:PRO:HA	1:D:122:LEU:HD12	1.97	0.46
1:B:114:PHE:CD1	1:B:114:PHE:C	2.94	0.46
1:B:186:ALA:HB3	1:B:195:LEU:HD22	1.98	0.46
1:A:40:THR:HG23	1:A:41:PRO:HD3	1.97	0.46
1:D:224:TYR:HB2	1:D:242:PHE:CD2	2.50	0.46
1:A:335:GLU:CG	1:A:336:GLU:N	2.63	0.46
1:C:147:TRP:O	1:C:148:LEU:C	2.57	0.46
1:D:67:TRP:CH2	1:D:291:LEU:HD23	2.50	0.46
1:A:222:GLY:O	1:A:225:ASN:HB2	2.15	0.46
1:A:243:GLN:HE21	1:A:246:ASN:HD22	1.64	0.46
1:D:17:LEU:HB2	1:D:152:LEU:CD1	2.45	0.46
1:A:199:ARG:HG3	1:A:282:PHE:CE1	2.51	0.46
1:B:283:ARG:HG3	1:B:283:ARG:HH21	1.81	0.46
1:C:47:VAL:HG12	1:C:47:VAL:O	2.14	0.46
1:C:332:ARG:HA	1:C:335:GLU:CG	2.46	0.46
1:D:100:GLU:O	1:D:101:ALA:C	2.58	0.46
1:D:228:TYR:OH	3:D:402:2LD:O16	2.30	0.46
1:A:133:PHE:C	1:A:133:PHE:CD2	2.94	0.46
1:D:53:GLN:HG2	3:D:402:2LD:H9	1.97	0.46
1:C:199:ARG:NH1	1:C:201:GLN:HE21	2.08	0.45
1:A:80:HIS:C	1:A:81:SER:O	2.55	0.45
1:D:139:LEU:HD11	1:D:144:TYR:CD1	2.51	0.45
1:B:7:GLY:O	1:B:12:GLY:HA3	2.16	0.45
1:A:298:THR:HG22	1:A:302:ASN:HA	1.98	0.45
1:D:140:GLU:OE1	1:D:233:THR:HB	2.17	0.45
1:D:162:ARG:O	2:D:401:FAD:H2A	2.17	0.45
1:D:227:PRO:CG	1:D:262:GLY:HA3	2.47	0.45
1:D:334:LEU:C	1:D:336:GLU:H	2.25	0.45
1:B:187:GLY:C	1:B:189:LEU:H	2.24	0.45
1:B:198:GLY:O	1:B:283:ARG:HG3	2.17	0.45
1:C:10:VAL:HB	1:C:45:THR:CG2	2.46	0.45
1:A:42:LEU:HD22	1:C:42:LEU:HD22	1.98	0.45
1:A:223:ILE:O	1:A:223:ILE:HG23	2.16	0.45
1:B:233:THR:HG23	1:B:234:GLN:N	2.32	0.45
1:C:117:LEU:HG	1:C:131:GLY:O	2.17	0.45
1:C:205:VAL:HG12	1:C:236:VAL:HB	1.98	0.45
1:C:215:LEU:N	1:C:215:LEU:HD23	2.32	0.45
1:C:27:LEU:HD11	1:C:334:LEU:HD11	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:233:THR:CG2	1:C:234:GLN:N	2.79	0.45
1:C:291:LEU:HA	1:C:307:HIS:O	2.17	0.45
1:C:316:LEU:O	1:C:319:HIS:HD2	1.99	0.45
1:D:102:ILE:HD13	1:D:103:PRO:HD2	1.99	0.45
1:D:114:PHE:O	1:D:115:ARG:HB3	2.15	0.45
1:A:10:VAL:HG13	1:A:11:ILE:HD13	2.00	0.44
1:B:168:GLU:O	1:B:172:ARG:HB2	2.18	0.44
1:D:144:TYR:OH	1:D:319:HIS:CE1	2.70	0.44
1:A:10:VAL:HB	1:A:45:THR:CG2	2.46	0.44
1:A:215:LEU:HD13	3:A:402:2LD:C6	2.47	0.44
1:C:224:TYR:HB2	1:C:242:PHE:CD2	2.50	0.44
1:C:5:VAL:O	1:C:34:VAL:HA	2.18	0.44
1:D:67:TRP:HB2	1:D:318:ILE:HD11	1.99	0.44
1:A:38:ARG:HD2	2:A:401:FAD:O2B	2.17	0.44
1:B:13:LEU:HB2	1:B:148:LEU:HD13	1.97	0.44
1:B:140:GLU:OE1	1:B:233:THR:HB	2.17	0.44
1:D:297:ARG:HG3	1:D:302:ASN:ND2	2.32	0.44
1:A:252:ASN:ND2	1:A:255:ASP:H	2.13	0.44
1:B:286:ARG:O	1:B:287:PRO:C	2.60	0.44
1:C:71:THR:OG1	1:C:320:TRP:HB3	2.18	0.44
1:D:55:TYR:CE1	1:D:224:TYR:CE2	3.05	0.44
1:B:293:ARG:NH2	1:B:304:GLU:OE1	2.42	0.44
1:D:58:ASP:O	1:D:59:PRO:C	2.57	0.44
1:D:180:ASN:ND2	1:D:307:HIS:HD2	2.15	0.44
1:D:36:ALA:HB3	1:D:39:PHE:CE1	2.53	0.44
1:D:40:THR:O	1:D:40:THR:OG1	2.31	0.44
1:A:265:ARG:HE	1:A:265:ARG:HB2	1.36	0.44
1:B:197:PRO:HG3	1:B:247:TRP:CE2	2.52	0.44
1:B:265:ARG:HE	1:B:265:ARG:HB2	1.49	0.44
1:C:114:PHE:HA	1:C:134:HIS:HB3	2.00	0.44
1:A:39:PHE:O	1:A:41:PRO:HD2	2.16	0.43
1:A:102:ILE:HG13	1:A:103:PRO:HD2	1.99	0.43
1:B:198:GLY:H	1:B:285:VAL:HG23	1.83	0.43
1:B:267:GLU:O	1:B:270:LEU:HB2	2.18	0.43
1:C:224:TYR:HD2	1:C:242:PHE:CE2	2.36	0.43
1:C:264:CYS:SG	1:C:271:LYS:HD2	2.54	0.43
1:D:11:ILE:HG21	1:D:308:ASN:O	2.18	0.43
1:D:40:THR:CG2	1:D:41:PRO:HD3	2.48	0.43
1:A:87:LEU:HB3	1:A:89:LEU:HB2	1.98	0.43
1:A:274:ARG:HH21	1:D:274:ARG:HH12	1.66	0.43
1:B:59:PRO:O	1:B:60:ASN:C	2.61	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:59:PRO:HG2	1:C:62:PRO:HA	2.00	0.43
1:C:200:GLY:HA2	1:C:241:ILE:O	2.18	0.43
1:A:298:THR:HG21	1:A:303:THR:HG23	1.99	0.43
1:B:332:ARG:HA	1:B:335:GLU:HG2	2.00	0.43
1:C:113:GLY:O	1:C:114:PHE:C	2.61	0.43
1:D:39:PHE:C	1:D:41:PRO:HD2	2.43	0.43
1:A:152:LEU:HD12	1:A:157:VAL:HG21	1.99	0.43
1:A:161:GLN:NE2	1:C:249:GLU:H	2.16	0.43
1:B:104:ASP:OD2	1:B:108:LYS:NZ	2.50	0.43
1:B:105:PRO:HG2	1:B:108:LYS:H	1.82	0.43
1:D:68:SER:N	1:D:318:ILE:HG13	2.33	0.43
1:A:199:ARG:HH12	1:A:201:GLN:NE2	2.17	0.43
1:B:38:ARG:NH1	1:B:249:GLU:OE2	2.52	0.43
1:C:206:ASP:OD1	1:C:208:PRO:HD3	2.18	0.43
1:D:56:LEU:H	1:D:56:LEU:HG	1.47	0.43
1:D:199:ARG:HG3	1:D:282:PHE:CE1	2.54	0.43
1:C:191:ARG:NH1	1:C:193:PRO:HG3	2.33	0.43
1:C:72:PHE:CD2	1:C:72:PHE:C	2.97	0.43
1:D:41:PRO:C	1:D:42:LEU:HD23	2.44	0.43
