



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 06:23 PM JST

PDB ID : 7DQX / pdb_00007dqx
Title : Crystal structure of xanthine dehydrogenase family protein
Authors : Lei, W.
Deposited on : 2020-12-24
Resolution : 3.44 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 : 1.8.5 (274361), CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

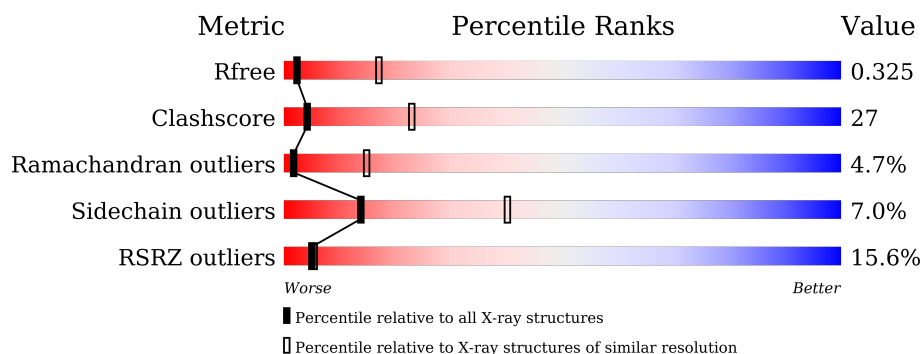
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.44 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	1736 (3.50-3.38)
Clashscore	190562	1808 (3.50-3.38)
Ramachandran outliers	187476	1776 (3.50-3.38)
Sidechain outliers	187428	1777 (3.50-3.38)
RSRZ outliers	180081	1736 (3.50-3.38)

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	794	19% 52% 35% 7% ..
1	D	794	19% 52% 37% 7% ..
2	B	296	8% 65% 26% 5% ..
3	C	160	7% 65% 32% ..
3	F	160	9% 72% 22% ..
4	E	296	7% 65% 26% 6% ..

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
8	FES	C	201	-	-	X	-
8	FES	C	202	-	-	X	-
8	FES	F	201	-	-	X	-
8	FES	F	202	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 18678 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-hydroxypseudooxynicotine dehydrogenase complex subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	765	Total	C	N	O	S	1	0	0
			5831	3665	1028	1122	16			
1	D	770	Total	C	N	O	S	1	0	0
			5867	3694	1027	1129	17			

- Molecule 2 is a protein called 6-hydroxypseudooxynicotine dehydrogenase complex subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	287	Total	C	N	O	S	0	0	0
			2135	1337	392	401	5			

- Molecule 3 is a protein called 6-hydroxypseudooxynicotine dehydrogenase complex subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	160	Total	C	N	O	S	0	0	0
			1229	750	227	240	12			
3	F	160	Total	C	N	O	S	0	0	0
			1229	750	227	240	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	53	ILE	LEU	conflict	UNP O87682
C	136	LEU	ILE	conflict	UNP O87682
F	53	ILE	LEU	conflict	UNP O87682
F	136	LEU	ILE	conflict	UNP O87682

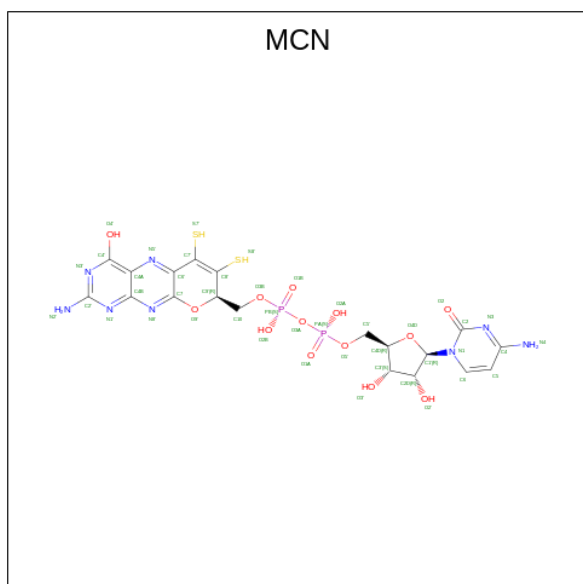
- Molecule 4 is a protein called 6-hydroxypseudooxynicotine dehydrogenase complex subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	293	Total	C	N	O	S	0	0	0
			2175	1361	400	409	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	201	LEU	ILE	conflict	UNP O87681

- Molecule 5 is PTERIN CYTOSINE DINUCLEOTIDE (CCD ID: MCN) (formula: $C_{19}H_{22}N_8O_{13}P_2S_2$).

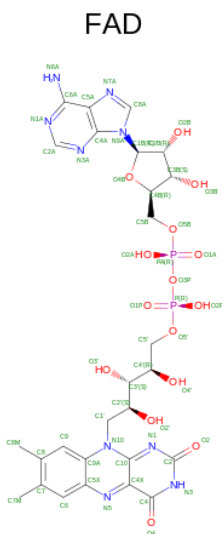


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 44	C 19	N 8	O 13	P 2	S 2	0	0
5	D	1	Total 44	C 19	N 8	O 13	P 2	S 2	0	0

- Molecule 6 is MOLYBDENUM ATOM (CCD ID: MO) (formula: Mo).

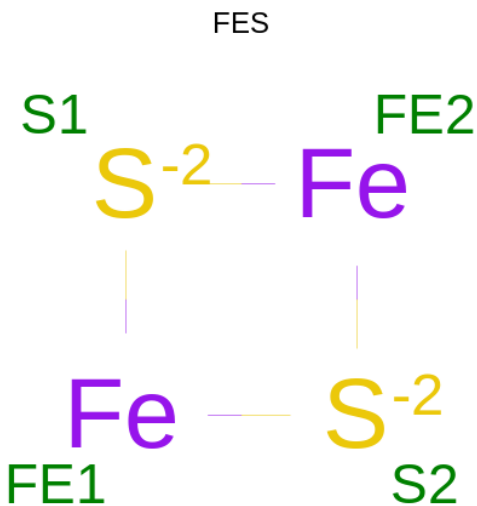
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mo	0	0
			1	1		
6	D	1	Total	Mo	0	0
			1	1		

- Molecule 7 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



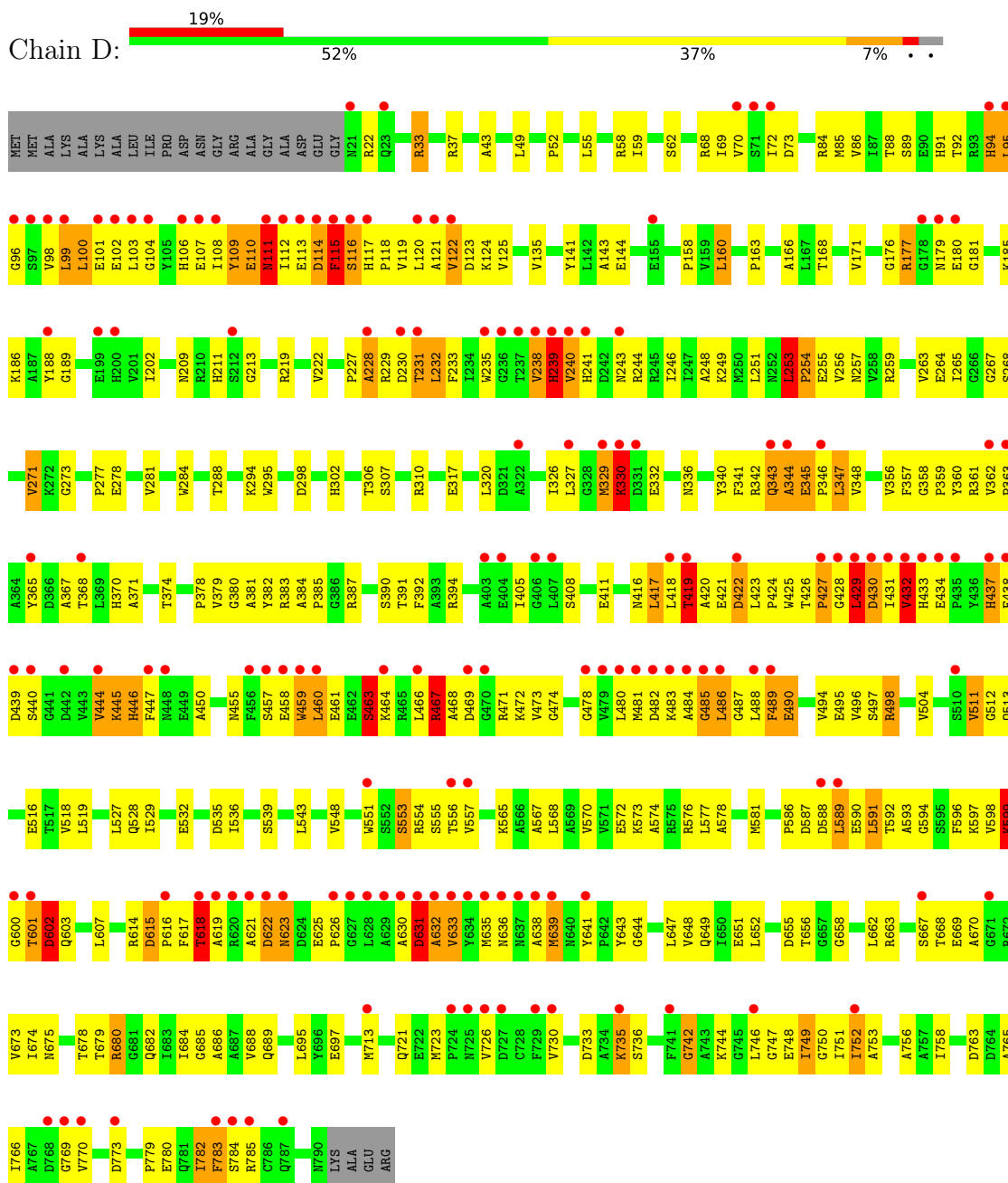
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total 4	Fe 2	S 2	0	0
8	C	1	Total 4	Fe 2	S 2	0	0

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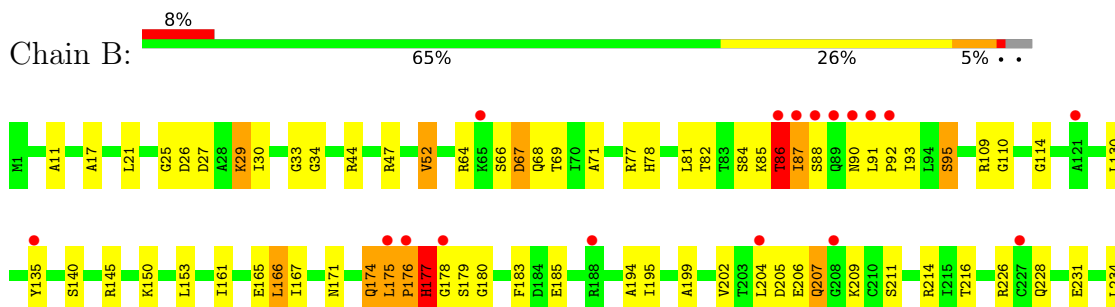
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	F	1	Total	Fe	S	0	0
			4	2	2		
8	F	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 1: 6-hydroxypseudooxynicotine dehydrogenase complex subunit gamma

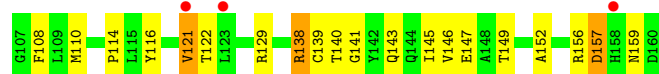


- Molecule 2: 6-hydroxypseudooxynicotine dehydrogenase complex subunit alpha

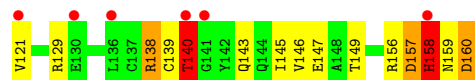
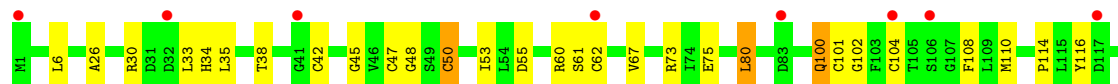




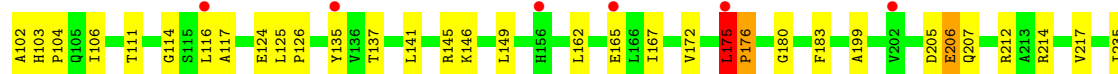
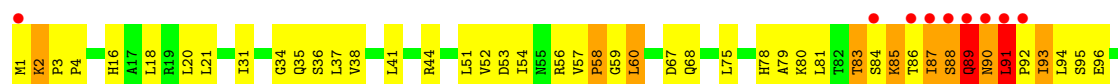
- Molecule 3: 6-hydroxypseudooxynicotine dehydrogenase complex subunit beta



- Molecule 3: 6-hydroxypseudooxynicotine dehydrogenase complex subunit beta



- Molecule 4: 6-hydroxypseudooxynicotine dehydrogenase complex subunit alpha



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.86Å 126.79Å 294.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	147.24 – 3.44 147.24 – 3.44	Depositor EDS
% Data completeness (in resolution range)	93.7 (147.24-3.44) 93.7 (147.24-3.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.287 , 0.326 0.286 , 0.325	Depositor DCC
R_{free} test set	2706 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	76.2	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	18678	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.39% 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: FES, MO, MCN, 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	0.59	0/5947	1.00	25/8084 (0.3%)
1	D	0.60	0/5986	1.02	25/8142 (0.3%)
2	B	0.62	0/2170	0.97	9/2950 (0.3%)
3	C	0.59	0/1247	0.90	4/1689 (0.2%)
3	F	0.62	0/1247	0.84	3/1689 (0.2%)
4	E	0.63	0/2211	0.94	7/3006 (0.2%)
All	All	0.60	0/18808	0.98	73/25560 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	D	0	10
2	B	0	2
3	C	0	1
3	F	0	2
4	E	0	2
All	All	0	26

There are no bond length outliers.

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	34	HIS	N-CA-C	-12.30	95.52	112.25
1	D	426	THR	CA-C-N	10.44	132.89	119.84
1	D	426	THR	C-N-CA	10.44	132.89	119.84
1	D	104	GLY	N-CA-C	-9.58	103.08	114.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	ASP	N-CA-C	8.99	123.80	109.86
2	B	175	LEU	C-N-CD	-8.75	101.35	120.60
1	D	239	HIS	N-CA-C	8.72	123.17	112.54
1	A	603	GLN	N-CA-C	8.72	121.00	110.19
1	D	464	LYS	N-CA-C	-8.70	101.26	112.23
1	D	784	SER	N-CA-C	-8.46	101.41	112.41
1	A	181	GLY	N-CA-C	8.12	119.76	111.56
4	E	91	LEU	CA-C-N	-7.98	110.46	120.51
4	E	91	LEU	C-N-CA	-7.98	110.46	120.51
2	B	273	ARG	N-CA-C	7.49	126.75	110.80
1	D	591	LEU	N-CA-C	6.93	120.20	107.73
3	C	33	LEU	N-CA-C	6.91	118.92	109.11
1	D	231	THR	N-CA-C	6.85	117.32	108.34
1	A	739	ASN	CA-C-N	6.74	128.26	119.84
1	A	739	ASN	C-N-CA	6.74	128.26	119.84
1	A	784	SER	N-CA-C	-6.68	104.87	113.16
1	D	467	ARG	N-CA-C	-6.68	104.99	113.01
2	B	175	LEU	CA-C-N	6.65	142.96	127.00
2	B	175	LEU	C-N-CA	6.65	142.96	127.00
1	D	332	GLU	N-CA-C	6.64	118.88	110.24
1	A	787	GLN	N-CA-C	-6.61	105.32	113.19
1	D	114	ASP	CA-C-N	6.56	133.51	121.70
1	D	114	ASP	C-N-CA	6.56	133.51	121.70
1	D	437	HIS	N-CA-C	6.50	118.83	109.14
2	B	274	THR	N-CA-C	-6.44	97.09	110.80
4	E	67	ASP	CB-CA-C	-6.41	109.17	116.54
2	B	275	MET	N-CA-C	-6.39	104.40	111.36
1	A	466	LEU	N-CA-C	-6.35	103.48	110.91
1	D	489	PHE	N-CA-C	6.18	118.85	109.95
3	F	140	THR	N-CA-C	6.15	120.96	112.90
1	D	253	LEU	CA-C-N	6.11	127.47	119.84
1	D	253	LEU	C-N-CA	6.11	127.47	119.84
1	A	109	TYR	N-CA-C	-6.09	101.18	109.95
1	A	588	ASP	N-CA-C	6.09	119.10	110.14
1	D	631	ASP	N-CA-C	6.06	123.71	110.80
1	A	100	LEU	N-CA-C	6.00	120.20	112.41
1	A	471	ARG	N-CA-C	5.90	123.37	110.80
1	A	768	ASP	N-CA-C	5.78	119.64	112.47
3	F	159	ASN	N-CA-CB	5.69	120.11	110.49
1	D	73	ASP	OD1-CG-OD2	-5.68	109.26	122.90
1	A	621	ALA	N-CA-C	5.64	117.76	110.65
1	D	115	PHE	N-CA-C	5.64	126.78	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	483	LYS	N-CA-C	5.63	122.80	110.80
1	A	770	VAL	N-CA-C	5.63	121.06	109.34
1	D	675	ASN	CA-C-N	5.63	125.74	119.32
1	D	675	ASN	C-N-CA	5.63	125.74	119.32
3	F	158	HIS	CB-CA-C	-5.63	101.04	110.56
4	E	59	GLY	N-CA-C	5.61	119.67	112.83
1	D	244	ARG	N-CA-C	-5.55	105.77	112.54
1	D	622	ASP	N-CA-C	5.44	116.54	108.60
2	B	67	ASP	CB-CA-C	-5.43	110.30	116.54
1	A	458	GLU	N-CA-C	5.42	116.87	110.97
1	A	418	LEU	N-CA-C	5.40	122.30	110.80
1	A	489	PHE	N-CA-C	5.37	116.44	108.86
1	A	555	SER	N-CA-C	5.36	118.04	111.82
1	D	344	ALA	N-CA-C	-5.35	104.33	111.87
1	A	578	ALA	N-CA-C	-5.34	106.82	113.38
1	A	472	LYS	N-CA-C	5.32	118.49	109.76
1	A	69	ILE	N-CA-C	5.31	117.71	108.90
4	E	88	SER	N-CA-C	-5.24	102.71	110.46
1	D	469	ASP	N-CA-C	-5.19	106.90	113.18
4	E	90	ASN	N-CA-C	5.17	117.07	108.02
3	C	87	HIS	CA-C-N	5.17	126.30	119.84
3	C	87	HIS	C-N-CA	5.17	126.30	119.84
4	E	85	LYS	N-CA-C	5.14	116.57	111.07
2	B	174	GLN	N-CA-C	5.13	116.87	111.28
1	A	108	ILE	N-CA-C	-5.06	108.57	113.53
2	B	204	LEU	N-CA-C	5.03	117.69	109.59
1	A	447	PHE	N-CA-C	5.03	116.84	111.36

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	114	ASP	Peptide
1	A	115	PHE	Peptide
1	A	243	ASN	Peptide
1	A	330	LYS	Peptide
1	A	466	LEU	Peptide
1	A	482	ASP	Peptide
1	A	587	ASP	Peptide
1	A	602	ASP	Peptide
1	A	603	GLN	Peptide
2	B	272	ILE	Peptide

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Mol	Chain	Res	Type	Group
2	B	273	ARG	Peptide
3	C	33	LEU	Peptide
1	D	110	GLU	Peptide
1	D	168	THR	Peptide
1	D	239	HIS	Peptide
1	D	330	LYS	Peptide
1	D	430	ASP	Peptide
1	D	445	LYS	Peptide
1	D	463	SER	Peptide
1	D	587	ASP	Peptide
1	D	590	GLU	Peptide
1	D	782	ILE	Peptide
4	E	89	GLN	Peptide
4	E	91	LEU	Peptide
3	F	140	THR	Peptide
3	F	158	HIS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5831	0	5717	371	0
1	D	5867	0	5754	409	0
2	B	2135	0	2188	97	0
3	C	1229	0	1187	47	0
3	F	1229	0	1187	45	0
4	E	2175	0	2219	82	0
5	A	44	0	17	14	0
5	D	44	0	17	15	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
7	B	53	0	31	11	0
7	E	53	0	31	9	0
8	C	8	0	0	6	0
8	F	8	0	0	6	0
All	All	18678	0	18348	1015	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 27.

