



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 15, 2026 – 09:52 AM UTC

PDB ID : 1O96 / pdb_00001o96
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:

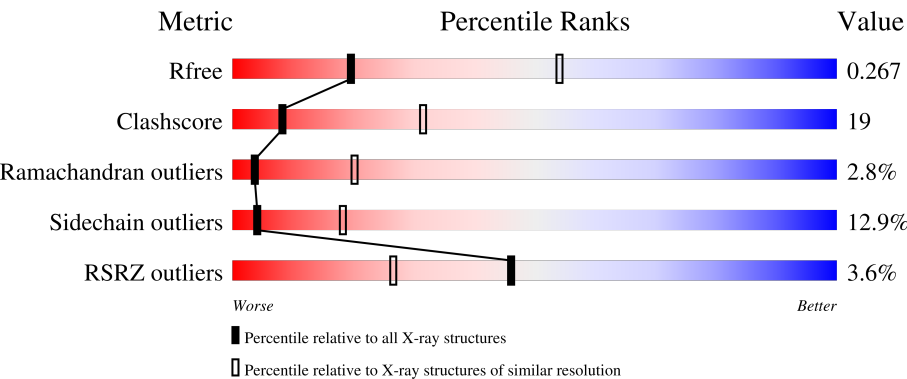
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	264	% 46%34%16% . .
1	C	264	2% 46%42%8% . .
1	E	264	% 44%39%14% . .
1	Q	264	8% 52%32%8% . 7%
2	B	320	% 49%36%9% . .

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Mol	Chain	Length	Quality of chain
2	D	320	2%39%41%14%. .
2	F	320	%43%38%14%. .
2	Z	320	11%75%19%. .

2 Entry composition

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.

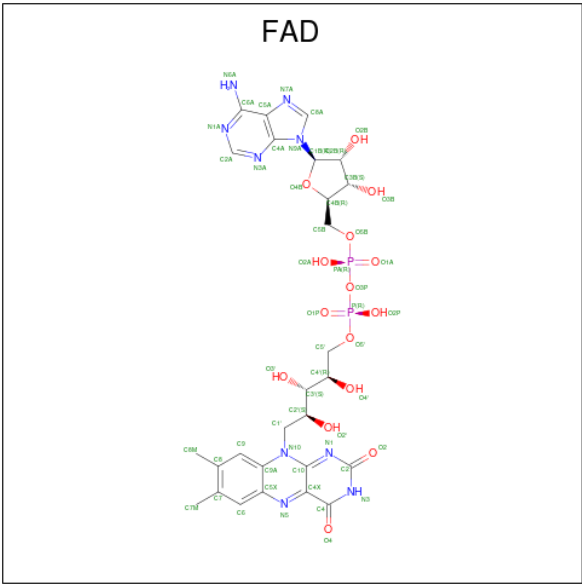
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	314	Total	C	N	O	S	0	0	0
			2287	1444	384	452	7			
2	D	314	Total	C	N	O	S	0	0	0
			2281	1440	383	451	7			
2	F	314	Total	C	N	O	S	0	0	0
			2281	1440	383	451	7			
2	Z	312	Total	C	N	O	S	0	0	0
			2265	1430	381	447	7			

- Molecule 3 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: C₁₀H₁₄N₅O₇P).



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 (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).

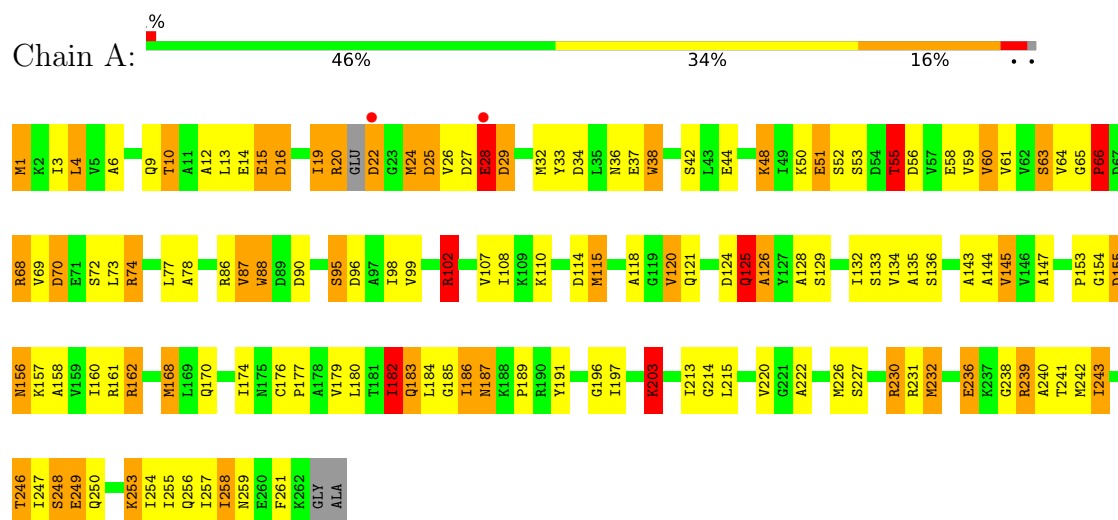


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	F	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
4	Z	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

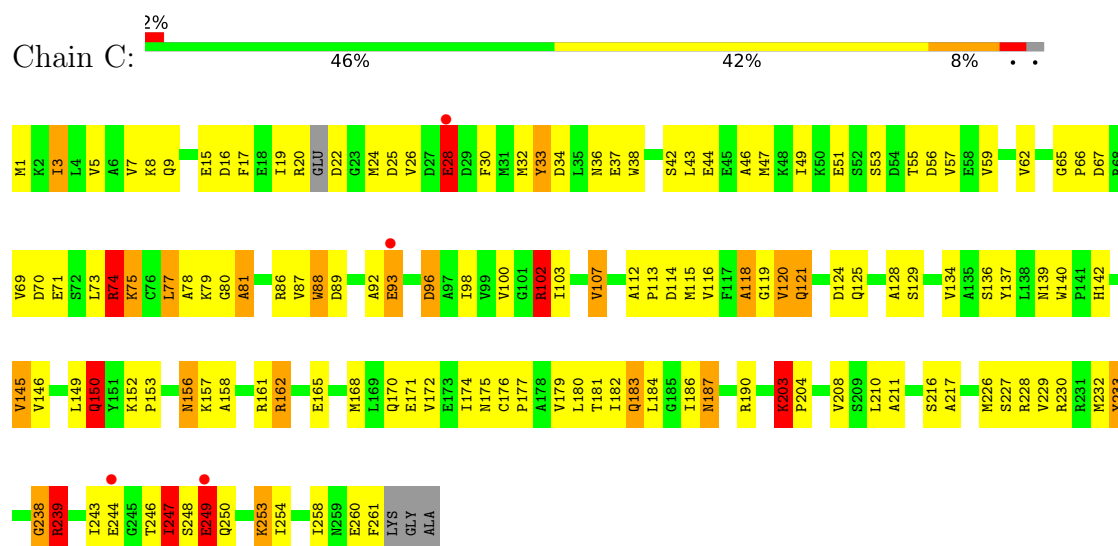
3 Residue-property plots [i](#)

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



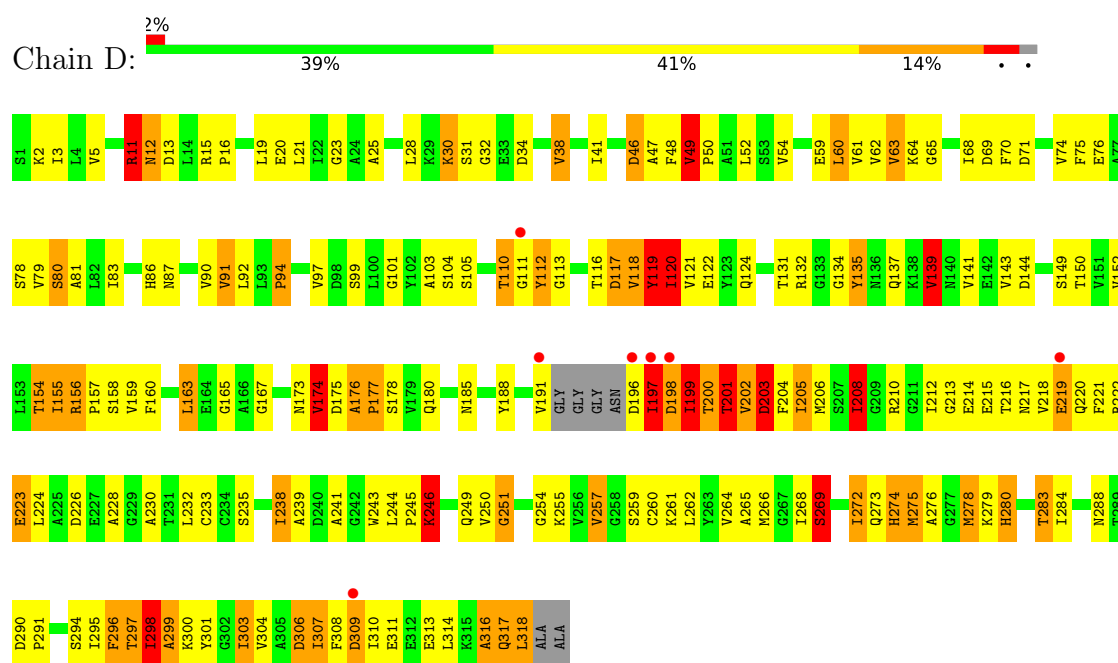
• Molecule 1: ELECTRON TRANSFERRING FLAVOPROTEIN BETA-SUBUNIT



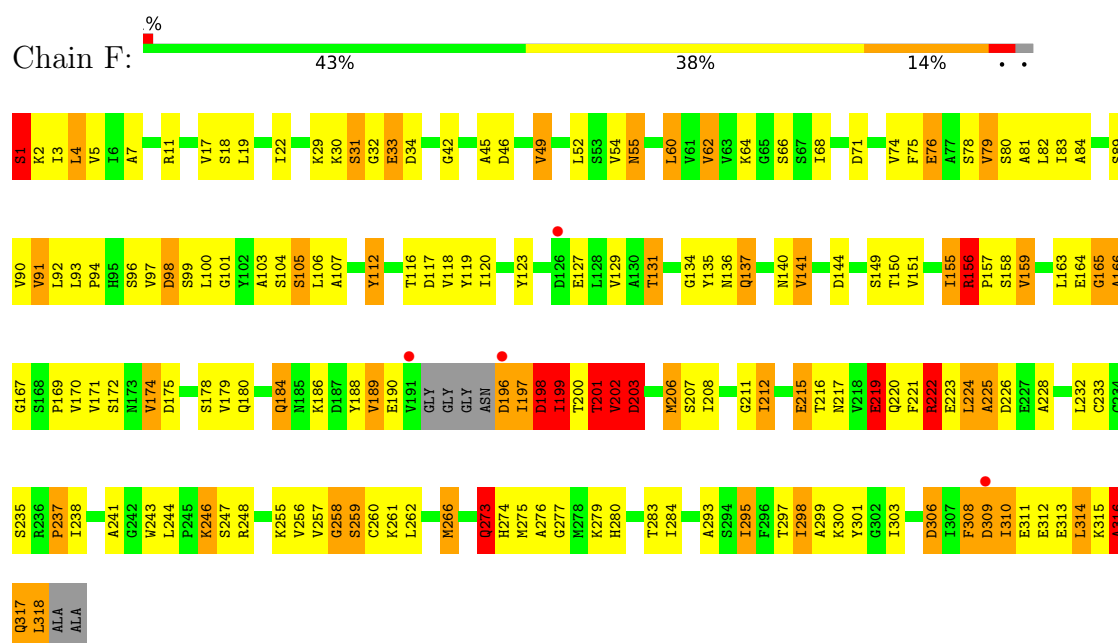
• Molecule 1: ELECTRON TRANSFERRING FLAVOPROTEIN BETA-SUBUNIT



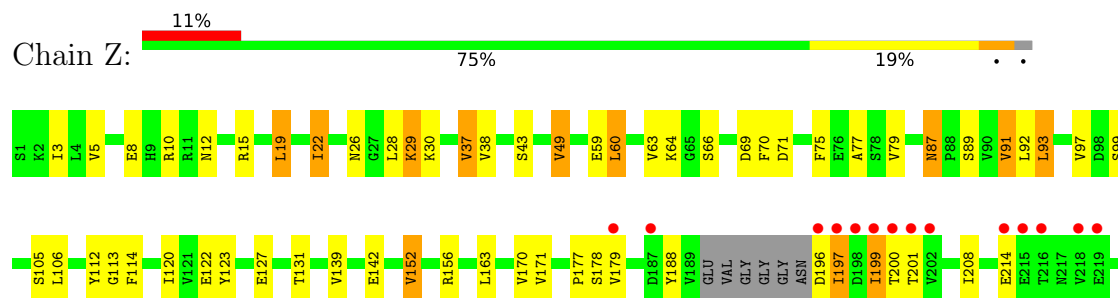


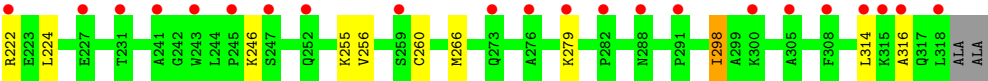


• Molecule 2: ELECTRON TRANSFERRING FLAVOPROTEIN ALPHA-SUBUNIT



• Molecule 2: ELECTRON TRANSFERRING FLAVOPROTEIN ALPHA-SUBUNIT





4 Data and refinement statistics

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 19.92 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.92-3.10) 97.4 (19.92-3.10)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 3.09Å)	Xtriage
Refinement program	REFMAC 5.1.08	Depositor
R, R_{free}	0.212 , 0.278 0.207 , 0.267	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 , 55.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.99	37/1986 (1.9%)	1.92	51/2688 (1.9%)
1	C	1.84	28/1965 (1.4%)	1.86	52/2660 (2.0%)
1	E	2.02	42/1962 (2.1%)	1.82	41/2657 (1.5%)
1	Q	1.66	28/1851 (1.5%)	1.58	18/2507 (0.7%)
2	B	1.87	34/2324 (1.5%)	1.90	63/3167 (2.0%)
2	D	1.96	48/2318 (2.1%)	1.94	76/3159 (2.4%)
2	F	1.98	55/2318 (2.4%)	1.97	74/3159 (2.3%)
2	Z	1.38	22/2302 (1.0%)	1.49	18/3137 (0.6%)
All	All	1.85	294/17026 (1.7%)	1.82	393/23134 (1.7%)