1:D:240:GLY:O	1:D:241:ILE:HD13	2.19	0.43
1:B:252:ASN:HD21	1:B:254:GLN:HB2	1.84	0.43
1:C:139:LEU:HD21	1:C:144:TYR:CE2	2.54	0.43
1:C:190:GLN:OE1	1:C:290:ARG:NH1	2.52	0.43
1:D:147:TRP:O	1:D:148:LEU:C	2.59	0.43
1:C:216:THR:OG1	1:C:226:SER:OG	2.36	0.42
1:D:55:TYR:CE1	1:D:224:TYR:OH	2.42	0.42
1:D:299:GLY:HA3	1:D:300:PRO:HD3	1.87	0.42
1:A:264:CYS:CB	1:A:271:LYS:NZ	2.73	0.42
1:B:102:ILE:HG12	1:B:103:PRO:O	2.18	0.42
1:D:202:ILE:HD11	1:D:279:ARG:HB2	2.01	0.42
1:D:218:ASP:OD2	1:D:221:ARG:NH2	2.47	0.42
1:A:118:THR:O	1:A:119:PRO:C	2.61	0.42
1:D:67:TRP:HB3	1:D:318:ILE:HG12	2.01	0.42
1:B:332:ARG:O	1:B:335:GLU:HG3	2.20	0.42
1:A:52:TRP:CE3	1:A:52:TRP:C	2.97	0.42
1:C:196:GLN:CG	1:C:244:LEU:HD21	2.49	0.42
1:C:253:ILE:HG22	1:C:254:GLN:NE2	2.35	0.42
1:C:293:ARG:HH21	1:C:304:GLU:CD	2.27	0.42
1:D:286:ARG:HG2	1:D:287:PRO:HD2	2.01	0.42
1:D:325:GLU:HA	1:D:328:LYS:HG3	2.02	0.42
1:B:190:GLN:NE2	1:B:294:GLU:OE1	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:ARG:HA	1:C:335:GLU:HG2	2.01	0.42
1:D:112:LEU:HB2	1:D:135:THR:HB	2.01	0.42
1:C:202:ILE:O	1:C:278:GLU:HG3	2.20	0.42
1:B:249:GLU:H	1:D:161:GLN:HG3	1.85	0.42
1:D:66:ASP:O	1:D:70:GLN:HG3	2.20	0.42
1:B:202:ILE:O	1:B:202:ILE:HD12	2.20	0.42
1:D:1:MET:HA	1:D:176:ASP:OD1	2.20	0.42
1:A:333:ILE:O	1:A:334:LEU:C	2.61	0.41
1:B:61:ASN:HB2	1:B:288:GLN:NE2	2.35	0.41
1:C:39:PHE:HE2	1:C:161:GLN:HA	1.84	0.41
1:C:233:THR:CG2	1:C:234:GLN:H	2.34	0.41
1:A:15:THR:HG22	1:A:19:ILE:HD12	2.02	0.41
1:A:40:THR:HG23	1:A:41:PRO:CD	2.50	0.41
1:A:150:GLU:HG3	1:A:151:ARG:HH22	1.85	0.41
1:C:67:TRP:HB3	1:C:321:GLY:HA3	2.02	0.41
1:C:325:GLU:O	1:C:326:ALA:C	2.63	0.41
2:C:401:FAD:H1'1	2:C:401:FAD:H9	1.78	0.41
1:D:8:ALA:CB	1:D:39:PHE:CD1	3.03	0.41
1:B:249:GLU:N	1:D:161:GLN:HG3	2.34	0.41
1:B:123:ASP:C	1:B:125:PHE:N	2.78	0.41
1:D:53:GLN:HG2	3:D:402:2LD:C3	2.50	0.41
1:D:149:THR:HG23	1:D:159:PHE:CE1	2.56	0.41
1:A:41:PRO:HB2	1:A:42:LEU:HD23	2.02	0.41
1:A:52:TRP:CD1	1:A:317:THR:HG23	2.55	0.41
1:B:118:THR:OG1	1:B:121:GLU:HG3	2.20	0.41
1:C:228:TYR:CZ	3:C:402:2LD:H3	2.55	0.41
1:C:286:ARG:HG2	1:C:287:PRO:HD2	2.01	0.41
1:D:300:PRO:HB2	1:D:301:SER:H	1.77	0.41
1:B:249:GLU:H	1:D:161:GLN:NE2	2.14	0.41
1:B:276:ILE:HD13	1:B:276:ILE:HA	1.84	0.41
1:D:20:HIS:CE1	1:D:155:ARG:HB3	2.55	0.41
1:D:61:ASN:HA	1:D:62:PRO:HD3	1.92	0.41
1:D:242:PHE:C	1:D:243:GLN:HG3	2.45	0.41
1:A:222:GLY:O	1:A:223:ILE:C	2.64	0.41
1:B:168:GLU:CD	1:B:168:GLU:H	2.29	0.41
1:B:280:THR:HG22	1:B:281:GLY:N	2.34	0.41
1:C:309:TYR:CD1	1:C:309:TYR:C	2.99	0.41
1:D:59:PRO:CG	1:D:65:ALA:HB2	2.42	0.41
1:D:133:PHE:CD2	1:D:133:PHE:C	2.99	0.41
1:B:39:PHE:O	1:B:41:PRO:CD	2.65	0.41
1:B:67:TRP:CH2	1:B:291:LEU:HD23	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:GLY:HA2	1:B:241:ILE:O	2.21	0.41
3:B:402:2LD:H2	3:B:402:2LD:H6	1.81	0.41
1:C:1:MET:CB	1:C:29:PRO:O	2.69	0.41
1:C:61:ASN:OD1	1:C:63:GLN:HB2	2.21	0.41
1:D:79:VAL:HA	1:D:89:LEU:CD1	2.50	0.41
1:D:223:ILE:HG13	1:D:224:TYR:CG	2.54	0.41
1:D:253:ILE:CG2	1:D:254:GLN:N	2.83	0.41
1:B:161:GLN:NE2	1:D:249:GLU:H	2.18	0.40
1:C:126:PRO:O	1:C:128:TYR:N	2.54	0.40
1:C:203:MET:HE3	1:C:203:MET:HB2	1.84	0.40
1:D:199:ARG:HB2	1:D:246:ASN:HB3	2.02	0.40
1:A:40:THR:O	1:A:46:ASP:OD2	2.39	0.40
1:C:139:LEU:HD11	1:C:144:TYR:CD1	2.56	0.40
1:C:224:TYR:CZ	1:C:313:GLY:HA3	2.56	0.40
1:C:286:ARG:C	1:C:288:GLN:N	2.77	0.40
1:A:252:ASN:ND2	1:A:254:GLN:HB2	2.33	0.40
1:B:100:GLU:OE1	1:B:100:GLU:HA	2.22	0.40
1:C:114:PHE:C	1:C:114:PHE:CD1	2.98	0.40
1:A:39:PHE:O	1:A:41:PRO:CD	2.70	0.40
1:B:1:MET:HG2	1:B:27:LEU:HD22	2.04	0.40
1:C:44:THR:O	1:C:45:THR:C	2.64	0.40
1:C:123:ASP:O	1:C:125:PHE:N	2.55	0.40
1:D:40:THR:HG23	1:D:41:PRO:HD3	2.02	0.40
1:D:161:GLN:O	1:D:162:ARG:HB3	2.22	0.40
1:B:52:TRP:CD1	1:B:317:THR:HG23	2.57	0.40
1:B:233:THR:CG2	1:B:234:GLN:N	2.85	0.40
1:C:56:LEU:HD23	1:C:56:LEU:N	2.37	0.40
1:C:98:PHE:HZ	1:C:132:TRP:CH2	2.39	0.40
1:D:93:SER:O	1:D:212:HIS:HA	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	338/347 (97%)	298 (88%)	33 (10%)	7 (2%)	5	9
1	B	338/347 (97%)	295 (87%)	34 (10%)	9 (3%)	4	6
1	C	338/347 (97%)	292 (86%)	35 (10%)	11 (3%)	3	4
1	D	338/347 (97%)	289 (86%)	41 (12%)	8 (2%)	4	7
All	All	1352/1388 (97%)	1174 (87%)	143 (11%)	35 (3%)	4	6

