Full wwPDB X-ray Structure Validation Report (i)

Dec 12, 2023 – 10:46 am GMT

PDB ID	:	4BBY
Title	:	MAMMALIAN ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE: WILD-TYPE
Authors	:	Nenci, S.; Piano, V.; Rosati, S.; Aliverti, A.; Pandini, V.; Fraaije, M.W.; Heck, A.J.R.; Edmondson, D.E.; Mattevi, A.
Deposited on	:	2012-09-28
Resolution	:	1.90 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

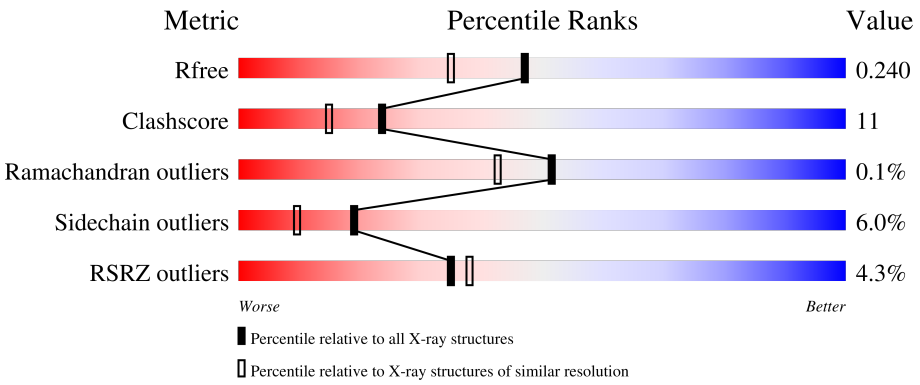
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	658	4% 65% 16% • 16%
1	B	658	4% 62% 17% • • 17%
1	C	658	3% 65% 17% • 15%
1	D	658	3% 65% 15% • • 16%

2 Entry composition (i)

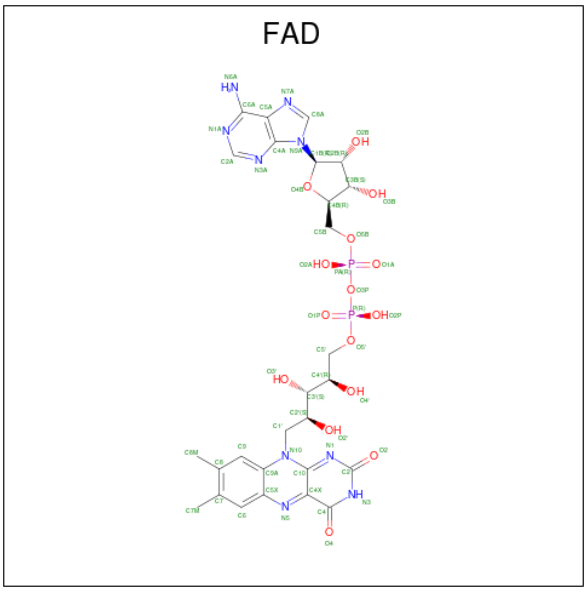
There are 4 unique types of molecules in this entry. The entry contains 18517 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	555	4413	2803	763	821	26	0	4	0
1	B	543	4301	2732	747	798	24	0	0	0
1	C	557	4418	2803	766	823	26	0	3	0
1	D	550	4363	2766	760	812	25	0	2	0

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



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

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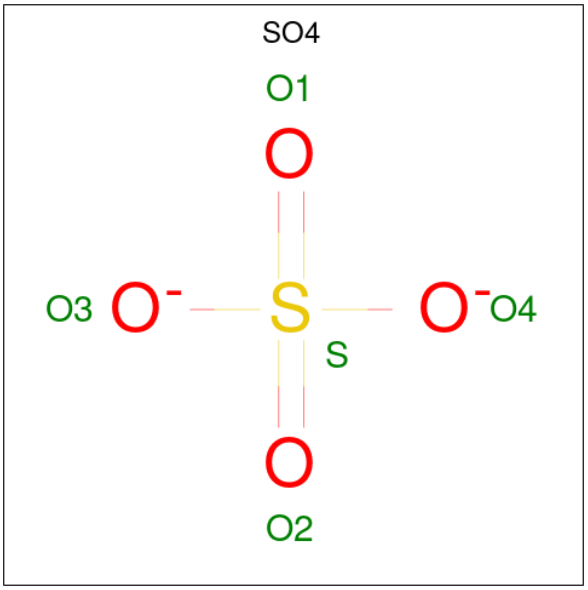
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	B	1	53	27	9	15	2	0	0
			Total	C	N	O	P		
2	C	1	53	27	9	15	2	0	0
			Total	C	N	O	P		
2	D	1	53	27	9	15	2	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
3	A	1	5	4	1	0	0
			Total	O	S		
3	A	1	5	4	1	0	0
			Total	O	S		
3	B	1	5	4	1	0	0
			Total	O	S		
3	D	1	5	4	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	227	227	227	0	0
			Total	O		
4	B	175	175	175	0	0

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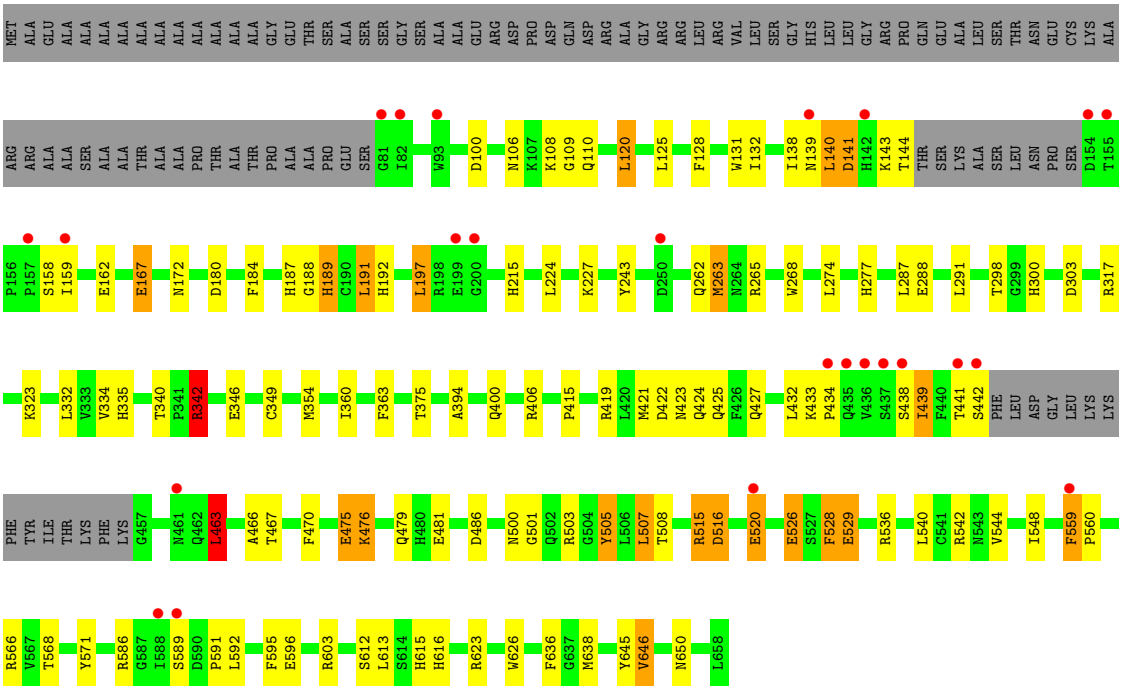
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	C	215	215	215	0	0
			Total	O		
4	D	173	173	173	0	0

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.

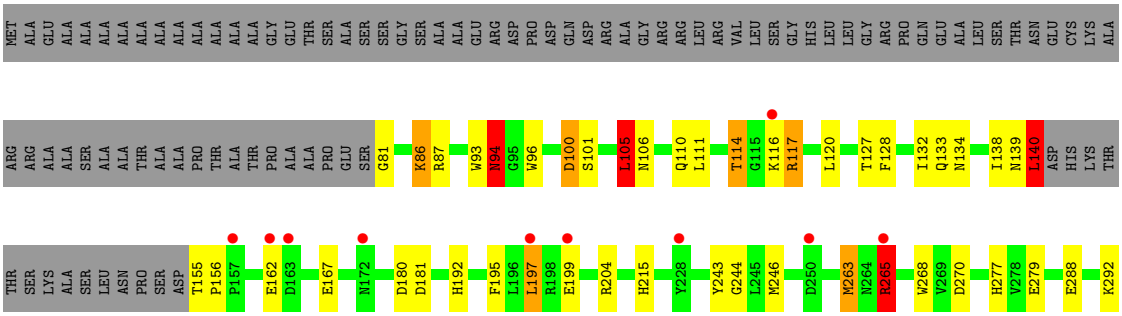
• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL

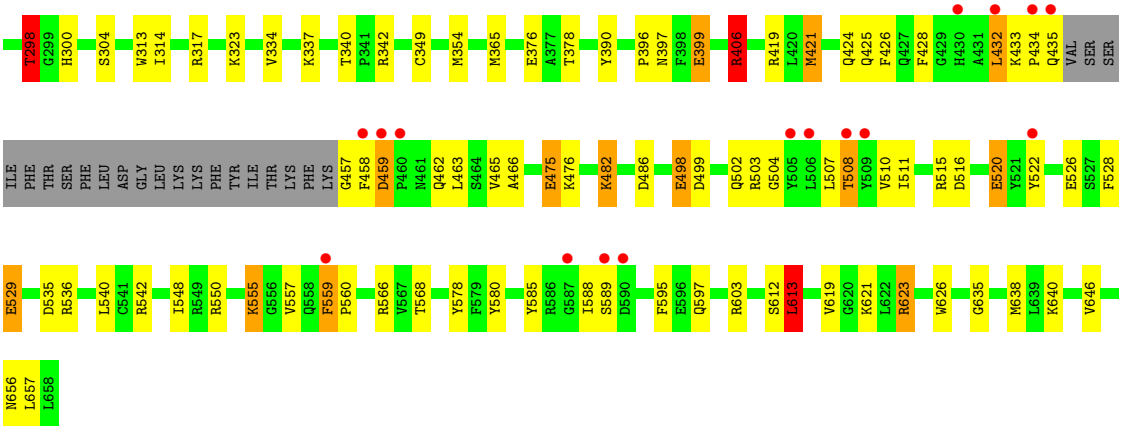
Chain A:



• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL

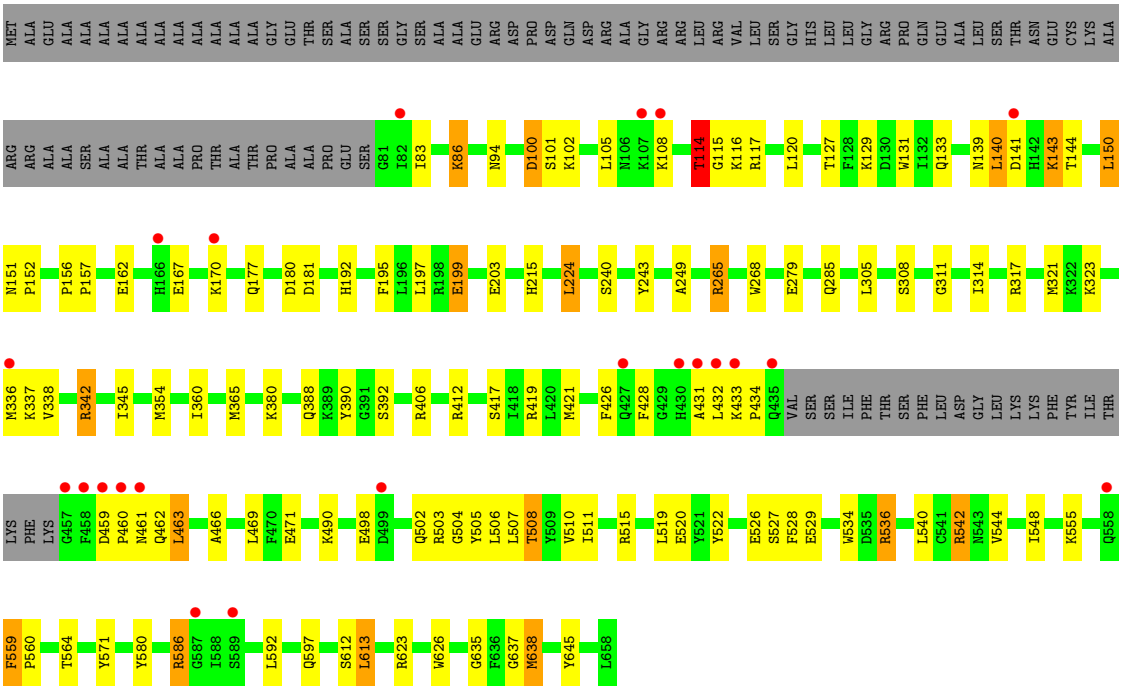
Chain B:





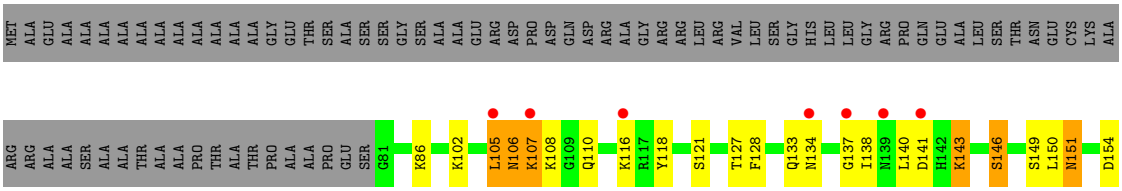
• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL

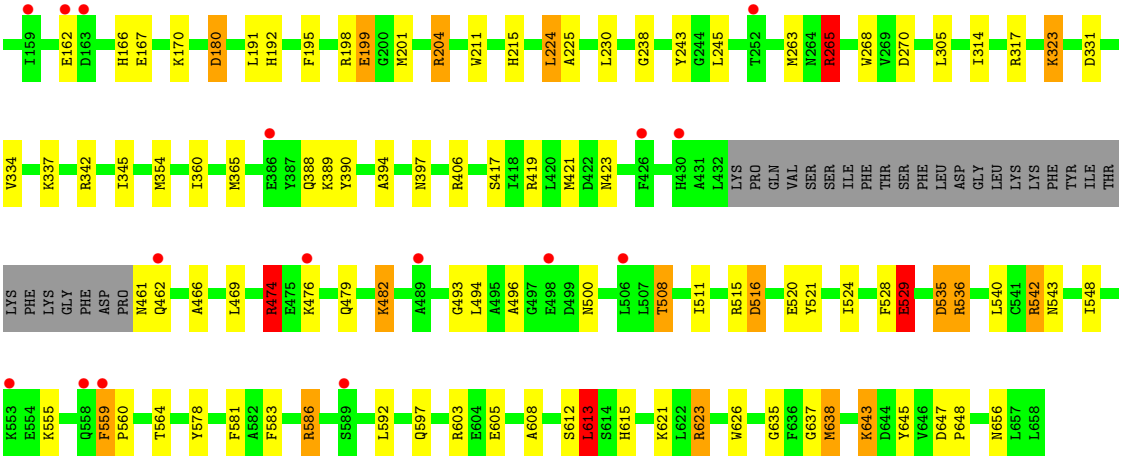
Chain C:



• Molecule 1: ALKYLDIHYDROXYACETONEPHOSPHATE SYNTHASE, PEROXISOMAL

Chain D:




I159
E162
D163
H166
E167
K170
D180
L191
H192
F195
R198
E199
G200
M201
R204
W211
H215
L224
A225
L230
G238
Y243
G244
L245
T252
M263
N264
R265
W268
V269
D270
L305
I314
R317
K323
D331
V334
K337
R342
I345
M354
I360
M365
E386
Y387
Q388
K389
Y390
A394
N397
R406
S417
I418
R419
L420
M421
D422
N423
F426
H430
A431
L432
LYS
PRO
GLN
VAL
SER
SER
ILE
PHE
THR
SER
PHE
LEU
ASP
GLY
LEU
LYS
LYS
PHE
TYR
ILE
THR
LYS
PHE
LYS
GLY
PHE
ASP
PRO
N461
Q462
A466
L469
R474
E475
K476
Q479
K482
A489
G493
L494
A495
A496
G497
E498
D499
N500
L506
L507
T508
I511
R515
D516
E520
Y521
I524
F528
E529
D535
R536
L540
C541
R542
N543
I548
K553
E554
K555
Q558
F559
P560
T564
Y578
F581
A582
F583
R586
S589
L592
Q597
R603
E604
E605
A608
S612
L613
S614
H615
K621
L622
R623
W626
G635
F636
G637
M638
K643
D644
Y645
V646
D647
P648
N656
L657
L658

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	61.30Å 99.17Å 107.83Å 90.43° 92.18° 94.92°	Depositor
Resolution (Å)	19.98 – 1.90 19.96 – 1.90	Depositor EDS
% Data completeness (in resolution range)	92.3 (19.98-1.90) 92.3 (19.96-1.90)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.7.0027	Depositor
R, R_{free}	0.191 , 0.240 0.192 , 0.240	Depositor DCC
R_{free} test set	2004 reflections (1.09%)	wwPDB-VP
Wilson B-factor (Å^2)	23.3	Xtriage
Anisotropy	0.126	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 54.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.040 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18517	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.35	34/4524 (0.8%)	1.34	51/6114 (0.8%)
1	B	1.15	14/4398 (0.3%)	1.19	32/5944 (0.5%)
1	C	1.15	13/4527 (0.3%)	1.19	31/6119 (0.5%)
1	D	1.14	9/4466 (0.2%)	1.27	40/6036 (0.7%)
All	All	1.20	70/17915 (0.4%)	1.25	154/24213 (0.6%)

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	B	1	1
1	D	0	1
All	All	1	2

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	542	ARG	CZ-NH1	-13.52	1.15	1.33
1	A	528	PHE	CG-CD2	-11.33	1.21	1.38
1	A	167	GLU	CD-OE1	-11.31	1.13	1.25
1	A	528	PHE	CG-CD1	-10.40	1.23	1.38
1	A	526	GLU	CD-OE1	-10.37	1.14	1.25
1	D	529	GLU	CD-OE2	-9.77	1.15	1.25
1	A	526	GLU	CD-OE2	-9.70	1.15	1.25
1	C	308	SER	CB-OG	9.28	1.54	1.42
1	A	536	ARG	CZ-NH1	-9.24	1.21	1.33
1	A	515	ARG	CZ-NH1	-9.00	1.21	1.33
1	A	363	PHE	CG-CD2	-8.94	1.25	1.38
1	A	167	GLU	CD-OE2	-8.89	1.15	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	184	PHE	CG-CD1	-8.88	1.25	1.38
1	A	636	PHE	CG-CD1	-8.87	1.25	1.38
1	A	363	PHE	CG-CD1	-8.48	1.26	1.38
1	A	636	PHE	CG-CD2	-8.45	1.26	1.38
1	A	184	PHE	CG-CD2	-8.42	1.26	1.38
1	C	240	SER	CB-OG	7.58	1.52	1.42
1	A	515	ARG	CZ-NH2	-7.36	1.23	1.33
1	A	603	ARG	CZ-NH2	-7.36	1.23	1.33
1	B	623	ARG	CZ-NH1	-7.34	1.23	1.33
1	A	529	GLU	CD-OE1	-6.92	1.18	1.25
1	A	184	PHE	CE2-CZ	-6.88	1.24	1.37
1	C	534	TRP	CD2-CE2	6.66	1.49	1.41
1	A	650	ASN	CG-ND2	-6.59	1.16	1.32
1	A	636	PHE	CE2-CZ	-6.47	1.25	1.37
1	C	571	TYR	CG-CD1	6.39	1.47	1.39
1	A	636	PHE	CE1-CZ	-6.38	1.25	1.37
1	C	177	GLN	CD-NE2	-6.36	1.17	1.32
1	D	417	SER	CB-OG	6.24	1.50	1.42
1	B	93	TRP	CD2-CE2	6.23	1.48	1.41
1	B	529	GLU	CD-OE1	-6.22	1.18	1.25
1	D	146	SER	CB-OG	6.21	1.50	1.42
1	C	529	GLU	CD-OE1	-6.17	1.18	1.25
1	A	262	GLN	CD-NE2	-6.12	1.17	1.32
1	A	131	TRP	CD2-CE2	6.05	1.48	1.41
1	A	528	PHE	CE2-CZ	-6.03	1.25	1.37
1	B	304	SER	CB-OG	5.98	1.50	1.42
1	B	334	VAL	CB-CG2	-5.95	1.40	1.52
1	A	400	GLN	CD-OE1	-5.86	1.11	1.24
1	A	172	ASN	CG-ND2	-5.86	1.18	1.32
1	B	406	ARG	CG-CD	-5.83	1.37	1.51
1	B	313	TRP	CD2-CE2	5.81	1.48	1.41
1	A	528	PHE	CE1-CZ	-5.79	1.26	1.37
1	B	94	ASN	CG-OD1	-5.75	1.11	1.24
1	A	529	GLU	CD-OE2	-5.66	1.19	1.25
1	A	626	TRP	CD2-CE2	5.63	1.48	1.41
1	C	626	TRP	CD2-CE2	5.63	1.48	1.41
1	A	189	HIS	CG-ND1	-5.58	1.26	1.38
1	B	96	TRP	CD2-CE2	5.58	1.48	1.41
1	C	177	GLN	CD-OE1	-5.57	1.11	1.24
1	D	211	TRP	CD2-CE2	5.55	1.48	1.41
1	D	268	TRP	CD2-CE2	5.54	1.48	1.41
1	D	529	GLU	CB-CG	-5.52	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	643	LYS	CD-CE	5.51	1.65	1.51
1	B	94	ASN	CG-ND2	-5.44	1.19	1.32
1	B	313	TRP	CG-CD1	5.43	1.44	1.36
1	B	626	TRP	CD2-CE2	5.39	1.47	1.41
1	A	172	ASN	CG-OD1	-5.36	1.12	1.24
1	B	529	GLU	CD-OE2	-5.33	1.19	1.25
1	D	626	TRP	CD2-CE2	5.29	1.47	1.41
1	D	180	ASP	CB-CG	-5.21	1.40	1.51
1	C	623	ARG	CZ-NH2	-5.12	1.26	1.33
1	A	603	ARG	CZ-NH1	-5.12	1.26	1.33
1	C	338	VAL	C-O	5.10	1.33	1.23
1	C	623	ARG	CD-NE	-5.10	1.37	1.46
1	C	311	GLY	N-CA	5.07	1.53	1.46
1	B	167	GLU	CD-OE1	-5.06	1.20	1.25
1	C	317	ARG	CZ-NH1	5.04	1.39	1.33
1	A	623	ARG	CZ-NH2	-5.03	1.26	1.33