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 (294) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	28	GLU	CD-OE2	18.09	1.59	1.25
1	E	232	MET	SD-CE	16.70	2.21	1.79
2	F	222	ARG	NE-CZ	16.04	1.50	1.33
1	E	195	ARG	NE-CZ	15.44	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	74	ARG	NE-CZ	15.34	1.50	1.33
1	A	74	ARG	CZ-NH2	15.10	1.53	1.33
1	E	242	MET	SD-CE	15.01	2.17	1.79
2	D	197	ILE	CA-CB	14.40	1.74	1.54
2	F	266	MET	SD-CE	13.64	2.13	1.79
2	B	197	ILE	CA-CB	13.63	1.73	1.54
1	E	226	MET	SD-CE	13.58	2.13	1.79
2	D	222	ARG	NE-CZ	13.41	1.47	1.33
1	E	168	MET	SD-CE	13.29	2.12	1.79
1	C	249	GLU	CD-OE1	12.99	1.50	1.25
2	F	201	THR	CA-C	12.82	1.69	1.52
1	A	232	MET	SD-CE	12.76	2.11	1.79
1	E	74	ARG	NE-CZ	12.08	1.46	1.33
2	D	275	MET	SD-CE	-12.07	1.49	1.79
2	Z	266	MET	SD-CE	11.28	2.07	1.79
2	F	103	ALA	CA-CB	-11.20	1.35	1.53
2	F	222	ARG	CZ-NH1	10.83	1.48	1.32
1	Q	232	MET	SD-CE	10.49	2.05	1.79
2	Z	71	ASP	CA-C	10.45	1.61	1.52
2	D	197	ILE	N-CA	10.35	1.59	1.46
2	B	5	VAL	CA-CB	-10.09	1.42	1.54
1	E	195	ARG	CZ-NH1	9.98	1.46	1.32
1	E	12	ALA	CA-CB	-9.91	1.38	1.53
2	B	304	VAL	CA-CB	-9.76	1.42	1.54
2	F	202	VAL	N-CA	9.71	1.58	1.46
2	D	197	ILE	C-O	9.60	1.35	1.24
1	Q	115	MET	SD-CE	9.49	2.03	1.79
2	D	222	ARG	CZ-NH1	8.96	1.45	1.32
2	D	309	ASP	CG-OD1	8.85	1.42	1.25
1	Q	74	ARG	CZ-NH1	8.78	1.45	1.32
1	Q	181	THR	CA-CB	8.61	1.64	1.53
2	D	306	ASP	CA-C	8.60	1.64	1.52
1	A	74	ARG	CZ-NH1	8.59	1.44	1.32
2	D	196	ASP	C-O	8.58	1.40	1.23
1	A	115	MET	SD-CE	8.57	2.00	1.79
2	F	238	ILE	CA-CB	-8.54	1.42	1.54
2	D	196	ASP	CA-C	8.52	1.70	1.52
2	D	250	VAL	CA-CB	-8.50	1.43	1.54
1	A	64	VAL	CA-CB	-8.31	1.44	1.53
1	Q	120	VAL	CA-CB	8.28	1.63	1.54
2	B	222	ARG	NE-CZ	8.21	1.42	1.33
2	D	201	THR	CA-C	8.08	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	GLU	CD-OE2	8.04	1.40	1.25
1	E	232	MET	CA-C	-7.96	1.43	1.52
2	B	201	THR	CA-C	7.86	1.63	1.53
2	B	225	ALA	CA-CB	-7.84	1.41	1.53
2	F	197	ILE	CA-CB	7.78	1.65	1.54
1	A	74	ARG	CG-CD	7.77	1.75	1.52
2	F	284	ILE	CA-CB	7.77	1.63	1.53
1	E	44	GLU	C-O	-7.67	1.14	1.24
1	C	93	GLU	CD-OE1	7.62	1.39	1.25
1	A	134	VAL	CA-CB	-7.60	1.45	1.54
1	E	24	MET	CA-CB	7.60	1.64	1.53
2	B	187	ASP	CA-C	-7.60	1.43	1.52
2	F	222	ARG	CZ-NH2	7.56	1.43	1.33
1	C	59	VAL	CA-CB	-7.55	1.45	1.54
1	C	247	ILE	CA-CB	-7.54	1.44	1.54
1	Q	74	ARG	CZ-NH2	7.52	1.43	1.33
2	B	202	VAL	N-CA	7.50	1.55	1.46
2	F	164	GLU	CA-C	7.49	1.62	1.52
1	A	6	ALA	CA-CB	-7.39	1.42	1.53
2	B	266	MET	CG-SD	-7.30	1.62	1.80
2	B	74	VAL	CA-C	-7.30	1.43	1.52
1	A	120	VAL	C-O	-7.26	1.16	1.24
2	D	219	GLU	CD-OE2	7.22	1.39	1.25
2	F	118	VAL	CA-CB	-7.21	1.45	1.54
2	B	292	GLY	C-O	-7.16	1.17	1.24
2	D	298	ILE	CA-CB	-7.13	1.46	1.54
2	D	276	ALA	CA-CB	-7.10	1.40	1.53
1	A	28	GLU	CG-CD	7.10	1.69	1.52
2	D	49	VAL	CA-CB	7.09	1.63	1.54
1	E	24	MET	CA-C	7.09	1.62	1.52
2	Z	256	VAL	CA-CB	7.05	1.62	1.54
1	Q	168	MET	SD-CE	7.00	1.97	1.79
2	B	6	ILE	CA-CB	-7.00	1.45	1.54
1	E	195	ARG	CD-NE	6.98	1.56	1.46
2	F	266	MET	CA-C	-6.90	1.44	1.52
2	B	202	VAL	CA-C	6.89	1.61	1.52
1	E	74	ARG	CA-C	6.88	1.61	1.52
1	A	182	ILE	N-CA	6.85	1.54	1.46
1	C	140	TRP	CA-CB	-6.83	1.45	1.54
1	E	74	ARG	CZ-NH2	6.81	1.42	1.33
2	D	196	ASP	N-CA	6.78	1.59	1.46
2	B	222	ARG	CD-NE	6.78	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	55	THR	CA-CB	6.77	1.64	1.53
2	F	303	ILE	CA-CB	-6.73	1.46	1.54
1	C	118	ALA	CA-CB	-6.73	1.41	1.53
1	C	93	GLU	CD-OE2	6.72	1.38	1.25
1	A	255	ILE	CA-CB	6.72	1.64	1.54
1	A	256	GLN	CA-C	-6.69	1.44	1.52
1	E	60	VAL	CA-CB	6.69	1.62	1.54
2	D	303	ILE	CA-C	-6.67	1.44	1.52
2	F	119	TYR	CA-C	-6.66	1.44	1.52
2	B	167	GLY	C-O	6.64	1.30	1.23
1	C	62	VAL	CA-CB	-6.62	1.45	1.54
1	C	244	GLU	CD-OE1	6.62	1.38	1.25
1	A	144	ALA	CA-CB	-6.61	1.42	1.53
2	F	137	GLN	C-O	6.59	1.33	1.23
1	A	38	TRP	C-O	-6.56	1.16	1.24
2	F	226	ASP	CB-CG	6.53	1.68	1.52
1	E	120	VAL	CA-CB	-6.52	1.47	1.54
2	F	123	TYR	CA-C	6.52	1.61	1.52
1	E	251	ALA	CA-CB	-6.52	1.43	1.53
2	F	179	VAL	CA-C	6.51	1.60	1.52
2	B	96	SER	CA-C	-6.51	1.44	1.52
2	B	30	LYS	CE-NZ	6.51	1.68	1.49
1	C	102	ARG	NE-CZ	6.48	1.40	1.33
1	C	3	ILE	CA-CB	-6.47	1.46	1.54
2	F	7	ALA	CA-CB	-6.44	1.43	1.53
1	A	242	MET	SD-CE	-6.40	1.63	1.79
2	F	293	ALA	CA-CB	6.38	1.64	1.53
2	D	54	VAL	CA-CB	-6.37	1.45	1.55
1	Q	55	THR	CA-CB	6.37	1.63	1.53
2	F	202	VAL	CA-CB	6.37	1.63	1.54
2	B	7	ALA	CA-CB	-6.36	1.43	1.53
1	C	56	ASP	CA-C	6.36	1.61	1.52
1	A	61	VAL	CA-CB	-6.33	1.46	1.54
2	F	129	VAL	CA-CB	-6.32	1.46	1.54
1	C	51	GLU	C-O	-6.31	1.16	1.24
1	C	233	TYR	CA-C	-6.30	1.45	1.52
1	A	78	ALA	CA-CB	-6.29	1.42	1.53
1	C	24	MET	CA-C	6.25	1.61	1.52
1	A	118	ALA	CA-CB	-6.25	1.42	1.53
2	Z	112	TYR	CA-C	-6.21	1.45	1.52
2	D	154	THR	CA-CB	6.20	1.61	1.53
2	D	196	ASP	C-N	6.19	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	6	ALA	C-O	6.19	1.31	1.24
1	E	64	VAL	CA-C	-6.18	1.45	1.52
2	D	103	ALA	C-O	-6.18	1.16	1.24
1	Q	100	VAL	CA-CB	6.15	1.61	1.54
2	F	299	ALA	CA-CB	-6.14	1.43	1.53
2	Z	179	VAL	CB-CG2	6.14	1.72	1.52
1	C	203	LYS	CA-C	6.14	1.60	1.52
1	Q	1	MET	CG-SD	6.12	1.96	1.80
1	E	51	GLU	CA-CB	6.12	1.64	1.53
1	E	53	SER	C-O	6.12	1.31	1.24
1	E	258	ILE	CA-CB	-6.11	1.46	1.54
2	F	62	VAL	CA-CB	-6.11	1.46	1.53
2	F	189	VAL	CA-CB	-6.11	1.46	1.54
2	D	11	ARG	CG-CD	6.10	1.70	1.52
2	B	49	VAL	CA-CB	6.09	1.58	1.53
1	A	12	ALA	CA-CB	-6.09	1.43	1.53
2	B	189	VAL	CA-CB	-6.09	1.46	1.54
2	F	273	GLN	N-CA	-6.07	1.38	1.46
2	D	299	ALA	CA-CB	-6.04	1.43	1.53
1	Q	178	ALA	CA-C	6.03	1.60	1.52
2	D	5	VAL	CA-CB	-6.00	1.47	1.54
2	B	243	TRP	C-O	-5.99	1.16	1.24
2	B	43	SER	C-O	-5.98	1.16	1.24
2	B	107	ALA	C-O	-5.95	1.17	1.24
2	F	140	ASN	CA-C	5.95	1.60	1.52
1	E	120	VAL	C-O	-5.94	1.17	1.24
2	D	303	ILE	N-CA	-5.92	1.38	1.46
1	Q	100	VAL	CA-C	5.91	1.60	1.52
2	Z	179	VAL	CA-CB	5.90	1.61	1.54
2	F	156	ARG	CA-C	-5.90	1.46	1.53
1	C	150	GLN	CA-CB	-5.90	1.45	1.53
1	Q	159	VAL	CA-CB	5.87	1.61	1.54
2	B	276	ALA	CA-CB	-5.86	1.43	1.53
1	Q	71	GLU	CD-OE2	5.85	1.36	1.25
2	Z	91	VAL	CA-CB	5.85	1.61	1.54
1	Q	234	ILE	CA-CB	5.84	1.59	1.53
2	Z	87	ASN	CA-C	5.82	1.60	1.52
1	A	20	ARG	CA-C	5.82	1.65	1.52
2	D	174	VAL	CA-CB	5.81	1.63	1.55
2	D	116	THR	CA-C	-5.80	1.45	1.52
1	Q	234	ILE	CA-C	5.80	1.57	1.53
2	F	116	THR	CA-C	-5.79	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	222	ARG	CZ-NH2	5.76	1.41	1.33
2	F	202	VAL	CA-C	5.75	1.60	1.52
2	Z	298	ILE	CA-CB	5.74	1.62	1.54
2	F	171	VAL	CA-CB	-5.73	1.47	1.54
2	F	261	LYS	CA-C	5.72	1.60	1.52
1	E	9	GLN	C-O	-5.72	1.17	1.24
2	B	228	ALA	CA-CB	-5.72	1.43	1.53
2	D	241	ALA	CA-CB	-5.70	1.44	1.53
2	F	219	GLU	CD-OE2	5.68	1.36	1.25
1	A	243	ILE	CA-CB	-5.66	1.47	1.54
2	B	5	VAL	C-O	-5.66	1.17	1.24
2	F	3	ILE	CA-CB	-5.65	1.47	1.53
2	D	308	PHE	C-O	5.65	1.30	1.24
1	Q	208	VAL	CA-CB	5.65	1.62	1.54
2	Z	64	LYS	N-CA	5.63	1.53	1.46
2	D	38	VAL	C-O	-5.62	1.18	1.24
2	Z	43	SER	CA-C	5.61	1.60	1.52
2	Z	22	ILE	CA-CB	5.60	1.62	1.54
1	Q	16	ASP	CG-OD2	5.60	1.35	1.25
1	C	3	ILE	C-O	-5.59	1.18	1.24
2	B	198	ASP	CB-CG	-5.58	1.38	1.52
2	F	316	ALA	CA-C	5.57	1.60	1.52
2	Z	63	VAL	CA-CB	5.57	1.60	1.53
2	D	119	TYR	CA-C	-5.55	1.45	1.52
1	A	50	LYS	CA-C	5.55	1.60	1.52
1	E	83	ARG	CA-C	-5.55	1.45	1.52
2	F	241	ALA	CA-CB	-5.53	1.44	1.53
2	D	301	TYR	CA-C	-5.52	1.45	1.52
1	Q	85	VAL	CA-CB	5.52	1.61	1.54
2	D	3	ILE	CA-CB	-5.50	1.47	1.54
2	D	272	ILE	C-O	5.49	1.30	1.24
1	E	232	MET	C-O	-5.49	1.17	1.24
2	Z	152	VAL	CA-CB	5.49	1.60	1.53
1	E	81	ALA	CA-CB	-5.48	1.44	1.53
1	C	28	GLU	CD-OE1	5.46	1.35	1.25
2	F	78	SER	C-O	-5.46	1.17	1.24
2	F	199	ILE	CA-CB	5.46	1.60	1.54
1	Q	75	LYS	CD-CE	5.46	1.68	1.52
1	C	137	TYR	C-O	-5.45	1.17	1.24
2	D	185	ASN	CB-CG	-5.44	1.38	1.52
1	C	96	ASP	CA-C	-5.43	1.45	1.53
1	A	143	ALA	CA-CB	-5.42	1.44	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	174	VAL	C-O	5.42	1.30	1.23
2	B	123	TYR	CA-C	5.42	1.59	1.52
2	B	2	LYS	CA-C	5.41	1.59	1.52
1	E	160	ILE	CA-C	-5.41	1.48	1.52
1	A	232	MET	N-CA	5.40	1.52	1.45
1	A	87	VAL	CA-CB	-5.40	1.47	1.54
2	F	266	MET	CG-SD	-5.39	1.67	1.80
1	A	28	GLU	N-CA	5.39	1.53	1.46
1	C	92	ALA	CA-CB	-5.38	1.44	1.53
1	E	147	ALA	CA-CB	-5.37	1.46	1.54
1	A	63	SER	CA-C	-5.37	1.46	1.52
1	Q	228	ARG	N-CA	5.37	1.52	1.46
1	C	28	GLU	CA-C	-5.35	1.45	1.52
1	E	17	PHE	N-CA	-5.34	1.39	1.45
2	F	84	ALA	CA-CB	-5.34	1.45	1.53
1	E	202	THR	CA-CB	5.34	1.61	1.53
2	D	139	VAL	CA-C	5.33	1.58	1.52
2	B	77	ALA	CA-C	5.32	1.59	1.52
2	F	169	PRO	CA-C	-5.32	1.45	1.52
2	B	211	GLY	C-O	-5.32	1.16	1.23
1	C	162	ARG	CB-CG	-5.31	1.36	1.52
2	F	79	VAL	CA-CB	-5.31	1.47	1.54
2	D	81	ALA	C-O	-5.31	1.18	1.24
2	Z	122	GLU	CD-OE1	5.30	1.35	1.25
1	E	47	MET	SD-CE	-5.30	1.66	1.79
1	C	100	VAL	CA-C	5.29	1.59	1.52
2	F	68	ILE	CA-C	-5.29	1.46	1.52
2	F	238	ILE	C-O	-5.29	1.17	1.24
1	E	5	VAL	CA-CB	-5.29	1.48	1.54
1	C	204	PRO	CA-C	5.29	1.57	1.52
2	D	191	VAL	CA-CB	5.28	1.68	1.54
1	E	74	ARG	CZ-NH1	5.28	1.40	1.32
2	F	206	MET	CA-C	-5.27	1.46	1.52
1	Q	160	ILE	CA-CB	5.26	1.63	1.54
1	E	9	GLN	CA-C	-5.25	1.46	1.52
1	E	103	ILE	CA-CB	-5.25	1.48	1.54
2	D	135	TYR	CA-C	5.25	1.60	1.53
2	D	112	TYR	CA-C	-5.24	1.46	1.52
2	B	307	ILE	CA-CB	-5.24	1.46	1.54
2	D	251	GLY	CA-C	-5.23	1.46	1.51
2	F	80	SER	N-CA	-5.22	1.40	1.46
1	A	95	SER	CA-C	-5.22	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Z	139	VAL	CA-C	5.22	1.58	1.52
1	A	48	LYS	CB-CG	5.22	1.68	1.52
1	Q	51	GLU	CA-C	5.22	1.59	1.52
2	Z	64	LYS	CA-CB	5.21	1.59	1.52
2	D	63	VAL	CA-C	-5.18	1.46	1.52
2	F	219	GLU	CA-CB	5.18	1.62	1.53
2	D	239	ALA	CA-CB	-5.17	1.45	1.53
1	E	74	ARG	CG-CD	5.14	1.67	1.52
2	F	246	LYS	CA-C	5.14	1.59	1.52
2	D	59	GLU	CA-C	-5.14	1.46	1.52
2	F	184	GLN	C-O	-5.13	1.18	1.23
1	A	102	ARG	NE-CZ	5.11	1.38	1.33
1	Q	32	MET	SD-CE	5.09	1.92	1.79
1	A	133	SER	C-O	5.09	1.30	1.24
2	B	10	ARG	CA-C	-5.09	1.46	1.52
2	D	202	VAL	CA-CB	5.09	1.61	1.54
1	Q	98	ILE	CA-CB	5.09	1.59	1.54
1	Q	31	MET	SD-CE	5.08	1.92	1.79
2	Z	199	ILE	CA-CB	5.08	1.60	1.53
1	E	11	ALA	CA-CB	-5.08	1.45	1.53
2	F	228	ALA	C-O	-5.08	1.17	1.24
2	F	22	ILE	C-O	-5.07	1.17	1.24
1	E	59	VAL	C-O	-5.07	1.18	1.24
1	E	126	ALA	CA-CB	-5.07	1.45	1.53
2	F	81	ALA	CA-CB	5.06	1.61	1.53
2	B	152	VAL	CA-CB	-5.06	1.48	1.54
2	Z	106	LEU	CA-C	5.06	1.59	1.52
2	F	283	THR	CA-CB	-5.06	1.46	1.53
2	Z	156	ARG	CA-C	5.06	1.58	1.53
1	Q	182	ILE	CA-CB	5.06	1.60	1.54
2	F	81	ALA	C-O	-5.05	1.18	1.24
2	Z	49	VAL	CA-CB	5.05	1.60	1.54
1	A	24	MET	CA-C	5.05	1.61	1.52
2	Z	170	VAL	CA-CB	5.04	1.59	1.54
1	E	118	ALA	CA-CB	-5.04	1.46	1.53
1	E	4	LEU	C-O	5.03	1.30	1.24
1	C	81	ALA	CA-CB	-5.01	1.45	1.53
1	A	135	ALA	CA-CB	-5.00	1.45	1.53

