Full wwPDB X-ray Structure Validation Report ⓘ

Jan 18, 2022 – 02:10 PM JST

PDB ID	:	7DQX
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 following versions of software and data (see references ⓘ) were used in the production of this report:

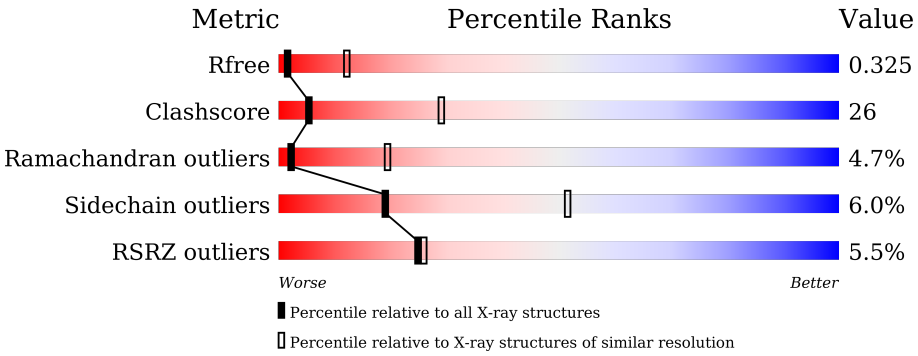
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.25
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.25

1 Overall quality at a glance (i)

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}	130704	1278 (3.50-3.38)
Clashscore	141614	1361 (3.50-3.38)
Ramachandran outliers	138981	1327 (3.50-3.38)
Sidechain outliers	138945	1328 (3.50-3.38)
RSRZ outliers	127900	1192 (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 <=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	6% 55% 34% 6%
1	D	794	7% 54% 36% 6%
2	B	296	4% 65% 27%
3	C	160	4% 68% 29%
3	F	160	3% 72% 24%
4	E	296	3% 69% 23% 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 (i)

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

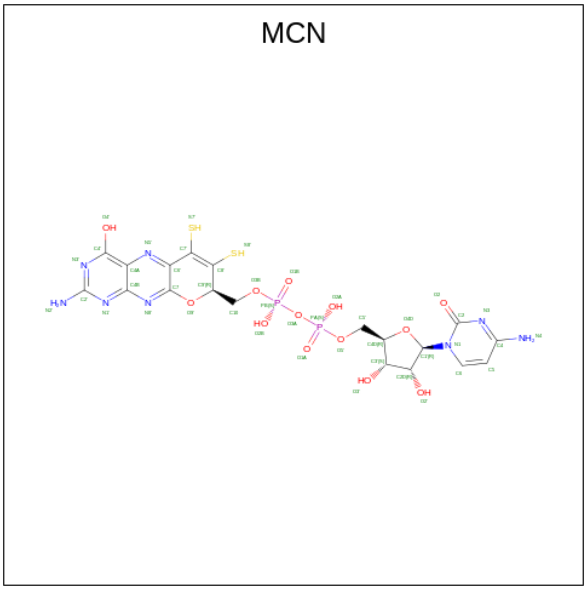
- Molecule 4 is a protein called 6-hydroxypseudooxynicotine dehydrogenase complex subunit alpha.

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 (three-letter code: MCN) (formula: $C_{19}H_{22}N_8O_{13}P_2S_2$).

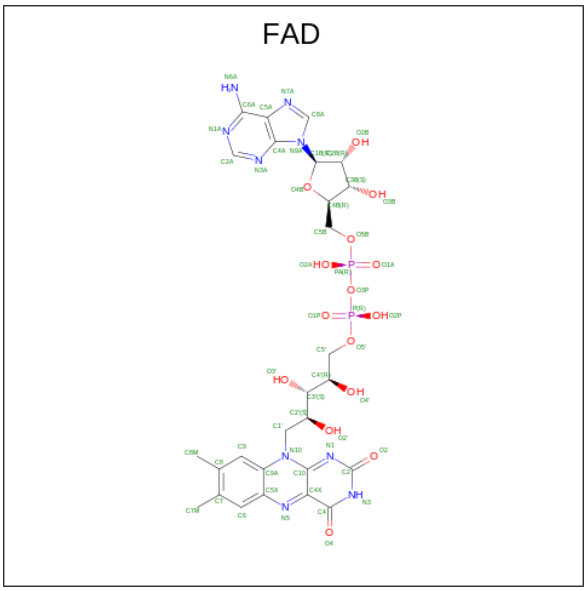


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			44	19	8	13	2	2		
5	D	1	Total	C	N	O	P	S	0	0
			44	19	8	13	2	2		

- Molecule 6 is MOLYBDENUM ATOM (three-letter code: MO) (formula: Mo).

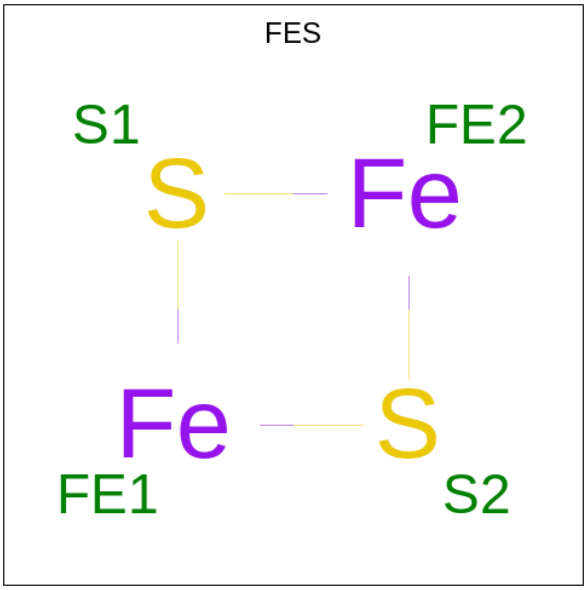
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mo	0	0
			1	1		
6	D	1	Total	Mo	0	0
			1	1		

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



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

- Molecule 8 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

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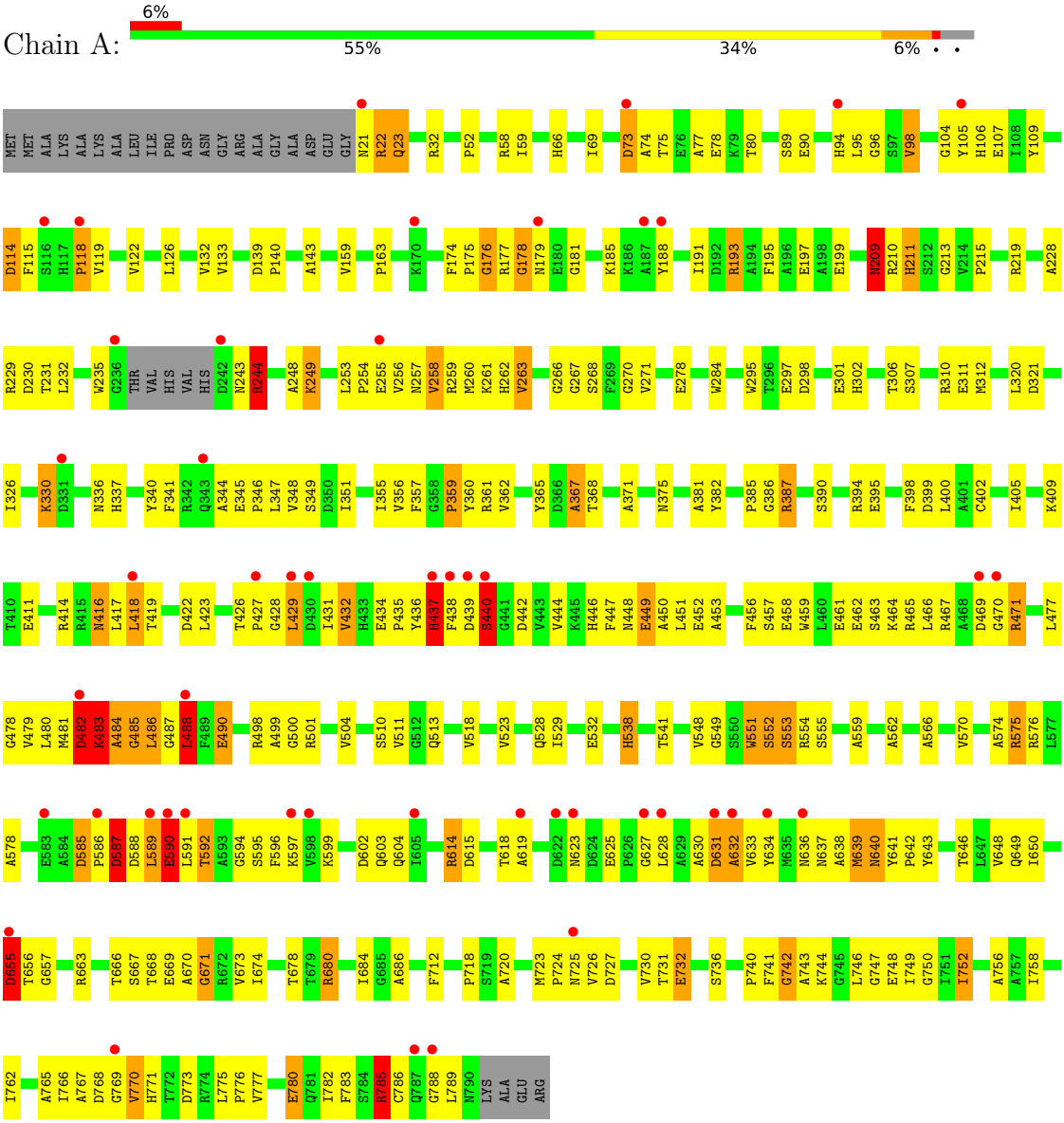
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	F	1	Total Fe S 4 2 2	0	0
8	F	1	Total Fe S 4 2 2	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