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	603	ARG	NE-CZ-NH1	26.51	133.56	120.30
1	B	265	ARG	NE-CZ-NH2	26.51	133.55	120.30
1	D	265	ARG	NE-CZ-NH2	-25.99	107.31	120.30
1	A	542	ARG	NE-CZ-NH2	25.05	132.83	120.30
1	C	623	ARG	NE-CZ-NH1	19.60	130.10	120.30
1	D	603	ARG	NE-CZ-NH2	-18.82	110.89	120.30
1	A	623	ARG	NE-CZ-NH1	17.94	129.27	120.30
1	C	623	ARG	NE-CZ-NH2	-17.52	111.54	120.30
1	D	623	ARG	NE-CZ-NH1	16.89	128.74	120.30
1	A	536	ARG	NE-CZ-NH2	15.65	128.13	120.30
1	A	542	ARG	NE-CZ-NH1	-15.61	112.50	120.30
1	A	526	GLU	OE1-CD-OE2	-15.44	104.78	123.30
1	A	515	ARG	NE-CZ-NH1	14.77	127.68	120.30
1	D	623	ARG	NE-CZ-NH2	-14.29	113.15	120.30
1	A	603	ARG	NE-CZ-NH1	13.65	127.12	120.30
1	A	180	ASP	CB-CG-OD1	12.62	129.66	118.30
1	A	167	GLU	OE1-CD-OE2	-12.50	108.30	123.30
1	A	623	ARG	NE-CZ-NH2	-12.49	114.06	120.30
1	C	317	ARG	NE-CZ-NH2	-12.45	114.08	120.30
1	B	265	ARG	NE-CZ-NH1	-12.33	114.13	120.30
1	C	536	ARG	NE-CZ-NH2	-12.09	114.26	120.30
1	A	191	LEU	CD1-CG-CD2	-11.89	74.83	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	180	ASP	CB-CG-OD2	11.55	128.70	118.30
1	C	536	ARG	NE-CZ-NH1	11.53	126.06	120.30
1	D	180	ASP	CB-CG-OD2	11.28	128.45	118.30
1	B	623	ARG	NE-CZ-NH2	11.18	125.89	120.30
1	B	536	ARG	NE-CZ-NH1	10.48	125.54	120.30
1	B	334	VAL	CG1-CB-CG2	-10.30	94.42	110.90
1	D	603	ARG	CD-NE-CZ	10.28	137.99	123.60
1	D	180	ASP	CB-CG-OD1	-10.26	109.07	118.30
1	A	515	ARG	NH1-CZ-NH2	-10.10	108.29	119.40
1	D	265	ARG	NE-CZ-NH1	-10.03	115.29	120.30
1	B	536	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	C	180	ASP	CB-CG-OD2	9.59	126.94	118.30
1	C	515	ARG	NE-CZ-NH1	8.97	124.78	120.30
1	B	204	ARG	NE-CZ-NH1	8.84	124.72	120.30
1	D	638	MET	CG-SD-CE	-8.83	86.07	100.20
1	C	536	ARG	CG-CD-NE	-8.63	93.69	111.80
1	B	536	ARG	CG-CD-NE	-8.47	94.02	111.80
1	A	603	ARG	NH1-CZ-NH2	-8.45	110.11	119.40
1	D	515	ARG	NE-CZ-NH1	8.37	124.49	120.30
1	A	224	LEU	CD1-CG-CD2	-8.35	85.47	110.50
1	A	100	ASP	CB-CG-OD1	8.28	125.75	118.30
1	B	542	ARG	NE-CZ-NH2	8.17	124.39	120.30
1	C	265	ARG	NE-CZ-NH1	-8.05	116.28	120.30
1	B	613	LEU	CB-CG-CD2	7.92	124.46	111.00
1	D	516	ASP	CB-CG-OD2	7.80	125.32	118.30
1	B	317	ARG	NE-CZ-NH2	-7.79	116.40	120.30
1	D	342	ARG	CG-CD-NE	-7.69	95.66	111.80
1	D	542	ARG	NE-CZ-NH2	7.58	124.09	120.30
1	C	638	MET	CG-SD-CE	-7.57	88.09	100.20
1	C	100	ASP	CB-CG-OD1	7.54	125.09	118.30
1	C	542	ARG	NE-CZ-NH2	7.53	124.06	120.30
1	C	564	THR	OG1-CB-CG2	-7.45	92.86	110.00
1	B	406	ARG	CG-CD-NE	7.33	127.18	111.80
1	D	536	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	D	331	ASP	CB-CG-OD1	-7.24	111.79	118.30
1	A	536	ARG	NH1-CZ-NH2	-7.16	111.53	119.40
1	A	334	VAL	CG1-CB-CG2	-7.16	99.45	110.90
1	D	536	ARG	CG-CD-NE	-7.09	96.92	111.80
1	D	613	LEU	CB-CG-CD1	7.06	123.01	111.00
1	D	331	ASP	CB-CG-OD2	6.97	124.58	118.30
1	A	342	ARG	CA-CB-CG	-6.93	98.15	113.40
1	D	317[A]	ARG	NE-CZ-NH2	-6.93	116.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	317[B]	ARG	NE-CZ-NH2	-6.93	116.84	120.30
1	D	224	LEU	CB-CG-CD1	6.85	122.64	111.00
1	C	623	ARG	CD-NE-CZ	6.84	133.18	123.60
1	B	265	ARG	NH1-CZ-NH2	-6.75	111.98	119.40
1	A	317	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	A	303	ASP	CB-CG-OD1	6.70	124.33	118.30
1	D	180	ASP	CB-CA-C	-6.65	97.10	110.40
1	A	623	ARG	CD-NE-CZ	6.63	132.88	123.60
1	A	528	PHE	CE1-CZ-CE2	-6.61	108.10	120.00
1	B	100	ASP	CB-CG-OD1	6.59	124.23	118.30
1	C	463	LEU	CA-CB-CG	6.57	130.41	115.30
1	C	224	LEU	CB-CG-CD1	6.55	122.13	111.00
1	A	363	PHE	CE1-CZ-CE2	-6.54	108.23	120.00
1	D	623	ARG	CD-NE-CZ	6.52	132.73	123.60
1	B	536	ARG	CD-NE-CZ	6.48	132.67	123.60
1	B	603	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	636	PHE	CE1-CZ-CE2	-6.36	108.56	120.00
1	A	638	MET	CG-SD-CE	6.34	110.35	100.20
1	B	623	ARG	NH1-CZ-NH2	-6.33	112.44	119.40
1	A	463	LEU	CA-CB-CG	6.28	129.74	115.30
1	B	535	ASP	CB-CG-OD1	6.26	123.93	118.30
1	A	363	PHE	CB-CG-CD1	6.22	125.16	120.80
1	A	303	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	C	140	LEU	CA-CB-CG	6.16	129.48	115.30
1	D	334	VAL	CG1-CB-CG2	-6.13	101.09	110.90
1	D	204	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	184	PHE	CB-CG-CD2	6.10	125.07	120.80
1	C	536	ARG	CD-NE-CZ	6.10	132.14	123.60
1	B	265	ARG	CD-NE-CZ	-6.09	115.07	123.60
1	C	342	ARG	CA-CB-CG	-6.06	100.06	113.40
1	B	342	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	D	494	LEU	CA-CB-CG	6.01	129.12	115.30
1	A	422	ASP	CB-CG-OD1	5.98	123.68	118.30
1	D	623	ARG	CG-CD-NE	-5.96	99.29	111.80
1	C	412	ARG	NE-CZ-NH2	-5.94	117.33	120.30
1	C	529	GLU	OE1-CD-OE2	-5.92	116.20	123.30
1	D	265	ARG	CB-CG-CD	-5.92	96.22	111.60
1	A	291	LEU	CD1-CG-CD2	-5.84	92.98	110.50
1	D	536	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	C	613	LEU	CB-CG-CD2	5.80	120.86	111.00
1	A	184	PHE	CD1-CG-CD2	-5.80	110.76	118.30
1	A	180	ASP	OD1-CG-OD2	-5.77	112.33	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	224	LEU	CA-CB-CG	5.76	128.55	115.30
1	C	180	ASP	OD1-CG-OD2	-5.76	112.36	123.30
1	A	515	ARG	CG-CD-NE	-5.76	99.71	111.80
1	D	342	ARG	CB-CG-CD	5.75	126.56	111.60
1	B	140	LEU	CA-CB-CG	5.70	128.42	115.30
1	C	380	LYS	CD-CE-NZ	-5.70	98.60	111.70
1	C	114	THR	N-CA-CB	-5.67	99.53	110.30
1	A	515	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	A	636	PHE	CZ-CE2-CD2	5.58	126.80	120.10
1	A	363	PHE	CD1-CG-CD2	-5.58	111.05	118.30
1	A	342	ARG	CB-CG-CD	5.57	126.09	111.60
1	D	516	ASP	CB-CG-OD1	-5.57	113.28	118.30
1	B	298	THR	OG1-CB-CG2	5.54	122.75	110.00
1	A	613	LEU	CD1-CG-CD2	-5.53	93.90	110.50
1	A	528	PHE	CZ-CE2-CD2	5.52	126.73	120.10
1	C	117	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	A	184	PHE	CE1-CZ-CE2	-5.48	110.14	120.00
1	C	623	ARG	CG-CD-NE	-5.47	100.31	111.80
1	D	265	ARG	CD-NE-CZ	-5.46	115.95	123.60
1	D	270	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	363	PHE	CZ-CE2-CD2	5.44	126.63	120.10
1	B	317	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	A	528	PHE	CD1-CG-CD2	-5.37	111.32	118.30
1	A	197	LEU	CA-CB-CG	5.34	127.58	115.30
1	B	117	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	A	636	PHE	CD1-CG-CD2	-5.33	111.38	118.30
1	A	505	TYR	CA-CB-CG	-5.32	103.30	113.40
1	B	87	ARG	NE-CZ-NH2	-5.31	117.64	120.30
1	A	636	PHE	CD1-CE1-CZ	5.29	126.45	120.10
1	B	399	GLU	OE1-CD-OE2	-5.29	116.96	123.30
1	C	265	ARG	CD-NE-CZ	-5.27	116.22	123.60
1	D	613	LEU	CB-CG-CD2	5.24	119.90	111.00
1	B	117	ARG	CG-CD-NE	-5.22	100.84	111.80
1	A	515	ARG	CD-NE-CZ	5.21	130.89	123.60
1	C	317	ARG	CG-CD-NE	-5.19	100.90	111.80
1	D	105	LEU	CA-CB-CG	5.19	127.23	115.30
1	A	636	PHE	CB-CG-CD2	5.16	124.41	120.80
1	D	474	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	C	515	ARG	NE-CZ-NH2	-5.09	117.75	120.30
1	B	270	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	A	528	PHE	CB-CG-CD2	5.07	124.34	120.80
1	A	486	ASP	CB-CG-OD2	5.06	122.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	515	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	D	265	ARG	CA-CB-CG	-5.06	102.28	113.40
1	C	542	ARG	NE-CZ-NH1	-5.03	117.78	120.30
1	D	535	ASP	CB-CG-OD1	5.01	122.81	118.30
1	B	105	LEU	CA-CB-CG	5.01	126.82	115.30
1	B	265	ARG	CB-CA-C	-5.00	100.39	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	298	THR	CB

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	406	ARG	Sidechain
1	D	265	ARG	Sidechain

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	4413	0	4359	98	0
1	B	4301	0	4242	117	7
1	C	4418	0	4365	106	6
1	D	4363	0	4313	95	0
2	A	53	0	31	0	0
2	B	53	0	31	0	0
2	C	53	0	31	1	0
2	D	53	0	31	0	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
3	D	5	0	0	0	0
4	A	227	0	0	14	0
4	B	175	0	0	22	0
4	C	215	0	0	14	1
4	D	173	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	18517	0	17403	392	7

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 11.

