Full wwPDB X-ray Structure Validation Report (i)

Nov 7, 2023 – 12:42 PM EST

PDB ID	:	3CUK
Title	:	Crystal structure of human D-amino acid oxidase: bound to an inhibitor
Authors	:	Prasad, S.; Munshi, S.
Deposited on	:	2008-04-16
Resolution	:	2.49 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:

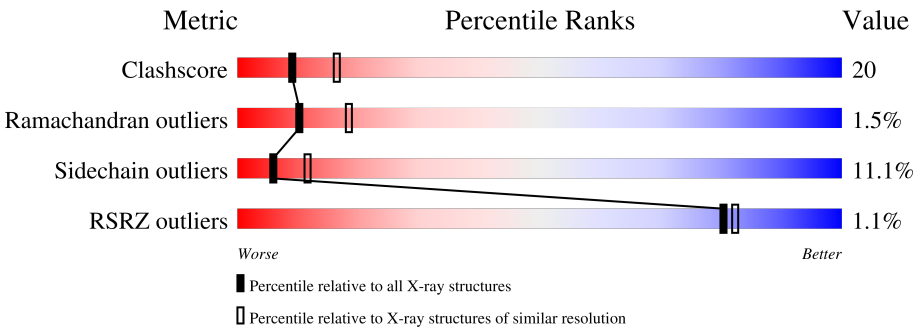
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.49 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	347	.% 60% 29% 5% 6%
1	B	347	2% 57% 30% 7% • 6%
1	C	347	.% 54% 32% 7% • 6%
1	D	347	52% 34% 9% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 10850 atoms, of which 0 are hydrogens and 0 are deuteriums.

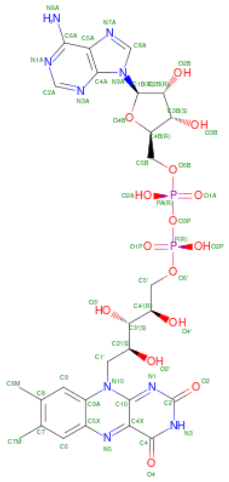
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called D-amino-acid oxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	327	2638	1696	460	473	9	0	0	0
1	B	327	2638	1696	460	473	9	0	0	0
1	C	327	2638	1696	460	473	9	0	0	0
1	D	327	2638	1696	460	473	9	0	0	0

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

FAD



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

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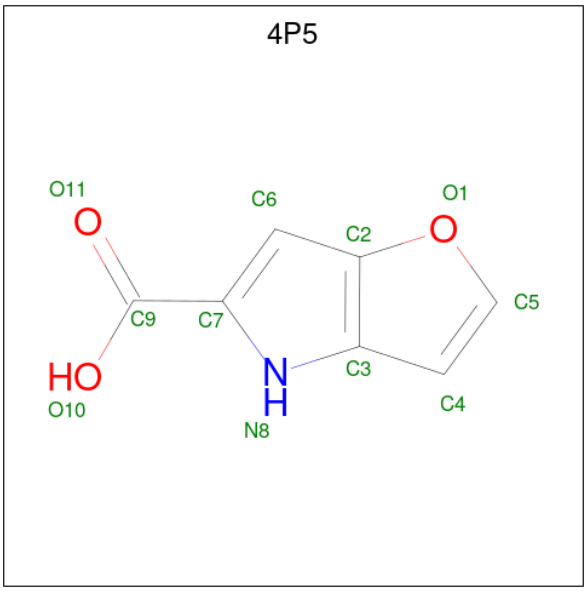
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	C	1	53	27	9	15	2	0	0
			Total	C	N	O	P		
2	D	1	53	27	9	15	2	0	0

- Molecule 3 is 4H-furo[3,2-b]pyrrole-5-carboxylic acid (three-letter code: 4P5) (formula: $C_7H_5NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	11	7	1	3	0	0
			Total	C	N	O		
3	B	1	11	7	1	3	0	0
			Total	C	N	O		
3	C	1	11	7	1	3	0	0
			Total	C	N	O		
3	D	1	11	7	1	3	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	13	13	13	0	0
			Total	O		
4	B	13	13	13	0	0
			Total	O		
4	C	7	7	7	0	0

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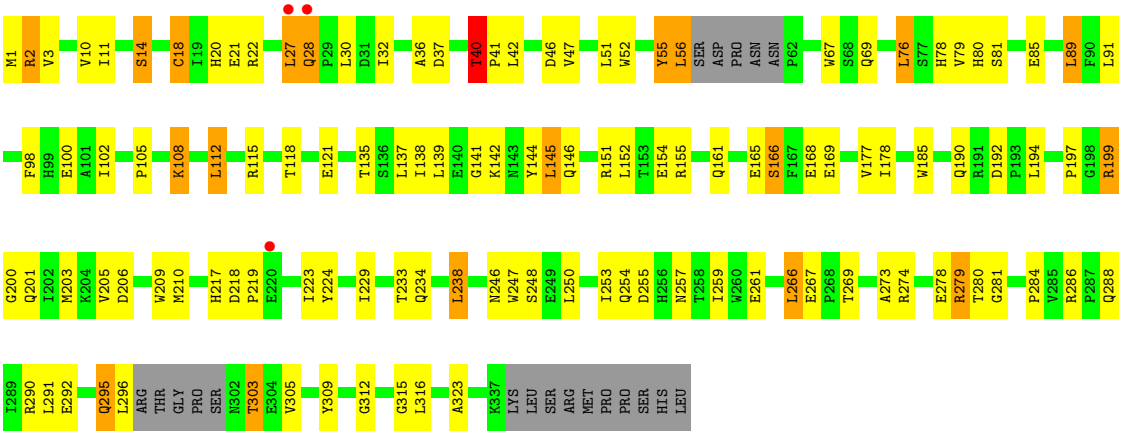
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	D	9	9	9	0	0

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.

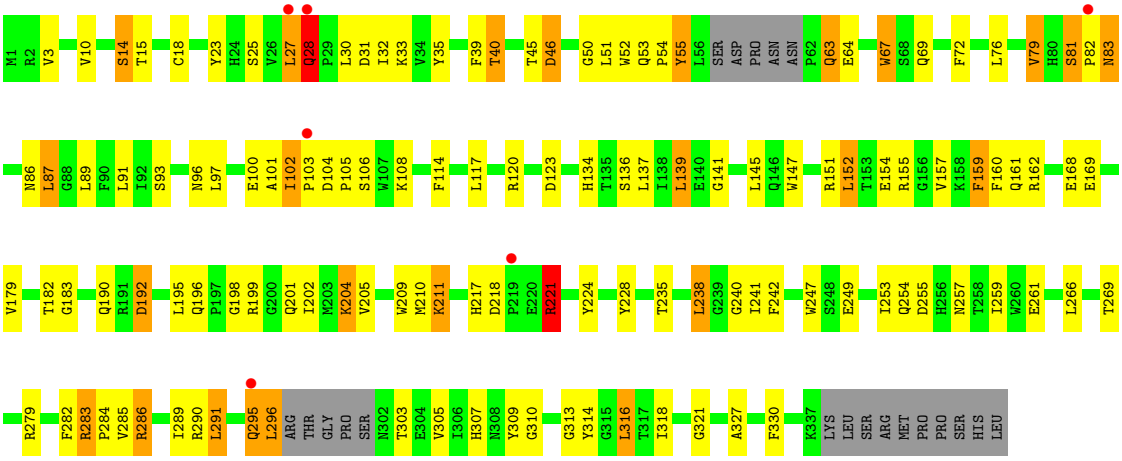
• Molecule 1: D-amino-acid oxidase

Chain A:



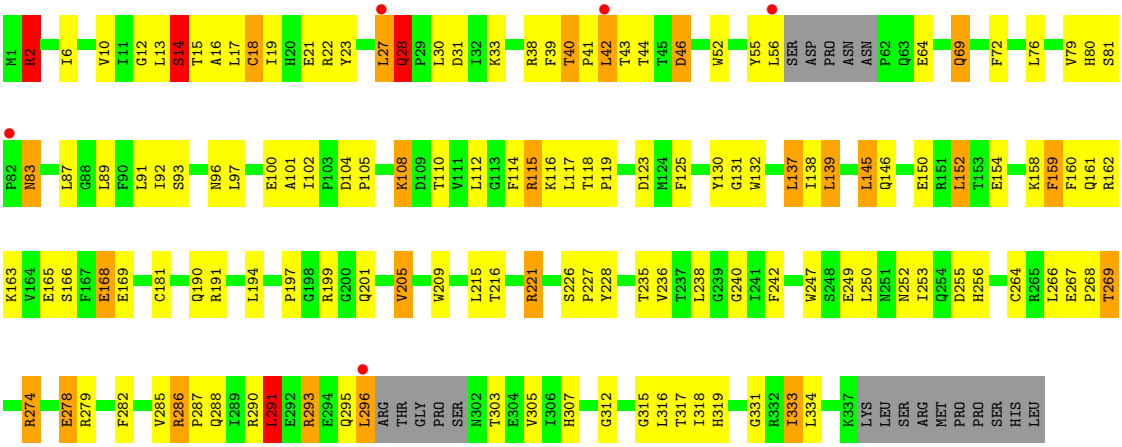
• Molecule 1: D-amino-acid oxidase

Chain B:



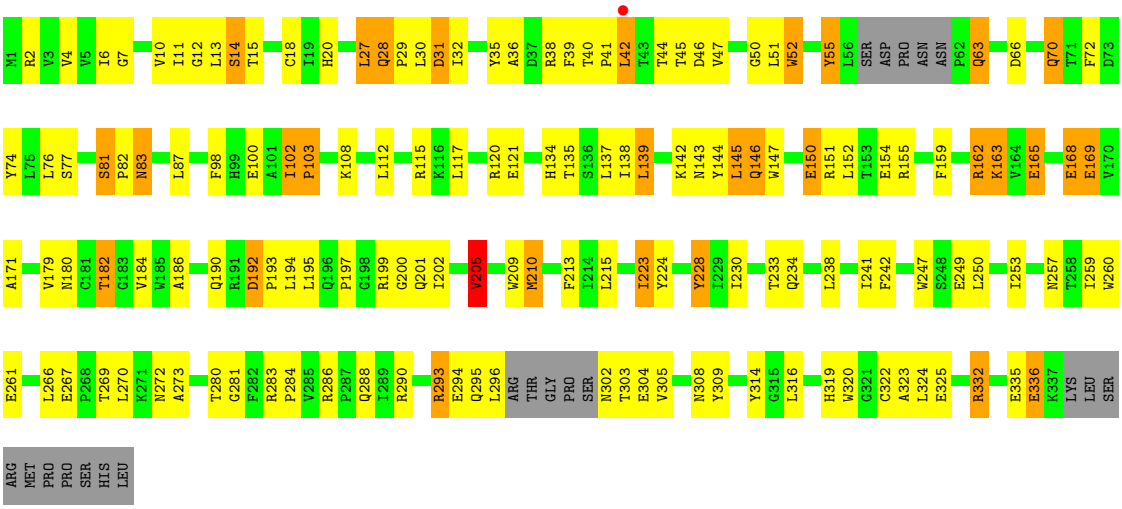
• Molecule 1: D-amino-acid oxidase

Chain C:



- Molecule 1: D-amino-acid oxidase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	187.73Å 51.15Å 153.29Å 90.00° 110.45° 90.00°	Depositor
Resolution (Å)	42.52 – 2.49 42.52 – 2.49	Depositor EDS
% Data completeness (in resolution range)	96.5 (42.52-2.49) 82.9 (42.52-2.49)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.79 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.239 , 0.329 0.237 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	31.4	Xtriage
Anisotropy	0.525	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 42.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10850	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 75.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3595e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: FAD, 4P5

