Full wwPDB X-ray Structure Validation Report ⓘ

Apr 29, 2024 – 01:28 am BST

PDB ID	:	1O96
Title	:	Structure of electron transferring flavoprotein for Methylophilus methylotrophus.
Authors	:	Leys, D.; Basran, J.; Talfournier, F.; Sutcliffe, M.J.; Scrutton, N.S.
Deposited on	:	2002-12-11
Resolution	:	3.10 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

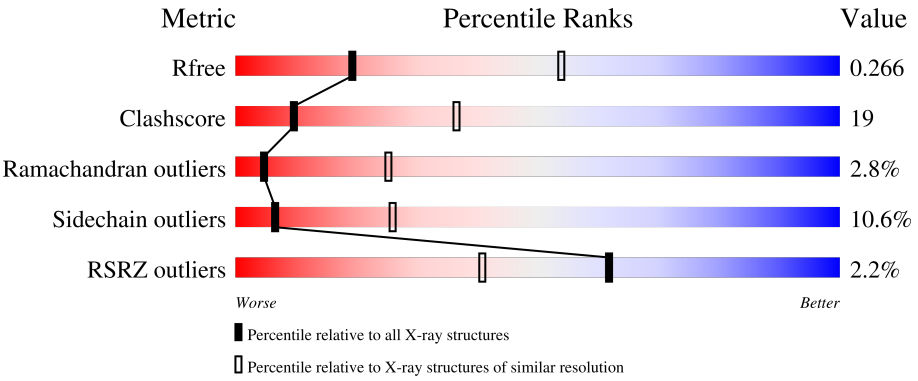
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	264	56% 30% 11%
1	C	264	55% 36% 6%
1	E	264	53% 31% 12%
1	Q	264	5% 56% 30% 5% 7%
2	B	320	% 61% 27% 8%

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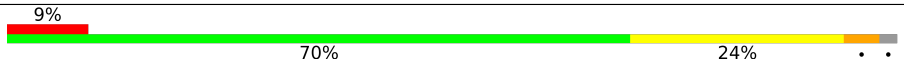
Mol	Chain	Length	Quality of chain
2	D	320	
2	F	320	
2	Z	320	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 17093 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.

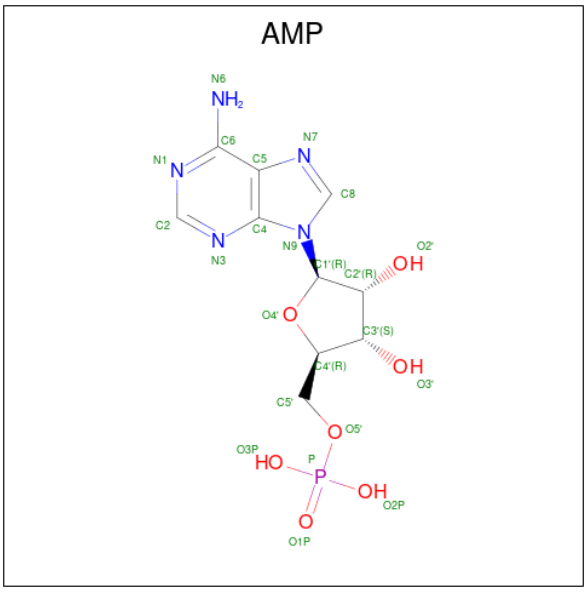
- Molecule 1 is a protein called ELECTRON TRANSFERRING FLAVOPROTEIN BETA-SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	261	Total	C	N	O	S	0	0	0
			1963	1227	336	389	11			
1	C	260	Total	C	N	O	S	0	0	0
			1942	1217	334	380	11			
1	E	260	Total	C	N	O	S	0	0	0
			1939	1216	331	381	11			
1	Q	246	Total	C	N	O	S	0	0	0
			1831	1147	311	363	10			

- Molecule 2 is a protein called ELECTRON TRANSFERRING FLAVOPROTEIN ALPHA-SUBUNIT.

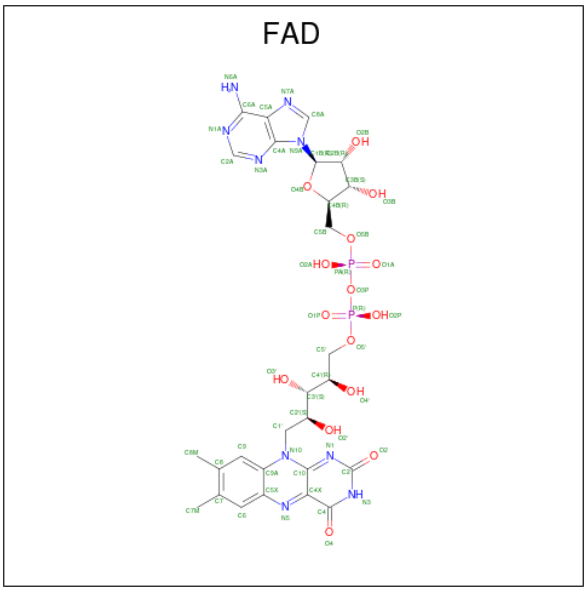
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	314	Total	C	N	O	S	0	0	0
			2287	1444	384	452	7			
2	D	314	Total	C	N	O	S	0	0	0
			2281	1440	383	451	7			
2	F	314	Total	C	N	O	S	0	0	0
			2281	1440	383	451	7			
2	Z	312	Total	C	N	O	S	0	0	0
			2265	1430	381	447	7			

- Molecule 3 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	C	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	E	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
3	Q	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



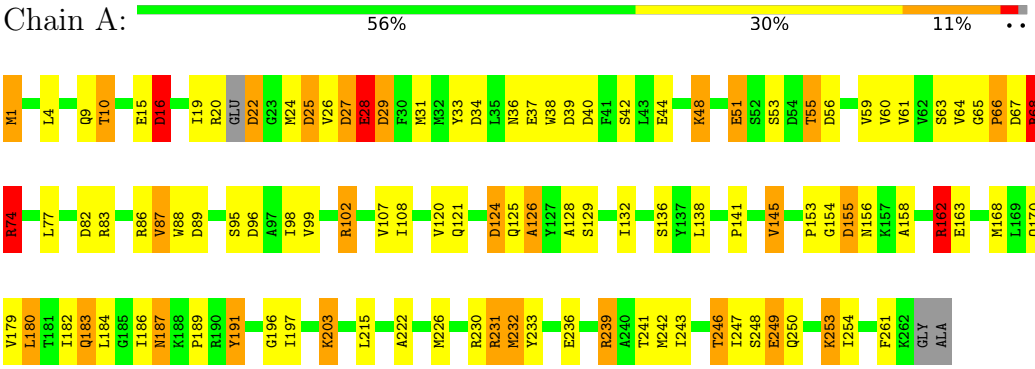
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	Z	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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.

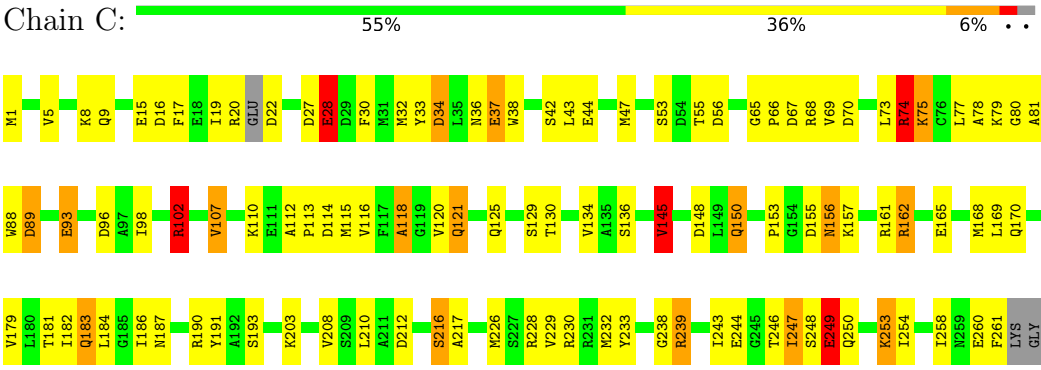
• Molecule 1: ELECTRON TRANSFERRING FLAVOPROTEIN BETA-SUBUNIT

Chain A:



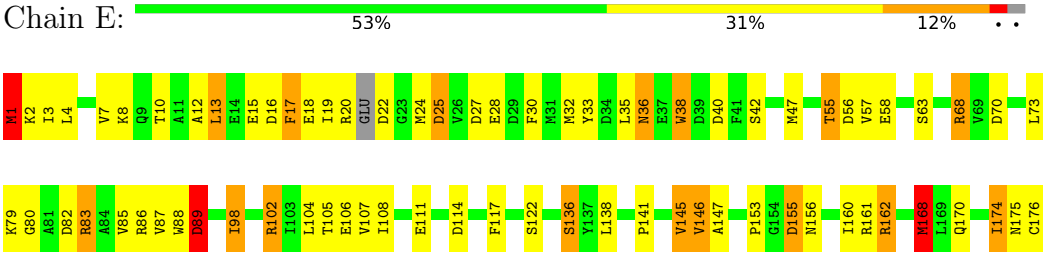
• Molecule 1: ELECTRON TRANSFERRING FLAVOPROTEIN BETA-SUBUNIT

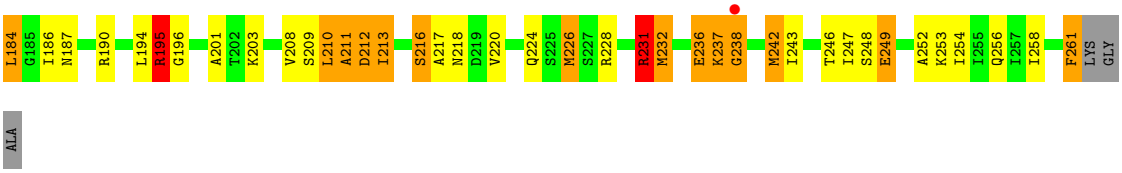
Chain C:



• Molecule 1: ELECTRON TRANSFERRING FLAVOPROTEIN BETA-SUBUNIT

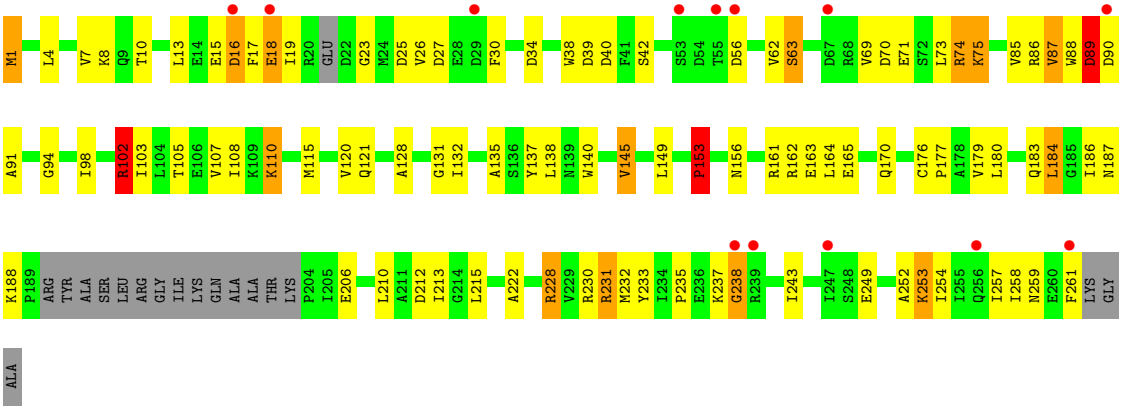
Chain E:





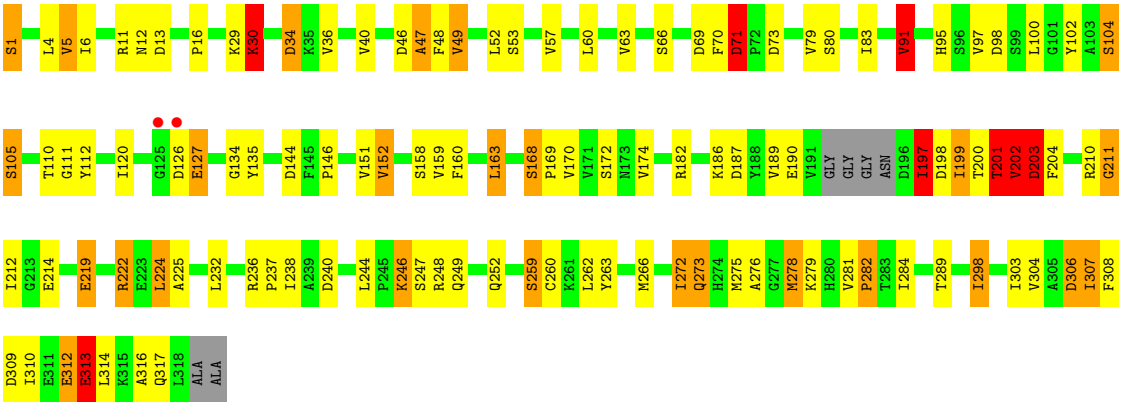
• Molecule 1: ELECTRON TRANSFERRING FLAVOPROTEIN BETA-SUBUNIT

Chain Q:



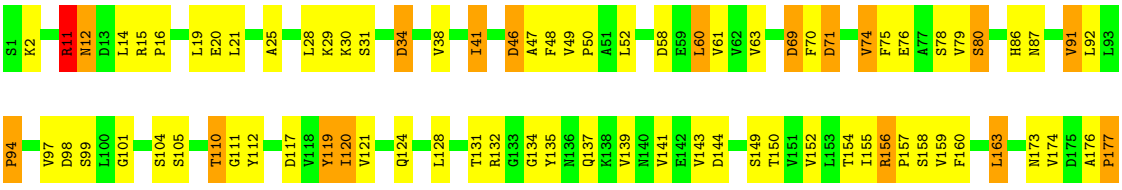
• Molecule 2: ELECTRON TRANSFERRING FLAVOPROTEIN ALPHA-SUBUNIT

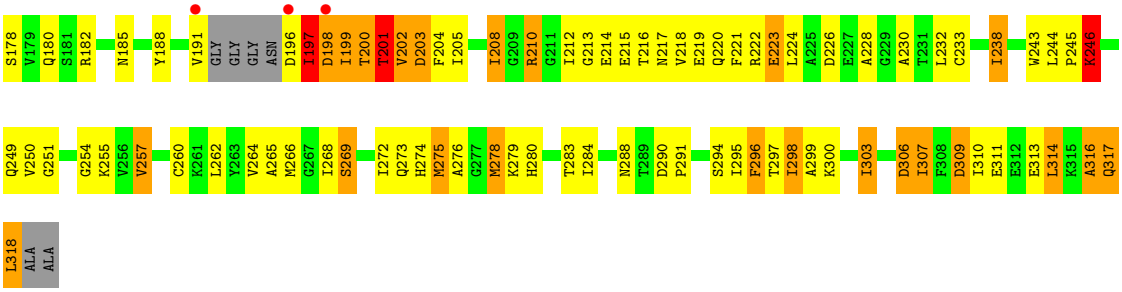
Chain B:



• Molecule 2: ELECTRON TRANSFERRING FLAVOPROTEIN ALPHA-SUBUNIT

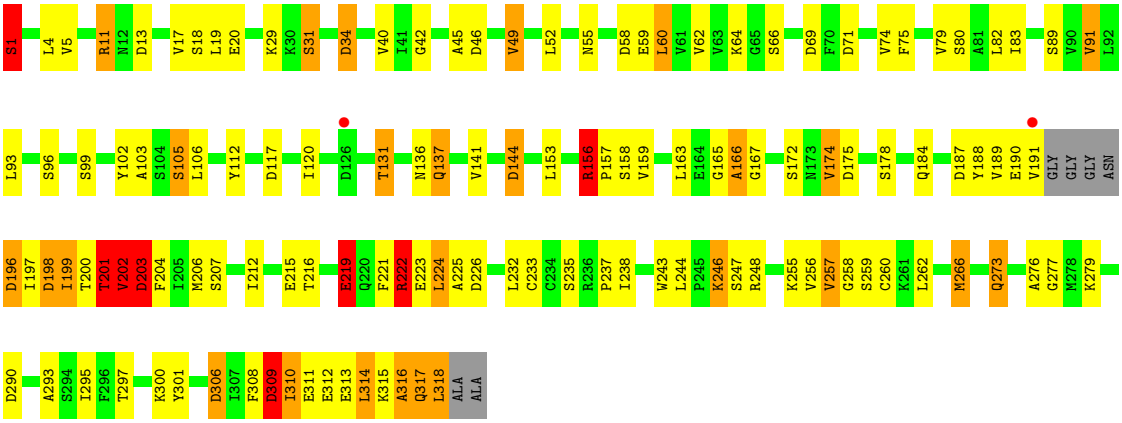
Chain D:





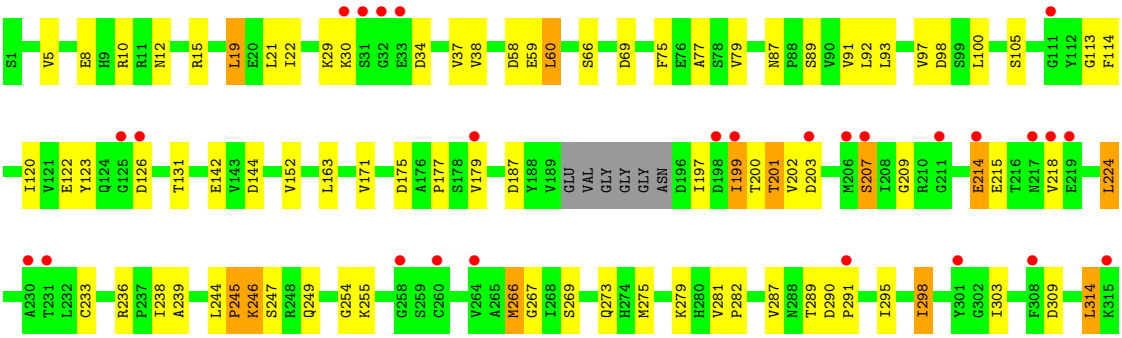
• Molecule 2: ELECTRON TRANSFERRING FLAVOPROTEIN ALPHA-SUBUNIT

Chain F:



• Molecule 2: ELECTRON TRANSFERRING FLAVOPROTEIN ALPHA-SUBUNIT

Chain Z:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	117.52Å 126.88Å 221.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 3.10 19.93 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.92-3.10) 97.8 (19.93-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.11 (at 3.09Å)	Xtriage
Refinement program	REFMAC 5.1.08	Depositor
R, R_{free}	0.212 , 0.278 0.207 , 0.266	Depositor DCC
R_{free} test set	2989 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	61.9	Xtriage
Anisotropy	0.422	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 56.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	17093	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.18% 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: FAD, AMP

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	1.69	17/1986 (0.9%)	1.59	26/2688 (1.0%)
1	C	1.72	20/1965 (1.0%)	1.53	24/2660 (0.9%)
1	E	1.55	19/1962 (1.0%)	1.51	31/2657 (1.2%)
1	Q	1.28	10/1851 (0.5%)	1.25	10/2507 (0.4%)
2	B	1.49	20/2324 (0.9%)	1.48	28/3167 (0.9%)
2	D	1.53	21/2318 (0.9%)	1.54	34/3159 (1.1%)
2	F	1.57	24/2318 (1.0%)	1.53	31/3159 (1.0%)
2	Z	1.06	6/2302 (0.3%)	1.17	11/3137 (0.4%)
All	All	1.50	137/17026 (0.8%)	1.46	195/23134 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	E	0	1
1	Q	0	1
2	B	0	3
2	D	0	2
2	F	0	2
All	All	0	10