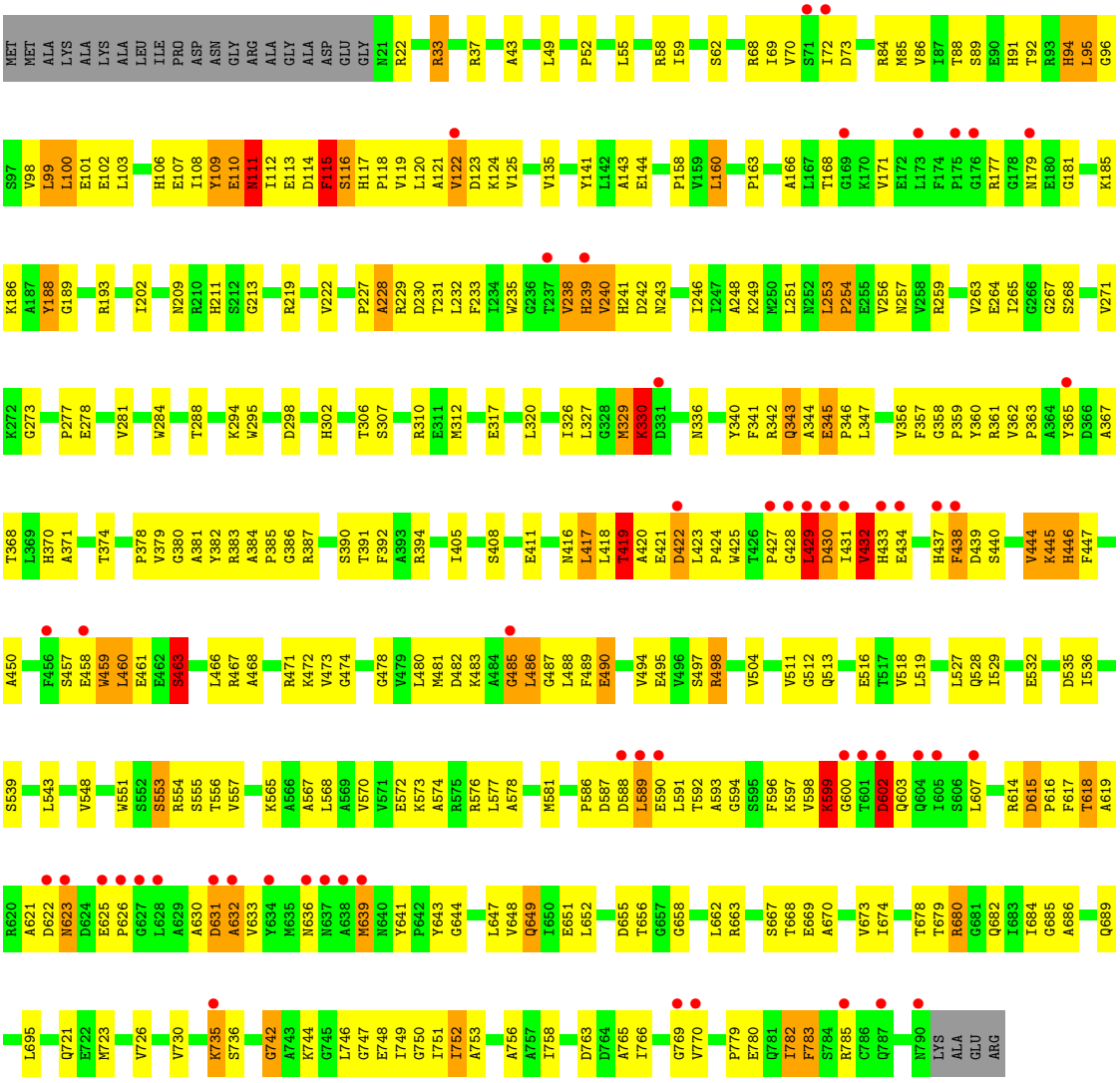
• Molecule 1: 6-hydroxypseudooxynicotine dehydrogenase complex subunit gamma

Chain A:



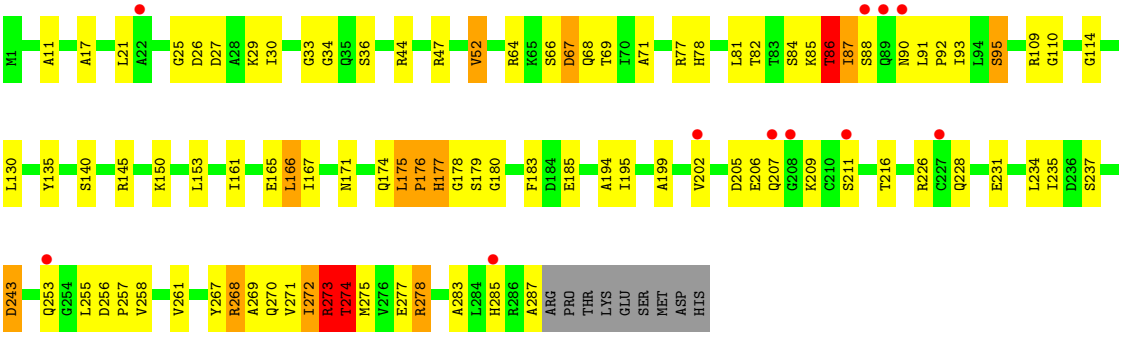
• Molecule 1: 6-hydroxypseudooxynicotine dehydrogenase complex subunit gamma

Chain D:



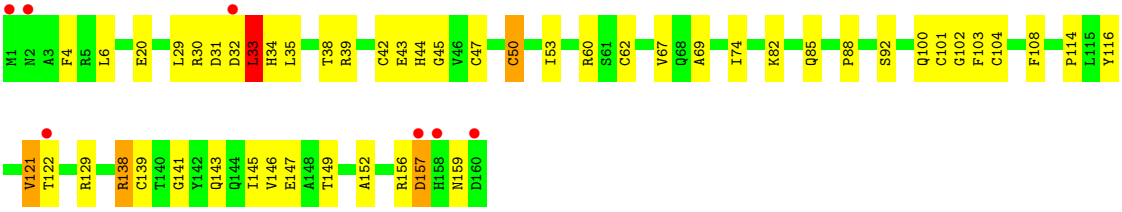
• Molecule 2: 6-hydroxypseudooxynicotine dehydrogenase complex subunit alpha

Chain B:

