



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:17 AM UTC

PDB ID : 1H7W / pdb_00001h7w
Title : Dihydropyrimidine dehydrogenase (DPD) from pig
Authors : Dobritsch, D.; Schneider, G.; Schnackerz, K.D.; Lindqvist, Y.
Deposited on : 2001-01-19
Resolution : 1.90 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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

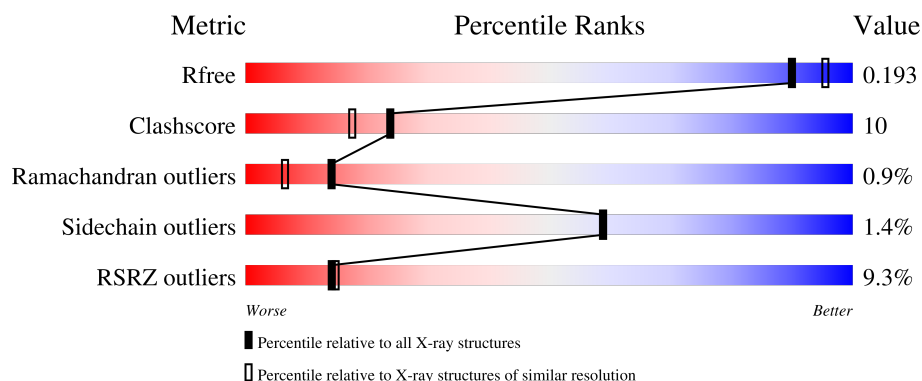
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7789 (1.90-1.90)
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1025	8% 78% 19% ..
1	B	1025	8% 81% 17% ..
1	C	1025	10% 78% 19% ..
1	D	1025	10% 80% 18% ..

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 36125 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.

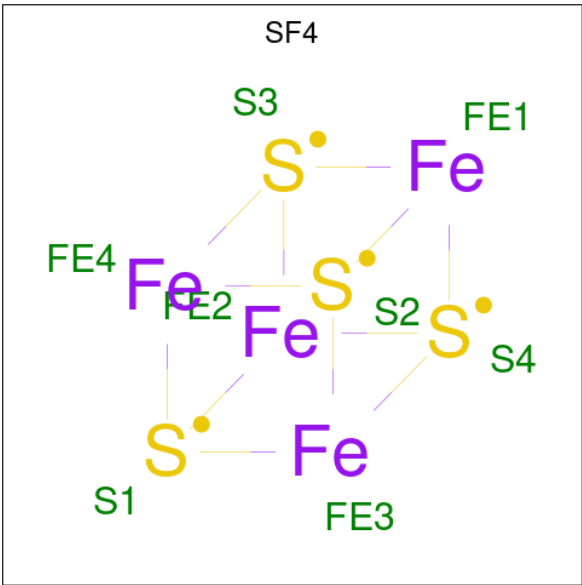
- Molecule 1 is a protein called DIHYDROPYRIMIDINE DEHYDROGENASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1016	Total	C	N	O	S	66	0	0
			7750	4913	1314	1467	56			
1	B	1017	Total	C	N	O	S	70	0	0
			7757	4918	1315	1468	56			
1	C	1016	Total	C	N	O	S	28	0	0
			7750	4913	1314	1467	56			
1	D	1018	Total	C	N	O	S	43	0	0
			7765	4924	1316	1469	56			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	ASP	GLY	conflict	UNP Q28943
B	60	ASP	GLY	conflict	UNP Q28943
C	60	ASP	GLY	conflict	UNP Q28943
D	60	ASP	GLY	conflict	UNP Q28943

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



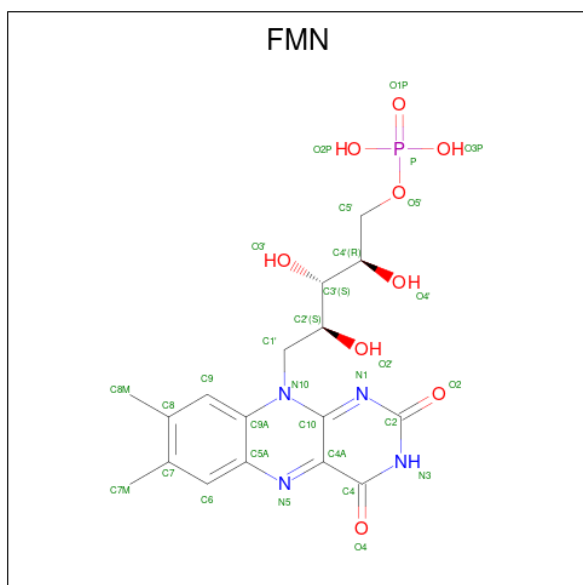
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		
2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

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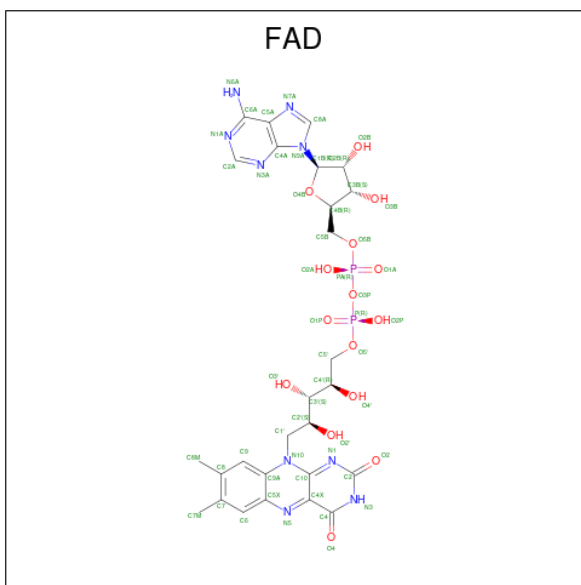
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	Fe	S	0	0
			8	4	4		
2	D	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	B	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	C	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	D	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

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



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

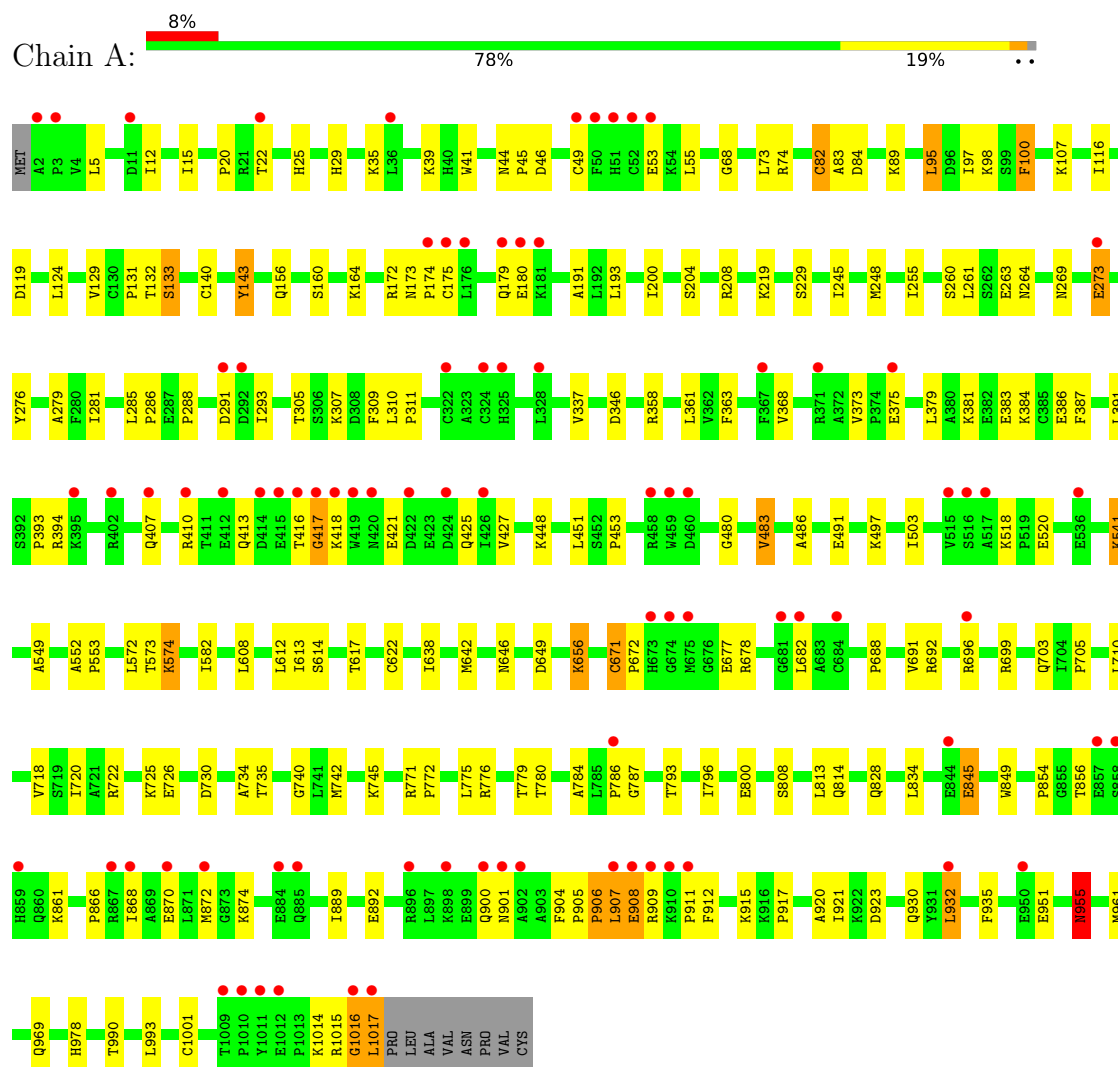
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1148	Total O 1148 1148	0	0
5	B	1125	Total O 1125 1125	0	0
5	C	1176	Total O 1176 1176	0	0
5	D	1190	Total O 1190 1190	0	0

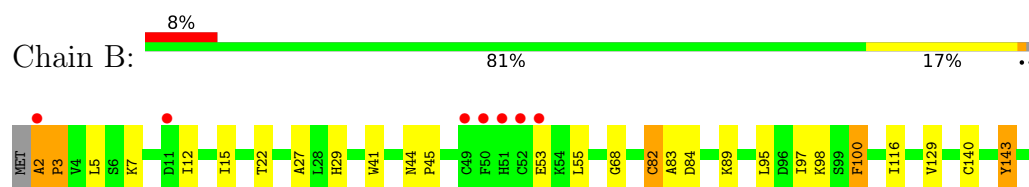
3 Residue-property plots

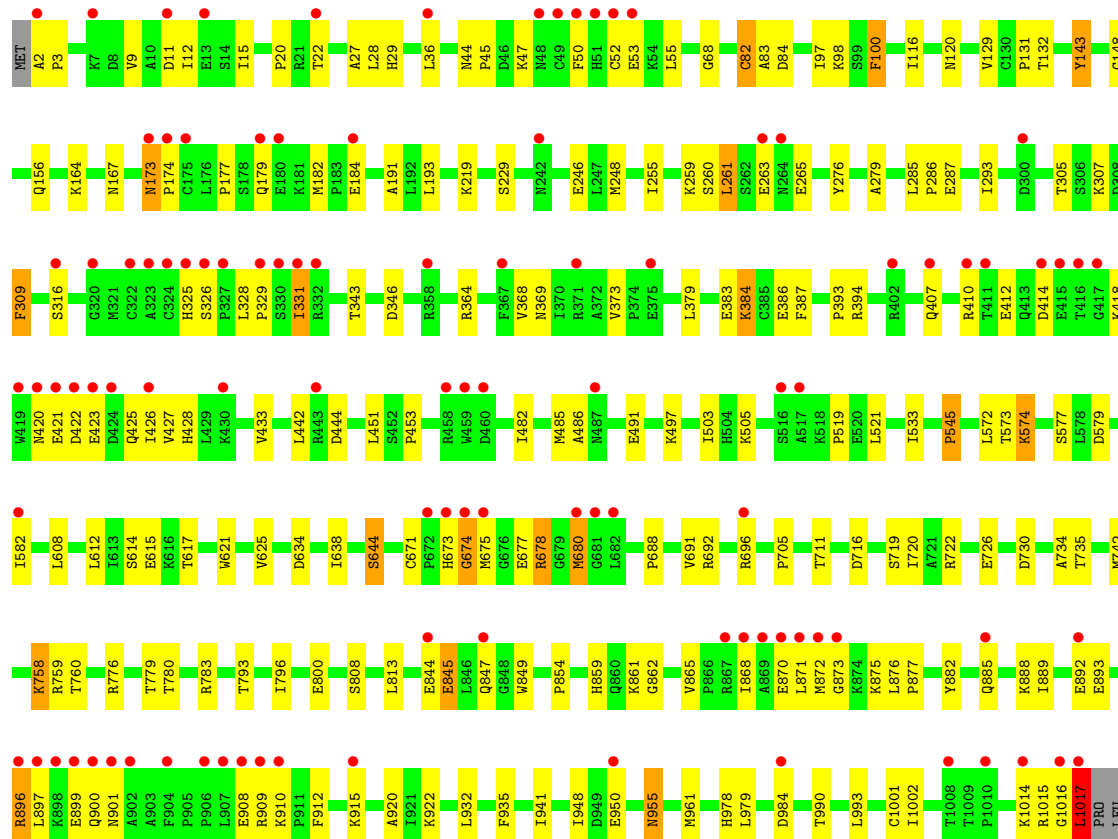
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DIHYDROPYRIMIDINE DEHYDROGENASE



• Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

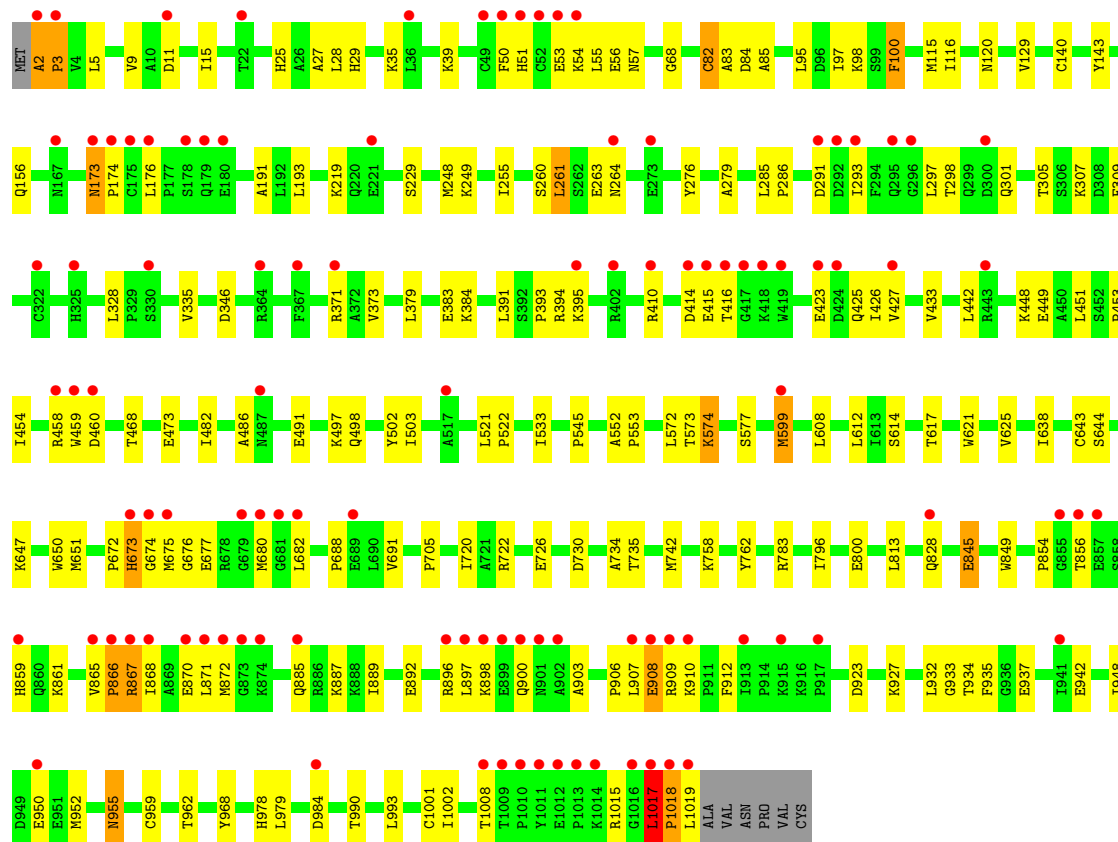




ALA
VAL
ASN
PRO
VAL
CYS

● Molecule 1: DIHYDROPYRIMIDINE DEHYDROGENASE

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.95Å 159.29Å 163.57Å 90.00° 96.04° 90.00°	Depositor
Resolution (Å)	19.97 – 1.90 19.97 – 1.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.97-1.90) 99.0 (19.97-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.83 (at 1.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.174 , 0.196 0.171 , 0.193	Depositor DCC
R_{free} test set	6485 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	12.7	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	36125	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.93% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: FMN, FAD, SF4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.40	0/7911	0.93	24/10721 (0.2%)
1	B	0.39	1/7919 (0.0%)	0.91	25/10733 (0.2%)
1	C	0.40	1/7911 (0.0%)	0.93	36/10721 (0.3%)
1	D	0.41	1/7927 (0.0%)	0.93	32/10744 (0.3%)
All	All	0.40	3/31668 (0.0%)	0.92	117/42919 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1017	LEU	C-O	-6.93	1.15	1.24
1	B	1017	LEU	C-O	-5.89	1.16	1.24
1	C	1017	LEU	CA-C	-5.24	1.42	1.52