All (1015) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:486:LEU:HD13	1:A:554:ARG:HB2	1.23	1.20
1:D:588:ASP:HB3	1:D:598:VAL:HA	1.23	1.18
1:A:439:ASP:HA	1:A:440:SER:CB	1.75	1.16
1:A:490:GLU:HG3	1:A:554:ARG:HH12	1.07	1.11
1:A:485:GLY:HA2	1:A:486:LEU:HB2	1.12	1.11
1:A:656:THR:HA	2:B:273:ARG:NH2	1.64	1.10
1:D:98:VAL:HB	1:D:118:PRO:HG2	1.32	1.07
1:A:667:SER:HA	1:A:730:VAL:HG21	1.35	1.07
1:A:95:LEU:HB3	1:A:96:GLY:HA2	1.36	1.06
2:B:273:ARG:HB3	2:B:275:MET:H	1.14	1.05
4:E:2:LYS:HD2	1:D:144:GLU:HB3	1.38	1.04
1:A:258:VAL:HB	1:A:259:ARG:CA	1.87	1.04
1:A:439:ASP:CA	1:A:440:SER:HB3	1.86	1.04
1:A:258:VAL:CB	1:A:259:ARG:HA	1.86	1.03
4:E:2:LYS:CD	1:D:144:GLU:HB3	1.91	1.01
1:A:485:GLY:CA	1:A:486:LEU:HB2	1.92	1.00
1:D:437:HIS:HB2	1:D:438:PHE:HA	1.44	0.97
1:A:667:SER:HA	1:A:730:VAL:CG2	1.93	0.97
1:A:439:ASP:HA	1:A:440:SER:HB3	0.97	0.97
3:F:143:GLN:OE1	1:D:726:VAL:HA	1.64	0.96
1:D:428:GLY:O	1:D:429:LEU:HB2	1.59	0.96
1:D:598:VAL:O	1:D:599:LYS:HD2	1.64	0.95
1:D:94:HIS:CG	1:D:95:LEU:H	1.84	0.95
1:D:112:ILE:HA	1:D:113:GLU:HB3	1.49	0.95
1:D:437:HIS:HB2	1:D:438:PHE:CA	1.96	0.95
1:A:95:LEU:HB3	1:A:96:GLY:CA	1.98	0.94
1:A:490:GLU:CG	1:A:554:ARG:HH12	1.80	0.94
2:B:274:THR:O	2:B:278:ARG:HG2	1.66	0.93
7:B:301:FAD:N1	7:B:301:FAD:H2'	1.83	0.93
1:A:486:LEU:HD13	1:A:554:ARG:CB	1.99	0.92
1:A:258:VAL:HB	1:A:259:ARG:HA	0.95	0.91
1:D:485:GLY:HA2	1:D:486:LEU:HG	1.51	0.91
1:D:593:ALA:H	1:D:594:GLY:HA2	1.33	0.91
4:E:175:LEU:HB2	4:E:176:PRO:HD2	1.50	0.91
4:E:175:LEU:HB2	4:E:176:PRO:CD	2.01	0.90
1:A:69:ILE:HD11	1:A:122:VAL:HA	1.52	0.89
1:D:615:ASP:HB2	1:D:616:PRO:HD2	1.52	0.89
1:D:598:VAL:HG13	1:D:599:LYS:HE3	1.53	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:LEU:HB3	1:A:447:PHE:CD1	2.07	0.89
1:D:106:HIS:H	1:D:107:GLU:HA	1.38	0.88
1:A:488:LEU:O	1:A:634:TYR:HB2	1.74	0.88
1:A:74:ALA:HA	1:A:75:THR:OG1	1.74	0.87
1:A:484:ALA:C	1:A:486:LEU:HG	1.99	0.87
1:A:94:HIS:HA	1:A:95:LEU:HG	1.56	0.87
1:A:490:GLU:HG3	1:A:554:ARG:NH1	1.89	0.86
1:A:417:LEU:HB3	1:A:447:PHE:CD2	2.09	0.86
1:A:486:LEU:CD1	1:A:554:ARG:HB2	2.04	0.86
2:B:271:VAL:HA	2:B:273:ARG:HD3	1.56	0.86
1:D:667:SER:HB2	1:D:730:VAL:HB	1.57	0.86
1:D:253:LEU:N	1:D:254:PRO:CD	2.39	0.86
1:A:666:THR:O	1:A:730:VAL:HG21	1.76	0.85
1:D:599:LYS:CD	1:D:600:GLY:H	1.87	0.85
1:D:779:PRO:HA	1:D:782:ILE:HG22	1.58	0.85
1:D:599:LYS:HD2	1:D:600:GLY:H	1.38	0.85
1:D:95:LEU:N	1:D:96:GLY:HA3	1.90	0.85
1:A:418:LEU:HG	1:A:419:THR:H	1.42	0.84
4:E:83:THR:HG22	4:E:84:SER:HB3	1.59	0.84
1:D:471:ARG:HB3	1:D:765:ALA:HB1	1.60	0.84
1:A:98:VAL:HA	1:A:118:PRO:HB2	1.59	0.84
1:A:670:ALA:HA	1:A:744:LYS:HD2	1.58	0.84
3:F:80:LEU:HD11	3:F:110:MET:HE3	1.61	0.83
1:D:437:HIS:HB2	1:D:438:PHE:CB	2.08	0.83
1:A:482:ASP:OD2	1:A:642:PRO:HD3	1.78	0.83
4:E:259:PRO:HB2	4:E:260:THR:HG23	1.58	0.83
1:A:219:ARG:HE	1:A:306:THR:HG22	1.41	0.82
1:D:239:HIS:CE1	1:D:265:ILE:HG21	2.14	0.82
1:A:656:THR:HA	2:B:273:ARG:HH21	1.42	0.82
1:D:94:HIS:CG	1:D:95:LEU:N	2.47	0.82
1:D:486:LEU:N	1:D:487:GLY:HA3	1.95	0.82
3:C:104:CYS:HB2	3:C:108:PHE:HE1	1.46	0.81
1:A:346:PRO:HB2	1:A:349:SER:HB2	1.61	0.81
1:A:486:LEU:CD1	1:A:554:ARG:CB	2.58	0.81
5:A:801:MCN:HN21	3:C:100:GLN:HB3	1.46	0.81
1:D:188:TYR:HD2	1:D:429:LEU:H	1.28	0.80
1:D:112:ILE:HA	1:D:113:GLU:CB	2.08	0.80
1:D:437:HIS:CB	1:D:438:PHE:HA	2.02	0.79
1:A:486:LEU:O	1:A:548:VAL:HG11	1.83	0.79
1:A:255:GLU:HB2	1:D:497:SER:HB2	1.63	0.79
1:A:74:ALA:HB1	1:A:77:ALA:H	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:PRO:N	1:A:587:ASP:HA	1.99	0.78
3:C:45:GLY:HA2	8:C:201:FES:S1	2.24	0.78
1:D:528:GLN:HG2	1:D:592:THR:HB	1.66	0.78
1:A:432:VAL:HB	1:A:440:SER:HB2	1.64	0.78
1:D:486:LEU:HD21	1:D:554:ARG:HD2	1.65	0.77
1:A:747:GLY:N	5:A:801:MCN:O2'	2.16	0.77
1:A:95:LEU:CB	1:A:96:GLY:HA2	2.14	0.77
1:A:485:GLY:HA2	1:A:486:LEU:CB	2.06	0.77
1:D:747:GLY:N	5:D:801:MCN:O2'	2.17	0.77
1:A:482:ASP:HB2	1:A:553:SER:HB2	1.67	0.77
1:D:111:ASN:O	1:D:113:GLU:HA	1.84	0.77
1:D:219:ARG:HE	1:D:306:THR:HG22	1.49	0.77
1:A:418:LEU:HD11	1:A:423:LEU:HD21	1.65	0.77
1:A:768:ASP:OD1	1:A:771:HIS:HE1	1.67	0.76
3:C:156:ARG:NE	3:C:157:ASP:OD1	2.16	0.76
1:D:485:GLY:CA	1:D:486:LEU:HG	2.15	0.76
1:D:490:GLU:HG2	1:D:554:ARG:NH2	2.00	0.76
2:B:30:ILE:HD11	7:B:301:FAD:C5A	2.14	0.76
1:A:312:MET:HE2	1:A:335:HIS:CD2	2.21	0.76
1:D:460:LEU:HD13	1:D:647:LEU:HD23	1.66	0.76
1:A:256:VAL:HB	1:A:258:VAL:HG22	1.68	0.75
3:F:104:CYS:HB2	3:F:108:PHE:HE1	1.50	0.75
1:D:241:HIS:HD2	1:D:539:SER:HB2	1.49	0.75
1:A:655:ASP:CA	2:B:273:ARG:HH22	1.98	0.75
1:A:666:THR:O	1:A:730:VAL:CG2	2.35	0.75
1:A:483:LYS:O	1:A:485:GLY:N	2.20	0.74
1:A:596:PHE:O	1:A:604:GLN:HB2	1.87	0.74
1:A:588:ASP:HB3	1:A:596:PHE:HZ	1.53	0.74
2:B:270:GLN:O	2:B:273:ARG:HD3	1.88	0.74
4:E:289:PRO:HA	4:E:290:THR:C	2.12	0.74
1:D:419:THR:O	1:D:422:ASP:HB2	1.87	0.74
1:A:640:ASN:OD1	1:A:744:LYS:HG2	1.88	0.74
1:D:615:ASP:HB2	1:D:616:PRO:CD	2.18	0.74
1:A:736:SER:HB3	1:A:742:GLY:HA3	1.70	0.73
1:D:329:MET:O	1:D:330:LYS:HB2	1.86	0.73
3:C:101:CYS:N	8:C:202:FES:S2	2.60	0.73
1:D:109:TYR:CD1	1:D:110:GLU:HB2	2.24	0.73
1:A:639:MET:O	1:A:640:ASN:HB3	1.88	0.73
4:E:86:THR:O	4:E:92:PRO:HD2	1.89	0.73
2:B:271:VAL:HA	2:B:273:ARG:CD	2.18	0.73
1:D:188:TYR:HD2	1:D:429:LEU:N	1.85	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:100:GLN:HG3	3:F:139:CYS:HB3	1.71	0.73
1:D:420:ALA:HA	1:D:421:GLU:C	2.14	0.73
4:E:21:LEU:HB3	4:E:52:VAL:HG21	1.69	0.72
1:A:447:PHE:CZ	1:A:448:ASN:HB2	2.24	0.72
1:A:747:GLY:N	5:A:801:MCN:HO2'	1.86	0.72
1:D:186:LYS:HB3	1:D:430:ASP:HB3	1.70	0.72
1:D:572:GLU:O	1:D:576:ARG:HB3	1.89	0.72
1:A:482:ASP:OD1	1:A:483:LYS:N	2.22	0.72
1:D:112:ILE:CA	1:D:113:GLU:HB3	2.19	0.72
1:D:241:HIS:CD2	1:D:539:SER:HB2	2.24	0.72
1:D:253:LEU:H	1:D:254:PRO:HD3	1.55	0.72
1:D:783:PHE:O	1:D:783:PHE:CD1	2.42	0.72
1:D:213:GLY:H	1:D:271:VAL:HG21	1.52	0.72
3:F:110:MET:HE2	3:F:110:MET:HA	1.70	0.72
1:A:418:LEU:HG	1:A:419:THR:N	2.04	0.72
1:A:213:GLY:H	1:A:271:VAL:HG21	1.54	0.71
1:D:238:VAL:O	1:D:241:HIS:ND1	2.20	0.71
1:A:486:LEU:N	1:A:487:GLY:HA3	2.05	0.71
1:D:37:ARG:HB3	1:D:43:ALA:HB2	1.71	0.71
1:D:783:PHE:O	1:D:783:PHE:HD1	1.73	0.71
1:A:302:HIS:CD2	1:A:306:THR:HG21	2.25	0.71
1:A:209:ASN:HD21	1:A:775:LEU:C	1.98	0.71
3:C:104:CYS:HB2	3:C:108:PHE:CE1	2.26	0.71
1:D:504:VAL:HB	1:D:536:ILE:HG12	1.73	0.71
1:A:219:ARG:HE	1:A:306:THR:CG2	2.04	0.71
3:C:139:CYS:HB2	8:C:202:FES:S2	2.31	0.71
1:A:215:PRO:HD2	1:A:302:HIS:HE1	1.55	0.70
1:D:239:HIS:HE1	1:D:265:ILE:HG21	1.55	0.70
1:A:471:ARG:HB2	1:A:765:ALA:HB1	1.74	0.70
3:F:156:ARG:NE	3:F:157:ASP:OD1	2.19	0.70
1:D:688:VAL:HG13	1:D:723:MET:HE2	1.74	0.70
2:B:34:GLY:N	7:B:301:FAD:O2A	2.25	0.70
3:F:100:GLN:HB2	1:D:512:GLY:O	1.92	0.70
4:E:259:PRO:HB2	4:E:260:THR:CG2	2.22	0.70
3:F:139:CYS:CB	8:F:202:FES:S2	2.79	0.70
1:A:766:ILE:H	1:A:767:ALA:HA	1.57	0.69
1:A:724:PRO:C	1:A:726:VAL:H	2.00	0.69
2:B:274:THR:HA	2:B:277:GLU:HB2	1.74	0.69
1:A:470:GLY:C	1:A:471:ARG:HG2	2.15	0.69
1:A:482:ASP:O	1:A:484:ALA:N	2.21	0.69
5:A:801:MCN:N2'	3:C:100:GLN:HB3	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:176:PRO:HD2	2:B:177:HIS:H	1.58	0.69
3:C:139:CYS:CB	8:C:202:FES:S2	2.81	0.68
1:D:573:LYS:O	1:D:577:LEU:HB2	1.92	0.68
2:B:273:ARG:HB3	2:B:275:MET:N	1.99	0.68
1:D:599:LYS:NZ	1:D:603:GLN:O	2.27	0.68
1:A:181:GLY:HA3	1:A:371:ALA:O	1.94	0.68
4:E:259:PRO:HB2	4:E:260:THR:HA	1.75	0.68
1:A:267:GLY:HA2	5:A:801:MCN:O4'	1.93	0.68
1:A:471:ARG:HB2	1:A:765:ALA:CB	2.24	0.68
1:A:266:GLY:HA2	3:C:101:CYS:HB2	1.74	0.68
1:A:326:ILE:HG12	1:A:416:ASN:OD1	1.93	0.68
1:A:485:GLY:C	1:A:487:GLY:HA3	2.18	0.68
1:D:433:HIS:HB3	1:D:437:HIS:ND1	2.07	0.68
1:D:432:VAL:O	1:D:437:HIS:HB3	1.94	0.68
4:E:291:LYS:HG2	4:E:292:GLU:N	2.08	0.67
1:D:365:TYR:CE2	1:D:367:ALA:HB2	2.29	0.67
1:D:211:HIS:CE1	1:D:310:ARG:HG2	2.29	0.67
1:A:785:ARG:HD2	1:A:786:CYS:N	2.10	0.67
1:D:89:SER:HB2	1:D:120:LEU:O	1.95	0.67
1:A:250:MET:HE2	1:A:280:VAL:HG11	1.76	0.67
1:A:419:THR:HB	1:A:422:ASP:HB3	1.77	0.67
4:E:103:HIS:HB3	4:E:104:PRO:HD2	1.77	0.67
1:D:320:LEU:HD13	1:D:405:ILE:HD11	1.77	0.67
1:D:181:GLY:HA3	1:D:371:ALA:O	1.94	0.66
1:D:384:ALA:HA	1:D:387:ARG:NH2	2.10	0.66
1:D:466:LEU:HB3	1:D:468:ALA:HB2	1.77	0.66
3:F:104:CYS:HB2	3:F:108:PHE:CE1	2.30	0.66
3:F:139:CYS:HB2	8:F:202:FES:S2	2.34	0.66
1:A:628:LEU:HD12	1:A:630:ALA:H	1.60	0.66
1:A:480:LEU:HD13	1:A:752:ILE:HD11	1.78	0.66
1:D:114:ASP:CB	1:D:340:TYR:HD1	2.08	0.66
1:D:483:LYS:HD2	1:D:553:SER:O	1.96	0.66
1:A:656:THR:HA	2:B:273:ARG:HH22	1.59	0.66
4:E:259:PRO:CB	4:E:260:THR:HA	2.26	0.66
1:D:99:LEU:HG	1:D:118:PRO:HB3	1.78	0.66
1:A:785:ARG:HD2	1:A:786:CYS:H	1.61	0.66
1:D:588:ASP:OD2	1:D:591:LEU:HD11	1.96	0.66
1:A:259:ARG:NH1	1:D:543:LEU:HD11	2.10	0.66
1:A:585:ASP:HB2	1:A:586:PRO:C	2.20	0.66
3:F:45:GLY:HA2	8:F:201:FES:S1	2.36	0.66
1:D:670:ALA:HA	1:D:744:LYS:HD2	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:518:VAL:HG11	1:D:556:THR:HG22	1.77	0.66
1:D:117:HIS:N	1:D:118:PRO:HA	2.11	0.66
1:A:597:LYS:HA	1:A:604:GLN:HB3	1.78	0.65
1:D:678:THR:OG1	5:D:801:MCN:N4	2.28	0.65
1:A:244:ARG:HH21	1:A:541:THR:HB	1.61	0.65
1:D:241:HIS:HD2	1:D:539:SER:CB	2.08	0.65
4:E:85:LYS:HB3	4:E:87:ILE:HA	1.78	0.65
1:D:240:VAL:HG13	1:D:243:ASN:HB2	1.77	0.65
1:D:108:ILE:HA	1:D:109:TYR:HB2	1.77	0.65
1:D:423:LEU:HD23	1:D:445:LYS:HA	1.79	0.65
1:A:89:SER:HB3	1:A:122:VAL:HG23	1.79	0.65
1:D:485:GLY:HA2	1:D:486:LEU:CG	2.26	0.65
1:A:213:GLY:O	3:C:138:ARG:NE	2.29	0.65
1:D:667:SER:CB	1:D:730:VAL:HB	2.26	0.64
1:A:399:ASP:HB3	1:A:770:VAL:HG11	1.78	0.64
1:A:588:ASP:CB	1:A:596:PHE:HZ	2.10	0.64
1:D:227:PRO:C	1:D:229:ARG:N	2.55	0.64
1:A:678:THR:OG1	5:A:801:MCN:N4	2.29	0.64
4:E:31:ILE:HG22	4:E:53:ASP:HA	1.80	0.64
1:D:267:GLY:HA2	5:D:801:MCN:O4'	1.97	0.64
2:B:273:ARG:CB	2:B:275:MET:H	2.00	0.64
1:D:227:PRO:C	1:D:229:ARG:H	2.03	0.64
1:D:253:LEU:N	1:D:254:PRO:HD2	2.12	0.64
1:D:494:VAL:O	1:D:622:ASP:OD1	2.16	0.64
3:C:29:LEU:O	3:C:33:LEU:O	2.15	0.63
1:D:209:ASN:O	1:D:310:ARG:HB3	1.98	0.63
1:D:599:LYS:CG	1:D:600:GLY:N	2.60	0.63
3:C:42:CYS:N	3:C:47:CYS:SG	2.69	0.63
1:A:513:GLN:O	5:A:801:MCN:H5	1.97	0.63
4:E:90:ASN:HA	4:E:92:PRO:HD3	1.79	0.63
1:D:114:ASP:CB	1:D:341:PHE:H	2.11	0.63
1:D:302:HIS:CD2	1:D:306:THR:HG21	2.34	0.63
4:E:284:LEU:O	4:E:286:ARG:N	2.31	0.63
1:D:256:VAL:O	1:D:257:ASN:HB2	1.99	0.63
1:D:329:MET:O	1:D:330:LYS:CB	2.46	0.63
1:D:518:VAL:HG13	1:D:674:ILE:HG21	1.81	0.63
1:D:591:LEU:HD22	1:D:596:PHE:HD1	1.64	0.63
4:E:259:PRO:HB2	4:E:260:THR:CA	2.29	0.62
1:D:365:TYR:CG	1:D:429:LEU:HD22	2.34	0.62
1:D:593:ALA:H	1:D:594:GLY:CA	2.11	0.62
1:A:667:SER:CA	1:A:730:VAL:HG21	2.21	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:668:THR:HG21	1:D:749:ILE:HG12	1.82	0.62
1:A:256:VAL:HA	1:A:257:ASN:HB2	1.80	0.62
1:A:592:THR:HG22	1:A:594:GLY:H	1.64	0.62
4:E:86:THR:H	4:E:90:ASN:CB	2.11	0.62
1:D:444:VAL:HG21	1:D:744:LYS:CE	2.30	0.62
3:F:33:LEU:O	3:F:35:LEU:N	2.33	0.62
4:E:35:GLN:HB2	7:E:301:FAD:H5'2	1.81	0.62
4:E:176:PRO:HD3	4:E:212:ARG:HH21	1.62	0.62
1:A:219:ARG:NE	1:A:306:THR:HG22	2.13	0.62
1:D:360:TYR:HE2	1:D:394:ARG:NH1	1.96	0.62
1:A:482:ASP:N	1:A:483:LYS:HE3	2.14	0.62
4:E:60:LEU:O	4:E:75:LEU:HB2	2.00	0.61
1:D:341:PHE:HE2	1:D:346:PRO:HD3	1.64	0.61
1:A:487:GLY:HA2	1:A:488:LEU:C	2.24	0.61
1:D:365:TYR:CD1	1:D:429:LEU:HD22	2.34	0.61
1:D:652:LEU:HD13	1:D:785:ARG:HH21	1.64	0.61
1:A:174:PHE:O	1:A:179:ASN:OD1	2.17	0.61
1:A:590:GLU:OE1	1:A:597:LYS:HB2	1.99	0.61
3:F:101:CYS:N	8:F:202:FES:S2	2.63	0.61
1:A:486:LEU:HD11	1:A:554:ARG:HB3	1.83	0.61
1:D:444:VAL:HG21	1:D:744:LYS:HE3	1.82	0.61
1:A:447:PHE:CE1	1:A:448:ASN:HB2	2.35	0.61
1:A:90:GLU:O	1:A:94:HIS:CE1	2.54	0.61
1:A:395:GLU:HB2	1:A:756:ALA:HB1	1.81	0.61
2:B:86:THR:HG22	2:B:86:THR:O	2.01	0.61
1:D:253:LEU:N	1:D:254:PRO:HD3	2.11	0.61
1:D:779:PRO:HA	1:D:782:ILE:CG2	2.31	0.61
1:A:478:GLY:O	1:A:643:TYR:HA	1.99	0.61
1:D:95:LEU:N	1:D:96:GLY:CA	2.64	0.61
1:D:106:HIS:N	1:D:107:GLU:HA	2.03	0.60
1:D:188:TYR:CE2	1:D:430:ASP:O	2.53	0.60
1:A:89:SER:HB3	1:A:122:VAL:CG2	2.31	0.60
4:E:180:GLY:HA3	4:E:283:ALA:O	2.01	0.60
5:A:801:MCN:HN21	3:C:100:GLN:CB	2.14	0.60
1:D:231:THR:HG22	1:D:257:ASN:HA	1.83	0.60
4:E:2:LYS:HD2	1:D:144:GLU:CB	2.23	0.60
1:A:667:SER:HA	1:A:730:VAL:HG23	1.83	0.60
4:E:145:ARG:HG2	4:E:146:LYS:N	2.16	0.60
1:A:268:SER:HB3	1:A:511:VAL:HG11	1.81	0.60
1:A:588:ASP:HB3	1:A:596:PHE:CZ	2.37	0.60
1:A:228:ALA:O	1:A:230:ASP:N	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:LEU:CD2	2:B:226:ARG:HG2	2.32	0.60
1:D:752:ILE:HD12	1:D:753:ALA:H	1.67	0.59
1:A:188:TYR:N	1:A:429:LEU:HA	2.18	0.59
1:D:22:ARG:NH1	1:D:592:THR:HG21	2.16	0.59
1:D:490:GLU:CG	1:D:554:ARG:NH2	2.66	0.59
3:F:6:LEU:HD21	3:F:67:VAL:HA	1.84	0.59
1:D:423:LEU:CD2	1:D:445:LYS:HA	2.32	0.59
1:D:599:LYS:HD3	1:D:602:ASP:N	2.16	0.59
1:A:253:LEU:N	1:A:254:PRO:CD	2.65	0.59
1:A:483:LYS:HZ3	1:A:641:TYR:HA	1.67	0.59
1:A:486:LEU:CD1	1:A:554:ARG:HB3	2.29	0.59
2:B:267:TYR:O	2:B:271:VAL:HG23	2.01	0.59
1:D:488:LEU:HD13	1:D:636:ASN:CG	2.28	0.59
1:D:593:ALA:N	1:D:594:GLY:HA2	2.12	0.59
1:A:98:VAL:HG22	1:A:118:PRO:HG2	1.82	0.59
1:A:471:ARG:HB2	1:A:765:ALA:CA	2.33	0.59
1:A:444:VAL:HG21	1:A:641:TYR:O	2.03	0.59
2:B:176:PRO:HD2	2:B:177:HIS:N	2.18	0.59
1:D:615:ASP:CB	1:D:616:PRO:HD2	2.28	0.59
1:A:193:ARG:O	1:A:197:GLU:HB2	2.03	0.59
1:A:485:GLY:CA	1:A:486:LEU:CB	2.73	0.59
5:A:801:MCN:H3'	5:A:801:MCN:O3A	2.03	0.58
1:D:188:TYR:CD2	1:D:429:LEU:N	2.70	0.58
1:D:635:MET:HE1	1:D:638:ALA:O	2.04	0.58
1:A:655:ASP:HA	2:B:273:ARG:HH22	1.68	0.58
1:D:695:LEU:HD11	1:D:758:ILE:HG21	1.85	0.58
1:A:365:TYR:CE2	1:A:367:ALA:HB2	2.38	0.58
3:C:42:CYS:SG	3:C:47:CYS:N	2.71	0.58
1:D:686:ALA:O	1:D:751:ILE:HG22	2.03	0.58
1:A:232:LEU:O	1:A:259:ARG:N	2.35	0.58
2:B:273:ARG:HG3	2:B:274:THR:HB	1.86	0.58
1:D:391:THR:HG22	1:D:394:ARG:HH21	1.69	0.58
1:A:209:ASN:ND2	1:A:775:LEU:C	2.62	0.58
1:A:262:HIS:CD2	1:A:538:HIS:HE1	2.21	0.58
4:E:38:VAL:HA	4:E:41:LEU:HD12	1.86	0.58
1:D:490:GLU:HG2	1:D:554:ARG:HH22	1.68	0.58
2:B:234:LEU:O	2:B:237:SER:HB3	2.03	0.58
2:B:257:PRO:HG2	2:B:269:ALA:HB2	1.85	0.58
1:D:648:VAL:HG11	1:D:758:ILE:HD13	1.86	0.58
1:A:320:LEU:HD13	1:A:405:ILE:HD11	1.86	0.58
1:D:417:LEU:HB3	1:D:447:PHE:HD2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:488:LEU:HD13	1:D:636:ASN:OD1	2.04	0.58
1:D:570:VAL:O	1:D:574:ALA:N	2.33	0.58
1:A:357:PHE:HB2	1:A:362:VAL:HG21	1.85	0.58
1:A:432:VAL:HB	1:A:440:SER:CB	2.32	0.58
4:E:92:PRO:O	4:E:94:LEU:N	2.37	0.58
1:D:599:LYS:HG2	1:D:600:GLY:N	2.18	0.58
2:B:243:ASP:OD1	2:B:243:ASP:N	2.36	0.57
1:D:622:ASP:CG	1:D:623:ASN:H	2.12	0.57
1:D:100:LEU:HD13	1:D:249:LYS:HD2	1.85	0.57
1:D:656:THR:HG23	1:D:658:GLY:H	1.70	0.57
1:A:570:VAL:HB	1:A:623:ASN:OD1	2.04	0.57
4:E:114:GLY:HA3	7:E:301:FAD:O1P	2.04	0.57
1:A:351:ILE:HG21	1:A:387:ARG:HH21	1.70	0.57
1:A:447:PHE:O	1:A:450:ALA:HB3	2.05	0.57