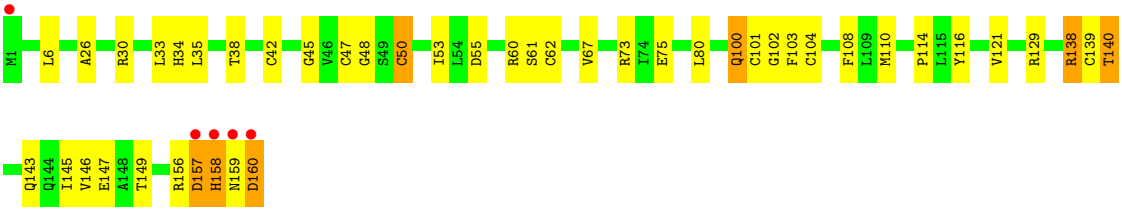


• Molecule 3: 6-hydroxypseudooxynicotine dehydrogenase complex subunit beta

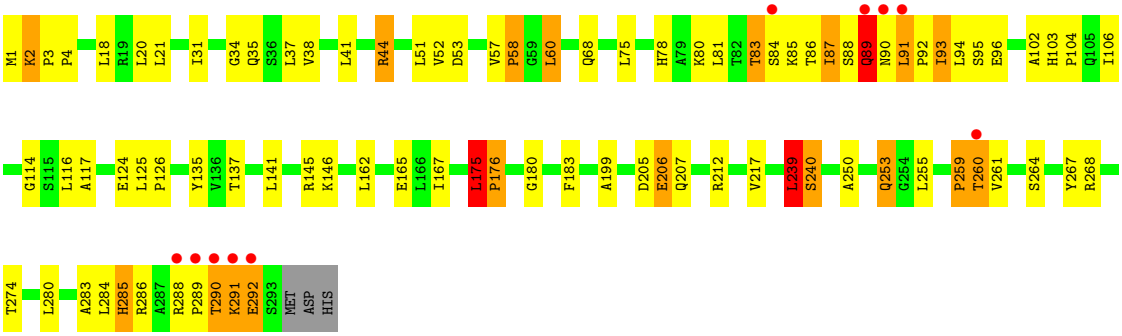
Chain C:



• Molecule 3: 6-hydroxypseudooxynicotine dehydrogenase complex subunit beta



• Molecule 4: 6-hydroxypseudooxynicotine dehydrogenase complex subunit alpha



4 Data and refinement statistics (i)

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 49.08 – 3.44	Depositor EDS
% Data completeness (in resolution range)	93.7 (147.24-3.44) 93.8 (49.08-3.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.08%)	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 , 27.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, FAD, MO, MCN

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	0.43	1/5947 (0.0%)	0.68	3/8084 (0.0%)
1	D	0.43	0/5986	0.69	3/8142 (0.0%)
2	B	0.40	0/2170	0.66	4/2950 (0.1%)
3	C	0.37	0/1247	0.58	2/1689 (0.1%)
3	F	0.40	0/1247	0.58	1/1689 (0.1%)
4	E	0.41	0/2211	0.61	0/3006
All	All	0.42	1/18808 (0.0%)	0.66	13/25560 (0.1%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	TRP	CD2-CE2	5.06	1.47	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	73	ASP	CB-CG-OD2	10.91	128.12	118.30
2	B	175	LEU	C-N-CD	-8.75	101.35	120.60
1	D	73	ASP	OD1-CG-OD2	-7.39	109.26	123.30
2	B	175	LEU	CA-CB-CG	6.77	130.86	115.30
1	D	115	PHE	N-CA-C	5.84	126.78	111.00
2	B	273	ARG	N-CA-C	5.83	126.75	111.00
3	C	33	LEU	CA-CB-CG	5.75	128.53	115.30
3	C	34	HIS	N-CA-C	-5.73	95.52	111.00
1	A	488	LEU	CA-CB-CG	5.42	127.76	115.30
1	A	73	ASP	CB-CG-OD2	5.41	123.17	118.30
3	F	159	ASN	N-CA-CB	5.29	120.11	110.60
2	B	274	THR	N-CA-C	-5.15	97.09	111.00
1	A	104	GLY	N-CA-C	-5.14	100.24	113.10

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
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

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Mol	Chain	Res	Type	Group
3	F	158	HIS	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	5831	0	5717	353	0
1	D	5867	0	5754	392	0
2	B	2135	0	2188	94	0
3	C	1229	0	1187	43	0
3	F	1229	0	1187	43	0
4	E	2175	0	2219	79	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	12	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	971	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 26.

All (971) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:484:ALA:C	1:A:486:LEU:HG	1.99	0.82
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
4:E:124:GLU:H	7:E:301:FAD:HM71	1.52	0.74
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
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
3:F:100:GLN:HG3	3:F:139:CYS:HB3	1.71	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
1:A:418:LEU:HG	1:A:419:THR:N	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:B:274:THR:HA	2:B:277:GLU:HB2	1.74	0.69
4:E:289:PRO:HA	4:E:290:THR:C	2.12	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
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:420:ALA:HA	1:D:421:GLU:C	2.14	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:89:SER:HB2	1:D:120:LEU:O	1.95	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:209:ASN:HD21	1:A:775:LEU:C	1.98	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
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
1:D:518:VAL:HG11	1:D:556:THR:HG22	1.77	0.66
1:A:470:GLY:C	1:A:471:ARG:HG2	2.15	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:A:724:PRO:C	1:A:726:VAL:H	2.00	0.65
1:D:599:LYS:CG	1:D:600:GLY:N	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:A:485:GLY:C	1:A:487:GLY:HA3	2.18	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
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:A:439:ASP:CA	1:A:440:SER:CB	2.62	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:585:ASP:HB2	1:A:586:PRO:C	2.20	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:D:227:PRO:C	1:D:229:ARG:H	2.03	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
2:B:130:LEU:CD2	2:B:226:ARG:HG2	2.32	0.60
1:D:227:PRO:C	1:D:229:ARG:N	2.55	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:360:TYR:CE1	1:A:398:PHE:HE2	2.23	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
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:A:487:GLY:HA2	1:A:488:LEU:C	2.24	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
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: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
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:483:LYS:HZ3	1:A:641:TYR:HA	1.72	0.55
1:A:575:ARG:CZ	1:A:596:PHE:HB2	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:488:LEU:HD13	1:D:636:ASN:CG	2.28	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
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: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: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:209:ASN:ND2	1:A:775:LEU:C	2.62	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:D:622:ASP:CG	1:D:623:ASN:H	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:724:PRO:C	1:A:726:VAL:N	2.61	0.53
4:E:88:SER:O	4:E:89:GLN:HG2	2.09	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: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
1:A:483:LYS:O	1:A:486:LEU:HD12	2.08	0.52
1:D:342:ARG:C	1:D:344:ALA:N	2.62	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: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: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
3:F:55:ASP:C	3:F:73:ARG:HH21	2.13	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
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:312:MET:HE3	1:A:386:GLY:HA2	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:527:LEU:HD22	1:D:607:LEU:HD21	1.91	0.51
1:A:95:LEU:HB3	1:A:96:GLY:C	2.30	0.51
1:A:122:VAL:HG12	1:A:122:VAL:O	2.11	0.51
1:A:655:ASP:C	2:B:273:ARG:HH22	2.13	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:111:ASN:CG	1:D:112:ILE:N	2.64	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:649:GLN:HG2	1:D:663:ARG:HB2	1.93	0.51
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
4:E:206:GLU:HA	4:E:207:GLN:C	2.31	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: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
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
2:B:86:THR:HG23	2:B:91:LEU:HD12	1.92	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:588:ASP:CB	1:D:598:VAL:HA	2.17	0.49
1:A:483:LYS:NZ	1:A:641:TYR:CD2	2.79	0.49
1:A:418:LEU:HD22	1:A:447:PHE:H	1.77	0.49
2:B:285:HIS:C	2:B:287:ALA:H	2.13	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:A:551:TRP:O	1:A:552:SER:C	2.50	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: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:A:215:PRO:HD2	1:A:302:HIS:CE1	2.43	0.48
1:A:351:ILE:HG21	1:A:387:ARG:NH2	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:488:LEU:HG	1:A:634:TYR:CD1	2.47	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
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
3:C:50:CYS:HB3	3:C:62:CYS:SG	2.52	0.48
1:D:116:SER:C	1:D:118:PRO:HA	2.33	0.48
1:D:163:PRO:HG3	1:D:336:ASN:HB2	1.96	0.48
1:D:273:GLY:C	1:D:342:ARG:HH22	2.16	0.48
1:D:357:PHE:HB2	1:D:362:VAL:HG21	1.94	0.48
1:D:430:ASP:HB2	1:D:431:ILE:C	2.32	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: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:D:219:ARG:HH12	1:D:278:GLU:CD	2.16	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
4:E:124:GLU:CD	7:E:301:FAD:HM72	2.34	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:113:GLU:HB2	1:D:114:ASP:C	2.35	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:448:ASN:C	1:A:450:ALA:N	2.66	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: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
2:B:211:SER:C	2:B:235:ILE:HD11	2.35	0.47
4:E:90:ASN:HA	4:E:91:LEU:C	2.35	0.47
4:E:124:GLU:N	7:E:301:FAD:HM71	2.27	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:262:HIS:CD2	1:A:538:HIS:CE1	3.03	0.46
1:A:483:LYS:HZ3	1:A:641:TYR:CA	2.28	0.46
2:B:64:ARG:HB3	2:B:71:ALA:HB3	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
1:A:786:CYS:C	1:A:788:GLY:N	2.68	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
3:F:60:ARG:C	3:F:62:CYS:H	2.20	0.45
1:D:231:THR:HG21	1:D:259:ARG:CZ	2.46	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: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:480:LEU:HD21	1:A:748:GLU:HB2	1.98	0.45
1:D:625:GLU:N	1:D:626:PRO:HD2	2.32	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
1:D:341:PHE:HD2	1:D:345:GLU:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:254:PRO:HA	1:A:255:GLU:C	2.37	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
1:A:786:CYS:C	1:A:788:GLY:H	2.20	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:228:ALA:C	1:D:230:ASP:H	2.21	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: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
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
3:C:141:GLY:C	3:C:143:GLN:H	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:92:THR:HA	1:D:94:HIS:CE1	2.52	0.44
1:D:111:ASN:OD1	1:D:112:ILE:N	2.49	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:430:ASP:CG	1:D:432:VAL:HA	2.38	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: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
3:F:110:MET:HA	3:F:110:MET:CE	2.48	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
4:E:205:ASP:O	4:E:206:GLU:C	2.56	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:D:480:LEU:HB3	1:D:482:ASP:CG	2.38	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
4:E:2:LYS:HZ3	4:E:44:ARG:CZ	2.31	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:H3'	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
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: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:D:342:ARG:O	1:D:343:GLN:C	2.57	0.43
1:D:459:TRP:CD1	1:D:459:TRP:C	2.91	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: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
2:B:285:HIS:C	2:B:287:ALA:N	2.73	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:423:LEU:HA	1:D:424:PRO:C	2.39	0.42
2:B:36:SER:HG	7:B:301:FAD:HO2'	1.66	0.42
3:C:129:ARG:HG2	3:C:146:VAL:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:261:LYS:HZ3	1:D:233:PHE:HE2	1.66	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: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:88:SER:C	2:B:90:ASN:H	2.22	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:312:MET:HE3	1:D:386:GLY:HA2	2.02	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:D:622:ASP:CG	1:D:623:ASN:N	2.73	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:268:SER:HB3	1:D:511:VAL:HG11	2.00	0.42
1:D:418:LEU:HD11	1:D:425:TRP:CE3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
4:E:2:LYS:HD3	1:D:144:GLU:CD	2.40	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
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:637:ASN:O	1:A:638:ALA:C	2.57	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: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:A:666:THR:O	1:A:730:VAL:HG22	2.19	0.41
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:431:ILE:HA	1:A:432:VAL:C	2.42	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: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:D:669:GLU:CD	1:D:735:LYS:HZ3	2.25	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
1:D:418:LEU:O	1:D:419:THR:C	2.58	0.41
1:D:459:TRP:HE1	1:D:463:SER:N	2.19	0.41
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:80:LEU:HD11	3:F:110:MET:CE	2.51	0.40
1:D:59:ILE:HD12	1:D:278:GLU:HG3	2.03	0.40
1:D:434:GLU:O	1:D:481:MET:HE1	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:484:ALA:O	1:A:485:GLY:C	2.59	0.40
4:E:96:GLU:OE2	4:E:183:PHE:N	2.54	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:105:TYR:C	1:A:107:GLU:H	2.24	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
1:D:277:PRO:O	1:D:281:VAL:HG23	2.21	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
3:C:33:LEU:C	3:C:35:LEU:N	2.75	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:229:ARG:HH22	1:D:253:LEU:CB	2.35	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	761/794 (96%)	612 (80%)	101 (13%)	48 (6%)	1 13
1	D	768/794 (97%)	616 (80%)	113 (15%)	39 (5%)	2 17
2	B	285/296 (96%)	250 (88%)	26 (9%)	9 (3%)	4 28
3	C	158/160 (99%)	129 (82%)	26 (16%)	3 (2%)	8 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	F	158/160 (99%)	135 (85%)	21 (13%)	2 (1%)	12 46
4	E	291/296 (98%)	251 (86%)	27 (9%)	13 (4%)	2 20
All	All	2421/2500 (97%)	1993 (82%)	314 (13%)	114 (5%)	2 19

