



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:44 AM UTC

PDB ID : 1TLL / pdb_00001tll
Title : CRYSTAL STRUCTURE OF RAT NEURONAL NITRIC-OXIDE SYNTHASE REDUCTASE MODULE AT 2.3 Å RESOLUTION.
Authors : Garcin, E.D.; Bruns, C.M.; Lloyd, S.J.; Hosfield, D.J.; Tiso, M.; Gachhui, R.; Stuehr, D.J.; Tainer, J.A.; Getzoff, E.D.
Deposited on : 2004-06-09
Resolution : 2.30 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

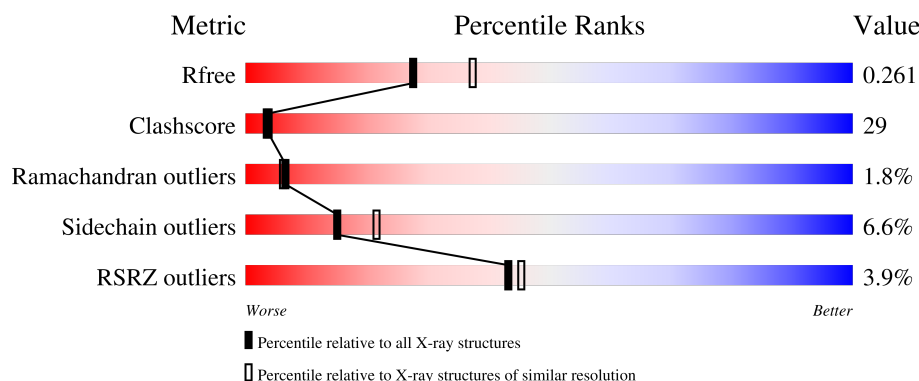
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	688	3% 52% 32% 6% • 8%
1	B	688	4% 43% 40% 7% 10%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10408 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.

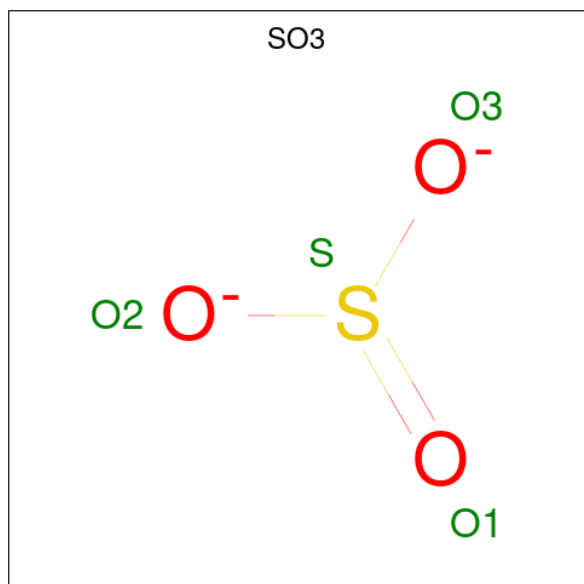
- Molecule 1 is a protein called Nitric-oxide synthase, brain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	630	Total	C	N	O	S	0	0	0
			5010	3170	882	932	26			
1	B	616	Total	C	N	O	S	0	0	0
			4903	3106	862	909	26			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1008	SER	PHE	SEE REMARK 999	UNP P29476
B	3008	SER	PHE	SEE REMARK 999	UNP P29476

- Molecule 2 is SULFITE ION (CCD ID: SO3) (formula: O₃S).



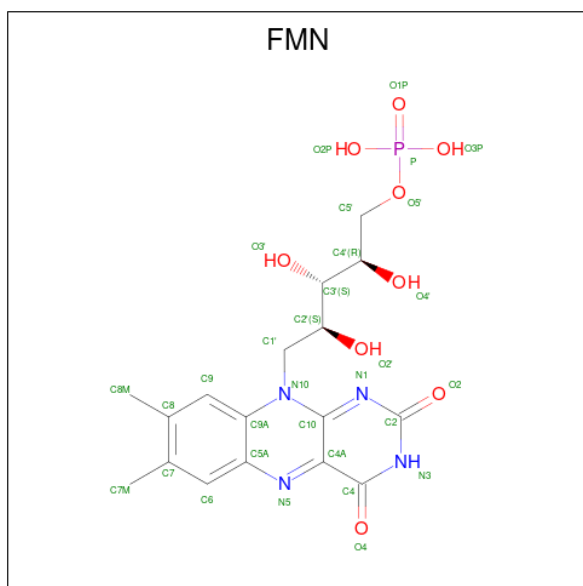
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			4	3	1		