1:A:159:VAL:HG13	1:A:375:ASN:HD22	1.69	0.57
1:A:361:ARG:NH1	1:A:419:THR:HG22	2.20	0.57
2:B:166:LEU:HD12	7:B:301:FAD:H62A	1.70	0.57
1:D:342:ARG:C	1:D:344:ALA:N	2.62	0.57
1:D:555:SER:N	5:D:801:MCN:O1A	2.30	0.57
2:B:85:LYS:O	2:B:87:ILE:HD13	2.05	0.57
1:D:68:ARG:HG3	1:D:123:ASP:O	2.05	0.57
3:C:53:ILE:HD11	3:C:114:PRO:HD3	1.87	0.57
1:D:110:GLU:HG2	1:D:111:ASN:HB3	1.87	0.57
1:A:417:LEU:O	1:A:418:LEU:O	2.24	0.56
1:A:548:VAL:HG13	1:A:551:TRP:CZ2	2.41	0.56
2:B:77:ARG:HA	2:B:110:GLY:O	2.04	0.56
3:F:55:ASP:C	3:F:73:ARG:HH21	2.13	0.56
1:D:513:GLN:N	1:D:513:GLN:OE1	2.38	0.56
3:C:4:PHE:CD1	3:C:67:VAL:HG23	2.41	0.56
1:A:418:LEU:HB3	1:A:447:PHE:CG	2.39	0.56
1:A:418:LEU:HD21	1:A:423:LEU:HD11	1.88	0.56
1:A:780:GLU:O	1:A:783:PHE:HB2	2.05	0.56
3:F:50:CYS:CB	3:F:62:CYS:SG	2.94	0.56
1:D:439:ASP:HB3	1:D:440:SER:HA	1.86	0.56
1:A:52:PRO:HD3	1:D:52:PRO:HD3	1.88	0.56
1:A:95:LEU:HB3	1:A:96:GLY:C	2.30	0.56
1:A:360:TYR:CE1	1:A:398:PHE:HE2	2.23	0.56
1:A:655:ASP:C	2:B:273:ARG:HH22	2.13	0.56
1:D:111:ASN:CG	1:D:112:ILE:N	2.64	0.56
1:D:278:GLU:HG2	1:D:295:TRP:CZ2	2.40	0.56
1:D:360:TYR:CE2	1:D:394:ARG:NH1	2.74	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:589:LEU:HD12	1:D:598:VAL:O	2.06	0.56
1:D:782:ILE:HG12	1:D:785:ARG:NH2	2.21	0.56
1:D:513:GLN:O	5:D:801:MCN:H5	2.06	0.56
1:D:652:LEU:HD22	1:D:782:ILE:HD11	1.88	0.56
4:E:4:PRO:HA	4:E:44:ARG:NH2	2.20	0.55
1:D:222:VAL:HG22	1:D:294:LYS:HD2	1.88	0.55
1:A:255:GLU:O	1:A:257:ASN:HB2	2.06	0.55
4:E:206:GLU:HA	4:E:207:GLN:C	2.31	0.55
1:A:59:ILE:HD12	1:A:278:GLU:HG3	1.89	0.55
1:A:511:VAL:HG12	5:A:801:MCN:O4'	2.07	0.55
1:A:724:PRO:C	1:A:726:VAL:N	2.61	0.55
1:D:188:TYR:CE2	1:D:428:GLY:N	2.74	0.55
2:B:176:PRO:CD	2:B:177:HIS:N	2.69	0.55
1:A:480:LEU:HD23	1:A:482:ASP:HB3	1.87	0.55
1:A:499:ALA:O	1:A:501:ARG:N	2.39	0.55
1:A:688:VAL:HG13	1:A:723:MET:HE2	1.88	0.55
2:B:30:ILE:HD11	7:B:301:FAD:C6A	2.36	0.55
3:F:100:GLN:HB2	5:D:801:MCN:HN21	1.71	0.55
1:A:417:LEU:HB3	1:A:447:PHE:HD2	1.69	0.55
1:A:575:ARG:CZ	1:A:596:PHE:HB2	2.36	0.55
2:B:285:HIS:C	2:B:287:ALA:H	2.13	0.55
1:D:383:ARG:NH1	1:D:689:GLN:OE1	2.39	0.55
1:D:387:ARG:HD2	1:D:480:LEU:HD23	1.88	0.55
1:A:648:VAL:HG11	1:A:758:ILE:HD13	1.89	0.55
4:E:183:PHE:HD1	4:E:199:ALA:HB2	1.72	0.55
3:F:53:ILE:HD11	3:F:114:PRO:HD3	1.89	0.55
1:D:116:SER:HA	1:D:340:TYR:CG	2.42	0.55
1:D:430:ASP:HB2	1:D:431:ILE:C	2.32	0.55
1:A:481:MET:SD	1:A:483:LYS:HD2	2.47	0.55
1:A:486:LEU:HD11	1:A:554:ARG:CB	2.36	0.55
1:A:551:TRP:H	1:A:554:ARG:CD	2.20	0.55
2:B:86:THR:O	2:B:86:THR:CG2	2.55	0.55
1:A:255:GLU:HG3	1:D:495:GLU:HG2	1.88	0.54
1:A:548:VAL:HG12	1:A:549:GLY:N	2.22	0.54
1:A:749:ILE:HD12	1:A:752:ILE:HG13	1.87	0.54
2:B:180:GLY:HA3	2:B:283:ALA:O	2.07	0.54
1:D:420:ALA:HB1	1:D:423:LEU:HD22	1.89	0.54
2:B:271:VAL:HG12	2:B:271:VAL:O	2.06	0.54
3:C:60:ARG:HB3	8:C:201:FES:S1	2.47	0.54
1:A:74:ALA:HA	1:A:75:THR:HG1	1.70	0.54
1:A:244:ARG:HG3	1:A:258:VAL:HG13	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:655:ASP:HB3	2:B:273:ARG:HH12	1.73	0.54
4:E:90:ASN:HA	4:E:92:PRO:CD	2.36	0.54
1:A:486:LEU:HD22	1:A:554:ARG:HD2	1.88	0.54
1:D:108:ILE:HA	1:D:109:TYR:CB	2.37	0.54
1:A:244:ARG:HE	1:A:258:VAL:CG1	2.21	0.54
1:A:586:PRO:CD	1:A:587:ASP:HA	2.38	0.54
1:D:471:ARG:HB2	1:D:651:GLU:HA	1.88	0.54
1:A:551:TRP:O	1:A:552:SER:C	2.50	0.54
1:A:566:ALA:O	1:A:623:ASN:ND2	2.40	0.54
1:A:411:GLU:HG3	1:A:414:ARG:HB3	1.91	0.53
3:C:82:LYS:O	3:C:85:GLN:HG2	2.08	0.53
1:D:268:SER:N	5:D:801:MCN:O4'	2.37	0.53
1:D:384:ALA:HA	1:D:387:ARG:HH22	1.73	0.53
1:D:746:LEU:N	5:D:801:MCN:O2'	2.36	0.53
1:A:256:VAL:HA	1:A:257:ASN:CB	2.38	0.53
2:B:30:ILE:HG22	2:B:52:VAL:HG23	1.89	0.53
2:B:271:VAL:CA	2:B:273:ARG:HD3	2.35	0.53
2:B:87:ILE:O	2:B:90:ASN:OD1	2.26	0.53
1:D:483:LYS:O	1:D:639:MET:HB3	2.08	0.53
2:B:78:HIS:HA	2:B:81:LEU:HD12	1.91	0.53
1:D:116:SER:C	1:D:118:PRO:HA	2.33	0.53
1:D:273:GLY:C	1:D:342:ARG:HH22	2.16	0.53
1:D:615:ASP:CB	1:D:616:PRO:CD	2.85	0.53
1:A:77:ALA:O	1:A:80:THR:OG1	2.27	0.53
2:B:258:VAL:O	2:B:268:ARG:NH2	2.41	0.53
1:D:186:LYS:HB3	1:D:430:ASP:CB	2.37	0.53
1:A:448:ASN:C	1:A:450:ALA:N	2.66	0.53
2:B:176:PRO:CD	2:B:177:HIS:H	2.18	0.53
1:D:482:ASP:O	1:D:553:SER:O	2.27	0.53
1:A:22:ARG:HG3	1:A:23:GLN:N	2.23	0.53
1:D:114:ASP:CB	1:D:340:TYR:CD1	2.92	0.53
1:D:360:TYR:HA	1:D:417:LEU:O	2.09	0.53
4:E:88:SER:O	4:E:89:GLN:HG2	2.09	0.53
4:E:124:GLU:H	7:E:301:FAD:HM73	1.74	0.53
1:D:432:VAL:HG21	1:D:439:ASP:O	2.09	0.53
1:D:478:GLY:HA3	1:D:752:ILE:HD13	1.91	0.53
2:B:25:GLY:O	2:B:27:ASP:N	2.42	0.52
1:D:219:ARG:HH12	1:D:278:GLU:CD	2.16	0.52
1:A:510:SER:HB3	1:A:538:HIS:NE2	2.25	0.52
1:D:357:PHE:HB3	1:D:429:LEU:HD23	1.90	0.52
1:A:446:HIS:ND1	1:A:449:GLU:HG2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:483:LYS:O	1:A:486:LEU:HD12	2.08	0.52
1:D:489:PHE:HA	1:D:633:VAL:O	2.10	0.52
1:A:344:ALA:CB	1:A:348:VAL:HG23	2.39	0.52
1:A:625:GLU:O	1:A:627:GLY:HA2	2.10	0.52
3:C:50:CYS:CB	3:C:62:CYS:SG	2.97	0.52
1:A:439:ASP:CA	1:A:440:SER:CB	2.62	0.52
1:A:766:ILE:N	1:A:767:ALA:HA	2.21	0.52
2:B:270:GLN:O	2:B:273:ARG:CD	2.55	0.52
1:D:113:GLU:HB2	1:D:114:ASP:C	2.35	0.52
1:D:219:ARG:NE	1:D:306:THR:HG22	2.22	0.52
1:D:359:PRO:HD2	1:D:394:ARG:HH12	1.75	0.52
1:A:177:ARG:NH1	1:A:178:GLY:O	2.43	0.52
1:A:631:ASP:HB3	1:A:634:TYR:CD2	2.44	0.52
3:F:100:GLN:HE21	3:F:139:CYS:HB3	1.74	0.52
1:D:431:ILE:HG22	1:D:431:ILE:O	2.10	0.52
1:D:439:ASP:HB3	1:D:641:TYR:OH	2.09	0.52
1:D:779:PRO:CA	1:D:782:ILE:HG22	2.36	0.52
1:A:114:ASP:CB	1:A:341:PHE:H	2.23	0.52
2:B:211:SER:C	2:B:235:ILE:HD11	2.35	0.52
1:D:307:SER:HB2	1:D:380:GLY:N	2.25	0.52
3:F:145:ILE:O	3:F:149:THR:HG23	2.10	0.52
1:D:482:ASP:HB3	1:D:553:SER:HB2	1.91	0.52
1:D:519:LEU:HB2	1:D:536:ILE:CD1	2.40	0.52
1:D:529:ILE:HD11	1:D:607:LEU:HD23	1.91	0.52
1:A:248:ALA:O	1:A:254:PRO:HD3	2.10	0.51
1:A:631:ASP:O	1:A:632:ALA:HB2	2.09	0.51
4:E:2:LYS:HD3	1:D:144:GLU:HB3	1.85	0.51
4:E:3:PRO:HD2	1:D:141:TYR:HE2	1.75	0.51
1:A:417:LEU:HB3	1:A:447:PHE:CE2	2.45	0.51
1:D:202:ILE:O	1:D:317:GLU:HA	2.11	0.51
1:D:527:LEU:HD22	1:D:607:LEU:HD21	1.91	0.51
1:A:122:VAL:HG12	1:A:122:VAL:O	2.11	0.51
2:B:33:GLY:O	2:B:109:ARG:NH1	2.40	0.51
2:B:91:LEU:N	2:B:92:PRO:HA	2.26	0.51
1:D:22:ARG:HH11	1:D:592:THR:HG21	1.74	0.51
1:D:341:PHE:CD2	1:D:345:GLU:HA	2.46	0.51
1:D:411:GLU:O	1:D:411:GLU:HG3	2.11	0.51
1:A:209:ASN:HD21	1:A:776:PRO:N	2.08	0.51
1:A:345:GLU:H	1:A:347:LEU:H	1.59	0.51
1:D:434:GLU:HB2	1:D:481:MET:HE3	1.91	0.51
1:D:649:GLN:HG2	1:D:663:ARG:HB2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:PHE:O	1:A:176:GLY:N	2.44	0.51
1:A:344:ALA:HB1	1:A:348:VAL:H	1.76	0.51
1:A:483:LYS:NZ	1:A:641:TYR:HA	2.26	0.51
1:A:231:THR:HG22	1:A:257:ASN:OD1	2.11	0.51
1:A:447:PHE:CG	1:A:448:ASN:N	2.79	0.51
1:A:122:VAL:O	1:A:122:VAL:CG1	2.59	0.51
2:B:167:ILE:N	7:B:301:FAD:H62A	2.08	0.51
1:D:113:GLU:HB2	1:D:114:ASP:HA	1.93	0.51
1:D:486:LEU:O	1:D:486:LEU:HD12	2.11	0.51
4:E:90:ASN:HA	4:E:91:LEU:C	2.35	0.50
4:E:291:LYS:CG	4:E:292:GLU:N	2.72	0.50
1:A:32:ARG:NH2	3:C:100:GLN:O	2.32	0.50
1:A:464:LYS:HB3	1:A:465:ARG:HA	1.93	0.50
3:F:50:CYS:HB3	3:F:62:CYS:SG	2.50	0.50
1:A:360:TYR:OH	1:A:477:LEU:HD12	2.11	0.50
1:D:256:VAL:O	1:D:257:ASN:CB	2.60	0.50
1:A:684:ILE:HD13	3:C:143:GLN:HG2	1.94	0.50
2:B:267:TYR:O	2:B:271:VAL:N	2.44	0.50
4:E:34:GLY:H	7:E:301:FAD:PA	2.35	0.50
1:D:92:THR:HA	1:D:94:HIS:ND1	2.26	0.50
1:D:342:ARG:O	1:D:342:ARG:NH1	2.37	0.50
1:D:357:PHE:HB3	1:D:429:LEU:CD2	2.41	0.50
3:F:60:ARG:C	3:F:62:CYS:H	2.20	0.50
1:D:618:THR:O	1:D:618:THR:CG2	2.58	0.50
3:C:30:ARG:NH1	3:C:38:THR:O	2.44	0.50
1:A:244:ARG:HE	1:A:258:VAL:HG13	1.76	0.50
1:A:786:CYS:C	1:A:788:GLY:N	2.68	0.50
2:B:86:THR:HG23	2:B:91:LEU:HD12	1.92	0.50
3:F:80:LEU:CD1	3:F:110:MET:HE3	2.39	0.50
1:D:188:TYR:CZ	1:D:430:ASP:O	2.64	0.50
1:D:357:PHE:CD1	1:D:429:LEU:HG	2.46	0.50
3:F:60:ARG:HD2	8:F:201:FES:S1	2.51	0.50
1:D:68:ARG:CZ	1:D:123:ASP:HB2	2.42	0.50
1:A:419:THR:CB	1:A:422:ASP:HB3	2.40	0.50
1:A:471:ARG:HB2	1:A:765:ALA:HA	1.93	0.50
1:A:486:LEU:N	1:A:487:GLY:CA	2.74	0.50
1:D:340:TYR:HB2	1:D:378:PRO:HG3	1.93	0.50
1:A:786:CYS:SG	1:A:789:LEU:HB2	2.52	0.49
3:C:116:TYR:O	3:C:156:ARG:NH1	2.44	0.49
1:D:457:SER:N	1:D:458:GLU:HA	2.26	0.49
1:D:483:LYS:CE	1:D:557:VAL:HG22	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:588:ASP:CB	1:D:598:VAL:HA	2.17	0.49
1:A:254:PRO:HA	1:A:255:GLU:C	2.37	0.49
1:A:483:LYS:NZ	1:A:641:TYR:CD2	2.79	0.49
1:A:786:CYS:C	1:A:788:GLY:H	2.20	0.49
1:A:418:LEU:HD22	1:A:447:PHE:H	1.77	0.49
1:D:228:ALA:C	1:D:230:ASP:H	2.21	0.49
1:D:490:GLU:CG	1:D:554:ARG:HH21	2.25	0.49
1:D:565:LYS:NZ	1:D:626:PRO:HB3	2.26	0.49
2:B:174:GLN:O	2:B:175:LEU:HB3	2.13	0.49
4:E:93:ILE:HD11	4:E:199:ALA:HB1	1.95	0.49
3:F:101:CYS:SG	3:F:102:GLY:N	2.85	0.49
1:D:43:ALA:HB1	1:D:264:GLU:HG3	1.94	0.49
1:D:519:LEU:HB2	1:D:536:ILE:HD13	1.94	0.49
1:D:673:VAL:HG13	1:D:679:THR:HG21	1.93	0.49
1:A:649:GLN:HE22	1:A:663:ARG:HH21	1.61	0.49
2:B:228:GLN:O	2:B:231:GLU:HB2	2.12	0.49
1:D:548:VAL:HB	1:D:554:ARG:HH22	1.77	0.49
1:D:598:VAL:CG1	1:D:599:LYS:HE3	2.36	0.49
1:D:365:TYR:CD2	1:D:429:LEU:HD13	2.47	0.49
1:D:467:ARG:HD3	1:D:467:ARG:N	2.28	0.49
1:A:432:VAL:CB	1:A:440:SER:HB2	2.37	0.49
1:A:528:GLN:HG2	1:A:592:THR:HB	1.95	0.49
1:D:326:ILE:HG12	1:D:416:ASN:ND2	2.27	0.49
1:A:712:PHE:HB2	3:C:44:HIS:NE2	2.28	0.49
4:E:37:LEU:HB2	7:E:301:FAD:H52A	1.93	0.49
4:E:80:LYS:O	4:E:80:LYS:HG2	2.13	0.49
3:F:42:CYS:H	3:F:47:CYS:CB	2.26	0.49
1:A:209:ASN:ND2	1:A:775:LEU:HB3	2.27	0.49
1:A:483:LYS:HZ3	1:A:641:TYR:CA	2.26	0.49
1:A:646:THR:HA	1:A:666:THR:HA	1.95	0.49
1:D:160:LEU:HD21	1:D:166:ALA:HA	1.94	0.49
1:D:430:ASP:CG	1:D:432:VAL:HA	2.38	0.49
1:A:215:PRO:HD2	1:A:302:HIS:CE1	2.43	0.48
1:A:329:MET:HE1	1:A:394:ARG:HD3	1.95	0.48
1:A:351:ILE:HG21	1:A:387:ARG:NH2	2.27	0.48
1:A:488:LEU:HG	1:A:634:TYR:CD1	2.47	0.48
3:C:141:GLY:C	3:C:143:GLN:H	2.21	0.48
4:E:239:LEU:O	4:E:240:SER:CB	2.61	0.48
1:D:68:ARG:HE	1:D:124:LYS:HB3	1.77	0.48
1:D:565:LYS:HE3	1:D:632:ALA:HB1	1.94	0.48
1:D:589:LEU:HB2	1:D:597:LYS:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:PRO:HG3	1:A:336:ASN:HB2	1.95	0.48
1:A:213:GLY:HA2	1:A:382:TYR:CE1	2.48	0.48
3:C:50:CYS:CB	8:C:201:FES:S1	3.01	0.48
1:A:633:VAL:CG2	1:A:635:MET:HE2	2.43	0.48
3:C:50:CYS:HB3	3:C:62:CYS:SG	2.52	0.48
4:E:2:LYS:HZ2	1:D:144:GLU:C	2.20	0.48
1:D:163:PRO:HG3	1:D:336:ASN:HB2	1.96	0.48
1:D:357:PHE:HB2	1:D:362:VAL:HG21	1.94	0.48
1:A:417:LEU:CB	1:A:447:PHE:CE2	2.96	0.48
1:D:213:GLY:HA2	1:D:382:TYR:CE1	2.48	0.48
1:D:485:GLY:N	1:D:486:LEU:HG	2.27	0.48
1:A:298:ASP:HB3	1:A:301:GLU:HG3	1.94	0.48
2:B:175:LEU:HG	2:B:176:PRO:HB3	1.94	0.48
1:D:599:LYS:CD	1:D:600:GLY:N	2.66	0.48
1:D:617:PHE:O	1:D:619:ALA:N	2.47	0.48
1:A:762:ILE:HD13	1:A:777:VAL:HG11	1.95	0.48
2:B:166:LEU:HD12	7:B:301:FAD:N6A	2.29	0.48
4:E:217:VAL:HG11	4:E:255:LEU:HD21	1.94	0.48
1:D:480:LEU:HB3	1:D:482:ASP:CG	2.38	0.48
1:A:456:PHE:O	1:A:457:SER:HB3	2.13	0.48
1:A:680:ARG:NH2	3:C:147:GLU:OE2	2.46	0.48
3:C:39:ARG:HD2	3:C:103:PHE:HA	1.96	0.48
1:D:59:ILE:CD1	1:D:278:GLU:HG3	2.44	0.48
1:A:417:LEU:CB	1:A:447:PHE:CD2	2.89	0.48
3:C:69:ALA:HB1	3:C:74:ILE:HD11	1.96	0.48
1:D:113:GLU:CB	1:D:114:ASP:HA	2.44	0.48
1:D:114:ASP:CB	1:D:341:PHE:N	2.77	0.48
1:D:614:ARG:HB2	1:D:621:ALA:HB2	1.95	0.48
1:A:58:ARG:HB2	1:A:143:ALA:HB1	1.96	0.47
2:B:167:ILE:H	7:B:301:FAD:H62A	1.60	0.47
2:B:183:PHE:HD2	2:B:199:ALA:HB2	1.79	0.47
3:F:50:CYS:CB	8:F:201:FES:S1	3.01	0.47
5:D:801:MCN:H3'	5:D:801:MCN:O3A	2.14	0.47
1:A:209:ASN:HD21	1:A:775:LEU:HB3	1.78	0.47
3:C:101:CYS:SG	3:C:102:GLY:N	2.87	0.47
4:E:2:LYS:CD	1:D:144:GLU:CB	2.80	0.47
3:F:116:TYR:O	3:F:156:ARG:NH1	2.46	0.47
1:D:106:HIS:H	1:D:107:GLU:CA	2.17	0.47
1:D:342:ARG:O	1:D:343:GLN:C	2.57	0.47
1:D:344:ALA:CB	1:D:379:VAL:O	2.62	0.47
1:D:432:VAL:O	1:D:437:HIS:CB	2.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:459:TRP:CD1	1:D:459:TRP:C	2.91	0.47
1:D:511:VAL:HG12	5:D:801:MCN:O4'	2.14	0.47
1:A:177:ARG:O	1:A:177:ARG:HD2	2.14	0.47
1:A:254:PRO:HB2	1:A:255:GLU:HA	1.96	0.47
3:C:145:ILE:O	3:C:149:THR:HG23	2.14	0.47
1:D:425:TRP:CZ2	1:D:428:GLY:HA3	2.49	0.47
1:D:565:LYS:HA	1:D:568:LEU:HB2	1.96	0.47
1:D:686:ALA:HB3	1:D:750:GLY:HA3	1.95	0.47
1:A:458:GLU:O	1:A:461:GLU:HB2	2.13	0.47
1:D:33:ARG:NH2	1:D:532:GLU:O	2.47	0.47
1:D:421:GLU:O	1:D:423:LEU:N	2.47	0.47
1:D:551:TRP:O	1:D:554:ARG:HG2	2.14	0.47
1:D:746:LEU:H	5:D:801:MCN:HO2'	1.56	0.47
1:A:724:PRO:HB2	1:A:726:VAL:O	2.13	0.47
1:A:746:LEU:N	5:A:801:MCN:O2'	2.38	0.47
2:B:206:GLU:HA	2:B:207:GLN:HA	1.48	0.47
1:D:95:LEU:H	1:D:96:GLY:HA3	1.75	0.47
1:D:384:ALA:HB2	1:D:748:GLU:HB3	1.96	0.47
1:A:555:SER:O	1:A:559:ALA:N	2.47	0.47
1:D:112:ILE:HG23	1:D:113:GLU:HB3	1.94	0.47
1:D:423:LEU:HA	1:D:424:PRO:C	2.39	0.47
1:A:105:TYR:HB3	1:A:436:TYR:CE2	2.49	0.47
1:A:785:ARG:HH12	2:B:270:GLN:HG2	1.77	0.47
2:B:195:ILE:HG21	2:B:267:TYR:HE2	1.80	0.47
4:E:205:ASP:O	4:E:206:GLU:C	2.56	0.47
1:D:241:HIS:CD2	1:D:539:SER:CB	2.92	0.47
1:D:356:VAL:O	1:D:394:ARG:HD3	2.15	0.47
1:D:391:THR:CG2	1:D:394:ARG:HH21	2.26	0.47
1:D:430:ASP:OD1	1:D:430:ASP:N	2.48	0.47
1:D:577:LEU:O	1:D:581:MET:HG3	2.15	0.47
1:D:598:VAL:O	1:D:599:LYS:CD	2.50	0.47
1:D:622:ASP:CG	1:D:623:ASN:N	2.73	0.47
1:A:518:VAL:HG13	1:A:674:ILE:HG21	1.95	0.47
2:B:179:SER:HB2	2:B:202:VAL:O	2.14	0.47
1:D:113:GLU:HB2	1:D:114:ASP:CA	2.45	0.47
1:A:249:LYS:HE3	1:D:498:ARG:HD3	1.96	0.47
1:A:483:LYS:HE2	1:A:640:ASN:O	2.15	0.47
2:B:145:ARG:HD3	2:B:165:GLU:OE2	2.15	0.47
4:E:135:TYR:HB3	4:E:146:LYS:HE2	1.96	0.47
1:A:504:VAL:HG21	1:A:523:VAL:HG21	1.97	0.47
3:C:33:LEU:C	3:C:35:LEU:H	2.17	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:2:LYS:HD3	1:D:144:GLU:CD	2.40	0.47
3:F:138:ARG:NE	1:D:213:GLY:O	2.47	0.47
1:D:160:LEU:HD22	1:D:374:THR:HG22	1.97	0.47
1:D:439:ASP:CB	1:D:440:SER:HA	2.44	0.47
1:D:763:ASP:HB3	1:D:770:VAL:HA	1.97	0.47
2:B:88:SER:C	2:B:90:ASN:H	2.22	0.46
1:D:256:VAL:HG22	1:D:257:ASN:H	1.80	0.46
1:D:387:ARG:HE	1:D:481:MET:HB3	1.80	0.46
2:B:185:GLU:HG3	2:B:194:ALA:HB2	1.96	0.46
1:D:248:ALA:O	1:D:254:PRO:HD3	2.15	0.46
1:D:358:GLY:HA3	1:D:394:ARG:NH1	2.29	0.46
1:D:158:PRO:HG2	1:D:171:VAL:HG13	1.96	0.46
1:D:327:LEU:HA	1:D:363:PRO:HG2	1.97	0.46
1:D:486:LEU:CD2	1:D:554:ARG:HD2	2.40	0.46
2:B:205:ASP:N	2:B:209:LYS:O	2.42	0.46
3:F:42:CYS:N	3:F:47:CYS:SG	2.80	0.46
1:D:466:LEU:CB	1:D:468:ALA:HB2	2.43	0.46
1:A:22:ARG:HG3	1:A:23:GLN:O	2.15	0.46
3:F:30:ARG:NH1	3:F:38:THR:O	2.48	0.46
1:A:105:TYR:C	1:A:107:GLU:H	2.24	0.46
1:A:262:HIS:CD2	1:A:538:HIS:CE1	3.03	0.46
1:A:637:ASN:O	1:A:638:ALA:C	2.57	0.46
2:B:64:ARG:HB3	2:B:71:ALA:HB3	1.98	0.46
2:B:285:HIS:C	2:B:287:ALA:N	2.73	0.46
4:E:57:VAL:HG13	4:E:58:PRO:HD2	1.98	0.46
4:E:285:HIS:O	4:E:288:ARG:HG2	2.16	0.46
1:D:418:LEU:HB3	1:D:447:PHE:HB3	1.98	0.46
1:D:570:VAL:HB	1:D:623:ASN:ND2	2.31	0.46
2:B:135:TYR:HD2	2:B:171:ASN:HB2	1.80	0.46