All (393) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	103	ILE	N-CA-C	-12.54	99.33	110.74
2	F	202	VAL	CB-CA-C	-12.20	91.29	111.29
2	D	198	ASP	CA-C-N	-11.44	108.08	122.37
2	D	198	ASP	C-N-CA	-11.44	108.08	122.37
2	D	202	VAL	CB-CA-C	-11.32	92.72	111.29
2	B	49	VAL	N-CA-CB	11.31	117.63	110.50
2	D	180	GLN	N-CA-C	-10.81	91.51	109.46
1	E	69	VAL	N-CA-C	-10.01	99.46	113.07
2	B	202	VAL	CB-CA-C	-9.95	94.98	111.29
2	F	1	SER	CA-C-N	-9.93	108.04	122.94
2	F	1	SER	C-N-CA	-9.93	108.04	122.94
2	F	30	LYS	N-CA-C	9.72	121.63	111.14
1	C	249	GLU	CB-CA-C	-9.11	96.83	110.95
2	B	313	GLU	N-CA-C	-9.07	102.00	113.43
2	F	167	GLY	CA-C-N	-9.02	112.26	122.00
2	F	167	GLY	C-N-CA	-9.02	112.26	122.00
2	F	203	ASP	N-CA-C	8.97	125.28	111.56
2	B	261	LYS	N-CA-C	-8.84	102.63	113.41
2	D	306	ASP	CB-CA-C	8.59	124.34	109.65
2	B	198	ASP	CA-C-N	-8.51	112.00	122.90
2	B	198	ASP	C-N-CA	-8.51	112.00	122.90
2	D	303	ILE	N-CA-C	-8.48	95.21	107.77
2	F	199	ILE	CB-CA-C	8.47	121.00	111.08
2	B	230	ALA	CA-C-N	-8.45	111.06	122.72
2	B	230	ALA	C-N-CA	-8.45	111.06	122.72
1	C	56	ASP	N-CA-C	8.44	121.31	109.15
1	C	168	MET	N-CA-C	8.42	122.71	110.42
2	F	201	THR	N-CA-CB	-8.38	97.86	110.35
2	D	201	THR	CA-C-N	8.36	137.01	121.97
2	D	201	THR	C-N-CA	8.36	137.01	121.97
2	B	113	GLY	N-CA-C	-8.31	101.42	112.14
1	E	24	MET	CB-CA-C	8.25	124.39	111.02
2	D	180	GLN	CB-CA-C	8.23	123.30	109.80
2	B	165	GLY	N-CA-C	8.22	122.22	111.70
2	B	274	HIS	N-CA-C	-8.21	101.38	111.40
2	F	159	VAL	N-CA-CB	-8.08	105.02	111.64
2	D	198	ASP	N-CA-C	8.06	121.64	108.26
1	A	168	MET	N-CA-C	8.05	120.98	110.43
1	C	92	ALA	N-CA-C	7.99	121.97	111.75
2	F	129	VAL	N-CA-C	7.98	119.28	108.11
2	Z	188	TYR	N-CA-C	-7.93	99.84	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	168	MET	CB-CA-C	-7.91	98.71	109.71
1	E	17	PHE	N-CA-C	-7.88	99.17	110.59
1	E	110	LYS	N-CA-C	7.88	119.94	111.36
2	D	46	ASP	CB-CA-C	-7.81	97.57	110.85
1	A	15	GLU	N-CA-C	7.77	121.76	110.42
1	A	48	LYS	N-CA-C	-7.76	102.77	111.07
1	A	236	GLU	CA-C-N	-7.73	110.69	123.37
1	A	236	GLU	C-N-CA	-7.73	110.69	123.37
2	F	201	THR	CA-C-N	7.73	135.89	121.97
2	F	201	THR	C-N-CA	7.73	135.89	121.97
2	D	198	ASP	N-CA-CB	-7.68	98.25	110.77
1	A	241	THR	OG1-CB-CG2	-7.66	93.97	109.30
2	F	220	GLN	N-CA-C	7.65	120.70	111.82
2	D	208	ILE	N-CA-C	7.57	119.50	108.53
1	A	48	LYS	CA-CB-CG	7.44	128.98	114.10
2	F	196	ASP	CA-C-N	7.42	135.32	121.97
2	F	196	ASP	C-N-CA	7.42	135.32	121.97
1	E	195	ARG	NH1-CZ-NH2	-7.36	109.73	119.30
1	A	214	GLY	N-CA-C	-7.36	104.61	115.72
1	Q	56	ASP	N-CA-C	7.31	120.00	108.67
2	F	186	LYS	N-CA-C	7.28	115.74	108.75
2	F	76	GLU	N-CA-C	-7.27	103.29	111.07
2	B	251	GLY	N-CA-C	7.25	119.53	111.85
1	Q	205	ILE	N-CA-C	7.16	118.29	108.84
1	C	174	ILE	N-CA-C	7.15	118.44	107.78
2	B	201	THR	CA-C-N	7.14	134.82	121.97
2	B	201	THR	C-N-CA	7.14	134.82	121.97
1	A	248	SER	N-CA-C	-7.09	103.60	111.82
2	F	211	GLY	CA-C-O	-7.08	113.23	120.45
2	B	203	ASP	N-CA-C	7.05	122.19	112.04
2	D	274	HIS	N-CA-C	-7.04	103.61	111.28
2	F	217	ASN	N-CA-C	7.03	121.71	113.20
2	F	97	VAL	CB-CA-C	-7.00	102.86	112.04
2	Z	106	LEU	N-CA-C	7.00	119.51	111.11
2	D	23	GLY	N-CA-C	6.97	121.07	112.64
2	F	90	VAL	CA-C-N	-6.96	114.56	123.19
2	F	90	VAL	C-N-CA	-6.96	114.56	123.19
1	Q	38	TRP	N-CA-C	6.96	119.75	111.33
1	A	182	ILE	N-CA-C	6.95	118.54	109.58
2	D	155	ILE	N-CA-C	6.95	118.06	108.89
1	C	172	VAL	CA-C-N	-6.92	113.17	122.72
1	C	172	VAL	C-N-CA	-6.92	113.17	122.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	118	VAL	N-CA-CB	-6.91	103.19	110.72
2	D	176	ALA	N-CA-C	-6.86	100.11	110.39
1	E	49	ILE	N-CA-C	6.85	117.00	110.42
1	A	156	ASN	N-CA-C	6.83	123.86	113.61
2	D	298	ILE	CB-CA-C	-6.83	103.24	110.62
2	F	189	VAL	N-CA-C	6.79	119.21	108.89
2	D	110	THR	O-C-N	-6.79	114.97	122.84
2	D	63	VAL	N-CA-C	-6.77	97.75	107.77
1	Q	87	VAL	CB-CA-C	-6.75	101.74	110.98
1	C	227	SER	N-CA-C	-6.74	98.28	108.52
1	E	185	GLY	N-CA-C	6.72	124.98	115.30
1	E	89	ASP	N-CA-C	-6.69	98.35	108.52
2	D	13	ASP	N-CA-C	6.69	120.94	110.17
1	C	49	ILE	N-CA-C	-6.68	104.66	110.74
2	D	199	ILE	N-CA-CB	6.66	118.59	111.00
2	Z	43	SER	N-CA-C	6.64	119.34	111.71
2	F	165	GLY	N-CA-C	6.62	120.40	111.72
2	F	1	SER	N-CA-C	-6.62	92.45	111.00
2	F	5	VAL	CB-CA-C	-6.59	101.88	110.84
2	F	98	ASP	N-CA-C	-6.59	104.02	111.07
2	F	274	HIS	N-CA-C	-6.54	104.23	111.36
2	D	297	THR	CA-C-N	-6.53	114.89	122.14
2	D	297	THR	C-N-CA	-6.53	114.89	122.14
1	Q	172	VAL	N-CA-C	-6.50	99.37	108.27
1	A	227	SER	N-CA-C	-6.46	98.09	108.55
2	B	82	LEU	N-CA-C	-6.43	104.12	112.23
1	C	25	ASP	N-CA-C	6.41	116.92	107.88
1	A	220	VAL	N-CA-C	6.40	119.53	108.90
2	D	296	PHE	N-CA-C	-6.40	104.73	112.54
1	C	74	ARG	CG-CD-NE	-6.36	98.00	112.00
2	B	316	ALA	N-CA-C	6.35	119.50	111.69
1	E	241	THR	CA-C-N	-6.35	114.03	122.85
1	E	241	THR	C-N-CA	-6.35	114.03	122.85
1	A	238	GLY	N-CA-C	6.34	117.97	111.95
2	F	306	ASP	N-CA-C	-6.33	100.66	110.10
2	B	197	ILE	N-CA-CB	6.33	121.68	111.23
2	F	298	ILE	CB-CA-C	-6.32	104.44	110.70
1	A	25	ASP	O-C-N	-6.31	117.33	123.26
1	C	77	LEU	N-CA-C	-6.30	104.46	111.71
1	E	158	ALA	CA-C-N	-6.29	114.69	123.13
1	E	158	ALA	C-N-CA	-6.29	114.69	123.13
2	B	147	GLY	N-CA-C	-6.29	105.94	115.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	167	GLY	CA-C-N	-6.28	115.85	122.89
2	D	167	GLY	C-N-CA	-6.28	115.85	122.89
2	Z	26	ASN	CA-C-N	6.28	127.06	120.03
2	Z	26	ASN	C-N-CA	6.28	127.06	120.03
2	D	259	SER	N-CA-C	-6.27	104.26	112.41
1	A	59	VAL	CA-C-N	-6.26	114.23	122.94
1	A	59	VAL	C-N-CA	-6.26	114.23	122.94
1	C	168	MET	CB-CG-SD	-6.26	93.91	112.70
1	E	48	LYS	N-CA-C	-6.26	104.54	111.36
2	D	254	GLY	N-CA-C	-6.25	98.36	113.18
2	D	213	GLY	N-CA-C	6.23	127.95	113.18
1	E	97	ALA	N-CA-C	-6.23	104.38	112.23
2	D	283	THR	N-CA-C	6.22	120.71	107.70
2	F	308	PHE	N-CA-C	6.21	120.66	111.04
2	F	295	ILE	N-CA-C	-6.19	103.36	111.09
1	C	161	ARG	CA-C-N	-6.17	113.68	122.94
1	C	161	ARG	C-N-CA	-6.17	113.68	122.94
2	F	80	SER	N-CA-C	-6.17	104.48	111.14
2	B	57	VAL	N-CA-C	6.15	117.27	107.98
1	E	258	ILE	CB-CA-C	-6.12	103.78	112.22
1	E	51	GLU	CB-CA-C	6.11	120.29	109.65
1	E	64	VAL	CB-CA-C	-6.11	102.75	111.31
2	F	198	ASP	CB-CA-C	-6.10	98.31	109.54
2	D	165	GLY	N-CA-C	6.10	123.20	112.83
1	E	238	GLY	N-CA-C	-6.09	98.74	113.18
2	F	127	GLU	N-CA-C	6.07	118.63	108.73
2	D	113	GLY	N-CA-C	-6.04	104.98	111.93
2	D	120	ILE	N-CA-C	6.03	116.77	107.78
1	C	149	LEU	CA-C-N	-6.02	115.01	122.84
1	C	149	LEU	C-N-CA	-6.02	115.01	122.84
2	F	32	GLY	CA-C-N	6.02	129.85	120.82
2	F	32	GLY	C-N-CA	6.02	129.85	120.82
1	Q	99	VAL	N-CA-C	6.01	116.67	110.36
1	A	182	ILE	CB-CA-C	-6.01	102.13	111.26
1	E	173	GLU	CA-C-N	-6.00	113.70	122.58
1	E	173	GLU	C-N-CA	-6.00	113.70	122.58
2	F	237	PRO	N-CA-C	-6.00	106.05	113.84
1	E	14	GLU	CA-C-O	-5.99	114.92	121.87
2	F	131	THR	OG1-CB-CG2	-5.99	97.33	109.30
1	C	162	ARG	CB-CA-C	5.98	120.80	109.37
1	C	124	ASP	N-CA-C	5.98	120.31	111.04
2	F	259	SER	CA-C-N	-5.98	112.63	121.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	259	SER	C-N-CA	-5.98	112.63	121.24
1	Q	260	GLU	N-CA-C	-5.97	105.70	112.87
2	B	74	VAL	CB-CA-C	-5.97	103.98	112.22
2	B	222	ARG	N-CA-C	-5.96	104.86	111.36
2	B	127	GLU	N-CA-C	5.96	119.36	107.62
1	C	88	TRP	N-CA-C	5.95	117.57	108.52
1	C	134	VAL	N-CA-C	-5.95	104.55	110.62
1	C	158	ALA	N-CA-C	-5.95	100.21	109.72
1	C	244	GLU	CB-CG-CD	-5.94	102.50	112.60
1	C	239	ARG	N-CA-C	5.93	119.25	109.94
1	E	17	PHE	N-CA-CB	-5.93	101.41	110.42
1	E	162	ARG	NE-CZ-NH1	-5.92	115.58	121.50
1	C	146	VAL	CB-CA-C	-5.92	103.40	111.33
2	D	222	ARG	N-CA-CB	5.92	119.34	110.22
2	D	261	LYS	N-CA-C	-5.92	106.68	114.31
2	D	16	PRO	N-CD-CG	-5.91	94.33	103.20
2	D	241	ALA	N-CA-C	-5.91	104.21	113.02
2	D	235	SER	N-CA-C	-5.91	101.72	110.46
1	C	249	GLU	CB-CG-CD	-5.90	102.57	112.60
2	D	203	ASP	N-CA-C	5.89	120.48	113.12
2	F	94	PRO	N-CA-C	-5.89	102.62	111.57
2	B	199	ILE	CB-CA-C	5.88	119.04	110.98
1	C	175	ASN	CB-CA-C	-5.88	100.32	109.61
1	C	152	LYS	CB-CA-C	5.88	117.60	108.61
1	A	240	ALA	CA-C-N	-5.85	114.99	122.77
1	A	240	ALA	C-N-CA	-5.85	114.99	122.77
2	D	62	VAL	N-CA-CB	-5.84	103.35	111.41
2	B	146	PRO	N-CD-CG	-5.81	94.48	103.20
2	F	197	ILE	N-CA-C	5.81	121.42	109.34
2	D	163	LEU	CA-CB-CG	5.81	136.62	116.30
2	B	311	GLU	N-CA-C	5.80	117.61	111.28
2	D	12	ASN	CB-CA-C	-5.80	98.88	110.42
2	D	94	PRO	N-CD-CG	-5.79	94.51	103.20
2	B	176	ALA	N-CA-C	-5.78	101.80	109.84
2	D	30	LYS	N-CA-C	5.77	120.45	112.90
2	Z	208	ILE	N-CA-C	5.75	117.28	108.71
2	B	313	GLU	N-CA-CB	-5.74	100.75	110.51
2	D	65	GLY	N-CA-C	5.74	121.94	112.30
2	B	90	VAL	CA-C-N	-5.74	115.63	123.14
2	B	90	VAL	C-N-CA	-5.74	115.63	123.14
1	A	203	LYS	N-CA-C	5.73	118.32	110.01
1	E	218	ASN	N-CA-C	-5.73	105.17	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	ASP	N-CA-C	5.72	116.94	107.73
1	E	125	GLN	N-CA-C	5.72	118.29	111.71
2	Z	49	VAL	N-CA-CB	5.71	119.21	111.21
1	C	187	ASN	N-CA-C	5.70	115.81	108.34
2	B	142	GLU	N-CA-C	-5.69	99.91	109.07
2	D	15	ARG	NE-CZ-NH1	-5.68	115.82	121.50
1	C	139	ASN	N-CA-C	5.67	118.11	111.02
2	B	129	VAL	N-CA-C	5.67	116.04	108.11
1	A	88	TRP	N-CA-C	5.66	117.72	108.55
2	F	198	ASP	N-CA-C	5.66	118.48	110.50
2	D	156	ARG	N-CA-C	5.66	117.63	109.48
2	D	280	HIS	N-CA-C	-5.66	106.25	114.12
2	B	105	SER	N-CA-CB	5.66	118.21	110.01
1	E	34	ASP	N-CA-C	5.65	115.85	107.88
2	B	128	LEU	N-CA-C	5.65	118.38	109.96
2	D	222	ARG	CB-CG-CD	5.64	124.27	111.30
1	A	29	ASP	CA-C-N	-5.64	113.75	122.49
1	A	29	ASP	C-N-CA	-5.64	113.75	122.49
1	E	106	GLU	N-CA-C	5.63	117.10	111.07
1	C	81	ALA	N-CA-C	5.63	118.18	110.24
2	F	112	TYR	CA-C-N	-5.63	114.99	120.34
2	F	112	TYR	C-N-CA	-5.63	114.99	120.34
2	F	203	ASP	CB-CA-C	-5.63	100.50	111.03
2	Z	93	LEU	N-CA-C	-5.62	101.50	110.10
1	A	19	ILE	N-CA-C	5.62	115.98	108.11
2	B	258	GLY	N-CA-C	5.61	119.43	112.64
2	B	120	ILE	N-CA-C	-5.61	100.95	108.35
1	Q	5	VAL	N-CA-C	5.59	115.64	107.37
2	D	61	VAL	CB-CA-C	-5.59	101.89	110.50
2	D	269	SER	N-CA-C	5.58	122.68	110.80
1	A	179	VAL	CA-C-N	-5.57	113.09	122.29
1	A	179	VAL	C-N-CA	-5.57	113.09	122.29
2	F	149	SER	N-CA-C	-5.57	105.29	111.36
2	Z	222	ARG	N-CA-C	-5.55	105.13	111.07
1	C	128	ALA	N-CA-C	-5.55	103.62	111.56
1	A	259	ASN	CB-CA-C	5.55	119.67	110.90
1	A	74	ARG	NE-CZ-NH2	-5.54	114.22	119.20
1	A	74	ARG	NH1-CZ-NH2	5.54	126.50	119.30
1	C	180	LEU	CA-C-N	-5.53	115.30	123.05
1	C	180	LEU	C-N-CA	-5.53	115.30	123.05
2	B	219	GLU	CB-CG-CD	5.52	121.98	112.60
2	D	208	ILE	CA-C-N	-5.51	117.56	122.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	208	ILE	C-N-CA	-5.51	117.56	122.47
2	D	219	GLU	CA-CB-CG	5.51	125.12	114.10
2	B	67	SER	N-CA-C	5.51	118.68	110.14
2	F	92	LEU	CB-CA-C	-5.51	101.16	110.19
2	B	70	PHE	N-CA-C	5.50	118.00	110.24
1	C	152	LYS	N-CA-C	-5.50	103.24	110.39
2	B	283	THR	N-CA-C	5.49	117.59	108.20
1	C	46	ALA	N-CA-C	-5.49	105.46	111.82
1	A	58	GLU	N-CA-C	5.48	117.69	107.99
1	C	7	VAL	N-CA-C	5.48	117.28	108.85
2	D	94	PRO	N-CA-C	-5.48	102.59	111.19
1	A	161	ARG	CA-C-N	-5.47	112.71	122.07
1	A	161	ARG	C-N-CA	-5.47	112.71	122.07
2	B	315	LYS	N-CA-C	-5.47	105.71	112.38
2	D	155	ILE	CB-CA-C	-5.46	104.05	111.15
2	Z	197	ILE	N-CA-C	5.46	120.70	109.34
1	E	227	SER	N-CA-C	-5.46	99.70	108.55
2	F	155	ILE	N-CA-CB	-5.46	103.82	111.25
2	B	303	ILE	CA-C-N	-5.45	115.92	122.90
2	B	303	ILE	C-N-CA	-5.45	115.92	122.90
1	C	203	LYS	N-CA-C	5.43	121.81	109.81
2	F	167	GLY	N-CA-C	-5.42	100.48	110.83
2	B	285	ILE	CA-C-N	-5.41	115.36	122.99
2	B	285	ILE	C-N-CA	-5.41	115.36	122.99
2	B	58	ASP	N-CA-C	5.41	118.35	111.69
1	C	119	GLY	N-CA-C	-5.41	102.86	112.54
2	Z	260	CYS	N-CA-C	5.41	117.53	109.25
2	Z	99	SER	N-CA-C	5.41	117.60	111.11
1	E	53	SER	O-C-N	5.40	129.37	123.27
2	D	117	ASP	CA-C-N	5.40	129.33	122.37
2	D	117	ASP	C-N-CA	5.40	129.33	122.37
1	A	66	PRO	N-CA-C	-5.39	101.36	112.47
2	F	107	ALA	N-CA-C	5.39	117.15	111.28
1	A	90	ASP	N-CA-C	-5.39	105.49	111.36
1	Q	123	SER	N-CA-C	5.38	117.57	111.11
1	A	70	ASP	N-CA-C	-5.38	105.42	111.28
2	B	234	CYS	N-CA-C	5.37	117.00	108.79
2	D	110	THR	CA-C-N	-5.37	110.89	121.41
2	D	110	THR	C-N-CA	-5.37	110.89	121.41
1	E	167	GLY	CA-C-N	-5.37	113.09	120.71
1	E	167	GLY	C-N-CA	-5.37	113.09	120.71
1	C	211	ALA	N-CA-C	-5.36	106.79	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	196	ASP	CA-C-N	5.36	131.61	121.97
2	Z	196	ASP	C-N-CA	5.36	131.61	121.97
1	C	107	VAL	N-CA-C	5.34	115.55	110.42
2	B	103	ALA	CA-C-N	-5.32	111.84	120.72
2	B	103	ALA	C-N-CA	-5.32	111.84	120.72
2	D	159	VAL	N-CA-C	-5.32	106.98	111.56
2	B	308	PHE	N-CA-C	5.31	117.98	111.82
2	Z	29	LYS	N-CA-C	5.31	117.78	110.35
2	F	199	ILE	N-CA-CB	5.31	116.90	110.95
1	A	157	LYS	N-CA-C	-5.30	101.35	109.41
2	Z	178	SER	CB-CA-C	-5.30	104.17	112.12
2	D	175	ASP	N-CA-C	-5.30	101.64	110.17
2	B	139	VAL	CA-C-O	-5.29	116.75	121.09
1	A	48	LYS	CB-CG-CD	-5.28	99.15	111.30
1	C	5	VAL	N-CA-C	5.27	115.55	108.17
1	E	53	SER	CA-C-N	5.27	128.07	120.38
1	E	53	SER	C-N-CA	5.27	128.07	120.38
2	D	175	ASP	N-CA-CB	5.26	119.20	110.63
1	A	256	GLN	N-CA-C	-5.25	104.99	111.40
2	B	254	GLY	N-CA-C	-5.25	100.73	113.18
2	D	94	PRO	CA-C-O	-5.25	115.02	121.31
2	F	215	GLU	CA-C-N	-5.25	111.96	120.72
2	F	215	GLU	C-N-CA	-5.25	111.96	120.72
1	Q	107	VAL	CB-CA-C	-5.24	105.15	112.02
2	F	2	LYS	CA-C-N	-5.24	116.07	122.93
2	F	2	LYS	C-N-CA	-5.24	116.07	122.93
2	B	73	ASP	N-CA-C	5.23	117.66	111.33
1	C	59	VAL	CB-CA-C	-5.23	103.82	110.98
1	E	83	ARG	CA-C-N	-5.22	114.27	122.73
1	E	83	ARG	C-N-CA	-5.22	114.27	122.73
2	F	4	LEU	N-CA-C	5.22	116.77	108.67
2	D	304	VAL	CB-CA-C	-5.22	106.73	112.68
2	Z	37	VAL	N-CA-C	5.22	115.09	107.37
2	F	258	GLY	CA-C-N	-5.21	114.34	122.73
2	F	258	GLY	C-N-CA	-5.21	114.34	122.73
2	F	156	ARG	CB-CA-C	-5.21	101.44	109.62
2	F	201	THR	CB-CA-C	5.21	120.15	111.30
1	A	60	VAL	CA-C-O	-5.21	114.84	120.67
2	B	83	ILE	N-CA-C	-5.20	105.31	110.62
1	A	52	SER	N-CA-C	5.20	119.25	113.01
2	D	64	LYS	CA-C-N	-5.20	114.11	121.54
2	D	64	LYS	C-N-CA	-5.20	114.11	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	213	ILE	N-CA-C	5.20	117.11	112.17
1	C	57	VAL	CB-CA-C	-5.19	103.38	110.96
1	Q	204	PRO	CA-C-N	5.19	128.96	121.18
1	Q	204	PRO	C-N-CA	5.19	128.96	121.18
2	B	112	TYR	N-CA-CB	5.19	117.64	110.17
1	C	142	HIS	N-CA-C	5.18	116.29	108.46
2	B	146	PRO	CB-CA-C	-5.18	103.01	111.56
2	D	122	GLU	N-CA-C	5.18	116.17	108.60
1	E	259	ASN	CB-CA-C	5.18	119.65	110.85
2	B	136	ASN	N-CA-C	5.18	118.27	111.28
2	F	180	GLN	N-CA-CB	5.18	118.31	109.87
1	Q	93	GLU	CB-CA-C	5.18	116.91	109.71
1	Q	154	GLY	N-CA-C	5.17	122.75	115.30
1	C	33	TYR	N-CA-C	5.16	117.70	109.96
1	C	244	GLU	N-CA-C	5.14	117.00	109.24
2	B	271	SER	CA-CB-OG	-5.12	100.85	111.10
2	F	165	GLY	CA-C-O	-5.12	117.37	121.77
2	F	219	GLU	N-CA-CB	5.12	118.23	110.14
2	Z	127	GLU	N-CA-C	5.12	117.00	107.99
2	B	201	THR	N-CA-C	5.12	117.27	107.75
2	F	223	GLU	CA-CB-CG	-5.12	103.87	114.10
1	C	244	GLU	CG-CD-OE1	-5.12	106.63	118.40
2	B	110	THR	CA-C-N	-5.11	111.39	121.41
2	B	110	THR	C-N-CA	-5.11	111.39	121.41
2	F	225	ALA	CA-C-N	5.11	127.89	120.79
2	F	225	ALA	C-N-CA	5.11	127.89	120.79
1	E	250	GLN	N-CA-C	-5.09	105.17	111.33
1	A	230	ARG	N-CA-C	-5.09	106.75	113.12
1	A	4	LEU	CA-C-N	-5.09	116.51	123.12
1	A	4	LEU	C-N-CA	-5.09	116.51	123.12
1	A	258	ILE	N-CA-C	-5.09	105.54	110.42
2	D	32	GLY	CA-C-N	5.08	127.35	120.44
2	D	32	GLY	C-N-CA	5.08	127.35	120.44
1	C	249	GLU	N-CA-C	5.08	116.67	111.03
1	Q	37	GLU	CA-C-N	5.08	127.33	120.38
1	Q	37	GLU	C-N-CA	5.08	127.33	120.38
2	F	280	HIS	N-CA-C	5.07	119.33	113.20
2	B	111	GLY	CA-C-N	-5.06	112.99	120.94
2	B	111	GLY	C-N-CA	-5.06	112.99	120.94
1	E	155	ASP	CB-CA-C	-5.06	100.35	110.42
2	F	92	LEU	N-CA-C	5.06	116.77	108.52
1	E	159	VAL	CA-C-N	-5.06	116.86	122.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	159	VAL	C-N-CA	-5.06	116.86	122.27
1	E	68	ARG	N-CA-C	5.04	118.90	112.34
1	A	125	GLN	CB-CA-C	5.04	119.40	109.72
2	F	33	GLU	N-CA-C	5.04	119.69	111.37
2	D	90	VAL	CB-CA-C	-5.04	102.33	110.28
1	A	61	VAL	CA-C-N	-5.03	114.35	122.25
1	A	61	VAL	C-N-CA	-5.03	114.35	122.25
1	C	238	GLY	N-CA-C	-5.03	101.25	113.18
2	D	159	VAL	N-CA-CB	-5.03	105.88	111.41
2	F	151	VAL	N-CA-C	5.02	115.20	108.17
1	Q	58	GLU	N-CA-C	5.02	116.49	108.41
2	D	12	ASN	N-CA-C	5.02	121.49	110.80
1	Q	118	ALA	N-CA-C	-5.01	101.79	109.41
2	D	206	MET	N-CA-C	-5.01	100.74	108.90
1	A	110	LYS	N-CA-C	5.00	116.42	111.07
2	F	170	VAL	CB-CA-C	-5.00	103.08	111.29