All (137) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	28	GLU	CD-OE2	30.98	1.59	1.25
1	C	249	GLU	CD-OE1	22.16	1.50	1.25
1	A	74	ARG	CZ-NH2	15.41	1.53	1.33
1	A	28	GLU	CD-OE2	13.61	1.40	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	222	ARG	NE-CZ	13.57	1.50	1.33
1	E	195	ARG	NE-CZ	13.06	1.50	1.33
1	Q	74	ARG	NE-CZ	12.98	1.50	1.33
1	C	93	GLU	CD-OE1	12.89	1.39	1.25
2	D	219	GLU	CD-OE2	12.20	1.39	1.25
1	A	28	GLU	CG-CD	11.90	1.69	1.51
2	F	222	ARG	CZ-NH1	11.43	1.48	1.33
2	D	222	ARG	NE-CZ	11.35	1.47	1.33
1	C	93	GLU	CD-OE2	11.34	1.38	1.25
1	C	244	GLU	CD-OE1	11.15	1.38	1.25
1	E	195	ARG	CZ-NH1	10.51	1.46	1.33
1	E	74	ARG	NE-CZ	10.22	1.46	1.33
1	Q	71	GLU	CD-OE2	9.84	1.36	1.25
2	F	219	GLU	CD-OE2	9.54	1.36	1.25
1	A	74	ARG	CG-CD	9.53	1.75	1.51
2	Z	179	VAL	CB-CG2	9.51	1.72	1.52
2	D	222	ARG	CZ-NH1	9.42	1.45	1.33
1	Q	74	ARG	CZ-NH1	9.22	1.45	1.33
1	C	28	GLU	CD-OE1	9.16	1.35	1.25
2	D	196	ASP	C-O	9.14	1.40	1.23
1	A	74	ARG	CZ-NH1	9.02	1.44	1.33
2	Z	122	GLU	CD-OE1	8.88	1.35	1.25
2	D	197	ILE	CA-CB	8.35	1.74	1.54
1	C	249	GLU	CD-OE2	8.16	1.34	1.25
2	B	30	LYS	CE-NZ	7.93	1.68	1.49
2	F	226	ASP	CB-CG	7.92	1.68	1.51
2	F	103	ALA	CA-CB	-7.92	1.35	1.52
2	B	197	ILE	CA-CB	7.89	1.73	1.54
2	F	222	ARG	CZ-NH2	7.87	1.43	1.33
1	Q	74	ARG	CZ-NH2	7.83	1.43	1.33
1	E	232	MET	SD-CE	7.76	2.21	1.77
2	F	219	GLU	CG-CD	7.75	1.63	1.51
2	B	40	VAL	CB-CG1	-7.73	1.36	1.52
1	A	179	VAL	CB-CG1	-7.71	1.36	1.52
2	D	11	ARG	CG-CD	7.52	1.70	1.51
2	D	309	ASP	CG-OD1	7.31	1.42	1.25
1	Q	71	GLU	CD-OE1	7.24	1.33	1.25
1	C	244	GLU	CD-OE2	7.18	1.33	1.25
2	B	266	MET	CG-SD	-7.17	1.62	1.81
2	F	40	VAL	CB-CG2	-7.13	1.37	1.52
1	E	74	ARG	CZ-NH2	7.12	1.42	1.33
2	Z	122	GLU	CD-OE2	7.08	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	145	VAL	CB-CG1	-7.04	1.38	1.52
1	Q	75	LYS	CD-CE	7.03	1.68	1.51
1	E	242	MET	SD-CE	7.00	2.17	1.77
2	B	170	VAL	CB-CG1	6.96	1.67	1.52
2	B	222	ARG	NE-CZ	6.95	1.42	1.33
2	D	196	ASP	CA-C	6.88	1.70	1.52
1	E	12	ALA	CA-CB	-6.86	1.38	1.52
1	A	28	GLU	CD-OE1	6.81	1.33	1.25
2	F	59	GLU	CD-OE1	6.76	1.33	1.25
2	D	191	VAL	CA-CB	6.65	1.68	1.54
1	E	122	SER	CB-OG	-6.59	1.33	1.42
2	B	198	ASP	CB-CG	-6.50	1.38	1.51
2	D	197	ILE	N-CA	6.47	1.59	1.46
2	D	197	ILE	C-O	6.39	1.35	1.23
2	F	266	MET	SD-CE	6.39	2.13	1.77
2	D	196	ASP	N-CA	6.39	1.59	1.46
1	C	93	GLU	CG-CD	6.37	1.61	1.51
1	E	74	ARG	CG-CD	6.37	1.67	1.51
1	E	226	MET	SD-CE	6.37	2.13	1.77
2	B	97	VAL	CB-CG2	-6.36	1.39	1.52
1	Q	163	GLU	CD-OE1	6.35	1.32	1.25
1	Q	140	TRP	CB-CG	6.32	1.61	1.50
2	B	152	VAL	CB-CG2	-6.27	1.39	1.52
1	E	168	MET	SD-CE	6.24	2.12	1.77
2	F	20	GLU	CD-OE1	6.23	1.32	1.25
2	F	201	THR	CA-C	6.22	1.69	1.52
1	A	87	VAL	CB-CG1	-6.21	1.39	1.52
1	C	107	VAL	CB-CG2	-6.18	1.39	1.52
2	B	5	VAL	CA-CB	-6.11	1.42	1.54
2	F	102	TYR	CE2-CZ	6.08	1.46	1.38
2	D	222	ARG	CZ-NH2	6.07	1.41	1.33
2	F	202	VAL	N-CA	6.07	1.58	1.46
1	A	232	MET	SD-CE	6.00	2.11	1.77
1	C	162	ARG	CB-CG	-5.94	1.36	1.52
2	F	257	VAL	CB-CG1	-5.82	1.40	1.52
1	A	163	GLU	CD-OE1	5.78	1.32	1.25
1	A	48	LYS	CB-CG	5.76	1.68	1.52
2	D	276	ALA	CA-CB	-5.76	1.40	1.52
1	Q	1	MET	CG-SD	5.73	1.96	1.81
2	B	304	VAL	CA-CB	-5.72	1.42	1.54
2	F	204	PHE	CD2-CE2	5.71	1.50	1.39
2	F	80	SER	CB-OG	-5.71	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	195	ARG	CD-NE	5.63	1.56	1.46
2	B	219	GLU	CG-CD	5.59	1.60	1.51
2	B	104	SER	CB-OG	-5.59	1.34	1.42
2	F	293	ALA	CA-CB	5.58	1.64	1.52
2	Z	187	ASP	CB-CG	5.57	1.63	1.51
1	E	75	LYS	CD-CE	5.55	1.65	1.51
2	D	219	GLU	CD-OE1	5.55	1.31	1.25
1	C	191	TYR	CD2-CE2	5.52	1.47	1.39
1	A	61	VAL	CB-CG2	-5.51	1.41	1.52
1	C	110	LYS	CD-CE	5.49	1.65	1.51
2	D	185	ASN	CB-CG	-5.48	1.38	1.51
1	C	102	ARG	NE-CZ	5.48	1.40	1.33
2	B	97	VAL	CB-CG1	-5.47	1.41	1.52
2	B	222	ARG	CD-NE	5.46	1.55	1.46
1	E	74	ARG	CZ-NH1	5.45	1.40	1.33
1	A	191	TYR	CB-CG	-5.43	1.43	1.51
2	B	91	VAL	CB-CG1	-5.43	1.41	1.52
2	B	225	ALA	CA-CB	-5.42	1.41	1.52
2	B	151	VAL	CB-CG2	-5.41	1.41	1.52
1	C	37	GLU	CD-OE1	5.39	1.31	1.25
1	C	5	VAL	CB-CG1	-5.38	1.41	1.52
1	Q	75	LYS	CE-NZ	5.38	1.62	1.49
1	E	38	TRP	CB-CG	-5.37	1.40	1.50
1	A	16	ASP	CB-CG	5.34	1.62	1.51
2	F	266	MET	CG-SD	-5.34	1.67	1.81
2	Z	266	MET	SD-CE	5.34	2.07	1.77
2	F	191	VAL	CB-CG1	5.32	1.64	1.52
2	F	238	ILE	CA-CB	-5.28	1.42	1.54
1	E	85	VAL	CB-CG2	-5.28	1.41	1.52
1	C	37	GLU	CD-OE2	5.27	1.31	1.25
2	D	74	VAL	CB-CG1	-5.27	1.41	1.52
2	D	250	VAL	CA-CB	-5.25	1.43	1.54
2	F	137	GLN	C-O	5.24	1.33	1.23
1	A	59	VAL	CB-CG2	-5.23	1.41	1.52
1	C	118	ALA	CA-CB	-5.22	1.41	1.52
1	E	195	ARG	CG-CD	5.20	1.65	1.51
2	B	144	ASP	CB-CG	5.18	1.62	1.51
2	B	127	GLU	CD-OE2	5.11	1.31	1.25
2	F	219	GLU	CB-CG	5.11	1.61	1.52
2	Z	122	GLU	CG-CD	5.11	1.59	1.51
1	E	36	ASN	CB-CG	5.09	1.62	1.51
2	D	275	MET	SD-CE	-5.08	1.49	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	233	TYR	CD1-CE1	5.07	1.47	1.39
1	A	64	VAL	CA-CB	-5.07	1.44	1.54
2	D	296	PHE	CB-CG	-5.07	1.42	1.51
1	C	134	VAL	CB-CG2	-5.06	1.42	1.52
2	F	223	GLU	CD-OE2	5.06	1.31	1.25
1	E	146	VAL	CB-CG1	5.04	1.63	1.52
2	D	159	VAL	CB-CG1	-5.04	1.42	1.52

All (195) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	74	ARG	NE-CZ-NH2	-12.17	114.22	120.30
2	D	198	ASP	CB-CG-OD2	11.85	128.97	118.30
1	C	56	ASP	CB-CG-OD2	11.16	128.35	118.30
1	Q	16	ASP	CB-CG-OD2	10.98	128.18	118.30
1	A	68	ARG	NE-CZ-NH1	10.87	125.73	120.30
2	F	202	VAL	CB-CA-C	-10.59	91.29	111.40
1	E	27	ASP	CB-CG-OD2	10.56	127.80	118.30
1	E	195	ARG	NE-CZ-NH1	10.54	125.57	120.30
2	D	202	VAL	CB-CA-C	-9.83	92.72	111.40
1	A	25	ASP	CB-CG-OD2	9.65	126.98	118.30
1	A	89	ASP	CB-CG-OD2	9.59	126.93	118.30
2	F	58	ASP	CB-CG-OD2	9.56	126.91	118.30
2	F	226	ASP	CB-CG-OD1	9.51	126.86	118.30
1	E	162	ARG	NE-CZ-NH1	-9.45	115.58	120.30
2	D	163	LEU	CA-CB-CG	9.27	136.62	115.30
2	B	187	ASP	CB-CG-OD1	-9.12	110.09	118.30
2	F	69	ASP	CB-CG-OD1	9.10	126.49	118.30
1	C	102	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	A	67	ASP	CB-CG-OD2	9.04	126.44	118.30
2	D	58	ASP	CB-CG-OD2	9.01	126.41	118.30
2	D	15	ARG	NE-CZ-NH1	-8.96	115.82	120.30
1	A	39	ASP	CB-CG-OD2	8.87	126.28	118.30
1	C	82	ASP	CB-CG-OD2	8.86	126.28	118.30
1	E	195	ARG	NH1-CZ-NH2	-8.79	109.73	119.40
2	Z	144	ASP	CB-CG-OD2	8.76	126.19	118.30
2	B	202	VAL	CB-CA-C	-8.64	94.98	111.40
1	C	28	GLU	OE1-CD-OE2	8.53	133.53	123.30
2	D	98	ASP	CB-CG-OD2	8.35	125.81	118.30
1	Q	27	ASP	CB-CG-OD2	8.30	125.77	118.30
1	C	27	ASP	CB-CG-OD2	8.27	125.75	118.30
2	Z	98	ASP	CB-CG-OD2	8.23	125.71	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	102	ARG	NE-CZ-NH1	8.12	124.36	120.30
2	Z	58	ASP	CB-CG-OD2	8.09	125.58	118.30
2	B	187	ASP	CB-CG-OD2	7.78	125.30	118.30
2	Z	34	ASP	CB-CG-OD2	7.74	125.26	118.30
2	F	156	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	E	68	ARG	NE-CZ-NH2	-7.47	116.56	120.30
2	B	126	ASP	CB-CG-OD2	7.28	124.86	118.30
1	C	68	ARG	NE-CZ-NH1	7.25	123.92	120.30
2	D	180	GLN	N-CA-C	-7.22	91.51	111.00
1	Q	16	ASP	CB-CG-OD1	-7.19	111.83	118.30
2	B	69	ASP	CB-CG-OD2	7.17	124.75	118.30
1	E	83	ARG	NE-CZ-NH1	-7.17	116.72	120.30
2	B	201	THR	CA-CB-CG2	-7.14	102.40	112.40
1	A	48	LYS	CA-CB-CG	7.08	128.98	113.40
2	Z	126	ASP	CB-CG-OD2	7.05	124.65	118.30
2	D	182	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	E	24	MET	CB-CA-C	6.99	124.39	110.40
2	D	306	ASP	CB-CA-C	6.97	124.34	110.40
1	A	241	THR	OG1-CB-CG2	-6.97	93.97	110.00
2	F	13	ASP	CB-CG-OD2	6.97	124.57	118.30
1	C	68	ARG	NE-CZ-NH2	-6.95	116.83	120.30
2	B	98	ASP	CB-CG-OD2	6.93	124.53	118.30
1	E	89	ASP	CB-CG-OD1	-6.91	112.08	118.30
1	A	29	ASP	CB-CG-OD2	6.89	124.50	118.30
1	E	70	ASP	CB-CG-OD2	6.88	124.49	118.30
1	E	89	ASP	CB-CG-OD2	6.88	124.49	118.30
1	C	244	GLU	OE1-CD-OE2	6.87	131.54	123.30
2	F	1	SER	N-CA-C	-6.87	92.45	111.00
2	D	198	ASP	N-CA-CB	-6.86	98.25	110.60
1	C	249	GLU	CB-CA-C	-6.78	96.83	110.40
2	F	156	ARG	NE-CZ-NH2	-6.78	116.91	120.30
2	F	34	ASP	CB-CG-OD2	6.77	124.39	118.30
1	A	162	ARG	NE-CZ-NH1	-6.75	116.93	120.30
1	Q	212	ASP	CB-CG-OD2	6.74	124.37	118.30
1	C	70	ASP	CB-CG-OD1	6.67	124.30	118.30
2	B	34	ASP	CB-CG-OD2	6.66	124.29	118.30
1	A	40	ASP	CB-CG-OD2	6.64	124.27	118.30
2	F	309	ASP	CB-CG-OD2	6.61	124.25	118.30
1	C	74	ARG	CG-CD-NE	-6.57	98.00	111.80
1	E	162	ARG	NE-CZ-NH2	6.57	123.58	120.30
2	F	11	ARG	NE-CZ-NH1	-6.55	117.02	120.30
2	F	201	THR	N-CA-CB	-6.55	97.86	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	74	ARG	NE-CZ-NH2	6.51	123.55	120.30
1	C	89	ASP	CB-CG-OD2	6.50	124.14	118.30
1	C	212	ASP	CB-CG-OD2	6.45	124.11	118.30
2	D	180	GLN	CB-CA-C	6.45	123.30	110.40
1	A	74	ARG	NH1-CZ-NH2	6.45	126.50	119.40
1	A	27	ASP	CB-CG-OD2	6.42	124.08	118.30
2	D	46	ASP	CB-CA-C	-6.42	97.57	110.40
2	B	163	LEU	CB-CG-CD2	-6.39	100.14	111.00
2	F	187	ASP	CB-CG-OD2	6.38	124.04	118.30
2	Z	175	ASP	CB-CG-OD2	6.36	124.03	118.30
1	E	102	ARG	NE-CZ-NH1	6.36	123.48	120.30
2	F	306	ASP	CB-CG-OD1	6.36	124.02	118.30
1	E	190	ARG	NE-CZ-NH1	6.34	123.47	120.30
2	D	198	ASP	CB-CG-OD1	-6.34	112.60	118.30
1	E	231	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	242	MET	CG-SD-CE	6.28	110.25	100.20
1	C	155	ASP	CB-CG-OD2	6.28	123.95	118.30
2	Z	309	ASP	CB-CG-OD2	6.19	123.87	118.30
1	C	168	MET	CB-CG-SD	-6.16	93.91	112.40
2	D	15	ARG	NE-CZ-NH2	6.16	123.38	120.30
2	D	69	ASP	CB-CG-OD1	6.16	123.84	118.30
2	Z	69	ASP	CB-CG-OD1	6.15	123.83	118.30
2	D	201	THR	C-N-CA	6.13	137.01	121.70
2	B	309	ASP	CB-CG-OD1	6.11	123.80	118.30
2	F	153	LEU	CB-CG-CD1	-6.10	100.63	111.00
1	C	148	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	180	LEU	CB-CG-CD2	-6.05	100.71	111.00
2	B	198	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	231	ARG	NE-CZ-NH2	-6.05	117.28	120.30
2	F	198	ASP	CB-CA-C	-6.04	98.31	110.40
2	F	144	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	124	ASP	CB-CG-OD2	6.00	123.70	118.30
1	E	190	ARG	NE-CZ-NH2	-5.96	117.32	120.30
2	F	318	LEU	CA-CB-CG	5.96	129.00	115.30
1	E	13	LEU	CB-CG-CD2	-5.95	100.88	111.00
2	D	213	GLY	N-CA-C	5.94	127.95	113.10
2	D	34	ASP	CB-CG-OD2	5.94	123.64	118.30
2	D	16	PRO	N-CD-CG	-5.91	94.33	103.20
2	D	254	GLY	N-CA-C	-5.90	98.36	113.10
2	D	210	ARG	NE-CZ-NH2	5.85	123.23	120.30
2	D	303	ILE	N-CA-C	-5.85	95.21	111.00
1	C	168	MET	CB-CA-C	-5.84	98.71	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	244	GLU	CG-CD-OE1	-5.83	106.63	118.30
2	B	146	PRO	N-CD-CG	-5.81	94.48	103.20
1	C	34	ASP	CB-CG-OD1	5.80	123.52	118.30
2	F	198	ASP	CB-CG-OD1	-5.80	113.08	118.30
2	D	94	PRO	N-CD-CG	-5.79	94.51	103.20
2	B	13	ASP	CB-CG-OD2	5.77	123.49	118.30
2	D	12	ASN	CB-CA-C	-5.76	98.88	110.40
1	A	67	ASP	CB-CG-OD1	-5.76	113.12	118.30
2	Z	100	LEU	CA-CB-CG	5.76	128.54	115.30
1	E	238	GLY	N-CA-C	-5.75	98.74	113.10
2	B	182	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	E	86	ARG	NE-CZ-NH1	-5.70	117.45	120.30
2	D	14	LEU	CB-CG-CD1	5.70	120.68	111.00
2	Z	98	ASP	CB-CG-OD1	-5.69	113.18	118.30
2	F	201	THR	C-N-CA	5.67	135.89	121.70
1	Q	184	LEU	CA-CB-CG	5.59	128.16	115.30
2	F	198	ASP	CB-CG-OD2	5.59	123.33	118.30
1	Q	40	ASP	CB-CG-OD2	5.58	123.32	118.30
2	D	314	LEU	CA-CB-CG	5.55	128.08	115.30
1	C	74	ARG	NE-CZ-NH2	-5.53	117.53	120.30
2	F	131	THR	OG1-CB-CG2	-5.51	97.33	110.00
1	A	31	MET	CG-SD-CE	-5.50	91.40	100.20
2	B	278	MET	CG-SD-CE	-5.49	91.41	100.20
2	B	71	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	138	LEU	CB-CG-CD1	-5.48	101.68	111.00
1	A	83	ARG	NE-CZ-NH1	5.47	123.04	120.30
2	B	313	GLU	N-CA-CB	-5.47	100.75	110.60
2	F	1	SER	C-N-CA	-5.46	108.04	121.70
2	D	198	ASP	C-N-CA	-5.45	108.08	121.70
2	F	196	ASP	C-N-CA	5.45	135.32	121.70
2	D	128	LEU	CB-CG-CD2	-5.44	101.76	111.00
2	D	110	THR	C-N-CA	-5.43	110.89	122.30
1	E	108	ILE	CG1-CB-CG2	-5.41	99.50	111.40
1	Q	228	ARG	NE-CZ-NH1	-5.41	117.59	120.30
2	D	41	ILE	CG1-CB-CG2	-5.40	99.52	111.40
2	B	73	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	70	ASP	CB-CG-OD1	5.38	123.14	118.30
2	B	272	ILE	CG1-CB-CG2	-5.37	99.59	111.40
1	C	161	ARG	NE-CZ-NH2	-5.35	117.62	120.30
2	D	71	ASP	CB-CG-OD2	5.35	123.11	118.30
2	D	219	GLU	CA-CB-CG	5.33	125.12	113.40
1	A	82	ASP	CB-CG-OD2	5.32	123.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	32	MET	CG-SD-CE	5.32	108.71	100.20
2	F	222	ARG	NE-CZ-NH2	5.30	122.95	120.30
2	F	203	ASP	N-CA-C	5.29	125.28	111.00
2	F	246	LYS	CD-CE-NZ	5.29	123.87	111.70
2	B	120	ILE	CG1-CB-CG2	-5.28	99.79	111.40
1	E	102	ARG	CG-CD-NE	5.27	122.86	111.80
2	B	201	THR	C-N-CA	5.25	134.82	121.70
2	B	222	ARG	NE-CZ-NH2	5.23	122.91	120.30
2	B	306	ASP	CB-CG-OD1	-5.23	113.60	118.30
1	A	180	LEU	CA-CB-CG	5.20	127.26	115.30
1	C	162	ARG	CB-CA-C	5.20	120.80	110.40
2	F	318	LEU	CB-CG-CD1	-5.20	102.16	111.00
2	B	110	THR	C-N-CA	-5.19	111.39	122.30
1	E	184	LEU	CB-CG-CD1	-5.18	102.19	111.00
1	A	68	ARG	NE-CZ-NH2	-5.17	117.72	120.30
2	B	240	ASP	CB-CG-OD2	5.17	122.95	118.30
2	B	203	ASP	CB-CG-OD2	5.17	122.95	118.30
1	E	161	ARG	NE-CZ-NH1	-5.15	117.73	120.30
2	B	105	SER	N-CA-CB	5.14	118.21	110.50
1	Q	25	ASP	CB-CG-OD2	5.14	122.92	118.30
1	E	98	ILE	CG1-CB-CG2	-5.13	100.12	111.40
1	A	40	ASP	CB-CG-OD1	-5.12	113.70	118.30
1	E	17	PHE	N-CA-CB	-5.10	101.41	110.60
2	D	156	ARG	NE-CZ-NH2	-5.10	117.75	120.30
2	Z	21	LEU	CA-CB-CG	5.10	127.03	115.30
1	Q	87	VAL	CB-CA-C	-5.09	101.74	111.40
1	E	184	LEU	CB-CG-CD2	5.06	119.60	111.00
1	E	195	ARG	NE-CZ-NH2	5.06	122.83	120.30
2	B	214	GLU	OE1-CD-OE2	-5.05	117.24	123.30
2	F	167	GLY	N-CA-C	-5.05	100.48	113.10
1	C	175	ASN	CB-CA-C	-5.04	100.32	110.40
1	E	155	ASP	CB-CA-C	-5.03	100.35	110.40
2	F	290	ASP	CB-CG-OD2	5.02	122.82	118.30
1	E	40	ASP	CB-CG-OD2	5.01	122.81	118.30
2	F	5	VAL	CB-CA-C	-5.01	101.88	111.40
1	C	169	LEU	CB-CG-CD2	-5.01	102.49	111.00
2	D	61	VAL	CB-CA-C	-5.00	101.89	111.40
1	E	1	MET	CB-CG-SD	5.00	127.41	112.40