3:C:33:LEU:O	3:C:35:LEU:HG	2.16	0.46
3:F:143:GLN:HG2	1:D:684:ILE:HD13	1.97	0.46
1:D:385:PRO:HD2	1:D:387:ARG:HH22	1.81	0.46
1:D:516:GLU:O	1:D:536:ILE:HD12	2.16	0.46
1:A:459:TRP:O	1:A:462:GLU:HB2	2.15	0.46
1:A:551:TRP:H	1:A:554:ARG:HD2	1.80	0.46
2:B:11:ALA:HB1	2:B:17:ALA:HB2	1.96	0.46
1:D:284:TRP:CH2	1:D:288:THR:HG21	2.51	0.46
1:D:686:ALA:O	1:D:751:ILE:CG2	2.64	0.46
1:A:235:TRP:HB3	1:A:263:VAL:HG21	1.97	0.46
1:D:459:TRP:CG	1:D:460:LEU:N	2.84	0.46
1:A:447:PHE:CE2	1:A:448:ASN:HB2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:ASP:HB3	1:A:634:TYR:HD2	1.79	0.46
2:B:177:HIS:HA	2:B:178:GLY:HA2	1.54	0.46
4:E:1:MET:O	4:E:2:LYS:HG3	2.16	0.46
4:E:176:PRO:CD	4:E:212:ARG:HH21	2.28	0.46
1:D:437:HIS:CB	1:D:438:PHE:CA	2.69	0.46
1:D:490:GLU:O	1:D:633:VAL:HG23	2.16	0.46
1:A:483:LYS:CB	1:A:639:MET:O	2.63	0.45
4:E:125:LEU:HB2	4:E:126:PRO:HD3	1.98	0.45
1:A:118:PRO:HA	1:A:119:VAL:HA	1.73	0.45
1:A:211:HIS:ND1	1:A:310:ARG:HG2	2.30	0.45
1:A:449:GLU:O	1:A:453:ALA:HB3	2.16	0.45
1:A:548:VAL:CG1	1:A:549:GLY:N	2.79	0.45
2:B:130:LEU:HB3	2:B:216:THR:HG21	1.99	0.45
1:D:231:THR:HG21	1:D:259:ARG:CZ	2.46	0.45
1:D:669:GLU:CD	1:D:735:LYS:HZ3	2.25	0.45
1:A:132:VAL:HG12	1:A:133:VAL:HG23	1.98	0.45
1:A:139:ASP:HB2	1:A:140:PRO:HD2	1.97	0.45
1:A:210:ARG:HD2	1:A:311:GLU:OE2	2.16	0.45
1:A:268:SER:N	5:A:801:MCN:O4'	2.45	0.45
1:A:554:ARG:HG3	1:A:555:SER:N	2.30	0.45
1:A:669:GLU:HA	1:A:732:GLU:HG3	1.98	0.45
2:B:85:LYS:O	2:B:87:ILE:N	2.49	0.45
2:B:145:ARG:NH1	2:B:165:GLU:OE2	2.41	0.45
3:C:121:VAL:HG12	3:C:122:THR:H	1.81	0.45
1:D:418:LEU:O	1:D:419:THR:C	2.58	0.45
1:D:599:LYS:HE2	1:D:603:GLN:H	1.81	0.45
1:A:66:HIS:HB2	1:A:375:ASN:ND2	2.32	0.45
1:A:209:ASN:O	1:A:311:GLU:HA	2.16	0.45
1:A:431:ILE:HA	1:A:432:VAL:C	2.42	0.45
1:A:480:LEU:HD21	1:A:748:GLU:HB2	1.98	0.45
1:D:599:LYS:HG3	1:D:602:ASP:CG	2.42	0.45
1:D:625:GLU:N	1:D:626:PRO:HD2	2.32	0.45
1:A:484:ALA:O	1:A:485:GLY:C	2.59	0.45
1:D:185:LYS:HG2	1:D:367:ALA:O	2.17	0.45
1:D:420:ALA:CB	1:D:423:LEU:HD22	2.46	0.45
1:A:344:ALA:HA	1:A:345:GLU:OE1	2.16	0.45
1:A:381:ALA:HB1	1:A:385:PRO:HG3	1.99	0.45
2:B:177:HIS:O	2:B:177:HIS:CG	2.68	0.45
1:D:117:HIS:N	1:D:118:PRO:CA	2.79	0.45
1:A:486:LEU:HD23	1:A:551:TRP:HE3	1.82	0.45
2:B:29:LYS:HD3	2:B:30:ILE:H	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:33:LEU:C	3:C:35:LEU:N	2.75	0.45
1:D:341:PHE:HD2	1:D:345:GLU:HA	1.81	0.45
1:D:365:TYR:CZ	1:D:367:ALA:HB2	2.52	0.45
1:D:553:SER:N	5:D:801:MCN:O2B	2.49	0.45
1:D:713:MET:HE2	1:D:713:MET:HA	1.98	0.45
1:A:428:GLY:O	1:A:429:LEU:CB	2.65	0.45
1:A:510:SER:H	1:A:538:HIS:CD2	2.34	0.45
1:A:718:PRO:HB3	1:A:723:MET:SD	2.57	0.45
4:E:106:ILE:HG21	7:E:301:FAD:N1	2.32	0.45
4:E:274:THR:HG21	1:D:655:ASP:O	2.16	0.45
1:D:459:TRP:O	1:D:461:GLU:N	2.50	0.45
1:A:423:LEU:HD22	1:A:442:ASP:O	2.17	0.45
1:A:655:ASP:CB	2:B:273:ARG:HH22	2.30	0.45
1:A:769:GLY:O	1:A:771:HIS:N	2.49	0.45
1:D:188:TYR:CE2	1:D:427:PRO:C	2.95	0.45
1:D:330:LYS:HE3	1:D:365:TYR:OH	2.17	0.45
1:A:400:LEU:HA	1:A:770:VAL:HG21	1.99	0.45
1:A:668:THR:O	1:A:731:THR:HA	2.17	0.45
2:B:86:THR:CG2	2:B:91:LEU:HD12	2.46	0.45
4:E:79:ALA:C	4:E:81:LEU:H	2.25	0.45
4:E:85:LYS:HD3	4:E:87:ILE:HG23	1.98	0.45
1:D:69:ILE:HG12	1:D:123:ASP:O	2.16	0.45
2:B:44:ARG:HB3	2:B:47:ARG:NH2	2.32	0.44
3:C:60:ARG:C	3:C:62:CYS:H	2.25	0.44
1:D:391:THR:HG22	1:D:394:ARG:NH2	2.31	0.44
1:D:488:LEU:HD23	1:D:631:ASP:HB2	2.00	0.44
1:D:232:LEU:N	1:D:257:ASN:O	2.50	0.44
1:D:574:ALA:O	1:D:578:ALA:N	2.49	0.44
1:A:185:LYS:HG2	1:A:368:THR:HB	1.98	0.44
1:A:209:ASN:N	1:A:209:ASN:HD22	2.15	0.44
1:A:640:ASN:HD21	1:A:744:LYS:HA	1.82	0.44
1:A:720:ALA:O	3:C:129:ARG:HD3	2.18	0.44
1:D:85:MET:HG2	1:D:86:VAL:N	2.33	0.44
1:D:428:GLY:O	1:D:429:LEU:CB	2.45	0.44
1:D:481:MET:O	1:D:481:MET:HG3	2.17	0.44
1:A:437:HIS:HA	1:A:438:PHE:HA	1.69	0.44
4:E:3:PRO:HB3	4:E:41:LEU:HB3	2.00	0.44
1:D:570:VAL:HB	1:D:623:ASN:OD1	2.18	0.44
1:A:209:ASN:ND2	1:A:775:LEU:CB	2.81	0.44
1:A:360:TYR:CE2	1:A:394:ARG:HD2	2.53	0.44
2:B:88:SER:C	2:B:90:ASN:N	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:LEU:HD21	2:B:226:ARG:HG2	1.98	0.44
1:D:381:ALA:HB1	1:D:385:PRO:HG3	2.00	0.44
1:A:355:ILE:HD11	1:A:387:ARG:HD2	2.00	0.44
1:A:446:HIS:CE1	1:A:449:GLU:HG2	2.53	0.44
2:B:140:SER:HB3	2:B:165:GLU:HA	2.00	0.44
2:B:274:THR:HA	2:B:277:GLU:CB	2.45	0.44
4:E:16:HIS:C	4:E:16:HIS:HD1	2.25	0.44
1:D:92:THR:HA	1:D:94:HIS:CE1	2.52	0.44
1:D:115:PHE:O	1:D:116:SER:O	2.35	0.44
1:D:330:LYS:NZ	1:D:367:ALA:HA	2.33	0.44
1:D:555:SER:HB2	5:D:801:MCN:H5'1	1.99	0.44
2:B:69:THR:O	2:B:174:GLN:NE2	2.50	0.44
7:B:301:FAD:N1	7:B:301:FAD:C2'	2.67	0.44
1:D:115:PHE:HA	1:D:341:PHE:O	2.18	0.44
1:D:736:SER:HB3	1:D:742:GLY:HA3	1.99	0.44
5:D:801:MCN:H3'	5:D:801:MCN:PA	2.58	0.44
1:A:270:GLY:HA3	1:A:381:ALA:O	2.18	0.44
2:B:274:THR:O	2:B:278:ARG:CG	2.53	0.44
1:D:599:LYS:HD3	1:D:601:THR:C	2.43	0.44
1:A:213:GLY:H	1:A:271:VAL:CG2	2.23	0.44
1:A:326:ILE:H	1:A:416:ASN:HD21	1.66	0.44
1:A:356:VAL:HA	1:A:390:SER:HB2	1.98	0.44
1:A:418:LEU:CB	1:A:447:PHE:CG	3.00	0.44
1:A:199:GLU:OE1	1:A:321:ASP:HA	2.17	0.43
1:A:359:PRO:HB3	1:A:479:VAL:HG23	1.99	0.43
2:B:114:GLY:HA2	7:B:301:FAD:N3A	2.33	0.43
4:E:78:HIS:HA	4:E:81:LEU:HD12	2.00	0.43
4:E:137:THR:HG22	4:E:146:LYS:HE3	1.99	0.43
1:D:361:ARG:N	1:D:417:LEU:O	2.50	0.43
1:A:344:ALA:CB	1:A:348:VAL:H	2.32	0.43
1:D:459:TRP:HE1	1:D:463:SER:H	1.65	0.43
1:A:258:VAL:HG12	1:A:260:MET:HG2	2.00	0.43
1:A:574:ALA:C	1:A:576:ARG:H	2.27	0.43
1:D:365:TYR:HE2	1:D:367:ALA:HB2	1.79	0.43
1:D:420:ALA:HB2	1:D:423:LEU:HD13	2.00	0.43
1:A:211:HIS:CE1	1:A:310:ARG:HG2	2.53	0.43
1:A:344:ALA:HB3	1:A:348:VAL:HG23	1.99	0.43
1:A:437:HIS:O	1:A:437:HIS:CG	2.71	0.43
1:A:449:GLU:HA	1:A:452:GLU:HB2	2.00	0.43
3:F:129:ARG:HH12	1:D:723:MET:HB2	1.82	0.43
1:D:88:THR:H	1:D:91:HIS:HD2	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:235:TRP:O	1:D:263:VAL:HG21	2.18	0.43
1:D:392:PHE:HA	1:D:756:ALA:HB2	1.99	0.43
1:A:482:ASP:H	1:A:483:LYS:HE3	1.81	0.43
1:A:486:LEU:HB3	1:A:554:ARG:HE	1.83	0.43
1:A:589:LEU:HD11	1:A:599:LYS:HA	2.01	0.43
5:A:801:MCN:HG3'	5:A:801:MCN:PA	2.59	0.43
2:B:82:THR:HA	2:B:95:SER:HB2	2.01	0.43
2:B:161:ILE:HG23	2:B:165:GLU:HB3	2.01	0.43
1:D:251:LEU:HB3	1:D:253:LEU:HD23	1.99	0.43
1:D:310:ARG:NH2	1:D:751:ILE:HD12	2.33	0.43
1:D:368:THR:O	1:D:370:HIS:HD2	2.01	0.43
2:B:235:ILE:O	2:B:236:ASP:CG	2.61	0.43
3:C:33:LEU:O	3:C:35:LEU:N	2.39	0.43
1:D:88:THR:H	1:D:91:HIS:CD2	2.36	0.43
1:D:365:TYR:HB3	1:D:429:LEU:O	2.19	0.43
1:D:471:ARG:HB3	1:D:765:ALA:CB	2.40	0.43
1:A:360:TYR:CE1	1:A:417:LEU:HD12	2.53	0.43
1:A:449:GLU:HG2	1:A:449:GLU:H	1.61	0.43
1:D:365:TYR:CD1	1:D:429:LEU:CD2	3.00	0.43
1:D:419:THR:HB	1:D:422:ASP:CG	2.43	0.43
1:A:631:ASP:O	1:A:632:ALA:CB	2.66	0.43
4:E:267:TYR:CE1	1:D:780:GLU:HA	2.54	0.43
1:D:106:HIS:N	1:D:107:GLU:CA	2.77	0.43
1:A:297:GLU:OE1	1:A:302:HIS:CD2	2.72	0.43
3:C:92:SER:OG	3:C:152:ALA:HB2	2.19	0.43
1:D:102:GLU:HG3	1:D:246:ILE:HD11	2.01	0.43
1:A:126:LEU:HD12	1:A:340:TYR:CZ	2.54	0.42
1:A:394:ARG:C	1:A:396:ARG:H	2.25	0.42
1:A:586:PRO:N	1:A:587:ASP:CA	2.76	0.42
4:E:264:SER:O	4:E:268:ARG:HG3	2.18	0.42
1:D:447:PHE:CD1	1:D:447:PHE:N	2.86	0.42
1:D:735:LYS:HB2	1:D:735:LYS:HE2	1.51	0.42
1:A:22:ARG:HB3	1:A:528:GLN:OE1	2.19	0.42
1:A:231:THR:HG22	1:A:257:ASN:HA	1.99	0.42
2:B:255:LEU:HD13	2:B:272:ILE:HD13	2.01	0.42
4:E:18:LEU:HB3	4:E:141:LEU:HG	2.01	0.42
4:E:162:LEU:O	4:E:165:GLU:HG2	2.19	0.42
1:D:58:ARG:HG2	1:D:144:GLU:CB	2.49	0.42
1:D:346:PRO:O	1:D:347:LEU:C	2.62	0.42
1:D:485:GLY:C	1:D:487:GLY:HA3	2.44	0.42
1:D:570:VAL:HB	1:D:623:ASN:CG	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ARG:HH12	1:A:301:GLU:CD	2.27	0.42
3:C:129:ARG:HG2	3:C:146:VAL:HG21	2.01	0.42
3:F:53:ILE:HB	3:F:75:GLU:HB2	2.01	0.42
3:F:160:ASP:OD1	3:F:160:ASP:N	2.51	0.42
1:D:114:ASP:HA	1:D:115:PHE:O	2.20	0.42
1:D:121:ALA:HB1	1:D:123:ASP:OD1	2.19	0.42
1:A:177:ARG:HG3	1:A:177:ARG:HH11	1.83	0.42
1:A:359:PRO:O	1:A:417:LEU:HG	2.19	0.42
1:A:448:ASN:O	1:A:451:LEU:N	2.52	0.42
1:A:592:THR:HG23	1:A:595:SER:O	2.20	0.42
2:B:84:SER:OG	2:B:85:LYS:N	2.51	0.42
4:E:91:LEU:HD23	4:E:95:SER:HB3	2.02	0.42
1:D:89:SER:HB3	1:D:122:VAL:HB	2.01	0.42
1:A:298:ASP:O	1:A:301:GLU:HB2	2.20	0.42
1:A:417:LEU:HD11	1:A:477:LEU:HD13	2.01	0.42
1:A:423:LEU:HA	1:A:424:PRO:C	2.45	0.42
1:A:666:THR:C	1:A:730:VAL:HG21	2.42	0.42
1:A:686:ALA:HB3	1:A:750:GLY:HA3	2.01	0.42
1:D:55:LEU:HD21	1:D:84:ARG:HD2	2.02	0.42
1:D:344:ALA:HB1	1:D:379:VAL:O	2.19	0.42
1:A:73:ASP:O	1:A:75:THR:HG23	2.19	0.42
1:A:74:ALA:O	1:A:78:GLU:HG3	2.19	0.42
1:A:418:LEU:HB3	1:A:447:PHE:CE1	2.51	0.42
5:A:801:MCN:N2'	3:C:100:GLN:CB	2.77	0.42
4:E:117:ALA:HB2	4:E:167:ILE:HD12	2.02	0.42
1:D:472:LYS:H	1:D:765:ALA:HB2	1.85	0.42
1:D:573:LYS:HD3	1:D:576:ARG:NH2	2.35	0.42
1:A:278:GLU:HG2	1:A:295:TRP:CZ2	2.55	0.42
1:A:574:ALA:O	1:A:578:ALA:N	2.45	0.42
1:A:574:ALA:O	1:A:576:ARG:N	2.53	0.42
2:B:174:GLN:O	2:B:175:LEU:CB	2.67	0.42
1:D:209:ASN:OD1	1:D:209:ASN:N	2.52	0.42
1:D:342:ARG:O	1:D:342:ARG:HG3	2.18	0.42
1:A:256:VAL:CA	1:A:257:ASN:HB2	2.48	0.42
1:A:417:LEU:HD11	1:A:477:LEU:CD1	2.49	0.42
1:D:383:ARG:O	1:D:751:ILE:HD11	2.20	0.42
1:A:394:ARG:NH1	1:A:395:GLU:OE2	2.53	0.42
2:B:235:ILE:HA	2:B:235:ILE:HD12	1.69	0.42
4:E:250:ALA:HA	4:E:253:GLN:OE1	2.20	0.42
1:D:176:GLY:O	1:D:177:ARG:C	2.63	0.42
1:D:268:SER:HB3	1:D:511:VAL:HG11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:418:LEU:HD11	1:D:425:TRP:CE3	2.55	0.42
1:D:427:PRO:HB2	1:D:428:GLY:C	2.45	0.42
1:D:437:HIS:HA	1:D:438:PHE:HA	1.86	0.42
1:D:450:ALA:HB2	1:D:643:TYR:HE1	1.85	0.42
1:D:614:ARG:CB	1:D:621:ALA:HB2	2.49	0.42
1:A:178:GLY:HA3	1:A:179:ASN:HA	1.63	0.41
1:A:402:CYS:SG	1:A:409:LYS:HA	2.60	0.41
1:A:470:GLY:O	1:A:650:ILE:O	2.37	0.41
4:E:111:THR:OG1	7:E:301:FAD:O2P	2.34	0.41
3:F:26:ALA:N	3:F:61:SER:O	2.50	0.41
1:D:211:HIS:NE2	1:D:310:ARG:HG2	2.35	0.41
1:D:341:PHE:CE2	1:D:346:PRO:HD3	2.50	0.41
1:A:412:PHE:CD1	1:A:412:PHE:C	2.98	0.41
1:A:418:LEU:CG	1:A:419:THR:H	2.22	0.41
1:A:426:THR:HA	1:A:427:PRO:HD3	1.84	0.41
1:A:483:LYS:HB2	1:A:639:MET:O	2.19	0.41
1:A:490:GLU:HG2	1:A:548:VAL:HB	2.01	0.41
3:C:110:MET:HE2	3:C:110:MET:HA	2.01	0.41
4:E:280:LEU:HA	4:E:283:ALA:HB3	2.03	0.41
3:F:104:CYS:O	3:F:108:PHE:HD1	2.03	0.41
1:D:471:ARG:HG3	1:D:652:LEU:H	1.86	0.41
1:D:486:LEU:HD13	1:D:554:ARG:CZ	2.50	0.41
1:A:385:PRO:HD2	1:A:387:ARG:NH1	2.35	0.41
1:A:538:HIS:HD1	1:A:538:HIS:C	2.28	0.41
1:A:740:PRO:C	1:A:742:GLY:N	2.78	0.41
3:F:139:CYS:O	1:D:685:GLY:HA3	2.20	0.41
1:D:382:TYR:CD1	1:D:383:ARG:N	2.89	0.41
1:A:419:THR:O	1:A:420:ALA:C	2.62	0.41
1:A:657:GLY:O	1:A:782:ILE:HD12	2.21	0.41
3:F:42:CYS:H	3:F:47:CYS:HB3	1.86	0.41
1:D:123:ASP:OD1	1:D:123:ASP:N	2.52	0.41
1:D:160:LEU:HD11	1:D:166:ALA:HA	2.01	0.41
1:D:416:ASN:ND2	1:D:416:ASN:O	2.54	0.41
1:D:599:LYS:HD2	1:D:600:GLY:N	2.19	0.41
1:D:644:GLY:HA3	1:D:668:THR:HG22	2.03	0.41
1:A:261:LYS:HZ3	1:D:233:PHE:HE2	1.67	0.41
1:A:434:GLU:HA	1:A:435:PRO:HA	1.86	0.41
3:C:43:GLU:HA	3:C:43:GLU:OE1	2.20	0.41
3:F:42:CYS:HB3	3:F:47:CYS:HB3	2.03	0.41
1:D:484:ALA:O	1:D:485:GLY:C	2.63	0.41
1:A:666:THR:O	1:A:730:VAL:HG22	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:31:ILE:O	7:E:301:FAD:O2A	2.38	0.41
1:D:135:VAL:HG21	1:D:143:ALA:O	2.21	0.41
1:D:345:GLU:HB2	1:D:346:PRO:HD2	2.03	0.41
1:D:450:ALA:CB	1:D:643:TYR:HE1	2.34	0.41
1:D:478:GLY:O	1:D:643:TYR:HA	2.21	0.41
1:A:48:ASP:CG	3:C:36:ARG:HB2	2.45	0.41
1:A:646:THR:HG22	1:A:666:THR:HB	2.02	0.41
1:A:762:ILE:O	1:A:765:ALA:HB3	2.21	0.41
4:E:102:ALA:HB1	4:E:106:ILE:HD13	2.03	0.41
3:F:143:GLN:NE2	3:F:147:GLU:OE2	2.54	0.41
3:F:147:GLU:OE2	1:D:680:ARG:NH2	2.54	0.41
1:D:58:ARG:NH2	1:D:298:ASP:OD2	2.53	0.41
1:D:385:PRO:HD2	1:D:387:ARG:NH2	2.36	0.41
1:D:591:LEU:HD22	1:D:596:PHE:CD1	2.50	0.41
1:D:630:ALA:O	1:D:631:ASP:O	2.38	0.41
1:A:177:ARG:O	1:A:178:GLY:C	2.63	0.41
1:A:486:LEU:HD22	1:A:554:ARG:CD	2.51	0.41
1:A:501:ARG:NH2	1:A:532:GLU:O	2.54	0.41
2:B:130:LEU:HD12	2:B:153:LEU:HD12	2.02	0.41
3:C:31:ASP:HA	3:C:32:ASP:HA	1.66	0.41
4:E:54:ILE:C	4:E:56:ARG:H	2.27	0.41
1:A:326:ILE:HB	1:A:361:ARG:O	2.21	0.41
1:A:344:ALA:HB1	1:A:347:LEU:HB3	2.02	0.41
1:A:444:VAL:HG11	1:A:641:TYR:N	2.36	0.41
1:A:448:ASN:O	1:A:452:GLU:N	2.35	0.41
1:A:614:ARG:NH1	1:A:619:ALA:HB3	2.36	0.41
1:A:671:GLY:HA3	1:A:743:ALA:HA	2.02	0.41
2:B:214:ARG:HA	2:B:231:GLU:CD	2.46	0.41
2:B:258:VAL:O	2:B:268:ARG:CZ	2.69	0.41
4:E:31:ILE:HD12	4:E:51:LEU:HD13	2.03	0.41
4:E:91:LEU:CD2	4:E:95:SER:HB3	2.51	0.41
3:F:48:GLY:HA2	3:F:60:ARG:NH1	2.36	0.41
3:F:129:ARG:HG2	3:F:146:VAL:HG21	2.03	0.41
1:D:62:SER:OG	1:D:125:VAL:HG11	2.21	0.41
1:D:554:ARG:HG3	1:D:555:SER:N	2.36	0.41
1:D:639:MET:H	1:D:639:MET:HG2	1.61	0.41
1:A:636:ASN:OD1	1:A:636:ASN:C	2.64	0.41
4:E:1:MET:HB3	4:E:2:LYS:H	1.63	0.41
1:D:239:HIS:HA	1:D:241:HIS:CE1	2.56	0.41
1:D:329:MET:O	1:D:329:MET:HG3	2.20	0.41
1:D:362:VAL:O	1:D:428:GLY:HA2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:459:TRP:HE1	1:D:463:SER:N	2.19	0.41
1:A:382:TYR:O	1:A:383:ARG:C	2.64	0.40
1:A:562:ALA:HB2	1:A:633:VAL:HG12	2.02	0.40
1:A:782:ILE:O	1:A:782:ILE:HG22	2.21	0.40
4:E:116:LEU:HD23	4:E:126:PRO:HG3	2.03	0.40
4:E:239:LEU:O	4:E:240:SER:HB3	2.21	0.40
3:F:138:ARG:HH22	1:D:697:GLU:CD	2.29	0.40
1:D:59:ILE:HD12	1:D:278:GLU:HG3	2.03	0.40
1:D:682:GLN:HE22	5:D:801:MCN:C7	2.34	0.40
1:A:449:GLU:O	1:A:453:ALA:CB	2.69	0.40
4:E:36:SER:OG	7:E:301:FAD:O2'	2.25	0.40
4:E:96:GLU:OE2	4:E:183:PHE:N	2.54	0.40
1:D:188:TYR:CD2	1:D:429:LEU:C	2.99	0.40
1:D:284:TRP:CZ3	1:D:288:THR:HG21	2.56	0.40
1:D:356:VAL:HG23	1:D:390:SER:HB2	2.04	0.40
1:A:366:ASP:O	1:A:367:ALA:C	2.64	0.40
1:A:656:THR:O	1:A:783:PHE:HE1	2.03	0.40
2:B:258:VAL:HG23	2:B:268:ARG:HH22	1.85	0.40
2:B:271:VAL:C	2:B:273:ARG:HB2	2.46	0.40
1:D:277:PRO:O	1:D:281:VAL:HG23	2.21	0.40
1:D:455:ASN:C	1:D:457:SER:H	2.28	0.40
1:D:473:VAL:HG12	1:D:474:GLY:N	2.37	0.40
1:A:191:ILE:O	1:A:195:PHE:HD1	2.03	0.40
1:A:259:ARG:HH12	1:D:543:LEU:HD11	1.86	0.40
1:A:484:ALA:CA	1:A:486:LEU:HG	2.51	0.40
1:D:565:LYS:HZ1	1:D:632:ALA:HB1	1.86	0.40
1:D:567:ALA:O	1:D:570:VAL:HG12	2.21	0.40
1:D:649:GLN:HG3	1:D:662:LEU:HB2	2.03	0.40
1:D:766:ILE:HG23	1:D:785:ARG:HG2	2.03	0.40
1:A:483:LYS:HE2	1:A:483:LYS:HB3	1.78	0.40
2:B:34:GLY:H	7:B:301:FAD:PA	2.45	0.40
2:B:67:ASP:HB3	2:B:68:GLN:H	1.44	0.40
1:D:111:ASN:OD1	1:D:112:ILE:N	2.49	0.40
1:D:229:ARG:HH22	1:D:253:LEU:CB	2.35	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	761/794 (96%)	612 (80%)	101 (13%)	48 (6%)	1	10
1	D	768/794 (97%)	616 (80%)	113 (15%)	39 (5%)	1	13
2	B	285/296 (96%)	250 (88%)	26 (9%)	9 (3%)	3	22
3	C	158/160 (99%)	129 (82%)	26 (16%)	3 (2%)	6	30
3	F	158/160 (99%)	135 (85%)	21 (13%)	2 (1%)	9	37
4	E	291/296 (98%)	251 (86%)	27 (9%)	13 (4%)	2	15
All	All	2421/2500 (97%)	1993 (82%)	314 (13%)	114 (5%)	2	15