All (392) 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:D:508:THR:HG22	4:D:2095:HOH:O	1.37	1.23
1:A:192:HIS:HB3	1:A:243:TYR:OH	1.43	1.15
1:C:192:HIS:HB3	1:C:243:TYR:OH	1.46	1.14
1:D:192:HIS:HB3	1:D:243:TYR:OH	1.44	1.14
1:A:559:PHE:HE2	1:D:608:ALA:CB	1.58	1.14
1:B:192:HIS:HB3	1:B:243:TYR:OH	1.46	1.13
1:A:419:ARG:HH22	1:A:508:THR:HG21	0.99	1.13
1:B:426:PHE:HE1	4:B:2139:HOH:O	1.29	1.13
1:B:457:GLY:HA3	4:B:2131:HOH:O	1.51	1.10
1:B:503:ARG:HG2	4:B:2140:HOH:O	1.50	1.10
1:C:586:ARG:HG3	1:C:586:ARG:HH11	1.00	1.09
1:C:421:MET:HE3	4:C:2158:HOH:O	1.52	1.08
1:C:426:PHE:HB2	4:C:2158:HOH:O	1.53	1.06
1:D:146:SER:HB2	4:D:2036:HOH:O	1.53	1.06
1:B:265:ARG:NH1	1:B:265:ARG:HB3	1.68	1.06
1:B:265:ARG:HB3	1:B:265:ARG:HH11	0.97	1.06
1:C:508:THR:HG22	4:C:2097:HOH:O	1.56	1.05
1:A:615:HIS:HD2	1:A:616:HIS:HD2	1.03	1.02
1:C:285:GLN:OE1	4:C:2015:HOH:O	1.76	1.02
1:A:559:PHE:HE2	1:D:608:ALA:HB1	1.22	1.01
1:C:419:ARG:HH12	1:C:508:THR:CG2	1.73	1.00
1:A:559:PHE:CE2	1:D:608:ALA:HB1	1.97	1.00
1:B:243:TYR:CD2	4:B:2060:HOH:O	2.14	1.00
1:B:426:PHE:CE1	4:B:2139:HOH:O	2.08	0.98
1:A:419:ARG:NH2	1:A:508:THR:HG21	1.79	0.96
1:A:559:PHE:CE2	1:D:608:ALA:CB	2.48	0.96
1:B:265:ARG:HH11	1:B:265:ARG:CB	1.80	0.94
1:C:586:ARG:HG3	1:C:586:ARG:NH1	1.79	0.94
1:A:349:CYS:SG	1:A:354[B]:MET:HE1	2.08	0.93
1:A:394:ALA:HB1	1:A:463:LEU:HD21	1.50	0.93
1:B:243:TYR:CE2	4:B:2060:HOH:O	2.21	0.91
1:D:586:ARG:HH11	1:D:586:ARG:HG3	1.35	0.91
1:A:476:LYS:HG2	4:A:2177:HOH:O	1.71	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:ARG:HH12	1:C:508:THR:HG21	1.35	0.91
1:A:615:HIS:HD2	1:A:616:HIS:CD2	1.90	0.89
1:B:139:ASN:O	1:B:140:LEU:CB	2.16	0.88
1:C:192:HIS:HB3	1:C:243:TYR:HH	1.38	0.88
1:B:424:GLN:NE2	4:B:2129:HOH:O	2.05	0.87
1:A:419:ARG:HH22	1:A:508:THR:CG2	1.85	0.86
1:A:615:HIS:CD2	1:A:616:HIS:HD2	1.94	0.85
1:B:100:ASP:O	1:B:114:THR:HG23	1.77	0.85
1:A:423:ASN:HD21	1:A:427:GLN:HE21	1.24	0.83
1:B:139:ASN:O	1:B:140:LEU:HB3	1.79	0.82
1:B:298:THR:HG23	1:B:300:HIS:H	1.44	0.81
1:D:192:HIS:CB	1:D:243:TYR:OH	2.28	0.81
1:B:426:PHE:CD1	1:B:465:VAL:HG21	2.17	0.80
1:C:586:ARG:HH11	1:C:586:ARG:CG	1.91	0.79
1:B:127:THR:HG22	1:B:127:THR:O	1.82	0.78
1:B:101:SER:HA	1:B:114:THR:HG22	1.64	0.78
1:A:159:ILE:HA	4:A:2030:HOH:O	1.82	0.77
1:B:555:LYS:NZ	1:B:597:GLN:HE21	1.82	0.77
1:B:246:MET:SD	4:B:2060:HOH:O	2.41	0.77
1:D:137:GLY:HA3	1:D:559:PHE:CE2	2.19	0.77
1:C:542:ARG:NH2	4:C:2180:HOH:O	2.16	0.77
1:C:360:ILE:HG12	4:C:2134:HOH:O	1.83	0.77
1:A:192:HIS:CB	1:A:243:TYR:OH	2.30	0.76
1:B:192:HIS:CB	1:B:243:TYR:OH	2.30	0.76
1:A:433:LYS:HB3	1:A:434:PRO:HD2	1.68	0.76
1:A:106[A]:ASN:HB2	1:A:110:GLN:O	1.86	0.76
1:A:349:CYS:SG	1:A:354[B]:MET:CE	2.74	0.76
1:B:100:ASP:O	1:B:114:THR:CG2	2.33	0.75
1:B:482:LYS:HE3	1:B:486:ASP:OD2	1.86	0.75
1:C:505:TYR:O	1:C:508:THR:OG1	2.01	0.75
1:C:83:ILE:HD12	4:C:2086:HOH:O	1.86	0.74
1:A:421[B]:MET:HE1	4:A:2167:HOH:O	1.86	0.74
1:A:559:PHE:HE2	1:D:608:ALA:HB2	1.52	0.74
1:D:496:ALA:O	1:D:500:ASN:ND2	2.21	0.74
1:C:508:THR:HA	1:C:511:ILE:HD13	1.70	0.74
1:D:154:ASP:O	1:D:201:MET:HG2	1.88	0.74
1:C:503:ARG:O	1:C:507:LEU:HB2	1.88	0.73
1:D:648:PRO:O	4:D:2167:HOH:O	2.05	0.73
1:C:388:GLN:NE2	1:C:471:GLU:OE1	2.22	0.73
1:D:133:GLN:HG2	1:D:138:ILE:O	1.89	0.72
1:C:139:ASN:HB2	1:C:141:ASP:OD1	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ALA:HB1	1:A:463:LEU:CD2	2.21	0.71
1:B:419:ARG:HH22	1:B:508:THR:HG21	1.55	0.71
1:B:457:GLY:C	1:B:458:PHE:HD1	1.94	0.70
1:D:215:HIS:CE1	1:D:337:LYS:HD3	2.27	0.70
1:B:550:ARG:HB2	4:B:2153:HOH:O	1.91	0.70
1:B:139:ASN:O	1:B:140:LEU:HB2	1.91	0.70
1:C:192:HIS:CB	1:C:243:TYR:OH	2.32	0.70
1:B:640:LYS:HD2	4:B:2169:HOH:O	1.93	0.69
1:A:158:SER:O	4:A:2030:HOH:O	2.10	0.69
1:A:143:LYS:HG3	1:A:144:THR:H	1.56	0.69
1:B:265:ARG:HG2	1:B:279:GLU:OE1	1.92	0.69
1:D:146:SER:CB	4:D:2036:HOH:O	2.24	0.68
1:A:139:ASN:HB3	1:A:141:ASP:OD1	1.93	0.68
1:C:131:TRP:CZ2	1:C:428:PHE:HD1	2.11	0.68
1:D:192:HIS:CE1	1:D:592:LEU:HD13	2.29	0.67
1:C:419:ARG:NH1	1:C:508:THR:HG21	2.08	0.67
1:D:419:ARG:HH12	1:D:508:THR:CG2	2.07	0.66
1:A:424:GLN:NE2	4:A:2170:HOH:O	2.15	0.66
1:C:428:PHE:HE2	1:C:507:LEU:HD21	1.61	0.66
1:B:498:GLU:O	1:B:502:GLN:N	2.24	0.66
1:D:474:ARG:HG3	4:D:2136:HOH:O	1.95	0.66
1:B:557:VAL:HG22	1:B:588:ILE:HD11	1.78	0.65
1:D:613:LEU:HD22	1:D:623:ARG:HD3	1.78	0.65
1:B:507:LEU:O	1:B:510:VAL:HG22	1.95	0.65
1:B:555:LYS:NZ	1:B:597:GLN:NE2	2.44	0.65
1:D:360:ILE:HG12	4:D:2122:HOH:O	1.96	0.65
1:A:438:SER:HB3	1:A:441:THR:HG22	1.78	0.65
1:D:555:LYS:NZ	1:D:597:GLN:HE21	1.94	0.65
1:B:613:LEU:HD22	1:B:623:ARG:HD2	1.79	0.65
1:C:462:GLN:HG2	4:C:2146:HOH:O	1.96	0.65
1:A:189:HIS:HE1	4:A:2043:HOH:O	1.79	0.64
1:B:425:GLN:HE22	1:B:566:ARG:HD3	1.62	0.64
1:D:586:ARG:HG3	4:D:2153:HOH:O	1.97	0.64
1:A:360:ILE:HG12	4:A:2138:HOH:O	1.96	0.63
1:A:571:TYR:OH	1:A:615:HIS:HE1	1.81	0.63
1:B:635:GLY:HA2	1:B:638:MET:HE2	1.81	0.62
1:A:442:SER:HB3	1:D:542:ARG:NH1	2.13	0.62
1:C:144:THR:HG22	1:C:520:GLU:HA	1.81	0.62
1:C:265:ARG:NH1	1:C:265:ARG:HG2	2.15	0.62
1:D:578:TYR:CE1	4:D:2152:HOH:O	2.51	0.62
1:B:555:LYS:HZ2	1:B:597:GLN:NE2	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:586:ARG:NH1	1:C:586:ARG:CG	2.57	0.62
1:B:265:ARG:HD3	4:B:2043:HOH:O	1.98	0.62
1:C:321:MET:HE1	1:C:469:LEU:CD2	2.30	0.61
1:A:467:THR:HB	1:A:505:TYR:HE1	1.64	0.61
1:B:508:THR:HA	1:B:511:ILE:HD13	1.82	0.61
1:C:129:LYS:O	1:C:133:GLN:HG3	2.01	0.61
1:D:578:TYR:HE1	4:D:2152:HOH:O	1.81	0.61
1:B:127:THR:O	1:B:127:THR:CG2	2.47	0.61
1:A:423:ASN:HD21	1:A:427:GLN:NE2	1.97	0.60
1:D:143:LYS:HG2	1:D:521:TYR:CE1	2.36	0.60
1:A:263:MET:HG2	4:A:2052:HOH:O	2.00	0.60
1:B:399:GLU:CD	1:B:399:GLU:H	2.04	0.60
1:A:439:ILE:HG13	1:D:535:ASP:HB2	1.84	0.59
1:C:580:TYR:HE1	4:C:2193:HOH:O	1.85	0.59
1:D:192:HIS:ND1	1:D:592:LEU:HD13	2.18	0.59
1:B:314:ILE:HG23	1:B:365:MET:HG2	1.83	0.59
1:C:139:ASN:O	1:C:140:LEU:HB2	2.02	0.59
1:D:529:GLU:OE2	1:D:615:HIS:N	2.33	0.58
1:B:557:VAL:HA	1:B:588:ILE:HD11	1.85	0.58
1:C:321:MET:CE	1:C:469:LEU:HD23	2.34	0.58
1:A:187:HIS:HD2	1:A:188:GLY:O	1.87	0.57
1:A:591:PRO:HD2	4:A:2205:HOH:O	2.04	0.57
1:D:419:ARG:HH12	1:D:508:THR:HG21	1.68	0.57
1:A:432:LEU:HD12	1:A:507:LEU:HD11	1.87	0.56
1:B:215:HIS:CE1	1:B:337:LYS:HD3	2.40	0.56
1:A:215:HIS:HD2	1:A:375:THR:OG1	1.89	0.56
1:B:94:ASN:HA	1:B:197:LEU:HD13	1.85	0.56
1:A:192:HIS:CE1	1:A:592:LEU:HD13	2.39	0.56
1:D:166:HIS:HD2	4:D:2047:HOH:O	1.86	0.56
1:B:277:HIS:HE1	1:B:376:GLU:OE1	1.87	0.56
1:C:508:THR:CB	4:C:2097:HOH:O	2.52	0.56
1:A:415:PRO:HB3	1:A:470:PHE:CE2	2.41	0.56
1:B:434:PRO:HG3	4:B:2130:HOH:O	2.05	0.56
1:C:505:TYR:C	1:C:507:LEU:H	2.08	0.56
1:D:146:SER:CA	4:D:2036:HOH:O	2.53	0.56
1:B:475:GLU:HB2	4:B:2134:HOH:O	2.06	0.56
1:C:345:ILE:HD13	1:D:638:MET:CE	2.36	0.56
1:C:555:LYS:NZ	1:C:597:GLN:HE21	2.02	0.55
1:D:107:LYS:NZ	4:D:2025:HOH:O	2.31	0.55
1:A:467:THR:HB	1:A:505:TYR:CE1	2.42	0.55
1:D:314:ILE:HG23	1:D:365:MET:HG2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:GLY:HA2	1:B:656:ASN:HD21	1.70	0.55
1:C:433:LYS:HE2	1:C:503:ARG:NH1	2.21	0.55
1:D:635:GLY:HA2	1:D:638:MET:HE3	1.88	0.55
1:D:540:LEU:C	1:D:540:LEU:HD23	2.27	0.55
1:B:550:ARG:HD3	4:B:2153:HOH:O	2.06	0.54
1:C:508:THR:CA	1:C:511:ILE:HD13	2.37	0.54
1:C:419:ARG:NH1	1:C:508:THR:CG2	2.58	0.54
1:C:507:LEU:O	1:C:510:VAL:HG22	2.08	0.54
1:B:457:GLY:O	1:B:458:PHE:HD1	1.90	0.53
1:D:586:ARG:HH11	1:D:586:ARG:CG	2.16	0.53
1:A:503:ARG:HG3	4:A:2184:HOH:O	2.09	0.53
1:A:612:SER:HB2	1:B:354:MET:HG2	1.90	0.53
1:A:120:LEU:CD2	1:A:125:LEU:HD21	2.39	0.53
1:B:106:ASN:HD21	1:B:110:GLN:HG2	1.73	0.53
1:C:156:PRO:HG2	4:C:2058:HOH:O	2.09	0.53
1:B:132:ILE:HG22	1:B:138:ILE:HD11	1.91	0.53
1:C:433:LYS:HE2	1:C:503:ARG:HH12	1.73	0.53
1:A:501:GLY:O	1:A:505:TYR:HD1	1.90	0.53
1:C:203:GLU:OE1	1:C:249:ALA:CB	2.56	0.53
1:C:508:THR:HA	1:C:511:ILE:CD1	2.38	0.53
1:D:108:LYS:HD3	1:D:110:GLN:NE2	2.24	0.52
1:C:144:THR:CG2	1:C:520:GLU:HA	2.39	0.52
1:C:321:MET:HE1	1:C:469:LEU:HD23	1.90	0.52
1:A:475:GLU:O	1:A:479:GLN:HG3	2.10	0.52
1:B:243:TYR:HD2	4:B:2060:HOH:O	1.69	0.52
1:A:433:LYS:CB	1:A:434:PRO:HD2	2.34	0.52
1:B:298:THR:CG2	1:B:300:HIS:H	2.19	0.52
1:D:105:LEU:HD13	1:D:521:TYR:OH	2.10	0.52
1:B:128:PHE:CD1	1:B:432:LEU:HD11	2.44	0.51
1:B:557:VAL:HG22	1:B:588:ILE:CD1	2.39	0.51
1:D:419:ARG:O	1:D:466:ALA:HA	2.09	0.51
1:D:586:ARG:HG3	1:D:586:ARG:NH1	2.14	0.51
1:C:265:ARG:HD2	1:C:279:GLU:OE1	2.10	0.51
1:C:345:ILE:CD1	1:D:638:MET:HE2	2.41	0.51
1:D:555:LYS:HZ1	1:D:597:GLN:HE21	1.58	0.51
1:B:155:THR:HG22	1:B:156:PRO:O	2.11	0.51
1:D:621:LYS:HG3	1:D:656:ASN:HD22	1.76	0.51
1:C:192:HIS:CB	1:C:243:TYR:HH	2.18	0.51
1:C:528:PHE:HZ	1:C:548:ILE:HD11	1.76	0.51
1:B:106:ASN:ND2	1:B:110:GLN:HG2	2.26	0.51
1:B:619:VAL:HB	1:B:657:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:ILE:HG23	1:C:365:MET:HG2	1.94	0.50
1:A:143:LYS:HE3	1:A:520:GLU:HB3	1.94	0.50
1:C:215:HIS:CE1	1:C:337:LYS:HD3	2.45	0.50