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	22	ASP	Peptide
2	B	201	THR	Peptide
2	B	312	GLU	Peptide
2	B	313	GLU	Peptide
2	D	197	ILE	Peptide
2	D	200	THR	Peptide
1	E	210	LEU	Peptide
2	F	196	ASP	Peptide
2	F	201	THR	Peptide
1	Q	231	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1963	0	1916	87	1
1	C	1942	0	1901	99	0
1	E	1939	0	1891	107	0
1	Q	1831	0	1768	68	0
2	B	2287	0	2250	81	0
2	D	2281	0	2237	125	0
2	F	2281	0	2237	85	1
2	Z	2265	0	2222	52	0
3	A	23	0	12	0	0
3	C	23	0	12	3	0
3	E	23	0	12	2	0
3	Q	23	0	12	2	0
4	B	53	0	31	1	0
4	D	53	0	31	8	0
4	F	53	0	31	0	0
4	Z	53	0	31	4	0
All	All	17093	0	16594	655	1

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 19.

All (655) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:ARG:CD	1:A:74:ARG:CG	1.75	1.56
2:B:30:LYS:CE	2:B:30:LYS:NZ	1.68	1.54
1:Q:115:MET:SD	1:Q:115:MET:CE	2.03	1.46
1:Q:232:MET:CE	1:Q:232:MET:SD	2.05	1.44
2:Z:266:MET:SD	2:Z:266:MET:CE	2.07	1.42
1:A:232:MET:SD	1:A:232:MET:CE	2.11	1.39
1:E:226:MET:SD	1:E:226:MET:CE	2.13	1.36
2:F:266:MET:SD	2:F:266:MET:CE	2.13	1.36
1:E:168:MET:SD	1:E:168:MET:CE	2.12	1.36
1:E:242:MET:SD	1:E:242:MET:CE	2.17	1.32
1:E:232:MET:SD	1:E:232:MET:CE	2.21	1.29
1:A:239:ARG:CG	1:A:239:ARG:O	1.80	1.27
1:C:53:SER:OG	1:C:55:THR:HG22	1.45	1.16
1:C:243:ILE:HD13	1:C:253:LYS:HG3	1.23	1.16
1:A:74:ARG:NH2	1:A:203:LYS:O	1.77	1.15
1:Q:235:PRO:HG2	1:Q:237:LYS:HG3	1.21	1.14
1:A:239:ARG:O	1:A:239:ARG:HG2	1.32	1.08
1:E:1:MET:HG3	1:E:153:PRO:HB3	1.27	1.08
2:D:202:VAL:HG12	2:D:203:ASP:H	0.93	1.06
2:F:202:VAL:HG12	2:F:203:ASP:N	1.67	1.05
1:E:236:GLU:O	1:E:237:LYS:HB2	1.52	1.03
1:C:47:MET:HE2	1:C:80:GLY:HA3	1.39	1.03
1:A:246:THR:H	1:A:249:GLU:HG3	1.19	1.03
1:E:246:THR:H	1:E:249:GLU:HG3	1.24	1.02
2:D:202:VAL:CG1	2:D:203:ASP:H	1.74	1.01
2:F:202:VAL:CG1	2:F:203:ASP:N	2.24	1.01
2:D:202:VAL:HG12	2:D:203:ASP:N	1.72	1.00
1:A:1:MET:HG3	1:A:153:PRO:HB3	1.43	1.00
2:B:313:GLU:O	2:B:317:GLN:HG3	1.61	0.99
2:B:202:VAL:HG12	2:B:203:ASP:N	1.72	0.98
2:D:310:ILE:HG22	2:D:314:LEU:HD22	1.45	0.96
2:F:1:SER:N	2:F:34:ASP:OD1	2.00	0.94
1:Q:235:PRO:HG2	1:Q:237:LYS:CG	1.97	0.94
2:F:202:VAL:CG1	2:F:203:ASP:H	1.79	0.94
2:D:205:ILE:HG13	2:D:260:CYS:SG	2.07	0.93
1:Q:102:ARG:HH11	1:Q:102:ARG:HG2	1.34	0.93
1:C:246:THR:H	1:C:249:GLU:HG3	1.34	0.92
2:Z:202:VAL:HG12	2:Z:203:ASP:N	1.85	0.92
1:Q:183:GLN:HE21	1:Q:184:LEU:H	0.93	0.91
2:F:31:SER:HA	1:Q:91:ALA:HA	1.53	0.91
1:Q:102:ARG:HG2	1:Q:102:ARG:NH1	1.83	0.91
2:Z:202:VAL:HG12	2:Z:203:ASP:H	1.37	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:202:VAL:CG1	2:Z:203:ASP:H	1.84	0.90
2:B:197:ILE:CD1	2:B:248:ARG:HE	1.84	0.89
1:E:168:MET:CE	1:E:168:MET:HB2	2.03	0.89
2:F:219:GLU:OE2	2:F:222:ARG:HD2	1.73	0.89
1:C:246:THR:O	1:C:247:ILE:C	2.10	0.89
1:A:246:THR:N	1:A:249:GLU:HG3	1.87	0.88
1:C:47:MET:CE	1:C:80:GLY:HA3	2.05	0.86
2:F:1:SER:N	2:F:34:ASP:CG	2.28	0.86
1:Q:183:GLN:NE2	1:Q:184:LEU:H	1.72	0.85
1:C:230:ARG:NH2	2:D:124:GLN:HE22	1.75	0.84
1:A:239:ARG:O	1:A:239:ARG:HG3	1.75	0.84
1:Q:183:GLN:HE21	1:Q:184:LEU:N	1.75	0.83
1:E:226:MET:HE3	2:F:112:TYR:O	1.77	0.83
1:C:243:ILE:CD1	1:C:253:LYS:HG3	2.05	0.83
2:B:202:VAL:HG12	2:B:203:ASP:H	1.41	0.83
2:Z:246:LYS:HE2	2:Z:249:GLN:HE22	1.44	0.82
1:C:74:ARG:NH2	1:C:203:LYS:O	2.13	0.82
2:B:202:VAL:CG1	2:B:203:ASP:N	2.42	0.81
1:C:66:PRO:O	1:C:86:ARG:HD2	1.80	0.81
1:A:28:GLU:OE2	1:A:33:TYR:OH	1.99	0.81
2:F:219:GLU:OE2	2:F:222:ARG:CD	2.28	0.81
2:B:197:ILE:HD13	2:B:248:ARG:HE	1.46	0.81
1:Q:102:ARG:HH11	1:Q:102:ARG:CG	1.92	0.80
2:F:120:ILE:HB	2:F:131:THR:HB	1.63	0.80
1:C:15:GLU:O	1:C:16:ASP:HB2	1.79	0.80
1:A:20:ARG:CB	1:A:22:ASP:HA	2.10	0.80
1:C:162:ARG:HE	1:C:170:GLN:NE2	1.79	0.80
1:A:102:ARG:HG3	1:A:102:ARG:HH11	1.48	0.80
1:A:246:THR:H	1:A:249:GLU:CG	1.93	0.79
2:D:243:TRP:O	2:D:244:LEU:HG	1.81	0.79
2:Z:202:VAL:CG1	2:Z:203:ASP:N	2.44	0.78
1:C:129:SER:HB3	2:D:104:SER:HB3	1.66	0.77
2:F:219:GLU:CD	2:F:222:ARG:HD2	2.03	0.77
1:Q:1:MET:HG3	1:Q:153:PRO:HB3	1.67	0.77
2:D:223:GLU:O	2:D:226:ASP:HB2	1.84	0.76
1:Q:108:ILE:HG21	1:Q:138:LEU:HD11	1.66	0.76
1:A:247:ILE:HG22	2:B:313:GLU:HG2	1.66	0.76
1:A:254:ILE:HD11	2:B:303:ILE:HD13	1.66	0.76
2:F:310:ILE:O	2:F:314:LEU:HB2	1.85	0.76
2:D:200:THR:HA	2:D:202:VAL:HG23	1.68	0.75
2:D:264:VAL:HG12	2:D:266:MET:HE2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:202:VAL:HG13	2:F:203:ASP:H	1.52	0.75
2:B:202:VAL:CG1	2:B:203:ASP:H	1.97	0.75
1:E:42:SER:HB2	1:E:182:ILE:HG13	1.67	0.75
1:E:15:GLU:O	1:E:16:ASP:HB2	1.86	0.74
1:Q:243:ILE:HD13	1:Q:253:LYS:HG3	1.70	0.74
2:F:313:GLU:O	2:F:316:ALA:N	2.21	0.73
2:D:204:PHE:CE1	2:D:230:ALA:HB2	2.22	0.73
1:E:232:MET:HG3	2:F:141:VAL:HG22	1.70	0.73
2:F:31:SER:HB3	1:Q:90:ASP:O	1.88	0.73
2:D:310:ILE:O	2:D:314:LEU:HB2	1.88	0.73
1:E:246:THR:N	1:E:249:GLU:HG3	2.02	0.73
1:C:53:SER:HG	1:C:55:THR:HG22	1.52	0.72
1:E:105:THR:HG23	1:E:138:LEU:HG	1.71	0.72
1:A:136:SER:HB2	2:B:105:SER:OG	1.88	0.72
2:B:313:GLU:HA	2:B:316:ALA:HB3	1.70	0.72
1:E:1:MET:CG	1:E:153:PRO:HB3	2.16	0.72
2:F:206:MET:SD	2:F:224:LEU:HD13	2.30	0.72
1:E:246:THR:H	1:E:249:GLU:CG	2.00	0.71
2:D:208:ILE:HG12	2:D:232:LEU:HD11	1.73	0.71
1:C:53:SER:OG	1:C:55:THR:CG2	2.35	0.70
2:D:278:MET:CE	2:D:284:ILE:HD13	2.22	0.69
1:A:20:ARG:HB2	1:A:22:ASP:HA	1.74	0.69
1:A:236:GLU:OE2	2:F:184:GLN:NE2	2.26	0.69
1:Q:105:THR:HG21	1:Q:137:TYR:HB3	1.75	0.69
2:D:21:LEU:HD11	2:D:94:PRO:HG3	1.74	0.69
2:B:95:HIS:CE1	2:B:100:LEU:HD21	2.27	0.68
2:D:204:PHE:CD2	2:D:262:LEU:HD23	2.27	0.68
1:E:20:ARG:O	1:E:22:ASP:CB	2.41	0.68
1:A:19:ILE:O	1:A:20:ARG:C	2.32	0.68
1:E:55:THR:OG1	1:E:56:ASP:N	2.28	0.67
2:Z:22:ILE:HD11	2:Z:38:VAL:HG21	1.74	0.67
1:A:25:ASP:OD1	1:A:26:VAL:N	2.24	0.67
1:E:10:THR:HG23	1:E:36:ASN:HB2	1.77	0.66
1:E:211:ALA:O	1:E:213:ILE:N	2.28	0.66
1:E:58:GLU:OE2	1:E:83:ARG:NH1	2.27	0.66
1:A:183:GLN:HE21	1:A:184:LEU:H	1.43	0.66
2:B:246:LYS:NZ	2:B:249:GLN:HE22	1.94	0.65
1:A:74:ARG:CG	1:A:74:ARG:NE	2.57	0.65
1:C:162:ARG:HE	1:C:170:GLN:HE21	1.44	0.65
2:D:25:ALA:HB2	2:D:92:LEU:HD12	1.78	0.65
2:F:313:GLU:O	2:F:314:LEU:C	2.35	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:162:ARG:HH21	1:Q:170:GLN:HE22	1.45	0.65
1:E:147:ALA:O	1:E:186:ILE:HG13	1.96	0.65
2:F:117:ASP:OD1	2:F:156:ARG:HD3	1.97	0.65
2:F:157:PRO:O	2:F:158:SER:HB2	1.97	0.65
1:Q:121:GLN:HB3	1:Q:128:ALA:HB2	1.78	0.65
2:B:46:ASP:O	2:B:48:PHE:N	2.29	0.64
2:D:173:ASN:O	2:D:174:VAL:HG12	1.97	0.64
1:C:87:VAL:HG21	1:C:107:VAL:HG21	1.78	0.64
1:Q:132:ILE:HG22	2:Z:105:SER:HB2	1.80	0.64
2:Z:8:GLU:O	2:Z:15:ARG:HB2	1.96	0.64
2:D:310:ILE:CG2	2:D:314:LEU:HD22	2.25	0.64
1:C:246:THR:OG1	1:C:249:GLU:HG2	1.98	0.64
1:A:38:TRP:HE1	1:A:183:GLN:NE2	1.95	0.64
1:A:176:CYS:HA	1:A:177:PRO:C	2.19	0.63
2:B:199:ILE:C	2:B:201:THR:H	2.00	0.63
2:D:257:VAL:HG23	2:D:257:VAL:O	1.99	0.63
1:E:63:SER:HA	3:E:1262:AMP:H2	1.64	0.63
1:Q:252:ALA:HA	2:Z:317:GLN:HE22	1.63	0.63
2:F:309:ASP:HA	2:F:312:GLU:HG2	1.81	0.62
2:B:189:VAL:HG12	2:B:190:GLU:N	2.14	0.62
2:D:63:VAL:HG22	2:D:174:VAL:HG22	1.80	0.62
1:Q:132:ILE:CG2	2:Z:105:SER:HB2	2.30	0.62
2:Z:30:LYS:HE3	2:Z:123:TYR:CD2	2.35	0.62
1:C:114:ASP:O	1:C:115:MET:HG2	2.00	0.61
1:C:230:ARG:HH22	2:D:124:GLN:HE22	1.47	0.61
2:B:199:ILE:O	2:B:201:THR:N	2.33	0.61
1:C:47:MET:HE2	1:C:80:GLY:CA	2.21	0.61
1:E:236:GLU:O	1:E:237:LYS:CB	2.39	0.61
1:C:9:GLN:HG2	1:C:33:TYR:HB3	1.81	0.61
2:B:197:ILE:HD11	2:B:247:SER:CB	2.31	0.61
2:D:11:ARG:HG3	2:D:188:TYR:CE1	2.35	0.61
2:D:313:GLU:O	2:D:317:GLN:HG3	2.00	0.61
2:Z:246:LYS:HE2	2:Z:249:GLN:NE2	2.14	0.61
2:D:275:MET:HG2	2:D:298:ILE:HD11	1.81	0.61
1:A:27:ASP:O	1:A:29:ASP:N	2.34	0.60
2:B:238:ILE:HG21	2:B:244:LEU:HD12	1.83	0.60
2:F:198:ASP:OD1	2:F:198:ASP:N	2.33	0.60
2:D:246:LYS:NZ	2:D:249:GLN:HE22	2.00	0.60
2:D:217:ASN:O	2:D:220:GLN:HG2	2.01	0.60
2:D:288:ASN:ND2	4:D:1319:FAD:H1B	2.16	0.60
1:E:1:MET:HG3	1:E:153:PRO:CB	2.18	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:87:VAL:HG21	1:Q:107:VAL:HG21	1.84	0.60
1:A:74:ARG:CD	1:A:74:ARG:CB	2.76	0.60
2:D:99:SER:C	2:D:101:GLY:H	2.05	0.60
2:Z:209:GLY:HA3	2:Z:267:GLY:O	2.01	0.60
1:A:20:ARG:HB3	1:A:22:ASP:HA	1.84	0.59
2:B:46:ASP:O	2:B:47:ALA:C	2.40	0.59
2:Z:114:PHE:HA	2:Z:152:VAL:O	2.03	0.59
1:C:65:GLY:O	1:C:88:TRP:HB2	2.02	0.59
1:C:249:GLU:O	1:C:253:LYS:N	2.29	0.59
1:C:1:MET:HG3	1:C:153:PRO:HB3	1.84	0.59
2:F:199:ILE:C	2:F:201:THR:H	2.05	0.59
2:Z:207:SER:HA	2:Z:233:CYS:O	2.02	0.59
2:F:79:VAL:HA	2:F:82:LEU:HD12	1.84	0.59
2:F:136:ASN:O	2:F:137:GLN:HB2	2.03	0.59
2:B:306:ASP:OD1	2:B:308:PHE:N	2.35	0.58
1:E:1:MET:HE2	1:E:2:LYS:N	2.17	0.58
2:F:316:ALA:O	2:F:317:GLN:C	2.42	0.58
1:C:98:ILE:O	1:C:98:ILE:CG2	2.52	0.58
1:Q:254:ILE:HD11	2:Z:303:ILE:HD13	1.86	0.58
2:D:76:GLU:O	2:D:80:SER:HB3	2.04	0.58
2:D:110:THR:HG21	2:D:112:TYR:CE2	2.38	0.58
2:B:91:VAL:HG13	2:B:152:VAL:HG22	1.84	0.58
2:F:266:MET:CE	2:F:266:MET:CG	2.81	0.58
1:E:1:MET:HE1	1:E:3:ILE:HG13	1.85	0.58
2:F:189:VAL:HG12	2:F:190:GLU:N	2.18	0.58
2:D:117:ASP:N	2:D:154:THR:O	2.35	0.58
1:A:158:ALA:HB2	1:A:176:CYS:SG	2.43	0.58
2:Z:120:ILE:HB	2:Z:131:THR:HB	1.86	0.58
1:A:186:ILE:O	1:A:187:ASN:HB3	2.02	0.57
1:E:1:MET:CE	1:E:3:ILE:HG13	2.34	0.57
1:C:47:MET:CE	1:C:80:GLY:CA	2.78	0.57
2:F:219:GLU:OE2	2:F:222:ARG:HD3	2.04	0.57
2:B:197:ILE:HD12	2:B:248:ARG:HE	1.67	0.57
1:E:25:ASP:HA	1:E:232:MET:SD	2.44	0.57
1:A:243:ILE:HD13	1:A:253:LYS:HG3	1.86	0.57
2:D:204:PHE:CD1	2:D:230:ALA:HB2	2.39	0.57
2:F:199:ILE:HG13	2:F:201:THR:OG1	2.04	0.57
2:F:316:ALA:O	2:F:318:LEU:N	2.38	0.57
2:Z:37:VAL:HG22	2:Z:59:GLU:HB2	1.85	0.57
1:Q:259:ASN:C	1:Q:261:PHE:N	2.58	0.57
1:E:145:VAL:HG12	1:E:145:VAL:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:269:SER:H	4:D:1319:FAD:H4B	1.70	0.56
2:B:134:GLY:O	2:B:135:TYR:C	2.43	0.56
2:D:46:ASP:O	2:D:49:VAL:HG13	2.04	0.56
1:Q:88:TRP:CG	1:Q:89:ASP:N	2.73	0.56
1:Q:230:ARG:HD3	2:Z:142:GLU:HG2	1.87	0.56
2:Z:254:GLY:C	2:Z:255:LYS:HE2	2.25	0.56
2:D:63:VAL:HG11	2:D:78:SER:HB3	1.87	0.56
2:D:91:VAL:HG13	2:D:152:VAL:HG22	1.87	0.56
2:B:312:GLU:O	2:B:316:ALA:N	2.39	0.56
2:D:157:PRO:O	2:D:158:SER:HB2	2.04	0.56
1:C:98:ILE:O	1:C:98:ILE:HG22	2.05	0.56
2:D:99:SER:C	2:D:101:GLY:N	2.57	0.56
2:F:232:LEU:O	2:F:248:ARG:HD2	2.05	0.56
1:A:247:ILE:N	1:A:247:ILE:HD13	2.19	0.56
1:C:89:ASP:OD2	1:C:210:LEU:HG	2.05	0.56
1:A:63:SER:HB2	1:A:73:LEU:HD21	1.88	0.55
1:A:102:ARG:HG3	1:A:102:ARG:NH1	2.21	0.55
2:D:99:SER:O	2:D:101:GLY:N	2.39	0.55
2:D:264:VAL:HG12	2:D:266:MET:CE	2.36	0.55
1:E:176:CYS:HA	1:E:177:PRO:C	2.27	0.55
1:E:17:PHE:HA	1:E:30:PHE:CD2	2.41	0.55
1:A:87:VAL:HG21	1:A:107:VAL:HG21	1.89	0.55
2:D:265:ALA:HB1	2:D:268:ILE:HD12	1.89	0.55
1:C:232:MET:HG2	2:D:141:VAL:HG22	1.89	0.55
2:D:246:LYS:HZ2	2:D:249:GLN:HE22	1.54	0.55
1:Q:186:ILE:HG23	1:Q:187:ASN:ND2	2.21	0.55
2:B:263:TYR:CE2	2:B:278:MET:HE2	2.42	0.55
1:C:246:THR:O	1:C:247:ILE:O	2.23	0.55
1:E:168:MET:HB2	1:E:168:MET:HE3	1.86	0.55
1:E:211:ALA:O	1:E:212:ASP:C	2.43	0.55
1:Q:259:ASN:C	1:Q:261:PHE:H	2.11	0.55
2:B:224:LEU:HD11	2:B:314:LEU:HD23	1.89	0.54
1:C:247:ILE:HG22	2:D:313:GLU:HG2	1.88	0.54
2:Z:239:ALA:HB3	2:Z:249:GLN:HE21	1.71	0.54
1:E:10:THR:CG2	1:E:36:ASN:HB2	2.37	0.54
2:F:309:ASP:O	2:F:312:GLU:N	2.37	0.54
1:C:75:LYS:O	1:C:79:LYS:HG3	2.08	0.54
2:F:219:GLU:OE1	2:F:222:ARG:HD2	2.07	0.54
1:C:246:THR:OG1	1:C:249:GLU:CG	2.55	0.54
2:D:266:MET:HG2	2:D:307:ILE:HG22	1.89	0.54
1:A:183:GLN:HG3	1:A:184:LEU:N	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:313:GLU:O	2:F:315:LYS:N	2.40	0.54
2:Z:60:LEU:HB3	2:Z:171:VAL:HG22	1.89	0.54
1:A:226:MET:CE	2:B:112:TYR:O	2.56	0.54
1:A:246:THR:HB	1:A:248:SER:H	1.73	0.54
2:Z:275:MET:HG2	2:Z:298:ILE:HD11	1.90	0.54
1:A:168:MET:CE	2:B:190:GLU:OE1	2.56	0.53
2:B:246:LYS:HZ1	2:B:249:GLN:HE22	1.53	0.53
1:E:63:SER:HA	3:E:1262:AMP:C2	2.43	0.53
2:B:273:GLN:H	2:B:273:GLN:NE2	2.06	0.53
1:C:38:TRP:HE1	1:C:183:GLN:NE2	2.07	0.53
2:D:200:THR:C	2:D:202:VAL:H	2.11	0.53
2:F:256:VAL:HG13	2:F:277:GLY:HA2	1.89	0.53
1:A:26:VAL:HG12	1:A:27:ASP:N	2.23	0.53
2:F:207:SER:HA	2:F:233:CYS:O	2.09	0.53
2:F:300:LYS:HG2	2:F:301:TYR:CE1	2.43	0.53
1:Q:94:GLY:HA3	1:Q:222:ALA:HB2	1.91	0.53
1:E:162:ARG:HE	1:E:170:GLN:NE2	2.06	0.53
1:E:209:SER:OG	1:E:211:ALA:HB3	2.09	0.53
1:A:10:THR:HG22	1:A:124:ASP:OD1	2.09	0.53
2:B:275:MET:HG2	2:B:298:ILE:HD13	1.89	0.53
1:E:237:LYS:O	1:E:238:GLY:C	2.47	0.53
2:B:79:VAL:O	2:B:83:ILE:HG13	2.10	0.52
2:F:309:ASP:OD1	2:F:309:ASP:N	2.41	0.52
2:Z:266:MET:HG2	2:Z:287:VAL:HB	1.90	0.52
1:E:254:ILE:O	1:E:258:ILE:HG13	2.10	0.52
1:C:230:ARG:NH2	2:D:124:GLN:NE2	2.53	0.52
1:Q:210:LEU:HB3	1:Q:215:LEU:HB2	1.91	0.52
1:C:28:GLU:OE2	1:C:33:TYR:OH	2.28	0.52
2:D:119:TYR:CE2	2:D:132:ARG:HA	2.44	0.52
1:E:226:MET:CE	2:F:112:TYR:O	2.56	0.52
2:B:36:VAL:HG12	2:B:36:VAL:O	2.09	0.52
2:Z:77:ALA:HB1	2:Z:177:PRO:HG2	1.92	0.52
2:D:251:GLY:HA3	4:D:1319:FAD:C4	2.40	0.52
1:E:183:GLN:HE21	1:E:184:LEU:H	1.57	0.52
1:E:252:ALA:HA	2:F:317:GLN:HE22	1.74	0.52
1:A:44:GLU:HG2	1:A:189:PRO:HA	1.92	0.51
2:D:290:ASP:O	2:D:296:PHE:HE1	1.92	0.51
1:C:77:LEU:HA	1:C:81:ALA:HB3	1.91	0.51
2:F:4:LEU:HB3	2:F:91:VAL:HB	1.92	0.51
1:Q:161:ARG:HA	1:Q:170:GLN:O	2.10	0.51
1:Q:17:PHE:HA	1:Q:30:PHE:CD1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:208:ILE:HG13	2:D:233:CYS:O	2.10	0.51
1:E:15:GLU:O	1:E:16:ASP:CB	2.54	0.51
1:A:187:ASN:C	1:A:187:ASN:OD1	2.49	0.51
2:D:25:ALA:HB2	2:D:92:LEU:CD1	2.40	0.51
1:Q:19:ILE:HD13	1:Q:26:VAL:HG22	1.92	0.51
2:Z:75:PHE:O	2:Z:79:VAL:HG23	2.10	0.51
1:C:38:TRP:NE1	1:C:184:LEU:HG	2.25	0.51
1:E:247:ILE:HD13	1:E:247:ILE:N	2.25	0.51
2:D:290:ASP:C	2:D:290:ASP:OD1	2.49	0.51
1:C:186:ILE:HG23	1:C:187:ASN:N	2.25	0.51
1:C:247:ILE:HD12	2:D:309:ASP:HB3	1.93	0.51
2:F:235:SER:OG	2:F:237:PRO:HD2	2.10	0.51
1:C:183:GLN:HA	1:C:183:GLN:HE21	1.77	0.50
1:A:33:TYR:CE1	1:A:68:ARG:HD2	2.46	0.50
2:F:17:VAL:O	2:F:18:SER:C	2.49	0.50
1:Q:63:SER:HB2	1:Q:73:LEU:HD21	1.93	0.50
1:C:233:TYR:O	2:D:139:VAL:HB	2.11	0.50
1:E:38:TRP:HE1	1:E:183:GLN:NE2	2.09	0.50
1:E:162:ARG:HE	1:E:170:GLN:HE21	1.59	0.50
1:E:183:GLN:HG3	1:E:184:LEU:N	2.25	0.50
2:F:314:LEU:O	2:F:318:LEU:HG	2.10	0.50
1:A:24:MET:O	1:A:25:ASP:HB2	2.10	0.50
1:A:102:ARG:HH11	1:A:102:ARG:CG	2.22	0.50
2:B:199:ILE:C	2:B:201:THR:N	2.64	0.50
1:E:243:ILE:HD11	2:F:301:TYR:HB3	1.93	0.50
2:Z:289:THR:H	4:Z:1319:FAD:C2A	2.23	0.50
1:E:186:ILE:HG23	1:E:187:ASN:ND2	2.27	0.50
2:D:20:GLU:HG2	2:D:160:PHE:O	2.11	0.50
2:Z:273:GLN:H	2:Z:273:GLN:NE2	2.10	0.50
2:D:202:VAL:CG1	2:D:203:ASP:N	2.45	0.50
1:E:216:SER:O	1:E:218:ASN:N	2.44	0.50