All (114) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	98	VAL
1	A	118	PRO
1	A	229	ARG
1	A	258	VAL
1	A	367	ALA
1	A	418	LEU
1	A	437	HIS
1	A	440	SER
1	A	482	ASP
1	A	483	LYS
1	A	484	ALA
1	A	486	LEU
1	A	552	SER
1	A	631	ASP
1	A	632	ALA
1	A	636	ASN
1	A	639	MET
2	B	86	THR
2	B	176	PRO

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Mol	Chain	Res	Type
2	B	177	HIS
2	B	273	ARG
2	B	274	THR
3	C	50	CYS
3	C	159	ASN
4	E	93	ILE
4	E	239	LEU
4	E	240	SER
4	E	285	HIS
4	E	291	LYS
4	E	292	GLU
3	F	34	HIS
3	F	50	CYS
1	D	111	ASN
1	D	115	PHE
1	D	116	SER
1	D	330	LYS
1	D	343	GLN
1	D	422	ASP
1	D	427	PRO
1	D	429	LEU
1	D	460	LEU
1	D	553	SER
1	D	602	ASP
1	D	615	ASP
1	D	631	ASP
1	A	178	GLY
1	A	209	ASN
1	A	429	LEU
1	A	463	SER
1	A	485	GLY
1	A	500	GLY
1	A	575	ARG
1	A	590	GLU
1	A	640	ASN
1	A	655	ASP
1	A	671	GLY
1	A	742	GLY
1	A	752	ILE
1	A	770	VAL
2	B	26	ASP
2	B	93	ILE