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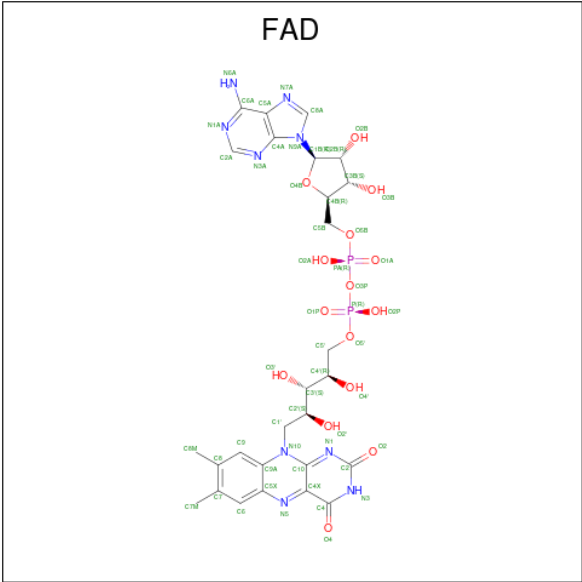
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			4	3	1		

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



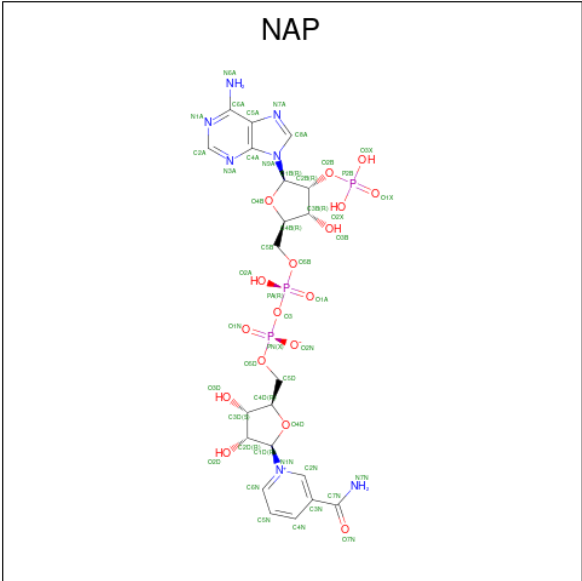
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 17	N 4	O 9	P 1	0	0
3	B	1	Total 31	C 17	N 4	O 9	P 1	0	0

- 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	C	N	O	P	0	0
			53	27	9	15	2		
4	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 5 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: C₂₁H₂₈N₇O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

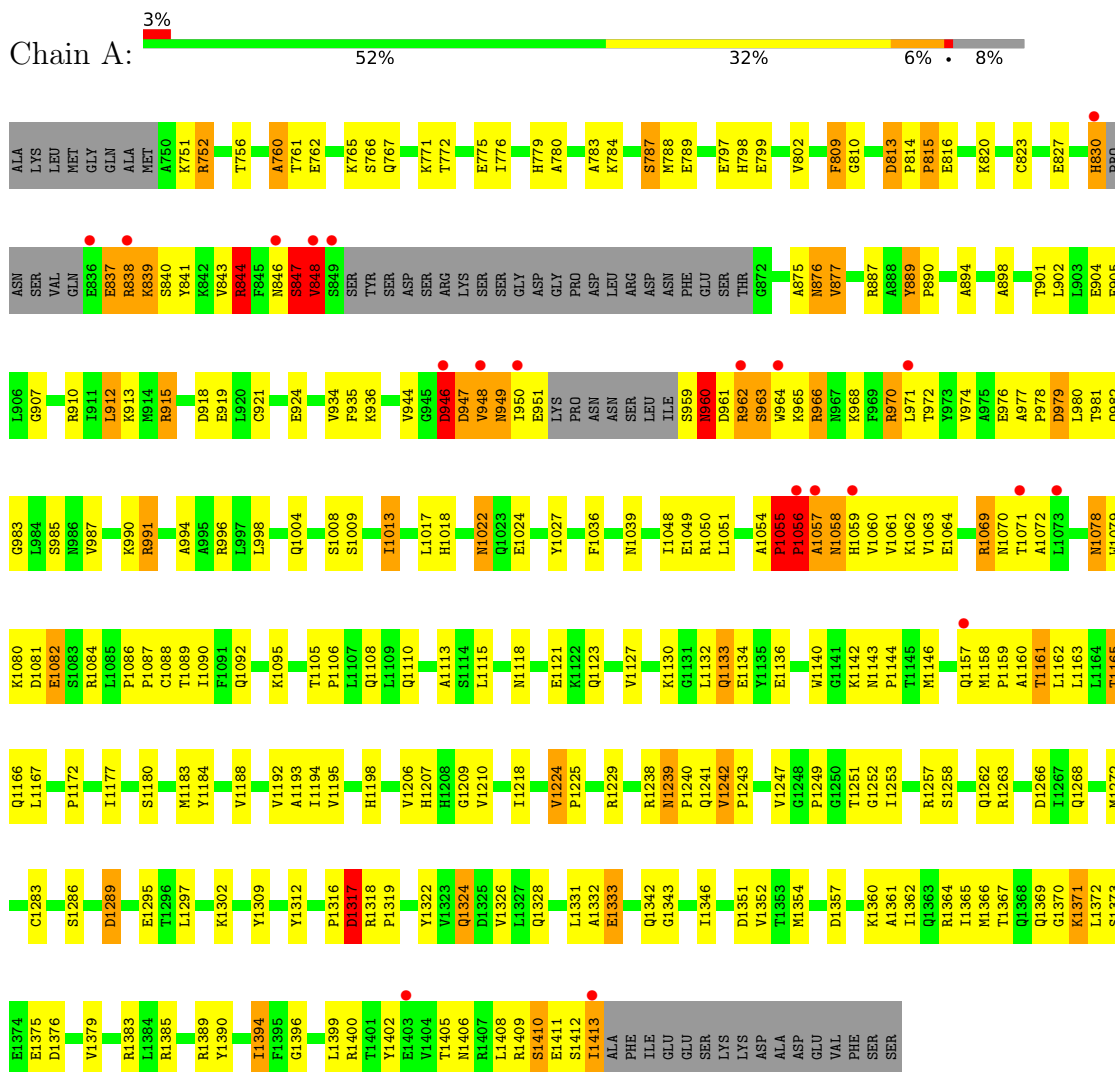
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	127	Total	O	0	0
			127	127		
6	B	96	Total	O	0	0
			96	96		