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	905	PRO	N-CA-C	12.18	125.56	110.70
1	C	305	THR	N-CA-C	-8.44	97.33	110.42
1	D	305	THR	N-CA-C	-8.24	97.65	110.42
1	B	305	THR	N-CA-C	-8.15	97.79	110.42
1	D	955	ASN	N-CA-C	7.97	122.42	111.90
1	A	305	THR	N-CA-C	-7.90	98.18	110.42
1	A	955	ASN	N-CA-C	7.70	122.07	111.90
1	A	309	PHE	N-CA-C	7.65	119.31	110.97
1	B	955	ASN	N-CA-C	7.64	121.98	111.90
1	C	955	ASN	N-CA-C	7.59	121.92	111.90
1	B	309	PHE	N-CA-C	7.58	119.45	111.03
1	D	574	LYS	N-CA-C	-7.54	99.87	110.50
1	C	574	LYS	N-CA-C	-7.50	99.92	110.50
1	C	309	PHE	N-CA-C	7.48	119.12	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	85	ALA	N-CA-C	7.38	118.65	109.57
1	D	309	PHE	N-CA-C	7.31	118.93	110.97
1	A	574	LYS	N-CA-C	-7.30	100.20	110.50
1	B	574	LYS	N-CA-C	-7.18	100.38	110.50
1	A	180	GLU	N-CA-C	7.00	119.77	111.71
1	C	1017	LEU	N-CA-C	7.00	130.59	111.00
1	A	82	CYS	N-CA-C	6.89	119.72	110.35
1	D	82	CYS	N-CA-C	6.76	119.54	110.35
1	C	900	GLN	N-CA-C	6.73	120.35	110.59
1	C	503	ILE	N-CA-C	-6.63	104.02	110.72
1	D	503	ILE	N-CA-C	-6.49	104.17	110.72
1	D	229	SER	N-CA-C	6.44	119.29	111.82
1	B	82	CYS	N-CA-C	6.41	119.54	110.50
1	A	132	THR	N-CA-C	6.35	119.01	111.33
1	A	285	LEU	CA-C-N	6.35	126.03	119.56
1	A	285	LEU	C-N-CA	6.35	126.03	119.56
1	D	865	VAL	CA-C-N	6.34	127.77	119.84
1	D	865	VAL	C-N-CA	6.34	127.77	119.84
1	C	82	CYS	N-CA-C	6.34	119.44	110.50
1	B	904	PHE	N-CA-C	6.33	123.81	109.81
1	A	229	SER	N-CA-C	6.32	119.14	111.82
1	C	1001	CYS	N-CA-C	-6.31	104.48	111.36
1	B	1001	CYS	N-CA-C	-6.30	104.49	111.36
1	D	285	LEU	CA-C-N	6.29	125.97	119.56
1	D	285	LEU	C-N-CA	6.29	125.97	119.56
1	A	143	TYR	N-CA-C	-6.26	104.90	112.54
1	D	677	GLU	N-CA-C	-6.22	103.10	111.87
1	C	173	ASN	CA-C-N	6.15	126.33	119.32
1	C	173	ASN	C-N-CA	6.15	126.33	119.32
1	D	1001	CYS	N-CA-C	-6.11	104.70	111.36
1	D	173	ASN	CA-C-N	6.11	125.59	119.24
1	D	173	ASN	C-N-CA	6.11	125.59	119.24
1	A	503	ILE	N-CA-C	-6.10	104.56	110.72
1	C	68	GLY	N-CA-C	-6.09	102.96	112.58
1	C	677	GLU	N-CA-C	6.07	117.11	108.74
1	B	423	GLU	N-CA-C	6.04	117.87	111.28
1	C	143	TYR	N-CA-C	-6.04	105.17	112.54
1	C	286	PRO	N-CA-C	6.04	121.69	113.84
1	B	68	GLY	N-CA-C	-6.03	103.05	112.58
1	D	286	PRO	N-CA-C	6.02	121.67	113.84
1	B	286	PRO	N-CA-C	5.97	121.61	113.84
1	D	143	TYR	N-CA-C	-5.97	105.25	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	503	ILE	N-CA-C	-5.94	104.72	110.72
1	B	2	ALA	CA-C-N	5.91	127.22	119.84
1	B	2	ALA	C-N-CA	5.91	127.22	119.84
1	A	1001	CYS	N-CA-C	-5.86	104.97	111.36
1	A	68	GLY	N-CA-C	-5.84	103.34	112.58
1	D	2	ALA	CA-C-N	5.84	127.14	119.84
1	D	2	ALA	C-N-CA	5.84	127.14	119.84
1	A	286	PRO	N-CA-C	5.83	121.42	113.84
1	B	285	LEU	CA-C-N	5.79	125.46	119.56
1	B	285	LEU	C-N-CA	5.79	125.46	119.56
1	B	143	TYR	N-CA-C	-5.75	105.36	112.38
1	C	285	LEU	CA-C-N	5.74	125.42	119.56
1	C	285	LEU	C-N-CA	5.74	125.42	119.56
1	C	644	SER	N-CA-C	-5.72	103.15	110.53
1	D	129	VAL	N-CA-C	5.70	119.64	113.43
1	B	678	ARG	N-CA-C	5.68	120.21	112.88
1	D	573	THR	N-CA-C	-5.66	102.91	110.55
1	A	129	VAL	N-CA-C	5.66	119.60	113.43
1	C	129	VAL	N-CA-C	5.64	119.58	113.43
1	A	573	THR	N-CA-C	-5.59	103.00	110.55
1	D	426	ILE	N-CA-C	5.57	117.20	109.29
1	D	423	GLU	N-CA-C	5.56	117.34	111.28
1	D	644	SER	N-CA-C	-5.56	102.68	110.35
1	C	384	LYS	N-CA-C	5.56	119.36	112.58
1	C	1017	LEU	CA-C-O	-5.55	111.36	120.80
1	B	129	VAL	N-CA-C	5.54	119.47	113.43
1	D	473	GLU	CA-C-N	5.53	125.62	119.32
1	D	473	GLU	C-N-CA	5.53	125.62	119.32
1	B	573	THR	N-CA-C	-5.52	103.10	110.55
1	C	617	THR	N-CA-C	5.52	117.81	110.53
1	C	573	THR	N-CA-C	-5.51	103.11	110.55
1	D	68	GLY	N-CA-C	-5.50	103.90	112.58
1	D	261	LEU	N-CA-C	-5.40	100.31	108.67
1	A	1016	GLY	N-CA-C	-5.40	108.57	115.42
1	B	148	GLY	N-CA-C	5.34	121.90	112.83
1	C	229	SER	N-CA-C	5.32	118.93	112.23
1	C	545	PRO	N-CA-C	5.32	120.21	114.68
1	C	120	ASN	CA-C-N	5.31	124.98	119.56
1	C	120	ASN	C-N-CA	5.31	124.98	119.56
1	C	132	THR	N-CA-C	5.31	118.54	111.75
1	A	671	CYS	CA-C-N	5.28	125.57	119.92
1	A	671	CYS	C-N-CA	5.28	125.57	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	617	THR	N-CA-C	5.28	117.50	110.53
1	D	120	ASN	CA-C-N	5.25	124.91	119.56
1	D	120	ASN	C-N-CA	5.25	124.91	119.56
1	C	261	LEU	N-CA-C	-5.24	100.54	108.67
1	A	617	THR	N-CA-C	5.24	117.44	110.53
1	B	594	THR	N-CA-C	-5.23	106.13	112.88
1	B	229	SER	N-CA-C	5.18	118.75	112.23
1	C	1016	GLY	N-CA-C	-5.17	108.70	115.47
1	A	384	LYS	N-CA-C	5.16	118.88	112.58
1	C	263	GLU	N-CA-C	5.12	121.71	110.80
1	B	384	LYS	N-CA-C	5.12	118.83	112.58
1	C	920	ALA	N-CA-C	-5.11	102.96	110.52
1	A	920	ALA	N-CA-C	-5.09	102.92	110.46
1	C	615	GLU	N-CA-C	-5.08	107.08	113.28
1	C	426	ILE	N-CA-C	5.06	116.48	109.29
1	C	148	GLY	N-CA-C	5.06	121.43	112.83
1	C	678	ARG	N-CA-C	-5.03	100.08	110.80
1	B	289	LYS	N-CA-C	-5.03	102.41	109.96
1	B	948	ILE	N-CA-C	5.02	115.53	108.36

There are no chirality outliers.

There are no planarity outliers.

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	7750	0	7775	186	0
1	B	7757	0	7782	140	1
1	C	7750	0	7775	190	0
1	D	7765	0	7793	181	1
2	A	32	0	0	1	0
2	B	32	0	0	2	0
2	C	32	0	0	1	0
2	D	32	0	0	2	0
3	A	31	0	19	0	0
3	B	31	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	31	0	19	0	0
3	D	31	0	19	0	0
4	A	53	0	31	1	0
4	B	53	0	31	2	0
4	C	53	0	31	2	0
4	D	53	0	31	1	0
5	A	1148	0	0	38	0
5	B	1125	0	0	35	0
5	C	1176	0	0	38	0
5	D	1190	0	0	41	0
All	All	36125	0	31325	629	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 10.