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	563 (94%)	39 (6%)	17	49
1	D	607/632 (96%)	569 (94%)	38 (6%)	18	50
2	B	225/234 (96%)	211 (94%)	14 (6%)	18	51
3	C	138/138 (100%)	133 (96%)	5 (4%)	35	66
3	F	138/138 (100%)	130 (94%)	8 (6%)	20	52
4	E	228/234 (97%)	216 (95%)	12 (5%)	22	55
All	All	1938/2008 (96%)	1822 (94%)	116 (6%)	19	51

All (116) 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	193	ARG
1	A	209	ASN
1	A	211	HIS
1	A	244	ARG
1	A	249	LYS
1	A	263	VAL
1	A	337	HIS
1	A	387	ARG
1	A	416	ASN
1	A	432	VAL
1	A	437	HIS
1	A	440	SER
1	A	449	GLU
1	A	469	ASP
1	A	471	ARG
1	A	483	LYS
1	A	488	LEU
1	A	490	GLU
1	A	529	ILE

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Mol	Chain	Res	Type
1	A	538	HIS
1	A	551	TRP
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	680	ARG
1	A	727	ASP
1	A	732	GLU
1	A	773	ASP
1	A	780	GLU
1	A	785	ARG
2	B	21	LEU
2	B	52	VAL
2	B	67	ASP
2	B	86	THR
2	B	87	ILE
2	B	95	SER
2	B	150	LYS
2	B	166	LEU
2	B	243	ASP
2	B	256	ASP
2	B	261	VAL
2	B	268	ARG
2	B	273	ARG
2	B	278	ARG
3	C	6	LEU
3	C	20	GLU
3	C	121	VAL
3	C	138	ARG
3	C	157	ASP
4	E	2	LYS
4	E	20	LEU
4	E	44	ARG
4	E	60	LEU
4	E	68	GLN
4	E	83	THR

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Mol	Chain	Res	Type
4	E	89	GLN
4	E	175	LEU
4	E	239	LEU
4	E	253	GLN
4	E	260	THR
4	E	261	VAL
3	F	100	GLN
3	F	103	PHE
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
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	188	TYR
1	D	193	ARG
1	D	240	VAL
1	D	242	ASP
1	D	329	MET
1	D	419	THR
1	D	429	LEU
1	D	432	VAL
1	D	438	PHE
1	D	444	VAL
1	D	446	HIS
1	D	459	TRP
1	D	463	SER
1	D	486	LEU
1	D	490	GLU
1	D	498	ARG
1	D	535	ASP
1	D	589	LEU

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Mol	Chain	Res	Type
1	D	599	LYS
1	D	602	ASP
1	D	623	ASN
1	D	639	MET
1	D	649	GLN
1	D	680	ARG
1	D	721	GLN
1	D	735	LYS
1	D	752	ILE
1	D	783	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	54	GLN
1	A	56	HIS
1	A	66	HIS
1	A	91	HIS
1	A	94	HIS
1	A	209	ASN
1	A	279	ASN
1	A	302	HIS
1	A	335	HIS
1	A	375	ASN
1	A	649	GLN
1	A	771	HIS
2	B	90	ASN
2	B	262	HIS
3	C	97	HIS
3	C	154	HIS
4	E	118	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

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
8	FES	C	202	3	0,4,4	-	-	-		
8	FES	F	201	3	0,4,4	-	-	-		
5	MCN	D	801	6	38,48,48	1.33	3 (7%)	40,74,74	1.91	9 (22%)
8	FES	C	201	3	0,4,4	-	-	-		
7	FAD	B	301	-	51,58,58	1.98	8 (15%)	60,89,89	2.09	11 (18%)
5	MCN	A	801	6	38,48,48	1.34	2 (5%)	40,74,74	1.79	9 (22%)
7	FAD	E	301	-	51,58,58	1.97	6 (11%)	60,89,89	1.94	12 (20%)
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
8	FES	C	202	3	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	FES	F	201	3	-	-	0/1/1/1
5	MCN	D	801	6	-	13/20/54/54	0/5/5/5
8	FES	C	201	3	-	-	0/1/1/1
7	FAD	B	301	-	-	19/30/50/50	0/6/6/6
5	MCN	A	801	6	-	11/20/54/54	0/5/5/5
7	FAD	E	301	-	-	12/30/50/50	0/6/6/6
8	FES	F	202	3	-	-	0/1/1/1