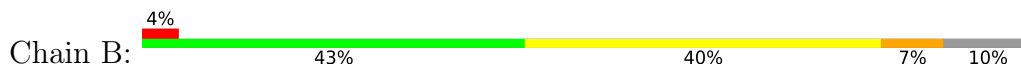
3 Residue-property plots

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: Nitric-oxide synthase, brain



• Molecule 1: Nitric-oxide synthase, brain



F3380	R3385	D3386	D3387	N3388	R3389	G3390	H3391	G3396	V3397	T3398	L3399	R3400	T3401	Y3402	E3403	V3404	T3405	N3406	L3407	L3408	R3409	S3410	E3411	S3412	I3413	ALA	PHE	ILE	GLU	GLU	SER	LYS	LYS	ASP	ALA	ASP	GLU	VAL	PHE	SER	SER																			
S3313	R3314	E3315	D3316	D3317	G3320	K3321	K3322	V3323	Q3324	Q3325	V3326	L3327	G3328	E3329	Q3330	L3331	A3332	V3335	R3336	R3337	A3338	E3341	Q3342	G3343	S3344	H3345	I3346	Y3347	V3348	D3266	M3272	V3280	F3281	G3282	C3283	R3284	Q3285	S3286	K3287	I3288	D3289	T3296	A3299	V3304	F3305	R3306	E3307	L3308	Y3309	Y3312										
I3218	Q3219	A3220	D3221	D3222	G3226	R3238	N3239	P3240	Q3241	V3242	P3243	G3244	I3245	L3246	V3247	G3248	P3249	G3250	T3251	G3252	I3253	A3254	R3257	S3258	F3259	V3260	Q3261	Q3262	D3266	M3272	V3280	F3281	G3282	C3283	R3284	Q3285	S3286	K3287	I3288	D3289	T3296	A3299	V3304	F3305	R3306	E3307	L3308	Y3309	Y3312											
H3040	Y3044	N3045	A3046	E3049	R3050	L3051	E3052	P3053	A3054	E3055	P3056	A3057	H3059	K3062	V3063	E3064	K3065	L3066	E3067	E3068	R3069	N3070	L3073	I3076	S3077	N3078	W3079	K3080	D3081	R3084	T3089	L3090	F3091	Q3092	P3103	F3104	L3107	Q3108	L3109	Q3110	Q3111	N3022	A3113	S3114	L3115	E3121	K3122	Q3123												
K2962	ASN	SER	LEU	ILE	S2969	N2960	D2961	R2962	W2963	W2964	R2965	R2966	K2967	F2968	F2969	R2970	L2971	Y2972	Y2973	V2974	E2976	A2977	D2978	D2979	L2980	T2981	A2994	L2998	S2999	R3000	Q3001	N3002	L3003	Q3004	S3008	S3009	R3010	F3014	V3015	T3019	N3020	G3021	A3113	S3114	L3115	E3121	K3122	Q3123												
LEU	ALA	ASN	V2877	R2878	ASN	F2879	S2880	V2881	F2882	G2883	L2884	Y2889	P2890	H2891	A2894	F2895	A2898	V2899	L2902	L2903	E2904	E2905	L2906	G2907	R2910	L2911	L2912	L2913	M2914	R2915	E2919	G2922	R2928	T2929	W2930	A2931	V2934	F2935	K2936	C2939	D2940	V2941	F2942	C2943	V2944	G2945	D2946	D2947	V2948	N2949										
G2812	F2815	E2816	N2817	G2818	F2821	G2822	C2823	A2824	L2825	W2826	E2827	M2828	R2829	HIS	PRO	ASN	SER	VAL	GLN	GLU	GLU	ARG	LYS	S2840	Y2841	F2842	L2843	R2844	F2845	N2846	SER	VAL	SER	SER	TYR	SER	ASP	M2786	S2787	ARG	LYS	SER	SER	GLY	ASP	D2792	Y2791	L2793	V2794	H2795	E2799	A2800	L2801	V2802	L2803	V2804	V2805	THR	GLY	PRO