All (629) 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:172:ARG:HD2	5:A:2301:HOH:O	1.29	1.28
1:C:427:VAL:HG13	1:D:410:ARG:CZ	1.78	1.12
1:A:373:VAL:HB	5:A:2254:HOH:O	1.57	1.02
1:C:427:VAL:HG13	1:D:410:ARG:NH1	1.75	1.01
1:C:680:MET:HE2	1:C:688:PRO:HD2	1.46	0.95
1:C:579:ASP:O	1:C:582:ILE:HG12	1.68	0.93
1:A:410:ARG:NH1	1:B:427:VAL:HG13	1.84	0.93
1:D:682:LEU:HA	5:D:2899:HOH:O	1.70	0.89
1:A:1017:LEU:O	5:A:3139:HOH:O	1.89	0.89
1:A:164:LYS:HG3	1:A:909:ARG:HH21	1.38	0.88
1:D:892:GLU:HG3	5:D:3065:HOH:O	1.72	0.88
1:D:51:HIS:HA	1:D:384:LYS:HG3	1.55	0.88
1:C:1017:LEU:HB3	5:C:2546:HOH:O	1.73	0.87
1:D:892:GLU:CG	5:D:3065:HOH:O	2.21	0.87
1:A:923:ASP:OD1	1:D:937:GLU:HG2	1.75	0.86
1:C:859:HIS:HD2	1:C:862:GLY:H	1.21	0.85
1:D:410:ARG:NH1	1:D:425:GLN:OE1	2.12	0.83
1:C:11:ASP:HB3	5:C:2028:HOH:O	1.78	0.83
1:D:856:THR:HG22	5:D:2184:HOH:O	1.78	0.82
1:A:1016:GLY:C	1:A:1017:LEU:HG	2.06	0.81
1:C:485:MET:HG2	1:D:35:LYS:HE3	1.62	0.80
1:D:54:LYS:HE3	1:D:56:GLU:HB2	1.64	0.79
1:A:427:VAL:CG2	1:B:410:ARG:CZ	2.61	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:LYS:HD2	5:B:2618:HOH:O	1.81	0.79
1:C:893:GLU:OE1	1:C:896:ARG:NH2	2.16	0.78
1:C:53:GLU:OE2	1:C:55:LEU:HD21	1.84	0.78
1:D:867:ARG:HG3	1:D:872:MET:CE	2.13	0.78
1:A:375:GLU:N	1:A:375:GLU:OE1	2.16	0.77
1:C:428:HIS:N	1:D:410:ARG:HH12	1.83	0.77
1:A:722:ARG:O	1:A:726:GLU:HG3	1.85	0.76
1:C:442:LEU:HD22	1:C:482:ILE:HD11	1.68	0.76
1:C:177:PRO:HG2	1:C:182:MET:SD	2.26	0.75
1:D:682:LEU:HD23	5:D:2899:HOH:O	1.86	0.75
1:D:54:LYS:HE3	1:D:56:GLU:CB	2.17	0.75
1:A:373:VAL:CG1	5:A:2254:HOH:O	2.35	0.75
1:C:164:LYS:O	1:C:909:ARG:NH2	2.21	0.74
1:C:410:ARG:CZ	1:D:427:VAL:HG22	2.17	0.74
1:D:867:ARG:HG3	1:D:872:MET:HE3	1.70	0.74
1:D:173:ASN:HB2	5:D:2372:HOH:O	1.89	0.73
1:D:896:ARG:O	1:D:900:GLN:HG3	1.87	0.73
1:D:984:ASP:HB3	5:D:3145:HOH:O	1.86	0.73
1:D:442:LEU:HD22	1:D:482:ILE:HD11	1.72	0.72
1:A:25:HIS:CD2	1:B:520:GLU:HG3	2.24	0.71
1:C:692:ARG:O	1:C:696:ARG:HG3	1.90	0.71
1:C:634:ASP:OD1	5:C:2793:HOH:O	2.07	0.71
1:D:53:GLU:HG3	1:D:887:LYS:HB3	1.71	0.71
1:B:673:HIS:CE1	1:B:682:LEU:HA	2.26	0.71
1:D:934:THR:OG1	1:D:937:GLU:HG3	1.91	0.71
1:D:1017:LEU:O	5:D:3179:HOH:O	2.08	0.71
1:A:427:VAL:CG2	1:B:410:ARG:NH2	2.54	0.70
1:A:410:ARG:CZ	1:B:427:VAL:HG13	2.21	0.70
1:D:950:GLU:HG3	1:D:979:LEU:HD22	1.74	0.70
1:C:859:HIS:CD2	1:C:862:GLY:H	2.08	0.69
1:D:722:ARG:O	1:D:726:GLU:HG3	1.93	0.69
1:A:1016:GLY:O	1:A:1017:LEU:HG	1.91	0.69
1:C:427:VAL:CG1	1:D:410:ARG:CZ	2.66	0.69
1:C:776:ARG:O	1:C:780:THR:HG23	1.93	0.69
1:D:173:ASN:HB3	1:D:176:LEU:HG	1.75	0.69
1:C:2:ALA:N	5:C:2002:HOH:O	2.26	0.69
1:C:316:SER:HA	1:C:325:HIS:CD2	2.27	0.69
1:C:9:VAL:HG23	1:C:11:ASP:OD1	1.93	0.69
1:C:910:LYS:HE2	5:C:3032:HOH:O	1.93	0.69
1:D:885:GLN:HG3	5:D:3057:HOH:O	1.93	0.69
1:D:9:VAL:HG23	1:D:11:ASP:OD1	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:THR:HA	5:A:2973:HOH:O	1.92	0.68
1:C:164:LYS:HG3	1:C:909:ARG:HH12	1.59	0.68
1:A:872:MET:HE1	1:A:951:GLU:HG3	1.76	0.68
5:C:2780:HOH:O	1:D:2:ALA:HB3	1.94	0.67
1:C:36:LEU:HD22	5:C:2093:HOH:O	1.93	0.67
1:A:12:ILE:O	1:A:15:ILE:HG22	1.93	0.67
1:C:2:ALA:HB3	5:C:2001:HOH:O	1.94	0.67
1:C:143:TYR:O	1:D:861:LYS:HE3	1.93	0.67
1:C:427:VAL:CG1	1:D:410:ARG:NH1	2.55	0.67
1:C:428:HIS:H	1:D:410:ARG:NH1	1.93	0.66
1:B:259:LYS:HE2	5:B:2415:HOH:O	1.96	0.66
1:C:950:GLU:OE2	1:C:979:LEU:HD13	1.95	0.66
1:A:427:VAL:HG21	1:B:410:ARG:CZ	2.25	0.66
1:C:680:MET:CE	1:C:688:PRO:HD2	2.23	0.66
1:A:692:ARG:O	1:A:696:ARG:HG3	1.94	0.66
1:A:915:LYS:O	1:C:675:MET:HB2	1.95	0.66
1:C:950:GLU:HG3	1:C:979:LEU:HD22	1.78	0.66
1:B:169:PRO:HG3	1:B:911:PRO:HB3	1.76	0.65
1:C:260:SER:HB2	1:C:265:GLU:OE1	1.95	0.65
1:D:1008:THR:HG22	5:D:3166:HOH:O	1.94	0.65
1:A:718:VAL:CG2	1:A:780:THR:HG22	2.26	0.65
1:C:12:ILE:O	1:C:15:ILE:HG22	1.96	0.65
1:D:414:ASP:O	1:D:416:THR:N	2.29	0.65
1:A:5:LEU:HD22	1:A:1017:LEU:HD12	1.77	0.65
1:B:343:THR:HG21	5:B:2602:HOH:O	1.96	0.65
1:D:54:LYS:CE	1:D:56:GLU:HB3	2.27	0.65
1:D:1017:LEU:HB3	1:D:1018:PRO:CD	2.26	0.65
1:A:5:LEU:CD2	1:A:1017:LEU:HD12	2.27	0.65
1:B:173:ASN:HB2	5:B:2297:HOH:O	1.97	0.65
1:D:263:GLU:O	1:D:264:ASN:HB3	1.97	0.65
1:B:442:LEU:HD22	1:B:482:ILE:HD11	1.79	0.64
1:C:909:ARG:HG3	5:C:2283:HOH:O	1.96	0.64
1:C:486:ALA:HB3	5:C:2658:HOH:O	1.98	0.64
1:A:483:VAL:HG23	5:A:2663:HOH:O	1.97	0.64
1:C:394:ARG:HH12	1:C:423:GLU:CD	2.06	0.64
1:A:261:LEU:HD21	1:A:451:LEU:HD21	1.81	0.63
1:A:1016:GLY:O	1:A:1017:LEU:CG	2.46	0.63
1:A:427:VAL:HG22	1:B:410:ARG:CZ	2.27	0.63
1:C:1017:LEU:CB	5:C:2546:HOH:O	2.35	0.63
1:B:722:ARG:O	1:B:726:GLU:HG3	1.98	0.63
1:C:428:HIS:N	1:D:410:ARG:NH1	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:ASN:HD22	1:A:174:PRO:CD	2.12	0.63
1:C:343:THR:HG21	5:C:2599:HOH:O	1.98	0.63
1:B:12:ILE:O	1:B:15:ILE:HG22	1.99	0.62
1:A:281:ILE:HD13	1:A:451:LEU:HD22	1.82	0.62
1:A:263:GLU:O	1:A:264:ASN:HB2	1.98	0.62
1:A:293:ILE:CD1	1:A:393:PRO:HB2	2.29	0.62
1:C:1015:ARG:HB2	1:C:1017:LEU:HG	1.80	0.62
1:A:293:ILE:HD11	1:A:393:PRO:HB2	1.82	0.62
1:A:416:THR:C	1:A:418:LYS:H	2.07	0.62
1:B:173:ASN:HB3	1:B:176:LEU:HG	1.81	0.62
1:D:897:LEU:HD23	1:D:900:GLN:OE1	2.00	0.62
1:C:922:LYS:HE3	5:C:3051:HOH:O	2.00	0.61
1:A:84:ASP:CG	1:A:89:LYS:HZ1	2.08	0.61
1:C:410:ARG:NH2	1:D:427:VAL:CG2	2.63	0.61
1:C:978:HIS:HE1	1:D:84:ASP:OD2	1.83	0.61
1:C:410:ARG:HG3	1:C:425:GLN:HB3	1.83	0.61
1:C:877:PRO:HD2	1:C:882:TYR:CG	2.36	0.61
1:C:293:ILE:HD11	1:C:393:PRO:HB2	1.82	0.61
1:D:219:LYS:HG3	1:D:260:SER:OG	2.00	0.61
1:A:990:THR:HG22	1:A:990:THR:O	2.00	0.61
1:B:857:GLU:O	1:B:859:HIS:HD2	1.84	0.61
1:C:688:PRO:HG3	1:C:720:ILE:HD13	1.82	0.61
1:D:54:LYS:CE	1:D:56:GLU:CB	2.78	0.60
1:A:745:LYS:HD2	5:A:2886:HOH:O	2.01	0.60
1:D:688:PRO:HG3	1:D:720:ILE:HD13	1.83	0.60
1:C:22:THR:HG22	5:D:2238:HOH:O	2.02	0.60
1:A:173:ASN:HD22	1:A:174:PRO:N	1.99	0.60
1:A:699:ARG:O	1:A:699:ARG:HD3	2.02	0.60
1:A:787:GLY:HA3	1:D:942:GLU:OE2	2.01	0.60
1:A:1014:LYS:HB3	5:A:3138:HOH:O	1.99	0.60
1:B:411:THR:HG22	1:B:421:GLU:OE1	2.02	0.59
1:C:1015:ARG:C	1:C:1017:LEU:H	2.10	0.59
1:A:219:LYS:HG3	1:A:260:SER:OG	2.02	0.59
1:A:646:ASN:HD22	1:A:649:ASP:CG	2.10	0.59
1:A:373:VAL:CB	5:A:2254:HOH:O	2.27	0.59
1:D:866:PRO:O	1:D:868:ILE:N	2.35	0.59
1:A:448:LYS:HD3	5:A:2611:HOH:O	2.01	0.59
1:A:911:PRO:HG2	5:A:2407:HOH:O	2.02	0.59
1:B:53:GLU:HG2	5:B:2124:HOH:O	2.02	0.58
1:C:1017:LEU:HD11	5:D:2379:HOH:O	2.03	0.58
1:C:844:GLU:O	1:C:847:GLN:HG3	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:990:THR:HG22	1:D:990:THR:O	2.02	0.58
1:A:173:ASN:HD22	1:A:173:ASN:C	2.10	0.58
1:A:900:GLN:O	1:A:900:GLN:HG2	2.03	0.58
1:C:783:ARG:HH11	1:C:932:LEU:HB3	1.68	0.58
1:C:716:ASP:OD2	1:C:719:SER:HB3	2.03	0.58
1:B:744:LEU:HD21	5:B:2430:HOH:O	2.03	0.58
1:C:410:ARG:CZ	1:D:427:VAL:CG2	2.81	0.58
1:D:923:ASP:O	1:D:927:LYS:HE3	2.04	0.58
1:B:410:ARG:HG3	1:B:425:GLN:HB3	1.85	0.58
1:C:173:ASN:OD1	1:C:174:PRO:HD2	2.04	0.58
1:A:12:ILE:HA	1:A:15:ILE:HG22	1.86	0.58
1:C:875:LYS:HA	1:C:950:GLU:OE2	2.04	0.58
1:A:427:VAL:HG21	1:B:410:ARG:NH2	2.19	0.57
1:C:722:ARG:O	1:C:726:GLU:HG3	2.04	0.57
1:C:410:ARG:NH1	5:C:2580:HOH:O	2.37	0.57
1:C:935:PHE:CE2	1:D:612:LEU:HD11	2.39	0.57
1:A:775:LEU:O	1:A:779:THR:HG23	2.05	0.57
1:A:410:ARG:NH1	1:A:425:GLN:OE1	2.28	0.57
1:A:410:ARG:NH1	1:B:427:VAL:CG1	2.64	0.57
1:C:845:GLU:HG3	1:C:912:PHE:CE1	2.39	0.57
1:C:990:THR:O	1:C:990:THR:HG22	2.02	0.57
1:D:486:ALA:HB3	5:D:2715:HOH:O	2.04	0.57
1:A:173:ASN:HD22	1:A:174:PRO:HD2	1.69	0.57
1:B:326:SER:HB3	5:B:2486:HOH:O	2.04	0.57
1:C:50:PHE:HD1	5:C:2116:HOH:O	1.88	0.57
1:D:907:LEU:O	1:D:908:GLU:C	2.48	0.56
1:B:2:ALA:HB3	5:B:2001:HOH:O	2.03	0.56
1:B:866:PRO:HG3	5:B:2962:HOH:O	2.05	0.56
1:C:36:LEU:HG	5:C:2086:HOH:O	2.05	0.56
1:A:22:THR:HG22	5:B:2211:HOH:O	2.04	0.56
1:A:703:GLN:HG3	5:A:2851:HOH:O	2.04	0.56
1:D:54:LYS:HE2	1:D:56:GLU:HB3	1.87	0.56
1:B:907:LEU:O	1:B:909:ARG:N	2.39	0.56
1:C:293:ILE:CD1	1:C:393:PRO:HB2	2.36	0.56
1:B:261:LEU:HD21	1:B:451:LEU:HD21	1.88	0.56
1:D:845:GLU:HG3	1:D:912:PHE:CE1	2.40	0.56
1:A:866:PRO:HG3	5:A:2142:HOH:O	2.05	0.55
1:C:892:GLU:HG3	5:C:3025:HOH:O	2.07	0.55
1:A:307:LYS:HE3	5:A:2481:HOH:O	2.05	0.55
1:C:410:ARG:HG3	1:C:425:GLN:CB	2.37	0.55
1:D:248:MET:HE1	1:D:255:ILE:HD11	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:859:HIS:CE1	1:D:952:MET:HE3	2.41	0.55
1:A:834:LEU:HD21	1:A:921:ILE:HD11	1.88	0.55
1:A:29:HIS:HB2	5:B:2197:HOH:O	2.07	0.55
1:D:379:LEU:O	1:D:383:GLU:HG3	2.07	0.55
1:A:179:GLN:HG3	5:A:2309:HOH:O	2.07	0.54
1:C:780:THR:HG22	1:D:762:TYR:CZ	2.41	0.54
1:C:612:LEU:HD11	1:D:935:PHE:CE2	2.43	0.54
1:A:779:THR:HG22	1:A:808:SER:HB3	1.89	0.54
1:C:505:LYS:HE2	5:C:2664:HOH:O	2.07	0.54
1:B:293:ILE:CD1	1:B:393:PRO:HB2	2.37	0.54
1:C:219:LYS:HG3	1:C:260:SER:OG	2.06	0.54
5:C:2196:HOH:O	1:D:29:HIS:HB2	2.07	0.54
1:D:307:LYS:HE3	5:D:2530:HOH:O	2.07	0.54
1:A:173:ASN:HB2	5:A:2347:HOH:O	2.08	0.54
1:C:711:THR:HG22	5:C:2843:HOH:O	2.07	0.54
1:C:783:ARG:NH1	1:C:932:LEU:HB3	2.22	0.54
1:A:646:ASN:ND2	1:A:649:ASP:H	2.06	0.53
1:A:688:PRO:HG3	1:A:720:ILE:HD13	1.88	0.53
1:C:680:MET:HE2	1:C:688:PRO:CD	2.28	0.53
1:B:7:LYS:NZ	5:B:2017:HOH:O	2.41	0.53
1:D:53:GLU:HG3	1:D:887:LYS:CB	2.37	0.53
1:A:779:THR:HG21	5:A:2931:HOH:O	2.07	0.53
1:B:1012:GLU:HG2	5:B:3108:HOH:O	2.07	0.53
1:C:27:ALA:O	1:D:497:LYS:HE2	2.08	0.53
1:C:287:GLU:OE2	1:C:444:ASP:HB2	2.07	0.53
1:C:868:ILE:HG22	1:C:870:GLU:H	1.73	0.53
1:D:674:GLY:HA2	5:D:2901:HOH:O	2.08	0.53
1:D:680:MET:CE	1:D:688:PRO:HD2	2.39	0.53
1:D:896:ARG:C	1:D:900:GLN:HG3	2.34	0.53
1:A:15:ILE:HD13	1:A:969:GLN:O	2.08	0.53
1:B:691:VAL:HG21	1:B:720:ILE:HG23	1.90	0.53
1:B:849:TRP:CH2	1:B:854:PRO:HG3	2.44	0.53
1:C:179:GLN:HG3	5:C:2301:HOH:O	2.08	0.53
1:B:990:THR:HG22	1:B:990:THR:O	2.07	0.53
1:C:845:GLU:HG3	1:C:912:PHE:CD1	2.43	0.53
1:A:776:ARG:HB2	1:B:740:GLY:HA2	1.89	0.53
1:C:796:ILE:HD13	1:C:813:LEU:HB3	1.91	0.53
1:B:173:ASN:O	1:B:176:LEU:HB2	2.08	0.52
1:C:410:ARG:HB2	1:C:422:ASP:HB2	1.90	0.52
1:D:115:MET:HE2	1:D:828:GLN:NE2	2.25	0.52
1:B:923:ASP:O	1:B:927:LYS:HE3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:261:LEU:HD21	1:C:451:LEU:HD21	1.91	0.52
1:C:410:ARG:NH2	1:D:427:VAL:HG22	2.24	0.52
1:D:82:CYS:O	1:D:98:LYS:HD2	2.08	0.52
1:A:845:GLU:HG3	1:A:912:PHE:CE1	2.45	0.52
1:B:82:CYS:O	1:B:98:LYS:HD2	2.09	0.52
1:B:455:LYS:HD3	1:B:463:GLU:OE1	2.09	0.52
1:B:699:ARG:HA	1:B:699:ARG:NE	2.24	0.52
1:D:845:GLU:HG3	1:D:912:PHE:CD1	2.45	0.52
1:A:874:LYS:NZ	5:A:2994:HOH:O	2.42	0.52
1:B:173:ASN:ND2	5:B:2298:HOH:O	2.37	0.52
1:A:46:ASP:HB3	1:A:49:CYS:SG	2.49	0.52
1:C:22:THR:HA	5:C:2063:HOH:O	2.10	0.52
1:C:1017:LEU:CD1	5:D:2379:HOH:O	2.58	0.52
1:D:867:ARG:HG3	1:D:872:MET:HE1	1.91	0.52
1:C:582:ILE:CD1	1:D:1019:LEU:HD21	2.40	0.52
1:C:691:VAL:HG21	1:C:720:ILE:HG23	1.92	0.51
1:A:172:ARG:HG3	5:A:2343:HOH:O	2.11	0.51
1:A:541:LYS:HD2	5:A:2715:HOH:O	2.10	0.51
1:C:82:CYS:O	1:C:98:LYS:HD2	2.11	0.51
1:D:263:GLU:HA	1:D:263:GLU:OE1	2.11	0.51
1:C:423:GLU:OE1	1:C:423:GLU:HA	2.09	0.51
1:C:485:MET:O	1:D:35:LYS:NZ	2.38	0.51
1:A:796:ILE:HD13	1:A:813:LEU:HB3	1.93	0.51
1:A:955:ASN:HB3	1:A:978:HIS:HB3	1.91	0.51
1:C:955:ASN:HB3	1:C:978:HIS:HB3	1.92	0.51
1:D:263:GLU:O	1:D:264:ASN:CB	2.59	0.51
1:D:909:ARG:NH2	5:D:3071:HOH:O	2.43	0.51
1:A:288:PRO:HG3	1:A:307:LYS:HB2	1.92	0.51
1:B:892:GLU:HG3	5:B:2981:HOH:O	2.11	0.51
1:C:978:HIS:HD2	5:D:2284:HOH:O	1.94	0.51
1:C:984:ASP:CG	5:C:3153:HOH:O	2.53	0.51
1:A:173:ASN:C	1:A:173:ASN:ND2	2.67	0.51
1:B:173:ASN:HB3	1:B:176:LEU:CG	2.40	0.51
1:A:705:PRO:HA	1:A:730:ASP:OD2	2.11	0.50
1:B:1014:LYS:HE3	5:B:3058:HOH:O	2.11	0.50
1:B:175:CYS:HB2	5:B:2300:HOH:O	2.11	0.50
1:C:410:ARG:HH22	1:D:391:LEU:HD21	1.76	0.50
1:A:725:LYS:HE3	5:A:2917:HOH:O	2.11	0.50
1:B:191:ALA:O	1:B:279:ALA:HA	2.12	0.50
1:C:394:ARG:NH2	1:C:423:GLU:OE2	2.38	0.50
1:D:796:ILE:HD13	1:D:813:LEU:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:935:PHE:CE2	1:B:612:LEU:HD11	2.47	0.50
1:B:358:ARG:NH2	5:B:2544:HOH:O	2.40	0.50
1:C:758:LYS:HD3	5:C:2902:HOH:O	2.11	0.50
1:A:82:CYS:O	1:A:98:LYS:HD2	2.12	0.50
1:B:915:LYS:HG3	5:B:2933:HOH:O	2.10	0.50
1:C:52:CYS:HB2	1:C:384:LYS:HB2	1.93	0.50
1:A:53:GLU:OE2	1:A:55:LEU:HD21	2.11	0.50
1:C:497:LYS:HE2	1:D:27:ALA:O	2.12	0.50
1:C:893:GLU:HA	1:C:896:ARG:HH21	1.77	0.50
1:D:100:PHE:CD1	1:D:100:PHE:C	2.90	0.50
1:B:845:GLU:HG3	1:B:912:PHE:CE1	2.46	0.50
1:C:1014:LYS:HB3	5:C:3167:HOH:O	2.12	0.50
1:D:115:MET:HE2	1:D:828:GLN:HE22	1.77	0.49
1:D:682:LEU:CD2	5:D:2899:HOH:O	2.54	0.49
1:A:572:LEU:HD13	1:A:638:ILE:HB	1.93	0.49
1:B:346:ASP:OD2	4:B:1031:FAD:H6	2.12	0.49
1:A:97:ILE:HA	1:A:100:PHE:CD2	2.47	0.49
1:C:364:ARG:NH1	5:C:2586:HOH:O	2.44	0.49
1:C:442:LEU:HD22	1:C:482:ILE:CD1	2.40	0.49
1:A:84:ASP:CG	1:A:89:LYS:NZ	2.71	0.49
1:A:386:GLU:HA	5:A:2574:HOH:O	2.12	0.49
1:A:672:PRO:HA	1:A:682:LEU:O	2.13	0.49
1:B:870:GLU:N	1:B:870:GLU:OE1	2.44	0.49
1:A:868:ILE:O	1:A:872:MET:HG2	2.13	0.49
1:A:909:ARG:NH1	5:A:3022:HOH:O	2.46	0.49
1:A:413:GLN:CG	1:A:417:GLY:HA2	2.42	0.49
1:B:193:LEU:N	1:B:193:LEU:HD22	2.28	0.49
1:B:442:LEU:HD22	1:B:482:ILE:CD1	2.42	0.49
1:B:430:LYS:HE2	5:B:2594:HOH:O	2.11	0.49
1:C:410:ARG:HD2	5:C:2579:HOH:O	2.13	0.49
1:A:35:LYS:NZ	5:A:2092:HOH:O	2.44	0.49
1:A:845:GLU:HG3	1:A:912:PHE:CD1	2.48	0.49
1:A:346:ASP:OD2	4:A:1031:FAD:H6	2.13	0.49
1:A:917:PRO:HG3	1:C:675:MET:HE3	1.95	0.49
1:B:621:TRP:O	1:B:625:VAL:HG23	2.12	0.49
1:A:95:LEU:HD12	1:A:119:ASP:HB2	1.95	0.49
1:A:281:ILE:HD13	1:A:451:LEU:CD2	2.42	0.49
1:A:699:ARG:NH2	1:A:730:ASP:OD2	2.46	0.49
1:A:784:ALA:C	1:A:786:PRO:HD3	2.38	0.49
1:B:410:ARG:HG3	1:B:425:GLN:CB	2.42	0.49
1:A:416:THR:C	1:A:418:LYS:N	2.71	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:673:HIS:O	1:C:674:GLY:O	2.30	0.48
1:D:993:LEU:C	1:D:993:LEU:HD23	2.38	0.48
1:A:379:LEU:O	1:A:383:GLU:HG3	2.13	0.48
1:B:219:LYS:HG3	1:B:260:SER:OG	2.12	0.48
1:C:407:GLN:NE2	5:C:2577:HOH:O	2.47	0.48
1:D:346:ASP:OD2	4:D:1031:FAD:H6	2.12	0.48
1:D:959:CYS:O	1:D:962:THR:HG22	2.12	0.48
1:A:427:VAL:HG22	1:B:410:ARG:NE	2.27	0.48
5:A:2209:HOH:O	1:B:29:HIS:HB2	2.12	0.48
1:C:779:THR:HG22	1:C:808:SER:HB3	1.95	0.48
1:C:246:GLU:OE1	1:C:908:GLU:OE1	2.32	0.48
1:C:412:GLU:OE1	1:C:422:ASP:OD2	2.31	0.48
1:C:418:LYS:HE2	1:C:420:ASN:OD1	2.14	0.48
1:D:451:LEU:O	1:D:454:ILE:HG12	2.14	0.48
1:B:320:GLY:O	1:B:321:MET:C	2.56	0.48
1:B:796:ILE:HD13	1:B:813:LEU:HB3	1.95	0.48
1:C:331:ILE:HG23	1:C:433:VAL:HG21	1.95	0.48
1:C:394:ARG:NH2	1:C:421:GLU:OE1	2.47	0.48
1:C:760:THR:CG2	1:D:932:LEU:HD23	2.44	0.48
1:C:780:THR:HG22	1:D:762:TYR:CE2	2.48	0.48
1:C:859:HIS:HA	1:C:865:VAL:HG23	1.96	0.48
1:D:758:LYS:HD3	5:D:2948:HOH:O	2.13	0.48
1:D:933:GLY:HA3	1:D:937:GLU:OE1	2.14	0.48
1:C:346:ASP:OD2	4:C:1031:FAD:H6	2.13	0.48
1:A:582:ILE:HD11	1:B:1015:ARG:CZ	2.43	0.48
1:B:845:GLU:HG3	1:B:912:PHE:CD1	2.48	0.48
1:C:47:LYS:HD3	1:D:373:VAL:HG12	1.96	0.48
1:C:167:ASN:OD1	1:C:909:ARG:NE	2.38	0.48
1:C:248:MET:HE1	1:C:255:ILE:HD11	1.95	0.48
1:D:193:LEU:N	1:D:193:LEU:HD22	2.28	0.48
1:D:458:ARG:HH21	1:D:459:TRP:HH2	1.62	0.48
1:B:859:HIS:CE1	1:B:864:PRO:HG3	2.48	0.48
1:C:191:ALA:O	1:C:279:ALA:HA	2.14	0.48
1:D:97:ILE:HD11	2:D:1026:SF4:S4	2.53	0.48
1:B:520:GLU:OE1	5:B:2674:HOH:O	2.20	0.47
1:D:673:HIS:HD2	1:D:675:MET:H	1.61	0.47
1:D:950:GLU:OE2	1:D:979:LEU:HD13	2.14	0.47
1:A:387:PHE:HD1	5:A:2574:HOH:O	1.97	0.47
1:B:291:ASP:OD1	1:B:293:ILE:HG12	2.13	0.47
1:B:1014:LYS:HB3	5:B:3114:HOH:O	2.15	0.47
1:C:364:ARG:CZ	5:C:2586:HOH:O	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:861:LYS:HE3	5:D:2286:HOH:O	2.13	0.47
1:B:5:LEU:HD21	1:B:1017:LEU:HD21	1.95	0.47
1:B:688:PRO:HG3	1:B:720:ILE:HD13	1.96	0.47
1:B:53:GLU:O	1:B:55:LEU:HG	2.14	0.47
1:B:872:MET:HE1	5:B:3043:HOH:O	2.14	0.47
1:C:993:LEU:HD23	1:C:993:LEU:C	2.40	0.47
1:C:1014:LYS:NZ	5:C:3164:HOH:O	2.32	0.47
1:B:608:LEU:HB2	1:B:742:MET:HE2	1.97	0.47
1:C:193:LEU:N	1:C:193:LEU:HD22	2.30	0.47
1:C:859:HIS:HD2	1:C:862:GLY:N	2.00	0.47
1:D:892:GLU:HG3	5:D:3063:HOH:O	2.15	0.47
1:B:1017:LEU:HB3	1:B:1018:PRO:CD	2.45	0.47
1:C:394:ARG:HD3	1:C:394:ARG:HA	1.68	0.47
1:C:870:GLU:OE1	1:C:889:ILE:HG23	2.14	0.47
1:D:83:ALA:O	1:D:84:ASP:C	2.58	0.47
1:A:1015:ARG:C	1:A:1017:LEU:H	2.22	0.47
1:C:2:ALA:HB3	5:D:2832:HOH:O	2.14	0.47
1:A:143:TYR:O	1:B:861:LYS:HE2	2.14	0.46
1:A:193:LEU:HD22	1:A:193:LEU:N	2.30	0.46
1:A:691:VAL:HG21	1:A:720:ILE:HG23	1.97	0.46
1:A:776:ARG:HD2	1:B:739:SER:OG	2.15	0.46
1:D:468:THR:HA	1:D:502:TYR:CD2	2.50	0.46
1:D:621:TRP:O	1:D:625:VAL:HG23	2.15	0.46
1:D:908:GLU:O	1:D:910:LYS:HG2	2.15	0.46
1:B:845:GLU:CD	1:B:845:GLU:H	2.23	0.46
1:B:870:GLU:O	1:B:889:ILE:HD13	2.15	0.46
1:D:845:GLU:CD	1:D:845:GLU:H	2.22	0.46
1:D:892:GLU:HG2	5:D:3065:HOH:O	2.01	0.46
1:A:116:ILE:HD13	1:A:156:GLN:HG3	1.97	0.46
1:A:413:GLN:HE21	1:A:417:GLY:CA	2.28	0.46
1:C:519:PRO:HB3	1:D:28:LEU:HD22	1.97	0.46
1:D:2:ALA:HB1	1:D:3:PRO:HD2	1.98	0.46
1:D:371:ARG:NH1	5:D:2615:HOH:O	2.49	0.46
1:D:552:ALA:HB3	1:D:553:PRO:HD3	1.96	0.46
1:B:955:ASN:HB3	1:B:978:HIS:HB3	1.97	0.46
1:D:2:ALA:HB3	5:D:2001:HOH:O	2.14	0.46
1:D:608:LEU:HB2	1:D:742:MET:HE2	1.97	0.46
1:D:672:PRO:HA	1:D:682:LEU:O	2.15	0.46
1:B:486:ALA:HB1	1:B:491:GLU:OE1	2.15	0.46
1:C:1015:ARG:C	1:C:1017:LEU:N	2.73	0.46
1:A:892:GLU:HG3	5:A:3013:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:LEU:HD13	1:B:638:ILE:HB	1.97	0.46
1:C:368:VAL:HG11	1:D:50:PHE:O	2.16	0.46
1:A:131:PRO:HB2	1:A:373:VAL:HG11	1.98	0.46
1:C:705:PRO:HA	1:C:730:ASP:OD2	2.15	0.46
1:C:849:TRP:CH2	1:C:854:PRO:HG3	2.51	0.46
1:D:173:ASN:O	1:D:176:LEU:HB2	2.15	0.46
1:D:486:ALA:HB1	1:D:491:GLU:OE1	2.16	0.46
1:A:907:LEU:O	1:A:908:GLU:C	2.59	0.46
1:D:574:LYS:HG3	1:D:614:SER:HB2	1.98	0.46
1:A:622:CYS:SG	1:A:656:LYS:HD2	2.56	0.46
1:B:375:GLU:OE1	1:B:375:GLU:HA	2.16	0.46
1:C:83:ALA:O	1:C:84:ASP:C	2.59	0.46
1:C:100:PHE:CD1	1:C:100:PHE:C	2.93	0.46
1:C:901:ASN:C	1:C:901:ASN:OD1	2.59	0.46
1:A:263:GLU:O	1:A:264:ASN:CB	2.64	0.45
1:A:486:ALA:HB1	1:A:491:GLU:OE1	2.15	0.45
1:D:53:GLU:HG3	1:D:887:LYS:HD3	1.98	0.45
1:A:164:LYS:O	1:A:909:ARG:NH2	2.47	0.45
1:B:307:LYS:HE3	5:B:2482:HOH:O	2.16	0.45
1:C:393:PRO:HD3	5:C:2562:HOH:O	2.15	0.45
1:D:394:ARG:HH11	1:D:394:ARG:HG2	1.80	0.45
1:D:955:ASN:HB3	1:D:978:HIS:HB3	1.97	0.45
1:B:896:ARG:NH2	5:B:2985:HOH:O	2.48	0.45
1:C:876:LEU:HD22	1:C:885:GLN:OE1	2.17	0.45
1:C:948:ILE:HG12	1:C:1002:ILE:HG12	1.98	0.45
1:D:950:GLU:CD	1:D:979:LEU:HD13	2.42	0.45
1:A:932:LEU:HD21	5:B:2430:HOH:O	2.16	0.45
1:B:410:ARG:HB2	1:B:422:ASP:HB2	1.99	0.45
1:C:680:MET:HE1	5:C:2400:HOH:O	2.15	0.45
1:D:293:ILE:CD1	1:D:393:PRO:HB2	2.46	0.45
1:D:414:ASP:C	1:D:416:THR:H	2.24	0.45
1:D:871:LEU:HG	1:D:889:ILE:HG21	1.98	0.45
5:A:2266:HOH:O	1:B:861:LYS:HE3	2.16	0.45
1:B:574:LYS:CG	1:B:614:SER:HB2	2.47	0.45
1:C:164:LYS:CG	1:C:909:ARG:HH12	2.29	0.45
1:C:915:LYS:HG2	5:C:3037:HOH:O	2.16	0.45
1:D:191:ALA:O	1:D:279:ALA:HA	2.16	0.45
1:A:164:LYS:HG3	1:A:909:ARG:NH2	2.19	0.45
1:A:281:ILE:CD1	1:A:451:LEU:HD22	2.46	0.45
1:A:381:LYS:NZ	5:A:2565:HOH:O	2.46	0.45
1:D:173:ASN:HA	1:D:174:PRO:HD3	1.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:291:ASP:OD1	1:D:293:ILE:HG12	2.16	0.45
1:B:577:SER:HB2	5:B:2718:HOH:O	2.15	0.45
1:D:328:LEU:HD12	5:D:2147:HOH:O	2.15	0.45
1:A:89:LYS:HE2	5:B:2043:HOH:O	2.16	0.45
1:B:293:ILE:HD11	1:B:393:PRO:HB2	1.99	0.45
1:B:705:PRO:HA	1:B:730:ASP:OD2	2.17	0.45
1:C:28:LEU:HD11	1:D:498:GLN:HA	1.99	0.45
1:C:1014:LYS:CE	5:C:3164:HOH:O	2.63	0.45
1:D:173:ASN:HB3	1:D:176:LEU:CG	2.44	0.45
1:B:83:ALA:O	1:B:84:ASP:C	2.59	0.45
1:A:41:TRP:CE2	1:B:89:LYS:HD2	2.51	0.44
1:A:173:ASN:OD1	5:A:2306:HOH:O	2.21	0.44
1:A:480:GLY:O	1:A:483:VAL:HG22	2.17	0.44
1:A:552:ALA:HB3	1:A:553:PRO:HD3	2.00	0.44
1:A:393:PRO:HD3	5:A:2578:HOH:O	2.16	0.44
1:A:413:GLN:HE21	1:A:417:GLY:HA2	1.82	0.44
1:A:710:LEU:HD22	1:A:720:ILE:HG22	2.00	0.44
1:A:870:GLU:O	1:A:874:LYS:HE3	2.17	0.44
1:D:54:LYS:HG3	1:D:55:LEU:N	2.32	0.44
1:A:107:LYS:NZ	5:A:2231:HOH:O	2.50	0.44
1:A:416:THR:O	1:A:418:LYS:N	2.50	0.44
1:A:613:ILE:HD13	1:A:642:MET:HE2	1.98	0.44
1:A:828:GLN:NE2	5:A:2942:HOH:O	2.50	0.44
1:B:97:ILE:HA	1:B:100:PHE:CD2	2.53	0.44
1:C:870:GLU:O	1:C:870:GLU:HG2	2.17	0.44
1:A:83:ALA:O	1:A:84:ASP:C	2.61	0.44
1:B:2:ALA:HB1	1:B:3:PRO:HD2	2.00	0.44
1:B:364:ARG:HA	1:B:391:LEU:O	2.17	0.44
1:C:97:ILE:HD11	2:C:1026:SF4:S4	2.58	0.44
1:C:410:ARG:NH2	1:D:427:VAL:HG21	2.33	0.44
1:A:849:TRP:CH2	1:A:854:PRO:HG3	2.52	0.44
1:A:191:ALA:O	1:A:279:ALA:HA	2.17	0.44
1:B:53:GLU:CG	5:B:2124:HOH:O	2.63	0.44
1:C:621:TRP:O	1:C:625:VAL:HG23	2.18	0.44
1:B:174:PRO:C	1:B:176:LEU:H	2.25	0.44
1:D:395:LYS:HD3	5:D:2643:HOH:O	2.18	0.44
1:A:930:GLN:HB3	5:D:3100:HOH:O	2.16	0.44
1:C:343:THR:HA	4:C:1031:FAD:HM73	1.98	0.44
1:C:871:LEU:O	1:C:873:GLY:N	2.48	0.44
1:D:116:ILE:HD13	1:D:156:GLN:HG3	1.99	0.44
1:D:572:LEU:HD13	1:D:638:ILE:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:CYS:HA	2:B:1027:SF4:S3	2.57	0.43
1:B:911:PRO:HG3	5:B:2133:HOH:O	2.17	0.43
1:C:29:HIS:HB2	5:D:2225:HOH:O	2.18	0.43
1:C:572:LEU:HD13	1:C:638:ILE:HB	1.99	0.43
1:C:845:GLU:HG3	1:C:912:PHE:CZ	2.53	0.43
1:C:870:GLU:O	1:C:889:ILE:HD13	2.18	0.43
1:C:888:LYS:HG2	1:C:892:GLU:OE2	2.18	0.43
1:B:868:ILE:HG22	1:B:870:GLU:H	1.83	0.43
1:C:386:GLU:HB2	5:C:2526:HOH:O	2.18	0.43
1:D:866:PRO:O	1:D:867:ARG:C	2.61	0.43
1:A:89:LYS:HD2	1:B:41:TRP:CE2	2.53	0.43
1:A:394:ARG:HA	1:A:394:ARG:HD3	1.80	0.43
1:B:779:THR:HG22	1:B:808:SER:HB3	2.00	0.43
1:B:916:LYS:HD3	5:B:3002:HOH:O	2.17	0.43
1:C:427:VAL:HG13	1:D:410:ARG:NH2	2.27	0.43
1:D:577:SER:HB2	5:D:2789:HOH:O	2.18	0.43
1:D:898:LYS:HE2	5:D:2259:HOH:O	2.17	0.43
1:A:248:MET:HE1	1:A:255:ILE:HD11	2.00	0.43
1:A:480:GLY:O	1:A:483:VAL:CG2	2.66	0.43
1:A:993:LEU:C	1:A:993:LEU:HD23	2.43	0.43
1:B:413:GLN:HG3	1:B:417:GLY:O	2.18	0.43
1:C:1017:LEU:O	1:C:1017:LEU:HD22	2.18	0.43
1:D:868:ILE:HG22	1:D:870:GLU:H	1.83	0.43
1:A:100:PHE:CD1	1:A:100:PHE:C	2.96	0.43
1:B:541:LYS:HB3	5:B:2697:HOH:O	2.18	0.43
1:D:691:VAL:HG21	1:D:720:ILE:HG23	1.99	0.43
1:D:948:ILE:HG12	1:D:1002:ILE:HG12	1.99	0.43
1:A:740:GLY:HA2	1:B:776:ARG:HB2	1.99	0.43
1:B:289:LYS:HG3	1:B:441:VAL:HG13	2.00	0.43
1:B:387:PHE:N	1:B:387:PHE:CD1	2.86	0.43
1:D:54:LYS:CE	1:D:56:GLU:HB2	2.42	0.43
1:D:219:LYS:HE2	5:D:3188:HOH:O	2.19	0.43
1:D:298:THR:HB	5:D:2520:HOH:O	2.19	0.43
1:D:391:LEU:HD21	1:D:427:VAL:HG21	2.00	0.43
1:D:734:ALA:HA	1:D:735:THR:HA	1.61	0.43
1:A:608:LEU:HB2	1:A:742:MET:HE2	2.01	0.43
1:C:191:ALA:HB2	1:C:276:TYR:CD2	2.54	0.43
1:D:297:LEU:HA	1:D:301:GLN:OE1	2.18	0.43
1:A:44:ASN:HB2	1:A:45:PRO:CD	2.49	0.43
1:A:870:GLU:HG2	1:A:889:ILE:HD13	2.01	0.43
1:A:909:ARG:NH1	5:A:3024:HOH:O	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1015:ARG:CZ	1:B:582:ILE:HD11	2.49	0.43
1:B:1009:THR:HB	1:B:1010:PRO:HD2	2.01	0.43
1:D:140:CYS:HA	2:D:1027:SF4:S3	2.59	0.43
1:A:612:LEU:HD11	1:B:935:PHE:CE2	2.53	0.43
1:B:173:ASN:HB3	1:B:176:LEU:CD1	2.49	0.43
1:B:367:PHE:O	1:B:370:ILE:HG13	2.19	0.43
1:A:5:LEU:HG	1:B:623:GLN:NE2	2.34	0.43
1:C:328:LEU:O	1:C:329:PRO:C	2.62	0.43
1:C:427:VAL:CG1	1:D:410:ARG:NH2	2.81	0.43
1:A:358:ARG:NH2	5:A:2535:HOH:O	2.51	0.42
1:B:734:ALA:HA	1:B:735:THR:HA	1.61	0.42
1:C:116:ILE:HD13	1:C:156:GLN:HG3	2.01	0.42
1:A:391:LEU:HD21	1:B:410:ARG:HH22	1.84	0.42
1:A:574:LYS:CG	1:A:614:SER:HB2	2.48	0.42
1:A:671:CYS:HA	1:A:672:PRO:HD3	1.80	0.42
1:B:834:LEU:HD21	1:B:921:ILE:HD11	2.00	0.42
1:A:861:LYS:CE	1:B:143:TYR:O	2.68	0.42
1:C:173:ASN:HB2	5:C:2333:HOH:O	2.19	0.42
1:D:249:LYS:NZ	5:D:2432:HOH:O	2.51	0.42
1:A:73:LEU:HD13	1:B:598:PRO:HB2	2.02	0.42
1:A:124:LEU:HD13	1:A:160:SER:HB2	2.02	0.42
1:B:643:CYS:HB2	1:B:650:TRP:CE2	2.54	0.42
1:C:309:PHE:CE1	1:C:331:ILE:HD11	2.55	0.42
1:D:849:TRP:CH2	1:D:854:PRO:HG3	2.54	0.42
1:A:363:PHE:CZ	1:A:387:PHE:HD2	2.37	0.42
1:C:307:LYS:HE3	5:C:2474:HOH:O	2.20	0.42
1:C:369:ASN:ND2	1:D:50:PHE:CD2	2.87	0.42
1:C:574:LYS:CG	1:C:614:SER:HB2	2.49	0.42
1:A:12:ILE:C	1:A:15:ILE:HG22	2.44	0.42
1:A:261:LEU:HD21	1:A:451:LEU:CD2	2.49	0.42
1:A:269:ASN:O	1:A:273:GLU:HB2	2.19	0.42
1:A:734:ALA:HA	1:A:735:THR:HA	1.62	0.42
1:A:786:PRO:C	1:D:942:GLU:HG2	2.44	0.42
1:D:705:PRO:HA	1:D:730:ASP:OD2	2.20	0.42
1:D:1017:LEU:HB3	1:D:1018:PRO:HD3	2.00	0.42
1:B:169:PRO:HG3	1:B:911:PRO:CB	2.45	0.42
1:B:220:GLN:O	1:B:257:CYS:HB3	2.19	0.42
1:C:760:THR:HG22	1:D:932:LEU:HD23	2.01	0.42
1:D:1015:ARG:HB2	5:D:3176:HOH:O	2.19	0.42
1:A:5:LEU:CD2	1:A:1017:LEU:CD1	2.97	0.42
1:A:291:ASP:OD1	1:A:293:ILE:HG12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:ARG:NH2	1:A:421:GLU:OE1	2.52	0.42
1:A:622:CYS:SG	1:A:656:LYS:CD	3.08	0.42
1:B:44:ASN:HB2	1:B:45:PRO:CD	2.50	0.42
1:A:191:ALA:HB2	1:A:276:TYR:CD2	2.55	0.41
1:A:200:ILE:CD1	1:A:245:ILE:HD11	2.50	0.41
1:B:162:VAL:HG12	1:B:166:MET:HE3	2.02	0.41
1:B:311:PRO:O	1:B:315:LYS:HG3	2.19	0.41
1:C:533:ILE:O	1:C:545:PRO:HD3	2.19	0.41
1:C:759:ARG:NH2	1:D:937:GLU:OE1	2.53	0.41
1:A:20:PRO:HG2	1:A:961:MET:SD	2.60	0.41
1:A:39:LYS:NZ	5:A:2103:HOH:O	2.52	0.41
1:B:22:THR:HA	5:B:2056:HOH:O	2.20	0.41
1:B:948:ILE:HG12	1:B:1002:ILE:HG12	2.02	0.41
1:C:20:PRO:HG2	1:C:961:MET:SD	2.60	0.41
1:D:97:ILE:HA	1:D:100:PHE:CD2	2.55	0.41
1:A:133:SER:OG	5:A:2254:HOH:O	2.22	0.41
1:D:448:LYS:NZ	1:D:460:ASP:OD2	2.45	0.41
1:A:771:ARG:N	1:A:772:PRO:CD	2.83	0.41
1:A:845:GLU:HG3	1:A:912:PHE:CZ	2.55	0.41
1:C:644:SER:HA	1:C:671:CYS:SG	2.61	0.41
1:A:204:SER:O	1:A:208:ARG:HG3	2.21	0.41
1:A:394:ARG:HG3	1:A:394:ARG:HH11	1.85	0.41
1:A:549:ALA:HB2	1:A:814:GLN:HB3	2.03	0.41
1:C:379:LEU:O	1:C:383:GLU:HG3	2.20	0.41
1:C:577:SER:HB2	5:C:2733:HOH:O	2.20	0.41
1:B:777:ALA:O	1:B:780:THR:HG22	2.20	0.41
1:C:608:LEU:HB2	1:C:742:MET:HE2	2.03	0.41
1:D:643:CYS:HB2	1:D:650:TRP:CE2	2.55	0.41
1:A:337:VAL:HB	1:A:361:LEU:HD23	2.02	0.41
1:B:901:ASN:OD1	1:B:902:ALA:N	2.53	0.41
1:C:97:ILE:HA	1:C:100:PHE:CD2	2.56	0.41
1:D:449:GLU:HG2	5:D:2675:HOH:O	2.19	0.41
1:D:533:ILE:O	1:D:545:PRO:HD3	2.20	0.41
1:D:968:TYR:CD1	1:D:968:TYR:N	2.88	0.41
1:A:140:CYS:HA	2:A:1027:SF4:S3	2.61	0.41
1:A:518:LYS:O	1:A:520:GLU:HG3	2.20	0.41
1:B:771:ARG:N	1:B:772:PRO:CD	2.84	0.41
1:C:387:PHE:N	1:C:387:PHE:CD1	2.88	0.41
1:C:486:ALA:HB1	1:C:491:GLU:OE1	2.21	0.41
1:C:582:ILE:HD11	1:D:1019:LEU:HD21	2.02	0.41
1:C:734:ALA:HA	1:C:735:THR:HA	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:VAL:CG2	1:D:11:ASP:OD1	2.67	0.41
1:D:261:LEU:HD21	1:D:451:LEU:HD21	2.03	0.41
1:D:599:MET:HB2	1:D:599:MET:HE2	1.81	0.41
1:D:680:MET:HE1	1:D:688:PRO:HD2	2.01	0.41
1:D:783:ARG:NE	5:D:2973:HOH:O	2.54	0.41
1:A:143:TYR:O	1:B:861:LYS:CE	2.69	0.41
1:D:335:VAL:HG22	1:D:433:VAL:HB	2.03	0.41
1:D:909:ARG:O	1:D:910:LYS:HD3	2.21	0.41
1:A:497:LYS:HE2	1:B:27:ALA:O	2.21	0.40
1:B:179:GLN:HG3	5:B:2306:HOH:O	2.21	0.40
1:B:343:THR:HA	4:B:1031:FAD:HM73	2.03	0.40
1:C:780:THR:HG22	1:D:762:TYR:OH	2.21	0.40
1:D:5:LEU:HD21	1:D:1017:LEU:HD21	2.03	0.40
1:D:191:ALA:HB2	1:D:276:TYR:CD2	2.56	0.40
1:D:647:LYS:O	1:D:651:MET:HG3	2.20	0.40
1:C:394:ARG:NH1	1:C:423:GLU:OE2	2.53	0.40
1:C:779:THR:CG2	1:C:808:SER:HB3	2.51	0.40
1:D:521:LEU:HA	1:D:522:PRO:HD3	1.91	0.40
1:B:97:ILE:HD11	2:B:1026:SF4:S4	2.61	0.40
1:B:470:GLN:HG2	5:B:2633:HOH:O	2.22	0.40
1:C:44:ASN:HB2	1:C:45:PRO:CD	2.51	0.40
1:D:39:LYS:HE2	5:D:2111:HOH:O	2.20	0.40
1:D:57:ASN:HB2	5:D:2147:HOH:O	2.20	0.40
1:B:100:PHE:CD1	1:B:100:PHE:C	3.00	0.40
1:B:552:ALA:HB3	1:B:553:PRO:HD3	2.03	0.40
1:C:131:PRO:HB2	1:C:373:VAL:HG11	2.03	0.40
1:C:897:LEU:C	1:C:899:GLU:N	2.76	0.40
1:D:892:GLU:CA	5:D:3065:HOH:O	2.68	0.40
1:A:310:LEU:HB2	1:A:311:PRO:HD3	2.04	0.40
1:A:1014:LYS:HE3	5:A:3082:HOH:O	2.21	0.40
1:B:116:ILE:HD13	1:B:156:GLN:HG3	2.03	0.40
1:C:521:LEU:O	1:D:25:HIS:HB3	2.21	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:B:460:ASP:OD1	1:D:395:LYS:NZ[1_656]	2.16	0.04