1:C:19:ILE:O	1:C:20:ARG:C	2.50	0.50
2:D:120:ILE:HG13	2:D:131:THR:HB	1.94	0.50
2:D:176:ALA:C	2:D:177:PRO:O	2.46	0.50
1:E:258:ILE:O	1:E:261:PHE:HB3	2.12	0.49
2:F:273:GLN:H	2:F:273:GLN:NE2	2.10	0.49
1:Q:131:GLY:O	1:Q:179:VAL:HG11	2.12	0.49
2:Z:236:ARG:HB2	4:Z:1319:FAD:C2	2.42	0.49
1:C:8:LYS:HG3	3:C:1262:AMP:N7	2.27	0.49
1:C:165:GLU:OE2	2:D:97:VAL:HG23	2.13	0.49
2:D:38:VAL:HG11	2:D:52:LEU:HD22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:ARG:NH2	1:E:201:ALA:O	2.37	0.49
1:E:146:VAL:HG22	1:E:160:ILE:HD13	1.94	0.49
1:A:65:GLY:HA3	1:A:69:VAL:HG21	1.94	0.49
2:F:71:ASP:OD1	2:F:74:VAL:HG23	2.12	0.49
2:B:49:VAL:O	2:B:53:SER:OG	2.13	0.49
2:D:134:GLY:O	2:D:135:TYR:C	2.50	0.49
1:E:246:THR:O	1:E:247:ILE:C	2.51	0.49
2:F:165:GLY:O	2:F:166:ALA:O	2.30	0.49
1:E:36:ASN:HD21	1:E:38:TRP:HB2	1.77	0.49
1:A:129:SER:HB3	2:B:104:SER:HB3	1.95	0.49
1:C:20:ARG:HB3	1:C:22:ASP:HA	1.95	0.49
1:Q:149:LEU:HD13	1:Q:180:LEU:CD1	2.43	0.49
2:D:46:ASP:O	2:D:47:ALA:C	2.52	0.49
2:D:238:ILE:HG21	2:D:244:LEU:HD12	1.95	0.49
2:D:269:SER:HB3	4:D:1319:FAD:O1P	2.12	0.49
1:A:230:ARG:O	1:A:231:ARG:HB3	2.12	0.48
2:D:264:VAL:HG12	2:D:264:VAL:O	2.13	0.48
2:B:57:VAL:HG12	2:B:169:PRO:HB3	1.95	0.48
2:B:310:ILE:O	2:B:314:LEU:HB2	2.12	0.48
1:Q:63:SER:HA	3:Q:1262:AMP:H2	1.78	0.48
1:A:26:VAL:CG1	1:A:27:ASP:N	2.76	0.48
1:A:183:GLN:NE2	1:A:184:LEU:H	2.09	0.48
2:F:199:ILE:C	2:F:201:THR:N	2.67	0.48
1:C:183:GLN:HE21	1:C:184:LEU:H	1.62	0.48
1:C:254:ILE:O	1:C:258:ILE:HG13	2.12	0.48
1:Q:252:ALA:CA	2:Z:317:GLN:HE22	2.27	0.48
1:A:231:ARG:O	1:A:231:ARG:HG3	2.11	0.48
1:Q:8:LYS:HB2	3:Q:1262:AMP:C5	2.48	0.48
1:Q:120:VAL:HG22	1:Q:145:VAL:HA	1.96	0.48
2:Z:202:VAL:HG13	2:Z:203:ASP:H	1.72	0.48
2:F:46:ASP:O	2:F:49:VAL:HG13	2.13	0.48
1:C:130:THR:OG1	3:C:1262:AMP:O2P	2.25	0.48
1:E:2:LYS:NZ	1:E:111:GLU:OE1	2.47	0.48
2:Z:5:VAL:HG22	2:Z:92:LEU:HB2	1.94	0.48
2:D:215:GLU:O	2:D:218:VAL:HG23	2.14	0.48
2:F:199:ILE:HG12	2:F:201:THR:HB	1.95	0.48
1:E:237:LYS:HA	2:F:297:THR:HG22	1.96	0.48
1:A:226:MET:HE2	2:B:112:TYR:O	2.14	0.47
1:C:102:ARG:HH11	1:C:102:ARG:HG2	1.78	0.47
2:F:189:VAL:CG1	2:F:190:GLU:N	2.77	0.47
1:E:4:LEU:C	1:E:4:LEU:HD23	2.34	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:237:LYS:C	1:E:238:GLY:O	2.51	0.47
1:Q:110:LYS:HD2	1:Q:213:ILE:HG22	1.95	0.47
2:F:219:GLU:OE1	2:F:222:ARG:NH1	2.46	0.47
2:B:201:THR:HG22	2:B:259:SER:OG	2.14	0.47
2:D:228:ALA:HA	2:D:318:LEU:CD1	2.45	0.47
1:Q:15:GLU:O	1:Q:16:ASP:HB2	2.14	0.47
1:C:102:ARG:HH11	1:C:102:ARG:CG	2.28	0.47
1:C:226:MET:HE1	2:D:111:GLY:HA2	1.95	0.47
2:D:205:ILE:HG13	2:D:260:CYS:HG	1.77	0.47
1:E:183:GLN:NE2	1:E:184:LEU:H	2.12	0.47
1:A:15:GLU:O	1:A:16:ASP:HB2	2.14	0.47
1:A:66:PRO:O	1:A:86:ARG:HD2	2.13	0.47
1:A:162:ARG:HH21	1:A:170:GLN:HE22	1.62	0.47
2:B:52:LEU:HA	2:B:52:LEU:HD23	1.81	0.47
2:B:168:SER:O	2:B:169:PRO:C	2.52	0.47
2:B:273:GLN:H	2:B:273:GLN:HE21	1.62	0.47
1:C:129:SER:HB3	2:D:104:SER:CB	2.41	0.47
1:C:176:CYS:HA	1:C:177:PRO:C	2.35	0.47
1:E:106:GLU:HB3	1:E:213:ILE:HB	1.96	0.47
1:A:77:LEU:HD23	1:A:77:LEU:HA	1.56	0.47
1:E:98:ILE:N	1:E:98:ILE:HD12	2.28	0.47
1:E:141:PRO:HG2	1:E:177:PRO:O	2.15	0.47
2:B:63:VAL:HG13	2:B:174:VAL:HG23	1.96	0.47
1:C:239:ARG:HG2	2:D:297:THR:HA	1.96	0.47
2:D:86:HIS:O	2:D:87:ASN:C	2.52	0.47
2:D:199:ILE:HG13	2:D:201:THR:HB	1.97	0.47
2:D:228:ALA:HA	2:D:318:LEU:HD12	1.97	0.47
1:E:1:MET:HA	1:E:114:ASP:OD1	2.14	0.47
2:B:238:ILE:CG2	2:B:244:LEU:HD12	2.45	0.47
1:C:36:ASN:O	1:C:37:GLU:C	2.52	0.47
1:C:156:ASN:ND2	1:C:157:LYS:HG3	2.29	0.47
2:F:215:GLU:HB2	2:F:243:TRP:CD2	2.50	0.47
1:C:102:ARG:HG2	1:C:102:ARG:NH1	2.29	0.46
1:C:112:ALA:N	1:C:113:PRO:CD	2.78	0.46
2:D:11:ARG:CG	2:D:188:TYR:CE1	2.98	0.46
2:F:215:GLU:HB2	2:F:243:TRP:CE2	2.50	0.46
1:A:102:ARG:NH1	1:A:102:ARG:CG	2.77	0.46
2:D:283:THR:HG23	2:D:300:LYS:HD3	1.96	0.46
2:B:163:LEU:HD22	2:B:163:LEU:H	1.80	0.46
1:E:210:LEU:O	1:E:213:ILE:HG13	2.16	0.46
2:Z:19:LEU:HA	2:Z:19:LEU:HD22	1.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Z:269:SER:HB3	4:Z:1319:FAD:O5B	2.16	0.46
1:A:247:ILE:N	1:A:247:ILE:CD1	2.75	0.46
1:C:67:ASP:C	1:C:69:VAL:H	2.17	0.46
2:D:278:MET:C	2:D:278:MET:HE2	2.35	0.46
1:E:170:GLN:HB2	2:F:188:TYR:CD2	2.50	0.46
1:Q:63:SER:HB3	1:Q:69:VAL:HG11	1.98	0.46
1:E:216:SER:C	1:E:218:ASN:N	2.67	0.46
1:Q:165:GLU:OE2	2:Z:97:VAL:HG23	2.15	0.46
2:B:272:ILE:HD13	2:B:272:ILE:HA	1.73	0.46
1:C:186:ILE:CG2	1:C:187:ASN:N	2.78	0.46
2:D:137:GLN:NE2	2:D:156:ARG:HH12	2.13	0.46
1:E:168:MET:HB2	1:E:168:MET:HE2	1.95	0.46
1:Q:164:LEU:HD13	2:Z:10:ARG:NE	2.31	0.46
2:B:1:SER:HB2	2:B:34:ASP:OD1	2.16	0.46
2:B:46:ASP:C	2:B:48:PHE:N	2.69	0.46
2:D:273:GLN:NE2	4:D:1319:FAD:O2'	2.49	0.46
1:Q:38:TRP:HE1	1:Q:183:GLN:HE22	1.64	0.46
2:D:284:ILE:HB	2:D:299:ALA:HA	1.98	0.46
1:A:65:GLY:O	1:A:88:TRP:HB2	2.16	0.45
2:F:212:ILE:HG22	2:F:221:PHE:CE1	2.51	0.45
1:A:36:ASN:O	1:A:37:GLU:C	2.53	0.45
1:A:182:ILE:N	1:A:182:ILE:HD13	2.31	0.45
1:E:98:ILE:N	1:E:98:ILE:CD1	2.79	0.45
1:E:168:MET:CE	1:E:168:MET:CB	2.85	0.45
2:F:1:SER:H3	2:F:34:ASP:CG	2.15	0.45
1:Q:4:LEU:HD22	1:Q:108:ILE:HG12	1.98	0.45
1:Q:164:LEU:HD13	2:Z:10:ARG:CZ	2.46	0.45
1:C:162:ARG:HH21	1:C:170:GLN:HE22	1.62	0.45
2:D:197:ILE:CB	2:D:198:ASP:CG	2.85	0.45
1:A:36:ASN:HD21	1:A:38:TRP:HB2	1.79	0.45
1:A:196:GLY:O	1:A:197:ILE:C	2.54	0.45
1:C:145:VAL:HG12	1:C:145:VAL:O	2.15	0.45
2:D:176:ALA:O	2:D:177:PRO:O	2.34	0.45
1:E:216:SER:O	1:E:217:ALA:C	2.54	0.45
1:Q:254:ILE:O	1:Q:258:ILE:HG13	2.17	0.45
2:B:260:CYS:O	2:B:281:VAL:HG13	2.17	0.45
1:C:44:GLU:HB3	1:C:187:ASN:ND2	2.31	0.45
1:C:183:GLN:NE2	1:C:184:LEU:H	2.14	0.45
2:D:204:PHE:CZ	2:D:230:ALA:HB2	2.51	0.45
1:Q:132:ILE:O	1:Q:135:ALA:HB3	2.17	0.45
2:D:264:VAL:CG1	2:D:266:MET:CE	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:73:LEU:O	1:E:76:CYS:HB2	2.16	0.45
2:D:92:LEU:HD22	2:D:155:ILE:HD11	1.99	0.45
2:D:251:GLY:HA3	4:D:1319:FAD:O4	2.16	0.45
2:B:189:VAL:CG1	2:B:190:GLU:N	2.76	0.45
2:B:197:ILE:HD13	2:B:248:ARG:NE	2.23	0.45
2:D:251:GLY:HA3	4:D:1319:FAD:N3	2.32	0.45
2:F:306:ASP:OD1	2:F:308:PHE:CD1	2.70	0.45
1:C:79:LYS:O	1:C:190:ARG:HD2	2.17	0.45
1:C:150:GLN:HE21	1:C:150:GLN:HB3	1.43	0.45
1:C:216:SER:O	1:C:217:ALA:C	2.54	0.45
2:D:69:ASP:O	2:D:70:PHE:C	2.51	0.45
2:F:174:VAL:HG23	2:F:175:ASP:N	2.32	0.45
1:A:20:ARG:HB3	1:A:22:ASP:CA	2.47	0.45
1:A:53:SER:OG	1:A:55:THR:HG23	2.17	0.45
2:D:41:ILE:HG12	2:D:63:VAL:HB	1.99	0.45
2:B:281:VAL:HG13	2:B:282:PRO:HD2	1.98	0.44
2:D:218:VAL:O	2:D:221:PHE:N	2.50	0.44
2:D:273:GLN:HG2	4:D:1319:FAD:C9A	2.47	0.44
2:B:284:ILE:HD13	2:B:284:ILE:HG21	1.64	0.44
1:C:183:GLN:HE21	1:C:183:GLN:CA	2.29	0.44
2:D:273:GLN:O	2:D:274:HIS:C	2.53	0.44
1:Q:102:ARG:NH1	1:Q:102:ARG:CG	2.54	0.44
1:Q:253:LYS:HD2	1:Q:257:ILE:HD11	1.97	0.44
1:A:124:ASP:OD1	1:A:124:ASP:N	2.50	0.44
2:D:112:TYR:CD1	2:D:150:THR:HB	2.53	0.44
2:F:260:CYS:SG	2:F:262:LEU:O	2.76	0.44
1:C:136:SER:HB2	2:D:105:SER:OG	2.17	0.44
2:D:208:ILE:HD11	2:D:244:LEU:HD11	1.98	0.44
2:F:60:LEU:HD23	2:F:60:LEU:HA	1.62	0.44
1:Q:231:ARG:CZ	1:Q:233:TYR:CE2	3.01	0.44
2:B:159:VAL:HG12	2:B:160:PHE:CD1	2.53	0.44
1:C:96:ASP:OD1	1:C:96:ASP:C	2.54	0.44
1:E:216:SER:C	1:E:218:ASN:H	2.21	0.44
2:Z:8:GLU:HG2	2:Z:15:ARG:HD3	2.00	0.44
2:B:263:TYR:CD2	2:B:278:MET:HE2	2.53	0.44
1:C:156:ASN:HD22	1:C:157:LYS:HG3	1.82	0.44
1:C:230:ARG:HH22	2:D:124:GLN:NE2	2.14	0.44
1:E:242:MET:CE	1:E:242:MET:CG	2.94	0.44
2:D:238:ILE:HD12	2:D:238:ILE:HA	1.93	0.44
1:E:75:LYS:O	1:E:79:LYS:HG3	2.18	0.44
1:Q:39:ASP:HA	1:Q:42:SER:HB3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:ARG:O	1:A:22:ASP:CB	2.65	0.44
2:B:314:LEU:HD12	2:B:314:LEU:HA	1.82	0.44
2:D:119:TYR:N	2:D:119:TYR:CD2	2.85	0.44
1:C:121:GLN:C	3:C:1262:AMP:H5'2	2.38	0.43
1:C:228:ARG:NH2	2:D:144:ASP:OD2	2.50	0.43
1:E:174:ILE:HG12	1:E:175:ASN:N	2.31	0.43
1:C:102:ARG:O	1:C:102:ARG:HD3	2.17	0.43
2:D:316:ALA:O	2:D:318:LEU:N	2.50	0.43
1:Q:23:GLY:O	1:Q:231:ARG:HA	2.18	0.43
2:Z:295:ILE:O	2:Z:295:ILE:HG13	2.17	0.43
1:C:120:VAL:HG23	1:C:182:ILE:O	2.18	0.43
1:E:88:TRP:CG	1:E:89:ASP:N	2.87	0.43
1:E:136:SER:HB2	2:F:105:SER:OG	2.19	0.43
1:E:246:THR:C	1:E:248:SER:N	2.71	0.43
1:A:168:MET:HE3	2:B:190:GLU:OE1	2.18	0.43
2:B:4:LEU:HB3	2:B:91:VAL:HB	1.98	0.43
2:D:49:VAL:HB	2:D:60:LEU:HD13	2.00	0.43
2:D:290:ASP:HA	2:D:291:PRO:HD3	1.77	0.43
1:E:252:ALA:O	1:E:256:GLN:HG3	2.19	0.43
2:Z:113:GLY:O	2:Z:114:PHE:HB2	2.17	0.43
1:C:243:ILE:HG22	1:C:250:GLN:HG2	2.00	0.43
1:E:47:MET:CE	1:E:80:GLY:HA3	2.48	0.43
1:E:87:VAL:HG21	1:E:107:VAL:HG21	2.00	0.43
1:Q:13:LEU:HD22	1:Q:26:VAL:HG11	2.01	0.43
1:Q:18:GLU:HG3	1:Q:30:PHE:CE1	2.52	0.43
1:A:243:ILE:HG21	1:A:253:LYS:HG3	1.99	0.43
1:C:249:GLU:HG2	1:C:249:GLU:H	1.44	0.43
1:E:33:TYR:CD1	1:E:68:ARG:HD2	2.53	0.43
1:E:117:PHE:N	1:E:117:PHE:CD1	2.85	0.43
2:B:163:LEU:HD22	2:B:163:LEU:N	2.34	0.43
2:B:222:ARG:HA	2:B:232:LEU:HD22	2.00	0.43
1:C:258:ILE:O	1:C:261:PHE:HB3	2.19	0.43
2:D:2:LYS:NZ	2:D:86:HIS:ND1	2.65	0.43
2:F:306:ASP:OD1	2:F:308:PHE:N	2.46	0.43
1:A:120:VAL:HG22	1:A:145:VAL:HA	2.01	0.43
2:D:264:VAL:HG11	2:D:266:MET:HE1	2.01	0.43
1:E:73:LEU:HA	1:E:73:LEU:HD23	1.56	0.43
1:Q:38:TRP:HE1	1:Q:183:GLN:NE2	2.17	0.43
1:A:226:MET:HE3	2:B:112:TYR:O	2.18	0.43
1:E:35:LEU:HD12	1:E:35:LEU:HA	1.77	0.43
2:Z:214:GLU:OE2	2:Z:214:GLU:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:GLU:OE2	2:B:127:GLU:HA	2.19	0.42
2:D:272:ILE:HD12	2:D:272:ILE:HG23	1.77	0.42
1:C:87:VAL:HG22	1:C:208:VAL:HB	2.01	0.42
1:C:182:ILE:HD12	1:C:182:ILE:HG23	1.76	0.42
2:B:11:ARG:O	2:B:12:ASN:HB2	2.19	0.42
1:E:253:LYS:O	1:E:254:ILE:C	2.56	0.42
2:B:6:ILE:HD12	2:B:79:VAL:HG22	2.01	0.42
1:C:20:ARG:CB	1:C:22:ASP:HA	2.50	0.42
1:E:104:LEU:HA	1:E:104:LEU:HD23	1.55	0.42
1:Q:7:VAL:HG12	1:Q:39:ASP:HB3	2.00	0.42
2:Z:199:ILE:C	2:Z:201:THR:H	2.23	0.42
1:A:162:ARG:HH11	1:A:162:ARG:HD2	1.59	0.42
2:B:186:LYS:HD2	2:B:186:LYS:HA	1.72	0.42
2:D:46:ASP:C	2:D:48:PHE:N	2.69	0.42
1:E:261:PHE:CD1	1:E:261:PHE:C	2.93	0.42
1:Q:103:ILE:HD13	1:Q:103:ILE:HG21	1.79	0.42
2:B:204:PHE:CE2	2:B:262:LEU:HD23	2.54	0.42
2:B:236:ARG:HB2	4:B:1319:FAD:C2	2.50	0.42
2:D:71:ASP:OD1	2:D:74:VAL:HG23	2.20	0.42
1:E:8:LYS:HD3	1:E:10:THR:HG22	2.01	0.42
2:F:42:GLY:O	2:F:64:LYS:HA	2.20	0.42
1:A:25:ASP:HA	1:A:232:MET:SD	2.59	0.42
2:B:210:ARG:O	2:B:212:ILE:N	2.53	0.42
2:D:28:LEU:HD13	2:D:121:VAL:HG13	2.01	0.42
2:D:266:MET:HB3	2:D:307:ILE:HG21	2.00	0.42
2:D:298:ILE:H	2:D:298:ILE:HG13	1.65	0.42
2:F:273:GLN:H	2:F:273:GLN:HE21	1.66	0.42
1:A:182:ILE:HG22	1:A:183:GLN:N	2.34	0.42
1:A:215:LEU:HA	1:A:215:LEU:HD23	1.85	0.42
1:E:38:TRP:NE1	1:E:184:LEU:HG	2.35	0.42
1:E:58:GLU:HA	1:E:82:ASP:OD2	2.20	0.42
1:C:116:VAL:O	1:C:179:VAL:HA	2.20	0.42
1:E:13:LEU:HA	1:E:13:LEU:HD23	1.81	0.42
2:Z:238:ILE:HG21	2:Z:244:LEU:HD12	2.02	0.42
1:E:17:PHE:HA	1:E:30:PHE:CG	2.55	0.42
1:C:73:LEU:HD23	1:C:73:LEU:HA	1.85	0.41
1:C:118:ALA:O	1:C:181:THR:HA	2.20	0.41
2:D:75:PHE:O	2:D:79:VAL:HG23	2.20	0.41
2:D:244:LEU:HA	2:D:245:PRO:HD2	1.79	0.41
2:F:75:PHE:O	2:F:79:VAL:HG23	2.20	0.41
1:A:9:GLN:OE1	1:A:68:ARG:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:252:GLN:HB3	2:B:273:GLN:HB3	2.01	0.41
1:C:53:SER:C	1:C:55:THR:H	2.23	0.41
2:F:45:ALA:HB3	2:F:62:VAL:CG1	2.50	0.41
2:F:106:LEU:HD12	2:F:106:LEU:HA	1.91	0.41
2:F:224:LEU:HA	2:F:224:LEU:HD23	1.83	0.41
1:A:70:ASP:OD1	1:A:86:ARG:NE	2.52	0.41
1:E:220:VAL:O	1:E:224:GLN:HG2	2.20	0.41
1:A:125:GLN:O	1:A:126:ALA:C	2.58	0.41
1:A:154:GLY:O	1:A:155:ASP:O	2.39	0.41
1:A:168:MET:HE2	2:B:190:GLU:OE1	2.20	0.41
1:E:19:ILE:H	1:E:19:ILE:HG12	1.62	0.41
1:E:87:VAL:HG22	1:E:208:VAL:HB	2.01	0.41
2:F:156:ARG:HG2	2:F:159:VAL:HG21	2.03	0.41
2:F:199:ILE:CG1	2:F:201:THR:HB	2.49	0.41
2:Z:245:PRO:C	2:Z:247:SER:N	2.74	0.41
1:A:226:MET:HE3	2:B:111:GLY:C	2.41	0.41
1:C:9:GLN:CG	1:C:33:TYR:HB3	2.49	0.41
1:C:16:ASP:C	1:C:17:PHE:O	2.58	0.41
1:E:194:LEU:HD23	1:E:194:LEU:HA	1.76	0.41
1:E:228:ARG:NH2	2:F:144:ASP:OD2	2.42	0.41
1:E:231:ARG:HG3	1:E:232:MET:N	2.36	0.41
1:E:246:THR:OG1	1:E:249:GLU:HG2	2.20	0.41
1:E:249:GLU:O	1:E:252:ALA:N	2.54	0.41
1:C:75:LYS:O	1:C:78:ALA:HB3	2.21	0.41
2:D:278:MET:O	2:D:280:HIS:N	2.54	0.41
2:D:278:MET:HE1	2:D:284:ILE:HD13	2.01	0.41
2:F:224:LEU:O	2:F:225:ALA:C	2.58	0.41
2:Z:215:GLU:O	2:Z:218:VAL:HG23	2.21	0.41
2:B:5:VAL:HG12	2:B:6:ILE:N	2.32	0.41
2:B:307:ILE:H	2:B:307:ILE:HG12	1.61	0.41
1:C:42:SER:O	1:C:43:LEU:C	2.59	0.41
2:D:49:VAL:N	2:D:50:PRO:HD2	2.35	0.41
2:D:197:ILE:CB	2:D:198:ASP:CB	2.99	0.41
1:E:7:VAL:O	1:E:7:VAL:HG23	2.20	0.41
2:F:244:LEU:HD23	2:F:244:LEU:HA	1.89	0.41
2:F:257:VAL:HG22	2:F:277:GLY:O	2.20	0.41
1:Q:176:CYS:HA	1:Q:177:PRO:C	2.41	0.41
1:Q:254:ILE:HD11	2:Z:303:ILE:CD1	2.50	0.41
2:Z:199:ILE:O	2:Z:201:THR:N	2.54	0.41
1:A:27:ASP:C	1:A:29:ASP:H	2.24	0.41
1:A:249:GLU:O	1:A:250:GLN:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:PHE:CG	2:B:71:ASP:N	2.89	0.41
2:B:102:TYR:O	2:B:105:SER:N	2.51	0.41
2:B:275:MET:HG2	2:B:298:ILE:CD1	2.51	0.41
1:C:87:VAL:CG2	1:C:107:VAL:HG21	2.49	0.41
2:D:197:ILE:CB	2:D:198:ASP:HB2	2.50	0.41
2:D:310:ILE:HG22	2:D:314:LEU:CD2	2.34	0.41
2:F:310:ILE:HD12	2:F:310:ILE:HG23	1.74	0.41
1:Q:18:GLU:HG3	1:Q:30:PHE:HE1	1.86	0.41
1:Q:89:ASP:CB	1:Q:210:LEU:HD12	2.51	0.41
1:Q:237:LYS:O	1:Q:238:GLY:C	2.59	0.41
1:A:121:GLN:HB3	1:A:128:ALA:HB2	2.03	0.40
1:C:17:PHE:HA	1:C:30:PHE:CD1	2.56	0.40
1:C:67:ASP:C	1:C:69:VAL:N	2.73	0.40
1:E:83:ARG:HH11	1:E:83:ARG:HD3	1.55	0.40
1:E:243:ILE:HG21	1:E:253:LYS:HG3	2.03	0.40
2:F:79:VAL:O	2:F:83:ILE:HG13	2.21	0.40
1:Q:162:ARG:HH21	1:Q:170:GLN:NE2	2.15	0.40
1:A:96:ASP:C	1:A:96:ASP:OD1	2.59	0.40
2:B:210:ARG:O	2:B:211:GLY:C	2.59	0.40
2:B:272:ILE:HD12	2:B:272:ILE:HG23	1.84	0.40
1:C:229:VAL:HA	2:D:143:VAL:HG12	2.03	0.40
2:D:120:ILE:HD13	2:D:120:ILE:HG21	1.62	0.40
1:E:57:VAL:HG12	1:E:58:GLU:N	2.36	0.40
2:F:52:LEU:HD23	2:F:52:LEU:HA	1.87	0.40
2:F:308:PHE:O	2:F:311:GLU:HB3	2.20	0.40
2:Z:281:VAL:HA	2:Z:282:PRO:HD3	1.86	0.40
2:Z:289:THR:HG23	4:Z:1319:FAD:N1A	2.36	0.40
2:D:316:ALA:O	2:D:317:GLN:C	2.60	0.40
2:F:96:SER:H	2:F:99:SER:HB2	1.87	0.40
1:Q:62:VAL:HG22	1:Q:85:VAL:HB	2.03	0.40
1:C:246:THR:N	1:C:249:GLU:HG3	2.17	0.40
2:D:278:MET:HE3	2:D:278:MET:HB2	1.92	0.40
1:Q:70:ASP:OD1	1:Q:86:ARG:NE	2.54	0.40
2:Z:290:ASP:HA	2:Z:291:PRO:HD2	1.79	0.40
1:A:4:LEU:HD22	1:A:108:ILE:HG12	2.03	0.40
1:A:95:SER:HB3	1:A:99:VAL:HB	2.04	0.40
1:C:77:LEU:HD23	1:C:81:ALA:HB3	2.03	0.40
1:C:246:THR:O	1:C:248:SER:N	2.54	0.40
2:Z:224:LEU:HD21	2:Z:314:LEU:HB3	2.03	0.40