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

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	93	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1942	0	1901	102	0
1	E	1939	0	1891	111	0
1	Q	1831	0	1768	59	0
2	B	2287	0	2250	85	0
2	D	2281	0	2237	127	0
2	F	2281	0	2237	95	1
2	Z	2265	0	2222	20	0
3	A	23	0	12	0	0
3	C	23	0	12	2	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	0	0
All	All	17093	0	16594	650	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 (650) 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
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:A:239:ARG:O	1:A:239:ARG:HG2	1.32	1.08
1:C:47:MET:HE2	1:C:80:GLY:HA3	1.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:A:1:MET:HG3	1:A:153:PRO:HB3	1.43	1.00
1:A:226:MET:HE3	2:B:112:TYR:O	1.62	1.00
2:D:202:VAL:HG12	2:D:203:ASP:N	1.72	0.99
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
2:F:202:VAL:CG1	2:F:203:ASP:H	1.79	0.94
1:C:246:THR:O	1:C:247:ILE:C	2.10	0.93
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
2:F:1:SER:N	2:F:34:ASP:CG	2.28	0.92
1:C:246:THR:H	1:C:249:GLU:HG3	1.34	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: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: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
1:Q:183:GLN:NE2	1:Q:184:LEU:H	1.72	0.85
1:C:47:MET:HE2	1:C:80:GLY:CA	2.07	0.84
1:E:1:MET:HE3	1:E:2:LYS:N	1.92	0.84
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: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
1:E:226:MET:HE3	2:F:112:TYR:O	1.78	0.82
2:F:219:GLU:CD	2:F:222:ARG:HD2	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:D:264:VAL:CG1	2:D:266:MET:HE2	2.11	0.79
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
1:C:129:SER:HB3	2:D:104:SER:HB3	1.66	0.77
1:Q:1:MET:HG3	1:Q:153:PRO:HB3	1.67	0.77
2:B:263:TYR:CE2	2:B:278:MET:HE3	2.20	0.76
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
1:E:1:MET:HE1	1:E:3:ILE:HG13	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:F:1:SER:H1	2:F:34:ASP:CG	1.93	0.75
2:F:275:MET:HE2	2:F:298:ILE:HD13	1.69	0.75
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
2:D:264:VAL:HG12	2:D:266:MET:HE2	1.69	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:A:19:ILE:O	1:A:20:ARG:C	2.32	0.72
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:275:MET:HE2	2:F:298:ILE:CD1	2.22	0.70
2:F:313:GLU:O	2:F:314:LEU:C	2.35	0.70
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
2:B:199:ILE:C	2:B:201:THR:H	2.00	0.68
1:A:176:CYS:HA	1:A:177:PRO:C	2.19	0.68
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
1:C:226:MET:HE1	2:D:111:GLY:HA2	1.79	0.65
1:C:226:MET:HE3	2:D:112:TYR:O	1.96	0.65
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
1:E:1:MET:HE1	1:E:3:ILE:CG1	2.27	0.64
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:E:55:THR:OG1	1:E:56:ASP:N	2.28	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:B:46:ASP:O	2:B:47:ALA:C	2.40	0.64
2:D:310:ILE:CG2	2:D:314:LEU:HD22	2.25	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:199:ILE:C	2:F:201:THR:H	2.05	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
2:D:99:SER:C	2:D:101:GLY:H	2.05	0.63
2:D:257:VAL:HG23	2:D:257:VAL:O	1.99	0.63
2:D:278:MET:C	2:D:278:MET:HE2	2.24	0.63
1:E:63:SER:HA	3:E:1262:AMP:H2	1.64	0.63
2:F:316:ALA:O	2:F:317:GLN:C	2.42	0.63
2:F:309:ASP:HA	2:F:312:GLU:HG2	1.81	0.62
2:D:264:VAL:HG11	2:D:266:MET:HE2	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:E:236:GLU:O	1:E:237:LYS:CB	2.39	0.61
2:B:134:GLY:O	2:B:135:TYR:C	2.43	0.61
1:C:9:GLN:HG2	1:C:33:TYR:HB3	1.81	0.61
1:Q:88:TRP:CG	1:Q:89:ASP:H	2.19	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: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:D:99:SER:C	2:D:101:GLY:N	2.57	0.60
2:B:238:ILE:HG21	2:B:244:LEU:HD12	1.83	0.60
1:A:14:GLU:HG3	1:A:32:MET:HE2	1.82	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
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
1:A:20:ARG:HB3	1:A:22:ASP:HA	1.84	0.59
1:E:211:ALA:O	1:E:212:ASP:C	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:HG3	1:C:153:PRO:HB3	1.84	0.59
1:E:176:CYS:HA	1:E:177:PRO:C	2.27	0.59
2:F:79:VAL:HA	2:F:82:LEU:HD12	1.84	0.59
2:B:306:ASP:OD1	2:B:308:PHE:N	2.35	0.58
1:E:168:MET:HB2	1:E:168:MET:HE3	1.82	0.58
1:C:98:ILE:O	1:C:98:ILE:CG2	2.52	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:D:200:THR:C	2:D:202:VAL:H	2.11	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
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
2:F:219:GLU:OE2	2:F:222:ARG:HD3	2.04	0.57
2:B:49:VAL:O	2:B:53:SER:OG	2.13	0.57
1:E:237:LYS:O	1:E:238:GLY:C	2.47	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
2:F:189:VAL:HG12	2:F:190:GLU:N	2.18	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
1:E:1:MET:HE3	1:E:2:LYS:H	1.70	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
2:D:269:SER:H	4:D:1319:FAD:H4B	1.70	0.56
2:F:136:ASN:O	2:F:137:GLN:HB2	2.03	0.56
1:E:145:VAL:HG12	1:E:145:VAL:O	2.03	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: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
1:A:187:ASN:C	1:A:187:ASN:OD1	2.49	0.56
2:F:232:LEU:O	2:F:248:ARG:HD2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:Q:1:MET:HE1	1:Q:3:ILE:CG1	2.36	0.56
2:D:290:ASP:C	2:D:290:ASP:OD1	2.49	0.55
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:17:PHE:HA	1:E:30:PHE:CD2	2.41	0.55
2:F:1:SER:H3	2:F:34:ASP:CG	2.15	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
2:F:17:VAL:O	2:F:18:SER:C	2.49	0.55
1:C:232:MET:HG2	2:D:141:VAL:HG22	1.89	0.55
2:B:199:ILE:C	2:B:201:THR:N	2.64	0.55
1:Q:186:ILE:HG23	1:Q:187:ASN:ND2	2.21	0.55
1:C:246:THR:O	1:C:247:ILE:O	2.23	0.55
2:B:224:LEU:HD11	2:B:314:LEU:HD23	1.89	0.54
1:C:19:ILE:O	1:C:20:ARG:C	2.50	0.54
1:C:247:ILE:HG22	2:D:313:GLU:HG2	1.88	0.54
2:D:176:ALA:C	2:D:177:PRO:O	2.46	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
2:F:313:GLU:O	2:F:315:LYS:N	2.40	0.54
2:D:134:GLY:O	2:D:135:TYR:C	2.50	0.54
1:E:246:THR:O	1:E:247:ILE:C	2.51	0.54
2:Z:60:LEU:HB3	2:Z:171:VAL:HG22	1.89	0.54
1:A:246:THR:HB	1:A:248:SER:H	1.73	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:46:ASP:O	2:D:47:ALA:C	2.52	0.53
2:F:256:VAL:HG13	2:F:277:GLY:HA2	1.89	0.53
2:F:199:ILE:C	2:F:201:THR:N	2.67	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:26:VAL:HG12	1:A:27:ASP:N	2.23	0.53
2:B:275:MET:HG2	2:B:298:ILE:HD13	1.89	0.53
1:C:47:MET:CE	1:C:80:GLY:CA	2.78	0.53
2:B:79:VAL:O	2:B:83:ILE:HG13	2.10	0.52
1:E:4:LEU:C	1:E:4:LEU:HD23	2.34	0.52
2:F:309:ASP:OD1	2:F:309:ASP:N	2.41	0.52
1:E:47:MET:HE2	1:E:80:GLY:HA3	1.91	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
1:C:176:CYS:HA	1:C:177:PRO:C	2.35	0.52
2:Z:77:ALA:HB1	2:Z:177:PRO:HG2	1.92	0.52
2:B:168:SER:O	2:B:169:PRO:C	2.52	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:D:86:HIS:O	2:D:87:ASN:C	2.52	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:C:36:ASN:O	1:C:37:GLU:C	2.52	0.51
1:Q:17:PHE:HA	1:Q:30:PHE:CD1	2.46	0.51
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
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:B:263:TYR:CD2	2:B:278:MET:HE3	2.45	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