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.76Å 69.17Å 82.63Å 76.80° 72.07° 67.14°	Depositor
Resolution (Å)	35.21 – 2.30 35.21 – 2.30	Depositor EDS
% Data completeness (in resolution range)	97.8 (35.21-2.30) 97.8 (35.21-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 2.18Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.244 , 0.272 0.236 , 0.261	Depositor DCC
R_{free} test set	1909 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å ²)	37.4	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 51.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10408	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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: FMN, NAP, SO3, 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	0.53	2/5122 (0.0%)	1.11	43/6932 (0.6%)
1	B	0.49	0/5014	1.10	46/6788 (0.7%)
All	All	0.51	2/10136 (0.0%)	1.11	89/13720 (0.6%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1133	GLN	CA-CB	-7.70	1.41	1.53
1	A	1133	GLN	CG-CD	-5.17	1.39	1.52

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2966	ARG	N-CA-C	11.98	126.37	112.72
1	A	946	ASP	N-CA-C	-9.76	98.97	113.61
1	B	2943	CYS	N-CA-C	9.73	124.67	111.24
1	B	2944	VAL	N-CA-C	-9.66	94.21	108.89
1	A	877	VAL	N-CA-C	9.53	122.17	109.21
1	B	3192	VAL	N-CA-C	8.86	120.69	107.75
1	B	3364	ARG	NE-CZ-NH1	8.59	130.09	121.50
1	A	1133	GLN	CB-CG-CD	-8.46	98.22	112.60
1	B	2844	ARG	N-CA-C	8.33	121.11	111.11
1	B	2889	TYR	CA-C-N	8.15	130.03	119.84
1	B	2889	TYR	C-N-CA	8.15	130.03	119.84
1	B	3364	ARG	NE-CZ-NH2	-8.03	111.97	119.20
1	B	3409	ARG	N-CA-C	-7.73	102.93	111.36
1	A	1133	GLN	N-CA-C	7.71	119.33	111.07
1	A	966	ARG	N-CA-C	7.66	121.72	112.38
1	A	944	VAL	N-CA-C	-7.65	97.47	108.42
1	A	815	PRO	N-CA-C	-7.65	99.48	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	949	ASN	N-CA-C	7.46	121.63	109.85
1	B	2968	LYS	N-CA-C	-7.34	104.35	113.38
1	A	1239	ASN	CA-C-N	7.29	127.14	119.05
1	A	1239	ASN	C-N-CA	7.29	127.14	119.05
1	B	3055	PRO	N-CA-C	7.29	119.59	110.70
1	B	3124	ARG	N-CA-C	-7.16	103.41	111.07
1	A	1009	SER	N-CA-C	-7.11	104.42	113.23
1	A	1289	ASP	N-CA-C	6.85	121.93	113.50
1	B	3387	ASP	N-CA-C	-6.80	104.98	113.28
1	A	752	ARG	N-CA-C	-6.72	103.05	110.91
1	B	2961	ASP	N-CA-C	6.68	119.12	111.11
1	B	3258	SER	N-CA-C	-6.60	105.36	113.41
1	A	837	GLU	N-CA-C	6.58	119.16	108.76
1	A	1082	GLU	N-CA-C	-6.57	103.23	111.11
1	B	2878	ARG	N-CA-C	-6.54	99.81	109.81
1	A	847	SER	N-CA-C	6.52	120.67	110.17
1	A	848	VAL	N-CA-C	6.52	122.89	109.34
1	B	3077	SER	N-CA-C	6.46	118.76	109.14
1	B	3289	ASP	N-CA-C	6.43	120.98	113.20
1	A	839	LYS	N-CA-C	6.34	124.31	110.80
1	A	948	VAL	N-CA-C	-6.34	99.11	109.12
1	B	3084	ARG	N-CA-C	-6.31	104.53	112.93
1	A	889	TYR	CA-C-N	6.23	127.63	119.84
1	A	889	TYR	C-N-CA	6.23	127.63	119.84
1	B	3261	GLN	N-CA-C	-6.02	104.64	112.23
1	B	3054	ALA	N-CA-C	5.96	122.99	109.81
1	B	3145	THR	N-CA-C	-5.94	102.87	110.53
1	A	1247	VAL	N-CA-C	5.92	116.39	107.80
1	A	1192	VAL	N-CA-C	5.92	116.69	107.28
1	B	3404	VAL	N-CA-C	5.92	116.10	110.42
1	B	3369	GLN	N-CA-C	5.88	118.47	111.71
1	B	2764	GLY	N-CA-C	5.85	124.09	115.08
1	B	3143	ASN	CA-C-N	5.81	125.57	119.76
1	B	3143	ASN	C-N-CA	5.81	125.57	119.76
1	A	1013	ILE	N-CA-C	5.79	116.92	108.53
1	A	783	ALA	N-CA-C	5.78	119.48	110.17
1	B	2977	ALA	CA-C-N	5.77	126.57	120.11
1	B	2977	ALA	C-N-CA	5.77	126.57	120.11
1	A	813	ASP	CA-C-N	5.75	123.80	119.66
1	A	813	ASP	C-N-CA	5.75	123.80	119.66
1	B	3050	ARG	N-CA-C	-5.69	106.00	113.17
1	B	3377	ALA	N-CA-C	-5.69	106.47	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1084	ARG	N-CA-C	-5.67	103.97	111.96
1	A	1252	GLY	N-CA-C	-5.56	108.42	115.31
1	B	3284	ARG	N-CA-C	5.55	118.40	111.24
1	B	3180	SER	N-CA-C	-5.45	103.20	110.07
1	A	1209	GLY	N-CA-C	-5.43	105.00	111.36
1	A	1394	ILE	N-CA-C	5.41	116.55	108.54
1	B	3153	PHE	CA-C-N	5.39	125.48	119.87
1	B	3153	PHE	C-N-CA	5.39	125.48	119.87
1	A	1210	VAL	N-CA-C	5.39	115.53	110.30
1	A	760	ALA	N-CA-C	-5.36	99.94	109.06
1	A	1258	SER	N-CA-C	-5.34	105.91	112.90
1	A	947	ASP	N-CA-C	-5.32	106.67	114.39
1	B	3296	THR	N-CA-C	-5.32	105.56	111.36
1	A	844	ARG	N-CA-C	5.30	116.86	111.14
1	A	921	CYS	N-CA-C	5.28	116.67	107.49
1	B	3222	ASP	N-CA-C	-5.27	103.52	110.43
1	A	1056	PRO	N-CA-C	-5.27	102.73	111.11
1	A	1317	ASP	N-CA-C	5.26	119.45	113.19
1	B	3254	ALA	N-CA-C	5.25	121.42	109.81
1	A	894	ALA	N-CA-C	5.23	116.67	111.07
1	A	1224	VAL	CA-C-N	5.22	126.03	119.98
1	A	1224	VAL	C-N-CA	5.22	126.03	119.98
1	B	3209	GLY	N-CA-C	-5.19	105.29	111.36
1	B	3009	SER	N-CA-C	-5.17	105.26	112.45
1	B	3152	GLU	N-CA-C	-5.17	106.48	112.89
1	B	3046	ALA	N-CA-C	-5.17	105.72	112.23
1	A	960	ASN	N-CA-C	5.12	121.70	110.80
1	B	2812	GLY	N-CA-C	-5.05	108.15	115.27
1	B	3344	GLY	N-CA-C	5.05	120.79	112.30
1	B	3144	PRO	N-CA-C	5.05	119.11	111.19