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	301	FAD	C4X-C10	10.47	1.49	1.38
7	E	301	FAD	C4X-C10	10.19	1.49	1.38
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	B	301	FAD	C4X-C4	4.47	1.49	1.41
7	E	301	FAD	C4X-C4	4.34	1.48	1.41
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	C9A-C5X	3.75	1.50	1.42
7	B	301	FAD	C9A-C5X	3.71	1.50	1.42
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	C9A-N10	2.68	1.42	1.38
7	E	301	FAD	C5A-C4A	2.59	1.47	1.40
7	B	301	FAD	C9A-N10	2.50	1.41	1.38
7	B	301	FAD	C5A-C4A	2.42	1.47	1.40
7	B	301	FAD	C10-N1	2.18	1.36	1.33
5	D	801	MCN	C7-N8'	2.04	1.35	1.30
7	B	301	FAD	C2A-N3A	2.03	1.35	1.32

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	301	FAD	C2-N3-C4	8.10	121.98	115.14
7	E	301	FAD	C2-N3-C4	8.10	121.98	115.14
7	B	301	FAD	C1'-N10-C10	7.37	125.01	118.41
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	B	301	FAD	P-O3P-PA	-4.40	117.72	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	801	MCN	PB-O3A-PA	-4.25	118.23	132.83
7	E	301	FAD	C1'-N10-C9A	4.21	121.60	118.29
7	B	301	FAD	C4X-N5-C5X	4.20	120.97	116.77
7	B	301	FAD	C10-C4X-C4	-4.07	117.26	119.95
7	E	301	FAD	C10-C4X-C4	-4.05	117.27	119.95
5	D	801	MCN	O9'-C7-N8'	3.99	120.25	115.30
7	E	301	FAD	C4X-N5-C5X	3.88	120.65	116.77
5	D	801	MCN	C4-N3-C2	3.80	120.19	116.34
5	A	801	MCN	O9'-C7-N8'	3.72	119.92	115.30
5	A	801	MCN	C4-N3-C2	3.69	120.08	116.34
7	E	301	FAD	P-O3P-PA	-3.66	120.26	132.83
7	E	301	FAD	C4X-C4-N3	-3.65	118.45	123.43
7	B	301	FAD	N3A-C2A-N1A	-3.58	123.08	128.68
7	E	301	FAD	N3A-C2A-N1A	-3.52	123.17	128.68
7	B	301	FAD	C4X-C4-N3	-3.52	118.62	123.43
5	D	801	MCN	N1'-C2'-N3'	-3.28	122.85	127.22
7	B	301	FAD	C9A-N10-C10	-3.12	117.83	121.91
5	A	801	MCN	N1'-C2'-N3'	-3.04	123.17	127.22
7	B	301	FAD	C5X-C9A-N10	3.02	119.90	117.72
7	E	301	FAD	C9A-N10-C10	-3.00	117.98	121.91
7	E	301	FAD	C3B-C2B-C1B	2.99	105.48	100.98
5	A	801	MCN	C3'-C2D-C1'	2.85	105.27	100.98
7	E	301	FAD	C4A-C5A-N7A	-2.68	106.61	109.40
5	A	801	MCN	N4-C4-N3	2.51	120.45	116.49
5	D	801	MCN	N4-C4-N3	2.49	120.43	116.49
7	E	301	FAD	C4-C4X-N5	2.43	121.37	118.60
5	D	801	MCN	N1'-C4B-N8'	2.42	121.70	115.97
7	B	301	FAD	C4-C4X-N5	2.34	121.28	118.60
5	D	801	MCN	C3'-C2D-C1'	2.33	104.49	100.98
5	D	801	MCN	C7-N8'-C4B	2.27	118.54	116.61
7	E	301	FAD	C1'-N10-C10	2.23	120.41	118.41
5	A	801	MCN	N1'-C4B-N8'	2.14	121.05	115.97
5	A	801	MCN	C7-N8'-C4B	2.01	118.33	116.61
7	B	301	FAD	C5'-C4'-C3'	-2.01	108.32	112.20

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	801	MCN	C2D-C1'-N1-C6
5	A	801	MCN	O4D-C1'-N1-C6
5	A	801	MCN	O4D-C4D-C5'-O5'

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Mol	Chain	Res	Type	Atoms
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	C2D-C1'-N1-C6
5	D	801	MCN	O4D-C1'-N1-C6
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
5	A	801	MCN	C3'-C4D-C5'-O5'
5	D	801	MCN	C3'-C4D-C5'-O5'
7	E	301	FAD	O4B-C4B-C5B-O5B
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	A	801	MCN	C5'-O5'-PA-O3A
7	B	301	FAD	O4B-C4B-C5B-O5B
5	A	801	MCN	C5'-O5'-PA-O2A

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Mol	Chain	Res	Type	Atoms
5	D	801	MCN	C10-O3B-PB-O1B
7	B	301	FAD	C5'-O5'-P-O2P
7	E	301	FAD	N10-C1'-C2'-O2'
7	E	301	FAD	C2'-C3'-C4'-O4'
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

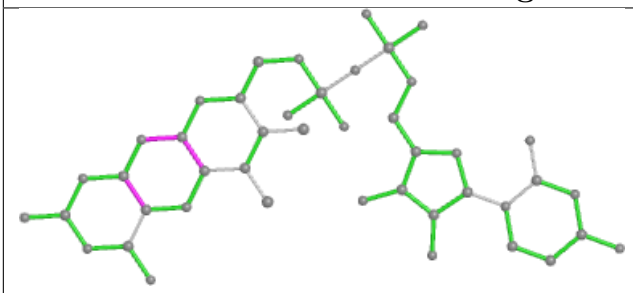
There are no ring outliers.

8 monomers are involved in 62 short contacts:

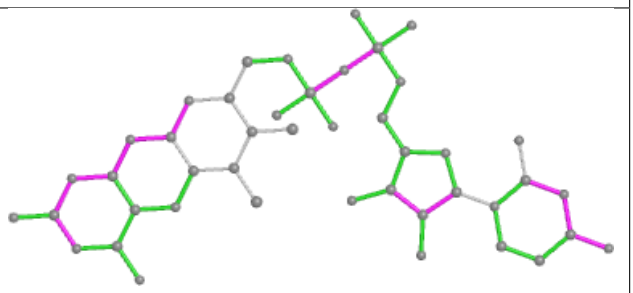
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	202	FES	3	0
8	F	201	FES	3	0
5	D	801	MCN	15	0
8	C	201	FES	3	0
7	B	301	FAD	12	0
5	A	801	MCN	14	0
7	E	301	FAD	9	0
8	F	202	FES	3	0

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 then 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.