1:A:265:ARG:NH1	1:A:265:ARG:HG2	2.26	0.50
1:C:638:MET:HE2	1:D:345:ILE:CD1	2.42	0.50
1:B:265:ARG:HD3	1:B:279:GLU:OE1	2.11	0.50
1:D:397:ASN:HA	1:D:462:GLN:O	2.12	0.50
1:C:345:ILE:HD13	1:D:638:MET:HE1	1.94	0.49
1:D:305:LEU:HD12	1:D:305:LEU:C	2.32	0.49
1:D:643:LYS:NZ	1:D:647:ASP:OD2	2.45	0.49
1:C:131:TRP:HB2	1:C:431:ALA:HB1	1.95	0.49
1:C:459:ASP:OD1	1:C:460:PRO:HD2	2.13	0.49
1:D:191:LEU:HD13	1:D:191:LEU:C	2.33	0.49
1:D:419:ARG:HH22	1:D:508:THR:HG21	1.77	0.49
1:C:195:PHE:CD1	1:C:592:LEU:HD11	2.47	0.49
1:A:566:ARG:HE	1:A:568:THR:HG22	1.77	0.49
1:B:101:SER:CA	1:B:114:THR:HG22	2.37	0.49
1:B:621:LYS:HG3	1:B:656:ASN:HD22	1.77	0.49
1:B:292:LYS:HB2	4:B:2073:HOH:O	2.11	0.49
1:A:120:LEU:HD21	1:A:125:LEU:HD21	1.95	0.48
1:B:458:PHE:HB2	1:B:463:LEU:HD12	1.94	0.48
1:C:86:LYS:HE3	1:C:181:ASP:OD1	2.12	0.48
1:C:100:ASP:O	1:C:114:THR:CG2	2.61	0.48
1:A:143:LYS:HG3	1:A:144:THR:N	2.25	0.48
1:A:106[B]:ASN:HD21	1:A:110:GLN:HB2	1.78	0.48
1:A:189:HIS:CE1	4:A:2043:HOH:O	2.59	0.48
1:A:612:SER:CB	1:B:354:MET:HG2	2.43	0.48
1:B:419:ARG:O	1:B:466:ALA:HA	2.13	0.48
1:C:305:LEU:C	1:C:305:LEU:HD12	2.34	0.48
1:B:397:ASN:HA	1:B:462:GLN:O	2.12	0.48
1:B:457:GLY:CA	4:B:2131:HOH:O	2.32	0.48
1:C:559:PHE:CD1	1:C:560:PRO:HD2	2.49	0.48
1:A:288:GLU:OE1	1:A:298[A]:THR:HG23	2.13	0.48
1:C:157:PRO:HA	4:C:2035:HOH:O	2.14	0.48
1:B:419:ARG:HH12	1:B:508:THR:CG2	2.28	0.47
1:B:94:ASN:HD22	1:B:94:ASN:H	1.63	0.47
1:A:215:HIS:HE1	4:A:2054:HOH:O	1.98	0.47
1:A:526:GLU:CB	1:A:595:PHE:HZ	2.27	0.47
1:C:144:THR:HG21	1:C:519:LEU:O	2.14	0.47
1:C:392:SER:HA	1:C:466:ALA:O	2.14	0.47
1:C:505:TYR:C	1:C:507:LEU:N	2.67	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:612:SER:HB2	1:D:354[A]:MET:HG2	1.96	0.47
1:B:105:LEU:HD13	1:B:111:LEU:HD23	1.97	0.46
1:B:528:PHE:HZ	1:B:548:ILE:HD11	1.80	0.46
1:C:526:GLU:HG3	1:C:527:SER:N	2.30	0.46
1:C:115:GLY:O	1:C:116:LYS:HD2	2.15	0.46
1:D:106:ASN:ND2	1:D:108:LYS:H	2.13	0.46
1:A:192:HIS:HB3	1:A:243:TYR:HH	1.72	0.46
1:A:419:ARG:NH2	1:A:508:THR:CG2	2.62	0.46
1:B:555:LYS:CE	1:B:597:GLN:HE21	2.28	0.46
1:C:342:ARG:HD2	1:C:645:TYR:CZ	2.50	0.46
1:A:189:HIS:HD2	4:A:2189:HOH:O	1.98	0.46
1:B:419:ARG:HH12	1:B:508:THR:HG21	1.81	0.46
1:D:394:ALA:O	1:D:493:GLY:HA2	2.15	0.46
1:C:505:TYR:O	1:C:508:THR:N	2.48	0.46
1:A:526:GLU:HB2	1:A:595:PHE:HZ	1.80	0.46
1:B:277:HIS:CE1	1:B:376:GLU:OE1	2.69	0.46
1:B:288:GLU:OE1	1:B:298:THR:HB	2.16	0.46
1:C:433:LYS:HD3	1:C:434:PRO:HD2	1.98	0.46
1:D:146:SER:HB3	1:D:198:ARG:HB3	1.98	0.46
1:C:314:ILE:HG21	1:C:336[B]:MET:SD	2.56	0.46
1:C:354[A]:MET:HG2	1:D:612:SER:HB2	1.98	0.45
1:D:586:ARG:NH1	4:D:2153:HOH:O	2.49	0.45
1:A:109:GLY:HA3	1:C:268:TRP:CE3	2.52	0.45
1:A:287:LEU:HD21	1:A:298[A]:THR:HG21	1.97	0.45
1:B:520:GLU:H	1:B:520:GLU:HG2	1.63	0.45
1:C:555:LYS:NZ	1:C:597:GLN:NE2	2.64	0.45
1:D:192:HIS:HB3	1:D:243:TYR:HH	1.72	0.45
1:A:340:THR:HB	1:A:646:VAL:HG13	1.98	0.45
1:A:354[A]:MET:HG2	1:B:612:SER:HB2	1.98	0.45
1:A:421[A]:MET:HB2	1:A:425:GLN:HB2	1.99	0.45
1:B:86:LYS:HE3	1:B:181:ASP:OD1	2.16	0.45
1:B:434:PRO:O	1:B:435:GLN:HG2	2.17	0.45
1:C:195:PHE:O	1:C:199:GLU:HB2	2.17	0.45
1:D:192:HIS:CB	1:D:243:TYR:HH	2.29	0.45
1:D:516:ASP:O	1:D:520:GLU:HG2	2.16	0.45
1:D:543:ASN:HB3	1:D:605:GLU:OE2	2.16	0.45
1:B:526:GLU:HB3	1:B:595:PHE:HZ	1.81	0.45
1:C:419:ARG:HH12	1:C:508:THR:HG22	1.71	0.45
1:D:559:PHE:CD1	1:D:560:PRO:HD2	2.52	0.45
1:C:203:GLU:OE1	1:C:249:ALA:HB2	2.16	0.45
1:A:342:ARG:HD2	1:A:645:TYR:CZ	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:94:ASN:HD22	1:B:94:ASN:N	2.15	0.45
1:B:578:TYR:HE2	1:B:580:TYR:CE1	2.34	0.45
1:A:559:PHE:CD1	1:A:560:PRO:HD2	2.52	0.45
1:A:187:HIS:CE1	1:A:197:LEU:HD11	2.52	0.44
1:B:265:ARG:NH1	1:B:265:ARG:CB	2.53	0.44
1:B:340:THR:HB	1:B:646:VAL:HG13	1.99	0.44
1:B:433:LYS:HA	1:B:434:PRO:HD3	1.75	0.44
1:C:559:PHE:HD1	1:C:560:PRO:HD2	1.82	0.44
1:A:354[B]:MET:HE1	1:B:612:SER:HB3	1.99	0.44
1:A:589:SER:O	1:A:591:PRO:HD3	2.17	0.44
1:A:442:SER:CB	1:D:542:ARG:NH1	2.79	0.44
1:B:244:GLY:HA2	1:B:656:ASN:ND2	2.32	0.44
1:C:101:SER:HA	1:C:114:THR:HG22	2.00	0.44
1:C:143:LYS:HE3	1:C:143:LYS:HB3	1.73	0.44
1:C:354[A]:MET:HG2	1:D:612:SER:CB	2.48	0.44
1:D:151:ASN:C	1:D:151:ASN:HD22	2.21	0.44
1:B:459:ASP:OD1	1:B:459:ASP:C	2.56	0.44
1:C:419:ARG:O	1:C:466:ALA:HA	2.17	0.44
1:B:81:GLY:HA3	4:B:2001:HOH:O	2.16	0.44
1:B:499:ASP:O	1:B:503:ARG:HB3	2.17	0.44
1:C:116:LYS:HD2	1:C:116:LYS:HA	1.79	0.44
1:C:504:GLY:O	1:C:508:THR:HG23	2.17	0.44
1:A:470:PHE:CZ	1:A:481:GLU:HA	2.53	0.44
1:B:128:PHE:CG	1:B:432:LEU:HD11	2.53	0.44
1:C:522:TYR:CB	1:C:586:ARG:HG2	2.48	0.44
1:D:524:ILE:HD11	1:D:583:PHE:CZ	2.53	0.43
1:C:133:GLN:NE2	1:C:139:ASN:O	2.51	0.43
1:D:423:ASN:CG	1:D:461:ASN:O	2.56	0.43
1:D:106:ASN:ND2	1:D:110:GLN:H	2.17	0.43
1:D:118:TYR:O	1:D:121:SER:HB2	2.18	0.43
1:D:204:ARG:HA	4:D:2063:HOH:O	2.18	0.43
1:A:433:LYS:HB3	1:A:434:PRO:CD	2.45	0.43
1:A:439:ILE:HG13	1:D:535:ASP:CB	2.47	0.43
1:D:482:LYS:HE3	1:D:482:LYS:HB2	1.86	0.43
1:D:419:ARG:NH1	1:D:508:THR:HG21	2.31	0.43
1:D:528:PHE:HZ	1:D:548:ILE:HD11	1.83	0.43
1:D:559:PHE:HD1	1:D:560:PRO:HD2	1.83	0.43
1:A:128:PHE:O	1:A:132:ILE:HG13	2.17	0.43
1:B:265:ARG:HD3	4:B:2044:HOH:O	2.18	0.43
1:B:559:PHE:CD1	1:B:560:PRO:HD2	2.54	0.43
1:B:421:MET:HG3	1:B:425:GLN:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:GLU:HA	1:C:170:LYS:HE3	2.01	0.42
1:B:132:ILE:CG2	1:B:138:ILE:HD11	2.48	0.42
1:C:94:ASN:HA	1:C:197:LEU:HD13	2.02	0.42
1:C:417:SER:HB3	1:C:469:LEU:HB3	2.01	0.42
1:D:108:LYS:HD3	1:D:110:GLN:HE22	1.84	0.42
1:A:268:TRP:CE2	1:A:277:HIS:HB2	2.55	0.42
1:D:195:PHE:O	1:D:199:GLU:HB2	2.20	0.42
1:A:167:GLU:OE2	1:A:227:LYS:NZ	2.50	0.42
1:B:277:HIS:HD2	1:B:378:THR:OG1	2.02	0.42
1:B:516:ASP:O	1:B:520:GLU:HG2	2.19	0.42
1:A:419:ARG:O	1:A:466:ALA:HA	2.19	0.42
1:B:292:LYS:HG3	4:B:2076:HOH:O	2.19	0.42
1:B:522:TYR:HD1	1:B:585:TYR:CE1	2.38	0.42
1:C:645:TYR:CZ	1:D:637:GLY:HA3	2.54	0.42
1:A:500:ASN:ND2	1:A:503:ARG:NH1	2.67	0.42
1:A:540:LEU:O	1:A:544:VAL:HG23	2.20	0.42
1:B:458:PHE:CB	1:B:463:LEU:HD12	2.49	0.42
1:D:106:ASN:C	1:D:106:ASN:HD22	2.22	0.42
1:D:238:GLY:HA2	1:D:245:LEU:HD11	2.02	0.42
1:D:323:LYS:HD2	1:D:323:LYS:C	2.40	0.42
1:B:635:GLY:HA2	1:B:638:MET:CE	2.47	0.42
1:C:265:ARG:NH1	1:C:265:ARG:CG	2.72	0.42
1:C:265:ARG:CG	1:C:265:ARG:HH11	2.33	0.42
1:B:432:LEU:HD23	1:B:507:LEU:HD21	2.01	0.42
1:B:504:GLY:N	4:B:2140:HOH:O	2.52	0.42
1:C:637:GLY:HA3	1:D:645:TYR:CZ	2.55	0.42
1:A:263:MET:HE2	1:A:263:MET:HB2	1.92	0.42
1:D:151:ASN:C	1:D:151:ASN:ND2	2.73	0.42
1:A:268:TRP:CZ2	1:A:277:HIS:HB2	2.55	0.41
1:B:263:MET:HE2	1:B:263:MET:HB2	1.81	0.41
1:D:225:ALA:HA	1:D:230:LEU:HD12	2.01	0.41
1:D:524:ILE:HD13	1:D:524:ILE:HG21	1.76	0.41
1:D:138:ILE:HD12	1:D:140:LEU:HD23	2.02	0.41
1:B:540:LEU:HD23	1:B:540:LEU:C	2.41	0.41
1:A:616:HIS:HE1	4:A:2203:HOH:O	2.02	0.41
1:B:265:ARG:HG2	1:B:279:GLU:CD	2.40	0.41
1:B:503:ARG:C	4:B:2140:HOH:O	2.58	0.41
1:C:141:ASP:OD1	1:C:141:ASP:N	2.53	0.41
1:C:265:ARG:HD2	4:C:2061:HOH:O	2.19	0.41
1:C:540:LEU:O	1:C:544:VAL:HG23	2.19	0.41
1:A:559:PHE:CE2	1:D:608:ALA:HB2	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:426:PHE:C	1:C:428:PHE:N	2.73	0.41
1:C:433:LYS:HA	1:C:434:PRO:HD2	1.91	0.41
1:A:300:HIS:HB2	1:A:332:LEU:HD13	2.03	0.41
1:A:516:ASP:O	1:A:520:GLU:HG2	2.21	0.41
1:A:615:HIS:CD2	1:A:616:HIS:CD2	2.82	0.41
1:B:390:TYR:CG	1:B:502:GLN:HA	2.56	0.41
2:C:999:FAD:H1'2	2:C:999:FAD:H9	1.86	0.41
1:A:139:ASN:OD1	1:D:536:ARG:NH2	2.54	0.41
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.90	0.41
1:A:335:HIS:HE1	1:A:346:GLU:OE2	2.04	0.41
1:A:423:ASN:ND2	1:A:427:GLN:HE21	2.04	0.41
1:A:528:PHE:HZ	1:A:548:ILE:HD11	1.86	0.41
1:B:419:ARG:NH2	1:B:508:THR:HG21	2.28	0.41
1:B:656:ASN:O	1:B:657:LEU:HB2	2.20	0.41
1:C:321:MET:HE3	1:C:469:LEU:HD23	2.02	0.41
1:C:635:GLY:HA2	1:C:638:MET:HE3	2.02	0.41
1:D:265:ARG:HH11	1:D:265:ARG:HD3	1.52	0.41
1:D:390:TYR:CE2	1:D:469:LEU:HD13	2.56	0.41
1:A:526:GLU:HB2	1:A:595:PHE:CZ	2.55	0.40
1:B:268:TRP:CE2	1:B:277:HIS:HB2	2.55	0.40
1:B:288:GLU:OE1	1:B:298:THR:HG22	2.20	0.40
1:A:559:PHE:HD1	1:A:560:PRO:HD2	1.86	0.40
1:B:117:ARG:HH11	1:B:117:ARG:HD3	1.67	0.40
1:C:390:TYR:CD2	1:C:502:GLN:HG3	2.56	0.40
1:C:508:THR:CA	4:C:2097:HOH:O	2.70	0.40
1:D:167:GLU:HA	1:D:170:LYS:HE3	2.02	0.40
1:C:342:ARG:HH11	1:C:342:ARG:HD3	1.65	0.40
1:C:555:LYS:HZ2	1:C:597:GLN:NE2	2.19	0.40
1:B:133:GLN:OE1	1:B:139:ASN:O	2.40	0.40
1:C:510:VAL:H	1:C:511:ILE:HD12	1.86	0.40
1:D:421:MET:HE2	1:D:421:MET:HB2	1.90	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ARG:NE	1:C:151:ASN:OD1[1_556]	1.55	0.65
1:B:265:ARG:NH2	1:C:152:PRO:CD[1_556]	1.67	0.53
1:B:134:ASN:OD1	4:C:2180:HOH:O[1_546]	1.85	0.35
1:B:265:ARG:NH2	1:C:151:ASN:CA[1_556]	1.98	0.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:ARG:NH2	1:C:150:LEU:O[1_556]	2.14	0.06
1:B:265:ARG:NH2	1:C:152:PRO:N[1_556]	2.16	0.04
1:B:139:ASN:ND2	1:C:536:ARG:NH2[1_546]	2.17	0.03