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	THR
1	A	297	ARG
1	B	40	THR
1	B	108	LYS
1	C	40	THR
1	C	127	ASP
1	D	335	GLU
1	A	299	GLY
1	B	191	ARG
1	C	21	GLU
1	C	124	MET
1	C	299	GLY
1	D	12	GLY
1	D	108	LYS
1	D	220	GLU
1	D	300	PRO
1	A	188	ALA
1	A	223	ILE
1	B	127	ASP
1	C	126	PRO
1	C	171	ALA
1	B	28	GLN
1	B	253	ILE
1	B	298	THR
1	C	300	PRO
1	D	223	ILE
1	A	300	PRO
1	B	172	ARG
1	C	105	PRO
1	B	104	ASP
1	D	29	PRO
1	A	240	GLY
1	C	28	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	240	GLY
1	D	240	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	292/299 (98%)	243 (83%)	49 (17%)	2	2
1	B	292/299 (98%)	258 (88%)	34 (12%)	5	10
1	C	292/299 (98%)	250 (86%)	42 (14%)	3	4
1	D	292/299 (98%)	241 (82%)	51 (18%)	2	2
All	All	1168/1196 (98%)	992 (85%)	176 (15%)	3	4

All (176) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ARG
1	A	6	ILE
1	A	28	GLN
1	A	31	ASP
1	A	32	ILE
1	A	38	ARG
1	A	56	LEU
1	A	81	SER
1	A	87	LEU
1	A	89	LEU
1	A	102	ILE
1	A	112	LEU
1	A	120	ARG
1	A	145	LEU
1	A	146	GLN
1	A	150	GLU
1	A	151	ARG
1	A	152	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	154	GLU
1	A	158	LYS
1	A	162	ARG
1	A	168	GLU
1	A	169	GLU
1	A	172	ARG
1	A	191	ARG
1	A	196	GLN
1	A	205	VAL
1	A	210	MET
1	A	221	ARG
1	A	235	THR
1	A	238	LEU
1	A	253	ILE
1	A	254	GLN
1	A	261	GLU
1	A	265	ARG
1	A	266	LEU
1	A	270	LEU
1	A	271	LYS
1	A	274	ARG
1	A	275	ILE
1	A	295	GLN
1	A	297	ARG
1	A	301	SER
1	A	305	VAL
1	A	335	GLU
1	A	337	LYS
1	A	338	LYS
1	A	339	LEU
1	B	22	ARG
1	B	28	GLN
1	B	31	ASP
1	B	56	LEU
1	B	89	LEU
1	B	102	ILE
1	B	108	LYS
1	B	112	LEU
1	B	145	LEU
1	B	151	ARG
1	B	152	LEU
1	B	158	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	164	VAL
1	B	168	GLU
1	B	169	GLU
1	B	173	GLU
1	B	196	GLN
1	B	211	LYS
1	B	215	LEU
1	B	221	ARG
1	B	235	THR
1	B	238	LEU
1	B	261	GLU
1	B	264	CYS
1	B	265	ARG
1	B	266	LEU
1	B	270	LEU
1	B	294	GLU
1	B	295	GLN
1	B	296	LEU
1	B	302	ASN
1	B	328	LYS
1	B	335	GLU
1	B	340	SER
1	C	18	CYS
1	C	22	ARG
1	C	27	LEU
1	C	56	LEU
1	C	63	GLN
1	C	85	GLU
1	C	87	LEU
1	C	89	LEU
1	C	120	ARG
1	C	145	LEU
1	C	151	ARG
1	C	152	LEU
1	C	161	GLN
1	C	168	GLU
1	C	172	ARG
1	C	173	GLU
1	C	182	THR
1	C	196	GLN
1	C	205	VAL
1	C	215	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	221	ARG
1	C	238	LEU
1	C	242	PHE
1	C	244	LEU
1	C	253	ILE
1	C	259	ILE
1	C	261	GLU
1	C	265	ARG
1	C	266	LEU
1	C	270	LEU
1	C	274	ARG
1	C	290	ARG
1	C	293	ARG
1	C	295	GLN
1	C	297	ARG
1	C	298	THR
1	C	301	SER
1	C	302	ASN
1	C	318	ILE
1	C	335	GLU
1	C	337	LYS
1	C	339	LEU
1	D	5	VAL
1	D	19	ILE
1	D	22	ARG
1	D	27	LEU
1	D	28	GLN
1	D	42	LEU
1	D	56	LEU
1	D	60	ASN
1	D	61	ASN
1	D	89	LEU
1	D	91	LEU
1	D	102	ILE
1	D	108	LYS
1	D	112	LEU
1	D	116	LYS
1	D	122	LEU
1	D	142	LYS
1	D	143	ASN
1	D	145	LEU
1	D	151	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	152	LEU
1	D	153	THR
1	D	164	VAL
1	D	168	GLU
1	D	176	ASP
1	D	179	VAL
1	D	184	VAL
1	D	195	LEU
1	D	202	ILE
1	D	205	VAL
1	D	215	LEU
1	D	221	ARG
1	D	225	ASN
1	D	235	THR
1	D	238	LEU
1	D	241	ILE
1	D	244	LEU
1	D	253	ILE
1	D	261	GLU
1	D	264	CYS
1	D	266	LEU
1	D	276	ILE
1	D	279	ARG
1	D	283	ARG
1	D	290	ARG
1	D	292	GLU
1	D	295	GLN
1	D	298	THR
1	D	301	SER
1	D	316	LEU
1	D	318	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
1	A	63	GLN
1	A	69	GLN
1	A	80	HIS
1	A	161	GLN
1	A	196	GLN
1	A	201	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	243	GLN
1	A	252	ASN
1	A	254	GLN
1	A	307	HIS
1	A	319	HIS
1	B	24	HIS
1	B	28	GLN
1	B	63	GLN
1	B	70	GLN
1	B	161	GLN
1	B	201	GLN
1	B	225	ASN
1	B	243	GLN
1	B	252	ASN
1	B	288	GLN
1	B	295	GLN
1	B	307	HIS
1	B	308	ASN
1	B	319	HIS
1	C	63	GLN
1	C	69	GLN
1	C	80	HIS
1	C	161	GLN
1	C	201	GLN
1	C	225	ASN
1	C	243	GLN
1	C	252	ASN
1	C	254	GLN
1	C	302	ASN
1	C	307	HIS
1	C	319	HIS
1	D	63	GLN
1	D	69	GLN
1	D	80	HIS
1	D	161	GLN
1	D	180	ASN
1	D	201	GLN
1	D	225	ASN
1	D	243	GLN
1	D	252	ASN
1	D	288	GLN
1	D	302	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	307	HIS
1	D	319	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 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	B	401	-	58,58,58	1.20	5 (8%)	85,89,89	1.46	12 (14%)
3	2LD	D	402	-	17,17,17	0.74	0	16,22,22	1.35	1 (6%)
3	2LD	C	402	-	17,17,17	0.73	0	16,22,22	1.36	1 (6%)
2	FAD	D	401	-	58,58,58	1.37	8 (13%)	85,89,89	1.76	20 (23%)
3	2LD	A	402	-	17,17,17	0.73	0	16,22,22	1.37	1 (6%)
3	2LD	B	402	-	17,17,17	0.74	0	16,22,22	1.46	1 (6%)
2	FAD	C	401	-	58,58,58	1.44	9 (15%)	85,89,89	1.53	17 (20%)
2	FAD	A	401	-	58,58,58	1.23	7 (12%)	85,89,89	1.66	20 (23%)