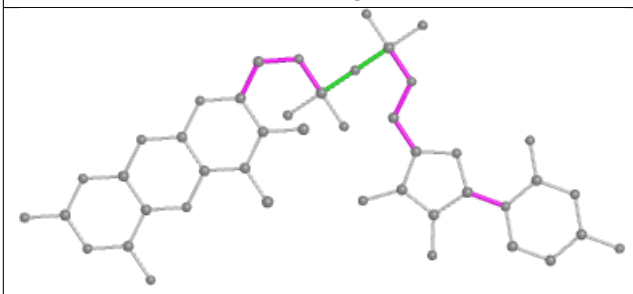
Ligand MCN D 801



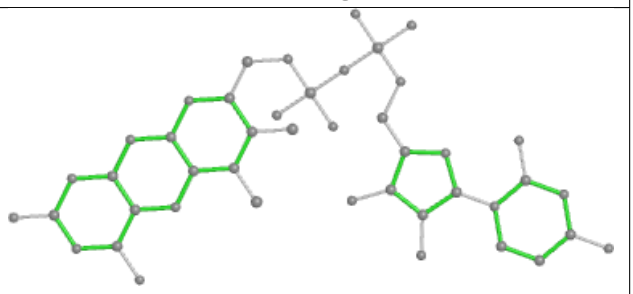
Bond lengths



Bond angles

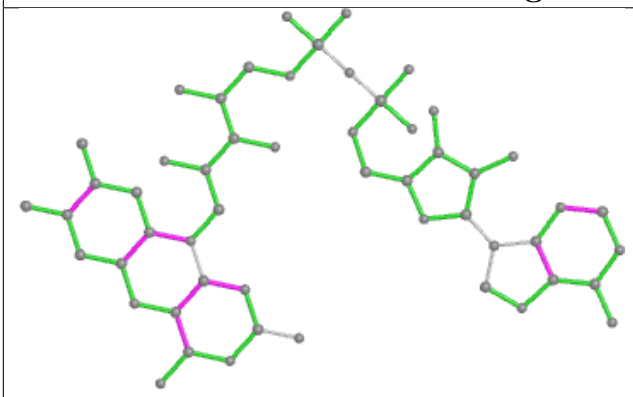


Torsions

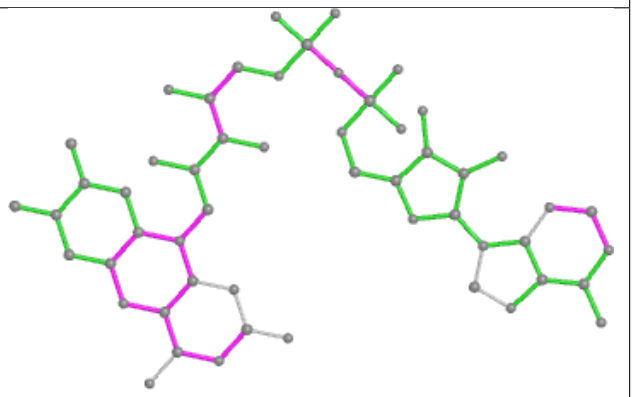


Rings

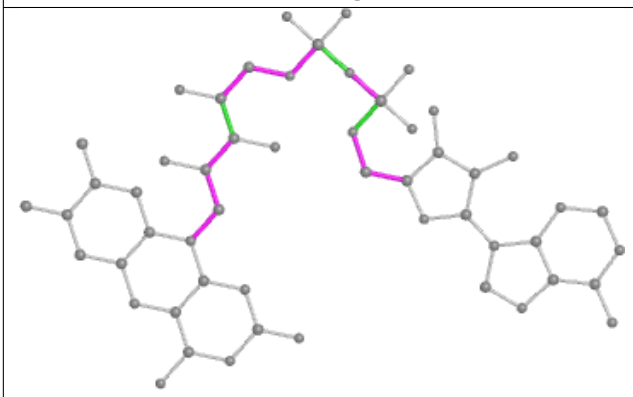
Ligand FAD B 301



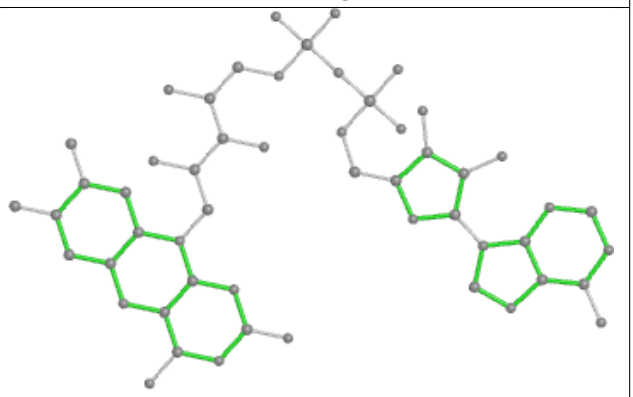
Bond lengths



Bond angles

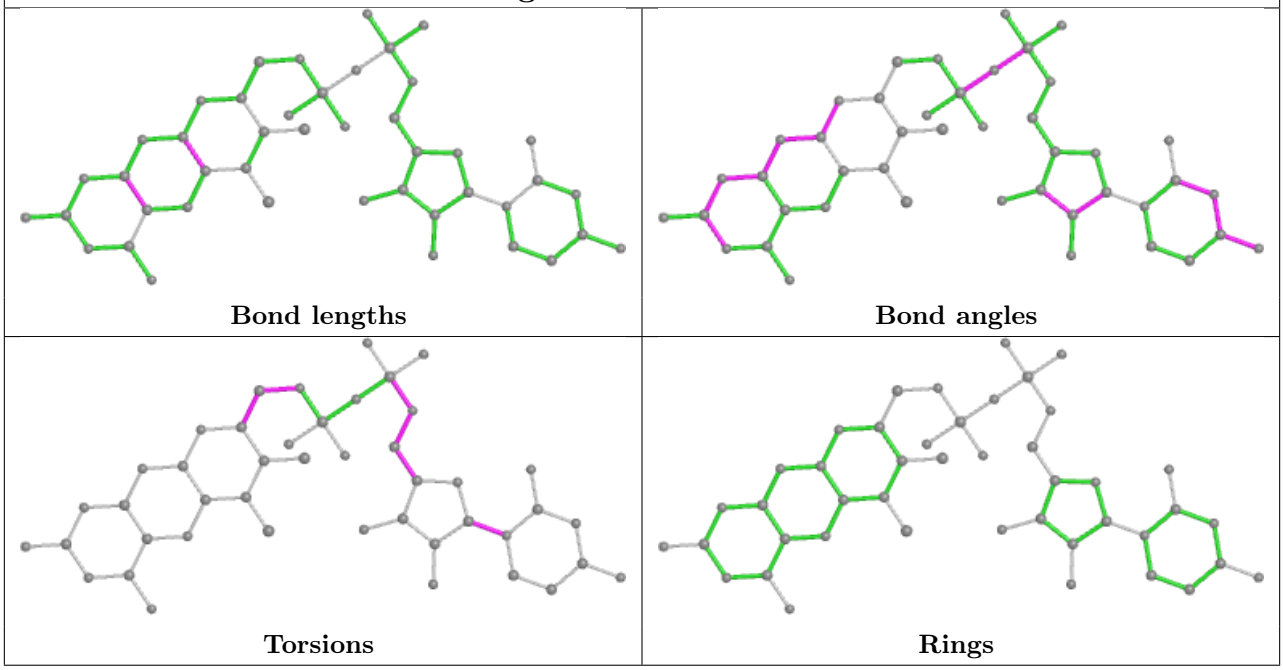


Torsions

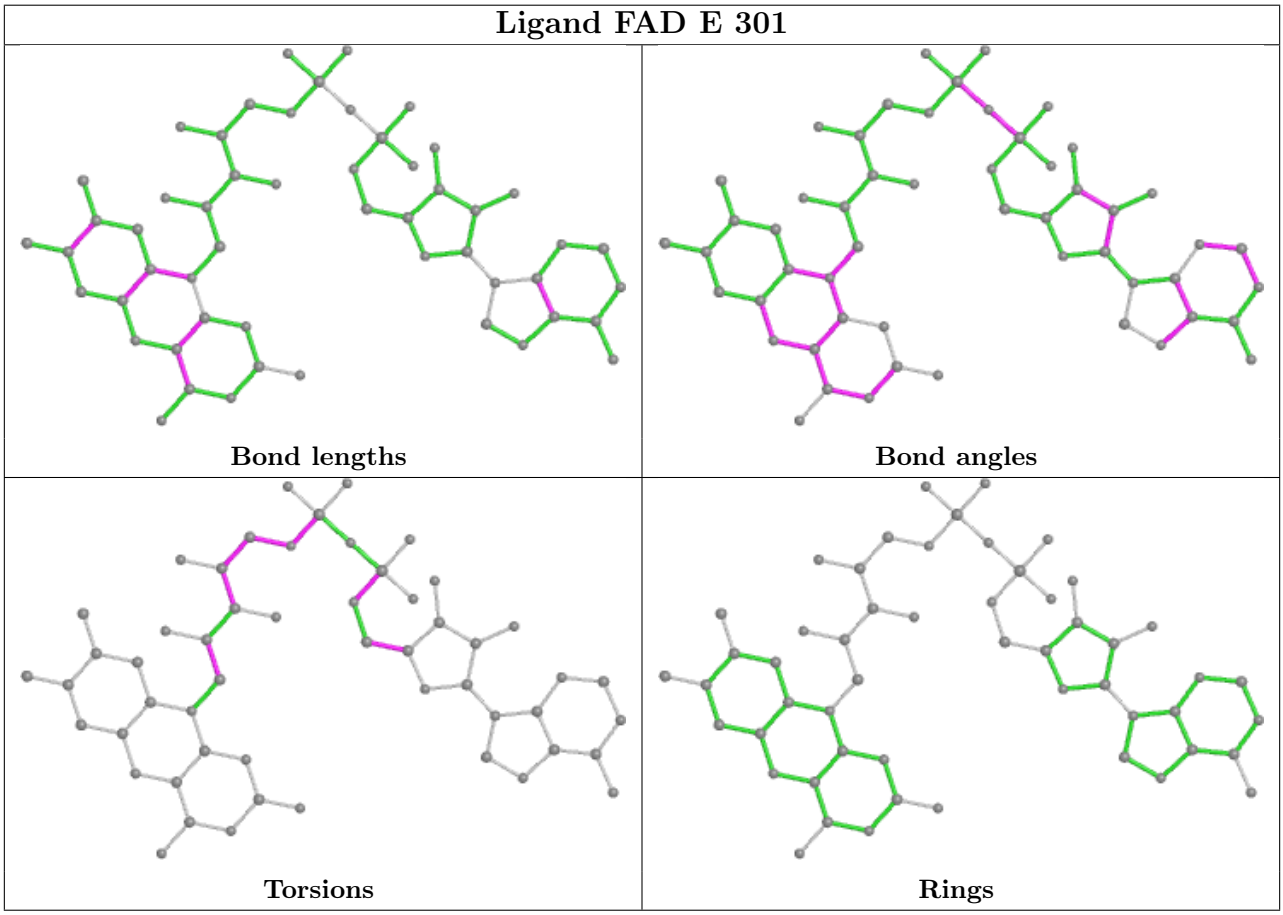


Rings

Ligand MCN A 801



Ligand FAD E 301



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, 95^{th} 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%)	0.38	49 (6%)	19	21	38, 60, 104, 150	1 (0%)
1	D	770/794 (96%)	0.47	53 (6%)	16	19	43, 64, 107, 148	1 (0%)
2	B	287/296 (96%)	0.28	11 (3%)	40	39	51, 71, 102, 116	0
3	C	160/160 (100%)	0.31	7 (4%)	34	33	38, 58, 89, 124	0
3	F	160/160 (100%)	0.25	5 (3%)	49	48	46, 56, 92, 137	0
4	E	293/296 (98%)	0.18	10 (3%)	45	44	43, 66, 92, 145	0
All	All	2435/2500 (97%)	0.36	135 (5%)	25	26	38, 63, 103, 150	2 (0%)

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	430	ASP	9.3
2	B	88	SER	8.4
4	E	289	PRO	6.3
1	D	428	GLY	6.3
1	A	627	GLY	6.1
1	A	439	ASP	6.1
1	D	179	ASN	5.8
1	A	628	LEU	5.6
1	D	438	PHE	5.1
1	D	627	GLY	5.1
1	A	73	ASP	4.7
1	D	769	GLY	4.6
1	A	589	LEU	4.5
4	E	290	THR	4.5
3	C	158	HIS	4.5
3	F	158	HIS	4.3
2	B	208	GLY	4.3
1	A	438	PHE	4.2
3	F	1	MET	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	591	LEU	4.1
1	D	601	THR	4.1
1	D	638	ALA	4.0
2	B	89	GLN	4.0
1	A	598	VAL	4.0
1	D	632	ALA	3.9
1	D	429	LEU	3.9
1	D	634	TYR	3.7
3	C	1	MET	3.7
1	D	636	ASN	3.7
1	A	631	ASP	3.5
1	D	625	GLU	3.5
1	D	589	LEU	3.5
2	B	227	CYS	3.4
2	B	207	GLN	3.4
1	A	179	ASN	3.4
1	D	72	ILE	3.3
1	A	430	ASP	3.3
1	A	725	ASN	3.3
1	A	482	ASP	3.3
1	D	433	HIS	3.2
1	A	590	GLU	3.2
1	D	485	GLY	3.2
1	A	619	ALA	3.2
1	A	343	GLN	3.1
1	D	427	PRO	3.1
1	A	255	GLU	3.1
1	D	431	ILE	3.1
3	F	159	ASN	3.1
1	D	602	ASP	3.1
1	D	600	GLY	3.0
1	D	628	LEU	3.0
1	D	588	ASP	3.0
1	A	236	GLY	3.0
3	C	160	ASP	3.0
1	D	735	LYS	3.0
1	A	187	ALA	2.9
2	B	202	VAL	2.9