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	553/658 (84%)	542 (98%)	10 (2%)	1 (0%)	47	38
1	B	537/658 (82%)	516 (96%)	21 (4%)	0	100	100
1	C	556/658 (84%)	536 (96%)	18 (3%)	2 (0%)	34	24
1	D	548/658 (83%)	534 (97%)	14 (3%)	0	100	100
All	All	2194/2632 (83%)	2128 (97%)	63 (3%)	3 (0%)	51	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	506	LEU
1	C	508	THR
1	A	140	LEU

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	480/545 (88%)	456 (95%)	24 (5%)	24	15
1	B	464/545 (85%)	430 (93%)	34 (7%)	14	6
1	C	480/545 (88%)	458 (95%)	22 (5%)	27	17
1	D	473/545 (87%)	439 (93%)	34 (7%)	14	6
All	All	1897/2180 (87%)	1783 (94%)	114 (6%)	19	9

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	108	LYS
1	A	120	LEU
1	A	138	ILE
1	A	140	LEU
1	A	141	ASP
1	A	162	GLU
1	A	191	LEU
1	A	263	MET
1	A	323	LYS
1	A	342	ARG
1	A	406	ARG
1	A	439	ILE
1	A	463	LEU
1	A	475	GLU
1	A	476	LYS
1	A	507	LEU
1	A	515	ARG
1	A	516	ASP
1	A	520	GLU
1	A	529	GLU
1	A	559	PHE
1	A	586	ARG
1	A	596	GLU
1	A	646	VAL
1	B	86	LYS
1	B	94	ASN
1	B	105	LEU
1	B	114	THR
1	B	116	LYS
1	B	120	LEU
1	B	140	LEU
1	B	162	GLU
1	B	195	PHE

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Mol	Chain	Res	Type
1	B	197	LEU
1	B	199	GLU
1	B	263	MET
1	B	265	ARG
1	B	298	THR
1	B	323	LYS
1	B	349	CYS
1	B	396	PRO
1	B	406	ARG
1	B	421	MET
1	B	428	PHE
1	B	432	LEU
1	B	459	ASP
1	B	475	GLU
1	B	476	LYS
1	B	482	LYS
1	B	498	GLU
1	B	508	THR
1	B	520	GLU
1	B	529	GLU
1	B	555	LYS
1	B	559	PHE
1	B	568	THR
1	B	589	SER
1	B	613	LEU
1	C	86	LYS
1	C	102	LYS
1	C	105	LEU
1	C	108	LYS
1	C	114	THR
1	C	120	LEU
1	C	127	THR
1	C	143	LYS
1	C	150	LEU
1	C	162	GLU
1	C	199	GLU
1	C	224	LEU
1	C	323	LYS
1	C	406	ARG
1	C	432	LEU
1	C	461	ASN
1	C	463	LEU

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Mol	Chain	Res	Type
1	C	490	LYS
1	C	498	GLU
1	C	559	PHE
1	C	586	ARG
1	C	613	LEU
1	D	86	LYS
1	D	102	LYS
1	D	106	ASN
1	D	107	LYS
1	D	116	LYS
1	D	127	THR
1	D	128	PHE
1	D	134	ASN
1	D	141	ASP
1	D	143	LYS
1	D	149	SER
1	D	150	LEU
1	D	151	ASN
1	D	162	GLU
1	D	180	ASP
1	D	199	GLU
1	D	224	LEU
1	D	263	MET
1	D	323	LYS
1	D	388	GLN
1	D	389	LYS
1	D	406	ARG
1	D	474	ARG
1	D	476	LYS
1	D	479	GLN
1	D	482	LYS
1	D	508	THR
1	D	511	ILE
1	D	529	GLU
1	D	559	PHE
1	D	564	THR
1	D	581	PHE
1	D	586	ARG
1	D	613	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	172	ASN
1	A	177	GLN
1	A	187	HIS
1	A	189	HIS
1	A	215	HIS
1	A	272	ASN
1	A	290	GLN
1	A	328	ASN
1	A	335	HIS
1	A	427	GLN
1	A	500	ASN
1	A	615	HIS
1	A	616	HIS
1	B	94	ASN
1	B	133	GLN
1	B	177	GLN
1	B	277	HIS
1	B	423	ASN
1	B	425	GLN
1	B	597	GLN
1	B	650	ASN
1	B	656	ASN
1	C	110	GLN
1	C	139	ASN
1	C	272	ASN
1	C	285	GLN
1	C	388	GLN
1	C	400	GLN
1	C	597	GLN
1	C	650	ASN
1	C	656	ASN
1	D	106	ASN
1	D	110	GLN
1	D	133	GLN
1	D	151	ASN
1	D	177	GLN
1	D	597	GLN
1	D	650	ASN
1	D	656	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	A	1660	-	4,4,4	0.69	0	6,6,6	0.50	0
3	SO4	A	1659	-	4,4,4	0.66	0	6,6,6	0.62	0
2	FAD	A	999	-	53,58,58	2.00	14 (26%)	68,89,89	1.99	19 (27%)
2	FAD	D	999	-	53,58,58	1.33	5 (9%)	68,89,89	1.68	15 (22%)
2	FAD	C	999	-	53,58,58	1.87	13 (24%)	68,89,89	1.97	22 (32%)
2	FAD	B	999	-	53,58,58	2.08	16 (30%)	68,89,89	1.91	20 (29%)
3	SO4	B	1659	-	4,4,4	0.39	0	6,6,6	0.50	0
3	SO4	D	1659	-	4,4,4	0.51	0	6,6,6	0.91	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	C	999	-	-	3/30/50/50	0/6/6/6
2	FAD	A	999	-	-	6/30/50/50	0/6/6/6
2	FAD	D	999	-	-	3/30/50/50	0/6/6/6
2	FAD	B	999	-	-	3/30/50/50	0/6/6/6

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	999	FAD	C1'-C2'	6.00	1.61	1.52
2	A	999	FAD	O4B-C1B	5.90	1.49	1.41
2	B	999	FAD	C5'-C4'	5.69	1.59	1.51
2	B	999	FAD	C4A-N3A	-5.49	1.28	1.35
2	A	999	FAD	C9A-C5X	5.28	1.50	1.41
2	B	999	FAD	C9A-C5X	4.98	1.49	1.41
2	A	999	FAD	C2A-N3A	4.46	1.39	1.32
2	D	999	FAD	C4X-N5	4.14	1.38	1.30
2	C	999	FAD	C2A-N3A	4.05	1.38	1.32
2	C	999	FAD	C5X-N5	-3.92	1.31	1.39
2	B	999	FAD	C4X-N5	3.91	1.38	1.30
2	B	999	FAD	C8-C7	3.63	1.49	1.40
2	A	999	FAD	C4X-N5	3.62	1.37	1.30
2	A	999	FAD	C2A-N1A	3.56	1.40	1.33
2	B	999	FAD	O4B-C1B	3.35	1.45	1.41
2	C	999	FAD	C4-N3	-3.30	1.32	1.38
2	A	999	FAD	PA-O2A	-3.30	1.39	1.55
2	A	999	FAD	C8-C7	3.29	1.49	1.40
2	C	999	FAD	C4X-N5	3.27	1.37	1.30
2	C	999	FAD	O4B-C1B	3.25	1.45	1.41
2	A	999	FAD	C6-C5X	-3.13	1.35	1.40
2	A	999	FAD	C5A-C4A	3.06	1.49	1.40
2	B	999	FAD	C5A-C4A	2.99	1.48	1.40
2	B	999	FAD	C1'-C2'	2.81	1.56	1.52
2	B	999	FAD	PA-O2A	-2.66	1.42	1.55
2	C	999	FAD	O2-C2	2.61	1.29	1.24
2	B	999	FAD	C9A-N10	2.52	1.45	1.41
2	B	999	FAD	C5A-N7A	-2.51	1.30	1.39
2	C	999	FAD	C8M-C8	2.49	1.56	1.51
2	A	999	FAD	C8M-C8	2.47	1.56	1.51
2	A	999	FAD	O4-C4	2.46	1.28	1.23
2	C	999	FAD	C5A-C4A	2.45	1.47	1.40
2	B	999	FAD	C2-N3	-2.44	1.33	1.39
2	A	999	FAD	C9-C9A	2.44	1.43	1.39
2	B	999	FAD	O2-C2	2.41	1.28	1.24
2	D	999	FAD	O4'-C4'	2.26	1.48	1.43
2	C	999	FAD	C6-C7	2.23	1.42	1.39
2	A	999	FAD	C6A-N6A	2.23	1.42	1.34
2	C	999	FAD	C10-N10	-2.21	1.32	1.37
2	D	999	FAD	C2-N3	-2.21	1.33	1.39
2	D	999	FAD	C8-C7	2.19	1.46	1.40
2	D	999	FAD	O4B-C1B	-2.17	1.38	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	999	FAD	C2-N1	-2.14	1.31	1.36
2	B	999	FAD	C10-N1	2.13	1.37	1.33
2	C	999	FAD	C8-C7	2.11	1.46	1.40
2	B	999	FAD	C5X-N5	-2.08	1.35	1.39
2	B	999	FAD	P-O5'	2.08	1.67	1.59
2	A	999	FAD	P-O1P	-2.01	1.43	1.50

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	999	FAD	N3A-C2A-N1A	-7.25	117.34	128.68
2	A	999	FAD	C4-C4X-N5	5.23	125.67	118.23
2	C	999	FAD	C4-C4X-N5	4.84	125.11	118.23
2	B	999	FAD	C4A-C5A-N7A	-4.83	104.37	109.40
2	C	999	FAD	C10-N1-C2	4.64	126.19	116.90
2	D	999	FAD	C5X-C9A-N10	4.55	122.65	117.95
2	C	999	FAD	C4X-C4-N3	4.50	124.63	113.19
2	C	999	FAD	C4-N3-C2	-4.46	117.41	125.64
2	B	999	FAD	C10-N1-C2	4.37	125.65	116.90
2	B	999	FAD	O4B-C1B-C2B	-4.15	100.86	106.93
2	C	999	FAD	C7M-C7-C6	-3.91	112.26	119.49
2	B	999	FAD	C5X-C9A-N10	3.88	121.96	117.95
2	D	999	FAD	C9A-C5X-N5	-3.80	118.30	122.43
2	D	999	FAD	O4-C4-C4X	-3.79	116.54	126.60
2	A	999	FAD	O2-C2-N1	-3.66	115.76	121.83
2	D	999	FAD	C1B-N9A-C4A	-3.56	120.38	126.64
2	C	999	FAD	C4X-C10-N1	-3.53	116.54	124.73
2	B	999	FAD	C9A-C5X-N5	-3.51	118.62	122.43
2	B	999	FAD	C4-C4X-N5	3.43	123.12	118.23
2	B	999	FAD	N3A-C2A-N1A	-3.24	123.61	128.68
2	B	999	FAD	C5A-C6A-N6A	3.22	125.24	120.35
2	A	999	FAD	C8M-C8-C9	3.17	125.36	119.49
2	C	999	FAD	O4-C4-C4X	-3.17	118.18	126.60
2	C	999	FAD	C7M-C7-C8	3.16	127.22	120.74
2	A	999	FAD	C4X-C4-N3	3.06	120.95	113.19
2	B	999	FAD	C3B-C2B-C1B	3.04	105.56	100.98
2	A	999	FAD	C2A-N1A-C6A	3.02	123.93	118.75
2	A	999	FAD	O4-C4-C4X	-3.01	118.61	126.60
2	B	999	FAD	C4X-C4-N3	3.00	120.80	113.19
2	C	999	FAD	O4'-C4'-C5'	-2.92	103.34	109.92
2	A	999	FAD	O4'-C4'-C5'	-2.87	103.46	109.92
2	D	999	FAD	O5'-C5'-C4'	-2.87	101.70	109.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	999	FAD	C7M-C7-C8	-2.86	114.88	120.74
2	D	999	FAD	O2-C2-N1	-2.83	117.14	121.83
2	B	999	FAD	C8M-C8-C9	-2.82	114.28	119.49
2	B	999	FAD	O2-C2-N3	2.81	124.10	118.65
2	C	999	FAD	C1B-N9A-C4A	-2.76	121.80	126.64
2	C	999	FAD	N6A-C6A-N1A	2.74	124.26	118.57
2	C	999	FAD	N3A-C2A-N1A	-2.71	124.45	128.68
2	A	999	FAD	C1B-N9A-C4A	-2.69	121.91	126.64
2	B	999	FAD	O3B-C3B-C4B	-2.66	103.35	111.05
2	B	999	FAD	C9A-N10-C10	-2.65	116.64	120.77
2	B	999	FAD	C4X-C10-N1	-2.56	118.78	124.73
2	C	999	FAD	C9A-C5X-N5	-2.55	119.66	122.43
2	C	999	FAD	O2-C2-N1	-2.53	117.63	121.83
2	D	999	FAD	O2A-PA-O1A	2.52	124.69	112.24
2	D	999	FAD	O4-C4-N3	2.51	124.93	120.12
2	B	999	FAD	O4-C4-C4X	-2.46	120.06	126.60
2	A	999	FAD	C3B-C2B-C1B	2.46	104.67	100.98
2	D	999	FAD	O4B-C1B-C2B	-2.45	103.35	106.93
2	B	999	FAD	O2-C2-N1	-2.44	117.79	121.83
2	C	999	FAD	C2A-N1A-C6A	2.37	122.80	118.75
2	A	999	FAD	C4A-C5A-N7A	-2.35	106.95	109.40
2	B	999	FAD	C4-C4X-C10	-2.34	112.86	116.79
2	B	999	FAD	C4X-C10-N10	2.27	119.80	116.48
2	D	999	FAD	O2'-C2'-C1'	2.24	115.21	109.80
2	D	999	FAD	O2B-C2B-C3B	-2.22	104.63	111.82
2	A	999	FAD	C5'-C4'-C3'	2.21	116.48	112.20
2	D	999	FAD	O4B-C4B-C3B	-2.20	100.77	105.11
2	A	999	FAD	O2-C2-N3	2.16	122.85	118.65
2	D	999	FAD	C3B-C2B-C1B	2.13	104.19	100.98
2	C	999	FAD	C4X-C10-N10	2.13	119.59	116.48
2	C	999	FAD	C3B-C2B-C1B	2.11	104.15	100.98
2	C	999	FAD	C5X-N5-C4X	2.10	121.57	118.07
2	A	999	FAD	C5X-N5-C4X	2.07	121.51	118.07
2	A	999	FAD	O4B-C1B-C2B	-2.07	103.91	106.93
2	A	999	FAD	C9-C8-C7	-2.05	116.73	119.67
2	C	999	FAD	C10-C4X-N5	-2.04	120.53	124.86
2	B	999	FAD	C8M-C8-C7	2.03	124.90	120.74
2	C	999	FAD	O3'-C3'-C4'	2.03	113.72	108.81
2	C	999	FAD	C8M-C8-C7	2.02	124.88	120.74
2	D	999	FAD	C4X-C4-N3	2.02	118.32	113.19
2	C	999	FAD	C4'-C3'-C2'	2.02	117.55	113.36
2	A	999	FAD	C10-C4X-N5	-2.01	120.59	124.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	999	FAD	N6A-C6A-N1A	2.01	122.74	118.57
2	A	999	FAD	O5'-C5'-C4'	-2.01	104.00	109.36

There are no chirality outliers.