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	5010	0	4925	275	1
1	B	4903	0	4814	302	1
2	A	4	0	0	0	0
2	B	4	0	0	0	0
3	A	31	0	18	0	0
3	B	31	0	18	0	0
4	A	53	0	28	0	0
4	B	53	0	28	0	0
5	A	48	0	24	9	0
5	B	48	0	24	13	0
6	A	127	0	0	2	0
6	B	96	0	0	6	0
All	All	10408	0	9879	576	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 29.

All (576) 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)
5:A:1453:NAP:O2A	5:A:1453:NAP:O3D	1.55	1.21
1:B:3360:LYS:O	1:B:3364:ARG:CD	1.98	1.11
1:B:3196:SER:N	6:B:6093:HOH:O	1.59	1.10
1:A:991:ARG:HG3	1:A:991:ARG:HH11	1.12	1.08
1:B:3053:ASP:HB2	1:B:3160:ALA:H	1.11	1.06
1:B:3360:LYS:O	1:B:3364:ARG:HD3	1.54	1.04
1:A:1161:THR:O	1:A:1165:THR:HG22	1.56	1.04
1:B:3324:GLN:H	1:B:3324:GLN:HE21	1.04	1.00
1:B:3398:THR:O	5:B:2453:NAP:O2D	1.80	1.00
1:A:1328:GLN:HE21	1:A:1361:ALA:HA	1.22	0.99
1:A:1078:ASN:N	1:A:1078:ASN:HD22	1.62	0.97
1:B:3313:SER:HB2	1:B:3320:LYS:HE2	1.45	0.96
1:A:1071:THR:HG22	1:A:1072:ALA:H	1.30	0.96
1:B:3360:LYS:HB3	1:B:3364:ARG:NH1	1.81	0.95
1:B:3019:THR:HG23	1:B:3025:LEU:HD12	1.50	0.94
1:B:2843:VAL:HG23	1:B:3386:ASP:OD2	1.68	0.94
1:A:1324:GLN:H	1:A:1324:GLN:HE21	1.08	0.93
1:B:2799:GLU:O	1:B:2877:VAL:HG22	1.70	0.92
1:B:3324:GLN:H	1:B:3324:GLN:NE2	1.68	0.92
1:B:3158:MET:HE3	1:B:3159:PRO:HD2	1.52	0.91
1:A:1324:GLN:HE22	5:A:1453:NAP:H2A	1.34	0.91
1:B:3193:ALA:HB1	5:B:2453:NAP:H51N	1.55	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:991:ARG:HH11	1:A:991:ARG:CG	1.87	0.88
1:A:1071:THR:HG22	1:A:1072:ALA:N	1.89	0.87
1:B:2930:TRP:O	1:B:2934:VAL:HG23	1.74	0.87
1:A:797:GLU:HG3	1:A:798:HIS:CD2	2.10	0.86
1:B:2881:VAL:HB	1:B:2914:MET:HG3	1.54	0.86
1:A:840:SER:OG	1:A:843:VAL:HG23	1.75	0.86
1:B:3283:CYS:HB2	1:B:3289:ASP:HB3	1.58	0.85
1:A:964:TRP:CZ2	1:A:966:ARG:HG3	2.11	0.85
1:A:1309:TYR:CZ	1:A:1331:LEU:HD21	2.11	0.84
1:A:912:LEU:HD22	1:A:915:ARG:HH12	1.41	0.84
1:A:1379:VAL:O	1:A:1383:ARG:HG2	1.77	0.83
1:B:2912:LEU:HD21	1:B:2915:ARG:NH1	1.93	0.83
1:A:775:GLU:HG2	1:A:961:ASP:CB	2.09	0.83
1:A:823:CYS:O	1:A:827:GLU:HG2	1.77	0.83
1:B:2922:GLY:N	1:B:3136:GLU:OE2	2.11	0.82
1:A:1069:ARG:HG2	1:A:1070:ASN:H	1.44	0.82
1:B:3353:THR:HG22	5:B:2453:NAP:H62A	1.44	0.81
1:A:972:THR:HG21	1:A:1064:GLU:OE1	1.80	0.81
1:A:1324:GLN:H	1:A:1324:GLN:NE2	1.79	0.81