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Mol	Chain	Res	Type
4	E	175	LEU
4	E	206	GLU
4	E	290	THR
1	D	94	HIS
1	D	99	LEU
1	D	109	TYR
1	D	177	ARG
1	D	189	GLY
1	D	347	LEU
1	D	446	HIS
1	D	618	THR
1	A	176	GLY
1	A	244	ARG
1	A	307	SER
1	A	467	ARG
1	A	740	PRO
1	A	741	PHE
1	A	785	ARG
2	B	253	GLN
1	D	103	LEU
1	D	254	PRO
1	D	345	GLU
1	D	408	SER
1	A	330	LYS
1	A	615	ASP
2	B	66	SER
4	E	176	PRO
1	D	228	ALA
1	D	417	LEU
1	D	419	THR
1	D	599	LYS
1	D	632	ALA
1	D	742	GLY
1	A	106	HIS
1	A	498	ARG
1	A	553	SER
1	A	673	VAL
4	E	58	PRO
1	D	586	PRO
1	A	175	PRO
1	A	359	PRO
1	A	725	ASN

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Mol	Chain	Res	Type
4	E	259	PRO
1	D	238	VAL
1	D	253	LEU
1	D	72	ILE
1	D	122	VAL
3	C	88	PRO
4	E	87	ILE
1	D	432	VAL
1	D	485	GLY
1	D	769	GLY

5.3.2 Protein sidechains [i](#)

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	602/632 (95%)	560 (93%)	42 (7%)	14	40
1	D	607/632 (96%)	560 (92%)	47 (8%)	12	38
2	B	225/234 (96%)	209 (93%)	16 (7%)	13	39
3	C	138/138 (100%)	131 (95%)	7 (5%)	21	49
3	F	138/138 (100%)	130 (94%)	8 (6%)	18	45
4	E	228/234 (97%)	213 (93%)	15 (7%)	15	42
All	All	1938/2008 (96%)	1803 (93%)	135 (7%)	14	40

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	22	ARG
1	A	109	TYR
1	A	123	ASP
1	A	193	ARG
1	A	202	ILE
1	A	209	ASN
1	A	211	HIS

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Mol	Chain	Res	Type
1	A	244	ARG
1	A	249	LYS
1	A	258	VAL
1	A	263	VAL
1	A	417	LEU
1	A	432	VAL
1	A	437	HIS
1	A	449	GLU
1	A	460	LEU
1	A	469	ASP
1	A	471	ARG
1	A	479	VAL
1	A	483	LYS
1	A	488	LEU
1	A	490	GLU
1	A	529	ILE
1	A	534	ILE
1	A	538	HIS
1	A	557	VAL
1	A	585	ASP
1	A	587	ASP
1	A	589	LEU
1	A	590	GLU
1	A	591	LEU
1	A	592	THR
1	A	614	ARG
1	A	618	THR
1	A	655	ASP
1	A	727	ASP
1	A	732	GLU
1	A	766	ILE
1	A	773	ASP
1	A	780	GLU
1	A	785	ARG
2	B	21	LEU
2	B	29	LYS
2	B	52	VAL
2	B	86	THR
2	B	87	ILE
2	B	95	SER
2	B	150	LYS
2	B	166	LEU

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Mol	Chain	Res	Type
2	B	177	HIS
2	B	207	GLN
2	B	235	ILE
2	B	243	ASP
2	B	256	ASP
2	B	261	VAL
2	B	268	ARG
2	B	273	ARG
3	C	6	LEU
3	C	20	GLU
3	C	81	GLN
3	C	121	VAL
3	C	138	ARG
3	C	140	THR
3	C	157	ASP
4	E	2	LYS
4	E	20	LEU
4	E	60	LEU
4	E	68	GLN
4	E	83	THR
4	E	89	GLN
4	E	149	LEU
4	E	172	VAL
4	E	175	LEU
4	E	214	ARG
4	E	235	ILE
4	E	239	LEU
4	E	253	GLN
4	E	260	THR
4	E	261	VAL
3	F	80	LEU
3	F	100	GLN
3	F	121	VAL
3	F	138	ARG
3	F	140	THR
3	F	157	ASP
3	F	158	HIS
3	F	160	ASP
1	D	33	ARG
1	D	49	LEU
1	D	70	VAL
1	D	95	LEU

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Mol	Chain	Res	Type
1	D	100	LEU
1	D	101	GLU
1	D	111	ASN
1	D	119	VAL
1	D	160	LEU
1	D	179	ASN
1	D	180	GLU
1	D	232	LEU
1	D	240	VAL
1	D	255	GLU
1	D	271	VAL
1	D	329	MET
1	D	348	VAL
1	D	419	THR
1	D	429	LEU
1	D	432	VAL
1	D	444	VAL
1	D	446	HIS
1	D	459	TRP
1	D	463	SER
1	D	467	ARG
1	D	486	LEU
1	D	490	GLU
1	D	496	VAL
1	D	498	ARG
1	D	511	VAL
1	D	535	ASP
1	D	589	LEU
1	D	599	LYS
1	D	601	THR
1	D	602	ASP
1	D	618	THR
1	D	623	ASN
1	D	633	VAL
1	D	639	MET
1	D	680	ARG
1	D	721	GLN
1	D	733	ASP
1	D	735	LYS
1	D	749	ILE
1	D	752	ILE
1	D	773	ASP

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Mol	Chain	Res	Type
1	D	783	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	23	GLN
1	A	54	GLN
1	A	56	HIS
1	A	66	HIS
1	A	94	HIS
1	A	111	ASN
1	A	130	GLN
1	A	204	HIS
1	A	209	ASN
1	A	302	HIS
1	A	335	HIS
1	A	375	ASN
1	A	416	ASN
1	A	533	ASN
1	A	649	GLN
1	A	721	GLN
1	A	739	ASN
1	A	771	HIS
2	B	90	ASN
2	B	103	HIS
2	B	262	HIS
3	C	81	GLN
3	C	97	HIS
3	C	143	GLN
3	C	144	GLN
3	C	154	HIS
4	E	35	GLN
4	E	118	HIS
4	E	174	GLN
3	F	34	HIS
3	F	100	GLN
3	F	144	GLN
1	D	91	HIS
1	D	239	HIS
1	D	343	GLN
1	D	416	ASN

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Mol	Chain	Res	Type
1	D	637	ASN
1	D	640	ASN
1	D	682	GLN
1	D	739	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 for Mogul analysis.

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	$\# Z > 2$
5	MCN	A	801	6	41,48,48	1.32	2 (4%)	49,74,74	1.54	8 (16%)
8	FES	C	201	3	0,4,4	-	-	-	-	-
7	FAD	B	301	-	56,58,58	1.48	10 (17%)	81,89,89	1.78	17 (20%)
7	FAD	E	301	-	56,58,58	1.51	10 (17%)	81,89,89	1.68	16 (19%)
8	FES	F	201	3	0,4,4	-	-	-	-	-
5	MCN	D	801	6	41,48,48	1.30	3 (7%)	49,74,74	1.64	6 (12%)
8	FES	C	202	3	0,4,4	-	-	-	-	-
8	FES	F	202	3	0,4,4	-	-	-	-	-

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
5	MCN	A	801	6	-	13/22/54/54	0/5/5/5
8	FES	C	201	3	-	-	0/1/1/1
7	FAD	B	301	-	-	21/34/50/50	0/6/6/6
7	FAD	E	301	-	-	12/34/50/50	0/6/6/6
8	FES	F	201	3	-	-	0/1/1/1
5	MCN	D	801	6	-	15/22/54/54	0/5/5/5
8	FES	C	202	3	-	-	0/1/1/1
8	FES	F	202	3	-	-	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	301	FAD	C9A-C5X	5.31	1.50	1.41
7	B	301	FAD	C9A-C5X	5.26	1.50	1.41
5	A	801	MCN	C4A-C4B	4.83	1.49	1.40
5	D	801	MCN	C4A-C4B	4.75	1.48	1.40
7	E	301	FAD	C5A-C4A	4.70	1.47	1.39
7	B	301	FAD	C5A-C4A	4.45	1.47	1.39
5	A	801	MCN	C6'-C7	4.22	1.49	1.43
5	D	801	MCN	C6'-C7	4.11	1.49	1.43
7	E	301	FAD	C8-C7	3.64	1.50	1.40
7	B	301	FAD	C8-C7	3.63	1.49	1.40
7	E	301	FAD	C5A-C6A	2.82	1.48	1.41
7	B	301	FAD	C10-N10	2.52	1.42	1.37
7	E	301	FAD	C8A-N7A	2.50	1.36	1.31
7	B	301	FAD	C5A-C6A	2.50	1.48	1.41
7	B	301	FAD	C4X-N5	2.45	1.35	1.30
7	E	301	FAD	C4-N3	-2.40	1.34	1.38
7	B	301	FAD	C4-N3	-2.40	1.34	1.38
7	B	301	FAD	C5A-N7A	-2.35	1.34	1.39
7	E	301	FAD	C4X-N5	2.24	1.35	1.30
7	B	301	FAD	C8A-N7A	2.19	1.35	1.31
7	E	301	FAD	C5X-N5	-2.17	1.35	1.39
7	E	301	FAD	C10-N10	2.15	1.42	1.37
7	E	301	FAD	C5A-N7A	-2.11	1.35	1.39
7	B	301	FAD	C5X-N5	-2.05	1.35	1.39
5	D	801	MCN	C7-N8'	2.04	1.35	1.30

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	301	FAD	C5A-C4A-N3A	-6.50	118.28	126.75
7	E	301	FAD	C5A-C4A-N3A	-6.00	118.93	126.75
7	B	301	FAD	N3A-C4A-N9A	5.62	136.34	127.08
5	D	801	MCN	C2'-N1'-C4B	5.06	121.14	115.36
5	A	801	MCN	C2'-N1'-C4B	4.90	120.96	115.36
5	D	801	MCN	PB-O3A-PA	-4.86	116.15	132.83
7	E	301	FAD	N3A-C4A-N9A	4.64	134.72	127.08
7	B	301	FAD	P-O3P-PA	-4.40	117.72	132.83
5	A	801	MCN	PB-O3A-PA	-4.25	118.23	132.83
7	B	301	FAD	C2A-N3A-C4A	4.15	121.56	111.75
5	D	801	MCN	O9'-C7-N8'	3.99	120.25	115.30
7	E	301	FAD	C2A-N3A-C4A	3.96	121.11	111.75
5	A	801	MCN	O9'-C7-N8'	3.72	119.92	115.30
7	E	301	FAD	P-O3P-PA	-3.66	120.26	132.83
7	B	301	FAD	N3A-C2A-N1A	-3.53	123.08	128.60
7	E	301	FAD	N3A-C2A-N1A	-3.47	123.17	128.60
7	B	301	FAD	C4X-C10-N1	-3.30	117.08	124.73
7	E	301	FAD	C4A-C5A-N7A	-3.30	106.61	110.62
5	D	801	MCN	N1'-C2'-N3'	-3.28	122.85	127.22
7	E	301	FAD	C4X-C10-N1	-3.07	117.61	124.73
5	A	801	MCN	N1'-C2'-N3'	-3.04	123.17	127.22
7	B	301	FAD	C10-N1-C2	2.79	122.47	116.90
7	B	301	FAD	C4A-N9A-C8A	2.76	108.72	105.73
7	E	301	FAD	C5A-N7A-C8A	2.71	107.36	103.51
7	E	301	FAD	C4A-N9A-C8A	2.49	108.43	105.73
7	B	301	FAD	C4A-C5A-N7A	-2.48	107.60	110.62
7	E	301	FAD	C10-N1-C2	2.45	121.80	116.90
7	E	301	FAD	C6A-C5A-N7A	2.43	136.54	132.02
7	B	301	FAD	C5A-N7A-C8A	2.43	106.95	103.51
5	D	801	MCN	N1'-C4B-N8'	2.42	121.70	115.97
5	D	801	MCN	C7-N8'-C4B	2.27	118.54	116.61
7	B	301	FAD	O4B-C1B-N9A	2.24	112.48	108.06
7	E	301	FAD	O4-C4-C4X	-2.23	120.69	126.60
7	B	301	FAD	O4-C4-C4X	-2.21	120.74	126.60
7	E	301	FAD	C4-C4X-N5	2.21	121.37	118.23
7	E	301	FAD	C4X-C10-N10	2.14	119.62	116.48
5	A	801	MCN	N1'-C4B-N8'	2.14	121.05	115.97
7	B	301	FAD	C4X-C4-N3	2.14	118.62	113.19
7	B	301	FAD	C4-C4X-N5	2.14	121.28	118.23
7	E	301	FAD	C3B-C2B-C1B	2.13	105.48	101.43
7	E	301	FAD	C4X-C4-N3	2.07	118.45	113.19
5	A	801	MCN	C3'-C2D-C1'	2.02	105.27	101.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	801	MCN	O2-C2-N3	-2.02	119.04	122.33
5	A	801	MCN	C7-N8'-C4B	2.01	118.33	116.61
7	B	301	FAD	C5A-C6A-N6A	-2.01	119.05	123.43
7	B	301	FAD	C5'-C4'-C3'	-2.01	108.32	112.20
7	B	301	FAD	C1'-N10-C9A	-2.01	117.17	120.51

There are no chirality outliers.