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	9/2711 (0.3%)	1.24	11/3685 (0.3%)
1	B	1.32	7/2711 (0.3%)	1.24	17/3685 (0.5%)
1	C	1.25	8/2711 (0.3%)	1.21	16/3685 (0.4%)
1	D	1.35	14/2711 (0.5%)	1.21	5/3685 (0.1%)
All	All	1.32	38/10844 (0.4%)	1.22	49/14740 (0.3%)

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	18	CYS	CB-SG	-10.74	1.64	1.82
1	A	18	CYS	CB-SG	-9.15	1.66	1.82
1	D	228	TYR	CG-CD1	8.01	1.49	1.39
1	A	168	GLU	CG-CD	7.96	1.63	1.51
1	A	55	TYR	CD1-CE1	7.85	1.51	1.39
1	D	322	CYS	CB-SG	7.85	1.95	1.82
1	D	52	TRP	CB-CG	7.37	1.63	1.50
1	D	314	TYR	CD1-CE1	7.30	1.50	1.39
1	C	228	TYR	CE2-CZ	6.89	1.47	1.38
1	D	228	TYR	CD2-CE2	6.55	1.49	1.39
1	D	228	TYR	CE1-CZ	6.37	1.46	1.38
1	B	18	CYS	CB-SG	-6.28	1.71	1.82
1	A	21	GLU	CG-CD	6.25	1.61	1.51
1	B	228	TYR	CD1-CE1	6.23	1.48	1.39
1	D	314	TYR	CD2-CE2	6.02	1.48	1.39
1	D	320	TRP	CB-CG	-5.88	1.39	1.50
1	A	185	TRP	CE3-CZ3	5.85	1.48	1.38
1	C	278	GLU	CG-CD	5.84	1.60	1.51
1	D	4	VAL	CB-CG1	5.74	1.65	1.52
1	B	67	TRP	CE3-CZ3	5.69	1.48	1.38
1	D	228	TYR	CE2-CZ	5.62	1.45	1.38
1	A	52	TRP	CB-CG	5.60	1.60	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	292	GLU	CG-CD	5.55	1.60	1.51
1	C	236	VAL	CB-CG2	5.53	1.64	1.52
1	B	23	TYR	CD2-CE2	5.40	1.47	1.39
1	D	154	GLU	CB-CG	5.37	1.62	1.52
1	A	295	GLN	CG-CD	5.34	1.63	1.51
1	C	205	VAL	CB-CG2	-5.30	1.41	1.52
1	B	295	GLN	CG-CD	5.29	1.63	1.51
1	B	247	TRP	CB-CG	5.25	1.59	1.50
1	D	213	PHE	CE2-CZ	5.24	1.47	1.37
1	C	255	ASP	CB-CG	5.21	1.62	1.51
1	D	74	TYR	CB-CG	-5.18	1.43	1.51
1	A	55	TYR	CD2-CE2	5.17	1.47	1.39
1	B	209	TRP	CB-CG	-5.16	1.41	1.50
1	C	146	GLN	CG-CD	5.13	1.62	1.51
1	D	260	TRP	CE3-CZ3	5.11	1.47	1.38
1	C	163	LYS	CB-CG	5.05	1.66	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	316	LEU	CA-CB-CG	-10.03	92.23	115.30
1	A	206	ASP	CB-CG-OD1	8.00	125.50	118.30
1	B	198	GLY	N-CA-C	-7.68	93.89	113.10
1	B	286	ARG	NE-CZ-NH1	-7.60	116.50	120.30
1	B	123	ASP	CB-CG-OD1	7.13	124.72	118.30
1	A	56	LEU	CA-CB-CG	-7.10	98.98	115.30
1	B	255	ASP	CB-CG-OD1	6.81	124.43	118.30
1	C	115	ARG	NE-CZ-NH2	6.81	123.70	120.30
1	D	31	ASP	CB-CG-OD1	6.80	124.42	118.30
1	B	27	LEU	CA-CB-CG	6.77	130.86	115.30
1	A	199	ARG	NE-CZ-NH1	-6.66	116.97	120.30
1	A	112	LEU	CB-CG-CD1	-6.53	99.91	111.00
1	C	46	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	A	274	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	89	LEU	CB-CG-CD2	-6.43	100.07	111.00
1	C	137	LEU	CB-CG-CD2	-6.38	100.15	111.00
1	D	192	ASP	CB-CG-OD1	6.10	123.79	118.30
1	B	28	GLN	C-N-CD	-6.04	107.31	120.60
1	C	221	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	A	40	THR	CB-CA-C	-6.00	95.40	111.60
1	C	2	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	B	296	LEU	CA-CB-CG	5.93	128.94	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	14	SER	N-CA-CB	-5.76	101.85	110.50
1	B	316	LEU	CB-CG-CD2	5.75	120.78	111.00
1	B	91	LEU	CA-CB-CG	5.72	128.45	115.30
1	A	203	MET	CB-CG-SD	-5.68	95.37	112.40
1	C	215	LEU	CA-CB-CG	-5.68	102.24	115.30
1	C	255	ASP	CB-CG-OD1	5.66	123.39	118.30
1	C	291	LEU	CA-CB-CG	5.65	128.30	115.30
1	B	266	LEU	CB-CG-CD1	-5.64	101.41	111.00
1	B	46	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	C	286	ARG	C-N-CD	5.64	140.24	128.40
1	C	291	LEU	CB-CG-CD2	-5.63	101.42	111.00
1	B	221	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	B	296	LEU	CB-CG-CD2	5.59	120.50	111.00
1	C	296	LEU	CA-CB-CG	5.58	128.14	115.30
1	B	286	ARG	NE-CZ-NH2	5.53	123.06	120.30
1	C	279	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	C	31	ASP	CB-CG-OD1	5.49	123.24	118.30
1	D	205	VAL	CG1-CB-CG2	5.47	119.65	110.90
1	D	139	LEU	CB-CG-CD2	5.44	120.25	111.00
1	D	27	LEU	C-N-CA	5.20	134.70	121.70
1	A	279	ARG	CG-CD-NE	-5.19	100.90	111.80
1	B	192	ASP	CB-CG-OD1	5.16	122.94	118.30
1	A	266	LEU	CA-CB-CG	5.06	126.95	115.30
1	B	283	ARG	NE-CZ-NH1	5.05	122.83	120.30
1	C	250	LEU	CB-CG-CD2	-5.03	102.45	111.00
1	C	123	ASP	CB-CG-OD1	5.02	122.81	118.30
1	C	293	ARG	NE-CZ-NH2	5.01	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

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	2638	0	2587	90	0
1	B	2638	0	2587	96	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2638	0	2587	116	0
1	D	2638	0	2587	128	0
2	A	53	0	31	2	0
2	B	53	0	31	1	0
2	C	53	0	31	2	0
2	D	53	0	31	2	0
3	A	11	0	4	1	0
3	B	11	0	4	1	0
3	C	11	0	4	0	0
3	D	11	0	4	3	0
4	A	13	0	0	2	0
4	B	13	0	0	2	0
4	C	7	0	0	0	0
4	D	9	0	0	2	0
All	All	10850	0	10488	427	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 20.