1:A:1146:MET:HE3	1:A:1167:LEU:HD21	1.62	0.81
1:B:3324:GLN:HE21	1:B:3324:GLN:N	1.76	0.81
1:A:1062:LYS:HE3	1:A:1087:PRO:HG3	1.62	0.80
1:B:3360:LYS:O	1:B:3364:ARG:HD2	1.78	0.80
1:A:1328:GLN:NE2	1:A:1361:ALA:HA	1.96	0.80
1:A:1324:GLN:HE21	1:A:1324:GLN:N	1.80	0.79
1:B:2842:LYS:HD3	1:B:2846:ASN:HD22	1.47	0.79
1:A:1146:MET:HE3	1:A:1167:LEU:CD2	2.11	0.79
1:A:876:ASN:C	1:A:876:ASN:HD22	1.91	0.79
1:A:1048:ILE:HG21	1:A:1057:ALA:HB2	1.64	0.79
1:A:1328:GLN:NE2	1:A:1364:ARG:HD2	1.98	0.79
1:B:2792:ASP:HB3	1:B:2794:VAL:HG12	1.66	0.78
1:A:1372:LEU:HB3	1:A:1376:ASP:HB2	1.63	0.78
1:B:3162:LEU:HD12	1:B:3166:GLN:HG2	1.66	0.78
1:A:1022:ASN:HD21	1:A:1024:GLU:HG2	1.48	0.77
1:A:1324:GLN:NE2	5:A:1453:NAP:H2A	1.98	0.77
1:A:1328:GLN:HE21	1:A:1361:ALA:CA	1.97	0.76
1:A:1158:MET:CE	1:A:1162:LEU:HB3	2.17	0.75
1:B:3053:ASP:HB2	1:B:3160:ALA:N	1.96	0.75
1:B:3322:TYR:HB3	1:B:3324:GLN:HE22	1.51	0.75
1:B:2760:ALA:HB3	1:B:2806:THR:OG1	1.87	0.75
1:B:2930:TRP:CE2	1:B:2934:VAL:HG21	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1180:SER:OG	1:A:1262:GLN:NE2	2.20	0.74
1:B:3162:LEU:HD12	1:B:3166:GLN:CG	2.17	0.74
1:A:1078:ASN:N	1:A:1078:ASN:ND2	2.36	0.74
1:B:3367:THR:HG23	1:B:3372:LEU:O	1.87	0.74
1:B:2912:LEU:CD2	1:B:2934:VAL:HG22	2.17	0.74
1:A:959:SER:O	1:A:960:ASN:HB3	1.86	0.74
1:A:1324:GLN:HG2	1:A:1357:ASP:HB3	1.70	0.73
1:A:1022:ASN:HD22	1:A:1024:GLU:H	1.36	0.73
1:A:775:GLU:HG2	1:A:961:ASP:HB3	1.71	0.73
1:A:1071:THR:CG2	1:A:1072:ALA:H	2.00	0.73
1:B:3285:GLN:HG2	1:B:3287:LYS:HG2	1.71	0.73
1:A:965:LYS:HD2	1:A:968:LYS:HD2	1.68	0.72
1:B:3198:HIS:HB2	1:B:3202:GLY:HA2	1.71	0.72
1:B:2889:TYR:OH	1:B:3396:GLY:HA2	1.89	0.72
1:A:1158:MET:HE3	1:A:1159:PRO:HD2	1.71	0.72
1:A:965:LYS:HG3	1:A:968:LYS:HB2	1.71	0.72
1:A:1243:PRO:HG3	1:A:1342:GLN:HE21	1.54	0.72
1:B:2966:ARG:HG3	1:B:2966:ARG:O	1.90	0.72
1:A:1062:LYS:HG3	1:A:1087:PRO:HG3	1.70	0.71
1:A:1158:MET:HE1	1:A:1162:LEU:HB3	1.72	0.71
1:A:780:ALA:HB2	1:A:948:VAL:HG21	1.70	0.71
1:B:2765:LYS:NZ	1:B:2919:GLU:OE1	2.24	0.71
1:B:2959:SER:HA	1:B:3110:GLN:HE22	1.55	0.71
1:B:3019:THR:HG23	1:B:3025:LEU:CD1	2.20	0.71
1:A:816:GLU:HB2	1:A:1229:ARG:NH2	2.06	0.70
1:A:961:ASP:C	1:A:963:SER:H	1.99	0.70
1:A:1127:VAL:HA	1:A:1130:LYS:HE3	1.73	0.70
1:A:962:ARG:O	1:A:963:SER:O	2.09	0.70