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	B	401	-	-	2/34/50/50	0/6/6/6
3	2LD	D	402	-	-	0/5/5/5	0/2/2/2
3	2LD	C	402	-	-	0/5/5/5	0/2/2/2
2	FAD	D	401	-	-	11/34/50/50	0/6/6/6
3	2LD	A	402	-	-	0/5/5/5	0/2/2/2
3	2LD	B	402	-	-	2/5/5/5	0/2/2/2
2	FAD	C	401	-	-	3/34/50/50	0/6/6/6
2	FAD	A	401	-	-	6/34/50/50	0/6/6/6

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	FAD	C9A-N10	-5.01	1.32	1.41
2	D	401	FAD	C9A-N10	-4.55	1.33	1.41
2	B	401	FAD	C5X-N5	-3.47	1.33	1.39
2	C	401	FAD	PA-O3P	3.40	1.63	1.59
2	A	401	FAD	C9A-N10	-3.22	1.35	1.41
2	D	401	FAD	C2'-C3'	3.21	1.59	1.53
2	D	401	FAD	C5X-N5	-3.19	1.33	1.39
2	B	401	FAD	C5'-C4'	3.17	1.56	1.51
2	D	401	FAD	C10-N1	3.15	1.39	1.33
2	C	401	FAD	C4-N3	-3.14	1.33	1.38
2	C	401	FAD	C10-N10	-3.03	1.30	1.37
2	B	401	FAD	C10-N1	2.94	1.39	1.33
2	C	401	FAD	C5X-N5	-2.93	1.34	1.39
2	A	401	FAD	C5X-N5	-2.85	1.34	1.39
2	B	401	FAD	C9A-N10	-2.77	1.36	1.41
2	C	401	FAD	C6A-N6A	2.57	1.40	1.34
2	A	401	FAD	C4-N3	-2.51	1.34	1.38
2	C	401	FAD	C4X-C10	-2.49	1.36	1.44
2	A	401	FAD	C10-N1	2.38	1.38	1.33
2	D	401	FAD	C8M-C8	-2.36	1.46	1.51
2	D	401	FAD	C4X-C10	-2.18	1.37	1.44
2	B	401	FAD	C4X-C10	-2.15	1.37	1.44
2	D	401	FAD	C4X-N5	2.15	1.35	1.30
2	A	401	FAD	C6A-N6A	2.12	1.39	1.34
2	D	401	FAD	C6A-N6A	2.11	1.39	1.34
2	A	401	FAD	C4X-C10	-2.04	1.38	1.44
2	C	401	FAD	C9-C9A	-2.02	1.36	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	FAD	P-O3P	2.01	1.61	1.59
2	A	401	FAD	C4X-N5	2.00	1.35	1.30