All (427) 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:41:PRO:CB	1:D:41:PRO:CG	1.74	1.44
1:B:117:LEU:HD12	4:B:1001:HOH:O	1.32	1.23
1:D:40:THR:HG22	1:D:46:ASP:OD2	1.40	1.18
1:B:10:VAL:O	1:B:14:SER:HB2	1.44	1.15
1:A:55:TYR:HE2	1:A:224:TYR:OH	1.30	1.15
1:B:40:THR:HG22	1:B:46:ASP:OD2	1.47	1.10
1:C:27:LEU:HA	1:C:28:GLN:HB3	1.22	1.10
1:C:10:VAL:O	1:C:14:SER:HB2	1.54	1.08
1:B:104:ASP:HB3	1:B:108:LYS:HE2	1.11	1.06
1:C:40:THR:HG22	1:C:46:ASP:OD2	1.59	1.03
1:A:40:THR:HG22	1:A:46:ASP:OD2	1.59	1.02
1:B:199:ARG:HH22	1:B:201:GLN:NE2	1.57	1.02
1:D:165:GLU:OE2	1:D:165:GLU:HA	1.62	0.99
1:C:209:TRP:HE1	1:C:269:THR:CG2	1.75	0.98
1:B:104:ASP:CB	1:B:108:LYS:HE2	1.97	0.94
1:C:201:GLN:HE22	1:C:252:ASN:H	1.15	0.92
1:D:192:ASP:OD2	1:D:286:ARG:NH1	2.02	0.92
1:D:55:TYR:HE2	1:D:224:TYR:OH	1.53	0.91
1:D:195:LEU:HD13	1:D:309:TYR:HE2	1.36	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:LEU:HD13	1:C:316:LEU:HD22	1.52	0.90
1:B:199:ARG:NH2	1:B:201:GLN:NE2	2.21	0.88
1:A:55:TYR:CE2	1:A:224:TYR:OH	2.10	0.88
1:C:201:GLN:NE2	1:C:252:ASN:H	1.72	0.87
1:D:209:TRP:NE1	1:D:269:THR:HG21	1.89	0.86
1:C:209:TRP:NE1	1:C:269:THR:CG2	2.38	0.86
1:C:27:LEU:CA	1:C:28:GLN:HB3	2.06	0.86
1:B:79:VAL:HG23	1:B:89:LEU:HG	1.58	0.86
1:A:27:LEU:HA	1:A:28:GLN:CB	2.04	0.85
1:B:190:GLN:HE22	1:B:290:ARG:HH22	1.24	0.85
1:C:291:LEU:HA	1:C:307:HIS:O	1.75	0.85
1:A:27:LEU:CA	1:A:28:GLN:HB3	2.05	0.85
1:D:195:LEU:HD13	1:D:309:TYR:CE2	2.12	0.85
1:C:40:THR:CG2	1:C:46:ASP:OD2	2.25	0.84
1:B:199:ARG:HH22	1:B:201:GLN:HE22	1.23	0.83
1:D:233:THR:HG22	1:D:234:GLN:NE2	1.94	0.82
1:D:209:TRP:HZ2	1:D:269:THR:HG22	1.44	0.82
1:B:10:VAL:O	1:B:14:SER:CB	2.28	0.82
1:B:97:LEU:HD23	4:B:1001:HOH:O	1.78	0.82
1:B:151:ARG:O	1:B:155:ARG:HG3	1.79	0.82
1:C:199:ARG:HH22	1:C:201:GLN:NE2	1.78	0.81
1:C:209:TRP:HE1	1:C:269:THR:HG21	1.42	0.81
1:D:209:TRP:CZ2	1:D:269:THR:HG22	2.15	0.81
1:C:209:TRP:NE1	1:C:269:THR:HG21	1.95	0.80
1:D:197:PRO:HG3	1:D:247:TRP:CE2	2.18	0.78
1:B:192:ASP:OD2	1:B:286:ARG:NH1	2.15	0.78
1:D:40:THR:CG2	1:D:46:ASP:OD2	2.29	0.78
1:D:55:TYR:HE2	1:D:224:TYR:HH	0.80	0.77
1:C:40:THR:HG22	1:C:46:ASP:CG	2.04	0.77
1:C:40:THR:HG23	1:C:145:LEU:HD23	1.66	0.76
1:D:190:GLN:HE22	1:D:290:ARG:HH22	1.31	0.76
1:D:20:HIS:CE1	1:D:155:ARG:HB3	2.22	0.75
1:C:92:ILE:HG21	1:C:138:ILE:HD12	1.67	0.75
1:C:27:LEU:CD1	1:C:30:LEU:HD13	2.18	0.74
1:D:209:TRP:CZ2	1:D:269:THR:CG2	2.70	0.74
1:A:27:LEU:CB	1:A:28:GLN:HB3	2.18	0.74
1:D:40:THR:HG22	1:D:46:ASP:CG	2.09	0.73
1:C:267:GLU:OE2	1:C:269:THR:HB	1.88	0.73
1:C:199:ARG:HH22	1:C:201:GLN:HE21	1.33	0.73
1:A:27:LEU:HA	1:A:28:GLN:HB3	1.64	0.73
1:B:199:ARG:NH2	1:B:201:GLN:HE21	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:ASP:OD2	1:B:221:ARG:HG2	1.90	0.72
1:C:104:ASP:CG	1:C:108:LYS:HE3	2.10	0.72
1:A:47:VAL:HG22	1:A:279:ARG:HG2	1.70	0.72
1:D:233:THR:CG2	1:D:234:GLN:HE21	2.02	0.72
1:A:27:LEU:HA	1:A:28:GLN:HB2	1.70	0.72
1:D:171:ALA:HB2	1:D:303:THR:HG21	1.73	0.71
1:A:192:ASP:OD2	1:A:286:ARG:NH1	2.24	0.71
1:C:27:LEU:HD12	1:C:30:LEU:HD13	1.73	0.69
1:A:55:TYR:HE2	1:A:224:TYR:CZ	2.10	0.69
1:D:142:LYS:O	1:D:146:GLN:HG3	1.93	0.68
1:D:134:HIS:HD2	4:D:1046:HOH:O	1.75	0.68
1:C:2:ARG:HH22	1:C:33:LYS:HE2	1.58	0.68
1:B:27:LEU:HA	1:B:28:GLN:HB2	1.74	0.68
1:C:150:GLU:O	1:C:154:GLU:HG3	1.95	0.67
1:D:184:VAL:HG22	1:D:184:VAL:O	1.93	0.67
1:C:139:LEU:CD1	1:C:316:LEU:HD22	2.24	0.67
1:D:209:TRP:HE1	1:D:269:THR:HG21	1.56	0.66
1:B:327:ALA:O	1:B:330:PHE:HB3	1.95	0.66
1:D:142:LYS:O	1:D:146:GLN:CG	2.44	0.66
1:D:134:HIS:CD2	4:D:1046:HOH:O	2.49	0.65
1:C:201:GLN:HE22	1:C:252:ASN:N	1.91	0.65
1:D:233:THR:CG2	1:D:234:GLN:NE2	2.58	0.65
1:C:190:GLN:HE22	1:C:290:ARG:HH22	1.43	0.65
1:D:209:TRP:CE2	1:D:269:THR:HG21	2.31	0.65
1:D:199:ARG:NH2	1:D:250:LEU:O	2.30	0.64
1:D:197:PRO:HG3	1:D:247:TRP:CZ2	2.31	0.64
1:A:112:LEU:HB2	1:A:135:THR:HB	1.79	0.64
1:A:255:ASP:O	1:A:259:ILE:HG13	1.98	0.64
1:A:151:ARG:O	1:A:155:ARG:HG3	1.97	0.64
1:A:47:VAL:CG2	1:A:279:ARG:HG2	2.27	0.64
1:B:291:LEU:HA	1:B:307:HIS:O	1.97	0.64
1:A:27:LEU:CA	1:A:28:GLN:CB	2.67	0.63
1:A:40:THR:HG23	1:A:145:LEU:HD23	1.80	0.63
1:C:38:ARG:HB2	2:C:401:FAD:O2B	1.98	0.63
1:B:45:THR:HG21	1:B:145:LEU:HD11	1.79	0.63
1:D:190:GLN:NE2	1:D:290:ARG:HH22	1.95	0.63
1:C:2:ARG:NH2	1:C:33:LYS:HE2	2.13	0.62
1:A:205:VAL:CG1	1:A:273:ALA:HB1	2.29	0.62
1:D:40:THR:CB	1:D:41:PRO:HA	2.23	0.62
1:C:101:ALA:O	1:C:102:ILE:CG2	2.47	0.62
1:C:226:SER:HB2	1:C:227:PRO:CD	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:55:TYR:HE2	1:B:224:TYR:HH	1.45	0.62
1:C:162:ARG:O	2:C:401:FAD:H2A	1.99	0.62
1:D:39:PHE:CE1	1:D:159:PHE:CD2	2.88	0.62
1:A:42:LEU:HD22	1:C:42:LEU:HD22	1.82	0.61
1:D:39:PHE:CE1	1:D:159:PHE:HD2	2.18	0.61
1:D:150:GLU:HB2	1:D:151:ARG:NH2	2.15	0.61
1:D:27:LEU:HA	1:D:28:GLN:HB2	1.83	0.61
1:A:190:GLN:HE22	1:A:290:ARG:HH22	1.49	0.61
1:A:279:ARG:NH1	1:A:279:ARG:HG3	2.14	0.61
1:B:190:GLN:HE22	1:B:290:ARG:NH2	1.96	0.61
1:D:18:CYS:SG	1:D:324:LEU:HD23	2.40	0.60
1:D:293:ARG:NH1	1:D:304:GLU:OE1	2.32	0.60
1:A:257:ASN:HB3	1:A:261:GLU:OE1	2.02	0.60
1:C:104:ASP:CB	1:C:108:LYS:HE3	2.31	0.60
1:C:209:TRP:NE1	1:C:269:THR:HG23	2.16	0.60
1:B:257:ASN:O	1:B:261:GLU:OE2	2.19	0.60
1:C:72:PHE:C	1:C:72:PHE:CD2	2.75	0.60
1:C:116:LYS:HE2	1:C:130:TYR:OH	2.01	0.60
1:D:165:GLU:OE2	1:D:165:GLU:CA	2.44	0.60
1:A:200:GLY:O	1:A:280:THR:HG23	2.02	0.60
1:B:242:PHE:CZ	1:B:285:VAL:HG21	2.37	0.59
1:C:226:SER:HB2	1:C:227:PRO:HD2	1.84	0.59
1:D:144:TYR:CE2	1:D:319:HIS:CE1	2.91	0.59
1:C:130:TYR:CG	1:C:131:GLY:N	2.68	0.59
1:B:224:TYR:HD2	1:B:242:PHE:CD2	2.19	0.59
1:C:104:ASP:HB3	1:C:108:LYS:HE3	1.83	0.58
1:A:161:GLN:HG3	1:C:249:GLU:O	2.02	0.58
1:A:233:THR:HG22	1:A:234:GLN:NE2	2.18	0.58
1:A:267:GLU:OE2	1:A:269:THR:HB	2.04	0.58
1:A:55:TYR:CE2	1:A:224:TYR:CZ	2.88	0.58
1:D:233:THR:HG21	1:D:234:GLN:HE21	1.69	0.57
1:D:209:TRP:CE2	1:D:269:THR:CG2	2.88	0.57
1:D:44:THR:OG1	2:D:401:FAD:O1A	2.17	0.57
1:B:314:TYR:O	1:B:318:ILE:HG22	2.05	0.57
1:A:224:TYR:HE1	4:A:1044:HOH:O	1.88	0.56
1:B:192:ASP:CG	1:B:286:ARG:HH12	2.08	0.56
1:C:267:GLU:OE2	1:C:267:GLU:C	2.43	0.56
1:B:67:TRP:HB3	1:B:321:GLY:HA3	1.87	0.56
1:C:249:GLU:HB2	1:C:282:PHE:CZ	2.41	0.56
1:D:138:ILE:HD11	1:D:230:ILE:CG2	2.36	0.56
1:A:199:ARG:NH2	1:A:250:LEU:O	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:THR:HG23	1:B:145:LEU:CD2	2.36	0.55