1:A:1036:PHE:HB2	1:A:1225:PRO:HB2	1.73	0.70
1:A:887:ARG:HG2	1:A:918:ASP:OD2	1.92	0.70
1:B:3249:PRO:HD2	1:B:3354:MET:HE2	1.73	0.69
1:A:946:ASP:OD1	1:A:946:ASP:O	2.09	0.69
1:B:3111:GLN:O	1:B:3115:LEU:HD12	1.92	0.69
1:B:3053:ASP:CB	1:B:3160:ALA:H	1.97	0.69
1:A:799:GLU:HG2	1:A:802:VAL:HG22	1.74	0.69
1:A:1062:LYS:HE3	1:A:1087:PRO:CG	2.21	0.69
1:A:1158:MET:HE2	1:A:1163:LEU:HG	1.73	0.69
1:A:1198:HIS:NE2	1:A:1206:VAL:HG22	2.08	0.69
1:B:3107:LEU:O	1:B:3110:GLN:HG2	1.93	0.69
1:B:3345:HIS:CE1	1:B:3389:ARG:HG2	2.28	0.69
1:B:3130:LYS:O	1:B:3132:LEU:N	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2878:ARG:HH12	1:B:2941:VAL:HG13	1.58	0.69
1:A:1058:ASN:CG	1:A:1058:ASN:O	2.36	0.68
1:B:3146:MET:HE2	1:B:3167:LEU:HD21	1.75	0.68
1:B:3247:VAL:HG12	1:B:3280:VAL:HB	1.75	0.68
1:B:3351:ASP:HB2	1:B:3399:LEU:HG	1.74	0.68
1:A:1048:ILE:HD13	1:A:1057:ALA:CB	2.23	0.68
1:B:3240:PRO:HG2	1:B:3241:GLN:HE21	1.57	0.68
1:A:1022:ASN:ND2	1:A:1024:GLU:HG2	2.07	0.68
1:B:3322:TYR:HB3	1:B:3324:GLN:NE2	2.07	0.68
1:A:779:HIS:CE1	1:A:951:GLU:OE2	2.47	0.68
1:B:2971:LEU:HD12	1:B:3055:PRO:HG2	1.75	0.68
1:A:1118:ASN:HB3	1:A:1121:GLU:HB3	1.76	0.67
1:A:976:GLU:OE2	1:B:2784:LYS:HD2	1.94	0.67
1:A:765:LYS:NZ	1:A:919:GLU:HG3	2.10	0.67
1:A:991:ARG:HG3	1:A:991:ARG:NH1	1.92	0.67
1:A:1161:THR:O	1:A:1165:THR:CG2	2.39	0.66
1:B:3314:ARG:O	1:B:3316:PRO:HD3	1.96	0.66
1:A:912:LEU:HD12	1:A:934:VAL:HA	1.78	0.66
1:A:1238:ARG:O	1:A:1240:PRO:HD3	1.95	0.66
1:A:848:VAL:HG12	1:A:848:VAL:O	1.94	0.66
1:A:1078:ASN:HD22	1:A:1078:ASN:H	1.44	0.66
1:A:1324:GLN:HE22	5:A:1453:NAP:C2A	2.07	0.66
1:B:2840:SER:HB2	1:B:3386:ASP:CG	2.21	0.66
1:B:3180:SER:OG	1:B:3262:GLN:NE2	2.30	0.65
1:B:2912:LEU:HD23	1:B:2934:VAL:HG22	1.78	0.65
1:A:1351:ASP:HB2	1:A:1399:LEU:HG	1.79	0.65
1:B:3193:ALA:HB2	1:B:3251:THR:HG21	1.79	0.65
1:B:2794:VAL:HG13	1:B:2795:HIS:HD2	1.62	0.65
1:B:2840:SER:HB2	1:B:3386:ASP:OD1	1.97	0.64
1:B:3242:VAL:HG11	1:B:3343:GLY:O	1.97	0.64
1:B:2947:ASP:O	1:B:2949:ASN:N	2.30	0.64
1:B:2878:ARG:NH1	1:B:2941:VAL:HG13	2.13	0.64
1:B:2757:ILE:HG12	1:B:2803:LEU:HD12	1.80	0.64
1:B:3158:MET:HE1	1:B:3162:LEU:CG	2.28	0.64
1:A:1239:ASN:HD22	1:A:1239:ASN:C	2.06	0.64
1:A:1268:GLN:HE21	1:A:1302:LYS:HD3	1.62	0.64
1:B:3283:CYS:HB2	1:B:3289:ASP:CB	2.27	0.64
1:B:2946:ASP:OD2	1:B:2946:ASP:N	2.30	0.63