5.3 Torsion angles

5.3.1 Protein backbone

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	1014/1025 (99%)	974 (96%)	32 (3%)	8 (1%)	16	8
1	B	1015/1025 (99%)	967 (95%)	36 (4%)	12 (1%)	10	4
1	C	1014/1025 (99%)	970 (96%)	38 (4%)	6 (1%)	21	13
1	D	1016/1025 (99%)	972 (96%)	34 (3%)	10 (1%)	12	5
All	All	4059/4100 (99%)	3883 (96%)	140 (3%)	36 (1%)	14	6

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	904	PHE
1	A	908	GLU
1	B	675	MET
1	B	677	GLU
1	B	906	PRO
1	C	678	ARG
1	C	872	MET
1	D	415	GLU
1	D	867	ARG
1	D	903	ALA
1	D	906	PRO
1	D	1017	LEU
1	A	901	ASN
1	B	416	THR
1	B	903	ALA
1	B	908	GLU
1	C	414	ASP
1	C	674	GLY
1	D	676	GLY
1	A	907	LEU
1	B	3	PRO
1	B	321	MET

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Mol	Chain	Res	Type
1	D	3	PRO
1	D	908	GLU
1	D	1018	PRO
1	A	417	GLY
1	A	678	ARG
1	B	905	PRO
1	C	680	MET
1	D	866	PRO
1	A	175	CYS
1	A	906	PRO
1	B	175	CYS
1	B	676	GLY
1	C	3	PRO
1	B	904	PHE

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	846/854 (99%)	827 (98%)	19 (2%)	45	42
1	B	847/854 (99%)	840 (99%)	7 (1%)	73	75
1	C	846/854 (99%)	833 (98%)	13 (2%)	57	56
1	D	848/854 (99%)	840 (99%)	8 (1%)	70	73
All	All	3387/3416 (99%)	3340 (99%)	47 (1%)	59	59

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	ARG
1	A	95	LEU
1	A	100	PHE
1	A	133	SER
1	A	273	GLU
1	A	368	VAL
1	A	407	GLN