1:D:280:THR:HG22	1:D:281:GLY:N	2.21	0.55
1:B:40:THR:HG21	1:B:145:LEU:HB2	1.89	0.55
1:A:210:MET:CE	1:A:267:GLU:HG2	2.35	0.55
1:C:56:LEU:HD22	1:C:132:TRP:HH2	1.71	0.55
1:C:118:THR:HB	1:C:119:PRO:HD2	1.89	0.55
1:C:296:LEU:HG	1:C:305:VAL:HG21	1.88	0.55
1:C:199:ARG:NH2	1:C:201:GLN:HE21	2.02	0.55
1:D:18:CYS:CB	1:D:323:ALA:HB1	2.36	0.55
1:C:56:LEU:HD22	1:C:132:TRP:CH2	2.42	0.55
1:D:184:VAL:HG22	1:D:247:TRP:CH2	2.42	0.54
1:A:56:LEU:N	1:A:56:LEU:HD23	2.18	0.54
1:B:211:LYS:HD2	1:B:211:LYS:N	2.22	0.54
1:A:199:ARG:HH22	1:A:201:GLN:NE2	2.04	0.54
1:B:242:PHE:HZ	1:B:285:VAL:HG21	1.72	0.54
1:D:180:ASN:ND2	1:D:182:THR:OG1	2.40	0.54
1:D:112:LEU:HB2	1:D:135:THR:HB	1.91	0.53
1:D:294:GLU:OE2	1:D:296:LEU:HD21	2.08	0.53
1:D:205:VAL:HG13	1:D:273:ALA:HB1	1.90	0.53
1:D:332:ARG:NH1	1:D:332:ARG:HB3	2.24	0.53
1:C:293:ARG:CZ	1:C:333:ILE:HG13	2.39	0.53
1:A:10:VAL:O	1:A:14:SER:OG	2.26	0.53
1:C:28:GLN:CG	1:C:28:GLN:O	2.56	0.53
1:C:27:LEU:HD13	1:C:30:LEU:CD1	2.39	0.53
1:A:284:PRO:O	1:A:312:GLY:N	2.37	0.52
1:A:79:VAL:HG13	1:A:80:HIS:CD2	2.44	0.52
1:A:279:ARG:HG3	1:A:279:ARG:HH11	1.74	0.52
1:C:39:PHE:O	1:C:40:THR:C	2.47	0.52
1:C:197:PRO:HG3	1:C:247:TRP:CE2	2.44	0.52
1:D:27:LEU:CD1	1:D:30:LEU:HD13	2.39	0.52
1:B:50:GLY:HA3	1:B:139:LEU:O	2.09	0.52
1:C:190:GLN:HE21	1:C:290:ARG:HH12	1.58	0.52
1:B:190:GLN:NE2	1:B:290:ARG:HH12	2.06	0.52
1:C:79:VAL:HG13	1:C:80:HIS:CD2	2.45	0.52
1:C:249:GLU:HB2	1:C:282:PHE:HZ	1.73	0.52
1:D:81:SER:CB	1:D:82:PRO:HD2	2.40	0.52
1:D:115:ARG:NH1	1:D:121:GLU:OE2	2.31	0.52
1:C:27:LEU:CD1	1:C:30:LEU:CD1	2.87	0.52
1:D:184:VAL:HG22	1:D:247:TRP:HH2	1.75	0.52
1:A:27:LEU:HB2	1:A:28:GLN:HB3	1.92	0.52
1:B:105:PRO:O	1:B:108:LYS:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:THR:CG2	1:D:145:LEU:HD21	2.40	0.52
1:C:108:LYS:HE2	1:C:114:PHE:CD2	2.44	0.51
1:D:144:TYR:HE2	1:D:319:HIS:CE1	2.26	0.51
1:D:197:PRO:CG	1:D:247:TRP:CE2	2.91	0.51
1:D:238:LEU:HD21	1:D:270:LEU:HD13	1.92	0.51
1:C:23:TYR:OH	1:C:331:GLY:HA3	2.11	0.51
1:D:286:ARG:O	1:D:288:GLN:N	2.44	0.51
1:B:151:ARG:O	1:B:155:ARG:CG	2.55	0.51
1:D:50:GLY:HA2	1:D:316:LEU:HD13	1.93	0.51
1:D:66:ASP:O	1:D:70:GLN:HB2	2.11	0.51
1:A:286:ARG:C	1:A:288:GLN:N	2.64	0.51
1:C:226:SER:CB	1:C:227:PRO:CD	2.89	0.51
1:D:223:ILE:HG13	1:D:224:TYR:CD2	2.46	0.51
1:C:79:VAL:HG13	1:C:80:HIS:HD2	1.75	0.51
1:D:294:GLU:N	1:D:305:VAL:O	2.40	0.51
1:A:37:ASP:HA	1:A:161:GLN:HE21	1.75	0.50
1:B:284:PRO:HB2	1:B:310:GLY:HA2	1.92	0.50
1:D:195:LEU:CD1	1:D:309:TYR:CE2	2.90	0.50
1:C:205:VAL:O	1:C:235:THR:HB	2.12	0.50
1:D:209:TRP:CD1	1:D:210:MET:HG2	2.46	0.50
1:B:27:LEU:HB3	1:B:28:GLN:HB3	1.94	0.50
1:B:64:GLU:CD	1:B:289:ILE:HD12	2.32	0.50
1:C:15:THR:HG22	1:C:19:ILE:HD12	1.94	0.50
1:C:159:PHE:N	1:C:159:PHE:HD1	2.09	0.50
1:C:286:ARG:HB3	1:C:288:GLN:O	2.12	0.50
1:B:40:THR:HG23	1:B:145:LEU:HD23	1.93	0.50
1:A:233:THR:HG22	1:A:234:GLN:HE21	1.77	0.50
1:D:36:ALA:HA	2:D:401:FAD:N3A	2.27	0.50
1:D:39:PHE:HE1	1:D:159:PHE:CD2	2.30	0.49
1:A:67:TRP:CH2	1:A:291:LEU:HD23	2.48	0.49
1:D:11:ILE:CG2	1:D:308:ASN:ND2	2.75	0.49
1:B:218:ASP:OD2	1:B:221:ARG:CG	2.60	0.49
1:C:83:ASN:O	1:C:87:LEU:HD12	2.12	0.49
1:A:137:LEU:C	1:A:137:LEU:HD12	2.32	0.49
1:A:192:ASP:O	1:A:194:LEU:N	2.46	0.49
1:B:96:ASN:ND2	1:B:217:HIS:NE2	2.60	0.49
1:A:1:MET:SD	1:A:177:VAL:HG23	2.52	0.49
1:B:51:LEU:HD12	1:B:137:LEU:O	2.12	0.49
1:C:10:VAL:HG21	1:C:316:LEU:HD23	1.95	0.49
1:A:79:VAL:HG13	1:A:80:HIS:HD2	1.78	0.49
1:C:158:LYS:C	1:C:159:PHE:HD1	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:THR:CG2	1:B:145:LEU:HB2	2.42	0.48
1:C:28:GLN:O	1:C:28:GLN:HG2	2.14	0.48
1:A:2:ARG:HB3	1:A:2:ARG:CZ	2.43	0.48
1:A:178:ILE:HB	1:A:305:VAL:HG22	1.95	0.48
1:B:81:SER:HB2	1:B:82:PRO:HD2	1.95	0.48
1:B:83:ASN:O	1:B:86:ASN:HB2	2.13	0.48
1:C:159:PHE:N	1:C:159:PHE:CD1	2.81	0.48
1:D:18:CYS:HB2	1:D:323:ALA:HB1	1.96	0.48
1:A:14:SER:HB2	1:A:323:ALA:HB2	1.96	0.48
1:C:14:SER:OG	1:C:319:HIS:HD2	1.97	0.48
1:B:157:VAL:O	1:B:159:PHE:CE1	2.66	0.48
1:A:209:TRP:NE1	1:A:269:THR:HG21	2.29	0.48
1:B:39:PHE:O	1:B:40:THR:C	2.51	0.48
1:B:81:SER:CB	1:B:82:PRO:HD2	2.44	0.48
1:B:159:PHE:N	1:B:159:PHE:CD1	2.80	0.48
1:B:224:TYR:CD2	1:B:242:PHE:CD2	3.00	0.48
1:C:101:ALA:O	1:C:102:ILE:HG22	2.12	0.48
1:D:10:VAL:HG13	1:D:11:ILE:N	2.29	0.48
1:A:205:VAL:CG1	1:A:273:ALA:CB	2.92	0.47
1:B:33:LYS:HD2	1:B:160:PHE:CE2	2.49	0.47
1:B:313:GLY:HA2	2:B:401:FAD:H1'1	1.96	0.47
1:A:118:THR:OG1	1:A:121:GLU:HG3	2.13	0.47
1:B:159:PHE:N	1:B:159:PHE:HD1	2.12	0.47
1:B:210:MET:C	1:B:211:LYS:HD2	2.35	0.47
1:C:89:LEU:HA	1:C:138:ILE:O	2.15	0.47
1:D:28:GLN:O	1:D:28:GLN:HG2	2.14	0.47
1:B:283:ARG:NE	3:B:402:4P5:O10	2.34	0.47
1:A:151:ARG:HH21	1:A:154:GLU:CD	2.18	0.47
1:C:96:ASN:O	1:C:131:GLY:HA3	2.15	0.47
1:A:286:ARG:C	1:A:288:GLN:H	2.17	0.47
1:B:83:ASN:O	1:B:87:LEU:HD13	2.15	0.47
1:B:168:GLU:OE2	1:B:168:GLU:N	2.41	0.47
1:D:28:GLN:N	1:D:29:PRO:HA	2.29	0.47
1:C:38:ARG:HG2	1:C:42:LEU:HB2	1.96	0.47
1:D:83:ASN:O	1:D:87:LEU:HD13	2.14	0.47
1:C:101:ALA:O	1:C:102:ILE:HG23	2.15	0.47
1:C:334:LEU:N	1:C:334:LEU:HD23	2.30	0.47
1:C:264:CYS:O	1:C:268:PRO:HA	2.14	0.46
1:C:44:THR:HG21	1:C:282:PHE:O	2.15	0.46
1:B:202:ILE:HD11	1:B:279:ARG:HB2	1.97	0.46
1:D:223:ILE:HG13	1:D:224:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:228:TYR:CE2	3:D:402:4P5:O11	2.68	0.46
1:A:280:THR:HG22	1:A:281:GLY:N	2.29	0.46
1:B:102:ILE:HG13	1:B:103:PRO:N	2.31	0.46
1:D:143:ASN:HA	1:D:146:GLN:HG3	1.98	0.46
1:D:184:VAL:O	1:D:184:VAL:CG2	2.62	0.46
1:B:195:LEU:HD12	1:B:196:GLN:H	1.81	0.46
1:C:267:GLU:O	1:C:269:THR:N	2.48	0.46
1:B:182:THR:O	1:B:183:GLY:C	2.54	0.46
1:D:201:GLN:HB3	1:D:259:ILE:HD11	1.97	0.46
1:B:63:GLN:H	1:B:63:GLN:HG3	1.57	0.46
1:B:241:ILE:HD12	1:B:241:ILE:HG23	1.71	0.46
1:A:20:HIS:CE1	1:A:155:ARG:HB3	2.51	0.45
1:A:41:PRO:HA	1:A:46:ASP:OD2	2.16	0.45
1:B:30:LEU:HG	1:B:32:ILE:HG13	1.96	0.45
1:A:139:LEU:HD13	1:A:144:TYR:CD2	2.52	0.45
1:B:40:THR:CG2	1:B:46:ASP:OD2	2.40	0.45
1:D:47:VAL:O	1:D:202:ILE:HD13	2.17	0.45
1:A:218:ASP:OD1	1:A:219:PRO:HD2	2.16	0.45
1:B:87:LEU:HD12	1:B:147:TRP:CD1	2.51	0.45
1:B:238:LEU:HB3	1:B:259:ILE:CG2	2.47	0.45
1:D:200:GLY:HA2	1:D:241:ILE:O	2.17	0.45
1:A:197:PRO:HD3	1:A:247:TRP:CZ2	2.51	0.45
1:C:209:TRP:CE2	1:C:269:THR:HG23	2.52	0.45