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	FAD	C5X-C9A-N10	5.33	122.78	117.97
2	B	401	FAD	O3'-C3'-C4'	-5.16	97.22	108.93
2	D	401	FAD	O2P-P-O3P	-4.31	95.63	107.27
2	D	401	FAD	N9A-C8A-N7A	-4.30	107.83	113.94
2	D	401	FAD	C4A-N9A-C8A	4.26	110.21	105.74
2	A	401	FAD	C5X-C9A-N10	4.13	121.70	117.97
2	A	401	FAD	O3'-C3'-C4'	-3.78	100.34	108.93
2	D	401	FAD	C9-C9A-N10	-3.75	116.81	121.85
2	A	401	FAD	C5X-N5-C4X	-3.67	112.14	118.09
2	C	401	FAD	C9-C9A-N10	-3.65	116.94	121.85
2	B	401	FAD	O4-C4-N3	3.46	126.61	120.11
2	B	401	FAD	C1'-N10-C9A	3.35	127.14	120.63
2	C	401	FAD	O3P-P-O1P	-3.32	100.72	110.70
2	A	401	FAD	C4-C4X-N5	-3.29	113.66	118.21
2	C	401	FAD	O3'-C3'-C4'	-3.25	101.56	108.93
2	C	401	FAD	O4B-C1B-N9A	3.18	114.19	108.09
2	C	401	FAD	O2A-PA-O3P	3.17	115.84	107.27
2	B	401	FAD	O4-C4-C4X	-3.15	118.21	126.53
2	C	401	FAD	C5X-C9A-N10	3.15	120.81	117.97
2	A	401	FAD	C2B-C1B-N9A	3.13	121.07	113.30
2	D	401	FAD	C5A-N7A-C8A	3.05	108.24	103.45
2	D	401	FAD	C8M-C8-C9	-3.04	114.21	119.57
2	D	401	FAD	C1'-C2'-C3'	3.04	117.89	109.66
2	A	401	FAD	O4B-C1B-N9A	-3.03	102.28	108.09
2	A	401	FAD	O3B-C3B-C2B	-2.96	102.32	111.82
2	A	401	FAD	O2'-C2'-C3'	-2.96	102.32	109.25
2	D	401	FAD	C4A-N9A-C1B	-2.94	119.75	126.63
2	A	401	FAD	O4-C4-N3	2.92	125.61	120.11
2	D	401	FAD	O3'-C3'-C4'	-2.90	102.34	108.93
2	C	401	FAD	C4X-C10-N10	2.87	120.59	116.48
2	D	401	FAD	C10-N1-C2	2.86	123.05	116.85
2	B	401	FAD	O2P-P-O5'	-2.81	94.82	107.57
2	C	401	FAD	O2-C2-N3	2.78	123.91	118.58
3	A	402	2LD	C1-C2-C4	-2.77	116.82	120.24
2	C	401	FAD	C5X-N5-C4X	-2.76	113.62	118.09
2	A	401	FAD	C1'-N10-C9A	2.76	126.00	120.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	2LD	C1-C2-C4	-2.74	116.85	120.24
3	B	402	2LD	C5-C6-C4	2.72	122.28	118.23
3	D	402	2LD	C1-C2-C4	-2.67	116.94	120.24
2	A	401	FAD	O3B-C3B-C4B	-2.63	103.52	111.08
2	C	401	FAD	O2-C2-N1	-2.60	117.48	121.80
2	A	401	FAD	O4-C4-C4X	-2.57	119.75	126.53
2	B	401	FAD	C6-C5X-C9A	2.46	122.43	119.05
2	C	401	FAD	C5A-C4A-N9A	2.40	108.42	105.81
2	C	401	FAD	C4A-C5A-N7A	-2.37	107.87	110.58
2	A	401	FAD	N3-C2-N1	-2.37	114.47	119.50
2	D	401	FAD	O3B-C3B-C2B	-2.36	104.24	111.82
2	A	401	FAD	C10-N1-C2	2.36	121.96	116.85
2	C	401	FAD	O4-C4-C4X	-2.31	120.42	126.53
2	B	401	FAD	C8M-C8-C9	-2.30	115.52	119.57
2	D	401	FAD	C5X-N5-C4X	-2.28	114.40	118.09
2	D	401	FAD	O2P-P-O1P	2.28	123.04	112.44
2	A	401	FAD	O3P-PA-O1A	2.24	117.44	110.70
2	D	401	FAD	C5'-C4'-C3'	2.23	116.43	112.22
2	D	401	FAD	C9A-N10-C10	-2.22	117.36	120.75
2	D	401	FAD	O4-C4-C4X	-2.19	120.74	126.53
2	A	401	FAD	C4-N3-C2	2.18	129.51	125.64
2	B	401	FAD	O2A-PA-O3P	2.17	113.15	107.27
2	A	401	FAD	C5A-N7A-C8A	2.17	106.85	103.45
2	D	401	FAD	O5B-PA-O1A	2.13	117.36	108.94
2	B	401	FAD	O2P-P-O1P	2.12	122.33	112.44
2	C	401	FAD	O2B-C2B-C3B	-2.12	105.03	111.82
2	C	401	FAD	O5'-P-O1P	2.12	117.32	108.94
2	C	401	FAD	C5B-C4B-C3B	-2.11	107.62	115.21
2	B	401	FAD	C3B-C2B-C1B	-2.08	97.52	101.46
2	A	401	FAD	C9A-N10-C10	-2.08	117.57	120.75
2	D	401	FAD	O5'-C5'-C4'	2.05	114.84	109.36
2	D	401	FAD	O3P-PA-O1A	-2.05	104.53	110.70
2	B	401	FAD	N9A-C8A-N7A	-2.05	111.03	113.94
2	A	401	FAD	N3A-C2A-N1A	2.04	131.67	128.58
2	C	401	FAD	C1'-N10-C9A	2.03	124.58	120.63
2	A	401	FAD	N6A-C6A-N1A	-2.01	113.91	118.38
2	B	401	FAD	C6-C7-C8	-2.00	116.75	119.69

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	FAD	C5B-O5B-PA-O2A
2	C	401	FAD	PA-O3P-P-O5'
2	D	401	FAD	C5B-O5B-PA-O1A
2	D	401	FAD	C5B-O5B-PA-O2A
2	D	401	FAD	C5B-O5B-PA-O3P
2	D	401	FAD	O4B-C4B-C5B-O5B
2	D	401	FAD	C3B-C4B-C5B-O5B
2	D	401	FAD	C5'-O5'-P-O1P
2	D	401	FAD	C5'-O5'-P-O2P
2	D	401	FAD	O4'-C4'-C5'-O5'
2	A	401	FAD	C3B-C4B-C5B-O5B
2	B	401	FAD	O4B-C4B-C5B-O5B
2	B	401	FAD	C3B-C4B-C5B-O5B
2	D	401	FAD	C3'-C4'-C5'-O5'
2	A	401	FAD	O4B-C4B-C5B-O5B
2	C	401	FAD	O4'-C4'-C5'-O5'
2	D	401	FAD	P-O3P-PA-O5B
2	A	401	FAD	C5B-O5B-PA-O1A
2	A	401	FAD	C5B-O5B-PA-O3P
2	D	401	FAD	C5'-O5'-P-O3P
3	B	402	2LD	C13-C12-C6-C5
3	B	402	2LD	C13-C12-C6-C4
2	C	401	FAD	O4B-C4B-C5B-O5B
2	A	401	FAD	PA-O3P-P-O2P