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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	0.51
1:E:247:ILE:HD13	1:E:247:ILE:N	2.25	0.51
1:A:168:MET:HE3	2:B:190:GLU:OE1	2.11	0.51
1:E:216:SER:C	1:E:218:ASN:N	2.67	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
2:B:46:ASP:C	2:B:48:PHE:N	2.69	0.50
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
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
1:C:67:ASP:C	1:C:69:VAL:H	2.17	0.50
2:D:197:ILE:CB	2:D:198:ASP:CG	2.85	0.50
1:E:243:ILE:HD11	2:F:301:TYR:HB3	1.93	0.50
1:E:186:ILE:HG23	1:E:187:ASN:ND2	2.27	0.50
1:A:196:GLY:O	1:A:197:ILE:C	2.54	0.50
2:D:20:GLU:HG2	2:D:160:PHE:O	2.11	0.50
1:E:216:SER:O	1:E:217:ALA:C	2.54	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
2:D:120:ILE:HG13	2:D:131:THR:HB	1.94	0.50
1:C:216:SER:O	1:C:217:ALA:C	2.54	0.49
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
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
2:D:69:ASP:O	2:D:70:PHE:C	2.51	0.49
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:C:121:GLN:C	3:C:1262:AMP:H5'2	2.38	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:96:ASP:OD1	1:C:96:ASP:C	2.54	0.49
1:Q:149:LEU:HD13	1:Q:180:LEU:CD1	2.43	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:E:216:SER:C	1:E:218:ASN:H	2.21	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
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:A:231:ARG:O	1:A:231:ARG:HG3	2.11	0.48
2:D:273:GLN:O	2:D:274:HIS:C	2.53	0.48
1:E:246:THR:C	1:E:248:SER:N	2.71	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:F:46:ASP:O	2:F:49:VAL:HG13	2.13	0.48
1:A:36:ASN:O	1:A:37:GLU:C	2.53	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
2:B:278:MET:HB2	2:B:278:MET:HE2	1.50	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:D:46:ASP:C	2:D:48:PHE:N	2.69	0.47
1:E:106:GLU:HB3	1:E:213:ILE:HB	1.96	0.47
1:E:261:PHE:C	1:E:261:PHE:CD1	2.93	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: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:156:ASN:ND2	1:C:157:LYS:HG3	2.29	0.47
2:D:246:LYS:HZ3	2:D:249:GLN:HE22	1.63	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
1:A:247:ILE:N	1:A:247:ILE:CD1	2.75	0.46
1:C:53:SER:C	1:C:55:THR:H	2.23	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:253:LYS:O	1:E:254:ILE:C	2.56	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:Q:164:LEU:HD13	2:Z:10:ARG:NE	2.31	0.46
1:A:125:GLN:O	1:A:126:ALA:C	2.58	0.46
2:B:1:SER:HB2	2:B:34:ASP:OD1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ASP:C	1:C:17:PHE:O	2.58	0.46
1:C:67:ASP:C	1:C:69:VAL:N	2.73	0.46
2:D:273:GLN:NE2	4:D:1319:FAD:O2'	2.49	0.46
2:F:224:LEU:O	2:F:225:ALA:C	2.58	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:Q:176:CYS:HA	1:Q:177:PRO:C	2.41	0.46
1:A:27:ASP:C	1:A:29:ASP:H	2.24	0.45
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:182:ILE:N	1:A:182:ILE:HD13	2.31	0.45
1:A:249:GLU:O	1:A:250:GLN:C	2.59	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
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:Q:168:MET:HB2	1:Q:168:MET:HE3	1.58	0.45
1:C:42:SER:O	1:C:43:LEU:C	2.59	0.45
1:C:162:ARG:HH21	1:C:170:GLN:HE22	1.62	0.45
1:A:36:ASN:HD21	1:A:38:TRP:HB2	1.79	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
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:316:ALA:O	2:D:317:GLN:C	2.60	0.45
1:E:73:LEU:O	1:E:76:CYS:HB2	2.16	0.45
2:B:210:ARG:O	2:B:211:GLY:C	2.59	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
1:A:96:ASP:C	1:A:96:ASP:OD1	2.59	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:54:VAL:O	2:F:55:ASN:C	2.60	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
1:Q:102:ARG:NH1	1:Q:102:ARG:CG	2.54	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
2:B:148:LYS:O	2:B:149:SER:C	2.59	0.44
1:C:136:SER:HB2	2:D:105:SER:OG	2.17	0.44
2:D:218:VAL:O	2:D:219:GLU:C	2.60	0.44
1:C:156:ASN:C	1:C:156:ASN:HD22	2.25	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
2:Z:8:GLU:HG2	2:Z:15:ARG:HD3	2.00	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:Z:69:ASP:O	2:Z:70:PHE:C	2.61	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
1:A:20:ARG:O	1:A:22:ASP:CB	2.65	0.44
1:A:114:ASP:C	1:A:115:MET:HG2	2.43	0.44
2:B:98:ASP:O	2:B:99:SER:C	2.61	0.44
2:B:314:LEU:HD12	2:B:314:LEU:HA	1.82	0.44
1:C:114:ASP:C	1:C:115:MET:HG2	2.41	0.44
2:D:119:TYR:N	2:D:119:TYR:CD2	2.85	0.44
2:B:275:MET:O	2:B:276:ALA:C	2.61	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:A:147:ALA:C	1:A:186:ILE:HD12	2.43	0.43
1:A:257:ILE:O	1:A:258:ILE:C	2.58	0.43
1:C:102:ARG:O	1:C:102:ARG:HD3	2.17	0.43
2:D:273:GLN:CD	2:D:273:GLN:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:316:ALA:O	2:D:318:LEU:N	2.50	0.43
1:E:103:ILE:O	1:E:104:LEU:C	2.60	0.43
2:F:98:ASP:O	2:F:99:SER:C	2.60	0.43
1:Q:23:GLY:O	1:Q:231:ARG:HA	2.18	0.43
1:A:246:THR:O	1:A:247:ILE:C	2.61	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
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: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
1:E:132:ILE:O	1:E:133:SER:C	2.60	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
1:E:47:MET:CE	1:E:80:GLY:HA3	2.48	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:E:35:LEU:HD12	1:E:35:LEU:HA	1.77	0.43
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
2:B:6:ILE:HD12	2:B:79:VAL:HG22	2.01	0.42
2:B:99:SER:C	2:B:101:GLY:N	2.77	0.42
2:B:280:HIS:CD2	2:B:280:HIS:C	2.97	0.42
1:C:20:ARG:CB	1:C:22:ASP:HA	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:F:134:GLY:O	2:F:135:TYR:C	2.61	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:154:GLY:O	1:A:155:ASP:C	2.63	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
2:D:246:LYS:HZ2	2:D:249:GLN:HE22	1.67	0.42
1:E:13:LEU:HA	1:E:13:LEU:HD23	1.81	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
1:A:160:ILE:HD12	1:A:160:ILE:C	2.45	0.41
1:A:185:GLY:C	1:A:187:ASN:H	2.28	0.41
2:B:252:GLN:HB3	2:B:273:GLN:HB3	2.01	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:B:31:SER:C	2:B:33:GLU:H	2.27	0.41
1:C:70:ASP:O	1:C:71:GLU:C	2.62	0.41
2:F:224:LEU:HA	2:F:224:LEU:HD23	1.83	0.41
1:A:69:VAL:O	1:A:70:ASP:C	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:154:GLY:O	1:A:155:ASP:O	2.39	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
1:C:9:GLN:CG	1:C:33:TYR:HB3	2.49	0.41
1:E:1:MET:HE2	1:E:57:VAL:HG13	2.01	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: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
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
2:F:75:PHE:O	2:F:76:GLU:C	2.62	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
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:217:ASN:O	2:D:218:VAL:C	2.62	0.41
2:D:310:ILE:HG22	2:D:314:LEU:CD2	2.34	0.41
2:F:99:SER:C	2:F:101:GLY:N	2.79	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: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: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
2:B:46:ASP:C	2:B:48:PHE:H	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:96:SER:H	2:F:99:SER:HB2	1.87	0.40
2:F:309:ASP:O	2:F:310:ILE:C	2.63	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:F:31:SER:C	2:F:33:GLU:N	2.78	0.40
1:Q:70:ASP:OD1	1:Q:86:ARG:NE	2.54	0.40
1:A:4:LEU:HD22	1:A:108:ILE:HG12	2.03	0.40
1:A:72:SER:O	1:A:73:LEU:C	2.64	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

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%)	4	20
1	C	256/264 (97%)	221 (86%)	29 (11%)	6 (2%)	5	23
1	E	256/264 (97%)	227 (89%)	20 (8%)	9 (4%)	3	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	Q	240/264 (91%)	221 (92%)	15 (6%)	4 (2%)	7	30
2	B	310/320 (97%)	269 (87%)	33 (11%)	8 (3%)	4	21
2	D	310/320 (97%)	272 (88%)	26 (8%)	12 (4%)	2	14
2	F	310/320 (97%)	272 (88%)	25 (8%)	13 (4%)	2	13
2	Z	308/320 (96%)	279 (91%)	24 (8%)	5 (2%)	7	30
All	All	2247/2336 (96%)	1989 (88%)	194 (9%)	64 (3%)	4	20

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
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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	169 (84%)	31 (16%)	2	12
1	C	196/216 (91%)	178 (91%)	18 (9%)	8	31
1	E	195/216 (90%)	171 (88%)	24 (12%)	4	20
1	Q	184/216 (85%)	166 (90%)	18 (10%)	7	29
2	B	245/258 (95%)	209 (85%)	36 (15%)	3	14
2	D	243/258 (94%)	203 (84%)	40 (16%)	2	11
2	F	243/258 (94%)	204 (84%)	39 (16%)	2	12
2	Z	241/258 (93%)	221 (92%)	20 (8%)	10	35
All	All	1747/1896 (92%)	1521 (87%)	226 (13%)	4	18

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	3	ILE
1	A	10	THR
1	A	13	LEU
1	A	16	ASP
1	A	34	ASP
1	A	42	SER
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	98	ILE
1	A	102	ARG
1	A	125	GLN
1	A	132	ILE
1	A	145	VAL
1	A	156	ASN
1	A	162	ARG
1	A	174	ILE
1	A	180	LEU
1	A	182	ILE
1	A	183	GLN
1	A	186	ILE
1	A	203	LYS
1	A	239	ARG

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Mol	Chain	Res	Type
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	19	LEU
2	B	29	LYS
2	B	30	LYS
2	B	36	VAL
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	127	GLU
2	B	158	SER
2	B	159	VAL
2	B	163	LEU
2	B	168	SER
2	B	172	SER
2	B	191	VAL
2	B	199	ILE
2	B	201	THR
2	B	203	ASP
2	B	216	THR
2	B	219	GLU
2	B	224	LEU
2	B	237	PRO
2	B	246	LYS
2	B	255	LYS
2	B	259	SER
2	B	273	GLN
2	B	279	LYS
2	B	285	ILE
2	B	289	THR
2	B	303	ILE
2	B	307	ILE
2	B	313	GLU
1	C	3	ILE
1	C	26	VAL

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Mol	Chain	Res	Type
1	C	32	MET
1	C	34	ASP
1	C	74	ARG
1	C	75	LYS
1	C	102	ARG
1	C	120	VAL
1	C	121	GLN
1	C	125	GLN
1	C	150	GLN
1	C	156	ASN
1	C	171	GLU
1	C	183	GLN
1	C	203	LYS
1	C	239	ARG
1	C	249	GLU
1	C	253	LYS
2	D	11	ARG
2	D	19	LEU
2	D	30	LYS
2	D	31	SER
2	D	49	VAL
2	D	60	LEU
2	D	68	ILE
2	D	80	SER
2	D	83	ILE
2	D	91	VAL
2	D	118	VAL
2	D	119	TYR
2	D	120	ILE
2	D	139	VAL
2	D	149	SER
2	D	163	LEU
2	D	174	VAL
2	D	178	SER
2	D	199	ILE
2	D	201	THR
2	D	203	ASP
2	D	205	ILE
2	D	208	ILE
2	D	212	ILE
2	D	214	GLU
2	D	216	THR

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Mol	Chain	Res	Type
2	D	223	GLU
2	D	224	LEU
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	19	ILE
1	E	28	GLU
1	E	50	LYS
1	E	55	THR
1	E	73	LEU
1	E	74	ARG
1	E	75	LYS
1	E	89	ASP
1	E	102	ARG
1	E	125	GLN
1	E	136	SER
1	E	156	ASN
1	E	168	MET
1	E	174	ILE
1	E	183	GLN
1	E	203	LYS
1	E	213	ILE
1	E	231	ARG
1	E	232	MET
1	E	243	ILE
1	E	249	GLU
1	E	258	ILE
2	F	1	SER
2	F	11	ARG
2	F	19	LEU
2	F	29	LYS

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Mol	Chain	Res	Type
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
2	F	100	LEU
2	F	104	SER
2	F	105	SER
2	F	141	VAL
2	F	150	THR
2	F	155	ILE
2	F	156	ARG
2	F	163	LEU
2	F	172	SER
2	F	174	VAL
2	F	178	SER
2	F	198	ASP
2	F	199	ILE
2	F	201	THR
2	F	203	ASP
2	F	208	ILE
2	F	212	ILE
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
2	F	318	LEU
1	Q	10	THR
1	Q	18	GLU
1	Q	34	ASP
1	Q	45	GLU
1	Q	56	ASP
1	Q	63	SER
1	Q	75	LYS

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Mol	Chain	Res	Type
1	Q	89	ASP
1	Q	98	ILE
1	Q	102	ARG
1	Q	110	LYS
1	Q	153	PRO
1	Q	188	LYS
1	Q	206	GLU
1	Q	213	ILE
1	Q	228	ARG
1	Q	249	GLU
1	Q	253	LYS
2	Z	3	ILE
2	Z	19	LEU
2	Z	28	LEU
2	Z	29	LYS
2	Z	49	VAL
2	Z	60	LEU
2	Z	66	SER
2	Z	89	SER
2	Z	91	VAL
2	Z	93	LEU
2	Z	163	LEU
2	Z	199	ILE
2	Z	201	THR
2	Z	214	GLU
2	Z	224	LEU
2	Z	246	LYS
2	Z	255	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 (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	150	GLN
1	A	170	GLN
1	A	175	ASN
1	A	183	GLN
1	A	199	GLN
1	A	218	ASN

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Mol	Chain	Res	Type
1	A	250	GLN
2	B	44	GLN
2	B	124	GLN
2	B	249	GLN
2	B	252	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	150	GLN
1	E	170	GLN
1	E	175	ASN
1	E	183	GLN
1	E	199	GLN
1	E	256	GLN
2	F	173	ASN
2	F	249	GLN
2	F	252	GLN
2	F	273	GLN
2	F	317	GLN
1	Q	121	GLN
1	Q	139	ASN
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

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Mol	Chain	Res	Type
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 oligosaccharides 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	$\# Z > 2$
4	FAD	F	1319	-	58,58,58	2.35	15 (25%)	85,89,89	1.64	16 (18%)
3	AMP	A	1263	-	25,25,25	1.73	5 (20%)	37,38,38	2.71	15 (40%)
4	FAD	Z	1319	-	58,58,58	1.79	10 (17%)	85,89,89	1.76	18 (21%)
3	AMP	Q	1262	-	25,25,25	1.52	5 (20%)	37,38,38	2.56	13 (35%)
3	AMP	E	1262	-	25,25,25	1.59	5 (20%)	37,38,38	2.60	15 (40%)
4	FAD	B	1319	-	58,58,58	2.32	13 (22%)	85,89,89	1.71	19 (22%)
3	AMP	C	1262	-	25,25,25	1.38	4 (16%)	37,38,38	2.47	13 (35%)
4	FAD	D	1319	-	58,58,58	2.42	18 (31%)	85,89,89	2.03	25 (29%)

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
4	FAD	F	1319	-	-	4/34/50/50	0/6/6/6
3	AMP	A	1263	-	-	4/10/26/26	0/3/3/3
4	FAD	Z	1319	-	-	4/34/50/50	0/6/6/6
3	AMP	Q	1262	-	-	0/10/26/26	0/3/3/3
3	AMP	E	1262	-	-	2/10/26/26	0/3/3/3
4	FAD	B	1319	-	-	3/34/50/50	0/6/6/6
3	AMP	C	1262	-	-	5/10/26/26	0/3/3/3
4	FAD	D	1319	-	-	2/34/50/50	0/6/6/6

All (75) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1319	FAD	PA-O3P	-10.82	1.47	1.59
4	F	1319	FAD	PA-O3P	-9.67	1.49	1.59
4	D	1319	FAD	P-O3P	8.59	1.68	1.59
4	Z	1319	FAD	PA-O3P	-7.35	1.51	1.59
4	B	1319	FAD	C5'-C4'	6.73	1.61	1.51
4	F	1319	FAD	P-O3P	5.82	1.65	1.59
4	D	1319	FAD	C8A-N7A	5.52	1.42	1.31
4	D	1319	FAD	C4X-N5	4.96	1.41	1.30
4	D	1319	FAD	C5'-C4'	4.92	1.58	1.51
4	F	1319	FAD	C5'-C4'	4.83	1.58	1.51
4	F	1319	FAD	C2A-N1A	4.70	1.42	1.33
4	F	1319	FAD	C4X-N5	4.66	1.40	1.30
4	B	1319	FAD	C4X-N5	4.48	1.40	1.30
4	Z	1319	FAD	C8A-N7A	4.47	1.40	1.31
3	E	1262	AMP	C2-N3	4.42	1.41	1.33
4	D	1319	FAD	C2A-N1A	4.42	1.41	1.33
4	D	1319	FAD	C2A-N3A	4.42	1.41	1.33
4	F	1319	FAD	C8A-N7A	4.21	1.39	1.31
3	A	1263	AMP	P-O1P	4.16	1.63	1.50
4	B	1319	FAD	C8A-N7A	4.11	1.39	1.31
4	D	1319	FAD	C1'-C2'	3.92	1.58	1.52
3	A	1263	AMP	C2-N3	3.78	1.40	1.33
4	B	1319	FAD	C9-C8	3.76	1.44	1.39
4	D	1319	FAD	PA-O1A	3.75	1.63	1.50
4	Z	1319	FAD	C2A-N3A	3.75	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1319	FAD	C1'-C2'	3.70	1.57	1.52
4	Z	1319	FAD	C5'-C4'	3.66	1.56	1.51
4	D	1319	FAD	PA-O3P	-3.49	1.55	1.59
3	Q	1262	AMP	C2-N1	3.47	1.40	1.33
4	F	1319	FAD	C2-N1	3.46	1.44	1.36
4	Z	1319	FAD	C4X-N5	3.44	1.38	1.30
4	B	1319	FAD	C10-N1	3.32	1.39	1.33
3	E	1262	AMP	P-O1P	3.15	1.60	1.50
4	Z	1319	FAD	C2A-N1A	3.13	1.39	1.33
4	F	1319	FAD	C9-C8	3.12	1.43	1.39
4	D	1319	FAD	C1'-N10	3.10	1.55	1.47
4	F	1319	FAD	C2A-N3A	3.06	1.39	1.33
4	Z	1319	FAD	C1'-C2'	2.99	1.56	1.52
4	B	1319	FAD	PA-O1A	2.96	1.61	1.50
4	F	1319	FAD	PA-O1A	2.94	1.61	1.50
4	D	1319	FAD	C8M-C8	2.89	1.56	1.51
3	Q	1262	AMP	C5-N7	-2.89	1.33	1.39
3	A	1263	AMP	C5-N7	-2.87	1.33	1.39
4	D	1319	FAD	P-O1P	2.86	1.60	1.50
3	A	1263	AMP	C2-N1	2.82	1.38	1.33
3	Q	1262	AMP	P-O1P	2.72	1.58	1.50
4	F	1319	FAD	C10-N1	2.67	1.38	1.33
4	Z	1319	FAD	C10-N1	2.58	1.38	1.33
3	C	1262	AMP	C2-N1	2.57	1.38	1.33
4	F	1319	FAD	C4A-N3A	2.54	1.39	1.34
4	D	1319	FAD	C2-N1	2.50	1.42	1.36
4	B	1319	FAD	C2A-N1A	2.43	1.38	1.33
4	B	1319	FAD	O2'-C2'	2.42	1.48	1.43
3	C	1262	AMP	C2-N3	2.39	1.38	1.33
4	D	1319	FAD	C3B-C4B	2.39	1.59	1.53
3	C	1262	AMP	O4'-C4'	-2.35	1.39	1.45
4	Z	1319	FAD	C9A-C5X	-2.31	1.37	1.41
3	E	1262	AMP	C2-N1	2.30	1.38	1.33
4	D	1319	FAD	C5B-C4B	2.28	1.58	1.51
3	Q	1262	AMP	C4-N3	2.21	1.38	1.34
3	Q	1262	AMP	C2-N3	2.21	1.37	1.33
4	Z	1319	FAD	C4X-C10	-2.17	1.37	1.44
4	F	1319	FAD	P-O1P	2.17	1.58	1.50
4	B	1319	FAD	C2A-N3A	2.16	1.37	1.33
4	F	1319	FAD	C5A-C4A	2.15	1.42	1.39
4	F	1319	FAD	O2'-C2'	2.15	1.47	1.43
4	B	1319	FAD	P-O1P	2.14	1.58	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1319	FAD	C5A-C6A	-2.14	1.35	1.41
3	A	1263	AMP	O4'-C4'	-2.11	1.40	1.45
3	C	1262	AMP	P-O2P	-2.11	1.47	1.54
4	D	1319	FAD	O4-C4	2.08	1.27	1.23
3	E	1262	AMP	C5-N7	-2.07	1.35	1.39
4	D	1319	FAD	P-O5'	2.06	1.67	1.59
4	D	1319	FAD	C6A-N1A	2.06	1.41	1.35
3	E	1262	AMP	C8-N7	2.05	1.35	1.31