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Mol	Chain	Res	Type
1	A	453	PRO
1	A	483	VAL
1	A	541	LYS
1	A	656	LYS
1	A	677	GLU
1	A	793	THR
1	A	800	GLU
1	A	845	GLU
1	A	906	PRO
1	A	932	LEU
1	A	955	ASN
1	A	1017	LEU
1	B	95	LEU
1	B	100	PHE
1	B	273	GLU
1	B	453	PRO
1	B	793	THR
1	B	845	GLU
1	B	907	LEU
1	C	100	PHE
1	C	184	GLU
1	C	259	LYS
1	C	326	SER
1	C	331	ILE
1	C	453	PRO
1	C	758	LYS
1	C	793	THR
1	C	800	GLU
1	C	845	GLU
1	C	896	ARG
1	C	941	ILE
1	C	1017	LEU
1	D	15	ILE
1	D	95	LEU
1	D	100	PHE
1	D	453	PRO
1	D	599	MET
1	D	673	HIS
1	D	800	GLU
1	D	845	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	ASN
1	A	295	GLN
1	A	413	GLN
1	A	623	GLN
1	A	646	ASN
1	A	693	ASN
1	A	878	ASN
1	A	900	GLN
1	A	930	GLN
1	B	23	GLN
1	B	242	ASN
1	B	413	GLN
1	B	494	ASN
1	B	623	GLN
1	B	847	GLN
1	B	878	ASN
1	B	930	GLN
1	C	57	ASN
1	C	295	GLN
1	C	407	GLN
1	C	623	GLN
1	C	828	GLN
1	C	859	HIS
1	C	930	GLN
1	C	972	GLN
1	C	978	HIS
1	D	242	ASN
1	D	498	GLN
1	D	623	GLN
1	D	673	HIS
1	D	878	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

24 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	SF4	C	1029	1	0,12,12	-	-	-		
2	SF4	C	1027	1	0,12,12	-	-	-		
2	SF4	B	1027	1	0,12,12	-	-	-		
2	SF4	B	1029	1	0,12,12	-	-	-		
2	SF4	C	1028	1	0,12,12	-	-	-		
2	SF4	D	1027	1	0,12,12	-	-	-		
2	SF4	C	1026	1	0,12,12	-	-	-		
2	SF4	A	1029	1	0,12,12	-	-	-		
2	SF4	B	1028	1	0,12,12	-	-	-		
2	SF4	D	1029	1	0,12,12	-	-	-		
2	SF4	A	1026	1	0,12,12	-	-	-		
4	FAD	B	1031	-	58,58,58	2.29	23 (39%)	85,89,89	1.65	8 (9%)
3	FMN	B	1030	-	33,33,33	1.92	9 (27%)	48,50,50	1.86	12 (25%)
2	SF4	A	1028	1	0,12,12	-	-	-		
3	FMN	D	1030	-	33,33,33	1.95	9 (27%)	48,50,50	1.84	11 (22%)
2	SF4	A	1027	1	0,12,12	-	-	-		
2	SF4	D	1028	1	0,12,12	-	-	-		
2	SF4	B	1026	1	0,12,12	-	-	-		
2	SF4	D	1026	1	0,12,12	-	-	-		
4	FAD	A	1031	-	58,58,58	2.27	25 (43%)	85,89,89	1.66	8 (9%)
4	FAD	C	1031	-	58,58,58	2.22	22 (37%)	85,89,89	1.63	9 (10%)
3	FMN	A	1030	-	33,33,33	1.94	10 (30%)	48,50,50	1.85	11 (22%)
3	FMN	C	1030	-	33,33,33	2.01	9 (27%)	48,50,50	1.85	12 (25%)
4	FAD	D	1031	-	58,58,58	2.31	22 (37%)	85,89,89	1.64	8 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SF4	C	1029	1	-	-	0/6/5/5
2	SF4	C	1027	1	-	-	0/6/5/5
2	SF4	C	1028	1	-	-	0/6/5/5
2	SF4	B	1027	1	-	-	0/6/5/5
2	SF4	B	1029	1	-	-	0/6/5/5
2	SF4	D	1027	1	-	-	0/6/5/5
2	SF4	C	1026	1	-	-	0/6/5/5
2	SF4	A	1029	1	-	-	0/6/5/5
2	SF4	B	1028	1	-	-	0/6/5/5
2	SF4	D	1029	1	-	-	0/6/5/5
2	SF4	A	1026	1	-	-	0/6/5/5
4	FAD	B	1031	-	-	5/34/50/50	0/6/6/6
3	FMN	B	1030	-	-	1/18/18/18	0/3/3/3
2	SF4	A	1028	1	-	-	0/6/5/5
3	FMN	D	1030	-	-	1/18/18/18	0/3/3/3
2	SF4	A	1027	1	-	-	0/6/5/5
2	SF4	D	1028	1	-	-	0/6/5/5
2	SF4	B	1026	1	-	-	0/6/5/5
2	SF4	D	1026	1	-	-	0/6/5/5
4	FAD	C	1031	-	-	4/34/50/50	0/6/6/6
4	FAD	A	1031	-	-	4/34/50/50	0/6/6/6
3	FMN	A	1030	-	-	1/18/18/18	0/3/3/3
3	FMN	C	1030	-	-	1/18/18/18	0/3/3/3
4	FAD	D	1031	-	-	5/34/50/50	0/6/6/6

All (129) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1031	FAD	PA-O3P	9.00	1.69	1.59
4	B	1031	FAD	PA-O3P	8.68	1.68	1.59
4	C	1031	FAD	PA-O3P	8.11	1.68	1.59
4	A	1031	FAD	PA-O3P	8.10	1.68	1.59
4	A	1031	FAD	P-O3P	-7.02	1.51	1.59
4	D	1031	FAD	P-O3P	-6.70	1.52	1.59
4	B	1031	FAD	P-O3P	-6.42	1.52	1.59
4	C	1031	FAD	P-O3P	-5.96	1.53	1.59
3	A	1030	FMN	C7M-C7	4.63	1.59	1.51
3	D	1030	FMN	C4A-N5	4.58	1.40	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1030	FMN	C7M-C7	4.57	1.59	1.51
3	C	1030	FMN	C4A-N5	4.55	1.40	1.30
3	A	1030	FMN	C4A-N5	4.53	1.40	1.30
3	C	1030	FMN	C7M-C7	4.50	1.59	1.51
3	D	1030	FMN	C7M-C7	4.32	1.59	1.51
4	D	1031	FAD	PA-O2A	-4.28	1.35	1.55
4	C	1031	FAD	PA-O2A	-4.26	1.35	1.55
3	B	1030	FMN	C4A-N5	4.24	1.39	1.30
4	B	1031	FAD	PA-O2A	-4.18	1.36	1.55
4	A	1031	FAD	PA-O2A	-4.13	1.36	1.55
3	C	1030	FMN	C9A-C5A	3.92	1.47	1.41
3	C	1030	FMN	C1'-N10	-3.76	1.38	1.47
3	A	1030	FMN	C1'-N10	-3.73	1.38	1.47
3	D	1030	FMN	C1'-N10	-3.70	1.38	1.47
3	B	1030	FMN	C1'-N10	-3.55	1.39	1.47
4	B	1031	FAD	C9A-N10	3.55	1.47	1.41
4	D	1031	FAD	P-O2P	-3.53	1.39	1.55
4	C	1031	FAD	C4X-N5	3.52	1.38	1.30
4	C	1031	FAD	C9A-N10	3.48	1.47	1.41
3	C	1030	FMN	C4'-C3'	3.45	1.59	1.53
4	A	1031	FAD	C4X-N5	3.43	1.38	1.30
4	A	1031	FAD	P-O2P	-3.43	1.39	1.55
4	A	1031	FAD	C9A-N10	3.42	1.47	1.41
4	B	1031	FAD	P-O2P	-3.42	1.39	1.55
4	D	1031	FAD	C4X-N5	3.40	1.38	1.30
4	C	1031	FAD	P-O2P	-3.40	1.39	1.55
3	B	1030	FMN	C9A-C5A	3.38	1.46	1.41
4	B	1031	FAD	C4X-N5	3.38	1.38	1.30
3	A	1030	FMN	C4'-C3'	3.29	1.59	1.53
4	D	1031	FAD	C9A-C5X	3.28	1.46	1.41
3	D	1030	FMN	C9A-C5A	3.21	1.46	1.41
3	D	1030	FMN	C4'-C3'	3.20	1.59	1.53
4	D	1031	FAD	C9A-N10	3.17	1.46	1.41
4	A	1031	FAD	C9A-C5X	3.13	1.46	1.41
3	B	1030	FMN	C4'-C3'	3.07	1.58	1.53
3	C	1030	FMN	C9A-N10	3.06	1.46	1.41
4	B	1031	FAD	C9A-C5X	3.06	1.46	1.41
4	A	1031	FAD	C8-C7	3.04	1.48	1.40
4	D	1031	FAD	C8-C7	3.02	1.48	1.40
4	B	1031	FAD	C8-C7	3.01	1.48	1.40
4	C	1031	FAD	C9A-C5X	2.96	1.46	1.41
3	A	1030	FMN	C9A-N10	2.91	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1030	FMN	C9A-C5A	2.87	1.45	1.41
4	A	1031	FAD	O5'-C5'	2.86	1.55	1.44
4	C	1031	FAD	C8-C7	2.85	1.47	1.40
3	D	1030	FMN	C9A-N10	2.79	1.46	1.41
4	C	1031	FAD	O5'-C5'	2.78	1.55	1.44
4	B	1031	FAD	C6-C5X	2.77	1.44	1.40
3	D	1030	FMN	C1'-C2'	2.76	1.56	1.52
4	B	1031	FAD	O5'-C5'	2.76	1.55	1.44
4	D	1031	FAD	O5'-C5'	2.74	1.55	1.44
4	A	1031	FAD	C6-C5X	2.66	1.44	1.40
4	B	1031	FAD	C10-N1	2.66	1.38	1.33
3	A	1030	FMN	C1'-C2'	2.61	1.56	1.52
3	B	1030	FMN	C9A-N10	2.60	1.45	1.41
4	D	1031	FAD	C4A-N3A	2.57	1.39	1.34
4	C	1031	FAD	C6-C5X	2.57	1.43	1.40
4	A	1031	FAD	C4A-N3A	2.56	1.39	1.34
4	C	1031	FAD	C4A-N3A	2.56	1.39	1.34
4	B	1031	FAD	O4B-C4B	2.53	1.50	1.45
4	A	1031	FAD	C9-C9A	2.52	1.43	1.39
4	C	1031	FAD	C5A-C4A	2.51	1.43	1.39
3	B	1030	FMN	C1'-C2'	2.51	1.56	1.52
4	B	1031	FAD	C9-C9A	2.49	1.43	1.39
4	C	1031	FAD	C10-N1	2.47	1.38	1.33
4	D	1031	FAD	C6-C5X	2.46	1.43	1.40
4	D	1031	FAD	C9-C9A	2.45	1.43	1.39
4	B	1031	FAD	C5A-C4A	2.43	1.43	1.39
3	C	1030	FMN	C1'-C2'	2.41	1.56	1.52
4	A	1031	FAD	C10-N1	2.41	1.38	1.33
4	C	1031	FAD	C5A-C6A	2.41	1.47	1.41
3	D	1030	FMN	C10-N1	2.39	1.38	1.33
4	D	1031	FAD	C5A-C6A	2.39	1.47	1.41
4	B	1031	FAD	C5A-C6A	2.38	1.47	1.41
4	B	1031	FAD	C4A-N3A	2.36	1.38	1.34
4	C	1031	FAD	C2A-N1A	2.36	1.38	1.33
4	C	1031	FAD	O4B-C4B	2.32	1.50	1.45
4	D	1031	FAD	O4B-C4B	2.30	1.50	1.45
4	D	1031	FAD	C5B-C4B	2.29	1.58	1.51
4	A	1031	FAD	C5A-C6A	2.29	1.47	1.41
4	C	1031	FAD	P-O5'	-2.27	1.50	1.59
4	D	1031	FAD	C2-N3	2.27	1.44	1.39
4	B	1031	FAD	C5B-C4B	2.26	1.58	1.51
4	C	1031	FAD	O4B-C1B	2.26	1.47	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1031	FAD	O4B-C4B	2.25	1.50	1.45
4	B	1031	FAD	O4B-C1B	2.24	1.47	1.42
4	B	1031	FAD	C2A-N1A	2.24	1.37	1.33
4	B	1031	FAD	C2-N3	2.23	1.43	1.39
4	D	1031	FAD	C10-N1	2.23	1.37	1.33
3	B	1030	FMN	C10-N1	2.23	1.37	1.33
4	C	1031	FAD	C2-N3	2.21	1.43	1.39
3	B	1030	FMN	C6-C7	2.21	1.42	1.39
4	D	1031	FAD	P-O5'	-2.20	1.50	1.59
4	C	1031	FAD	C5B-C4B	2.19	1.58	1.51
3	C	1030	FMN	C10-N1	2.19	1.37	1.33
4	B	1031	FAD	P-O5'	-2.19	1.50	1.59
4	A	1031	FAD	C2A-N1A	2.18	1.37	1.33
4	A	1031	FAD	C5A-C4A	2.18	1.43	1.39
4	D	1031	FAD	C2A-N1A	2.14	1.37	1.33
4	D	1031	FAD	C9-C8	2.14	1.42	1.39
4	A	1031	FAD	C9-C8	2.13	1.42	1.39
4	A	1031	FAD	C2-N3	2.12	1.43	1.39
3	D	1030	FMN	C6-C7	2.10	1.42	1.39
4	C	1031	FAD	C3B-C4B	2.10	1.58	1.53
4	A	1031	FAD	C3B-C4B	2.08	1.58	1.53
4	B	1031	FAD	C9-C8	2.08	1.42	1.39
4	A	1031	FAD	C5B-C4B	2.08	1.57	1.51
4	D	1031	FAD	C5A-C4A	2.08	1.42	1.39
3	A	1030	FMN	C10-N1	2.07	1.37	1.33
3	C	1030	FMN	C6-C7	2.07	1.42	1.39
4	C	1031	FAD	C9-C9A	2.06	1.43	1.39
4	D	1031	FAD	C3B-C4B	2.06	1.58	1.53
3	A	1030	FMN	C8M-C8	2.05	1.54	1.51
3	A	1030	FMN	C6-C7	2.05	1.42	1.39
4	A	1031	FAD	O2-C2	-2.04	1.20	1.24
4	A	1031	FAD	P-O5'	-2.01	1.51	1.59
4	B	1031	FAD	C3B-C4B	2.01	1.58	1.53
4	A	1031	FAD	PA-O5B	-2.01	1.51	1.59
4	A	1031	FAD	O4B-C1B	2.00	1.46	1.42

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1031	FAD	O3P-PA-O1A	-8.60	84.84	110.70
4	D	1031	FAD	O3P-PA-O1A	-8.54	85.00	110.70
4	B	1031	FAD	O3P-PA-O1A	-8.48	85.20	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	1031	FAD	O3P-PA-O1A	-8.25	85.88	110.70
4	C	1031	FAD	O2A-PA-O3P	-7.05	88.22	107.27
4	B	1031	FAD	O2A-PA-O3P	-7.01	88.33	107.27
4	A	1031	FAD	O2A-PA-O3P	-6.86	88.74	107.27
4	D	1031	FAD	O2A-PA-O3P	-6.77	88.98	107.27
3	B	1030	FMN	C10-N1-C2	4.72	127.07	116.85
3	D	1030	FMN	C10-N1-C2	4.71	127.05	116.85
3	C	1030	FMN	C10-N1-C2	4.69	127.01	116.85
3	A	1030	FMN	C10-N1-C2	4.66	126.93	116.85
3	C	1030	FMN	C4A-C10-N1	-4.02	114.74	124.59
3	C	1030	FMN	O4'-C4'-C3'	3.98	118.56	109.25
3	D	1030	FMN	C4A-C10-N1	-3.97	114.85	124.59
3	D	1030	FMN	O3'-C3'-C2'	-3.97	99.91	108.93
3	B	1030	FMN	C4-C4A-C10	3.96	123.72	116.93
3	A	1030	FMN	O3'-C3'-C2'	-3.96	99.94	108.93
3	A	1030	FMN	C4A-C10-N1	-3.95	114.90	124.59
3	C	1030	FMN	C4-C4A-C10	3.94	123.69	116.93
3	B	1030	FMN	C4A-C10-N1	-3.93	114.94	124.59
3	A	1030	FMN	O4'-C4'-C3'	3.93	118.44	109.25
3	D	1030	FMN	C4-C4A-C10	3.91	123.64	116.93
3	A	1030	FMN	C4-C4A-C10	3.91	123.63	116.93
3	D	1030	FMN	O4'-C4'-C3'	3.83	118.20	109.25
3	B	1030	FMN	O3'-C3'-C2'	-3.82	100.26	108.93
3	B	1030	FMN	O4'-C4'-C3'	3.79	118.13	109.25
4	D	1031	FAD	O2A-PA-O1A	3.77	129.99	112.44
4	A	1031	FAD	O2A-PA-O1A	3.72	129.75	112.44
4	B	1031	FAD	O2A-PA-O1A	3.69	129.62	112.44
3	C	1030	FMN	O3'-C3'-C2'	-3.66	100.62	108.93
4	C	1031	FAD	O2A-PA-O1A	3.53	128.89	112.44
3	C	1030	FMN	C5'-C4'-C3'	-3.15	106.27	112.22
3	A	1030	FMN	C5'-C4'-C3'	-3.15	106.28	112.22
3	D	1030	FMN	C5'-C4'-C3'	-3.07	106.42	112.22
3	B	1030	FMN	C5'-C4'-C3'	-3.04	106.48	112.22
4	B	1031	FAD	C5'-C4'-C3'	-2.96	106.62	112.22
4	A	1031	FAD	O4B-C1B-N9A	-2.84	102.64	108.09
4	B	1031	FAD	O4B-C1B-N9A	-2.83	102.65	108.09
4	C	1031	FAD	O4B-C1B-N9A	-2.82	102.67	108.09
4	D	1031	FAD	O4B-C1B-N9A	-2.82	102.67	108.09
4	C	1031	FAD	C5'-C4'-C3'	-2.82	106.90	112.22
4	D	1031	FAD	C5'-C4'-C3'	-2.78	106.97	112.22
3	C	1030	FMN	C4A-C10-N10	2.76	120.43	116.48
3	D	1030	FMN	C4A-C10-N10	2.69	120.33	116.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1030	FMN	C4A-C10-N10	2.69	120.33	116.48
3	B	1030	FMN	C4A-C10-N10	2.67	120.31	116.48
4	A	1031	FAD	C2A-N1A-C6A	2.65	123.09	118.73
4	A	1031	FAD	C5'-C4'-C3'	-2.65	107.22	112.22
3	B	1030	FMN	O3'-C3'-C4'	2.63	114.92	108.93
4	B	1031	FAD	C2A-N1A-C6A	2.52	122.87	118.73
4	D	1031	FAD	C2A-N1A-C6A	2.47	122.79	118.73
3	D	1030	FMN	O3'-C3'-C4'	2.43	114.45	108.93
4	C	1031	FAD	C2A-N1A-C6A	2.42	122.71	118.73
3	A	1030	FMN	O3'-C3'-C4'	2.41	114.40	108.93
4	A	1031	FAD	C5X-C9A-N10	-2.34	115.85	117.97
3	C	1030	FMN	O3'-C3'-C4'	2.33	114.23	108.93
3	C	1030	FMN	C4-C4A-N5	-2.25	115.10	118.21
4	A	1031	FAD	C4-N3-C2	-2.22	121.70	125.64
4	B	1031	FAD	C5X-C9A-N10	-2.19	115.99	117.97
4	C	1031	FAD	C5X-C9A-N10	-2.18	116.00	117.97
4	D	1031	FAD	C5X-C9A-N10	-2.18	116.00	117.97
4	B	1031	FAD	C4-N3-C2	-2.16	121.81	125.64
3	C	1030	FMN	C6-C5A-C9A	2.15	122.01	119.05
3	C	1030	FMN	N10-C10-N1	2.14	124.80	118.51
3	D	1030	FMN	N10-C10-N1	2.14	124.80	118.51
3	B	1030	FMN	C6-C5A-C9A	2.14	121.98	119.05
3	A	1030	FMN	N10-C10-N1	2.13	124.77	118.51
3	B	1030	FMN	C4-C4A-N5	-2.12	115.27	118.21
4	C	1031	FAD	C4-N3-C2	-2.12	121.87	125.64
3	B	1030	FMN	N10-C10-N1	2.12	124.75	118.51
3	A	1030	FMN	C6-C5A-C9A	2.11	121.95	119.05
4	C	1031	FAD	O2A-PA-O5B	2.10	117.11	107.57
3	B	1030	FMN	N3-C2-N1	-2.10	115.05	119.50
4	D	1031	FAD	C4-N3-C2	-2.09	121.94	125.64
3	D	1030	FMN	N3-C2-N1	-2.08	115.07	119.50
3	D	1030	FMN	C4-C4A-N5	-2.06	115.36	118.21
3	C	1030	FMN	O4'-C4'-C5'	2.01	114.43	109.99
3	A	1030	FMN	N3-C2-N1	-2.00	115.25	119.50