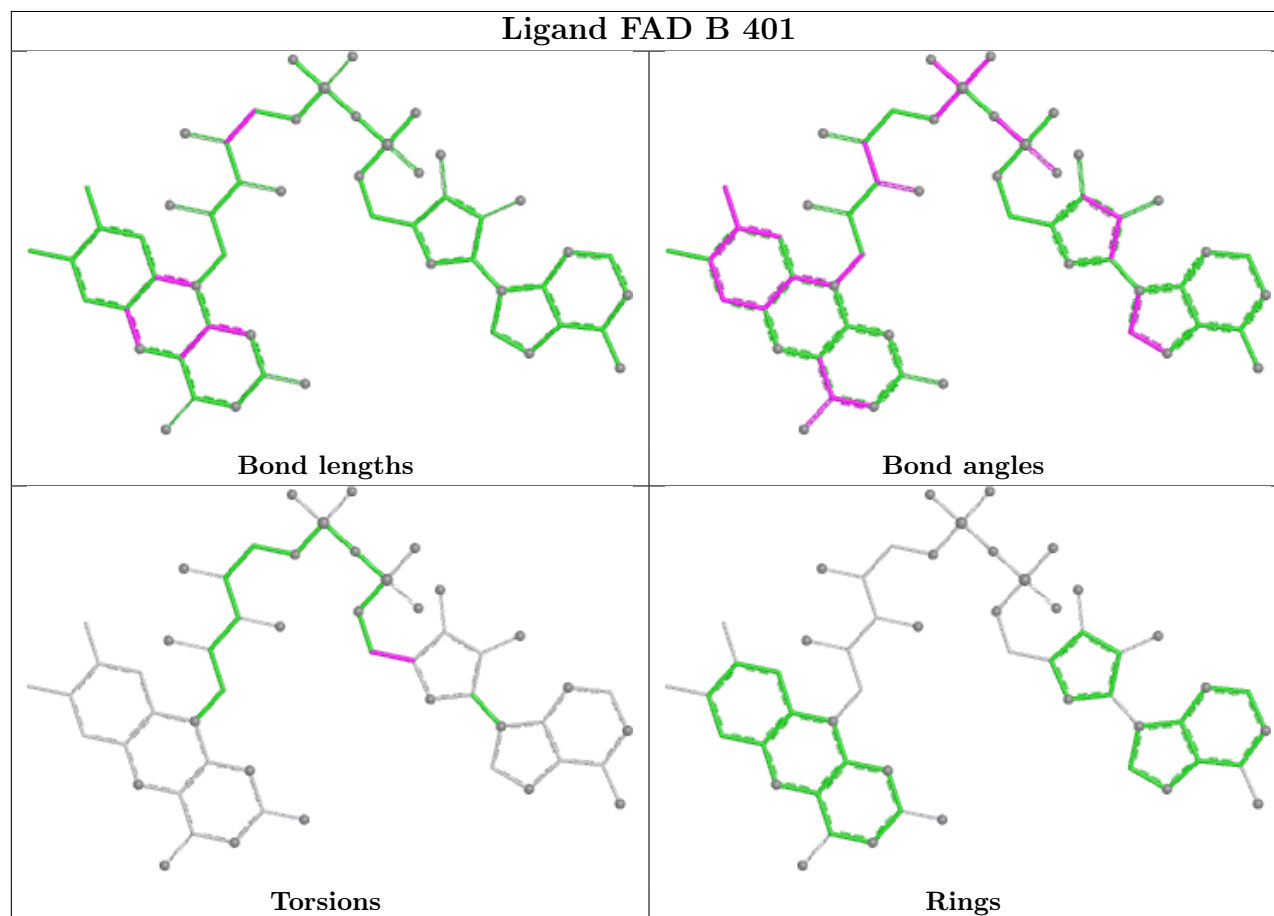
There are no ring outliers.

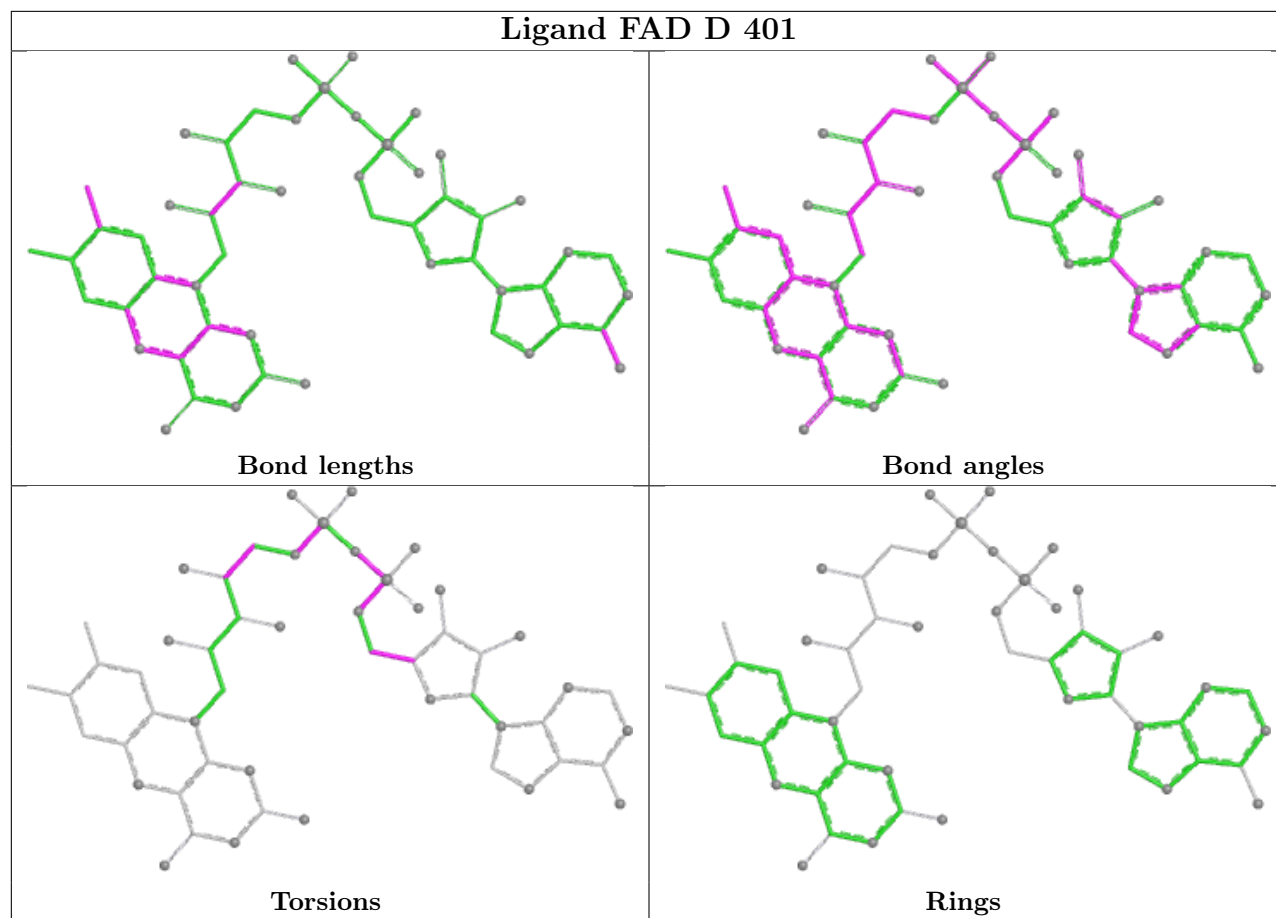
8 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	FAD	1	0
3	D	402	2LD	6	0
3	C	402	2LD	1	0
2	D	401	FAD	2	0
3	A	402	2LD	1	0
3	B	402	2LD	1	0
2	C	401	FAD	5	0
2	A	401	FAD	3	0