1	A	655	ASP	2.9
3	C	2	ASN	2.9
4	E	292	GLU	2.9
1	D	71	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	105	TYR	2.9
1	A	634	TYR	2.9
1	D	590	GLU	2.9
4	E	288	ARG	2.9
3	F	157	ASP	2.9
1	A	605	ILE	2.8
1	A	440	SER	2.8
1	D	175	PRO	2.8
1	D	437	HIS	2.8
1	D	604	GLN	2.7
1	D	770	VAL	2.7
3	C	122	THR	2.7
1	A	636	ASN	2.7
3	F	160	ASP	2.7
1	A	437	HIS	2.7
1	A	170	LYS	2.6
1	A	632	ALA	2.6
1	A	788	GLY	2.6
4	E	89	GLN	2.6
1	A	623	ASN	2.6
1	D	169	GLY	2.5
1	A	586	PRO	2.5
1	D	626	PRO	2.5
1	D	623	ASN	2.5
4	E	91	LEU	2.5
1	D	237	THR	2.5
1	D	434	GLU	2.5
1	A	787	GLN	2.5
1	D	176	GLY	2.5
2	B	211	SER	2.5
1	D	790	ASN	2.4
1	A	469	ASP	2.4
1	D	331	ASP	2.4
1	D	422	ASP	2.4
1	D	122	VAL	2.4
1	D	239	HIS	2.4
3	C	157	ASP	2.4
1	D	605	ILE	2.4
1	D	785	ARG	2.4
4	E	84	SER	2.4
1	A	94	HIS	2.4
1	D	787	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	331	ASP	2.3
1	D	365	TYR	2.3
1	A	116	SER	2.3
1	A	583	GLU	2.3
1	A	769	GLY	2.2
1	D	458	GLU	2.2
1	D	622	ASP	2.2
1	A	188	TYR	2.2
1	D	631	ASP	2.2
1	D	637	ASN	2.2
2	B	22	ALA	2.2
1	A	21	ASN	2.2
2	B	90	ASN	2.2
4	E	291	LYS	2.2
1	A	597	LYS	2.2
1	A	429	LEU	2.1
1	A	470	GLY	2.1
1	A	242	ASP	2.1
1	D	456	PHE	2.1
3	C	32	ASP	2.1
1	A	488	LEU	2.1
1	A	622	ASP	2.1
1	D	639	MET	2.1
1	A	418	LEU	2.1
1	D	173	LEU	2.1
1	D	607	LEU	2.1
2	B	285	HIS	2.1
1	A	118	PRO	2.0
1	A	427	PRO	2.0
4	E	260	THR	2.0
2	B	253	GLN	2.0
4	E	90	ASN	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 monosaccharides in this entry.

6.4 Ligands

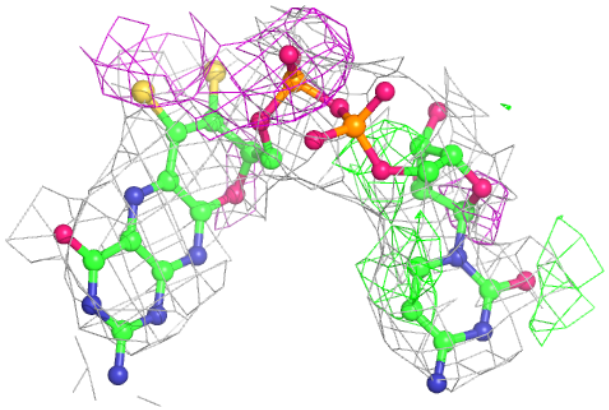
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

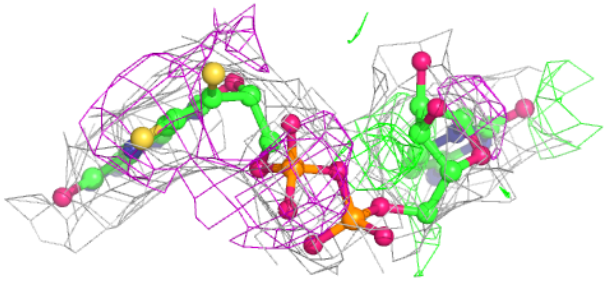
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	MO	A	802	1/1	0.73	0.16	96,96,96,96	0
6	MO	D	802	1/1	0.78	0.17	105,105,105,105	0
5	MCN	A	801	44/44	0.82	0.29	53,69,82,87	0
5	MCN	D	801	44/44	0.83	0.31	54,74,89,93	0
8	FES	F	202	4/4	0.87	0.21	46,48,50,51	0
8	FES	C	201	4/4	0.91	0.16	64,64,65,66	0
7	FAD	B	301	53/53	0.92	0.23	57,60,70,71	0
7	FAD	E	301	53/53	0.93	0.21	50,57,63,64	0
8	FES	C	202	4/4	0.95	0.17	43,47,47,49	0
8	FES	F	201	4/4	0.96	0.16	54,55,57,58	0