All (134) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	1262	AMP	N3-C2-N1	-9.29	114.52	128.58
3	A	1263	AMP	O4'-C1'-N9	-7.47	93.75	108.09
3	E	1262	AMP	N3-C2-N1	-7.00	117.99	128.58
3	C	1262	AMP	N3-C2-N1	-6.46	118.81	128.58
4	Z	1319	FAD	N3A-C2A-N1A	-6.31	119.03	128.58
3	A	1263	AMP	N9-C8-N7	-6.27	105.05	113.94
3	E	1262	AMP	C5-C4-N3	-5.96	118.52	126.72
3	C	1262	AMP	O2P-P-O1P	-5.93	87.74	110.83
4	D	1319	FAD	O2A-PA-O3P	5.86	123.11	107.27
4	B	1319	FAD	N3A-C2A-N1A	-5.67	120.00	128.58
4	D	1319	FAD	N3A-C2A-N1A	-5.38	120.44	128.58
4	D	1319	FAD	C4-N3-C2	-5.28	116.27	125.64
3	A	1263	AMP	C5-N7-C8	5.14	111.53	103.45
3	C	1262	AMP	C5-C4-N3	-5.09	119.71	126.72
4	B	1319	FAD	N9A-C8A-N7A	-4.97	106.89	113.94
4	D	1319	FAD	N9A-C8A-N7A	-4.94	106.92	113.94
3	E	1262	AMP	O5'-P-O1P	-4.92	93.16	106.44
3	C	1262	AMP	O2P-P-O5'	4.79	119.16	106.67
4	F	1319	FAD	C4-N3-C2	-4.76	117.19	125.64
3	Q	1262	AMP	C2-N3-C4	4.69	123.29	111.83
3	E	1262	AMP	O4'-C1'-N9	-4.66	99.15	108.09
3	E	1262	AMP	C2-N3-C4	4.49	122.80	111.83
4	Z	1319	FAD	C5A-C4A-N3A	-4.41	120.65	126.72
3	A	1263	AMP	C4-N9-C8	4.34	110.29	105.74
4	D	1319	FAD	C5'-C4'-C3'	-4.26	104.19	112.22
3	Q	1262	AMP	O2P-P-O5'	4.23	117.69	106.67
3	C	1262	AMP	C2-N3-C4	4.21	122.11	111.83
3	A	1263	AMP	O5'-C5'-C4'	4.07	122.87	108.99
4	F	1319	FAD	C9A-C5X-N5	-4.05	118.15	122.45
4	Z	1319	FAD	C2A-N3A-C4A	4.00	121.60	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	1262	AMP	C5-C4-N3	-3.90	121.34	126.72
4	F	1319	FAD	C5'-C4'-C3'	-3.86	104.94	112.22
3	A	1263	AMP	O2P-P-O5'	3.84	116.68	106.67
3	E	1262	AMP	N3-C4-N9	3.81	133.65	127.17
3	A	1263	AMP	C5-C4-N3	-3.81	121.48	126.72
3	E	1262	AMP	O3P-P-O5'	3.75	116.44	106.67
3	Q	1262	AMP	N3-C4-N9	3.72	133.50	127.17
4	F	1319	FAD	C4X-C4-N3	3.71	122.71	113.25
4	D	1319	FAD	C5A-C4A-N3A	-3.71	121.61	126.72
3	Q	1262	AMP	N9-C8-N7	-3.69	108.70	113.94
3	Q	1262	AMP	O5'-P-O1P	-3.56	96.83	106.44
4	D	1319	FAD	C4A-N9A-C8A	3.53	109.44	105.74
3	C	1262	AMP	N3-C4-N9	3.50	133.12	127.17
4	F	1319	FAD	C5X-C9A-N10	3.50	121.13	117.97
4	Z	1319	FAD	N9A-C8A-N7A	-3.49	108.99	113.94
4	Z	1319	FAD	C10-C4X-N5	-3.43	117.81	124.81
4	D	1319	FAD	O3P-PA-O1A	-3.41	100.45	110.70
4	F	1319	FAD	O4-C4-C4X	-3.41	117.54	126.53
3	C	1262	AMP	N9-C8-N7	-3.40	109.11	113.94
4	B	1319	FAD	C5X-C9A-N10	3.38	121.02	117.97
4	B	1319	FAD	O3P-PA-O1A	-3.37	100.56	110.70
4	D	1319	FAD	C5A-C6A-N6A	-3.35	115.00	123.29
4	B	1319	FAD	C5A-C4A-N3A	-3.27	122.22	126.72
4	Z	1319	FAD	C9A-C5X-N5	-3.26	119.00	122.45
4	Z	1319	FAD	O3P-P-O1P	-3.25	100.94	110.70
4	B	1319	FAD	C4-N3-C2	-3.25	119.88	125.64
3	A	1263	AMP	C4-C5-N7	-3.23	106.89	110.58
3	C	1262	AMP	C5-N7-C8	3.22	108.51	103.45
4	Z	1319	FAD	O2P-P-O3P	3.19	115.89	107.27
4	D	1319	FAD	C2A-N3A-C4A	3.16	119.54	111.83
3	Q	1262	AMP	C2'-C3'-C4'	-3.13	96.57	102.61
4	Z	1319	FAD	C4-N3-C2	-3.10	120.14	125.64
4	Z	1319	FAD	C4-C4X-N5	3.06	122.43	118.21
3	C	1262	AMP	O3P-P-O2P	3.06	119.26	107.80
4	B	1319	FAD	C5A-N7A-C8A	3.05	108.24	103.45
3	E	1262	AMP	N9-C8-N7	-3.04	109.62	113.94
4	D	1319	FAD	C4X-C4-N3	3.02	120.94	113.25
3	A	1263	AMP	N3-C4-N9	3.01	132.29	127.17
4	B	1319	FAD	C2A-N3A-C4A	2.94	119.02	111.83
4	D	1319	FAD	C4X-C10-N10	2.92	120.66	116.48
4	F	1319	FAD	N9A-C8A-N7A	-2.90	109.82	113.94
4	Z	1319	FAD	C5X-N5-C4X	2.86	122.71	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	1262	AMP	O3P-P-O5'	2.83	114.05	106.67
3	E	1262	AMP	C5-N7-C8	2.80	107.86	103.45
4	D	1319	FAD	C9-C8-C7	-2.77	115.62	119.69
3	A	1263	AMP	N3-C2-N1	-2.77	124.39	128.58
4	D	1319	FAD	C5A-N7A-C8A	2.75	107.77	103.45
4	B	1319	FAD	C4X-C4-N3	2.71	120.15	113.25
3	Q	1262	AMP	C5-C6-N6	-2.71	116.58	123.29
3	Q	1262	AMP	C5-N7-C8	2.68	107.67	103.45
4	F	1319	FAD	O4B-C4B-C3B	2.66	110.44	105.15
4	F	1319	FAD	C5A-N7A-C8A	2.65	107.61	103.45
4	B	1319	FAD	C5'-C4'-C3'	-2.62	107.28	112.22
4	D	1319	FAD	O2B-C2B-C1B	-2.62	101.10	110.10
4	B	1319	FAD	O4'-C4'-C5'	2.61	115.75	109.99
3	E	1262	AMP	O4'-C4'-C3'	-2.59	100.02	105.15
4	F	1319	FAD	C4A-C5A-N7A	-2.57	107.65	110.58
4	B	1319	FAD	C9-C8-C7	-2.55	115.95	119.69
4	Z	1319	FAD	C4X-C10-N10	2.54	120.11	116.48
4	D	1319	FAD	C10-C4X-N5	-2.53	119.65	124.81
4	B	1319	FAD	C5A-C6A-N6A	-2.52	117.05	123.29
4	Z	1319	FAD	N3A-C4A-N9A	2.50	131.41	127.17
3	A	1263	AMP	O3P-P-O5'	-2.49	100.17	106.67
3	A	1263	AMP	C2'-C3'-C4'	-2.49	97.80	102.61
4	F	1319	FAD	C5A-C4A-N3A	-2.49	123.29	126.72
4	B	1319	FAD	C4A-N9A-C8A	2.47	108.33	105.74
4	Z	1319	FAD	C4X-C4-N3	2.47	119.53	113.25
4	F	1319	FAD	C4B-O4B-C1B	-2.45	104.05	109.47
3	A	1263	AMP	C5-C6-N6	-2.44	117.24	123.29
3	A	1263	AMP	C6-C5-C4	2.43	120.49	117.18
4	D	1319	FAD	O4-C4-C4X	-2.42	120.14	126.53
3	E	1262	AMP	C5-C6-N1	2.39	123.57	117.51
4	B	1319	FAD	C9A-C9-C8	2.38	124.01	119.22
4	D	1319	FAD	O4'-C4'-C5'	2.36	115.20	109.99
4	F	1319	FAD	C9-C8-C7	-2.33	116.26	119.69
4	D	1319	FAD	N3A-C4A-N9A	2.32	131.12	127.17
4	Z	1319	FAD	C5'-C4'-C3'	-2.30	107.88	112.22
3	C	1262	AMP	O2'-C2'-C1'	-2.29	102.22	110.10
3	A	1263	AMP	C5'-C4'-C3'	2.29	123.45	115.21
3	C	1262	AMP	O3P-P-O5'	2.27	112.60	106.67
3	E	1262	AMP	O3P-P-O1P	2.25	119.58	110.83
3	C	1262	AMP	O5'-P-O1P	-2.23	100.41	106.44
4	F	1319	FAD	O2-C2-N3	-2.18	114.41	118.58
4	Z	1319	FAD	O3P-PA-O1A	2.17	117.25	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1319	FAD	O5B-C5B-C4B	-2.17	101.61	108.99
4	Z	1319	FAD	C5A-N7A-C8A	2.16	106.84	103.45
4	B	1319	FAD	C7M-C7-C6	-2.16	115.77	119.57
4	Z	1319	FAD	O2A-PA-O3P	-2.16	101.44	107.27
4	D	1319	FAD	O3P-P-O1P	2.16	117.19	110.70
3	E	1262	AMP	O2P-P-O5'	2.15	112.27	106.67
3	E	1262	AMP	C4-C5-N7	-2.11	108.17	110.58
3	C	1262	AMP	C4-C5-N7	-2.11	108.17	110.58
3	Q	1262	AMP	C4'-O4'-C1'	-2.10	104.83	109.47
3	Q	1262	AMP	C2-N1-C6	2.10	122.17	118.73
4	B	1319	FAD	C1'-C2'-C3'	2.09	115.33	109.66
4	F	1319	FAD	O3P-PA-O1A	-2.07	104.48	110.70
4	D	1319	FAD	C6-C5X-N5	2.06	121.87	118.44
4	D	1319	FAD	N6A-C6A-N1A	2.06	122.96	118.38
4	F	1319	FAD	C4A-N9A-C8A	2.04	107.88	105.74
4	D	1319	FAD	C9A-C9-C8	2.04	123.33	119.22
4	B	1319	FAD	C4X-C10-N10	2.03	119.39	116.48
3	E	1262	AMP	C5'-C4'-C3'	2.02	122.48	115.21
4	D	1319	FAD	C9A-C5X-N5	-2.01	120.33	122.45
4	B	1319	FAD	C3B-C2B-C1B	2.00	105.25	101.46

There are no chirality outliers.

All (24) 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'
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	Z	1319	FAD	C2'-C3'-C4'-O4'
4	F	1319	FAD	PA-O3P-P-O1P

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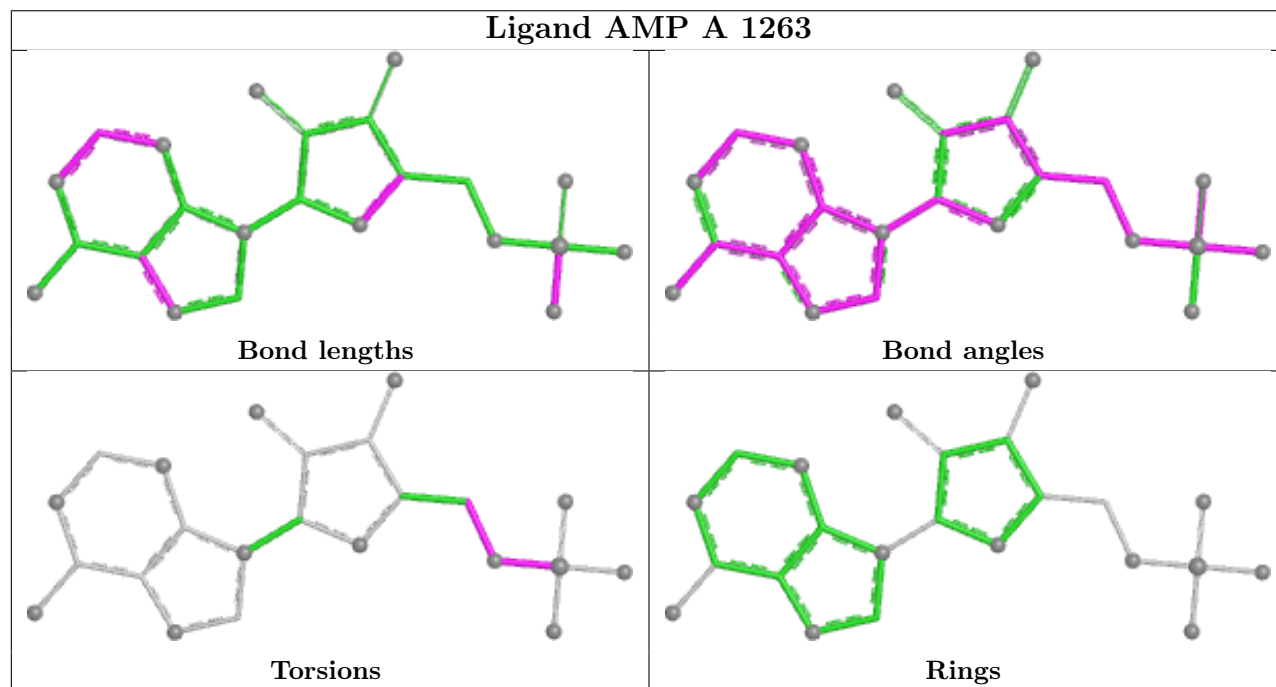
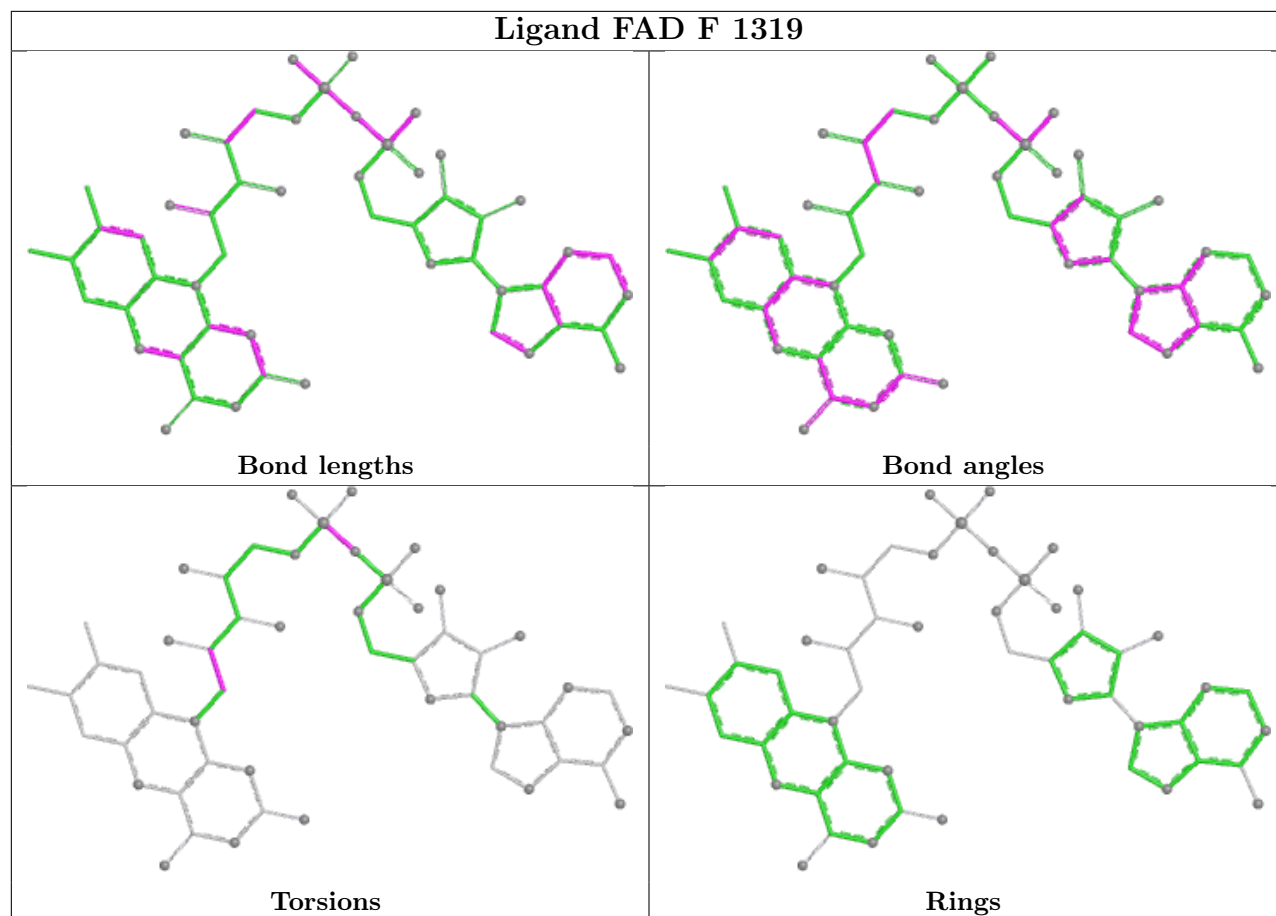
Mol	Chain	Res	Type	Atoms
3	C	1262	AMP	C4'-C5'-O5'-P
4	B	1319	FAD	PA-O3P-P-O2P
4	F	1319	FAD	PA-O3P-P-O2P
4	B	1319	FAD	N10-C1'-C2'-O2'
4	F	1319	FAD	N10-C1'-C2'-O2'
4	F	1319	FAD	N10-C1'-C2'-C3'
4	Z	1319	FAD	N10-C1'-C2'-O2'