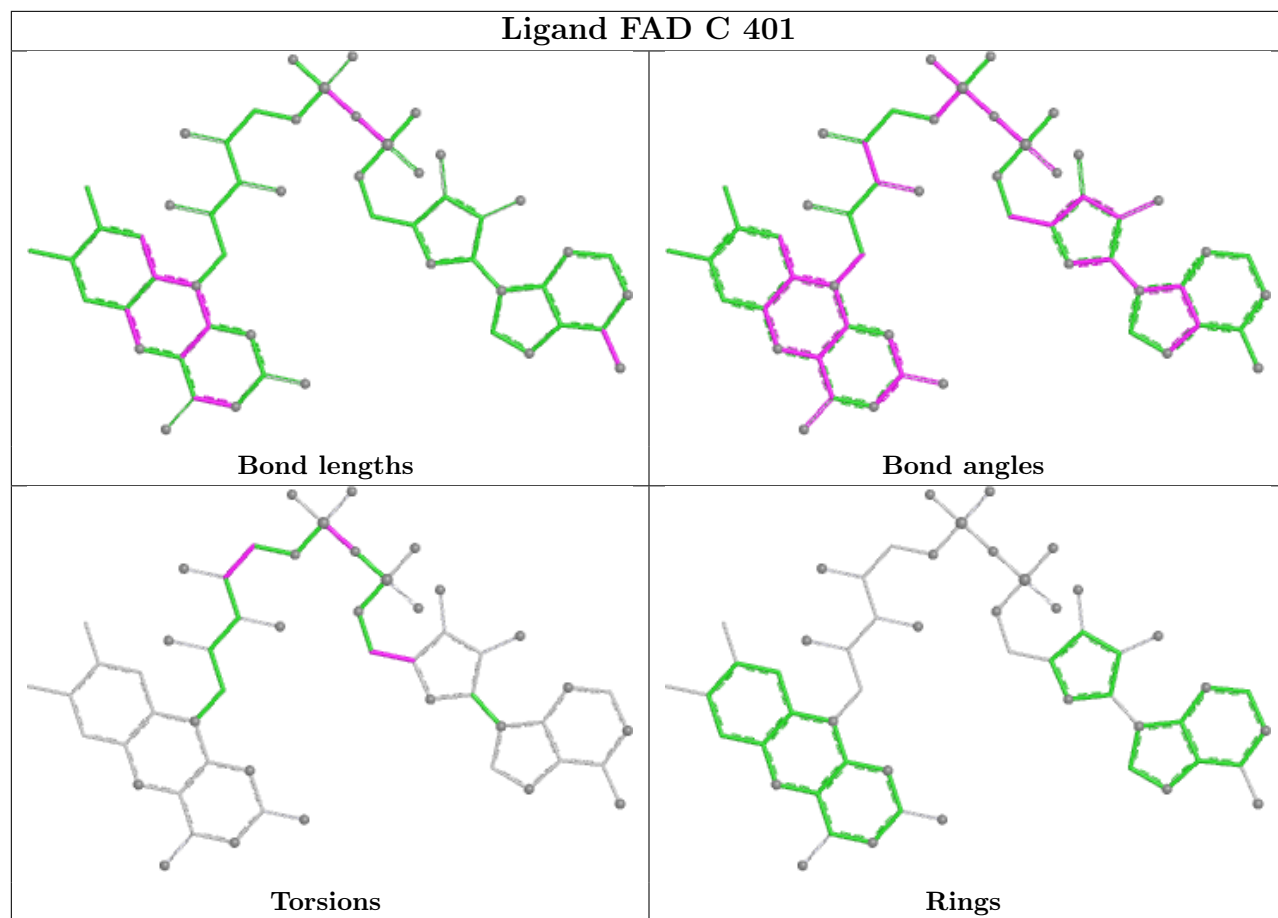
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

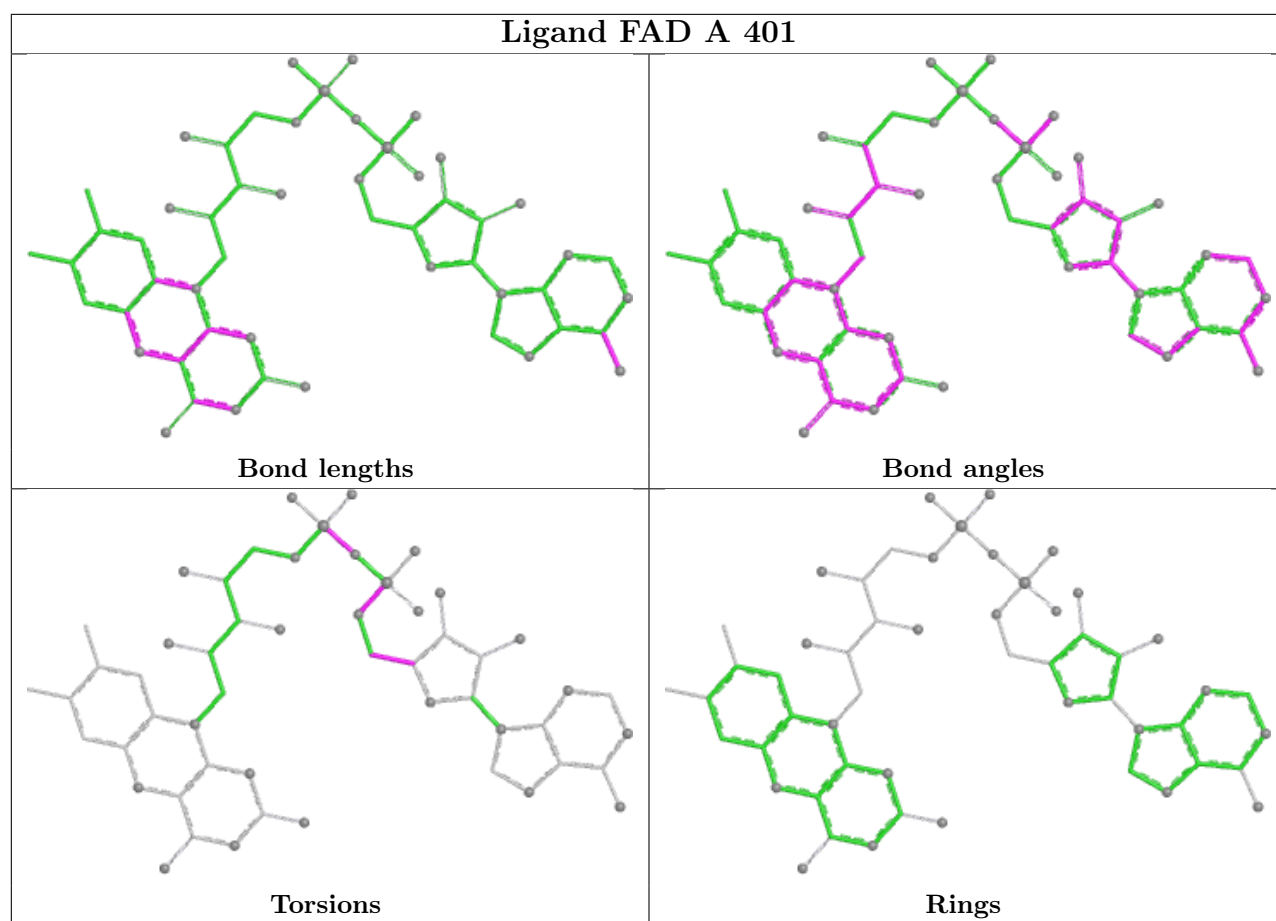
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