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1031	FAD	C5B-O5B-PA-O1A
4	A	1031	FAD	PA-O3P-P-O5'
4	B	1031	FAD	C5B-O5B-PA-O1A

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Mol	Chain	Res	Type	Atoms
4	B	1031	FAD	PA-O3P-P-O5'
4	C	1031	FAD	C5B-O5B-PA-O1A
4	C	1031	FAD	PA-O3P-P-O5'
4	D	1031	FAD	C5B-O5B-PA-O1A
4	D	1031	FAD	PA-O3P-P-O5'
3	C	1030	FMN	C4'-C5'-O5'-P
3	A	1030	FMN	C4'-C5'-O5'-P
3	D	1030	FMN	C4'-C5'-O5'-P
4	A	1031	FAD	C2B-C1B-N9A-C8A
4	B	1031	FAD	C2B-C1B-N9A-C8A
4	C	1031	FAD	C2B-C1B-N9A-C8A
4	D	1031	FAD	C2B-C1B-N9A-C8A
3	B	1030	FMN	C4'-C5'-O5'-P
4	B	1031	FAD	P-O3P-PA-O1A
4	D	1031	FAD	P-O3P-PA-O1A
4	D	1031	FAD	P-O3P-PA-O2A
4	A	1031	FAD	P-O3P-PA-O2A
4	B	1031	FAD	P-O3P-PA-O2A
4	C	1031	FAD	P-O3P-PA-O2A

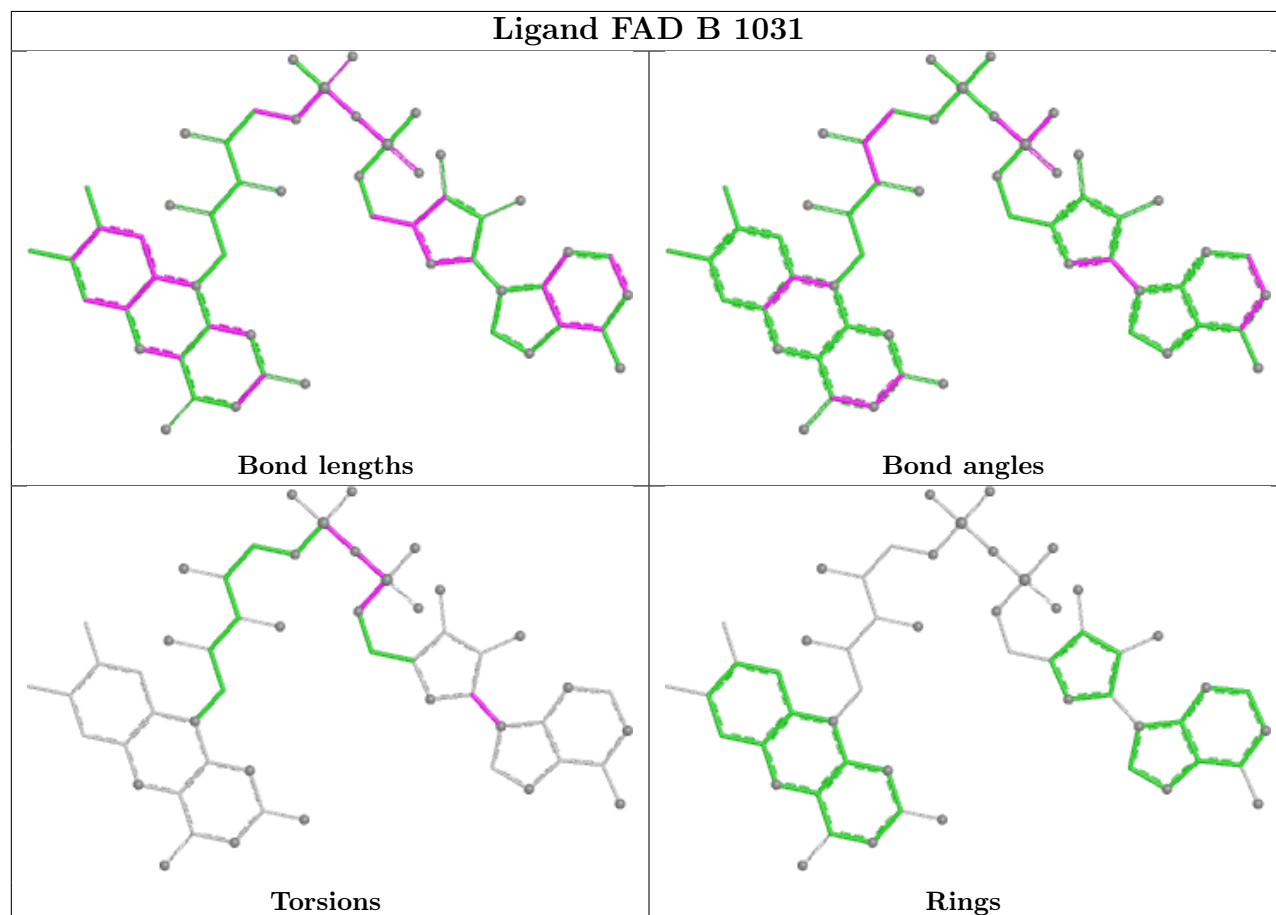
There are no ring outliers.

10 monomers are involved in 12 short contacts:

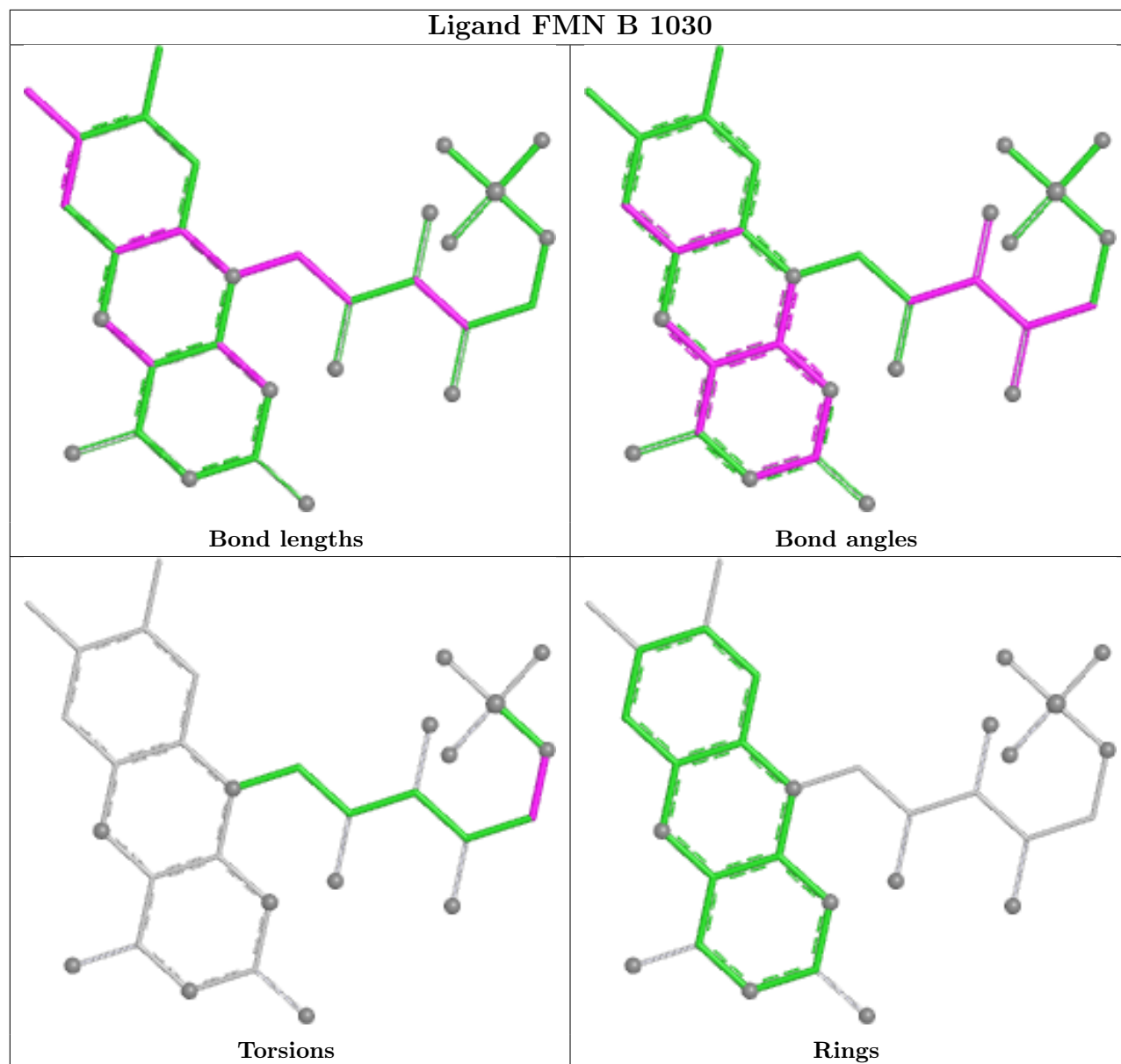
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1027	SF4	1	0
2	D	1027	SF4	1	0
2	C	1026	SF4	1	0
4	B	1031	FAD	2	0
2	A	1027	SF4	1	0
2	B	1026	SF4	1	0
2	D	1026	SF4	1	0
4	A	1031	FAD	1	0
4	C	1031	FAD	2	0
4	D	1031	FAD	1	0

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

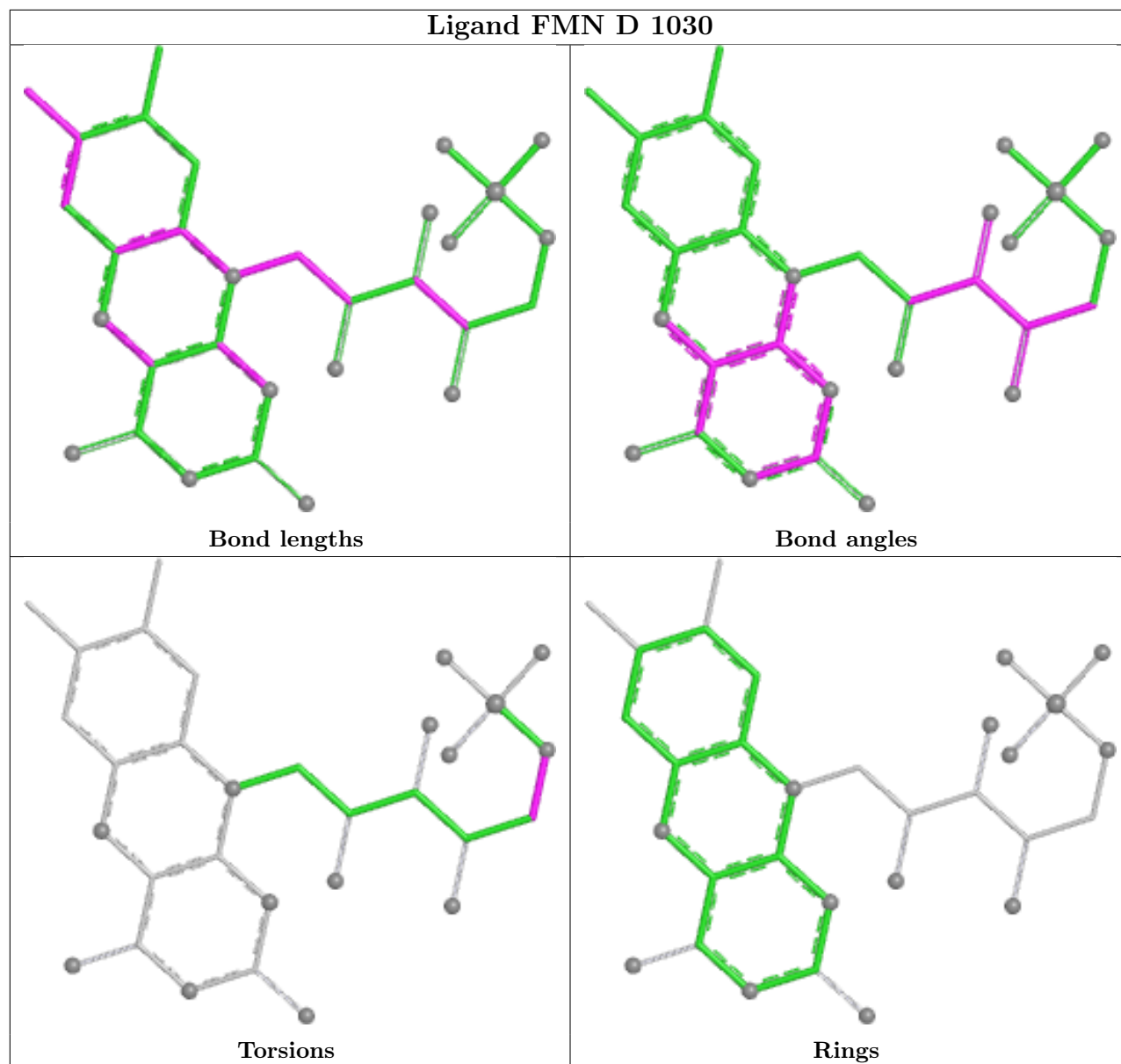
in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