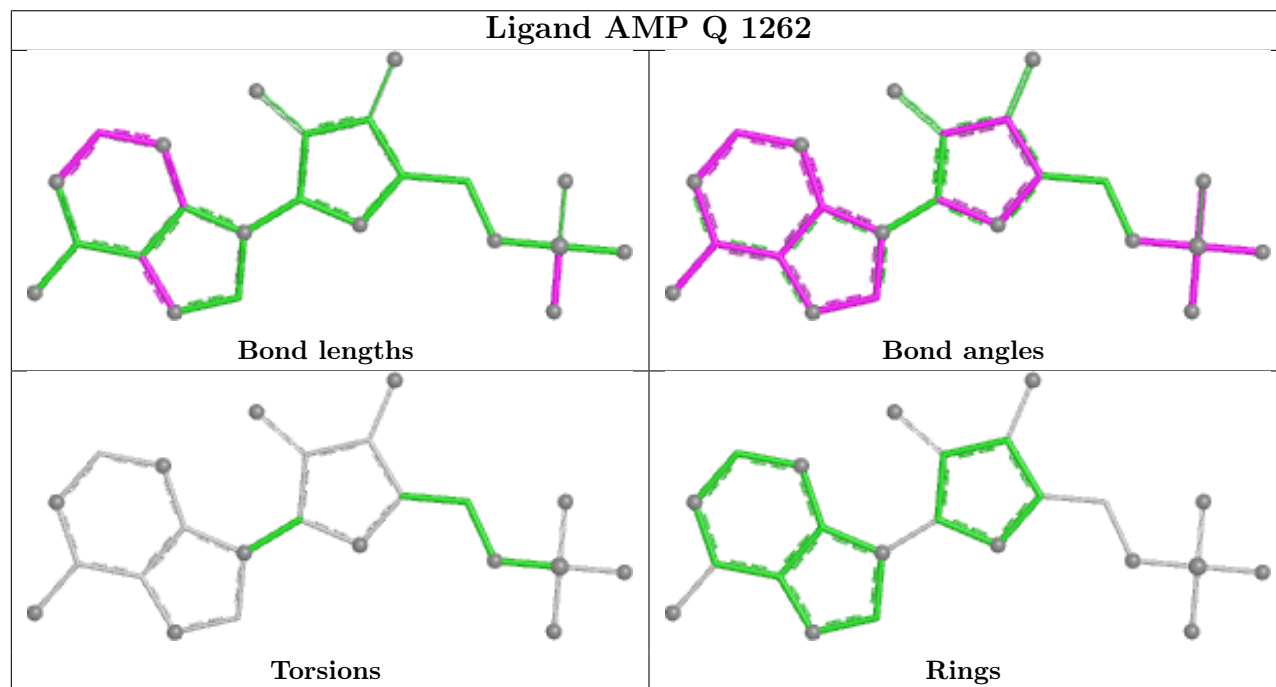
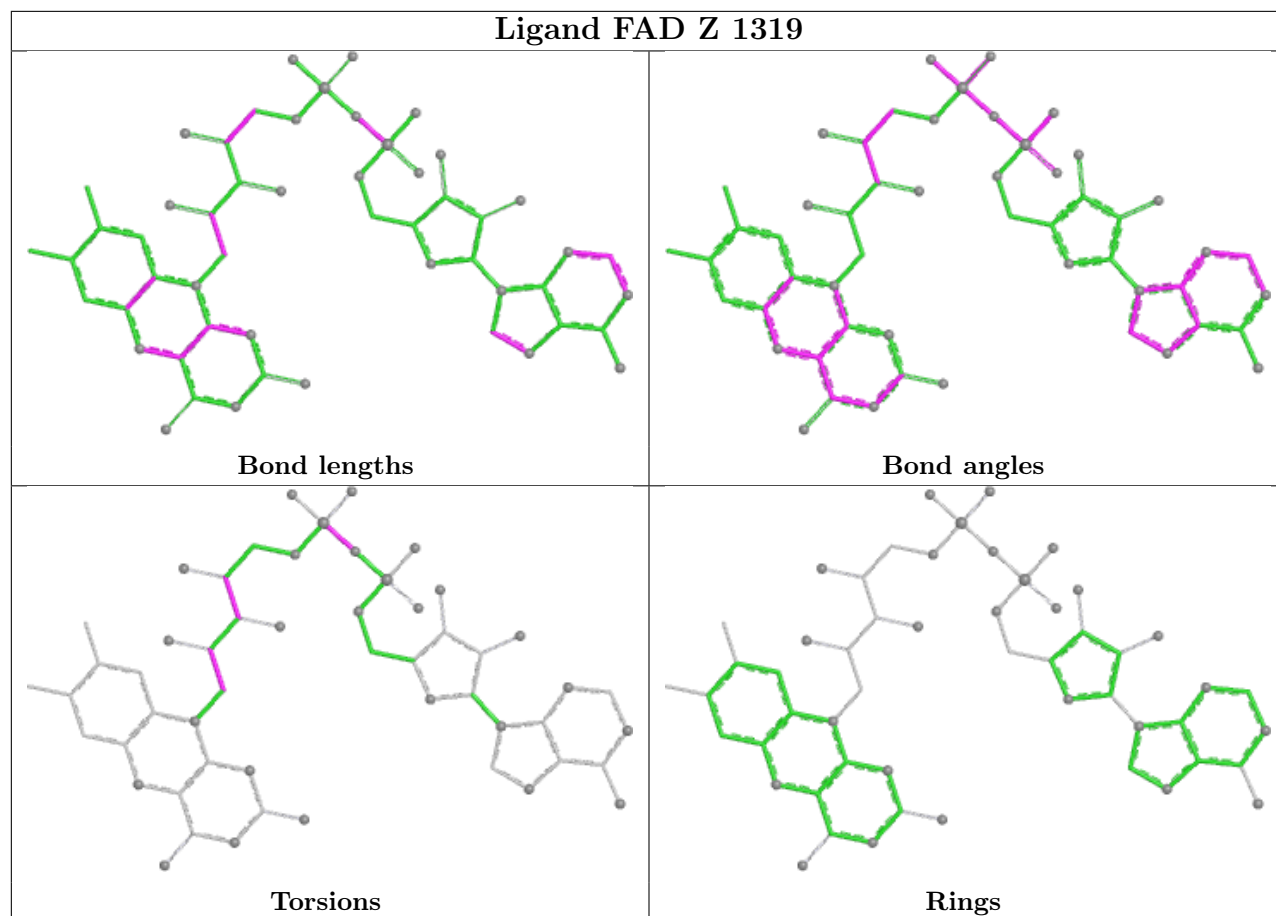
There are no ring outliers.

5 monomers are involved in 15 short contacts:

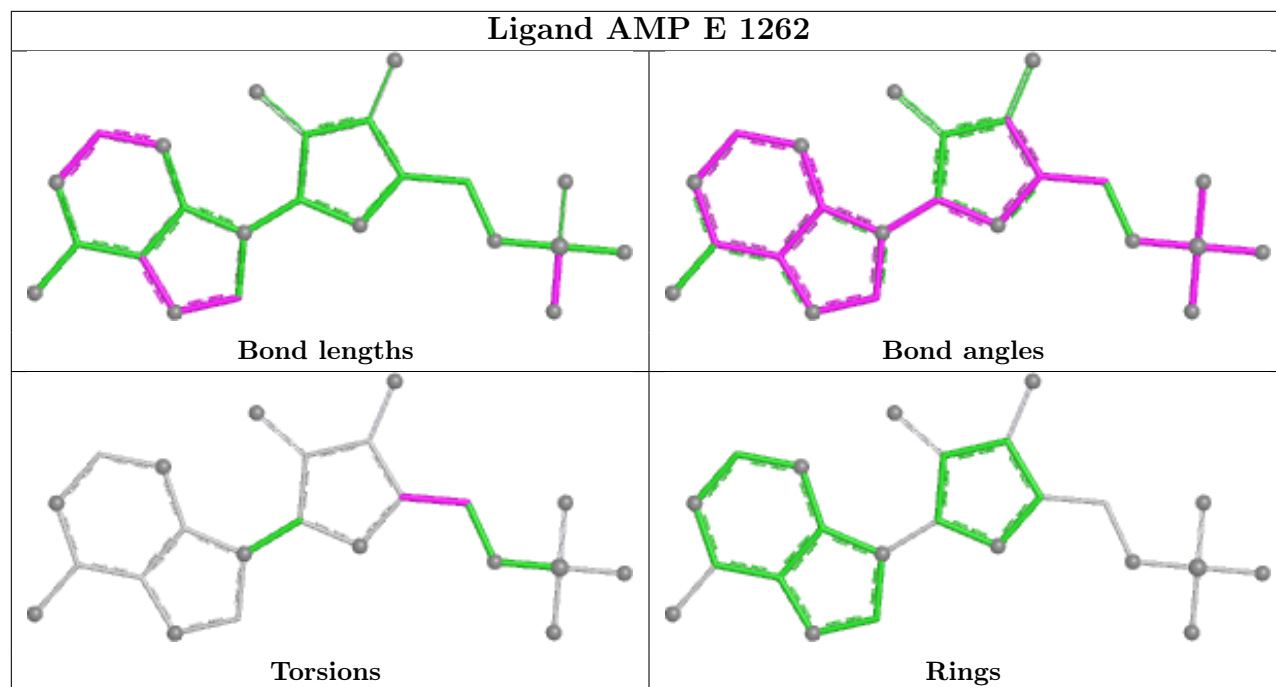
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	Q	1262	AMP	2	0
3	E	1262	AMP	2	0
4	B	1319	FAD	1	0
3	C	1262	AMP	2	0
4	D	1319	FAD	8	0

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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

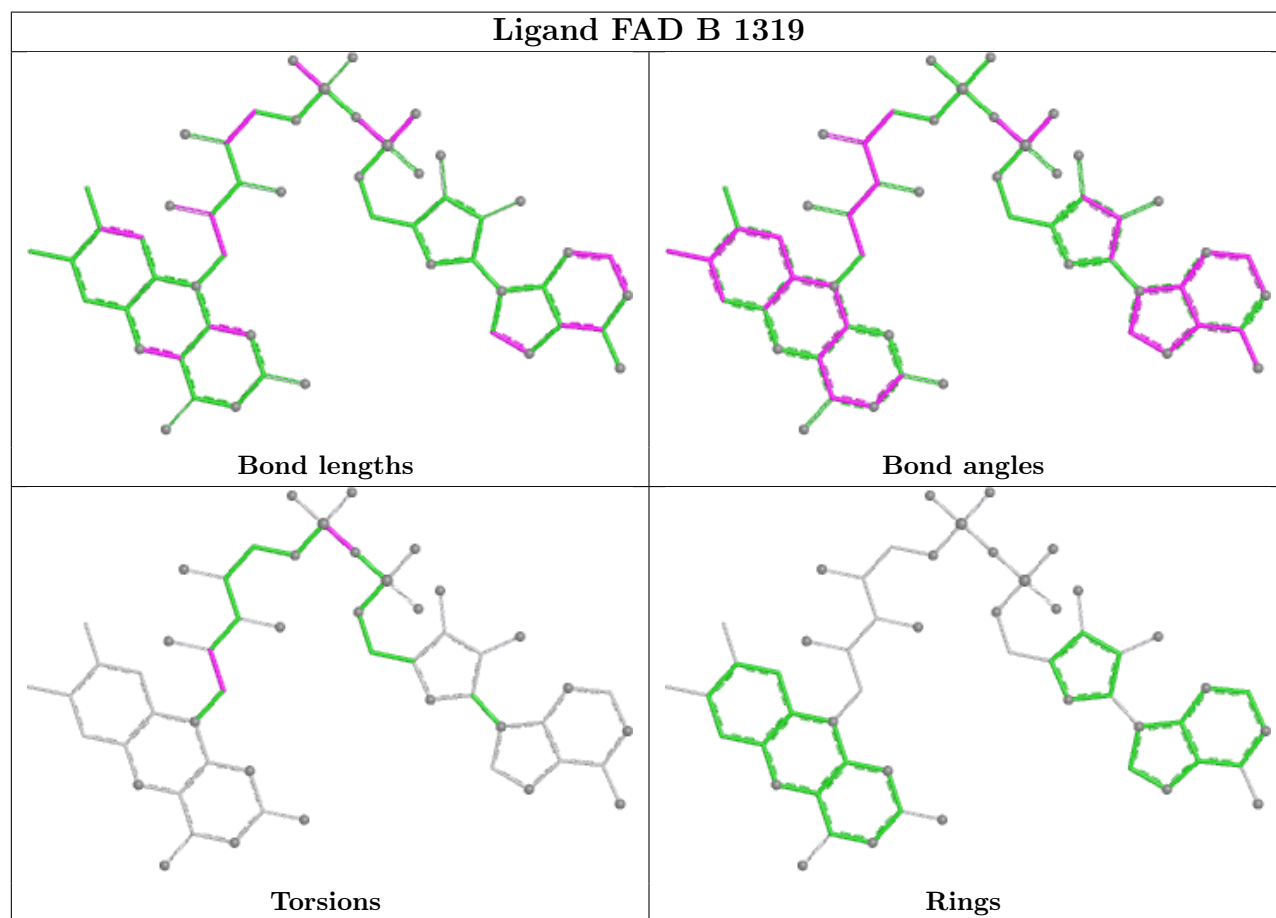


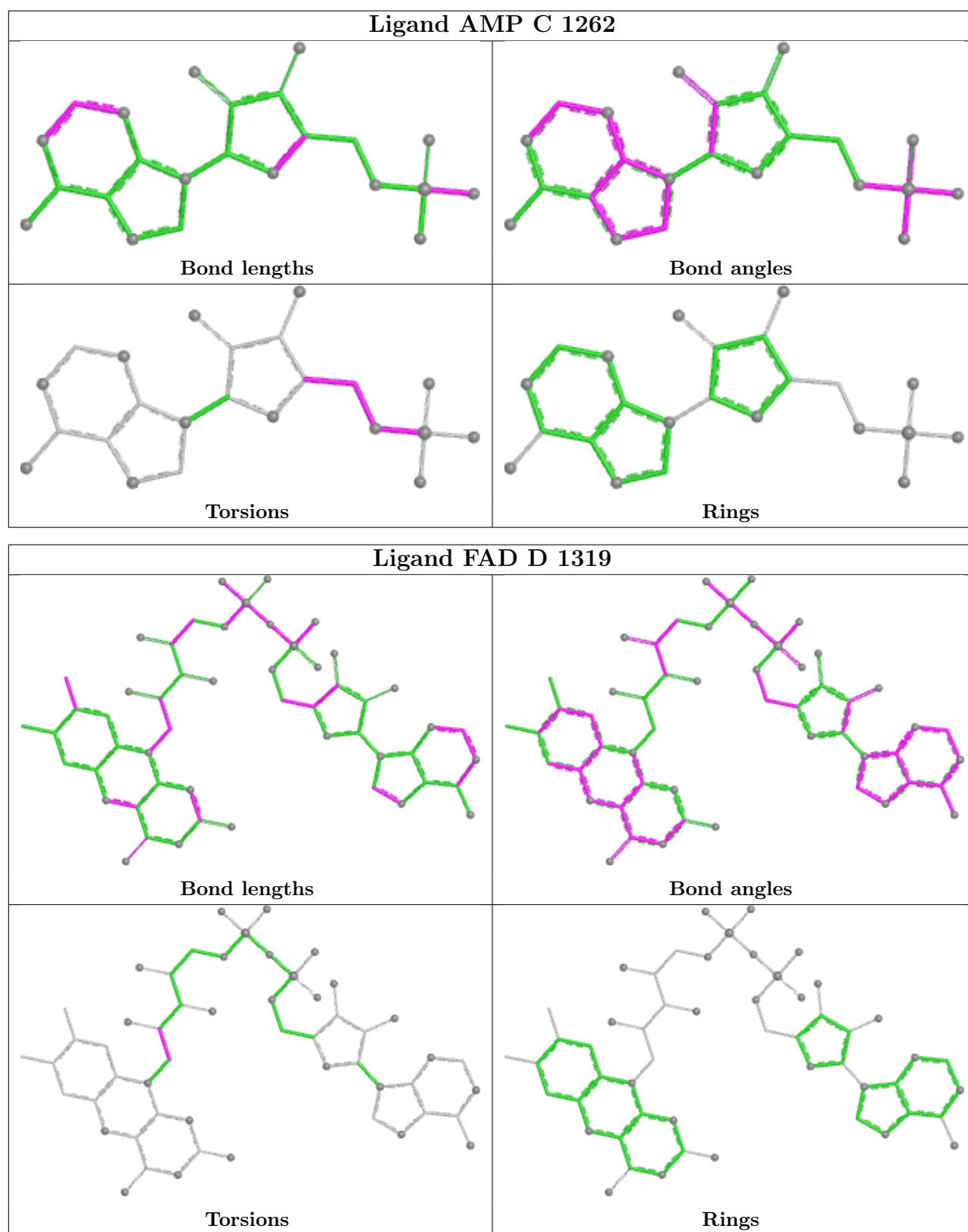


Ligand AMP E 1262



Ligand FAD B 1319





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	261/264 (98%)	-0.56	2 (0%) 82 65	20, 43, 65, 83	0
1	C	260/264 (98%)	-0.35	4 (1%) 72 52	29, 52, 90, 112	0
1	E	260/264 (98%)	-0.42	3 (1%) 76 58	27, 52, 77, 88	0
1	Q	246/264 (93%)	0.45	22 (8%) 15 8	37, 73, 93, 102	27 (10%)
2	B	314/320 (98%)	-0.56	4 (1%) 75 56	25, 47, 68, 86	0
2	D	314/320 (98%)	-0.38	7 (2%) 62 41	2, 50, 83, 98	0
2	F	314/320 (98%)	-0.48	4 (1%) 75 56	31, 49, 70, 88	0
2	Z	312/320 (97%)	0.77	36 (11%) 9 5	23, 73, 95, 114	123 (39%)
All	All	2281/2336 (97%)	-0.19	82 (3%) 46 26	2, 51, 86, 114	150 (6%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	236	GLU	8.0
1	Q	235	PRO	7.5
1	Q	259	ASN	6.6
2	D	196	ASP	5.7
2	D	198	ASP	5.5
1	Q	260	GLU	4.5
2	Z	196	ASP	4.5
1	Q	237	LYS	4.2
2	Z	218	VAL	4.0
2	Z	227	GLU	4.0
1	Q	248	SER	3.9
1	A	28	GLU	3.8
1	Q	16	ASP	3.8
2	B	126	ASP	3.8
2	Z	202	VAL	3.7
2	Z	179	VAL	3.6