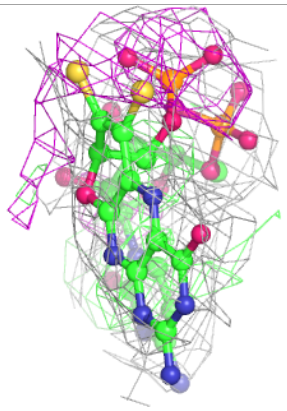
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

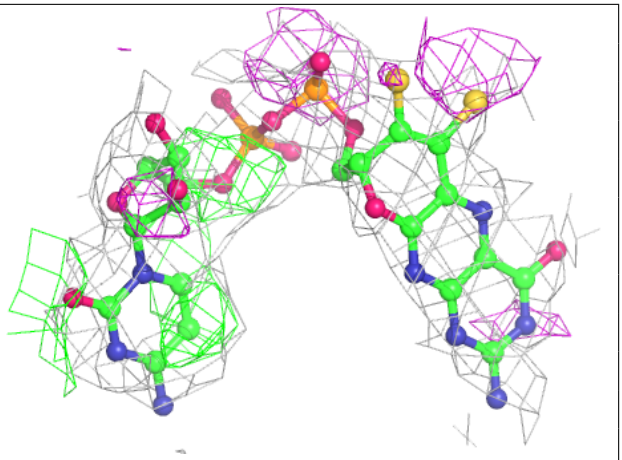


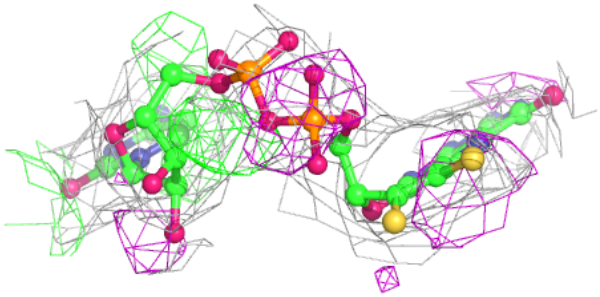


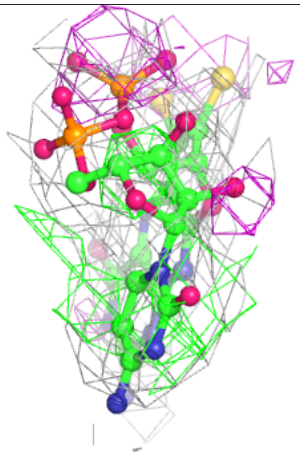


Electron density around MCN D 801:

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

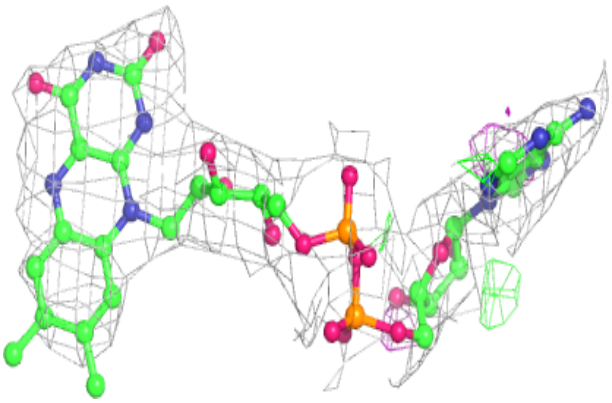


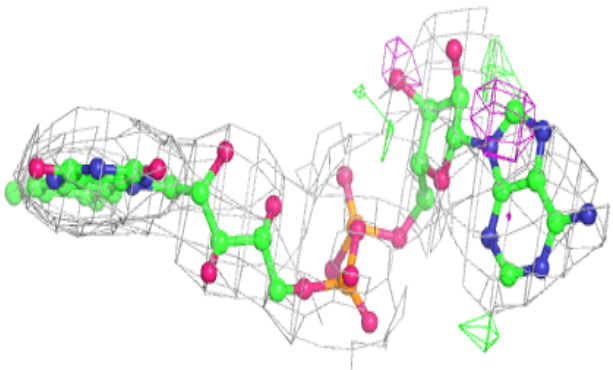


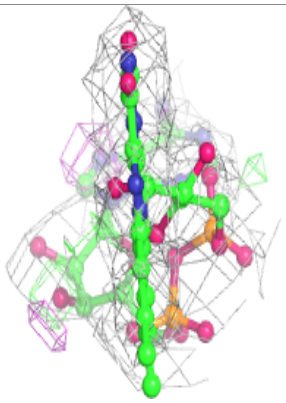


Electron density around FAD B 301:

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

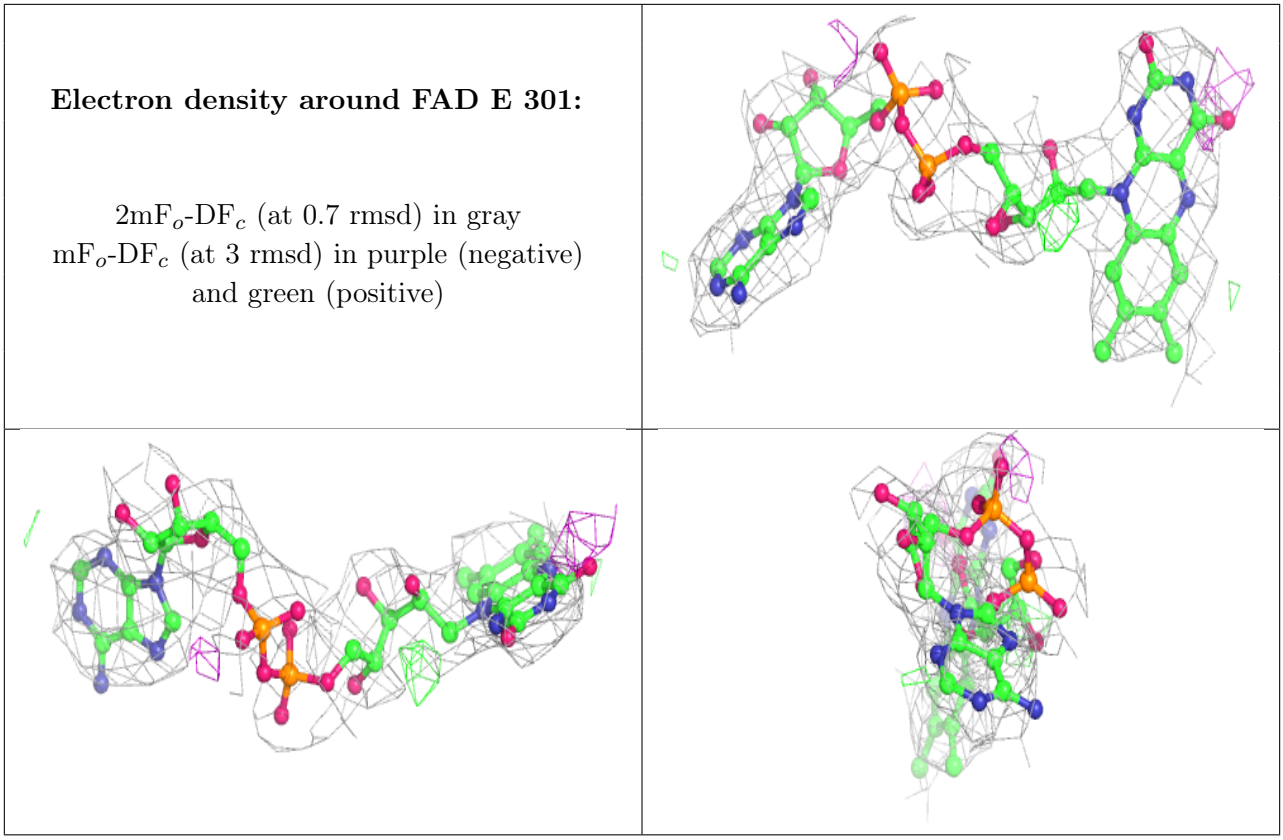






Electron density around FAD E 301:

$2mF_o$-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.