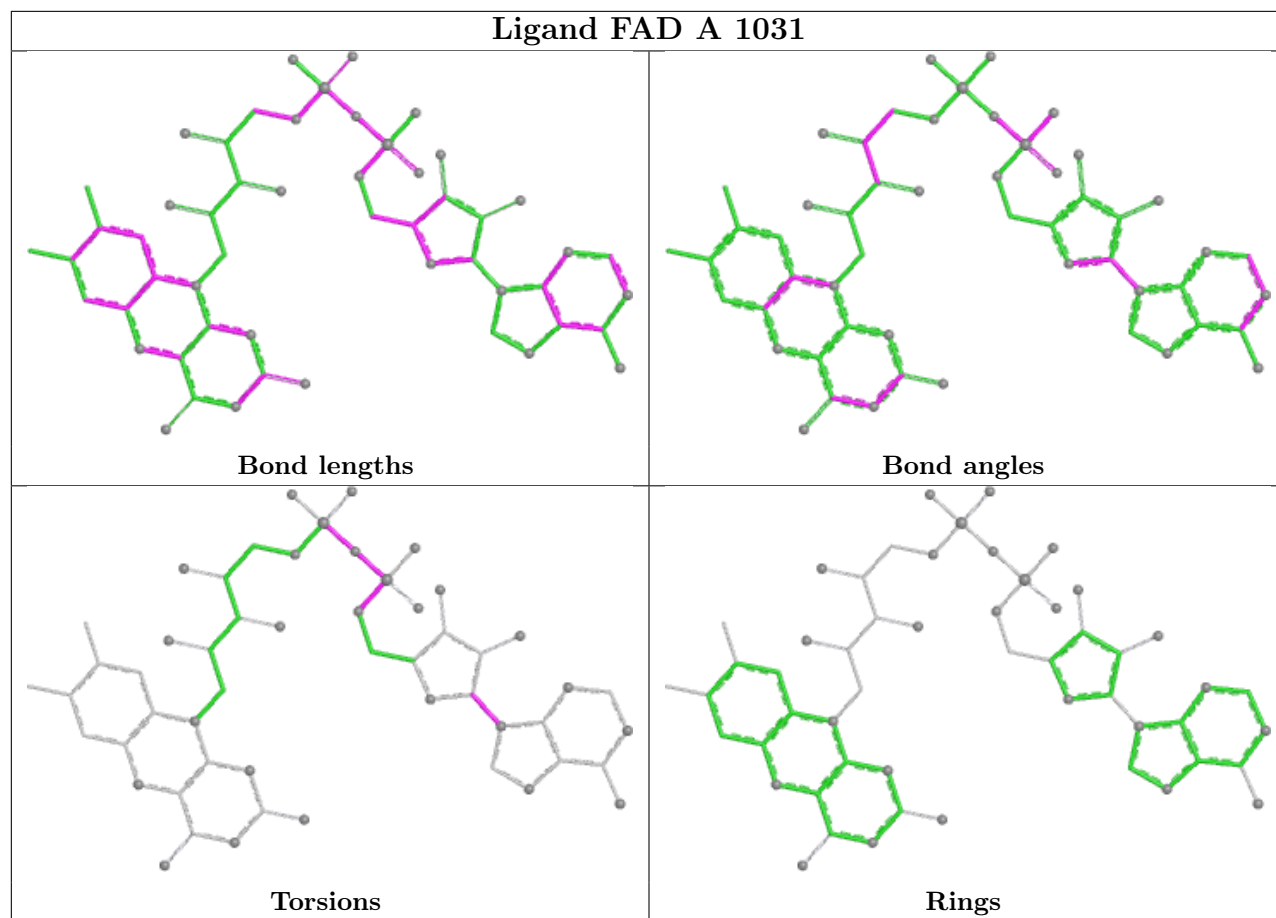


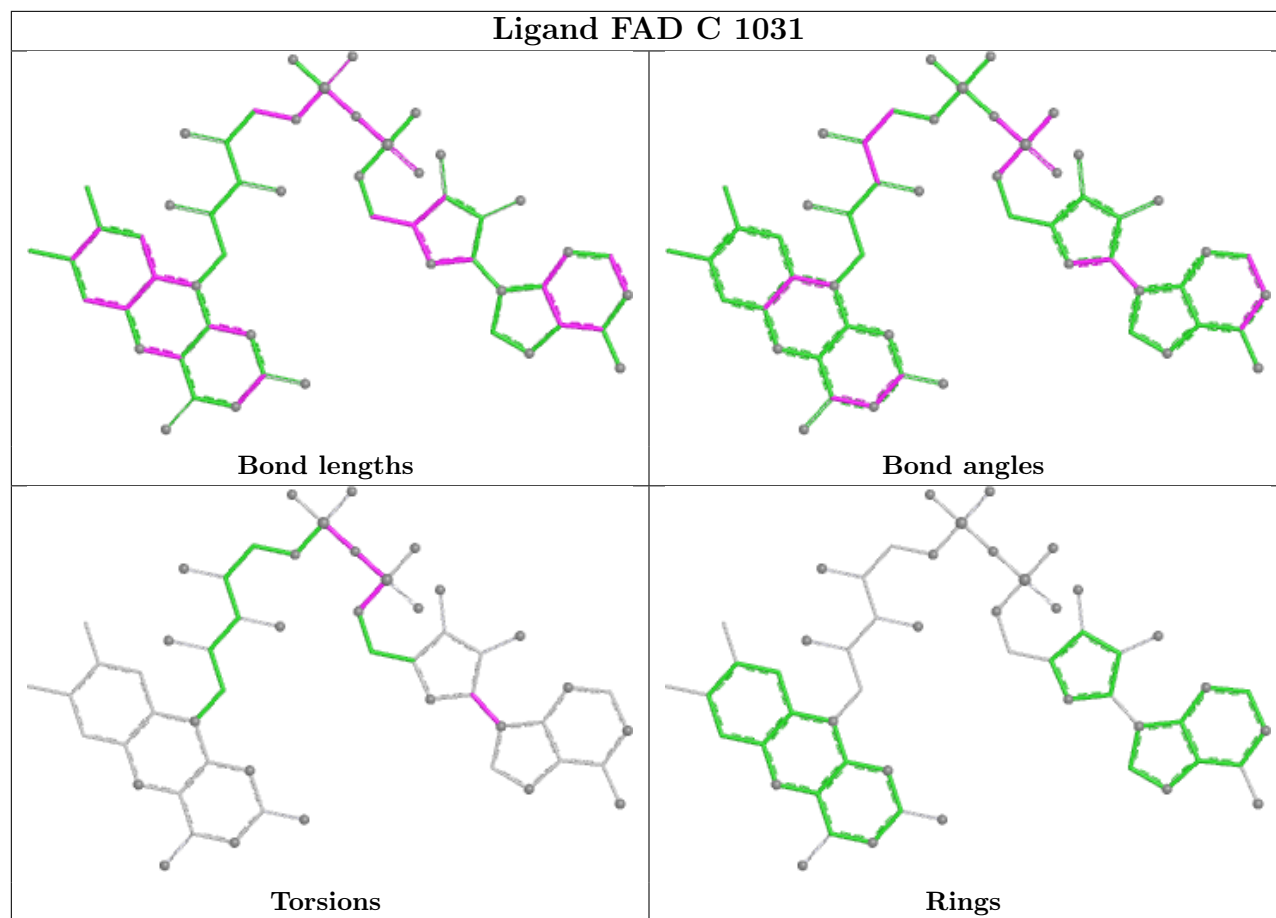
Ligand FMN B 1030



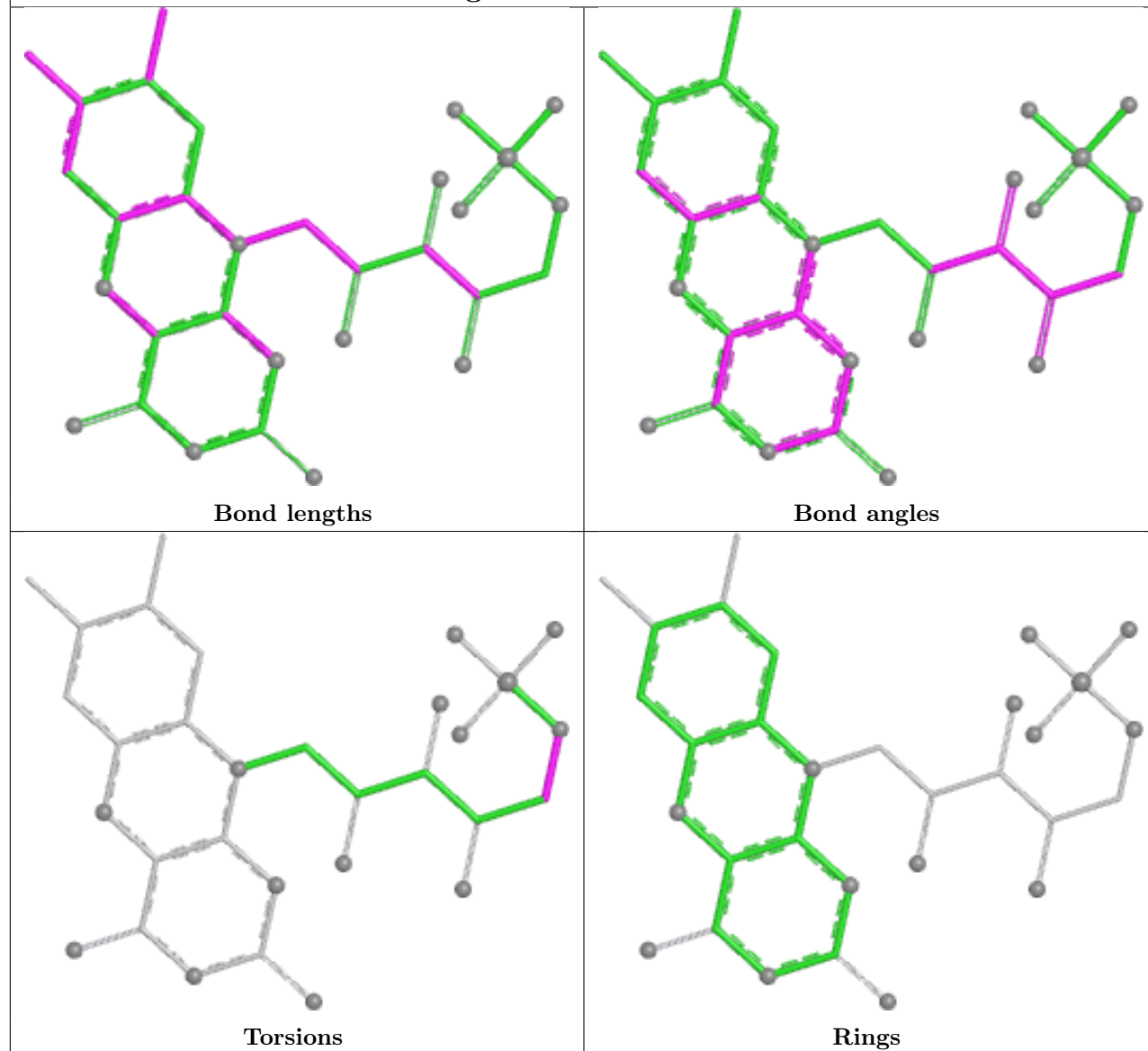
Ligand FMN D 1030



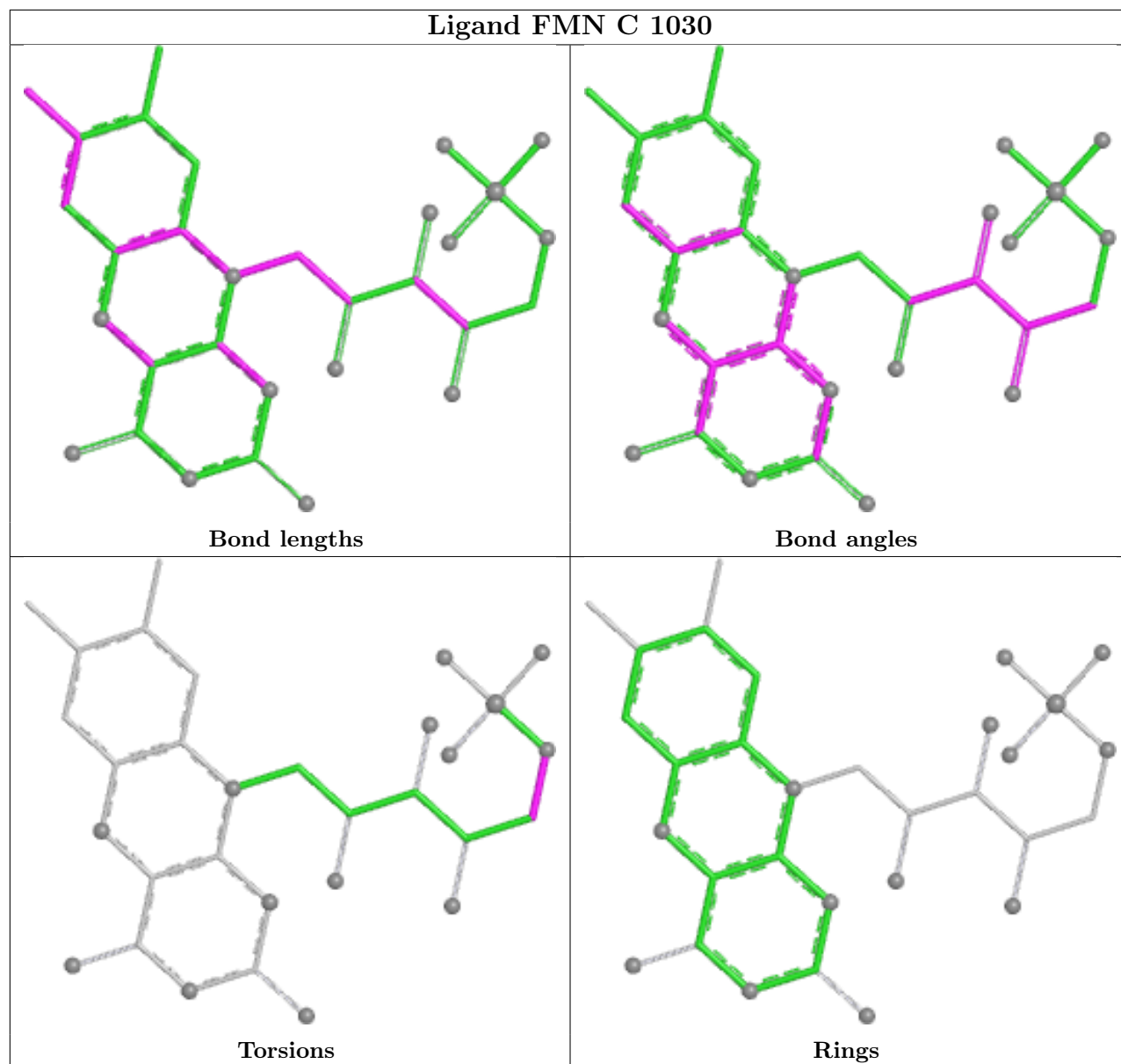


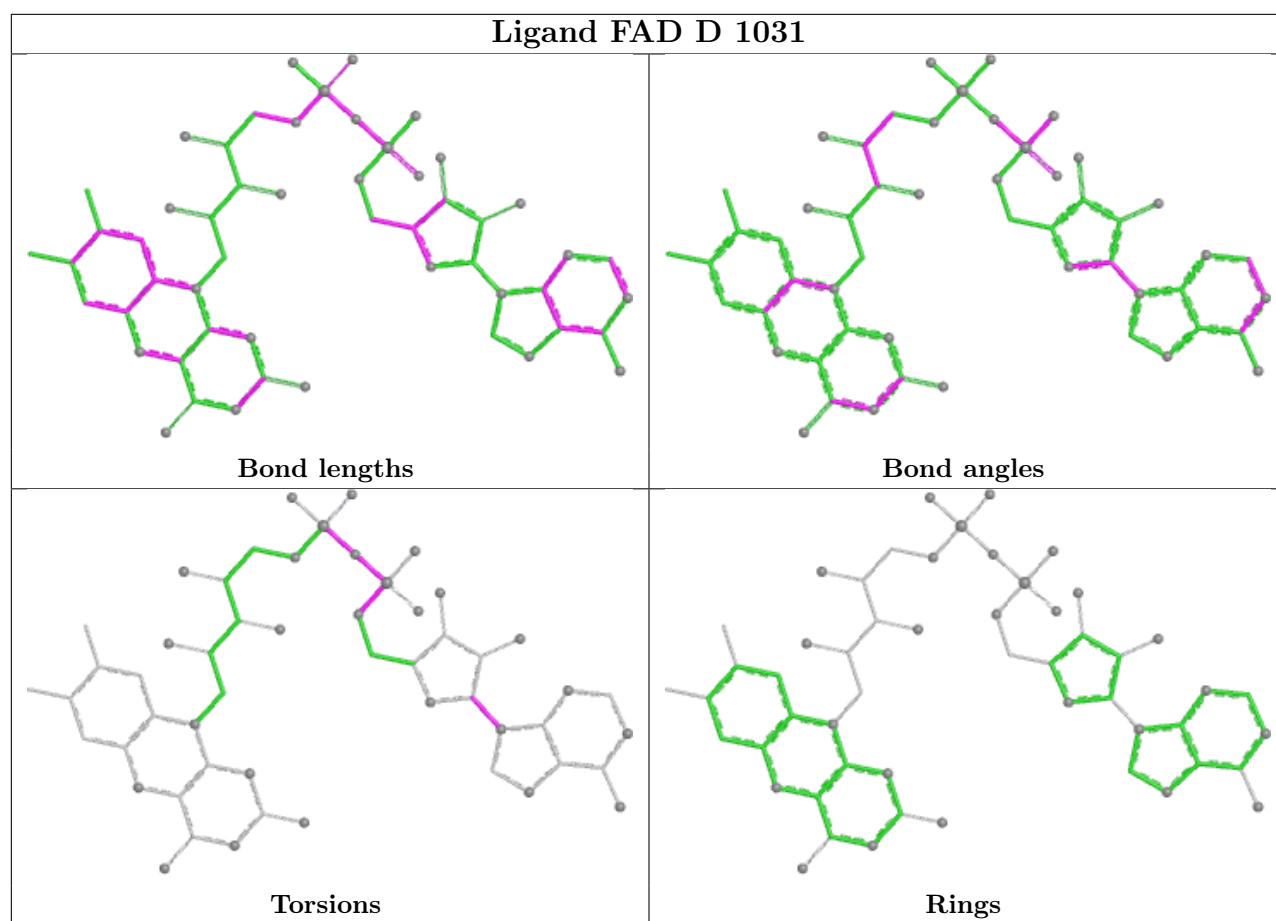


Ligand FMN A 1030



Ligand FMN C 1030





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	1007/1025 (98%)	0.22	84 (8%)	17 18	7, 14, 36, 56	0
1	B	1007/1025 (98%)	0.23	84 (8%)	17 18	6, 14, 36, 55	0
1	C	1012/1025 (98%)	0.24	102 (10%)	12 13	6, 14, 38, 54	0
1	D	1012/1025 (98%)	0.24	104 (10%)	12 12	6, 14, 37, 55	0
All	All	4038/4100 (98%)	0.23	374 (9%)	14 15	6, 14, 37, 56	0

All (374) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1017	LEU	11.3
1	A	2	ALA	11.2
1	A	1017	LEU	10.5
1	B	2	ALA	10.4
1	D	1017	LEU	9.9
1	D	2	ALA	9.6
1	D	52	CYS	9.1
1	C	2	ALA	9.0
1	C	53	GLU	8.2
1	A	52	CYS	7.4
1	B	417	GLY	7.4
1	B	1017	LEU	7.2
1	A	1016	GLY	6.7
1	D	901	ASN	6.6
1	D	51	HIS	6.5
1	C	674	GLY	6.4
1	C	410	ARG	6.2
1	D	902	ALA	6.2
1	C	423	GLU	6.1
1	D	674	GLY	6.0
1	A	902	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	175	CYS	5.8
1	D	50	PHE	5.8
1	C	417	GLY	5.8
1	B	52	CYS	5.6
1	D	868	ILE	5.6
1	B	51	HIS	5.6
1	C	681	GLY	5.5
1	D	679	GLY	5.5
1	B	326	SER	5.5
1	D	866	PRO	5.5
1	D	415	GLU	5.5
1	A	675	MET	5.4
1	A	458	ARG	5.4
1	D	907	LEU	5.4
1	B	415	GLU	5.3
1	C	52	CYS	5.3
1	C	325	HIS	5.3
1	B	907	LEU	5.3
1	C	415	GLU	5.2
1	B	1018	PRO	5.2
1	D	175	CYS	5.2
1	D	53	GLU	5.0
1	B	367	PHE	5.0
1	D	459	TRP	4.9
1	C	869	ALA	4.9
1	B	1011	TYR	4.9
1	B	416	THR	4.8
1	D	909	ARG	4.8
1	A	417	GLY	4.8
1	C	324	CYS	4.7
1	C	180	GLU	4.7
1	A	907	LEU	4.7
1	B	680	MET	4.7
1	C	675	MET	4.7
1	B	175	CYS	4.7
1	C	51	HIS	4.6
1	A	49	CYS	4.6
1	C	326	SER	4.6
1	B	1010	PRO	4.6
1	B	902	ALA	4.6
1	A	324	CYS	4.6
1	D	900	GLN	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	410	ARG	4.6
1	C	459	TRP	4.5
1	C	50	PHE	4.5
1	C	422	ASP	4.5
1	D	1009	THR	4.5
1	B	908	GLU	4.5
1	D	1018	PRO	4.4
1	D	49	CYS	4.3
1	D	367	PHE	4.3
1	A	322	CYS	4.3
1	D	867	ARG	4.3
1	B	459	TRP	4.3
1	B	901	ASN	4.3
1	D	1016	GLY	4.2
1	A	179	GLN	4.2
1	C	682	LEU	4.2
1	D	859	HIS	4.2
1	A	174	PRO	4.2
1	C	873	GLY	4.1
1	A	51	HIS	4.1
1	D	870	GLU	4.1
1	A	416	THR	4.1
1	C	680	MET	4.1
1	D	54	LYS	4.1
1	B	410	ARG	4.0
1	D	908	GLU	4.0
1	B	50	PHE	4.0
1	A	1009	THR	4.0
1	C	175	CYS	3.9
1	A	908	GLU	3.9
1	C	872	MET	3.9
1	C	867	ARG	3.9
1	B	173	ASN	3.9
1	D	899	GLU	3.9
1	B	868	ILE	3.9
1	A	682	LEU	3.8
1	A	11	ASP	3.8
1	B	900	GLN	3.8
1	A	410	ARG	3.8
1	C	909	ARG	3.8
1	D	1011	TYR	3.8
1	B	673	HIS	3.7