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Mol	Chain	Res	Type	RSRZ
1	Q	241	THR	3.5
1	Q	227	SER	3.5
1	Q	246	THR	3.5
2	Z	199	ILE	3.4
1	Q	238	GLY	3.4
2	D	197	ILE	3.4
1	C	249	GLU	3.4
2	Z	247	SER	3.2
2	F	309	ASP	3.2
2	Z	197	ILE	3.2
2	Z	216	THR	3.1
2	Z	198	ASP	3.1
2	Z	201	THR	3.1
2	Z	318	LEU	3.1
2	D	219	GLU	3.0
1	Q	245	GLY	3.0
2	B	312	GLU	3.0
2	D	309	ASP	2.9
2	B	125	GLY	2.9
2	Z	259	SER	2.9
1	Q	255	ILE	2.9
2	Z	252	GLN	2.8
1	Q	242	MET	2.8
1	Q	247	ILE	2.8
2	Z	282	PRO	2.7
2	Z	219	GLU	2.7
2	Z	300	LYS	2.7
2	Z	215	GLU	2.7
2	Z	241	ALA	2.7
1	C	28	GLU	2.6
1	E	22	ASP	2.6
1	Q	261	PHE	2.6
2	Z	214	GLU	2.6
2	Z	316	ALA	2.5
2	F	126	ASP	2.5
2	Z	273	GLN	2.5
2	D	191	VAL	2.5
1	E	24	MET	2.4
2	Z	231	THR	2.4
1	Q	90	ASP	2.4
1	Q	258	ILE	2.3
2	Z	279	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
2	Z	308	PHE	2.3
2	D	111	GLY	2.3
1	A	22	ASP	2.3
1	C	244	GLU	2.3
2	Z	314	LEU	2.2
1	C	93	GLU	2.2
2	Z	245	PRO	2.2
2	Z	243	TRP	2.2
2	Z	200	THR	2.2
2	Z	187	ASP	2.2
1	Q	239	ARG	2.2
1	Q	22	ASP	2.1
1	E	195	ARG	2.1
2	Z	276	ALA	2.1
2	Z	305	ALA	2.1
2	Z	288	ASN	2.1
1	Q	71	GLU	2.1
2	Z	291	PRO	2.0
2	F	191	VAL	2.0
2	Z	222	ARG	2.0
2	B	309	ASP	2.0
2	F	196	ASP	2.0
1	Q	204	PRO	2.0
2	Z	315	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

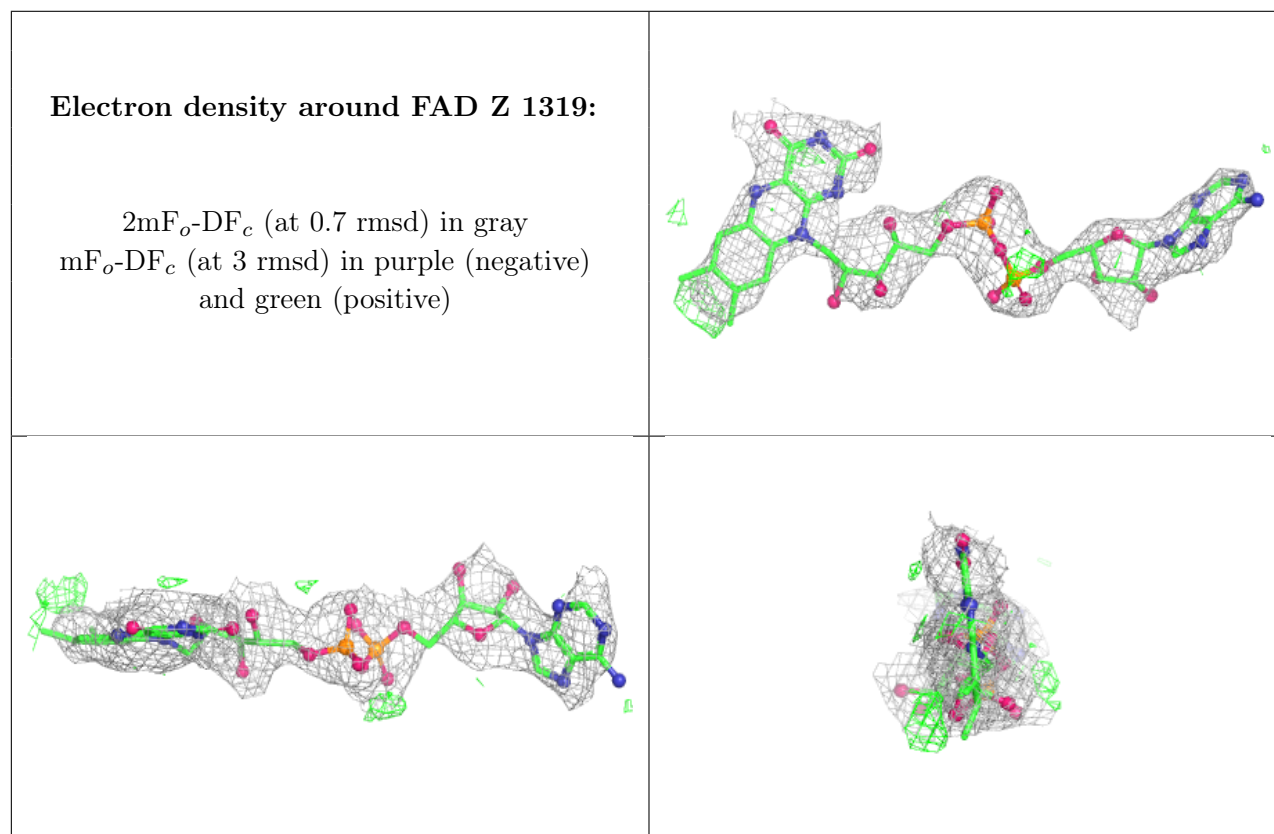
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

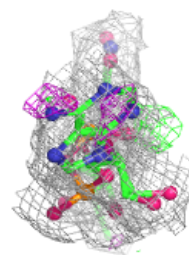
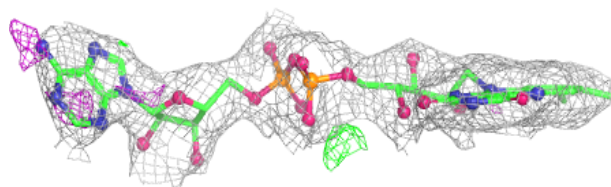
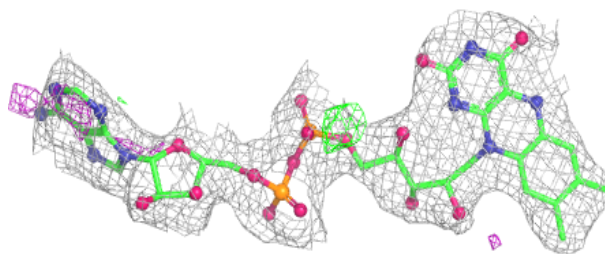
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	FAD	Z	1319	53/53	0.85	0.12	17,28,36,42	53
4	FAD	D	1319	53/53	0.94	0.08	21,28,38,42	0
3	AMP	Q	1262	23/23	0.94	0.07	57,62,69,74	0
4	FAD	B	1319	53/53	0.97	0.07	17,24,31,33	0
3	AMP	E	1262	23/23	0.97	0.06	25,33,38,39	0
4	FAD	F	1319	53/53	0.97	0.07	17,24,29,35	0
3	AMP	A	1263	23/23	0.97	0.05	23,28,34,37	0
3	AMP	C	1262	23/23	0.99	0.05	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.



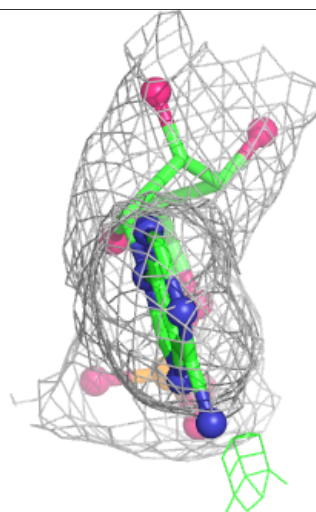
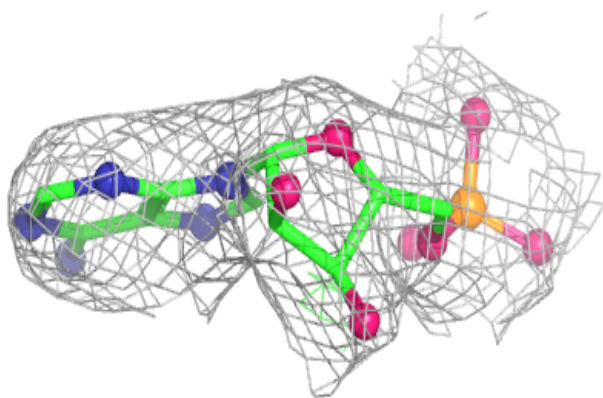
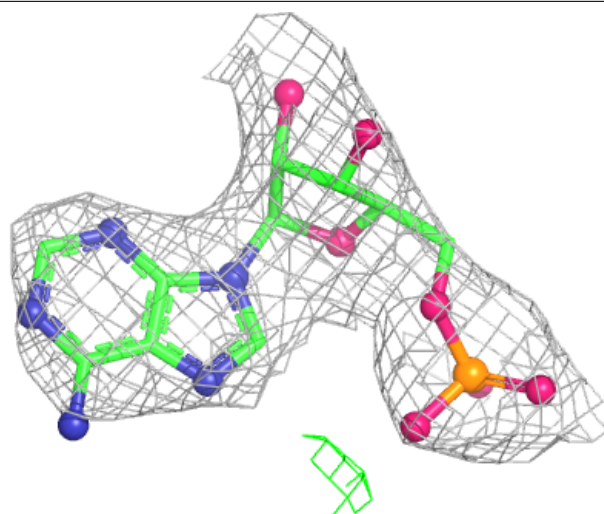
Electron density around FAD D 1319:

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



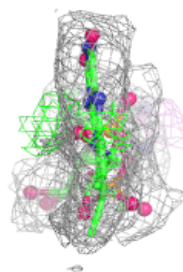
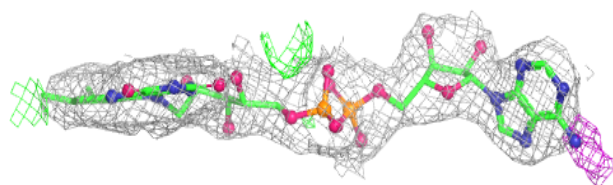
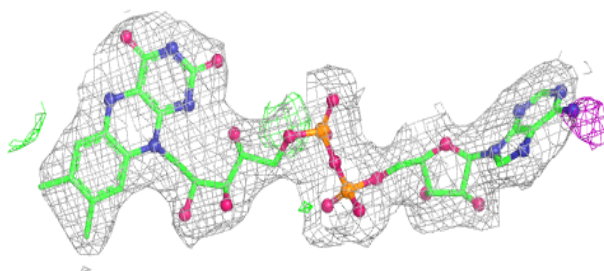
Electron density around AMP Q 1262:

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

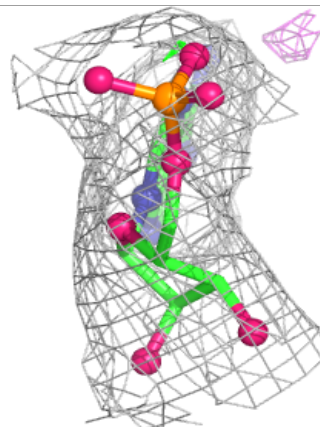
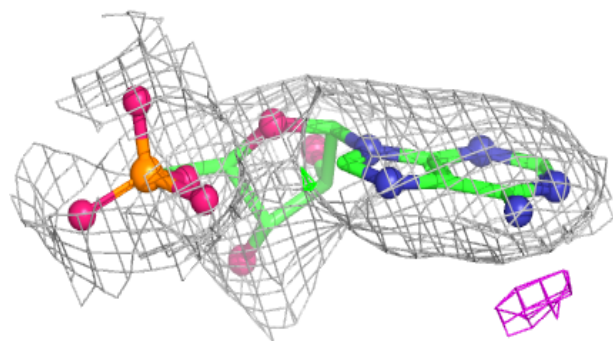
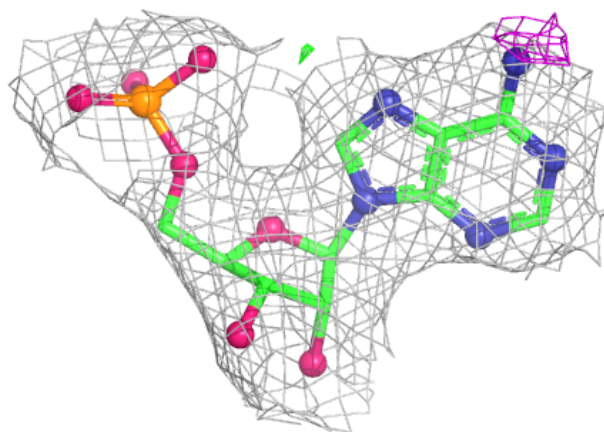


Electron density around FAD B 1319:

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

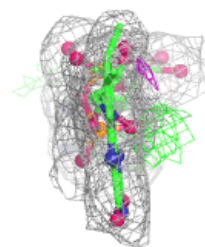
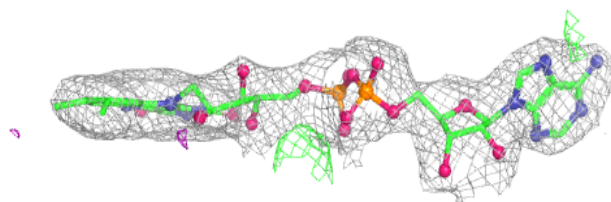
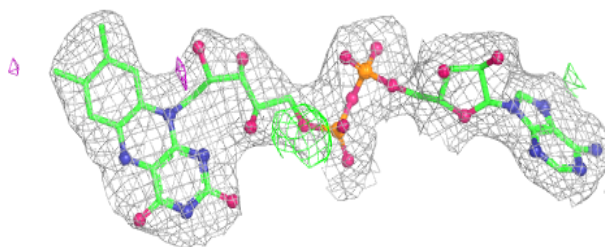
**Electron density around AMP E 1262:**

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



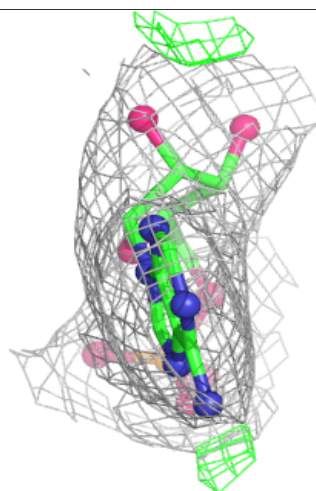
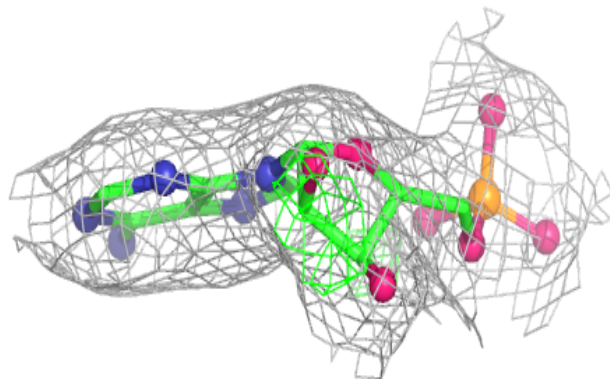
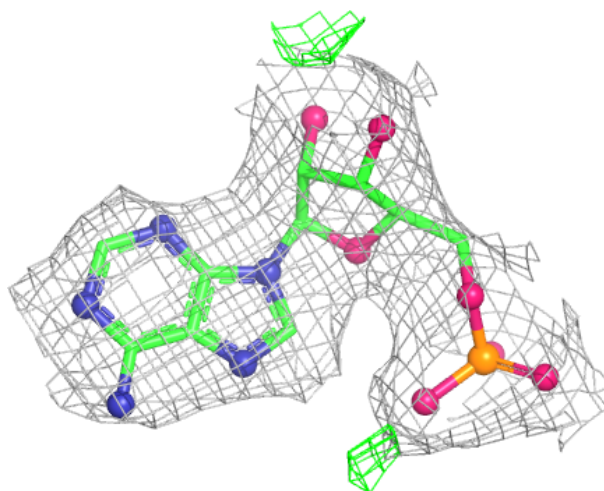
Electron density around FAD F 1319:

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



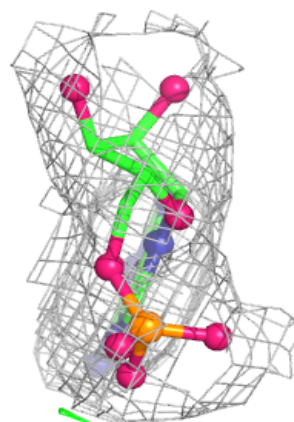
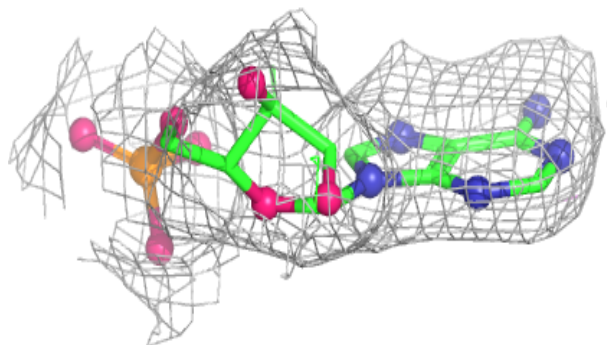
Electron density around AMP A 1263:

$2mF_o-DF_c$ (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 [i](#)

There are no such residues in this entry.