1:D:38:ARG:NH1	1:D:42:LEU:O	2.45	0.45
1:D:81:SER:HB2	1:D:82:PRO:HD2	1.99	0.45
1:A:224:TYR:CE1	4:A:1044:HOH:O	2.56	0.45
1:B:33:LYS:HD2	1:B:160:PHE:HE2	1.81	0.45
1:D:257:ASN:HB3	1:D:261:GLU:OE1	2.16	0.45
1:B:3:VAL:N	1:B:31:ASP:O	2.49	0.45
1:B:87:LEU:N	1:B:87:LEU:CD1	2.80	0.45
1:B:296:LEU:HD23	1:B:305:VAL:HG21	1.97	0.45
1:B:114:PHE:HA	1:B:134:HIS:HB3	1.98	0.44
1:B:289:ILE:HG22	1:B:290:ARG:N	2.31	0.44
1:D:137:LEU:HD12	1:D:137:LEU:O	2.17	0.44
1:A:141:GLY:O	1:A:145:LEU:HB2	2.16	0.44
1:B:35:TYR:CD2	1:B:162:ARG:HD3	2.52	0.44
1:C:13:LEU:O	1:C:16:ALA:HB3	2.16	0.44
1:A:142:LYS:O	1:A:146:GLN:HG3	2.18	0.44
1:B:52:TRP:O	1:B:53:GLN:HB2	2.17	0.44
1:C:315:GLY:O	1:C:319:HIS:HB3	2.16	0.44
1:A:55:TYR:CE2	1:A:224:TYR:CE2	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:87:LEU:HD11	1:D:147:TRP:CE2	2.52	0.44
1:D:115:ARG:HH22	1:D:121:GLU:CD	2.20	0.44
1:A:144:TYR:HD1	1:A:144:TYR:HA	1.70	0.44
1:A:288:GLN:HE21	1:A:288:GLN:HB3	1.48	0.44
1:C:115:ARG:O	1:C:132:TRP:HA	2.17	0.44
1:C:194:LEU:HB3	1:C:287:PRO:HD2	2.00	0.44
1:D:51:LEU:HD22	1:D:230:ILE:HD13	2.00	0.44
1:C:256:HIS:ND1	1:C:278:GLU:OE1	2.31	0.44
1:A:76:LEU:C	1:A:78:HIS:H	2.21	0.44
1:C:165:GLU:O	1:C:166:SER:HB3	2.18	0.44
1:C:242:PHE:CZ	1:C:285:VAL:HG21	2.53	0.44
1:D:293:ARG:HE	1:D:293:ARG:HB3	1.70	0.44
1:C:91:LEU:HD23	1:C:91:LEU:HA	1.77	0.44
1:C:253:ILE:O	1:C:256:HIS:HB3	2.18	0.44
1:D:168:GLU:H	1:D:168:GLU:CD	2.20	0.44
1:D:324:LEU:HD23	1:D:324:LEU:HA	1.91	0.44
1:B:87:LEU:HD11	1:B:147:TRP:CE2	2.53	0.43
1:C:6:ILE:O	1:C:181:CYS:HB2	2.17	0.43
1:A:76:LEU:C	1:A:78:HIS:N	2.71	0.43
1:A:210:MET:HE1	1:A:267:GLU:HG2	1.99	0.43
1:D:325:GLU:OE1	1:D:325:GLU:HA	2.18	0.43
1:A:315:GLY:HA3	2:A:401:FAD:H4'	1.99	0.43
1:B:296:LEU:N	1:B:303:THR:O	2.33	0.43
1:B:27:LEU:CA	1:B:28:GLN:HB2	2.44	0.43
1:D:210:MET:HE2	1:D:210:MET:HB3	1.84	0.43
1:C:242:PHE:HZ	1:C:285:VAL:HG21	1.84	0.43
1:A:165:GLU:HB2	1:A:169:GLU:OE1	2.19	0.43
1:A:246:ASN:OD1	1:A:246:ASN:C	2.55	0.43
1:C:190:GLN:NE2	1:C:290:ARG:HH22	2.14	0.43
1:A:51:LEU:HB3	3:A:402:4P5:C5	2.49	0.43
1:B:204:LYS:HG3	1:B:235:THR:OG1	2.18	0.43
1:B:224:TYR:HD2	1:B:242:PHE:CE2	2.36	0.43
1:D:233:THR:HB	1:D:234:GLN:HG2	2.00	0.43
1:B:53:GLN:HA	1:B:54:PRO:HD3	1.72	0.43
1:C:296:LEU:HG	1:C:305:VAL:CG2	2.47	0.43
1:D:7:GLY:O	1:D:12:GLY:HA3	2.18	0.43
1:D:145:LEU:HD12	1:D:145:LEU:HA	1.95	0.43
1:D:47:VAL:O	1:D:47:VAL:HG12	2.19	0.43
1:B:249:GLU:HB2	1:B:282:PHE:CE2	2.54	0.43
1:B:283:ARG:HA	1:B:284:PRO:HD3	1.63	0.43
1:D:163:LYS:HB2	1:D:163:LYS:HE2	1.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:VAL:HG13	1:A:11:ILE:N	2.34	0.42
1:A:98:PHE:CE1	1:A:217:HIS:CD2	3.07	0.42
1:A:248:SER:OG	1:A:250:LEU:HB3	2.19	0.42
1:B:242:PHE:HZ	1:B:285:VAL:CG2	2.32	0.42
1:C:64:GLU:HB3	1:C:318:ILE:HD11	2.01	0.42
1:C:286:ARG:CZ	1:C:290:ARG:HB2	2.49	0.42
1:B:145:LEU:CD1	1:B:145:LEU:N	2.82	0.42
1:B:161:GLN:HG3	1:D:249:GLU:O	2.19	0.42
1:D:52:TRP:CD2	1:D:72:PHE:HD1	2.37	0.42
1:A:210:MET:CE	1:A:229:ILE:HG21	2.50	0.42
1:B:152:LEU:HB3	1:B:159:PHE:HZ	1.85	0.42
1:C:168:GLU:O	1:C:169:GLU:C	2.58	0.42
1:C:52:TRP:CD1	1:C:317:THR:HA	2.54	0.42
1:D:15:THR:HG21	1:D:179:VAL:HG11	2.02	0.42
1:D:102:ILE:HA	1:D:103:PRO:HD2	1.65	0.42
1:D:223:ILE:HD12	1:D:224:TYR:H	1.84	0.42
1:A:108:LYS:HE3	1:A:108:LYS:HB2	1.84	0.42
1:C:17:LEU:O	1:C:21:GLU:HB2	2.19	0.42
1:D:137:LEU:HD12	1:D:137:LEU:C	2.40	0.42
1:A:56:LEU:HD23	1:A:56:LEU:HA	1.53	0.42
1:D:63:GLN:H	1:D:63:GLN:HG3	1.55	0.42
1:A:309:TYR:CD2	1:A:309:TYR:C	2.92	0.42
1:B:309:TYR:C	1:B:309:TYR:CD2	2.93	0.42
1:D:168:GLU:O	1:D:169:GLU:C	2.58	0.42
1:A:36:ALA:O	1:A:161:GLN:HA	2.20	0.42
1:C:274:ARG:HH11	1:C:274:ARG:HB3	1.83	0.42
1:A:253:ILE:HG23	1:A:254:GLN:NE2	2.35	0.42
1:C:17:LEU:HA	1:C:152:LEU:HD11	2.00	0.42
1:C:40:THR:HA	1:C:41:PRO:HA	1.83	0.42
1:C:69:GLN:HG3	1:C:110:THR:HG23	2.02	0.42
1:D:184:VAL:N	1:D:284:PRO:HB3	2.35	0.42
1:D:335:GLU:O	1:D:336:GLU:C	2.58	0.42
1:B:87:LEU:HD12	1:B:147:TRP:CG	2.55	0.41
1:C:160:PHE:CD2	1:C:160:PHE:N	2.87	0.41
1:C:216:THR:HG23	1:C:266:LEU:HD11	2.02	0.41
1:D:27:LEU:HD13	1:D:30:LEU:HD13	2.02	0.41
1:D:35:TYR:CG	1:D:162:ARG:HD2	2.55	0.41
1:A:178:ILE:HD12	1:A:303:THR:HG21	2.02	0.41
1:A:205:VAL:HG21	1:A:238:LEU:CD2	2.50	0.41
1:B:55:TYR:HE2	1:B:224:TYR:OH	1.99	0.41
1:C:97:LEU:HD11	1:C:125:PHE:CD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:TRP:CD2	1:B:72:PHE:HD1	2.38	0.41
1:C:27:LEU:HD13	1:C:30:LEU:HD12	2.02	0.41
1:D:192:ASP:HA	1:D:193:PRO:HD2	1.88	0.41
1:D:228:TYR:HE2	3:D:402:4P5:O11	2.04	0.41
1:D:283:ARG:HH21	3:D:402:4P5:C9	2.32	0.41
1:D:286:ARG:C	1:D:288:GLN:N	2.73	0.41
1:A:105:PRO:O	1:A:108:LYS:HE2	2.21	0.41
1:C:92:ILE:HG21	1:C:138:ILE:CD1	2.46	0.41
1:D:40:THR:HG22	1:D:41:PRO:HA	2.02	0.41
1:A:192:ASP:C	1:A:194:LEU:H	2.24	0.41
1:C:12:GLY:O	1:C:16:ALA:HB2	2.21	0.41
1:C:105:PRO:O	1:C:108:LYS:HG3	2.21	0.41
1:C:118:THR:HB	1:C:119:PRO:CD	2.50	0.41
1:D:2:ARG:NH1	1:D:31:ASP:OD2	2.54	0.41
1:D:55:TYR:CE2	1:D:224:TYR:OH	2.42	0.41
1:D:242:PHE:CD1	1:D:242:PHE:C	2.93	0.41
1:A:36:ALA:HA	2:A:401:FAD:N3A	2.35	0.41
1:B:27:LEU:CA	1:B:28:GLN:CB	2.99	0.41
1:B:108:LYS:HB2	1:B:108:LYS:HE3	1.88	0.41
1:D:286:ARG:C	1:D:288:GLN:H	2.24	0.41
1:D:309:TYR:CD2	1:D:309:TYR:C	2.93	0.41
1:D:332:ARG:HB3	1:D:332:ARG:HH11	1.86	0.41
1:B:211:LYS:N	1:B:211:LYS:CD	2.82	0.41
1:C:190:GLN:NE2	1:C:290:ARG:HH12	2.18	0.41
1:C:293:ARG:NE	1:C:333:ILE:HD11	2.36	0.41
1:D:11:ILE:O	1:D:12:GLY:C	2.57	0.41
1:D:102:ILE:O	1:D:102:ILE:HG13	2.17	0.41
1:D:117:LEU:HA	1:D:117:LEU:HD23	1.58	0.41
1:A:3:VAL:O	1:A:32:ILE:HA	2.21	0.41
1:C:117:LEU:HA	1:C:117:LEU:HD23	1.79	0.41
1:D:186:ALA:HB3	1:D:195:LEU:HD22	2.03	0.40
1:B:15:THR:HG21	1:B:179:VAL:HG11	2.03	0.40
1:C:274:ARG:HH11	1:C:274:ARG:CB	2.34	0.40
1:A:89:LEU:HA	1:A:138:ILE:O	2.21	0.40
1:D:13:LEU:O	1:D:14:SER:C	2.58	0.40
1:A:286:ARG:HH11	1:A:286:ARG:HD2	1.73	0.40
1:C:267:GLU:OE2	1:C:269:THR:N	2.43	0.40
1:A:115:ARG:NH1	1:A:121:GLU:OE2	2.46	0.40
1:D:194:LEU:O	1:D:286:ARG:HA	2.21	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	321/347 (92%)	291 (91%)	27 (8%)	3 (1%)	17 31
1	B	321/347 (92%)	293 (91%)	23 (7%)	5 (2%)	9 17
1	C	321/347 (92%)	294 (92%)	21 (6%)	6 (2%)	8 13
1	D	321/347 (92%)	289 (90%)	27 (8%)	5 (2%)	9 17
All	All	1284/1388 (92%)	1167 (91%)	98 (8%)	19 (2%)	10 18