All (61) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	801	MCN	O4D-C4D-C5'-O5'
5	A	801	MCN	C5'-O5'-PA-O1A
5	A	801	MCN	O3B-C10-C9'-C8'
5	A	801	MCN	O3B-C10-C9'-O9'
5	D	801	MCN	O4D-C4D-C5'-O5'
5	D	801	MCN	C5'-O5'-PA-O1A
5	D	801	MCN	C5'-O5'-PA-O2A
5	D	801	MCN	C10-O3B-PB-O3A
5	D	801	MCN	O3B-C10-C9'-C8'
7	B	301	FAD	C4B-C5B-O5B-PA
7	B	301	FAD	C2'-C1'-N10-C9A
7	B	301	FAD	C2'-C1'-N10-C10
7	B	301	FAD	N10-C1'-C2'-O2'
7	B	301	FAD	N10-C1'-C2'-C3'
7	B	301	FAD	C1'-C2'-C3'-O3'
7	B	301	FAD	C1'-C2'-C3'-C4'
7	B	301	FAD	O2'-C2'-C3'-O3'
7	B	301	FAD	O2'-C2'-C3'-C4'
7	B	301	FAD	C3'-C4'-C5'-O5'
7	B	301	FAD	O4'-C4'-C5'-O5'
7	B	301	FAD	C5'-O5'-P-O1P
7	E	301	FAD	N10-C1'-C2'-C3'
7	E	301	FAD	O4'-C4'-C5'-O5'
7	E	301	FAD	C5'-O5'-P-O1P
7	E	301	FAD	C5'-O5'-P-O2P
7	B	301	FAD	C3B-C4B-C5B-O5B
7	B	301	FAD	O4B-C1B-N9A-C8A
7	B	301	FAD	O4B-C1B-N9A-C4A
5	A	801	MCN	C3'-C4D-C5'-O5'
5	D	801	MCN	C3'-C4D-C5'-O5'
5	A	801	MCN	C2D-C1'-N1-C6
7	E	301	FAD	O4B-C4B-C5B-O5B

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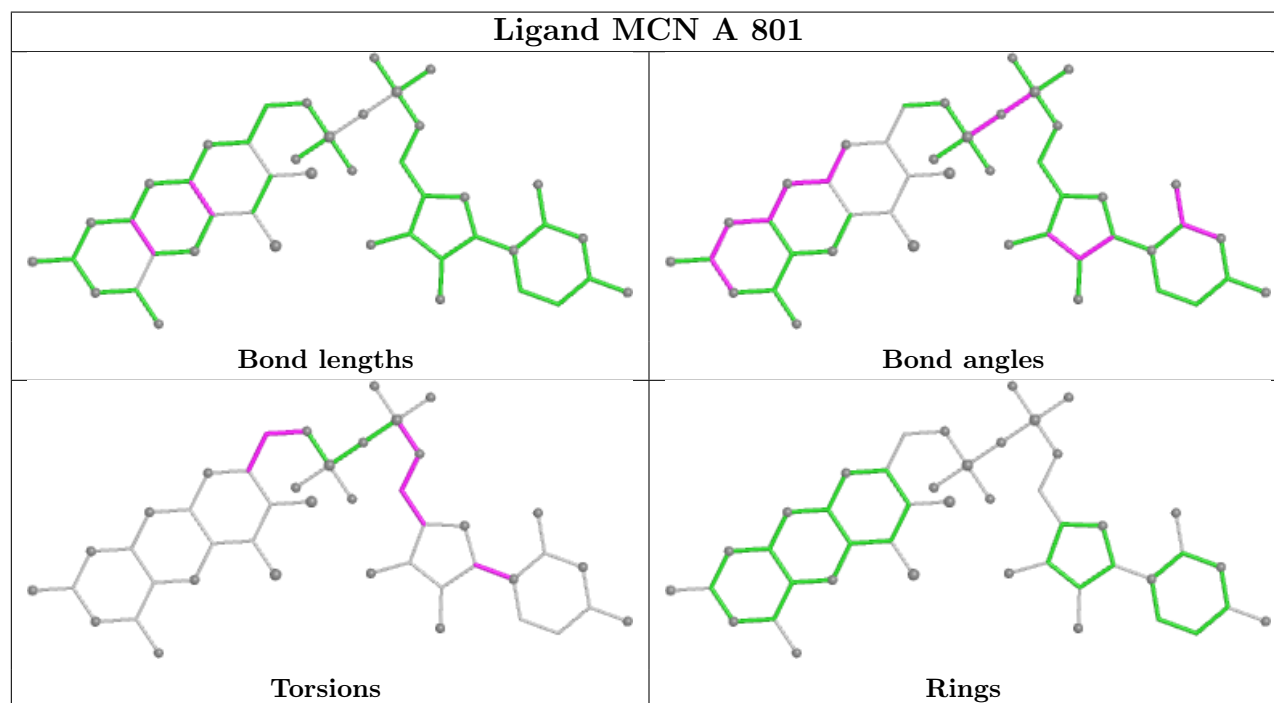
Mol	Chain	Res	Type	Atoms
7	E	301	FAD	C3'-C4'-C5'-O5'
7	E	301	FAD	C3B-C4B-C5B-O5B
5	A	801	MCN	C4D-C5'-O5'-PA
5	D	801	MCN	C9'-C10-O3B-PB
5	D	801	MCN	O3B-C10-C9'-O9'
5	A	801	MCN	C9'-C10-O3B-PB
5	D	801	MCN	C4D-C5'-O5'-PA
7	B	301	FAD	C4'-C5'-O5'-P
7	E	301	FAD	C4'-C5'-O5'-P
5	D	801	MCN	C2D-C1'-N1-C6
5	A	801	MCN	C5'-O5'-PA-O3A
7	B	301	FAD	O4B-C4B-C5B-O5B
5	A	801	MCN	C5'-O5'-PA-O2A
5	D	801	MCN	C10-O3B-PB-O1B
7	B	301	FAD	C5'-O5'-P-O2P
7	E	301	FAD	N10-C1'-C2'-O2'
5	A	801	MCN	C2D-C1'-N1-C2
5	A	801	MCN	O4D-C1'-N1-C6
5	D	801	MCN	C2D-C1'-N1-C2
5	A	801	MCN	O4D-C1'-N1-C2
5	D	801	MCN	O4D-C1'-N1-C6
7	E	301	FAD	C2'-C3'-C4'-O4'
5	D	801	MCN	O4D-C1'-N1-C2
7	B	301	FAD	P-O3P-PA-O1A
5	D	801	MCN	C5'-O5'-PA-O3A
7	B	301	FAD	C5'-O5'-P-O3P
7	E	301	FAD	C5B-O5B-PA-O3P
7	E	301	FAD	C5'-O5'-P-O3P
7	B	301	FAD	P-O3P-PA-O2A

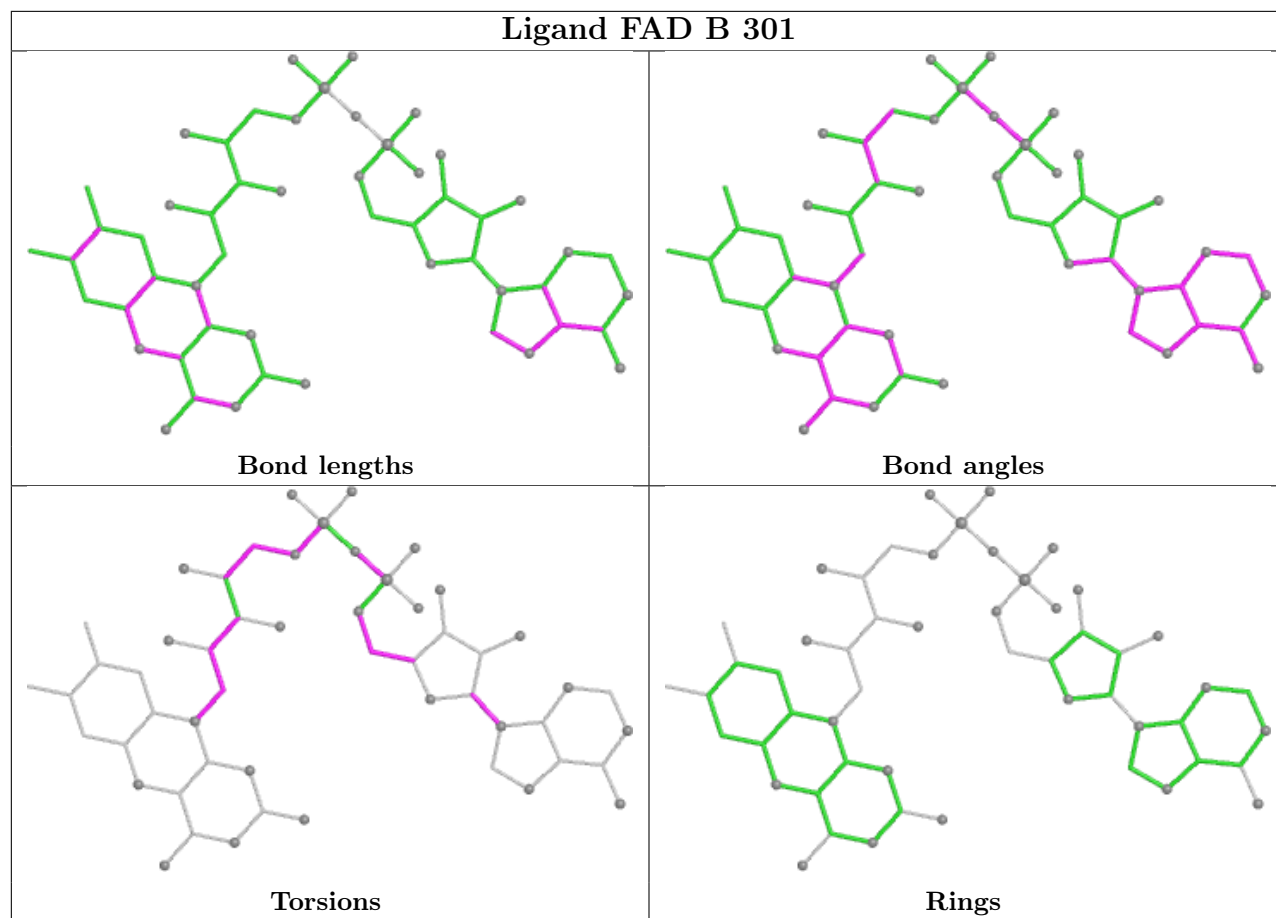
There are no ring outliers.

8 monomers are involved in 61 short contacts:

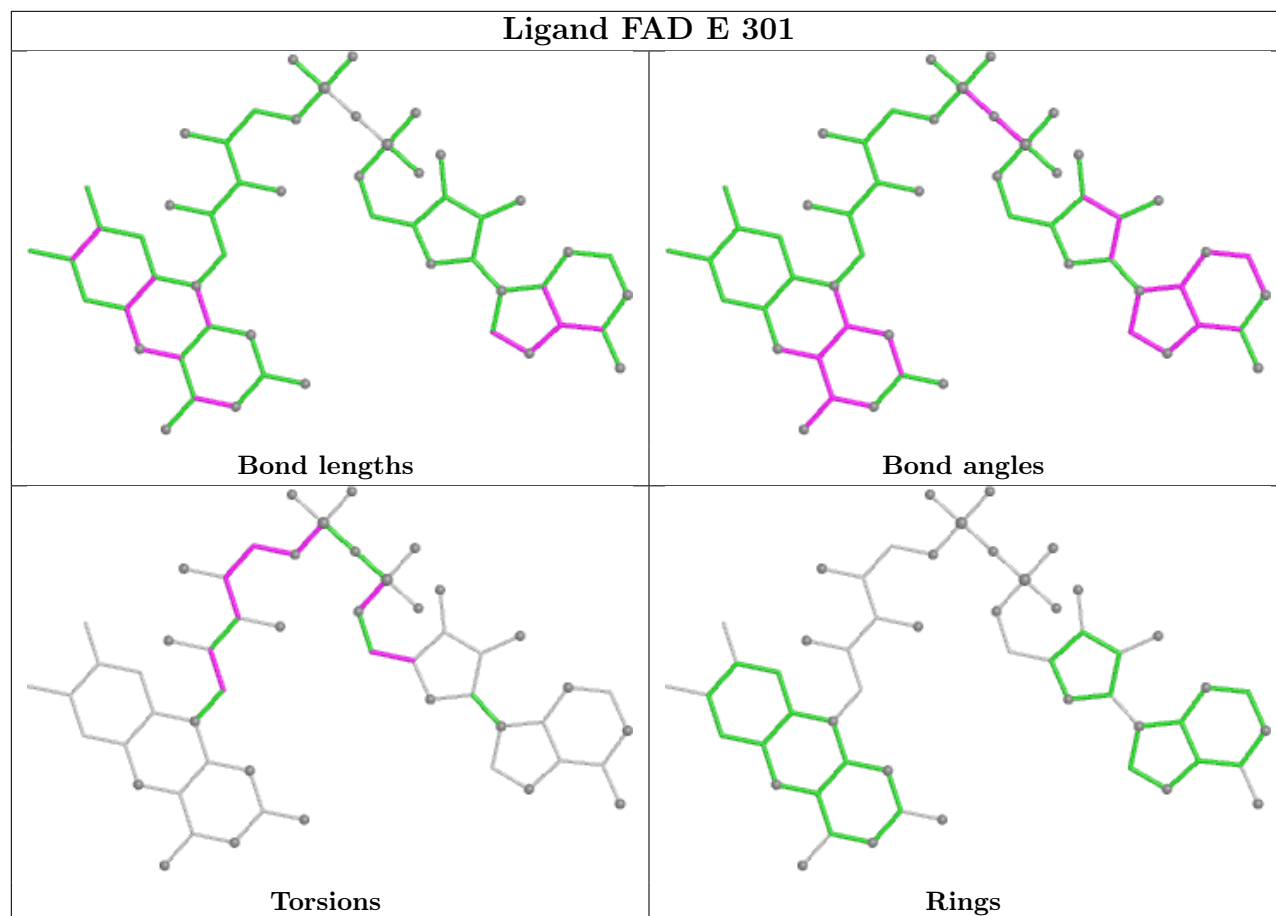
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	801	MCN	14	0
8	C	201	FES	3	0
7	B	301	FAD	11	0
7	E	301	FAD	9	0
8	F	201	FES	3	0
5	D	801	MCN	15	0
8	C	202	FES	3	0
8	F	202	FES	3	0

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.

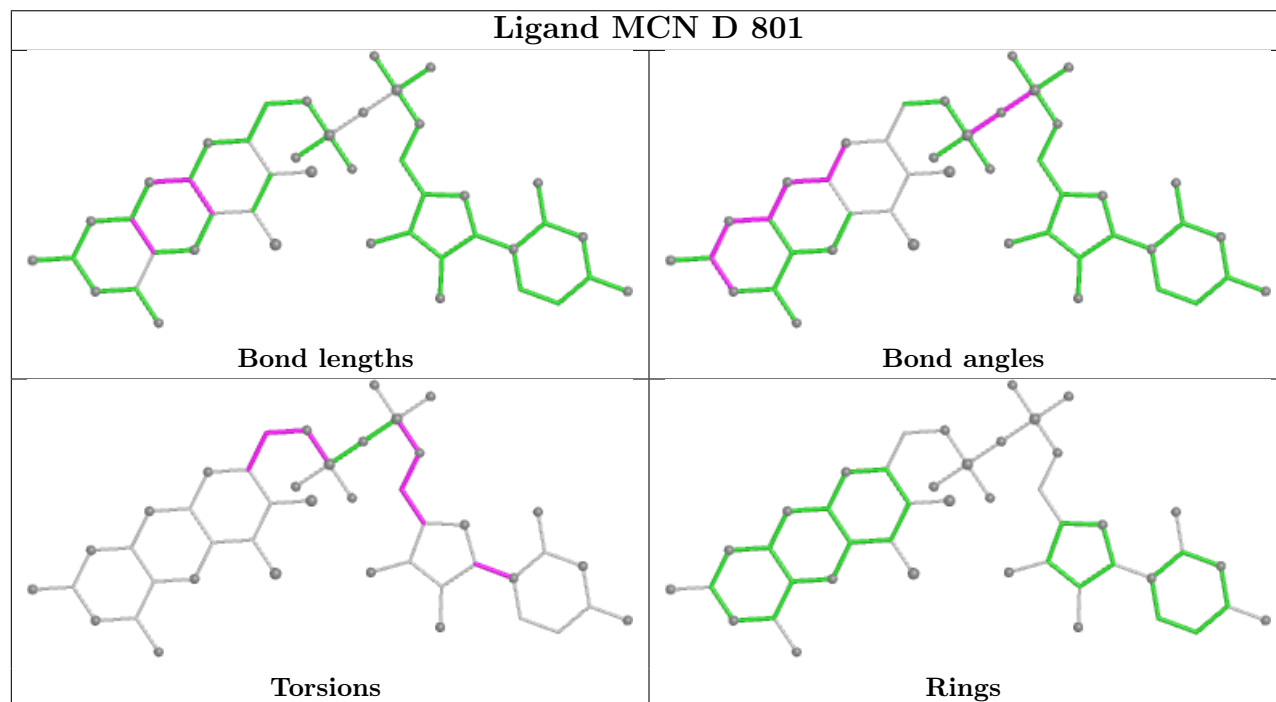




Ligand FAD E 301



Ligand MCN D 801



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	765/794 (96%)	1.14	154 (20%) 3 3	38, 60, 104, 150	1 (0%)
1	D	770/794 (96%)	1.21	154 (20%) 3 3	43, 64, 107, 148	1 (0%)
2	B	287/296 (96%)	0.79	24 (8%) 17 13	51, 71, 102, 116	0
3	C	160/160 (100%)	0.72	11 (6%) 23 17	38, 58, 89, 124	0
3	F	160/160 (100%)	0.77	14 (8%) 15 12	46, 56, 92, 137	0
4	E	293/296 (98%)	0.73	22 (7%) 20 15	43, 66, 92, 145	0
All	All	2435/2500 (97%)	1.02	379 (15%) 5 5	38, 63, 103, 150	2 (0%)

All (379) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	430	ASP	11.0
1	D	428	GLY	8.6
1	A	482	ASP	7.7
1	D	237	THR	7.5
1	D	239	HIS	7.2
1	A	619	ALA	7.1
1	A	430	ASP	6.6
1	A	627	GLY	6.4
1	A	255	GLU	6.0
1	A	116	SER	5.9
1	D	638	ALA	5.9
1	A	440	SER	5.8
1	D	770	VAL	5.8
1	D	621	ALA	5.7
2	B	88	SER	5.7
1	D	429	LEU	5.7
1	D	238	VAL	5.6
1	A	432	VAL	5.5
3	C	62	CYS	5.5