All (1) 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:A:191:TYR:OH	2:F:216:THR:CG2[4_456]	2.19	0.01

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	257/264 (97%)	228 (89%)	22 (9%)	7 (3%)	5	25
1	C	256/264 (97%)	221 (86%)	29 (11%)	6 (2%)	6	28
1	E	256/264 (97%)	227 (89%)	20 (8%)	9 (4%)	3	20
1	Q	240/264 (91%)	221 (92%)	15 (6%)	4 (2%)	9	36
2	B	310/320 (97%)	269 (87%)	33 (11%)	8 (3%)	5	26
2	D	310/320 (97%)	272 (88%)	26 (8%)	12 (4%)	3	18
2	F	310/320 (97%)	272 (88%)	25 (8%)	13 (4%)	3	16
2	Z	308/320 (96%)	279 (91%)	24 (8%)	5 (2%)	9	37
All	All	2247/2336 (96%)	1989 (88%)	194 (9%)	64 (3%)	5	25

All (64) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	155	ASP
2	B	211	GLY
1	C	247	ILE
2	D	197	ILE
2	D	201	THR
2	D	269	SER
2	D	316	ALA
1	E	155	ASP
1	E	211	ALA
1	E	237	LYS
2	F	166	ALA
2	F	197	ILE

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Mol	Chain	Res	Type
2	F	202	VAL
2	F	314	LEU
1	Q	145	VAL
2	B	47	ALA
2	B	202	VAL
1	C	28	GLU
2	D	257	VAL
2	D	279	LYS
1	E	145	VAL
1	E	212	ASP
2	F	222	ARG
2	F	247	SER
2	F	276	ALA
2	F	310	ILE
2	F	316	ALA
2	F	317	GLN
1	Q	238	GLY
1	A	28	GLU
2	B	200	THR
2	B	276	ALA
1	C	93	GLU
1	C	145	VAL
2	D	12	ASN
2	D	34	ASP
2	D	177	PRO
1	E	195	ARG
1	E	236	GLU
2	F	258	GLY
2	Z	12	ASN
2	Z	316	ALA
1	A	126	ALA
1	A	187	ASN
2	B	197	ILE
1	E	196	GLY
2	F	55	ASN
2	F	200	THR
1	Q	89	ASP
2	Z	200	THR
1	A	222	ALA
1	C	260	GLU
2	D	246	LYS
1	E	25	ASP

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Mol	Chain	Res	Type
1	A	51	GLU
1	A	66	PRO
2	D	210	ARG
2	D	317	GLN
1	Q	153	PRO
2	B	298	ILE
2	Z	87	ASN
1	C	238	GLY
2	Z	197	ILE
2	B	282	PRO

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	200/216 (93%)	173 (86%)	27 (14%)	4 16
1	C	196/216 (91%)	181 (92%)	15 (8%)	13 41
1	E	195/216 (90%)	176 (90%)	19 (10%)	8 30
1	Q	184/216 (85%)	166 (90%)	18 (10%)	8 29
2	B	245/258 (95%)	220 (90%)	25 (10%)	7 27
2	D	243/258 (94%)	209 (86%)	34 (14%)	3 15
2	F	243/258 (94%)	213 (88%)	30 (12%)	4 19
2	Z	241/258 (93%)	223 (92%)	18 (8%)	13 42
All	All	1747/1896 (92%)	1561 (89%)	186 (11%)	6 26

All (186) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	10	THR
1	A	16	ASP
1	A	34	ASP
1	A	42	SER

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Mol	Chain	Res	Type
1	A	48	LYS
1	A	51	GLU
1	A	55	THR
1	A	56	ASP
1	A	60	VAL
1	A	68	ARG
1	A	74	ARG
1	A	98	ILE
1	A	102	ARG
1	A	132	ILE
1	A	141	PRO
1	A	145	VAL
1	A	156	ASN
1	A	162	ARG
1	A	180	LEU
1	A	183	GLN
1	A	203	LYS
1	A	239	ARG
1	A	246	THR
1	A	249	GLU
1	A	253	LYS
1	A	261	PHE
2	B	1	SER
2	B	16	PRO
2	B	29	LYS
2	B	30	LYS
2	B	49	VAL
2	B	60	LEU
2	B	66	SER
2	B	71	ASP
2	B	80	SER
2	B	91	VAL
2	B	158	SER
2	B	168	SER
2	B	172	SER
2	B	199	ILE
2	B	201	THR
2	B	203	ASP
2	B	219	GLU
2	B	224	LEU
2	B	237	PRO
2	B	246	LYS