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	GLN
1	B	28	GLN
1	B	55	TYR
1	C	28	GLN
1	C	55	TYR
1	D	28	GLN
1	D	108	LYS
1	A	108	LYS
1	C	108	LYS
1	D	55	TYR
1	B	101	ALA
1	D	103	PRO
1	D	77	SER
1	A	166	SER
1	B	240	GLY
1	C	14	SER
1	C	312	GLY
1	B	141	GLY
1	C	240	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	280/299 (94%)	256 (91%)	24 (9%)	10 20
1	B	280/299 (94%)	249 (89%)	31 (11%)	6 11
1	C	280/299 (94%)	248 (89%)	32 (11%)	5 11
1	D	280/299 (94%)	243 (87%)	37 (13%)	4 7
All	All	1120/1196 (94%)	996 (89%)	124 (11%)	6 11

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ARG
1	A	14	SER
1	A	18	CYS
1	A	22	ARG
1	A	27	LEU
1	A	30	LEU
1	A	40	THR
1	A	69	GLN
1	A	76	LEU
1	A	81	SER
1	A	85	GLU
1	A	91	LEU
1	A	100	GLU
1	A	102	ILE
1	A	145	LEU
1	A	152	LEU
1	A	166	SER
1	A	223	ILE
1	A	238	LEU
1	A	266	LEU
1	A	278	GLU
1	A	295	GLN
1	A	296	LEU
1	A	303	THR

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Mol	Chain	Res	Type
1	B	25	SER
1	B	40	THR
1	B	63	GLN
1	B	69	GLN
1	B	76	LEU
1	B	79	VAL
1	B	81	SER
1	B	83	ASN
1	B	87	LEU
1	B	93	SER
1	B	100	GLU
1	B	102	ILE
1	B	106	SER
1	B	120	ARG
1	B	136	SER
1	B	139	LEU
1	B	152	LEU
1	B	154	GLU
1	B	159	PHE
1	B	169	GLU
1	B	204	LYS
1	B	205	VAL
1	B	211	LYS
1	B	221	ARG
1	B	238	LEU
1	B	253	ILE
1	B	254	GLN
1	B	269	THR
1	B	291	LEU
1	B	295	GLN
1	B	316	LEU
1	C	2	ARG
1	C	14	SER
1	C	18	CYS
1	C	22	ARG
1	C	27	LEU
1	C	28	GLN
1	C	40	THR
1	C	42	LEU
1	C	43	THR
1	C	69	GLN
1	C	76	LEU

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Mol	Chain	Res	Type
1	C	81	SER
1	C	83	ASN
1	C	93	SER
1	C	100	GLU
1	C	112	LEU
1	C	137	LEU
1	C	139	LEU
1	C	145	LEU
1	C	152	LEU
1	C	159	PHE
1	C	161	GLN
1	C	168	GLU
1	C	191	ARG
1	C	221	ARG
1	C	238	LEU
1	C	269	THR
1	C	274	ARG
1	C	291	LEU
1	C	295	GLN
1	C	303	THR
1	C	333	ILE
1	D	6	ILE
1	D	14	SER
1	D	32	ILE
1	D	42	LEU
1	D	63	GLN
1	D	70	GLN
1	D	76	LEU
1	D	81	SER
1	D	83	ASN
1	D	98	PHE
1	D	100	GLU
1	D	102	ILE
1	D	120	ARG
1	D	139	LEU
1	D	145	LEU
1	D	146	GLN
1	D	150	GLU
1	D	152	LEU
1	D	162	ARG
1	D	163	LYS
1	D	165	GLU

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Mol	Chain	Res	Type
1	D	168	GLU
1	D	169	GLU
1	D	182	THR
1	D	205	VAL
1	D	210	MET
1	D	215	LEU
1	D	223	ILE
1	D	253	ILE
1	D	266	LEU
1	D	267	GLU
1	D	272	ASN
1	D	293	ARG
1	D	295	GLN
1	D	302	ASN
1	D	332	ARG
1	D	336	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	A	134	HIS
1	A	143	ASN
1	A	161	GLN
1	A	180	ASN
1	A	190	GLN
1	A	196	GLN
1	A	201	GLN
1	A	234	GLN
1	A	256	HIS
1	A	288	GLN
1	A	311	HIS
1	B	53	GLN
1	B	80	HIS
1	B	96	ASN
1	B	180	ASN
1	B	190	GLN
1	B	201	GLN
1	C	80	HIS
1	C	180	ASN
1	C	190	GLN
1	C	201	GLN