Ligand FAD C 401





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	340/347 (97%)	-0.17	2 (0%) 85 85	28, 48, 72, 89	0
1	B	340/347 (97%)	-0.14	1 (0%) 90 91	29, 49, 73, 81	0
1	C	340/347 (97%)	0.06	8 (2%) 59 56	40, 58, 82, 100	0
1	D	340/347 (97%)	0.02	10 (2%) 53 51	39, 58, 84, 99	0
All	All	1360/1388 (97%)	-0.06	21 (1%) 72 69	28, 53, 79, 100	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	299	GLY	3.3
1	D	339	LEU	3.2
1	C	339	LEU	3.0
1	D	340	SER	2.8
1	D	56	LEU	2.7
1	A	340	SER	2.7
1	D	224	TYR	2.6
1	C	300	PRO	2.5
1	C	298	THR	2.5
1	D	299	GLY	2.4
1	D	338	LYS	2.3
1	C	55	TYR	2.2
1	D	29	PRO	2.2
1	C	56	LEU	2.2
1	C	219	PRO	2.1
1	D	55	TYR	2.1
1	D	82	PRO	2.1
1	A	55	TYR	2.1
1	B	55	TYR	2.1
1	C	224	TYR	2.1
1	D	300	PRO	2.1

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

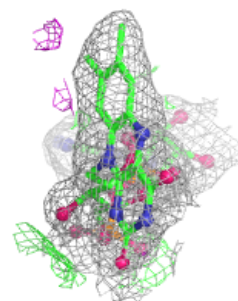
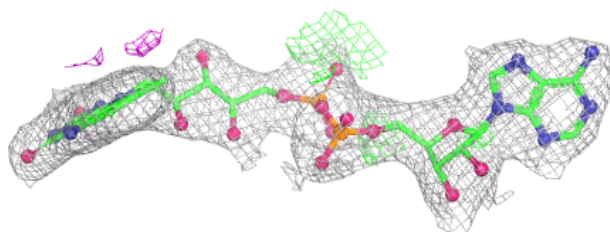
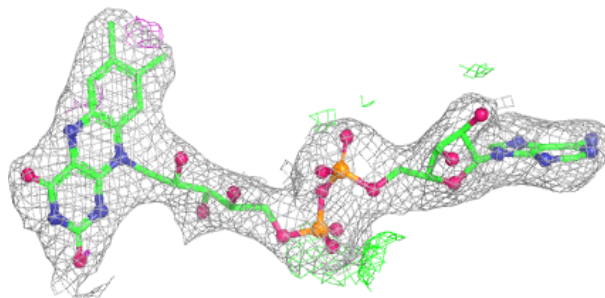
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	2LD	C	402	16/16	0.86	0.12	32,36,43,43	0
3	2LD	D	402	16/16	0.86	0.12	32,36,43,43	0
3	2LD	B	402	16/16	0.94	0.07	34,39,45,45	0
2	FAD	D	401	53/53	0.95	0.07	31,39,49,52	0
2	FAD	C	401	53/53	0.96	0.06	35,39,48,50	0
2	FAD	B	401	53/53	0.96	0.07	29,34,44,50	0
3	2LD	A	402	16/16	0.96	0.07	32,36,43,43	0
2	FAD	A	401	53/53	0.97	0.06	26,36,43,46	0

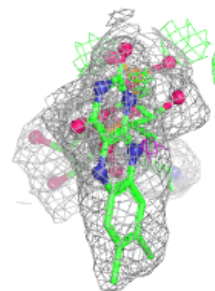
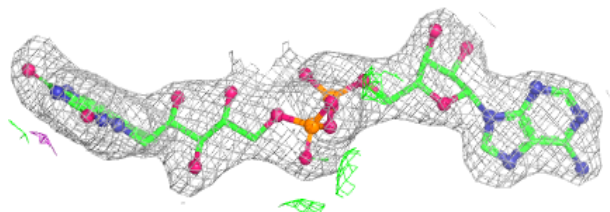
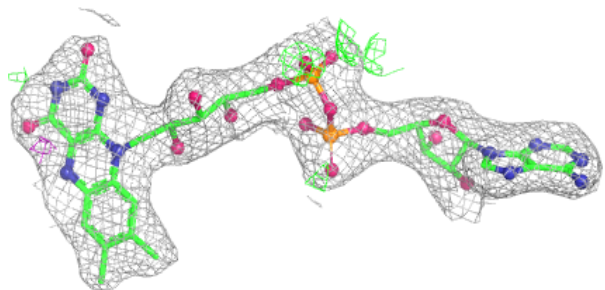
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD D 401:

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

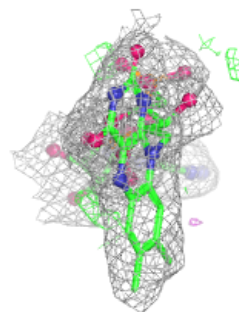
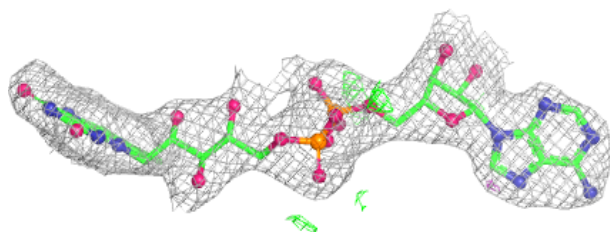
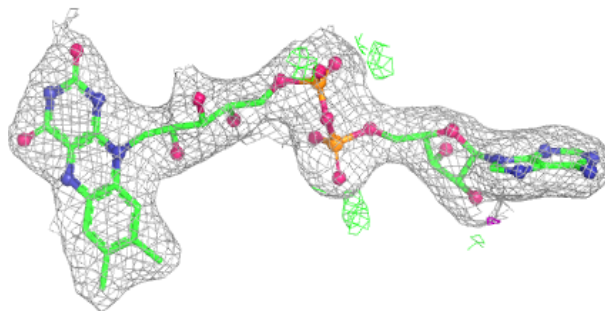
**Electron density around FAD C 401:**

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

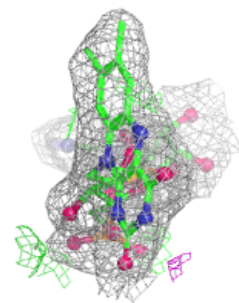
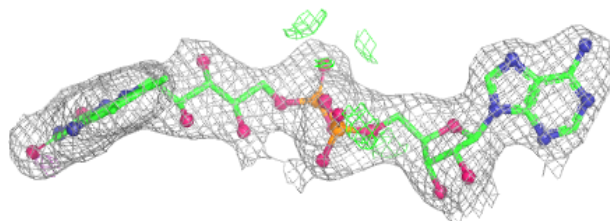
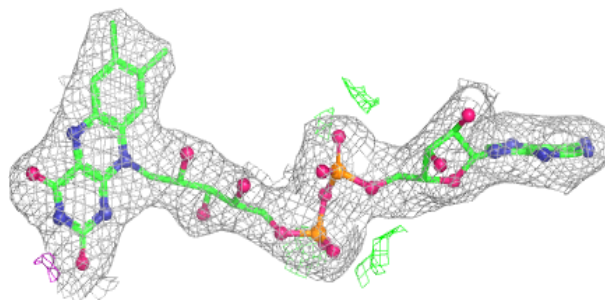


Electron density around FAD B 401:

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

**Electron density around FAD A 401:**

$2mF_o-DF_c$ (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.