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Mol	Chain	Res	Type
2	B	259	SER
2	B	273	GLN
2	B	279	LYS
2	B	289	THR
2	B	307	ILE
1	C	32	MET
1	C	34	ASP
1	C	74	ARG
1	C	75	LYS
1	C	102	ARG
1	C	121	GLN
1	C	125	GLN
1	C	150	GLN
1	C	156	ASN
1	C	183	GLN
1	C	193	SER
1	C	216	SER
1	C	239	ARG
1	C	249	GLU
1	C	253	LYS
2	D	11	ARG
2	D	19	LEU
2	D	29	LYS
2	D	30	LYS
2	D	31	SER
2	D	60	LEU
2	D	80	SER
2	D	91	VAL
2	D	119	TYR
2	D	120	ILE
2	D	149	SER
2	D	163	LEU
2	D	178	SER
2	D	199	ILE
2	D	201	THR
2	D	203	ASP
2	D	208	ILE
2	D	212	ILE
2	D	214	GLU
2	D	216	THR
2	D	223	GLU
2	D	224	LEU

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Mol	Chain	Res	Type
2	D	238	ILE
2	D	246	LYS
2	D	255	LYS
2	D	278	MET
2	D	294	SER
2	D	295	ILE
2	D	298	ILE
2	D	303	ILE
2	D	306	ASP
2	D	307	ILE
2	D	311	GLU
2	D	318	LEU
1	E	1	MET
1	E	18	GLU
1	E	28	GLU
1	E	55	THR
1	E	74	ARG
1	E	89	ASP
1	E	102	ARG
1	E	136	SER
1	E	156	ASN
1	E	168	MET
1	E	174	ILE
1	E	183	GLN
1	E	195	ARG
1	E	203	LYS
1	E	213	ILE
1	E	216	SER
1	E	231	ARG
1	E	249	GLU
1	E	261	PHE
2	F	1	SER
2	F	11	ARG
2	F	19	LEU
2	F	29	LYS
2	F	31	SER
2	F	49	VAL
2	F	60	LEU
2	F	66	SER
2	F	89	SER
2	F	91	VAL
2	F	93	LEU

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Mol	Chain	Res	Type
2	F	105	SER
2	F	156	ARG
2	F	163	LEU
2	F	172	SER
2	F	174	VAL
2	F	178	SER
2	F	199	ILE
2	F	201	THR
2	F	203	ASP
2	F	219	GLU
2	F	222	ARG
2	F	224	LEU
2	F	246	LYS
2	F	255	LYS
2	F	259	SER
2	F	273	GLN
2	F	279	LYS
2	F	295	ILE
2	F	309	ASP
1	Q	10	THR
1	Q	18	GLU
1	Q	34	ASP
1	Q	56	ASP
1	Q	63	SER
1	Q	74	ARG
1	Q	75	LYS
1	Q	89	ASP
1	Q	98	ILE
1	Q	102	ARG
1	Q	110	LYS
1	Q	153	PRO
1	Q	156	ASN
1	Q	188	LYS
1	Q	206	GLU
1	Q	228	ARG
1	Q	249	GLU
1	Q	253	LYS
2	Z	19	LEU
2	Z	29	LYS
2	Z	60	LEU
2	Z	66	SER
2	Z	89	SER

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Mol	Chain	Res	Type
2	Z	91	VAL
2	Z	93	LEU
2	Z	163	LEU
2	Z	199	ILE
2	Z	201	THR
2	Z	207	SER
2	Z	214	GLU
2	Z	224	LEU
2	Z	245	PRO
2	Z	246	LYS
2	Z	279	LYS
2	Z	298	ILE
2	Z	314	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	A	175	ASN
1	A	183	GLN
1	A	199	GLN
1	A	250	GLN
2	B	124	GLN
2	B	173	ASN
2	B	249	GLN
2	B	273	GLN
2	B	317	GLN
1	C	121	GLN
1	C	150	GLN
1	C	156	ASN
1	C	170	GLN
1	C	175	ASN
1	C	183	GLN
1	C	199	GLN
1	C	250	GLN
2	D	124	GLN
2	D	137	GLN
2	D	249	GLN
2	D	273	GLN
2	D	317	GLN
1	E	121	GLN
1	E	170	GLN

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Mol	Chain	Res	Type
1	E	175	ASN
1	E	183	GLN
1	E	199	GLN
1	E	250	GLN
1	E	256	GLN
2	F	124	GLN
2	F	173	ASN
2	F	249	GLN
2	F	273	GLN
2	F	317	GLN
1	Q	121	GLN
1	Q	150	GLN
1	Q	156	ASN
1	Q	170	GLN
1	Q	175	ASN
1	Q	183	GLN
1	Q	250	GLN
1	Q	256	GLN
2	Z	44	GLN
2	Z	173	ASN
2	Z	249	GLN
2	Z	273	GLN
2	Z	317	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	AMP	A	1263	-	22,25,25	1.97	5 (22%)	25,38,38	1.94	9 (36%)
3	AMP	E	1262	-	22,25,25	1.81	3 (13%)	25,38,38	2.38	7 (28%)
4	FAD	Z	1319	-	53,58,58	1.54	9 (16%)	68,89,89	1.58	12 (17%)
4	FAD	F	1319	-	53,58,58	1.92	15 (28%)	68,89,89	1.63	12 (17%)
3	AMP	C	1262	-	22,25,25	1.54	5 (22%)	25,38,38	2.43	8 (32%)
3	AMP	Q	1262	-	22,25,25	1.59	4 (18%)	25,38,38	2.49	6 (24%)
4	FAD	B	1319	-	53,58,58	1.90	12 (22%)	68,89,89	1.56	13 (19%)
4	FAD	D	1319	-	53,58,58	2.19	17 (32%)	68,89,89	1.85	18 (26%)

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
3	AMP	A	1263	-	-	4/6/26/26	0/3/3/3
3	AMP	E	1262	-	-	2/6/26/26	0/3/3/3
4	FAD	Z	1319	-	-	5/30/50/50	0/6/6/6
4	FAD	F	1319	-	-	5/30/50/50	0/6/6/6
3	AMP	C	1262	-	-	5/6/26/26	0/3/3/3
3	AMP	Q	1262	-	-	0/6/26/26	0/3/3/3
4	FAD	B	1319	-	-	4/30/50/50	0/6/6/6
4	FAD	D	1319	-	-	3/30/50/50	0/6/6/6

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1319	FAD	C5'-C4'	6.48	1.61	1.51
3	E	1262	AMP	C2-N3	6.01	1.41	1.32
4	D	1319	FAD	C2A-N3A	6.00	1.41	1.32
4	D	1319	FAD	C4X-N5	5.51	1.41	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1263	AMP	C2-N3	5.31	1.40	1.32
4	Z	1319	FAD	C2A-N3A	5.27	1.40	1.32
4	F	1319	FAD	C4X-N5	5.17	1.40	1.30
4	B	1319	FAD	C4X-N5	4.97	1.40	1.30
4	D	1319	FAD	C5'-C4'	4.73	1.58	1.51
4	F	1319	FAD	C5'-C4'	4.65	1.58	1.51
4	F	1319	FAD	C2A-N3A	4.51	1.39	1.32
4	F	1319	FAD	C2A-N1A	4.50	1.42	1.33
4	D	1319	FAD	C8A-N7A	4.26	1.42	1.34
4	D	1319	FAD	C2A-N1A	4.23	1.41	1.33
3	A	1263	AMP	P-O1P	3.98	1.63	1.50
4	D	1319	FAD	C1'-C2'	3.87	1.58	1.52
4	Z	1319	FAD	C4X-N5	3.83	1.38	1.30
3	C	1262	AMP	C2-N3	3.78	1.38	1.32
4	B	1319	FAD	C1'-C2'	3.65	1.57	1.52
4	D	1319	FAD	PA-O1A	3.64	1.63	1.50
3	Q	1262	AMP	C2-N3	3.58	1.37	1.32
4	Z	1319	FAD	C5'-C4'	3.53	1.56	1.51
4	B	1319	FAD	C9-C8	3.52	1.44	1.39
4	B	1319	FAD	C2A-N3A	3.52	1.37	1.32
3	Q	1262	AMP	C2-N1	3.32	1.40	1.33
3	A	1263	AMP	C2'-C1'	-3.29	1.48	1.53
4	B	1319	FAD	C10-N1	3.29	1.39	1.33
4	F	1319	FAD	C2-N1	3.25	1.44	1.36
4	Z	1319	FAD	C8A-N7A	3.13	1.40	1.34
4	D	1319	FAD	O4B-C1B	3.05	1.45	1.41
3	E	1262	AMP	P-O1P	3.01	1.60	1.50
4	Z	1319	FAD	C2A-N1A	3.01	1.39	1.33
4	Z	1319	FAD	C1'-C2'	2.95	1.56	1.52
4	F	1319	FAD	C9-C8	2.93	1.43	1.39
4	B	1319	FAD	PA-O1A	2.87	1.61	1.50
4	F	1319	FAD	PA-O1A	2.85	1.61	1.50
4	F	1319	FAD	C8A-N7A	2.84	1.39	1.34
4	D	1319	FAD	C1'-N10	2.84	1.55	1.48
4	D	1319	FAD	P-O1P	2.77	1.60	1.50
4	B	1319	FAD	C8A-N7A	2.74	1.39	1.34
3	A	1263	AMP	C2-N1	2.71	1.38	1.33
4	D	1319	FAD	C8M-C8	2.70	1.56	1.51
4	F	1319	FAD	C10-N1	2.64	1.38	1.33
3	Q	1262	AMP	P-O1P	2.60	1.58	1.50
4	F	1319	FAD	C2B-C1B	-2.59	1.49	1.53
4	Z	1319	FAD	C10-N1	2.55	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1319	FAD	C4A-N3A	2.55	1.39	1.35
3	C	1262	AMP	C2-N1	2.47	1.38	1.33
4	B	1319	FAD	O2'-C2'	2.39	1.48	1.43
4	D	1319	FAD	C3B-C4B	2.37	1.59	1.53
3	C	1262	AMP	O4'-C4'	-2.34	1.39	1.45
4	B	1319	FAD	C2A-N1A	2.33	1.38	1.33
4	D	1319	FAD	C2-N1	2.33	1.42	1.36
3	C	1262	AMP	C2'-C1'	-2.29	1.50	1.53
4	F	1319	FAD	O4B-C1B	2.27	1.44	1.41
4	B	1319	FAD	C6A-C5A	-2.22	1.35	1.43
3	E	1262	AMP	C2-N1	2.21	1.38	1.33
4	D	1319	FAD	C5B-C4B	2.19	1.58	1.51
4	Z	1319	FAD	C9A-C5X	-2.18	1.37	1.41
4	D	1319	FAD	C2B-C1B	-2.17	1.50	1.53
4	Z	1319	FAD	C4X-C10	-2.15	1.37	1.44
4	F	1319	FAD	O2'-C2'	2.12	1.47	1.43
3	Q	1262	AMP	C4-N3	2.11	1.38	1.35
3	A	1263	AMP	O4'-C4'	-2.10	1.40	1.45
4	F	1319	FAD	P-O1P	2.09	1.58	1.50
4	B	1319	FAD	P-O1P	2.07	1.58	1.50
4	D	1319	FAD	O4-C4	2.06	1.27	1.23
3	C	1262	AMP	P-O2P	-2.04	1.47	1.54
4	D	1319	FAD	P-O5'	2.02	1.67	1.59
4	F	1319	FAD	O3B-C3B	2.00	1.47	1.43

All (85) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Q	1262	AMP	N3-C2-N1	-9.06	114.52	128.68
3	E	1262	AMP	N3-C2-N1	-6.84	117.99	128.68
3	C	1262	AMP	N3-C2-N1	-6.32	118.81	128.68
4	Z	1319	FAD	N3A-C2A-N1A	-6.18	119.03	128.68
3	C	1262	AMP	O2P-P-O1P	-5.86	87.74	110.68
4	B	1319	FAD	N3A-C2A-N1A	-5.55	120.00	128.68
4	D	1319	FAD	N3A-C2A-N1A	-5.27	120.44	128.68
4	D	1319	FAD	C4-N3-C2	-5.07	116.27	125.64
3	E	1262	AMP	O5'-P-O1P	-4.75	93.16	106.47
3	C	1262	AMP	O2P-P-O5'	4.67	119.16	106.73
4	F	1319	FAD	C4-N3-C2	-4.57	117.19	125.64
3	E	1262	AMP	P-O5'-C5'	4.18	129.82	118.30
4	D	1319	FAD	C5'-C4'-C3'	-4.15	104.19	112.20
3	Q	1262	AMP	O2P-P-O5'	4.12	117.69	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	1263	AMP	O5'-C5'-C4'	4.03	122.87	108.99
4	D	1319	FAD	P-O3P-PA	-4.00	119.11	132.83
4	F	1319	FAD	C9A-C5X-N5	-3.94	118.15	122.43
4	F	1319	FAD	C5'-C4'-C3'	-3.76	104.94	112.20
4	F	1319	FAD	C4X-C4-N3	3.75	122.71	113.19
3	A	1263	AMP	O2P-P-O5'	3.74	116.68	106.73
3	C	1262	AMP	P-O5'-C5'	3.72	128.53	118.30
3	E	1262	AMP	O3P-P-O5'	3.65	116.44	106.73
4	D	1319	FAD	C5A-C6A-N6A	-3.52	115.00	120.35
4	Z	1319	FAD	P-O3P-PA	-3.48	120.89	132.83
3	Q	1262	AMP	O5'-P-O1P	-3.44	96.83	106.47
4	F	1319	FAD	O4-C4-C4X	-3.41	117.54	126.60
4	Z	1319	FAD	C10-C4X-N5	-3.32	117.81	124.86
4	Z	1319	FAD	C9A-C5X-N5	-3.16	119.00	122.43
3	Q	1262	AMP	C2'-C3'-C4'	-3.12	96.57	102.64
4	B	1319	FAD	C4-N3-C2	-3.12	119.88	125.64
4	F	1319	FAD	C5X-C9A-N10	3.07	121.13	117.95
4	D	1319	FAD	C4X-C4-N3	3.05	120.94	113.19
3	C	1262	AMP	O3P-P-O2P	3.04	119.26	107.64
4	Z	1319	FAD	C4-N3-C2	-2.98	120.14	125.64
4	B	1319	FAD	C5X-C9A-N10	2.97	121.02	117.95
4	Z	1319	FAD	C4-C4X-N5	2.95	122.43	118.23
4	D	1319	FAD	C4X-C10-N10	2.86	120.66	116.48
4	B	1319	FAD	C3B-C2B-C1B	2.84	105.25	100.98
4	D	1319	FAD	C9-C8-C7	-2.83	115.62	119.67
4	Z	1319	FAD	C5X-N5-C4X	2.79	122.71	118.07
3	Q	1262	AMP	O3P-P-O5'	2.75	114.05	106.73
3	A	1263	AMP	N3-C2-N1	-2.74	124.39	128.68
4	B	1319	FAD	C4X-C4-N3	2.74	120.15	113.19
4	F	1319	FAD	O4B-C4B-C3B	2.69	110.44	105.11
4	D	1319	FAD	O2B-C2B-C1B	-2.64	101.10	110.85
4	B	1319	FAD	C9-C8-C7	-2.60	115.95	119.67
4	B	1319	FAD	O4'-C4'-C5'	2.60	115.75	109.92
3	E	1262	AMP	O4'-C4'-C3'	-2.57	100.02	105.11
4	D	1319	FAD	C1B-N9A-C4A	-2.56	122.15	126.64
4	B	1319	FAD	C5'-C4'-C3'	-2.55	107.28	112.20
3	A	1263	AMP	C3'-C2'-C1'	2.52	104.78	100.98
4	Z	1319	FAD	C4X-C4-N3	2.50	119.53	113.19
3	A	1263	AMP	C2'-C3'-C4'	-2.49	97.80	102.64
4	Z	1319	FAD	C4X-C10-N10	2.49	120.11	116.48
3	Q	1262	AMP	C5-C6-N6	-2.48	116.58	120.35
3	A	1263	AMP	O3P-P-O5'	-2.47	100.17	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1319	FAD	C10-C4X-N5	-2.45	119.65	124.86
4	D	1319	FAD	O4-C4-C4X	-2.43	120.14	126.60
3	A	1263	AMP	C4-C5-N7	-2.41	106.89	109.40
4	F	1319	FAD	C9-C8-C7	-2.38	116.26	119.67
4	D	1319	FAD	O4'-C4'-C5'	2.35	115.20	109.92
4	B	1319	FAD	C9A-C9-C8	2.34	124.01	119.30
3	C	1262	AMP	O2'-C2'-C1'	-2.34	102.22	110.85
4	F	1319	FAD	C1B-N9A-C4A	-2.30	122.59	126.64
4	F	1319	FAD	P-O3P-PA	-2.30	124.94	132.83
4	Z	1319	FAD	O4B-C1B-C2B	-2.29	103.58	106.93
3	E	1262	AMP	O3P-P-O1P	2.27	119.58	110.68
4	Z	1319	FAD	C5'-C4'-C3'	-2.24	107.88	112.20
3	A	1263	AMP	C5'-C4'-C3'	2.21	123.45	115.18
3	C	1262	AMP	O3P-P-O5'	2.20	112.60	106.73
4	F	1319	FAD	O2-C2-N3	-2.18	114.41	118.65
4	B	1319	FAD	C5A-C6A-N6A	-2.17	117.05	120.35
3	C	1262	AMP	O5'-P-O1P	-2.16	100.41	106.47
4	D	1319	FAD	O5B-C5B-C4B	-2.14	101.61	108.99
4	D	1319	FAD	N6A-C6A-N1A	2.11	122.96	118.57
4	B	1319	FAD	O4B-C1B-C2B	-2.11	103.84	106.93
4	B	1319	FAD	N3-C2-N1	2.09	123.49	119.38
4	F	1319	FAD	N3-C2-N1	2.08	123.47	119.38
3	E	1262	AMP	O2P-P-O5'	2.08	112.27	106.73
4	Z	1319	FAD	C1B-N9A-C4A	-2.07	123.01	126.64
4	D	1319	FAD	N3-C2-N1	2.07	123.44	119.38
3	A	1263	AMP	C5-C6-N6	-2.05	117.24	120.35
4	D	1319	FAD	C4-C4X-C10	2.04	120.22	116.79
4	B	1319	FAD	C7M-C7-C6	-2.01	115.77	119.49
4	D	1319	FAD	C9A-C9-C8	2.00	123.33	119.30

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1263	AMP	C5'-O5'-P-O1P
3	A	1263	AMP	C5'-O5'-P-O2P
3	A	1263	AMP	C5'-O5'-P-O3P
3	C	1262	AMP	C5'-O5'-P-O3P
4	D	1319	FAD	N10-C1'-C2'-O2'
3	C	1262	AMP	O4'-C4'-C5'-O5'
3	E	1262	AMP	O4'-C4'-C5'-O5'
3	C	1262	AMP	C3'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
3	E	1262	AMP	C3'-C4'-C5'-O5'
3	A	1263	AMP	C4'-C5'-O5'-P
4	B	1319	FAD	PA-O3P-P-O1P
4	D	1319	FAD	N10-C1'-C2'-C3'
3	C	1262	AMP	C5'-O5'-P-O1P
4	Z	1319	FAD	PA-O3P-P-O1P
4	Z	1319	FAD	PA-O3P-P-O2P
4	F	1319	FAD	PA-O3P-P-O1P
3	C	1262	AMP	C4'-C5'-O5'-P
4	B	1319	FAD	O4B-C4B-C5B-O5B
4	F	1319	FAD	O4B-C4B-C5B-O5B
4	Z	1319	FAD	O4B-C4B-C5B-O5B
4	B	1319	FAD	PA-O3P-P-O2P
4	F	1319	FAD	PA-O3P-P-O2P
4	Z	1319	FAD	C2'-C3'-C4'-O4'
4	D	1319	FAD	O4B-C4B-C5B-O5B
4	B	1319	FAD	N10-C1'-C2'-O2'
4	F	1319	FAD	N10-C1'-C2'-O2'
4	F	1319	FAD	N10-C1'-C2'-C3'
4	Z	1319	FAD	N10-C1'-C2'-O2'

There are no ring outliers.