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Mol	Chain	Res	Type
1	D	24	HIS
1	D	69	GLN
1	D	78	HIS
1	D	99	HIS
1	D	134	HIS
1	D	180	ASN
1	D	190	GLN
1	D	196	GLN
1	D	201	GLN
1	D	234	GLN
1	D	295	GLN

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	$\#\|Z\| > 2$
2	FAD	C	401	-	53,58,58	1.42	8 (15%)	68,89,89	1.85	15 (22%)
3	4P5	D	402	-	8,12,12	1.67	2 (25%)	7,17,17	2.94	3 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	FAD	B	401	-	53,58,58	1.38	6 (11%)	68,89,89	1.94	21 (30%)
3	4P5	C	402	-	8,12,12	2.91	2 (25%)	7,17,17	2.45	4 (57%)
3	4P5	B	402	-	8,12,12	1.53	2 (25%)	7,17,17	1.80	3 (42%)
2	FAD	A	401	-	53,58,58	1.54	7 (13%)	68,89,89	1.67	18 (26%)
2	FAD	D	401	-	53,58,58	1.62	8 (15%)	68,89,89	1.78	17 (25%)
3	4P5	A	402	-	8,12,12	1.89	3 (37%)	7,17,17	2.77	3 (42%)

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	401	-	-	1/30/50/50	0/6/6/6
3	4P5	D	402	-	-	0/2/4/4	0/2/2/2
2	FAD	B	401	-	-	2/30/50/50	0/6/6/6
3	4P5	C	402	-	-	0/2/4/4	0/2/2/2
3	4P5	B	402	-	-	0/2/4/4	0/2/2/2
2	FAD	A	401	-	-	2/30/50/50	0/6/6/6
2	FAD	D	401	-	-	8/30/50/50	0/6/6/6
3	4P5	A	402	-	-	0/2/4/4	0/2/2/2

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	4P5	C7-C9	-6.79	1.41	1.50
2	A	401	FAD	C2A-N3A	5.33	1.40	1.32
2	D	401	FAD	C2A-N3A	5.20	1.40	1.32
2	D	401	FAD	C4X-N5	5.05	1.40	1.30
2	B	401	FAD	C2A-N3A	4.93	1.40	1.32
2	A	401	FAD	C4X-N5	4.46	1.39	1.30
2	C	401	FAD	C2A-N3A	3.92	1.38	1.32
2	B	401	FAD	O4B-C1B	3.71	1.46	1.41
2	A	401	FAD	C10-N1	3.63	1.40	1.33
2	D	401	FAD	C10-N1	3.62	1.40	1.33
2	C	401	FAD	C4X-N5	3.59	1.37	1.30
3	C	402	4P5	O10-C9	-3.56	1.19	1.30
2	D	401	FAD	C2A-N1A	3.43	1.40	1.33
2	A	401	FAD	C2A-N1A	3.38	1.40	1.33
3	D	402	4P5	O11-C9	3.34	1.32	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	FAD	C9-C8	3.17	1.44	1.39
2	B	401	FAD	C2A-N1A	3.15	1.39	1.33
2	B	401	FAD	C4X-N5	3.13	1.36	1.30
2	A	401	FAD	O4B-C1B	-3.05	1.36	1.41
2	C	401	FAD	C4X-C10	-2.93	1.35	1.44
3	A	402	4P5	O11-C9	2.79	1.31	1.22
3	D	402	4P5	C3-N8	-2.77	1.29	1.38
2	D	401	FAD	O2-C2	2.65	1.29	1.24
2	A	401	FAD	C2B-C1B	-2.62	1.49	1.53
3	A	402	4P5	C3-N8	-2.62	1.30	1.38
2	D	401	FAD	C2B-C1B	-2.54	1.49	1.53
3	B	402	4P5	O11-C9	2.52	1.30	1.22
2	C	401	FAD	C9A-C5X	-2.50	1.37	1.41
2	B	401	FAD	O4B-C4B	-2.49	1.39	1.45
2	D	401	FAD	O4B-C1B	-2.48	1.37	1.41
3	A	402	4P5	C7-C9	-2.43	1.47	1.50
2	C	401	FAD	C5X-N5	-2.32	1.35	1.39
2	D	401	FAD	C5'-C4'	2.27	1.55	1.51
2	C	401	FAD	C8A-N7A	2.27	1.38	1.34
2	A	401	FAD	C2-N1	2.19	1.42	1.36
3	B	402	4P5	C3-N8	-2.10	1.32	1.38
2	B	401	FAD	C4X-C10	-2.03	1.38	1.44
2	C	401	FAD	O4B-C1B	2.01	1.43	1.41

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	FAD	N3A-C2A-N1A	-7.29	117.29	128.68
3	D	402	4P5	C6-C2-C3	6.21	111.64	106.24
3	A	402	4P5	C6-C2-C3	5.97	111.43	106.24
2	C	401	FAD	N3A-C2A-N1A	-5.29	120.41	128.68
2	D	401	FAD	C1B-N9A-C4A	-4.92	117.99	126.64
2	D	401	FAD	N3A-C2A-N1A	-4.46	121.71	128.68
2	A	401	FAD	C4A-C5A-N7A	-4.26	104.96	109.40
2	C	401	FAD	C4X-C10-N10	4.26	122.71	116.48
3	C	402	4P5	C6-C2-C3	4.08	109.79	106.24
2	D	401	FAD	C9A-C5X-N5	-3.94	118.15	122.43
2	B	401	FAD	C4X-C10-N10	3.84	122.10	116.48
2	B	401	FAD	O4B-C1B-C2B	-3.81	101.36	106.93
2	D	401	FAD	O5'-C5'-C4'	-3.79	99.25	109.36
2	C	401	FAD	C4-C4X-N5	3.75	123.57	118.23
2	C	401	FAD	C10-C4X-N5	-3.67	117.07	124.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	FAD	C10-N1-C2	3.66	124.21	116.90
2	A	401	FAD	C4X-C10-N10	3.54	121.65	116.48
2	A	401	FAD	N3A-C2A-N1A	-3.53	123.15	128.68
2	D	401	FAD	C4A-C5A-N7A	-3.48	105.77	109.40
2	A	401	FAD	C10-C4X-N5	-3.48	117.47	124.86
2	D	401	FAD	C4-C4X-N5	3.42	123.10	118.23
3	D	402	4P5	O10-C9-C7	-3.36	107.02	114.69
2	A	401	FAD	C4-N3-C2	-3.31	119.53	125.64
2	D	401	FAD	C5'-C4'-C3'	3.30	118.58	112.20
2	A	401	FAD	O4'-C4'-C5'	-3.27	102.57	109.92
2	C	401	FAD	O4-C4-N3	-3.22	113.95	120.12
2	B	401	FAD	C4-N3-C2	-3.19	119.74	125.64
2	B	401	FAD	C4-C4X-C10	3.08	121.96	116.79
2	B	401	FAD	C10-C4X-N5	-3.06	118.36	124.86
2	D	401	FAD	C9-C9A-N10	-3.02	117.75	121.84
3	C	402	4P5	O10-C9-C7	3.00	121.51	114.69
2	C	401	FAD	C4X-C4-N3	2.99	120.79	113.19
2	C	401	FAD	C4A-C5A-N7A	-2.99	106.29	109.40
2	C	401	FAD	C4X-C10-N1	-2.99	117.80	124.73
2	B	401	FAD	O3B-C3B-C2B	-2.97	102.20	111.82
2	A	401	FAD	C1B-N9A-C4A	-2.97	121.42	126.64
2	D	401	FAD	C5X-C9A-N10	2.96	121.01	117.95
3	D	402	4P5	O11-C9-C7	2.95	127.23	121.24
2	A	401	FAD	C4X-C10-N1	-2.94	117.91	124.73
2	B	401	FAD	O3'-C3'-C4'	-2.88	101.86	108.81
2	C	401	FAD	C4-N3-C2	-2.87	120.33	125.64
3	B	402	4P5	C6-C2-C3	2.81	108.69	106.24
2	B	401	FAD	C9A-C5X-N5	-2.66	119.54	122.43
2	B	401	FAD	C2B-C3B-C4B	2.65	107.78	102.64
2	A	401	FAD	C4X-C4-N3	2.64	119.88	113.19
3	C	402	4P5	C6-C7-C9	-2.63	120.57	128.31
2	A	401	FAD	C4-C4X-N5	2.58	121.91	118.23
2	D	401	FAD	C4'-C3'-C2'	-2.57	108.02	113.36
2	B	401	FAD	C2A-N1A-C6A	2.54	123.10	118.75
2	B	401	FAD	C1'-N10-C9A	2.53	124.73	120.51
2	A	401	FAD	O2-C2-N1	-2.51	117.66	121.83
2	D	401	FAD	C4X-C4-N3	2.51	119.57	113.19
3	A	402	4P5	O10-C9-C7	-2.50	108.99	114.69
2	B	401	FAD	C5A-C6A-N6A	2.50	124.15	120.35
3	A	402	4P5	O10-C9-O11	2.46	128.81	123.35
2	C	401	FAD	C5X-N5-C4X	2.46	122.16	118.07
2	B	401	FAD	C6-C5X-C9A	2.45	122.40	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	FAD	C5X-N5-C4X	2.39	122.05	118.07
2	C	401	FAD	P-O3P-PA	-2.36	124.74	132.83
3	B	402	4P5	C6-C7-C9	-2.35	121.37	128.31
2	C	401	FAD	C5'-C4'-C3'	2.35	116.74	112.20
2	D	401	FAD	C3B-C2B-C1B	-2.35	97.44	100.98
2	B	401	FAD	C4A-C5A-N7A	-2.33	106.97	109.40
2	B	401	FAD	O4'-C4'-C5'	2.31	115.12	109.92
2	C	401	FAD	C6-C7-C8	-2.28	116.40	119.67
2	B	401	FAD	C9-C9A-N10	2.27	124.90	121.84
2	A	401	FAD	O4-C4-C4X	-2.26	120.61	126.60
2	D	401	FAD	C6-C5X-N5	2.25	122.45	118.51
2	A	401	FAD	C4-C4X-C10	2.25	120.58	116.79
3	C	402	4P5	O11-C9-C7	-2.24	116.69	121.24
2	A	401	FAD	C10-N1-C2	2.23	121.36	116.90
2	D	401	FAD	O4-C4-C4X	-2.23	120.69	126.60
2	B	401	FAD	C4X-C10-N1	-2.20	119.61	124.73
2	A	401	FAD	C8M-C8-C7	-2.20	116.22	120.74
2	A	401	FAD	C5A-C6A-N6A	2.20	123.69	120.35
2	B	401	FAD	C3B-C2B-C1B	-2.17	97.71	100.98
3	B	402	4P5	O10-C9-C7	2.15	119.58	114.69
2	A	401	FAD	C5X-N5-C4X	2.10	121.56	118.07
2	D	401	FAD	C10-C4X-N5	-2.09	120.43	124.86
2	A	401	FAD	O4B-C1B-C2B	-2.08	103.89	106.93
2	C	401	FAD	C5A-C6A-N6A	2.07	123.50	120.35
2	B	401	FAD	C4'-C3'-C2'	-2.07	109.07	113.36
2	D	401	FAD	O2A-PA-O5B	-2.03	98.30	107.75
2	D	401	FAD	C4X-C10-N10	2.03	119.44	116.48

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	FAD	N10-C1'-C2'-O2'
2	D	401	FAD	C5B-O5B-PA-O1A
2	D	401	FAD	N10-C1'-C2'-O2'
2	D	401	FAD	O3'-C3'-C4'-O4'
2	D	401	FAD	C2'-C3'-C4'-O4'
2	D	401	FAD	C5B-O5B-PA-O3P
2	D	401	FAD	C5'-O5'-P-O3P
2	C	401	FAD	O4B-C4B-C5B-O5B
2	A	401	FAD	O4B-C4B-C5B-O5B
2	D	401	FAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
2	B	401	FAD	O4B-C4B-C5B-O5B
2	B	401	FAD	C3B-C4B-C5B-O5B
2	D	401	FAD	O3'-C3'-C4'-C5'

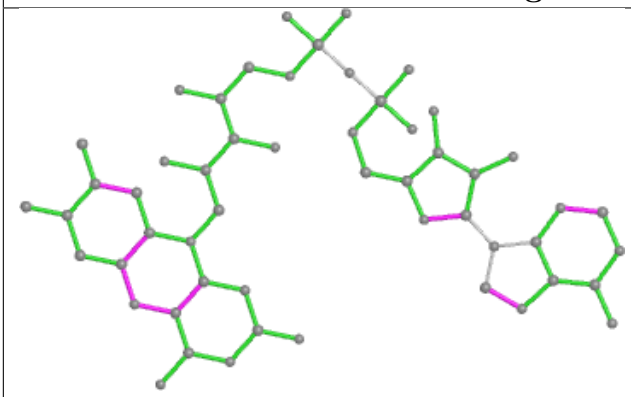
There are no ring outliers.