All (15) torsion outliers are listed below:

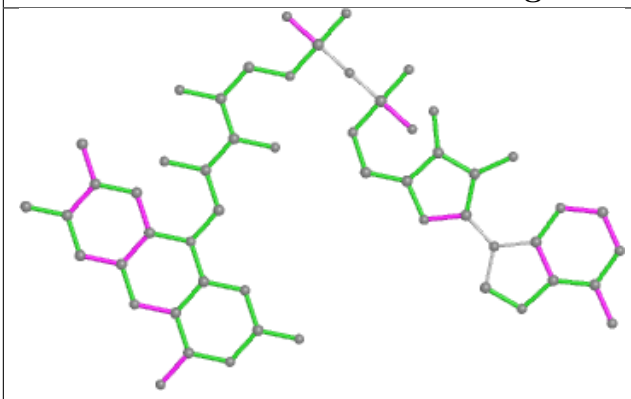
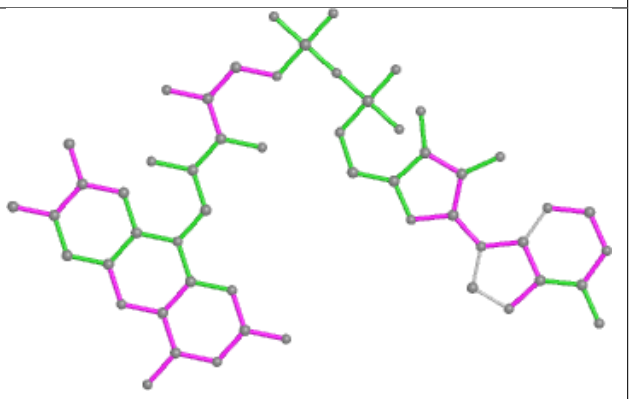
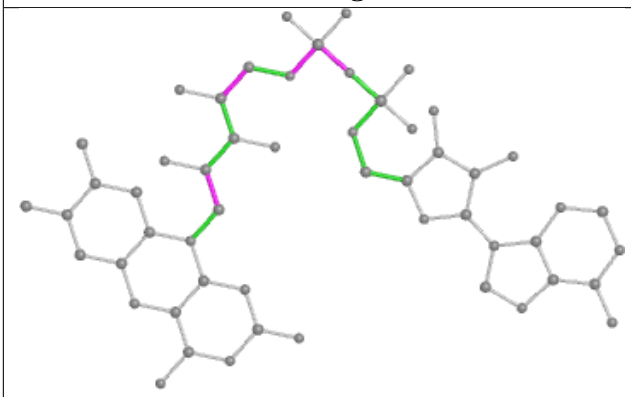
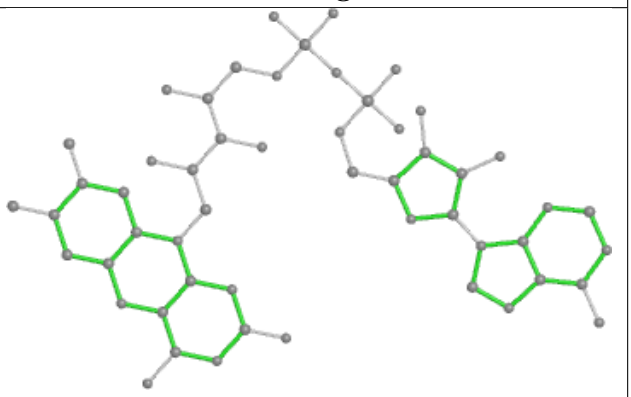
Mol	Chain	Res	Type	Atoms
2	A	999	FAD	N10-C1'-C2'-O2'
2	A	999	FAD	N10-C1'-C2'-C3'
2	B	999	FAD	N10-C1'-C2'-O2'
2	B	999	FAD	N10-C1'-C2'-C3'
2	C	999	FAD	N10-C1'-C2'-O2'
2	C	999	FAD	N10-C1'-C2'-C3'
2	D	999	FAD	N10-C1'-C2'-O2'
2	D	999	FAD	N10-C1'-C2'-C3'
2	A	999	FAD	O4'-C4'-C5'-O5'
2	A	999	FAD	PA-O3P-P-O2P
2	B	999	FAD	PA-O3P-P-O1P
2	C	999	FAD	PA-O3P-P-O2P
2	A	999	FAD	C3'-C4'-C5'-O5'
2	A	999	FAD	C5'-O5'-P-O1P
2	D	999	FAD	C5'-O5'-P-O1P

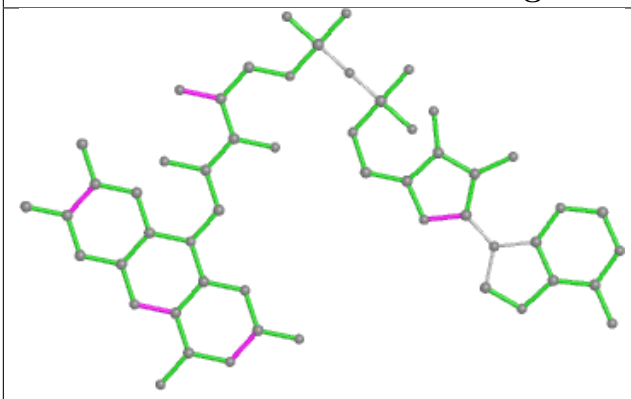
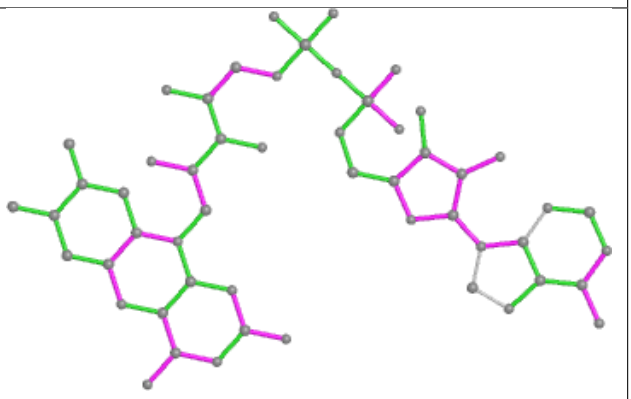
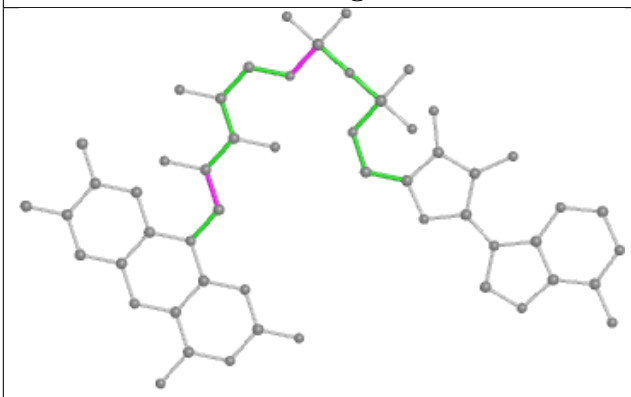
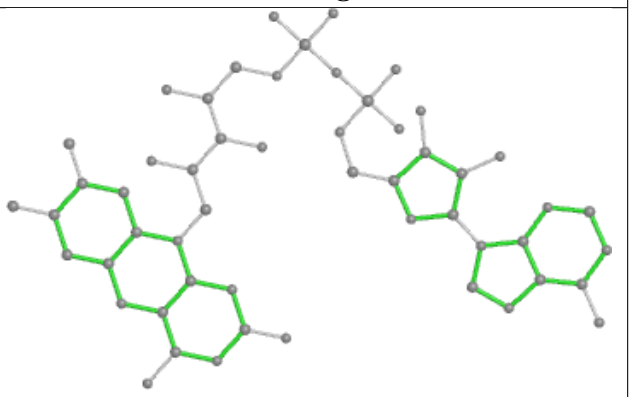
There are no ring outliers.

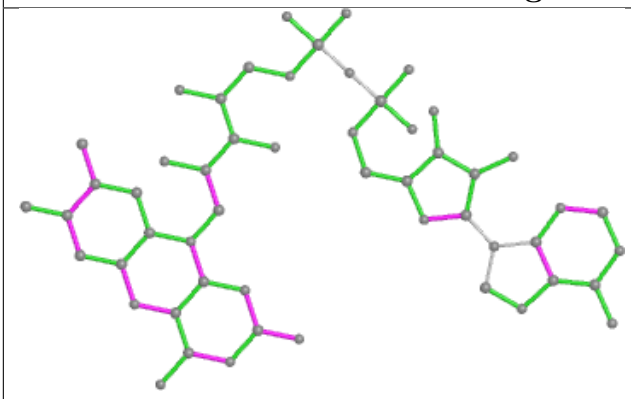
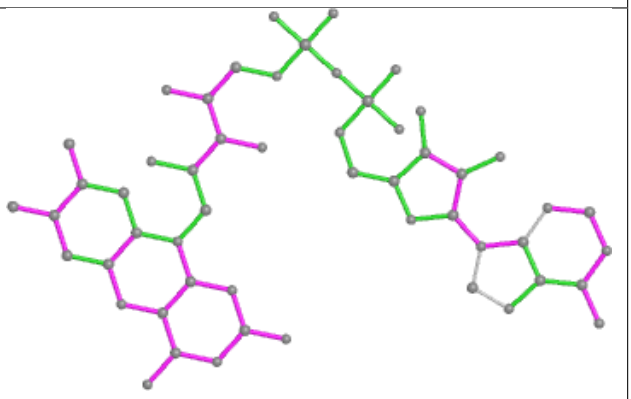
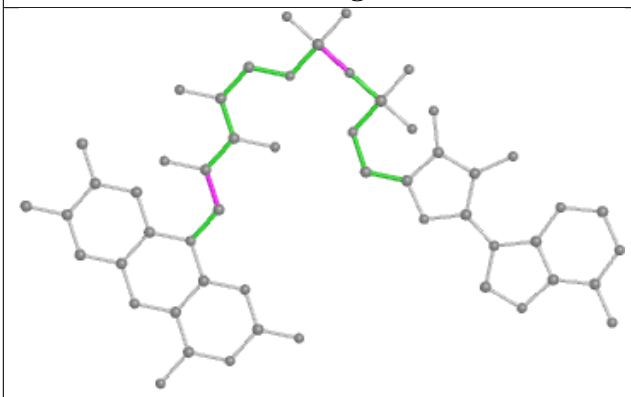
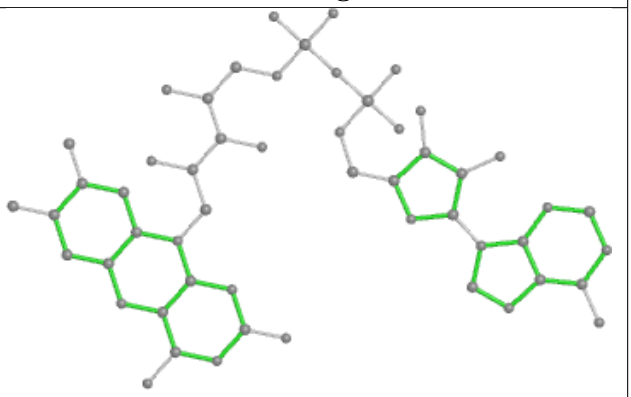
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	999	FAD	1	0