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Mol	Chain	Res	Type	RSRZ
1	D	675	MET	3.7
1	D	423	GLU	3.7
1	D	3	PRO	3.7
1	C	870	GLU	3.7
1	C	174	PRO	3.7
1	D	416	THR	3.7
1	C	458	ARG	3.7
1	C	426	ILE	3.7
1	A	909	ARG	3.7
1	B	421	GLU	3.6
1	B	323	ALA	3.6
1	A	53	GLU	3.6
1	B	520	GLU	3.6
1	C	1010	PRO	3.6
1	D	872	MET	3.6
1	B	53	GLU	3.5
1	B	859	HIS	3.5
1	B	174	PRO	3.5
1	A	867	ARG	3.5
1	A	870	GLU	3.5
1	B	375	GLU	3.5
1	B	869	ALA	3.5
1	B	681	GLY	3.5
1	C	49	CYS	3.5
1	B	443	ARG	3.5
1	C	332	ARG	3.5
1	A	292	ASP	3.5
1	C	899	GLU	3.5
1	D	273	GLU	3.5
1	B	872	MET	3.5
1	C	420	ASN	3.4
1	A	367	PHE	3.4
1	A	414	ASP	3.4
1	A	375	GLU	3.4
1	D	857	GLU	3.4
1	C	673	HIS	3.4
1	D	1014	LYS	3.4
1	A	415	GLU	3.4
1	C	402	ARG	3.4
1	B	419	TRP	3.4
1	C	367	PHE	3.4
1	C	904	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	900	GLN	3.3
1	B	413	GLN	3.3
1	B	424	ASP	3.3
1	A	681	GLY	3.3
1	B	176	LEU	3.3
1	C	910	LYS	3.3
1	D	856	THR	3.3
1	B	49	CYS	3.3
1	C	330	SER	3.3
1	D	680	MET	3.3
1	B	395	LYS	3.3
1	C	242	ASN	3.3
1	D	913	ILE	3.3
1	A	325	HIS	3.3
1	D	264	ASN	3.3
1	C	264	ASN	3.2
1	C	320	GLY	3.2
1	D	296	GLY	3.2
1	C	419	TRP	3.2
1	A	426	ILE	3.2
1	C	11	ASP	3.2
1	D	176	LEU	3.2
1	C	487	ASN	3.2
1	C	1016	GLY	3.2
1	B	322	CYS	3.2
1	D	414	ASP	3.2
1	D	1019	LEU	3.2
1	A	419	TRP	3.1
1	A	36	LEU	3.1
1	D	865	VAL	3.1
1	D	173	ASN	3.1
1	D	295	GLN	3.1
1	D	419	TRP	3.1
1	D	417	GLY	3.1
1	B	180	GLU	3.1
1	B	458	ARG	3.1
1	C	323	ALA	3.1
1	C	517	ALA	3.1
1	A	1012	GLU	3.1
1	D	291	ASP	3.1
1	D	984	ASP	3.1
1	B	327	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	582	ILE	3.0
1	B	324	CYS	3.0
1	A	674	GLY	3.0
1	D	917	PRO	3.0
1	C	871	LEU	3.0
1	A	859	HIS	3.0
1	A	1010	PRO	3.0
1	C	322	CYS	3.0
1	D	1010	PRO	3.0
1	C	898	LYS	3.0
1	D	896	ARG	3.0
1	D	689	GLU	3.0
1	B	11	ASP	3.0
1	C	908	GLU	3.0
1	A	176	LEU	2.9
1	A	872	MET	2.9
1	A	868	ILE	2.9
1	C	407	GLN	2.9
1	C	414	ASP	2.9
1	D	11	ASP	2.9
1	D	36	LEU	2.9
1	B	418	LYS	2.9
1	B	910	LYS	2.9
1	D	910	LYS	2.9
1	C	329	PRO	2.8
1	D	517	ALA	2.8
1	D	1012	GLU	2.8
1	A	459	TRP	2.8
1	B	899	GLU	2.8
1	C	316	SER	2.8
1	B	847	GLN	2.8
1	C	844	GLU	2.8
1	A	1011	TYR	2.8
1	C	901	ASN	2.8
1	B	696	ARG	2.8
1	C	331	ILE	2.8
1	C	984	ASP	2.8
1	A	901	ASN	2.7
1	D	458	ARG	2.7
1	C	184	GLU	2.7
1	C	902	ALA	2.7
1	B	325	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	423	GLU	2.7
1	A	673	HIS	2.7
1	D	292	ASP	2.7
1	D	599	MET	2.7
1	C	906	PRO	2.7
1	D	330	SER	2.7
1	D	418	LYS	2.7
1	A	273	GLU	2.6
1	C	7	LYS	2.6
1	C	424	ASP	2.6
1	C	179	GLN	2.6
1	C	885	GLN	2.6
1	C	421	GLU	2.6
1	D	874	LYS	2.6
1	A	3	PRO	2.6
1	C	868	ILE	2.6
1	C	896	ARG	2.6
1	B	179	GLN	2.6
1	D	673	HIS	2.6
1	A	402	ARG	2.6
1	D	221	GLU	2.6
1	C	847	GLN	2.5
1	B	682	LEU	2.5
1	A	910	LYS	2.5
1	D	681	GLY	2.5
1	C	22	THR	2.5
1	D	22	THR	2.5
1	D	828	GLN	2.5
1	C	375	GLU	2.5
1	D	180	GLU	2.5
1	B	671	CYS	2.5
1	D	300	ASP	2.5
1	C	430	LYS	2.5
1	A	932	LEU	2.5
1	C	907	LEU	2.5
1	D	293	ILE	2.5
1	D	487	ASN	2.5
1	C	443	ARG	2.5
1	B	427	VAL	2.5
1	A	328	LEU	2.5
1	A	896	ARG	2.5
1	D	371	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	857	GLU	2.5
1	A	422	ASP	2.5
1	A	696	ARG	2.4
1	C	173	ASN	2.4
1	B	428	HIS	2.4
1	C	950	GLU	2.4
1	A	911	PRO	2.4
1	C	897	LEU	2.4
1	D	682	LEU	2.4
1	A	371	ARG	2.4
1	D	885	GLN	2.4
1	D	915	LYS	2.4
1	A	291	ASP	2.4
1	C	371	ARG	2.4
1	D	402	ARG	2.4
1	D	1008	THR	2.4
1	B	873	GLY	2.4
1	A	395	LYS	2.4
1	D	395	LYS	2.4
1	A	424	ASP	2.3
1	A	50	PHE	2.3
1	B	874	LYS	2.3
1	C	516	SER	2.3
1	B	867	ARG	2.3
1	D	179	GLN	2.3
1	C	1008	THR	2.3
1	A	516	SER	2.3
1	B	896	ARG	2.3
1	B	273	GLU	2.3
1	C	13	GLU	2.3
1	A	517	ALA	2.3
1	B	177	PRO	2.3
1	B	1016	GLY	2.3
1	D	167	ASN	2.3
1	A	181	LYS	2.3
1	A	418	LYS	2.3
1	C	36	LEU	2.3
1	A	536	GLU	2.2
1	A	786	PRO	2.2
1	A	844	GLU	2.2
1	B	329	PRO	2.2
1	D	855	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	426	ILE	2.2
1	D	460	ASP	2.2
1	A	515	VAL	2.2
1	C	1014	LYS	2.2
1	D	322	CYS	2.2
1	B	856	THR	2.2
1	B	857	GLU	2.2
1	C	263	GLU	2.2
1	C	300	ASP	2.2
1	D	941	ILE	2.2
1	C	358	ARG	2.2
1	A	412	GLU	2.2
1	D	871	LEU	2.2
1	C	460	ASP	2.2
1	D	174	PRO	2.2
1	D	1013	PRO	2.2
1	B	915	LYS	2.2
1	B	909	ARG	2.2
1	C	696	ARG	2.2
1	A	884	GLU	2.2
1	A	950	GLU	2.2
1	D	950	GLU	2.2
1	C	900	GLN	2.2
1	B	292	ASP	2.2
1	B	1012	GLU	2.1
1	A	22	THR	2.1
1	B	411	THR	2.1
1	C	411	THR	2.1
1	D	424	ASP	2.1
1	D	427	VAL	2.1
1	D	178	SER	2.1
1	A	684	CYS	2.1
1	B	519	PRO	2.1
1	C	48	ASN	2.1
1	B	320	GLY	2.1
1	D	898	LYS	2.1
1	B	221	GLU	2.1
1	D	325	HIS	2.1
1	A	407	GLN	2.1
1	A	885	GLN	2.1
1	A	858	SER	2.1
1	D	364	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	517	ALA	2.1
1	A	898	LYS	2.0
1	B	293	ILE	2.0
1	C	915	LYS	2.0
1	D	873	GLY	2.0
1	A	420	ASN	2.0
1	B	1013	PRO	2.0
1	D	897	LEU	2.0
1	A	460	ASP	2.0
1	B	422	ASP	2.0
1	A	180	GLU	2.0
1	C	892	GLU	2.0
1	C	416	THR	2.0
1	C	327	PRO	2.0
1	C	672	PRO	2.0
1	B	396	VAL	2.0
1	D	443	ARG	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
2	SF4	B	1026	8/8	0.95	0.07	10,10,12,12	0
2	SF4	C	1026	8/8	0.95	0.07	10,10,12,12	0
2	SF4	A	1028	8/8	0.96	0.07	9,11,11,13	0
2	SF4	A	1029	8/8	0.96	0.07	10,11,13,13	0
2	SF4	A	1026	8/8	0.96	0.07	10,10,12,12	0
2	SF4	B	1027	8/8	0.96	0.07	8,9,11,11	0

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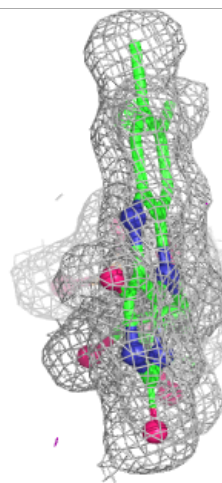
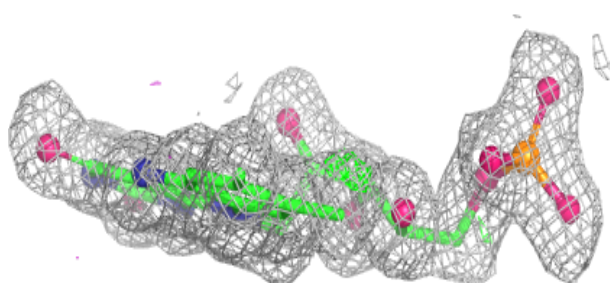
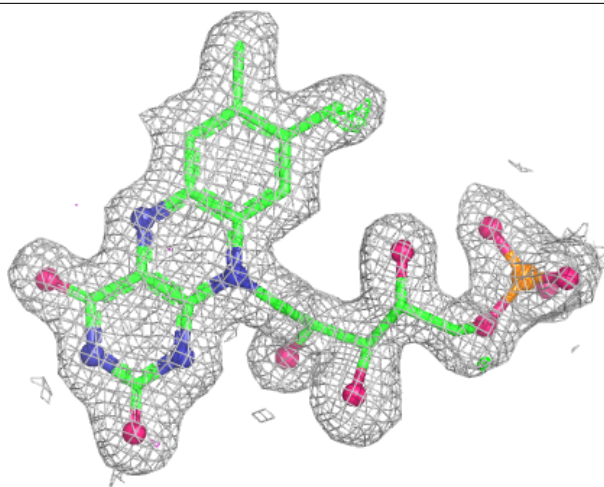
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SF4	B	1028	8/8	0.96	0.07	10,11,12,13	0
2	SF4	B	1029	8/8	0.96	0.07	10,11,13,13	0
2	SF4	A	1027	8/8	0.96	0.07	8,9,11,12	0
2	SF4	C	1027	8/8	0.96	0.07	8,9,11,11	0
2	SF4	C	1028	8/8	0.96	0.06	8,9,10,12	0
2	SF4	C	1029	8/8	0.96	0.07	9,10,12,12	0
2	SF4	D	1026	8/8	0.96	0.07	9,10,11,12	0
2	SF4	D	1027	8/8	0.96	0.07	7,8,10,11	0
2	SF4	D	1028	8/8	0.96	0.07	9,10,12,12	0
2	SF4	D	1029	8/8	0.96	0.07	10,11,12,13	0
3	FMN	A	1030	31/31	0.96	0.07	8,10,13,13	0
3	FMN	B	1030	31/31	0.96	0.07	7,10,12,15	0
3	FMN	C	1030	31/31	0.96	0.06	8,9,12,15	0
4	FAD	A	1031	53/53	0.96	0.06	8,11,13,14	0
4	FAD	B	1031	53/53	0.96	0.07	9,12,14,15	0
4	FAD	D	1031	53/53	0.96	0.06	8,11,13,14	0
4	FAD	C	1031	53/53	0.97	0.06	7,11,14,15	0
3	FMN	D	1030	31/31	0.97	0.06	7,10,12,13	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.

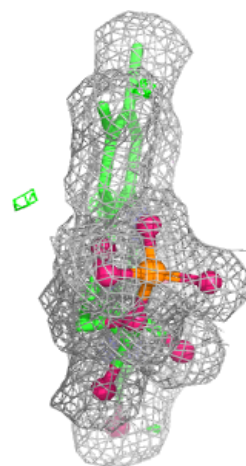
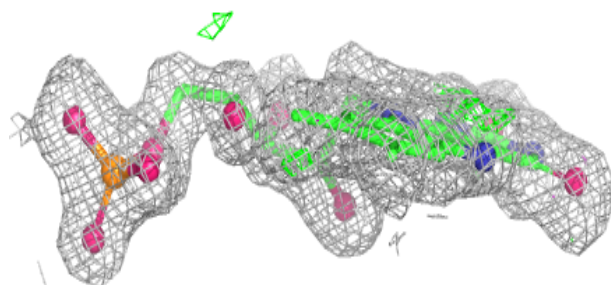
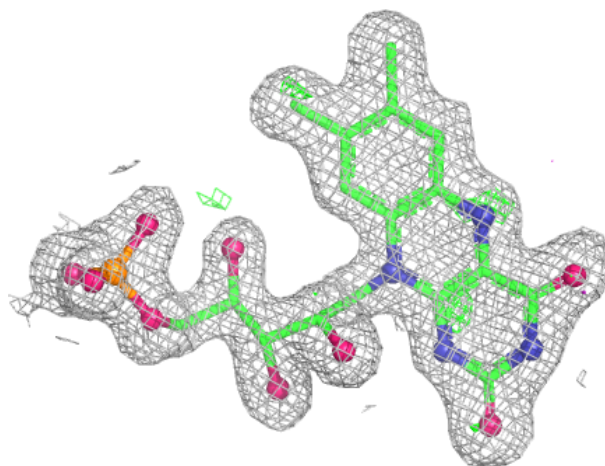
Electron density around FMN A 1030:

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



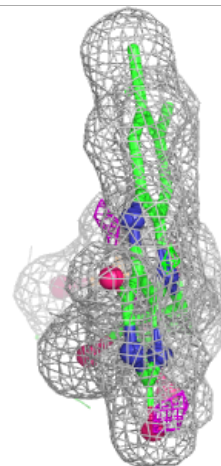
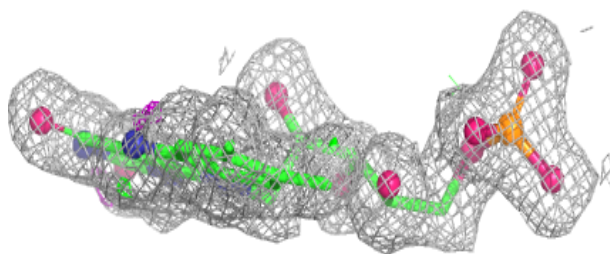
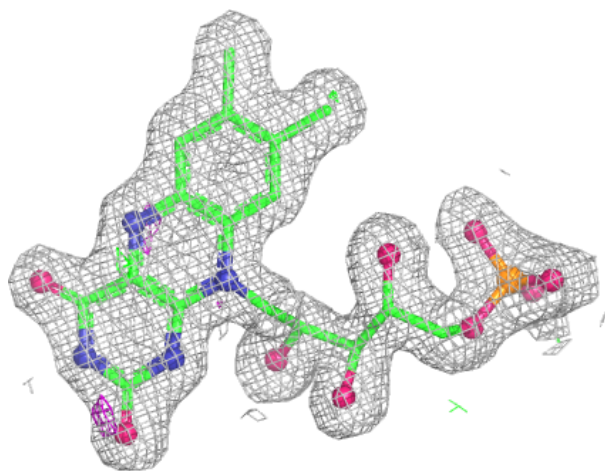
Electron density around FMN B 1030:

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



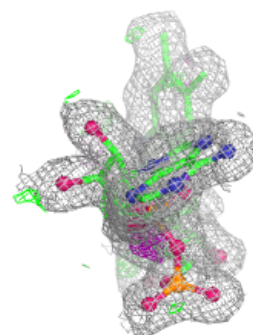
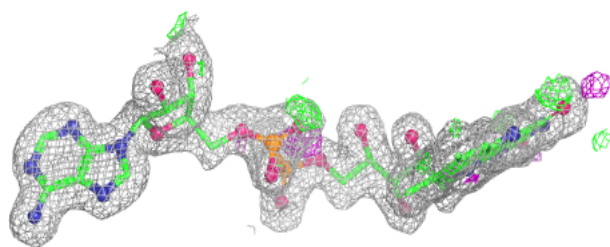
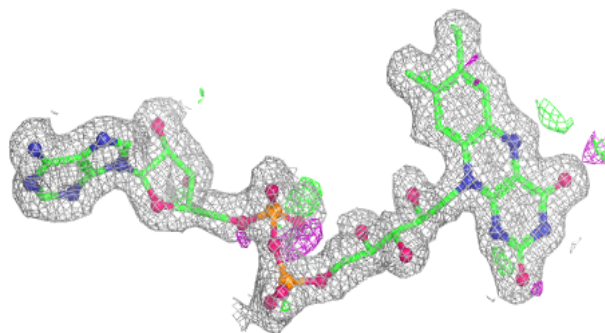
Electron density around FMN C 1030:

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

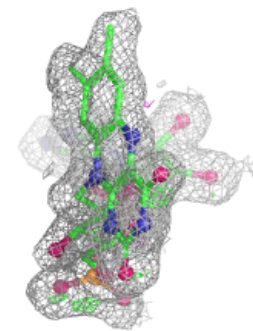
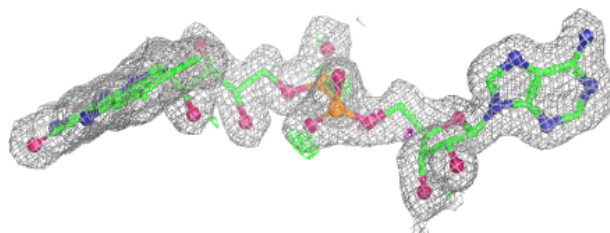
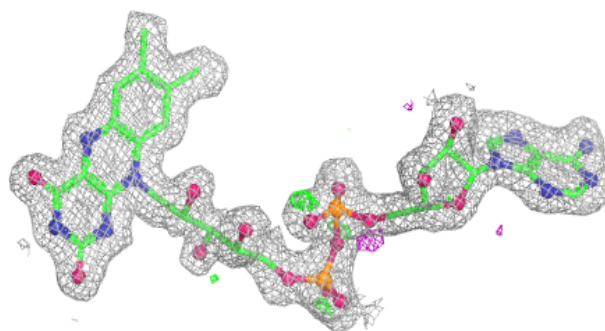


Electron density around FAD A 1031:

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

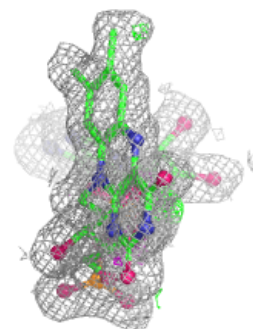
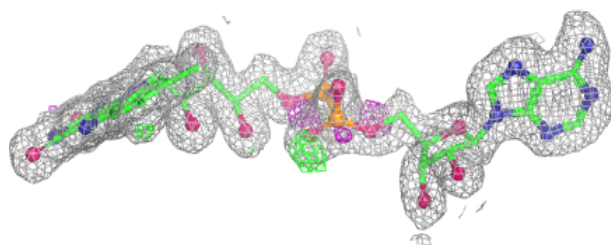
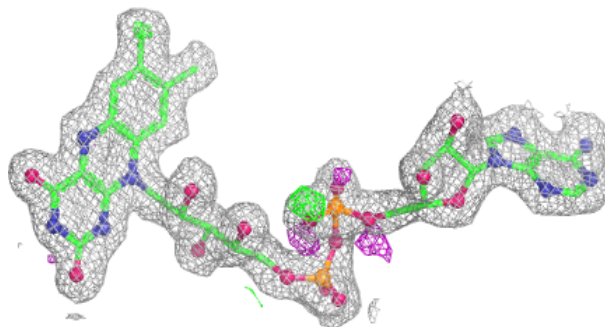
**Electron density around FAD B 1031:**

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

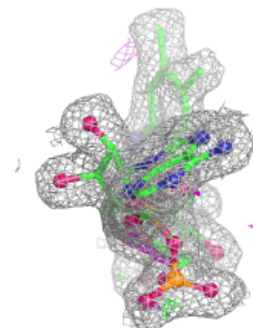
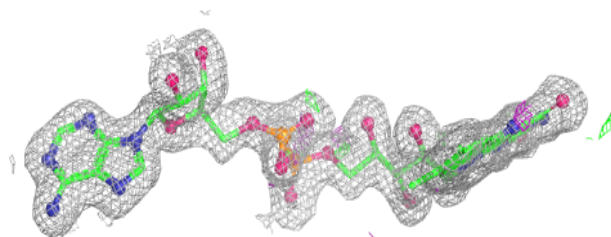
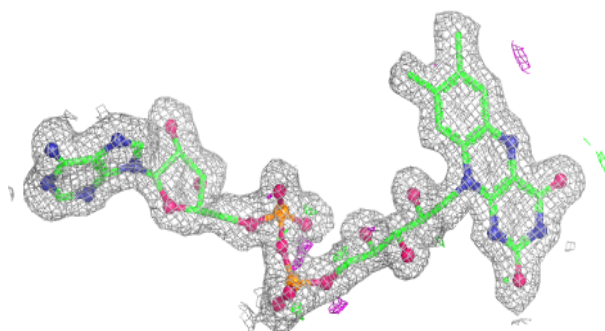


Electron density around FAD D 1031:

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

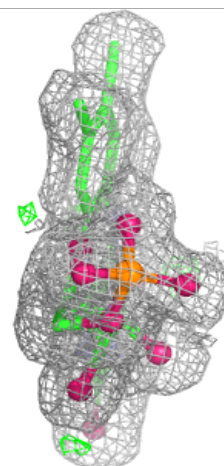
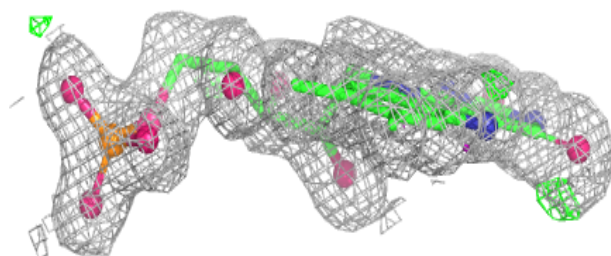
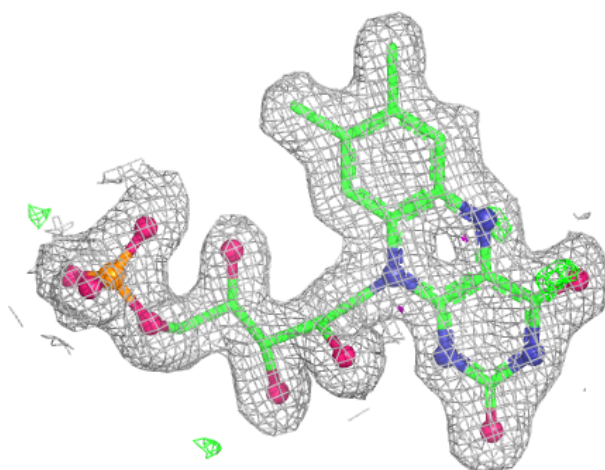
**Electron density around FAD C 1031:**

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



Electron density around FMN D 1030:

$2mF_o-DF_c$ (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.