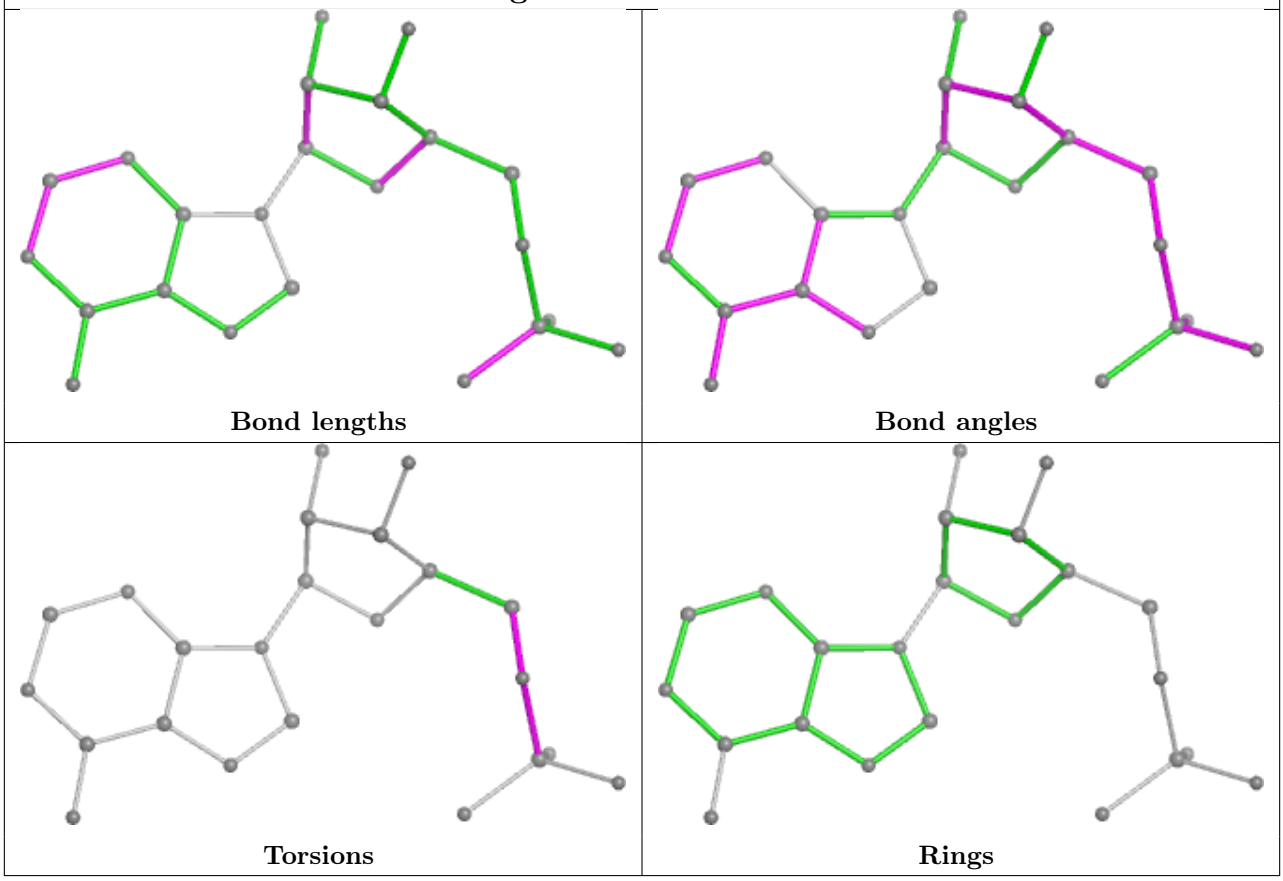
6 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	1262	AMP	2	0
4	Z	1319	FAD	4	0
3	C	1262	AMP	3	0
3	Q	1262	AMP	2	0
4	B	1319	FAD	1	0
4	D	1319	FAD	8	0

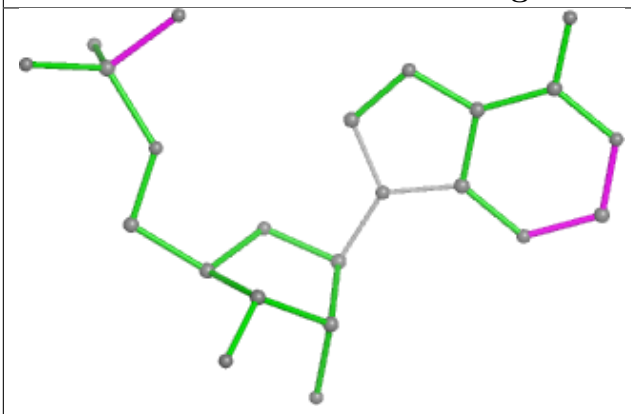
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

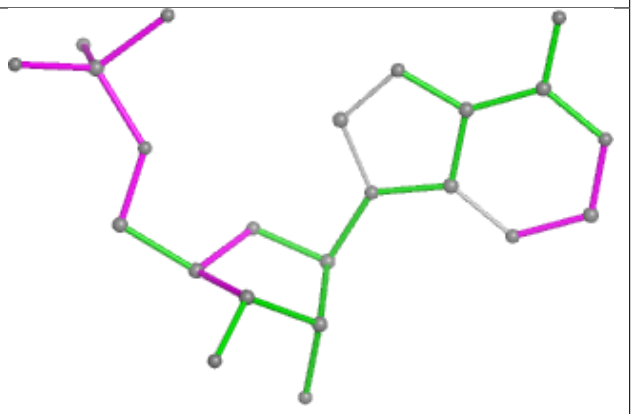
Ligand AMP A 1263



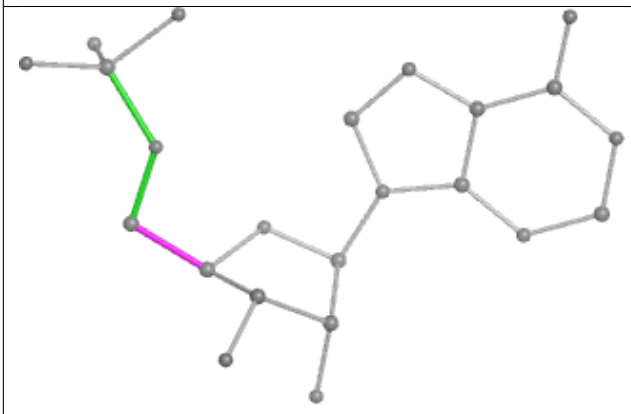
Ligand AMP E 1262



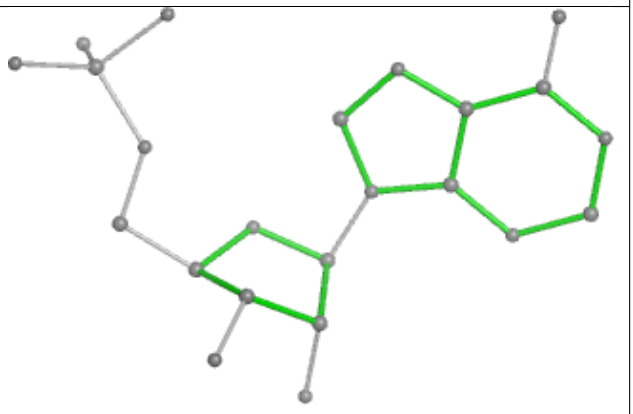
Bond lengths



Bond angles

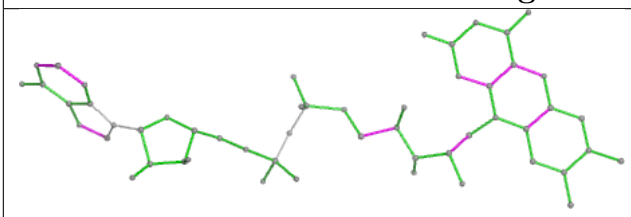


Torsions

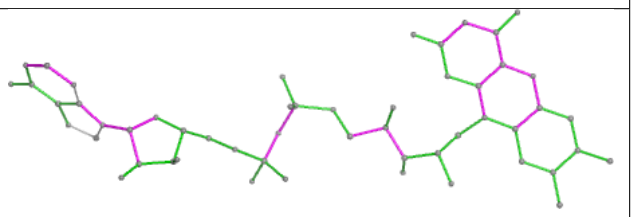


Rings

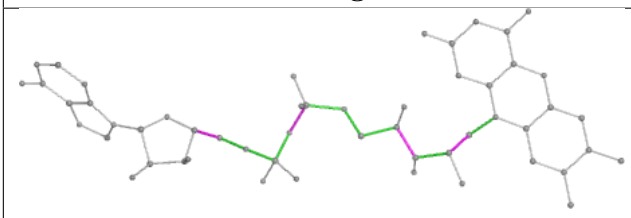
Ligand FAD Z 1319



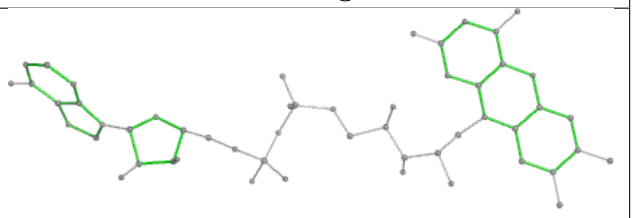
Bond lengths



Bond angles

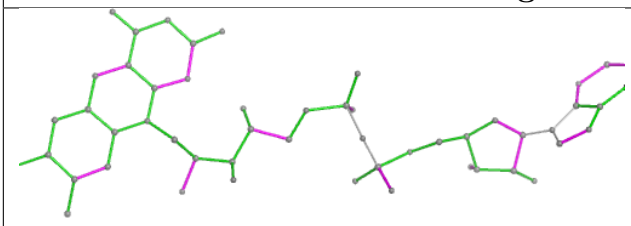


Torsions

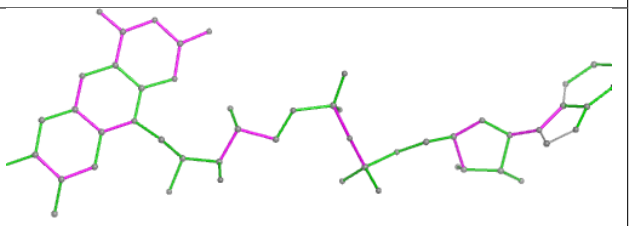


Rings

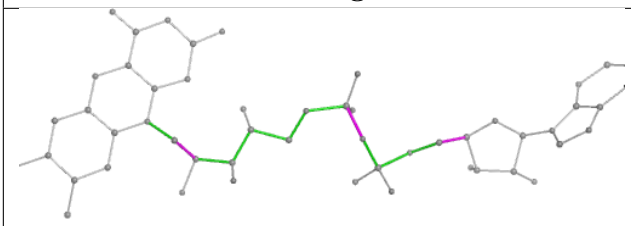
Ligand FAD F 1319



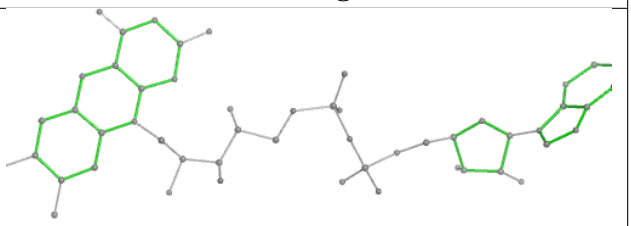
Bond lengths



Bond angles

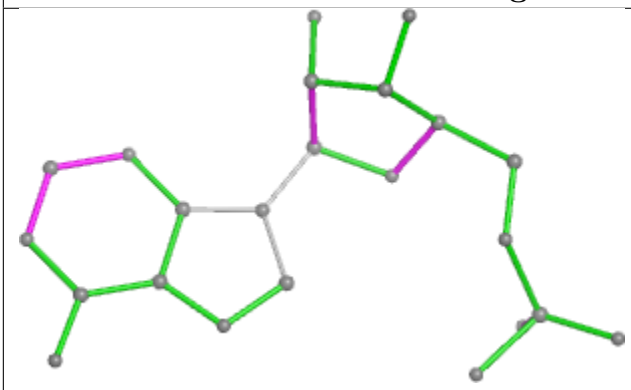


Torsions

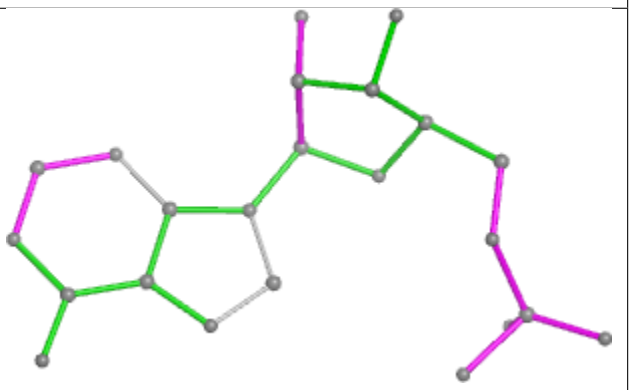


Rings

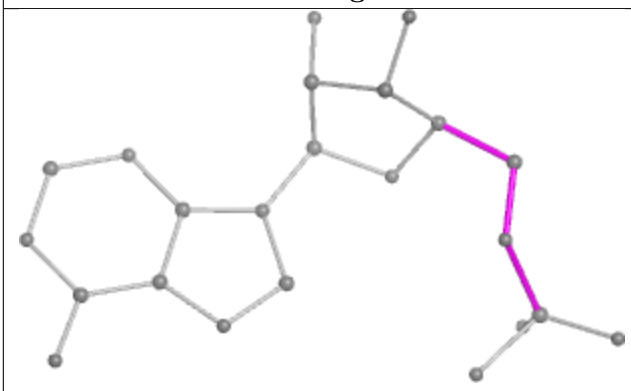
Ligand AMP C 1262



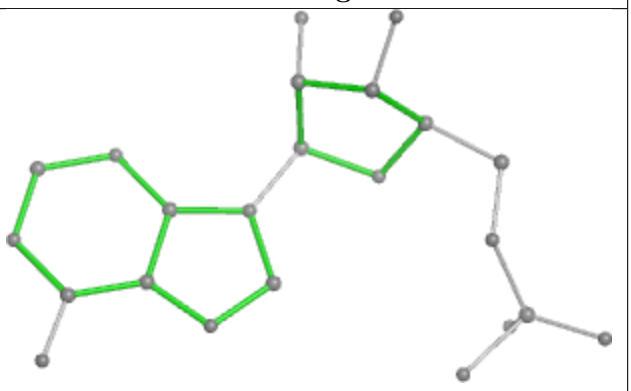
Bond lengths



Bond angles

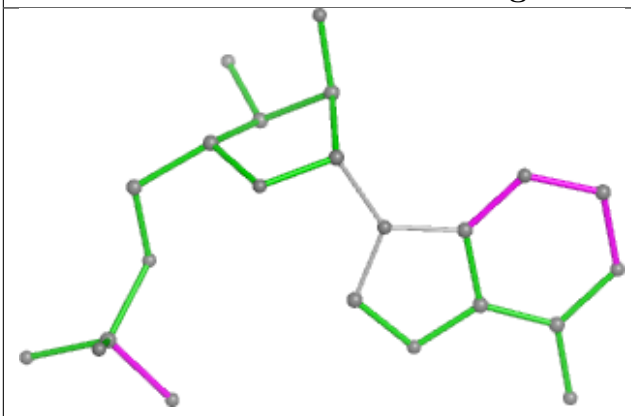


Torsions

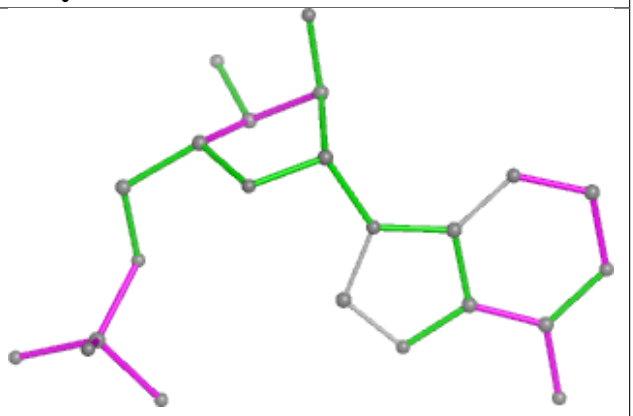


Rings

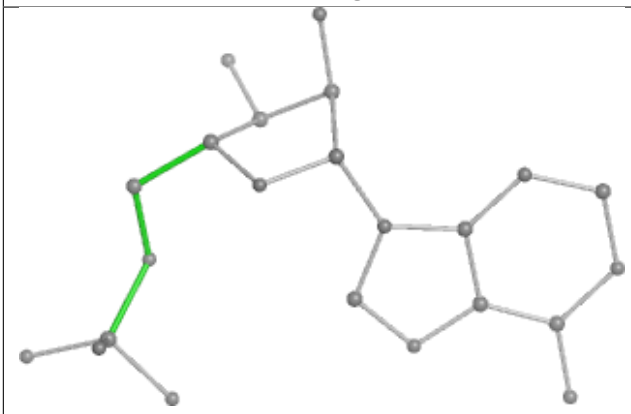
Ligand AMP Q 1262



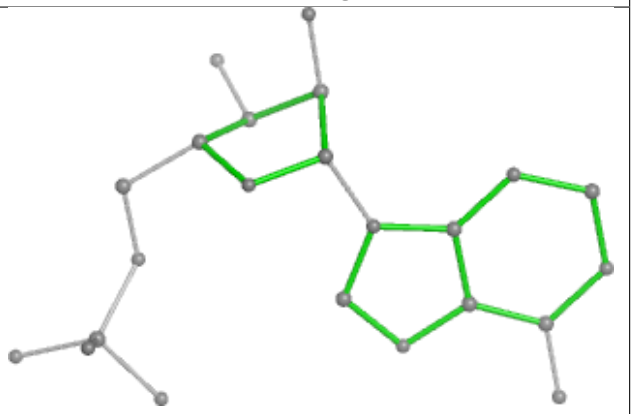
Bond lengths



Bond angles

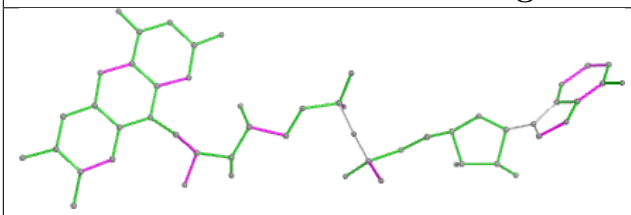


Torsions

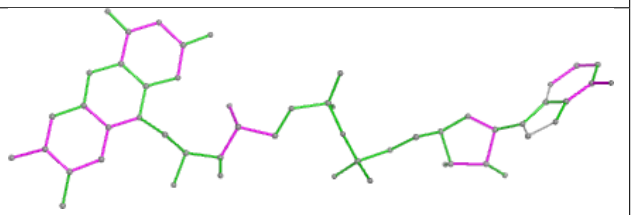


Rings

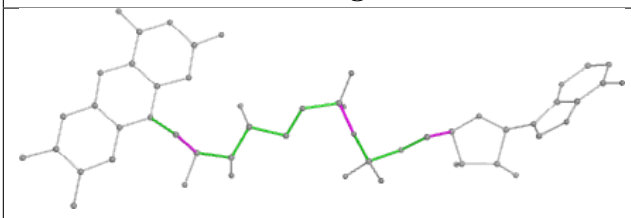
Ligand FAD B 1319



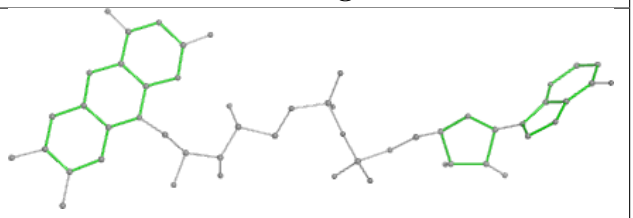
Bond lengths



Bond angles

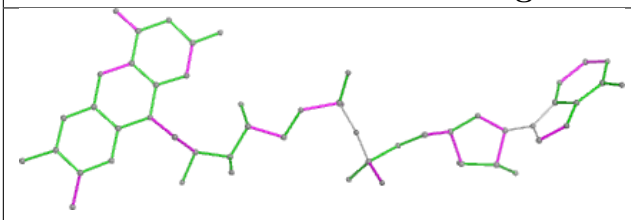


Torsions

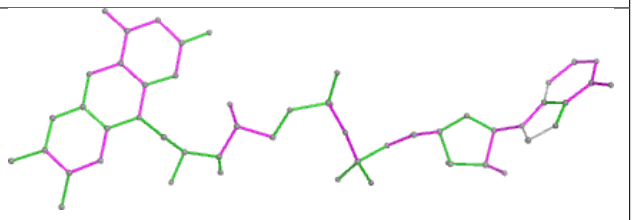


Rings

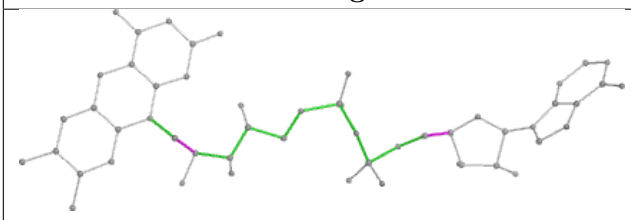
Ligand FAD D 1319



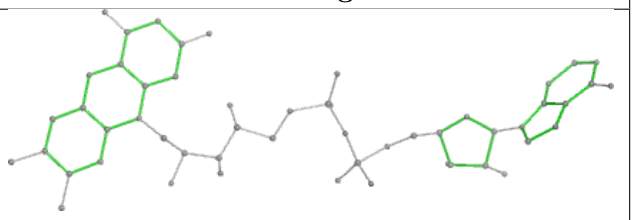
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	261/264 (98%)	-0.74	0 100 100	20, 43, 65, 83	0
1	C	260/264 (98%)	-0.60	0 100 100	29, 52, 90, 112	0
1	E	260/264 (98%)	-0.60	1 (0%) 92 84	27, 52, 77, 88	0
1	Q	246/264 (93%)	0.09	13 (5%) 26 12	41, 76, 93, 102	27 (10%)
2	B	314/320 (98%)	-0.65	2 (0%) 89 78	25, 47, 68, 86	0
2	D	314/320 (98%)	-0.58	3 (0%) 82 67	2, 50, 83, 98	0
2	F	314/320 (98%)	-0.66	2 (0%) 89 78	31, 49, 70, 88	0
2	Z	312/320 (97%)	0.44	30 (9%) 8 2	46, 77, 95, 114	123 (39%)
All	All	2281/2336 (97%)	-0.41	51 (2%) 62 41	2, 54, 86, 114	150 (6%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Z	198	ASP	7.8
2	Z	315	LYS	5.2
2	Z	203	ASP	5.1
2	Z	316	ALA	4.9
2	Z	219	GLU	4.6
2	B	126	ASP	4.2
1	Q	238	GLY	3.9
1	Q	239	ARG	3.8
2	Z	317	GLN	3.7
2	Z	218	VAL	3.7
2	D	196	ASP	3.6
2	D	191	VAL	3.6
2	Z	231	THR	3.5
2	Z	126	ASP	3.4
1	Q	247	ILE	3.4
2	Z	206	MET	3.2