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Mol	Chain	Res	Type	RSRZ
1	D	785	ARG	5.5
1	D	632	ALA	5.4
1	A	343	GLN	5.3
1	D	434	GLU	5.3
1	A	484	ALA	5.2
1	D	589	LEU	5.1
1	D	438	PHE	5.1
1	D	769	GLY	5.1
1	A	632	ALA	5.0
1	A	470	GLY	5.0
4	E	89	GLN	5.0
1	D	422	ASP	4.9
1	D	179	ASN	4.9
1	A	439	ASP	4.9
1	D	114	ASP	4.8
1	A	436	TYR	4.8
1	A	344	ALA	4.7
1	D	435	PRO	4.7
2	B	92	PRO	4.7
1	A	438	PHE	4.7
1	A	629	ALA	4.7
1	A	428	GLY	4.6
1	D	241	HIS	4.6
1	A	73	ASP	4.6
1	D	116	SER	4.6
1	D	117	HIS	4.6
1	A	726	VAL	4.5
1	D	178	GLY	4.5
1	A	616	PRO	4.5
4	E	90	ASN	4.5
1	A	95	LEU	4.5
1	A	725	ASN	4.4
1	A	117	HIS	4.4
1	D	431	ILE	4.4
1	A	729	PHE	4.4
1	D	479	VAL	4.4
1	A	448	ASN	4.4
1	D	619	ALA	4.3
4	E	91	LEU	4.3
1	D	484	ALA	4.3
1	D	95	LEU	4.2
1	D	783	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	655	ASP	4.2
4	E	289	PRO	4.2
4	E	87	ILE	4.2
1	D	98	VAL	4.1
1	A	97	SER	4.1
3	C	43	GLU	4.1
1	A	236	GLY	4.1
1	D	485	GLY	4.1
1	A	622	ASP	4.1
1	A	630	ALA	4.1
1	A	487	GLY	4.0
1	D	330	LYS	4.0
2	B	90	ASN	4.0
1	A	628	LEU	4.0
1	D	444	VAL	4.0
1	D	633	VAL	4.0
1	D	726	VAL	4.0
1	D	628	LEU	3.9
3	C	121	VAL	3.8
1	D	231	THR	3.8
1	D	470	GLY	3.8
1	A	331	ASP	3.8
1	D	440	SER	3.8
1	A	118	PRO	3.8
1	A	230	ASP	3.8
1	A	620	ARG	3.8
1	A	623	ASN	3.8
2	B	287	ALA	3.8
1	A	483	LYS	3.8
1	D	727	ASP	3.7
1	A	99	LEU	3.7
1	D	122	VAL	3.7
1	D	329	MET	3.7
1	D	626	PRO	3.7
1	D	634	TYR	3.7
1	D	103	LEU	3.7
1	A	242	ASP	3.7
1	A	591	LEU	3.7
3	F	106	SER	3.6
1	D	631	ASP	3.6
1	A	72	ILE	3.6
1	A	418	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	D	623	ASN	3.6
1	D	427	PRO	3.6
1	A	497	SER	3.6
1	D	433	HIS	3.6
1	D	729	PHE	3.6
2	B	272	ILE	3.6
1	A	420	ALA	3.6
1	A	188	TYR	3.6
1	D	510	SER	3.6
4	E	84	SER	3.6
1	D	331	ASP	3.6
1	D	629	ALA	3.5
1	A	615	ASP	3.5
3	C	57	GLN	3.5
1	D	407	LEU	3.5
1	A	105	TYR	3.5
1	A	713	MET	3.5
1	D	365	TYR	3.5
4	E	290	THR	3.4
1	D	94	HIS	3.4
1	A	626	PRO	3.4
1	D	622	ASP	3.4
1	D	344	ALA	3.4
1	D	482	ASP	3.4
1	A	488	LEU	3.4
2	B	208	GLY	3.4
1	A	187	ALA	3.4
1	A	638	ALA	3.4
1	D	641	TYR	3.4
1	A	179	ASN	3.3
1	D	418	LEU	3.3
1	A	631	ASP	3.3
1	A	634	TYR	3.3
1	D	106	HIS	3.3
1	A	668	THR	3.3
1	D	616	PRO	3.3
1	D	724	PRO	3.3
1	A	783	PHE	3.3
4	E	175	LEU	3.3
1	D	235	TRP	3.3
1	A	481	MET	3.3
4	E	288	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	437	HIS	3.2
1	D	343	GLN	3.2
1	D	432	VAL	3.2
4	E	260	THR	3.2
1	D	635	MET	3.2
1	A	94	HIS	3.2
1	D	481	MET	3.2
1	D	627	GLY	3.2
2	B	285	HIS	3.2
1	A	466	LEU	3.2
1	A	639	MET	3.2
3	C	32	ASP	3.2
1	A	728	CYS	3.2
1	D	636	ASN	3.2
1	A	635	MET	3.2
1	D	639	MET	3.2
1	D	70	VAL	3.1
1	A	434	GLU	3.1
3	F	121	VAL	3.1
4	E	86	THR	3.1
1	A	229	ARG	3.1
1	D	437	HIS	3.1
1	A	636	ASN	3.1
4	E	239	LEU	3.1
1	A	96	GLY	3.1
1	A	747	GLY	3.1
1	D	667	SER	3.1
1	A	459	TRP	3.1
1	A	427	PRO	3.1
1	D	466	LEU	3.0
1	A	98	VAL	3.0
1	A	479	VAL	3.0
1	D	72	ILE	3.0
1	D	630	ALA	3.0
2	B	227	CYS	3.0
2	B	65	LYS	3.0
2	B	91	LEU	3.0
1	A	478	GLY	3.0
1	D	96	GLY	3.0
1	A	598	VAL	3.0
1	D	21	ASN	3.0
1	D	741	PHE	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	621	ALA	3.0
1	D	121	ALA	3.0
1	A	770	VAL	3.0
1	A	456	PHE	3.0
1	D	486	LEU	2.9
1	D	199	GLU	2.9
1	D	97	SER	2.9
4	E	135	TYR	2.9
1	D	200	HIS	2.9
3	F	62	CYS	2.9
1	A	259	ARG	2.9
2	B	176	PRO	2.9
1	A	100	LEU	2.9
2	B	89	GLN	2.9
1	A	121	ALA	2.9
1	A	180	GLU	2.9
1	D	346	PRO	2.9
1	D	115	PHE	2.9
1	D	230	ASP	2.8
1	A	593	ALA	2.8
1	D	556	THR	2.8
1	A	279	ASN	2.8
1	A	103	LEU	2.8
1	D	730	VAL	2.8
1	A	101	GLU	2.8
1	A	637	ASN	2.8
1	A	109	TYR	2.8
2	B	188	ARG	2.8
1	A	596	PHE	2.7
1	A	480	LEU	2.7
1	D	101	GLU	2.7
2	B	274	THR	2.7
1	A	178	GLY	2.7
1	D	236	GLY	2.7
3	F	140	THR	2.7
1	A	617	PHE	2.7
1	A	471	ARG	2.7
1	D	228	ALA	2.7
1	A	108	ILE	2.7
1	D	735	LYS	2.7
1	D	419	THR	2.7
1	D	442	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	769	GLY	2.6
1	D	107	GLU	2.6
3	F	141	GLY	2.6
1	A	589	LEU	2.6
1	A	625	GLU	2.6
1	D	180	GLU	2.6
1	A	443	VAL	2.6
1	A	469	ASP	2.6
1	D	104	GLY	2.6
1	D	113	GLU	2.6
1	D	120	LEU	2.6
1	A	429	LEU	2.6
3	F	130	GLU	2.6
1	A	735	LYS	2.6
1	D	456	PHE	2.6
1	D	488	LEU	2.6
1	A	464	LYS	2.6
1	D	551	TRP	2.5
1	A	447	PHE	2.5
3	C	158	HIS	2.5
1	A	600	GLY	2.5
1	D	102	GLU	2.5
1	D	322	ALA	2.5
4	E	165	GLU	2.5
1	D	112	ILE	2.5
1	A	106	HIS	2.5
3	F	158	HIS	2.5
2	B	271	VAL	2.5
1	A	113	GLU	2.5
1	A	749	ILE	2.5
3	C	45	GLY	2.5
1	A	552	SER	2.5
1	D	212	SER	2.5
1	A	112	ILE	2.5
1	A	575	ARG	2.5
1	D	752	ILE	2.4
1	A	590	GLU	2.4
1	D	458	GLU	2.4
1	A	445	LYS	2.4
1	A	618	THR	2.4
1	D	618	THR	2.4
1	A	256	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	557	VAL	2.4
4	E	88	SER	2.4
1	A	486	LEU	2.4
1	D	108	ILE	2.4
3	C	1	MET	2.4
1	D	620	ARG	2.4
1	A	111	ASN	2.4
1	A	114	ASP	2.4
3	F	41	GLY	2.4
1	D	489	PHE	2.4
1	A	449	GLU	2.4
1	D	459	TRP	2.4
1	A	614	ARG	2.3
1	D	469	ASP	2.3
1	D	99	LEU	2.3
1	A	102	GLU	2.3
1	D	155	GLU	2.3
1	D	601	THR	2.3
1	D	671	GLY	2.3
2	B	87	ILE	2.3
1	D	448	ASN	2.3
1	A	787	GLN	2.3
1	A	119	VAL	2.3
1	A	419	THR	2.3
1	D	71	SER	2.3
2	B	86	THR	2.3
1	D	713	MET	2.3
1	A	442	ASP	2.3
1	D	439	ASP	2.3
1	D	588	ASP	2.3
1	D	773	ASP	2.3
1	A	345	GLU	2.3
4	E	202	VAL	2.3
1	A	181	GLY	2.3
4	E	156	HIS	2.3
1	D	111	ASN	2.3
1	A	588	ASP	2.3
2	B	273	ARG	2.3
1	D	460	LEU	2.3
3	F	136	LEU	2.3
1	D	447	PHE	2.3
1	A	123	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	243	ASN	2.2
3	C	42	CYS	2.2
1	D	478	GLY	2.2
1	D	480	LEU	2.2
1	D	368	THR	2.2
1	A	258	VAL	2.2
1	D	327	LEU	2.2
1	D	406	GLY	2.2
1	D	746	LEU	2.2
2	B	175	LEU	2.2
3	C	123	LEU	2.2
1	A	633	VAL	2.2
1	A	457	SER	2.2
1	A	326	ILE	2.2
4	E	1	MET	2.2
4	E	116	LEU	2.2
1	A	687	ALA	2.2
1	A	727	ASP	2.2
3	F	83	ASP	2.2
3	F	117	ASP	2.2
1	A	362	VAL	2.2
1	D	188	TYR	2.2
1	D	464	LYS	2.2
1	D	637	ASN	2.2
1	D	768	ASP	2.2
3	F	104	CYS	2.2
1	D	240	VAL	2.1
1	A	120	LEU	2.1
1	A	577	LEU	2.1
1	D	457	SER	2.1
2	B	269	ALA	2.1
3	C	106	SER	2.1
1	A	542	GLU	2.1
1	D	600	GLY	2.1
1	D	483	LYS	2.1
3	F	1	MET	2.1
1	D	404	GLU	2.1
1	A	640	ASN	2.1
1	D	362	VAL	2.1
4	E	285	HIS	2.1
1	A	431	ILE	2.1
1	A	592	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	121	ALA	2.1
4	E	92	PRO	2.1
1	A	115	PHE	2.1
3	F	32	ASP	2.1
2	B	135	TYR	2.1
1	A	584	ALA	2.1
1	D	23	GLN	2.1
1	A	254	PRO	2.1
1	A	22	ARG	2.1
1	A	203	ARG	2.1
1	A	721	GLN	2.1
1	A	788	GLY	2.1
2	B	178	GLY	2.1
1	D	363	PRO	2.1
1	D	784	SER	2.0
1	A	753	ALA	2.0
1	D	403	ALA	2.0
1	A	657	GLY	2.0
1	A	730	VAL	2.0
1	A	408	SER	2.0
1	D	725	ASN	2.0
1	D	787	GLN	2.0
2	B	204	LEU	2.0
4	E	284	LEU	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](#)

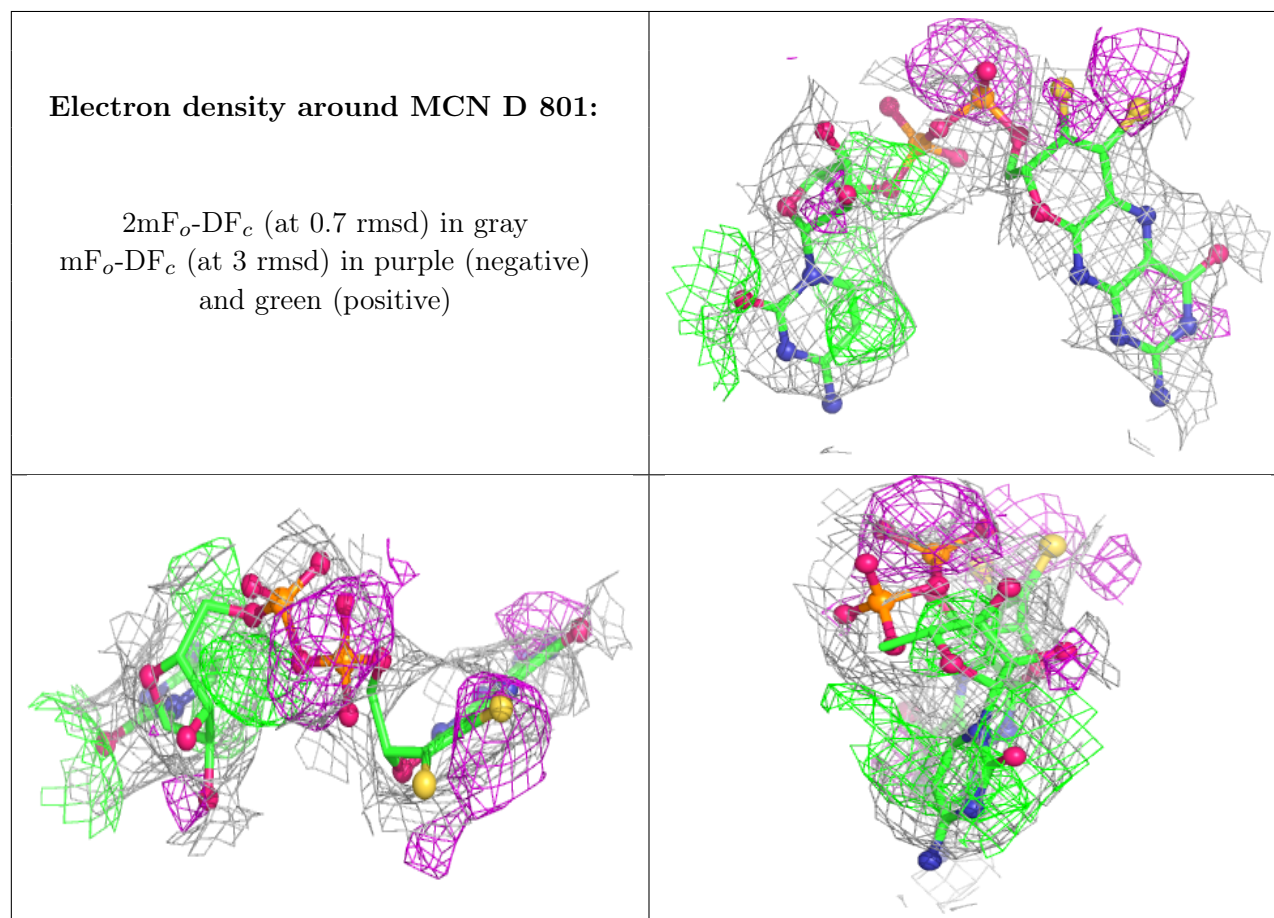
There are no oligosaccharides in this entry.

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.

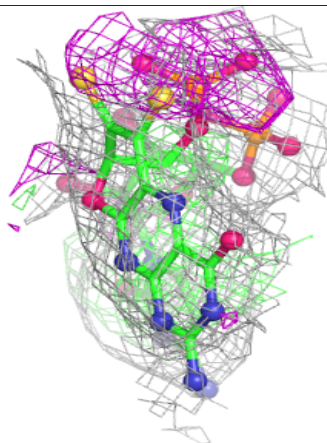
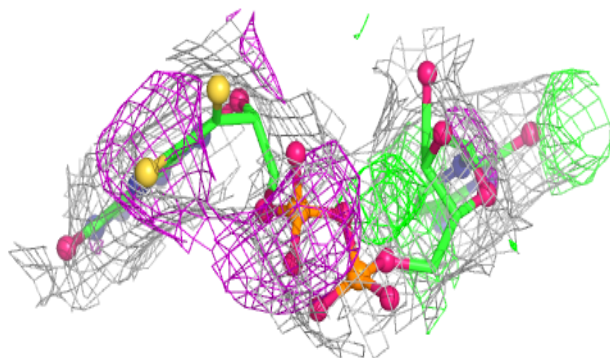
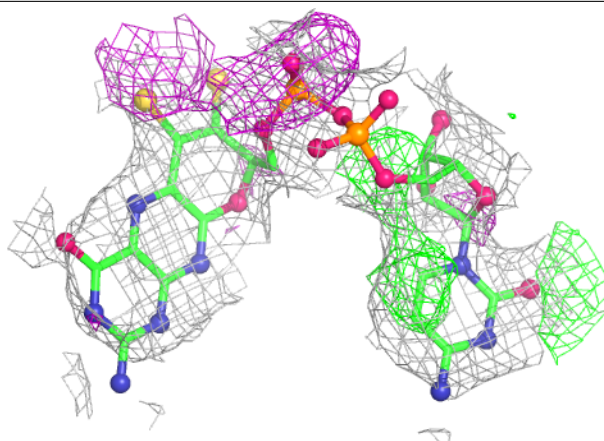
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MCN	D	801	44/44	0.68	0.21	54,74,89,93	0
5	MCN	A	801	44/44	0.73	0.18	53,69,82,87	0
6	MO	D	802	1/1	0.76	0.21	105,105,105,105	0
6	MO	A	802	1/1	0.88	0.19	96,96,96,96	0
8	FES	F	202	4/4	0.89	0.13	46,48,50,51	0
7	FAD	E	301	53/53	0.90	0.13	50,57,63,64	0
7	FAD	B	301	53/53	0.91	0.12	57,60,70,71	0
8	FES	C	201	4/4	0.92	0.10	64,64,65,66	0
8	FES	C	202	4/4	0.95	0.08	43,47,47,49	0
8	FES	F	201	4/4	0.96	0.07	54,55,57,58	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.

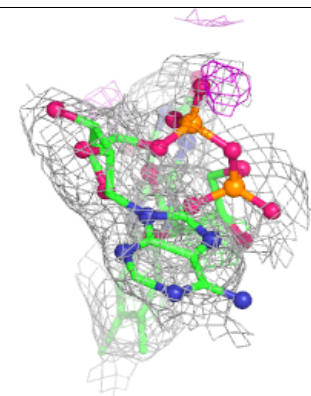
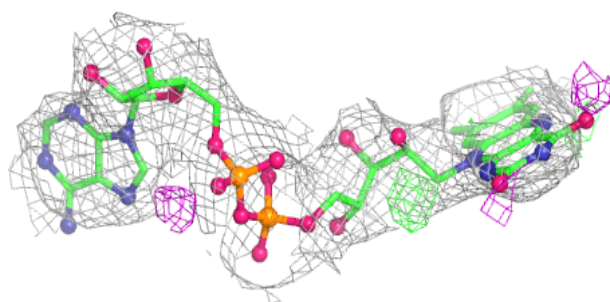
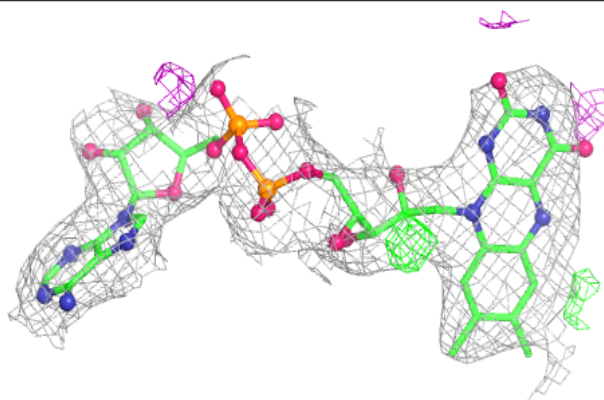


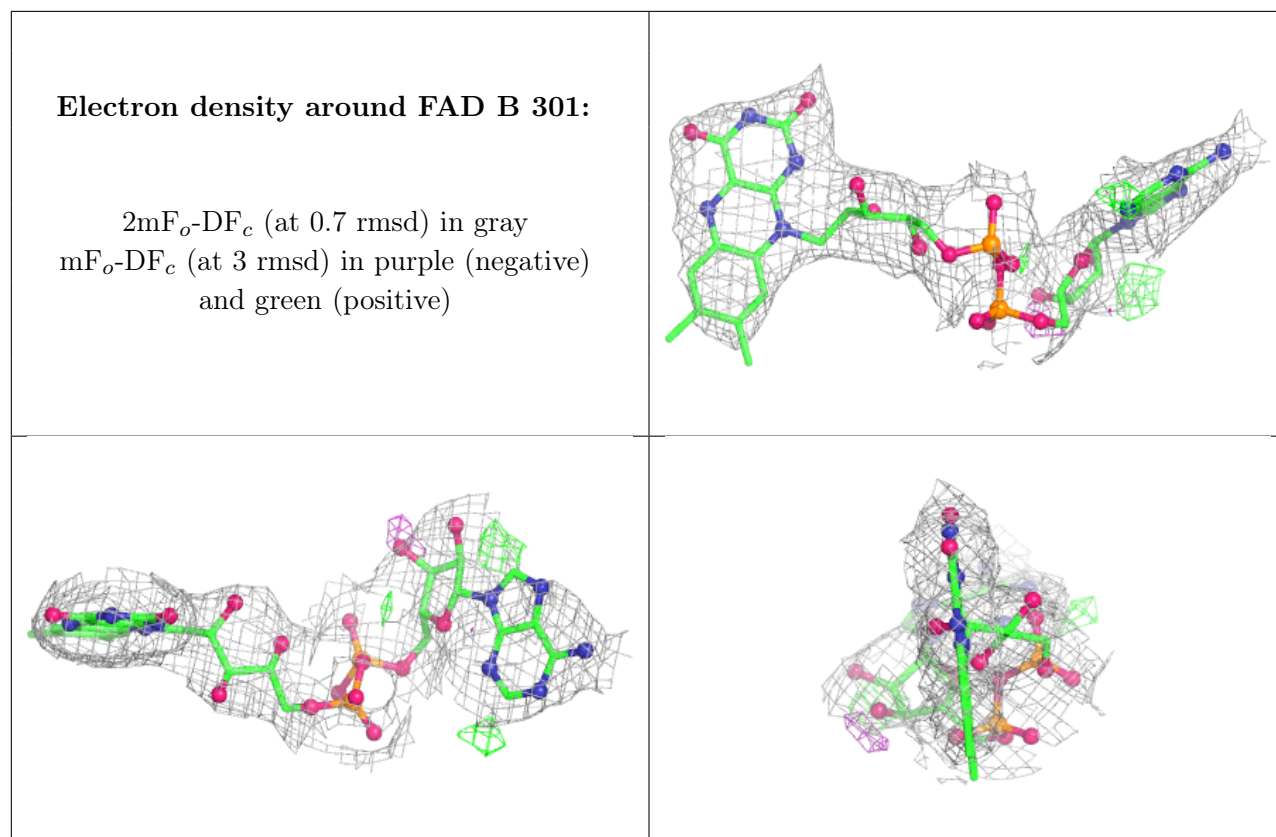
Electron density around MCN A 801:

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

**Electron density around FAD E 301:**

$2mF_o-DF_c$ (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.