7 monomers are involved in 12 short contacts:

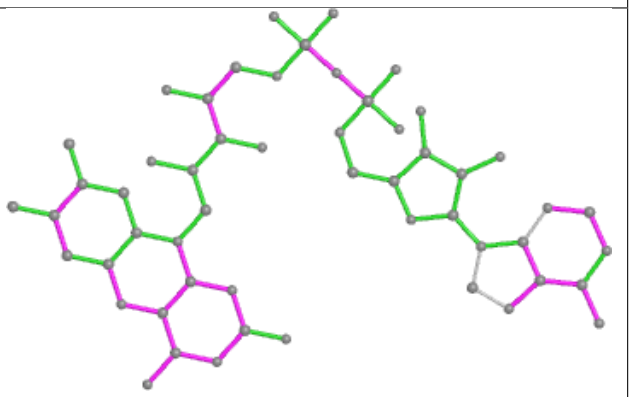
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	FAD	2	0
3	D	402	4P5	3	0
2	B	401	FAD	1	0
3	B	402	4P5	1	0
2	A	401	FAD	2	0
2	D	401	FAD	2	0
3	A	402	4P5	1	0

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.

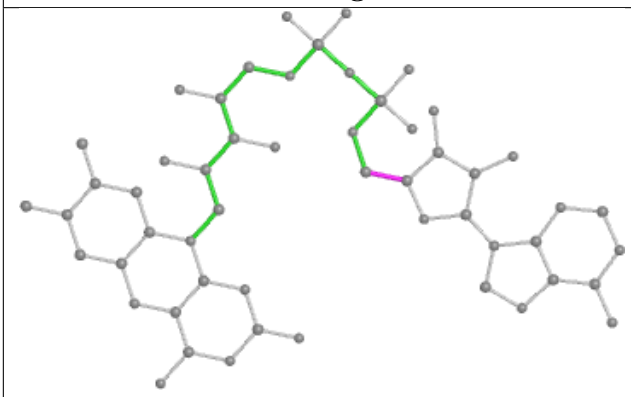
Ligand FAD C 401



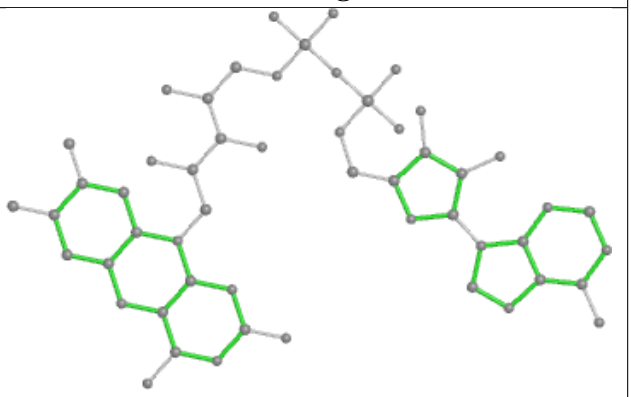
Bond lengths



Bond angles

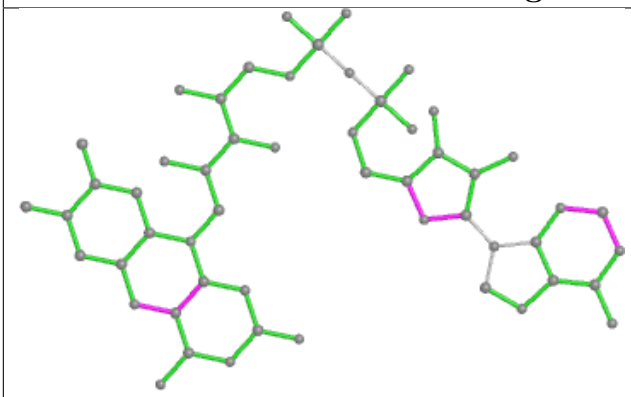


Torsions

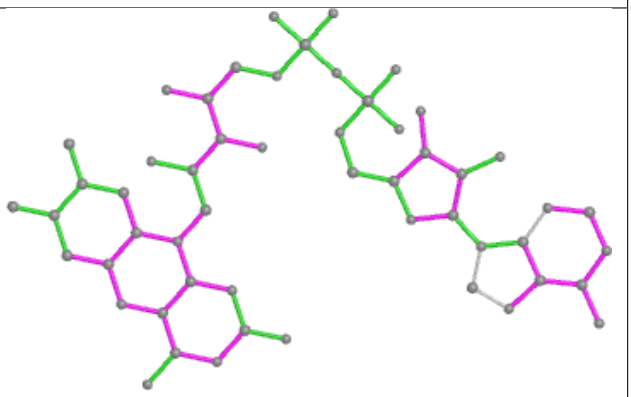


Rings

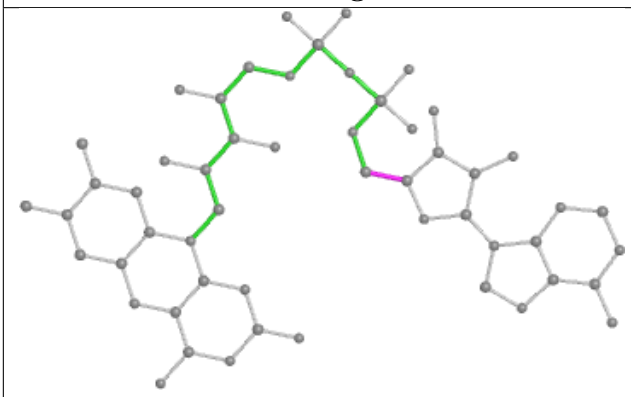
Ligand FAD B 401



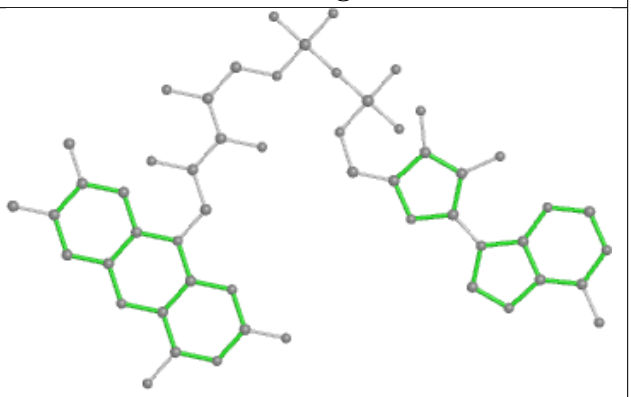
Bond lengths



Bond angles

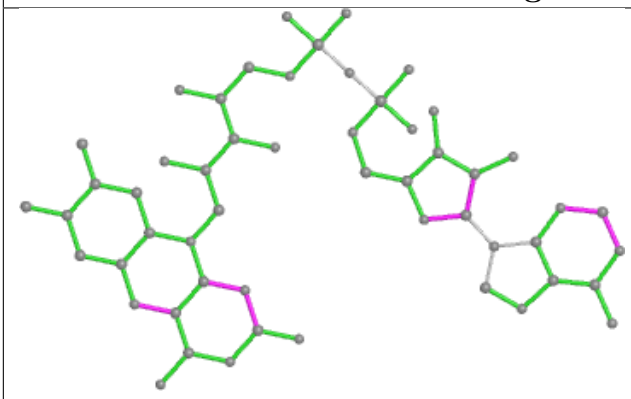


Torsions

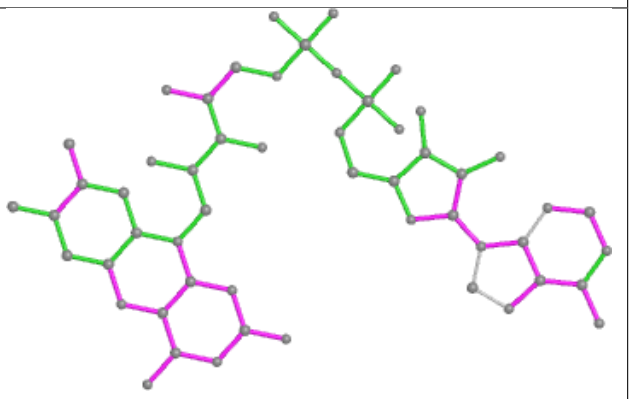


Rings

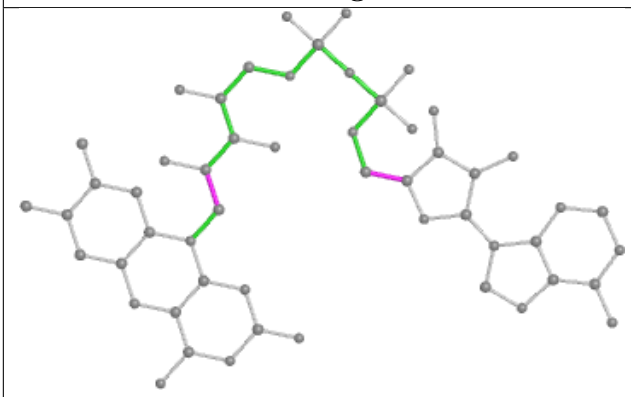
Ligand FAD A 401



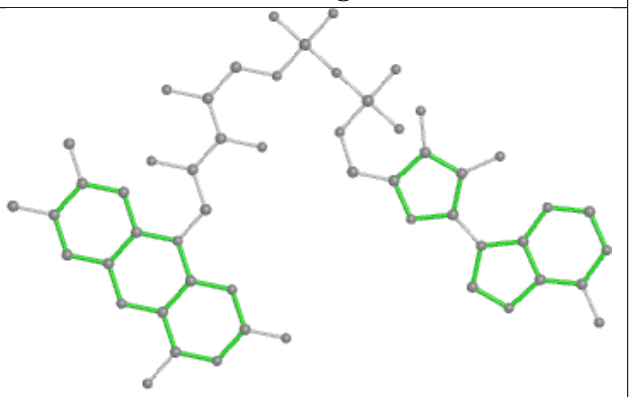
Bond lengths



Bond angles

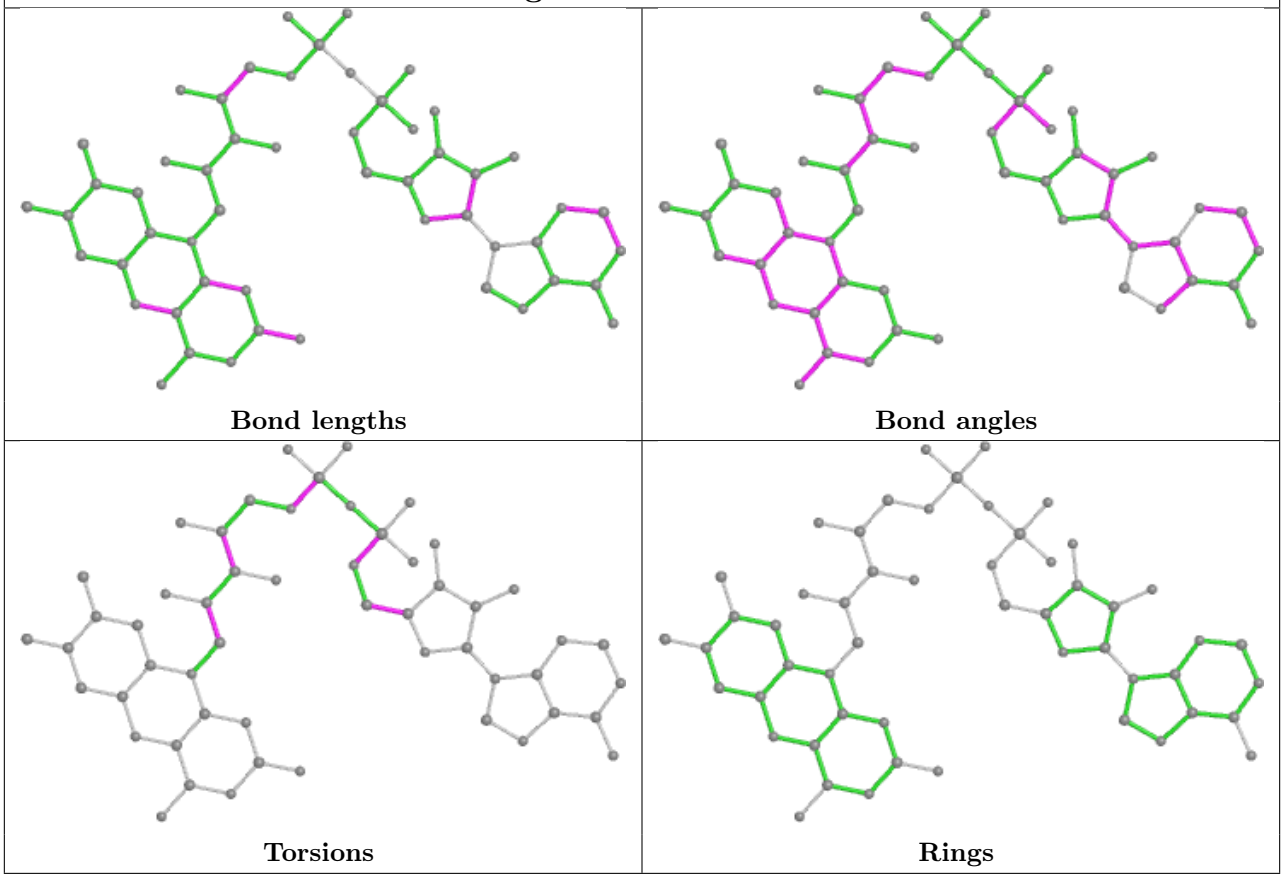


Torsions



Rings

Ligand FAD D 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	327/347 (94%)	-0.04	3 (0%)	84	86	11, 21, 34, 44	0
1	B	327/347 (94%)	0.00	6 (1%)	68	71	11, 22, 34, 44	0
1	C	327/347 (94%)	0.01	5 (1%)	73	75	10, 22, 33, 46	0
1	D	327/347 (94%)	0.08	1 (0%)	94	94	11, 22, 34, 45	0
All	All	1308/1388 (94%)	0.01	15 (1%)	80	82	10, 22, 34, 46	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	82	PRO	3.5
1	C	82	PRO	3.4
1	B	28	GLN	3.0
1	C	27	LEU	3.0
1	A	28	GLN	2.7
1	A	220	GLU	2.6
1	C	42	LEU	2.5
1	B	103	PRO	2.5
1	C	296	LEU	2.4
1	B	295	GLN	2.4
1	A	27	LEU	2.3
1	B	27	LEU	2.2
1	C	56	LEU	2.2
1	D	42	LEU	2.1
1	B	219	PRO	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)

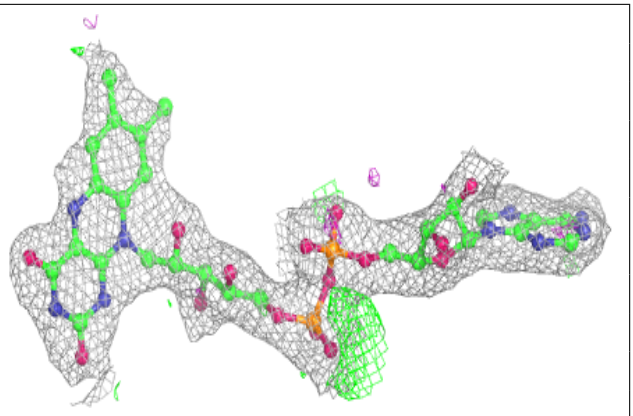
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

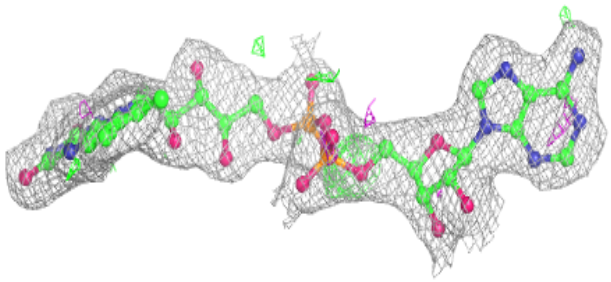
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	4P5	D	402	11/11	0.91	0.15	26,28,29,30	0
2	FAD	B	401	53/53	0.95	0.13	10,19,24,26	0
2	FAD	C	401	53/53	0.95	0.14	12,22,24,29	0
2	FAD	A	401	53/53	0.95	0.12	7,19,27,32	0
3	4P5	A	402	11/11	0.96	0.11	15,25,26,28	0
3	4P5	B	402	11/11	0.96	0.12	14,18,19,19	0
2	FAD	D	401	53/53	0.96	0.11	11,19,23,26	0
3	4P5	C	402	11/11	0.97	0.10	10,11,16,21	0

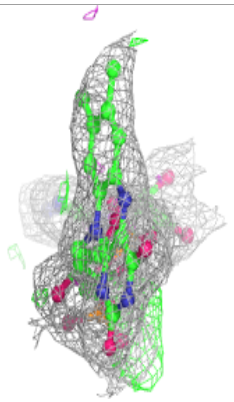
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 401:

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

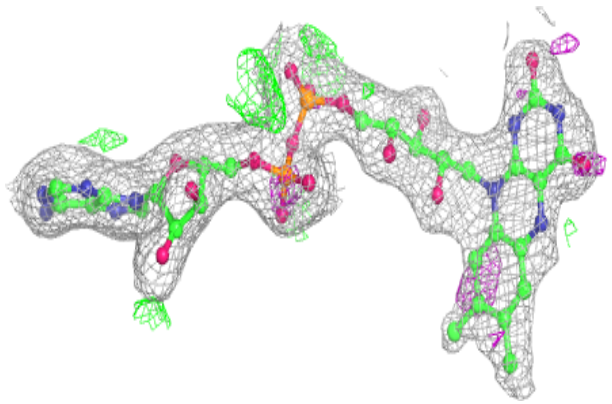


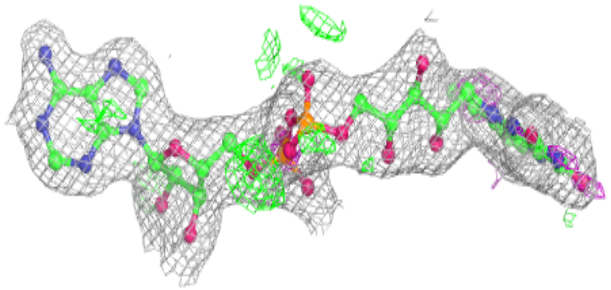


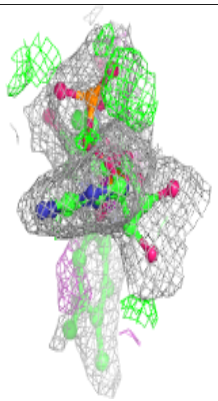


Electron density around FAD C 401:

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

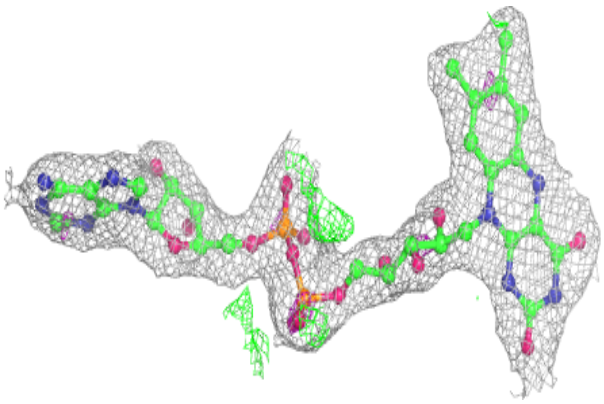


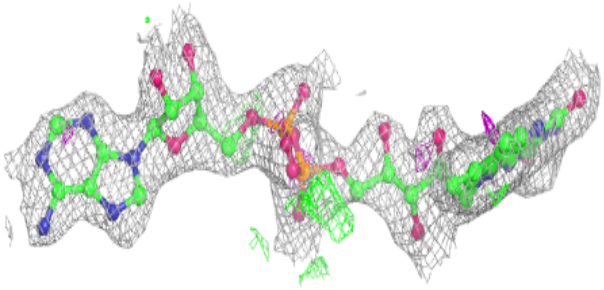


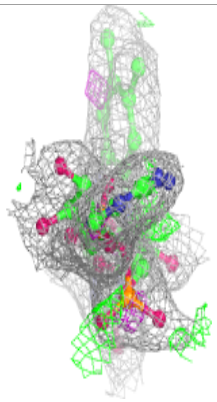


Electron density around FAD A 401:

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

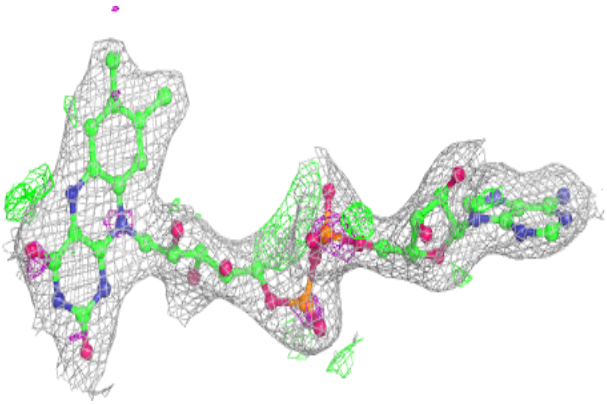


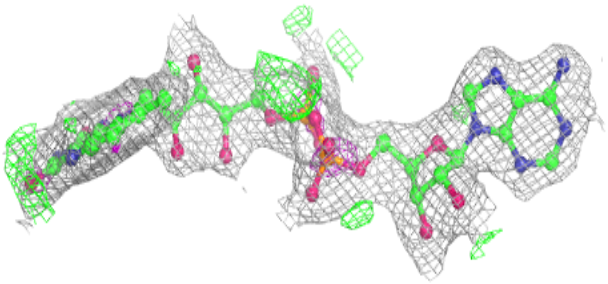


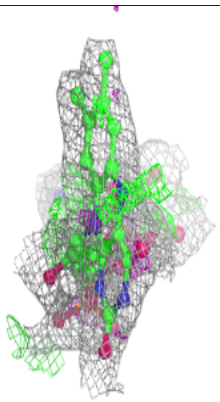


Electron density around FAD D 401:

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







6.5 Other polymers (i)

There are no such residues in this entry.