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Mol	Chain	Res	Type	RSRZ
2	Z	111	GLY	3.2
2	Z	264	VAL	3.2
2	Z	32	GLY	3.2
2	Z	30	LYS	2.9
2	D	198	ASP	2.9
2	Z	207	SER	2.8
2	Z	214	GLU	2.8
2	Z	318	LEU	2.7
2	Z	258	GLY	2.7
2	F	126	ASP	2.7
1	Q	16	ASP	2.6
1	Q	90	ASP	2.6
1	Q	261	PHE	2.5
2	Z	199	ILE	2.5
1	Q	256	GLN	2.5
2	Z	291	PRO	2.5
2	B	125	GLY	2.4
2	Z	211	GLY	2.4
2	Z	125	GLY	2.3
2	Z	260	CYS	2.3
2	Z	308	PHE	2.3
2	Z	301	TYR	2.3
2	Z	33	GLU	2.3
2	Z	179	VAL	2.3
1	Q	67	ASP	2.2
1	Q	18	GLU	2.2
1	E	238	GLY	2.2
2	Z	31	SER	2.1
1	Q	29	ASP	2.1
2	Z	230	ALA	2.1
1	Q	56	ASP	2.1
1	Q	53	SER	2.1
1	Q	55	THR	2.0
2	Z	217	ASN	2.0
2	F	191	VAL	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)

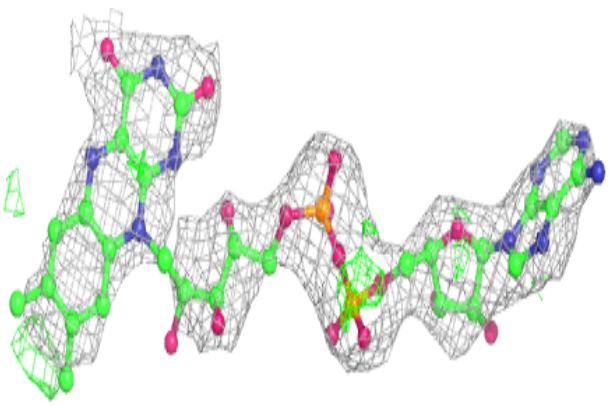
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

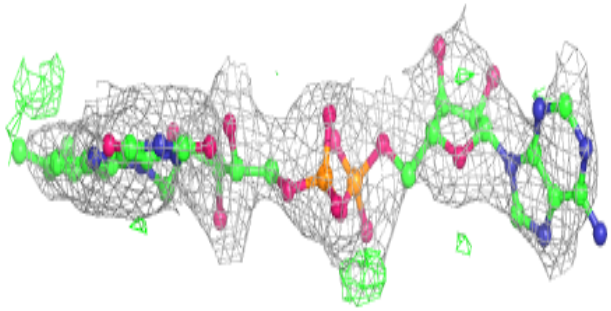
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	FAD	Z	1319	53/53	0.89	0.22	17,28,36,42	53
4	FAD	D	1319	53/53	0.95	0.15	21,28,38,42	0
3	AMP	Q	1262	23/23	0.96	0.13	57,62,69,74	0
4	FAD	B	1319	53/53	0.96	0.14	17,24,31,33	0
4	FAD	F	1319	53/53	0.97	0.12	17,24,29,35	0
3	AMP	E	1262	23/23	0.98	0.11	25,33,38,39	0
3	AMP	A	1263	23/23	0.98	0.12	23,28,34,37	0
3	AMP	C	1262	23/23	0.99	0.12	30,46,52,52	0

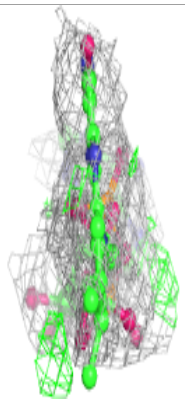
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD Z 1319:

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

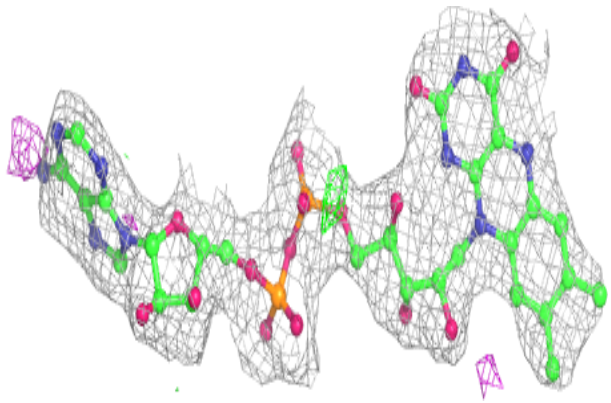


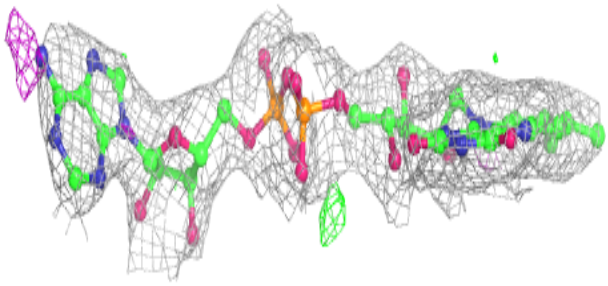


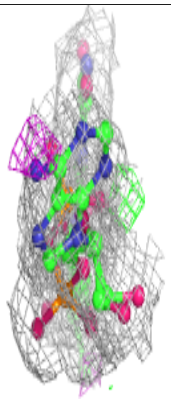


Electron density around FAD D 1319:

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

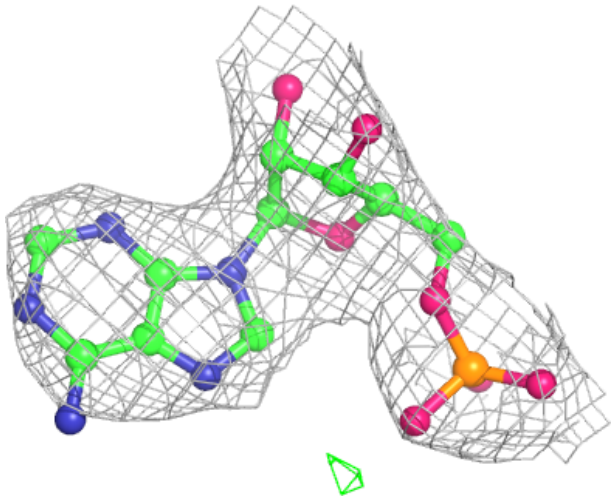


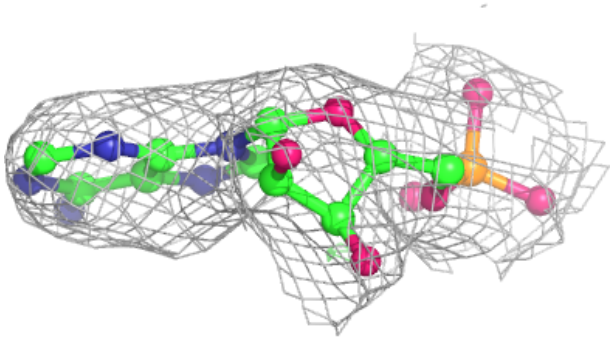


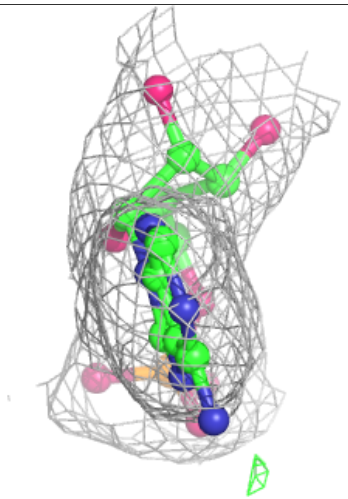


Electron density around AMP Q 1262:

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

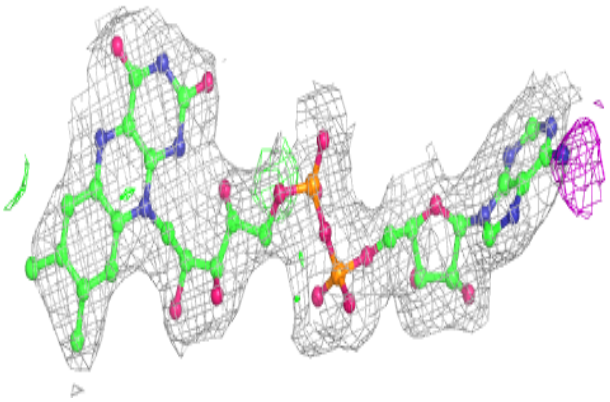


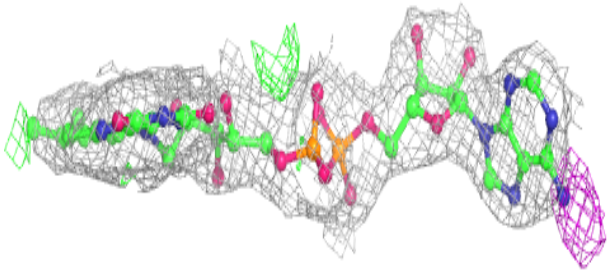


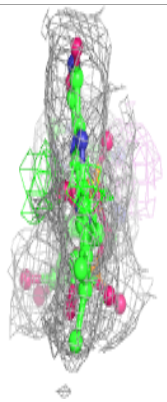


Electron density around FAD B 1319:

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

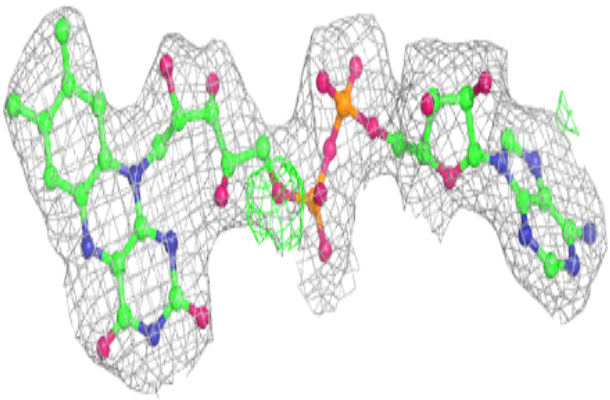


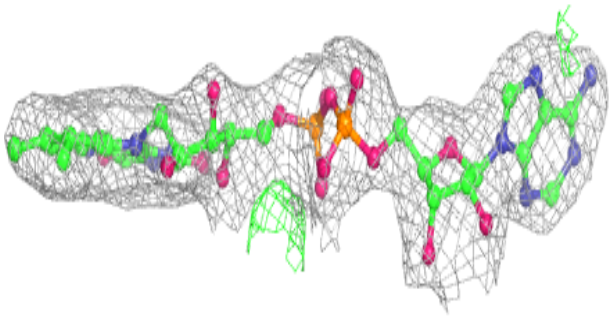


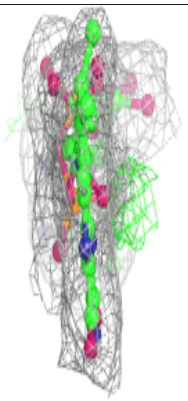


Electron density around FAD F 1319:

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

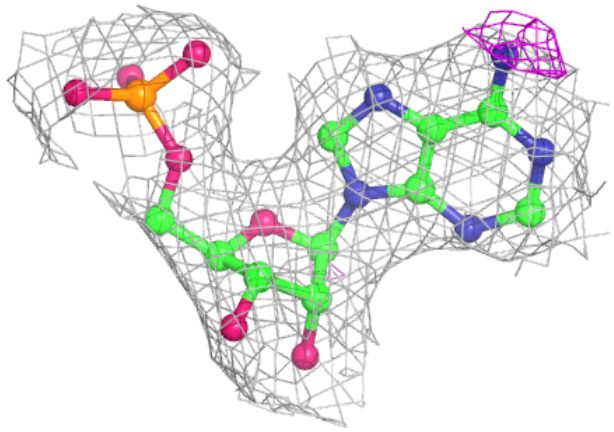


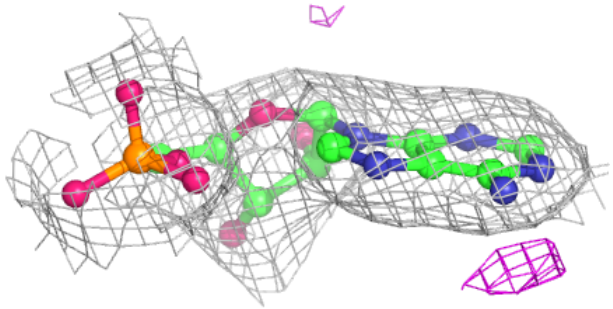


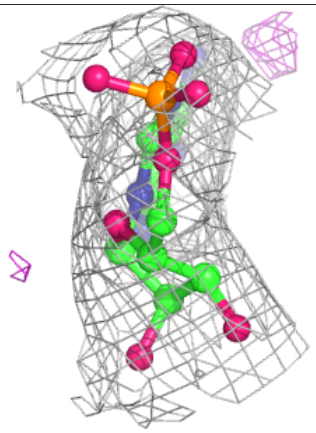


Electron density around AMP E 1262:

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

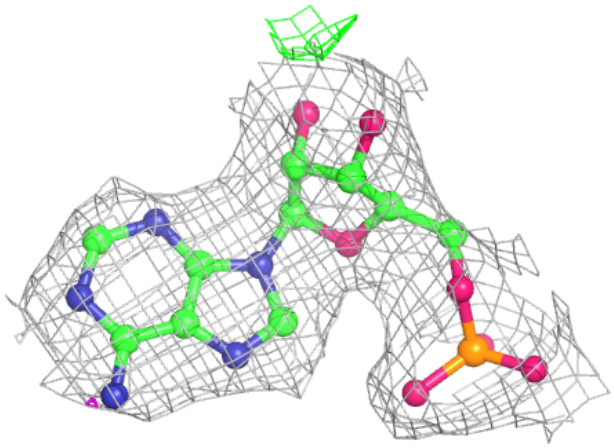


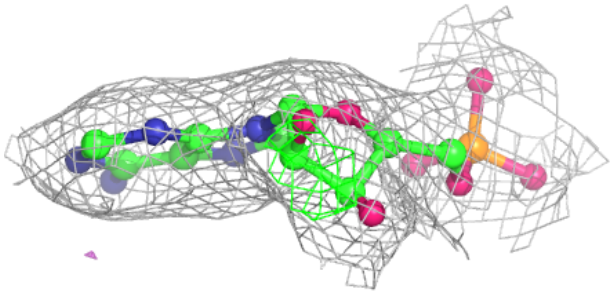


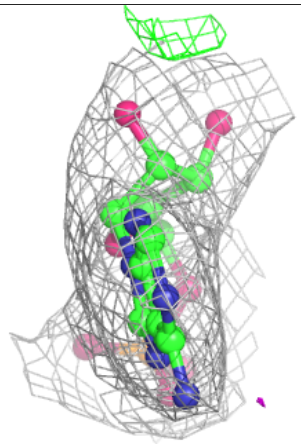


Electron density around AMP A 1263:

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

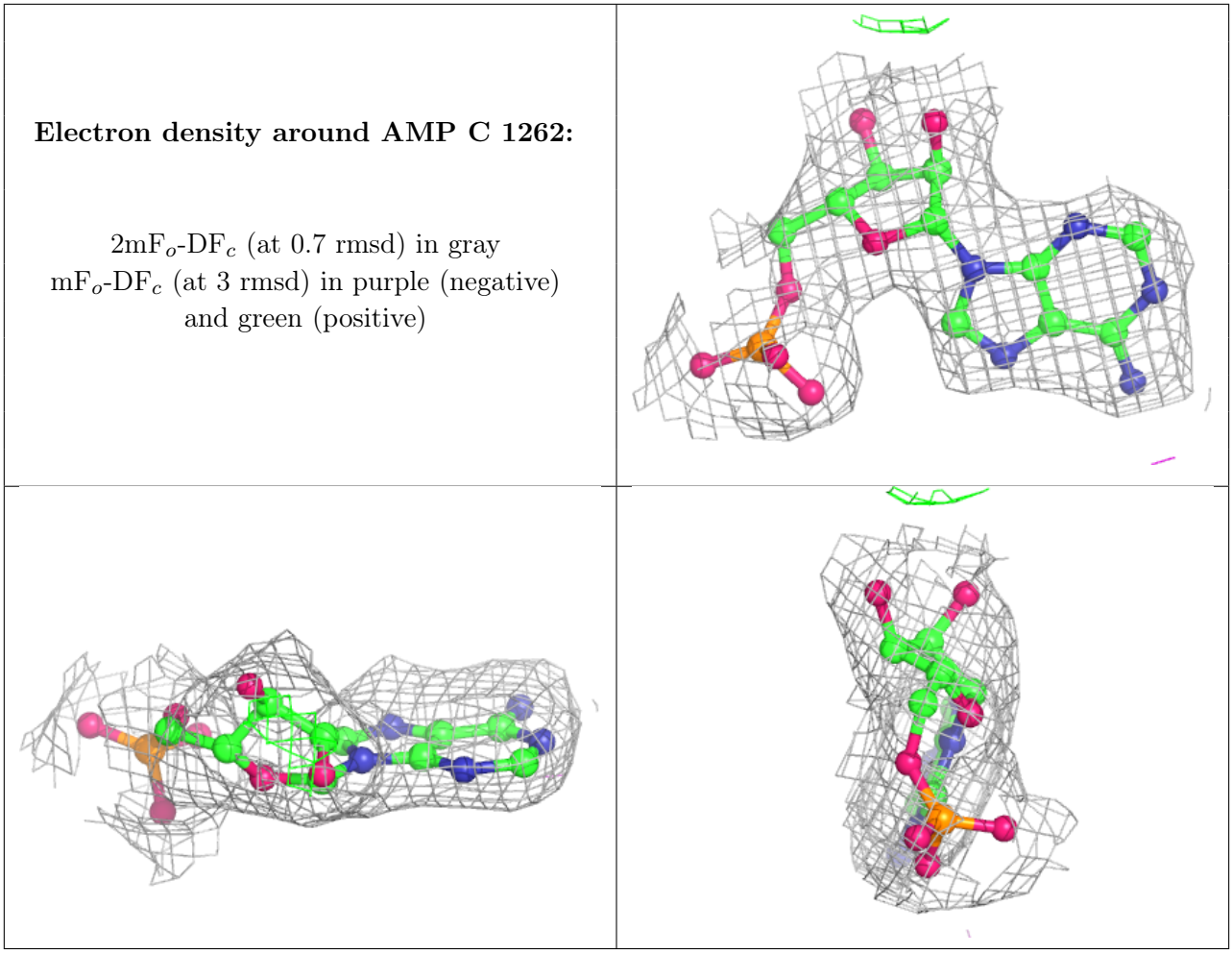






Electron density around AMP C 1262:

$2mF_o$-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

There are no such residues in this entry.