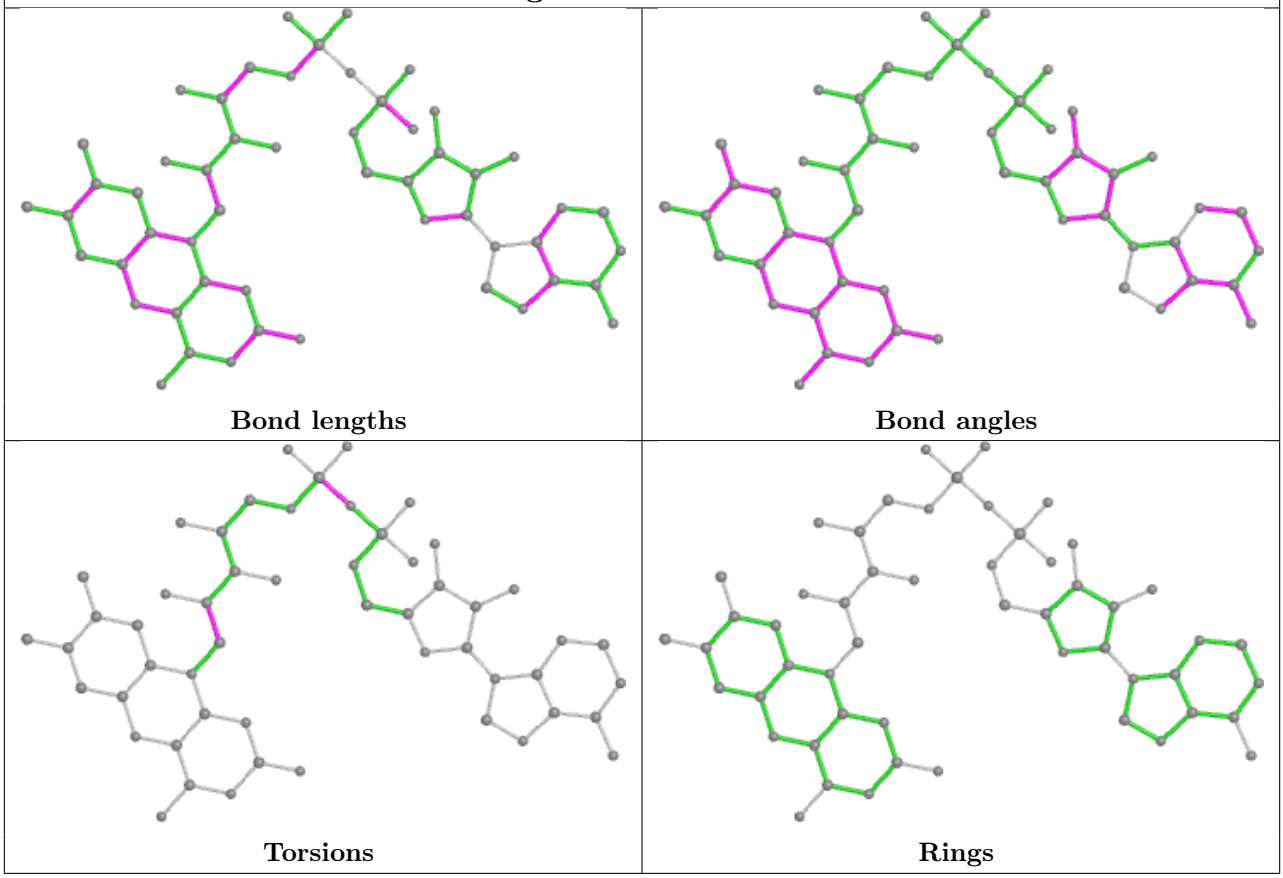
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 FAD A 999	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FAD D 999	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FAD C 999	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand FAD B 999



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	555/658 (84%)	0.01	24 (4%)	35	38	11, 26, 55, 88	0
1	B	543/658 (82%)	0.16	26 (4%)	30	33	14, 30, 59, 84	0
1	C	557/658 (84%)	0.05	22 (3%)	39	42	11, 27, 55, 75	1 (0%)
1	D	550/658 (83%)	0.18	23 (4%)	36	39	12, 32, 60, 78	0
All	All	2205/2632 (83%)	0.10	95 (4%)	35	38	11, 29, 58, 88	1 (0%)

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	460	PRO	6.0
1	B	458	PHE	6.0
1	A	559	PHE	4.8
1	D	559	PHE	4.7
1	B	435	GLN	4.6
1	B	434	PRO	4.5
1	A	155	THR	4.2
1	B	559	PHE	4.2
1	A	435	GLN	4.0
1	B	522	TYR	4.0
1	B	587	GLY	4.0
1	C	460	PRO	3.9
1	D	137	GLY	3.8
1	D	589	SER	3.8
1	C	107	LYS	3.6
1	D	107	LYS	3.6
1	A	81	GLY	3.6
1	C	431	ALA	3.6
1	A	441	THR	3.4
1	A	142	HIS	3.4
1	A	442	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	162	GLU	3.3
1	C	587	GLY	3.3
1	B	459	ASP	3.3
1	D	159	ILE	3.2
1	C	457	GLY	3.2
1	D	116	LYS	3.2
1	A	589	SER	3.1
1	C	461	ASN	3.1
1	A	159	ILE	3.1
1	D	553	LYS	3.1
1	C	141	ASP	3.0
1	A	437	SER	3.0
1	C	435	GLN	3.0
1	D	430	HIS	3.0
1	B	163	ASP	2.9
1	D	462	GLN	2.9
1	A	154	ASP	2.9
1	B	250	ASP	2.9
1	A	438	SER	2.9
1	A	157	PRO	2.9
1	C	433	LYS	2.9
1	D	139	ASN	2.8
1	C	336[A]	MET	2.8
1	B	506	LEU	2.8
1	C	430	HIS	2.8
1	C	499	ASP	2.7
1	A	434	PRO	2.7
1	B	197	LEU	2.7
1	C	82	ILE	2.6
1	C	170	LYS	2.6
1	B	509	TYR	2.6
1	A	82	ILE	2.6
1	A	436	VAL	2.6
1	B	157	PRO	2.6
1	D	558	GLN	2.6
1	B	172	ASN	2.5
1	C	558	GLN	2.5
1	C	589	SER	2.5
1	D	252	THR	2.5
1	D	163	ASP	2.5
1	B	508	THR	2.5
1	A	139	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	116	LYS	2.5
1	D	498	GLU	2.5
1	D	506	LEU	2.5
1	B	589	SER	2.5
1	C	166	HIS	2.5
1	B	590	ASP	2.5
1	B	265	ARG	2.4
1	B	228	TYR	2.4
1	A	250	ASP	2.3
1	D	141	ASP	2.3
1	A	588	ILE	2.3
1	D	426	PHE	2.3
1	C	459	ASP	2.3
1	A	93	TRP	2.3
1	B	199	GLU	2.3
1	C	432	LEU	2.3
1	A	200	GLY	2.2
1	A	199	GLU	2.2
1	A	461	ASN	2.2
1	C	427	GLN	2.2
1	A	520	GLU	2.2
1	C	458	PHE	2.2
1	B	505	TYR	2.1
1	B	430	HIS	2.1
1	D	134	ASN	2.1
1	B	432	LEU	2.1
1	D	489	ALA	2.1
1	D	105	LEU	2.1
1	D	162	GLU	2.0
1	D	386	GLU	2.0
1	C	108	LYS	2.0
1	D	476	LYS	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 (i)

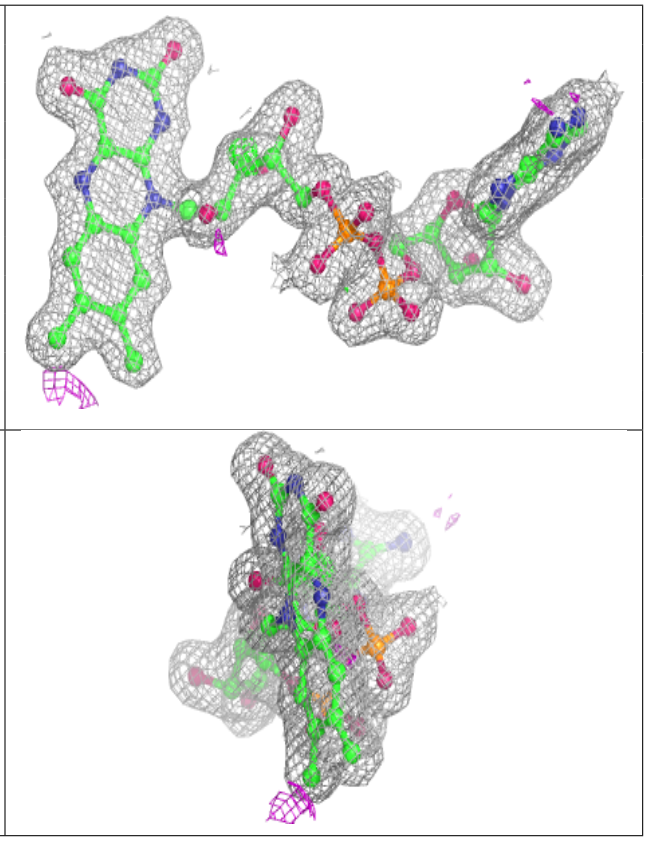
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	B	1659	5/5	0.94	0.23	41,51,57,66	0
3	SO4	D	1659	5/5	0.95	0.15	39,40,44,58	0
3	SO4	A	1659	5/5	0.96	0.17	34,37,43,59	0
3	SO4	A	1660	5/5	0.96	0.19	47,51,61,62	0
2	FAD	B	999	53/53	0.98	0.08	13,15,19,20	0
2	FAD	D	999	53/53	0.98	0.07	10,13,17,21	0
2	FAD	A	999	53/53	0.98	0.07	10,14,17,18	0
2	FAD	C	999	53/53	0.99	0.07	9,12,16,19	0

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

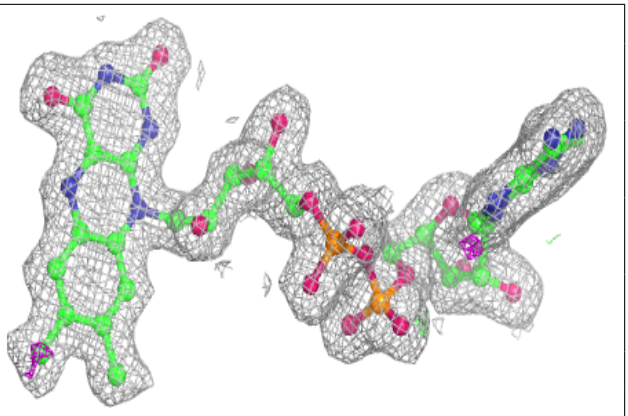
Electron density around FAD B 999:

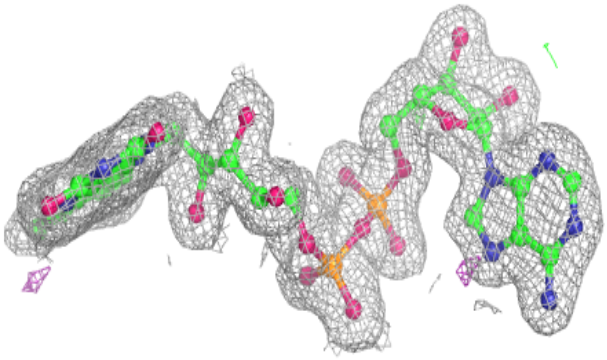
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

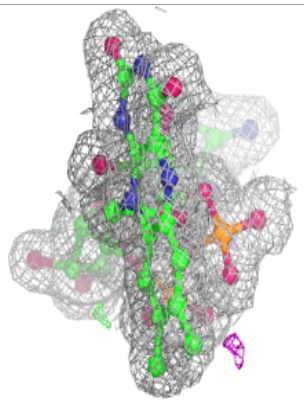


Electron density around FAD D 999:

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

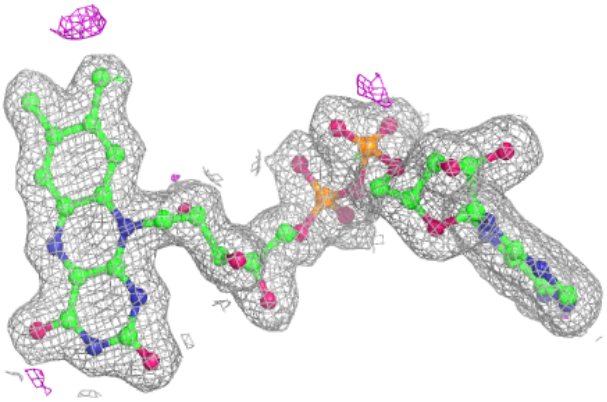


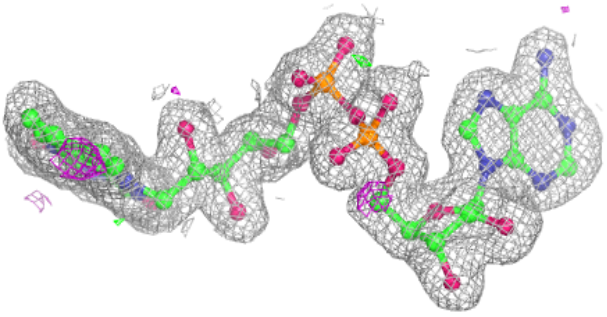


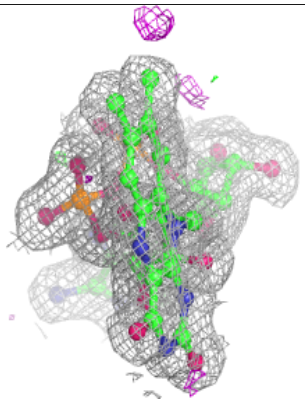


Electron density around FAD A 999:

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

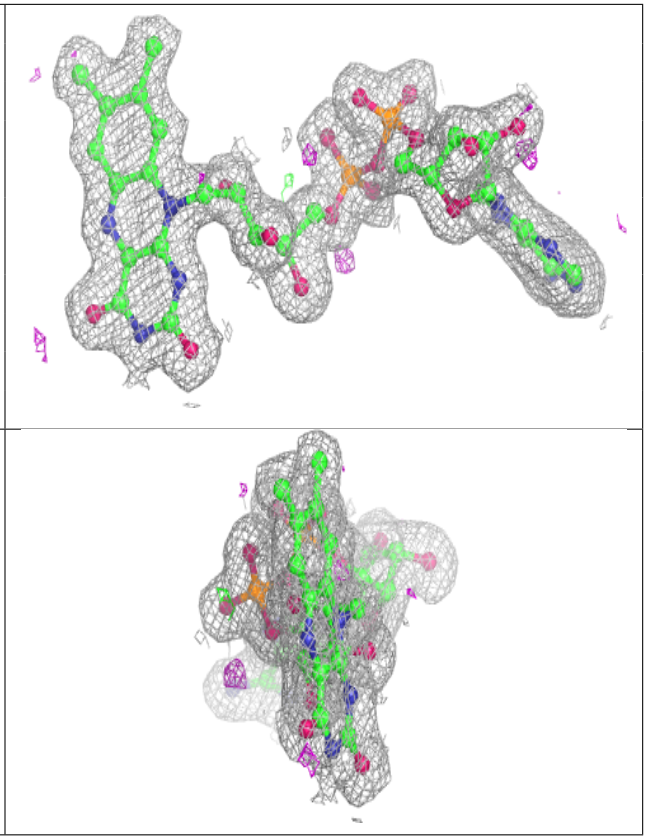






Electron density around FAD C 999:

$2mF_o$-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.