1:B:3019:THR:CG2	1:B:3025:LEU:HB2	2.28	0.63
1:A:1328:GLN:HE22	1:A:1364:ARG:HD2	1.61	0.63
1:A:1373:SER:C	1:A:1375:GLU:H	2.05	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:ILE:HD13	1:A:1057:ALA:HB1	1.79	0.63
1:A:1069:ARG:HG2	1:A:1070:ASN:N	2.12	0.63
1:A:1322:TYR:HB3	1:A:1324:GLN:NE2	2.13	0.63
1:B:3158:MET:CE	1:B:3162:LEU:HB3	2.29	0.63
1:B:3242:VAL:HG13	1:B:3243:PRO:HD2	1.80	0.63
1:B:3195:VAL:HA	6:B:6093:HOH:O	1.99	0.63
1:B:3363:GLN:HE21	1:B:3378:GLY:CA	2.12	0.62
1:B:2915:ARG:HD2	1:B:2930:TRP:HB2	1.79	0.62
1:B:2905:GLU:O	1:B:2906:LEU:HD23	1.99	0.62
1:B:2884:LEU:N	1:B:2884:LEU:HD12	2.14	0.62
1:B:3286:SER:HB3	1:B:3312:TYR:CZ	2.34	0.62
1:A:1283:CYS:HB2	1:A:1289:ASP:HB3	1.82	0.62
1:B:2774:CYS:O	1:B:2778:LYS:HG2	2.00	0.62
1:B:2971:LEU:CD1	1:B:3055:PRO:HG2	2.29	0.62
1:B:3312:TYR:H	1:B:3321:LYS:HE3	1.64	0.62
1:B:3165:THR:OG1	1:B:3166:GLN:NE2	2.30	0.61
1:A:991:ARG:CG	1:A:991:ARG:NH1	2.55	0.61
1:B:3002:ASN:HB3	6:B:6013:HOH:O	2.00	0.61
1:A:987:VAL:CG2	1:A:1086:PRO:HD3	2.31	0.61
1:B:2878:ARG:NH1	1:B:2941:VAL:CG1	2.64	0.61
1:A:1022:ASN:HD21	1:A:1024:GLU:CG	2.14	0.60
1:A:1158:MET:HE3	1:A:1159:PRO:CD	2.31	0.60
1:B:2760:ALA:HB1	1:B:2815:PRO:HG3	1.82	0.60
1:B:2974:VAL:HG12	1:B:2976:GLU:H	1.67	0.60
1:A:1402:TYR:O	1:A:1406:ASN:HB2	2.02	0.60
5:B:2453:NAP:H1D	6:B:6095:HOH:O	2.01	0.60
1:A:1057:ALA:HA	1:A:1090:ILE:HD11	1.83	0.60
1:A:1162:LEU:HD12	1:A:1166:GLN:HG2	1.84	0.59
1:B:3193:ALA:CB	5:B:2453:NAP:H51N	2.30	0.59
1:B:3353:THR:HG22	5:B:2453:NAP:N6A	2.16	0.59
1:B:2912:LEU:HD22	1:B:2934:VAL:HG22	1.82	0.59
1:A:1056:PRO:C	1:A:1058:ASN:H	2.11	0.59
1:A:1123:GLN:O	1:A:1127:VAL:HG23	2.02	0.59
1:B:2828:MET:SD	1:B:2906:LEU:HD13	2.43	0.59
1:B:2973:TYR:HE2	1:B:3059:HIS:CD2	2.21	0.59
1:A:1361:ALA:O	1:A:1365:ILE:HG13	2.02	0.58
1:B:3161:THR:O	1:B:3165:THR:HG23	2.03	0.58
1:B:2757:ILE:CG1	1:B:2803:LEU:HD12	2.34	0.58
1:A:1268:GLN:NE2	1:A:1302:LYS:HD3	2.17	0.58
1:B:2842:LYS:HD3	1:B:2846:ASN:ND2	2.16	0.58
1:B:3019:THR:O	1:B:3022:ASN:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2973:TYR:HE2	1:B:3059:HIS:HD2	1.52	0.58
1:B:3247:VAL:HG23	1:B:3348:VAL:HA	1.85	0.58
1:A:924:GLU:HG3	1:A:1106:PRO:HD2	1.85	0.58
1:B:3324:GLN:NE2	5:B:2453:NAP:H2A	2.18	0.58
1:B:3033:LEU:HD22	1:B:3188:VAL:HG11	1.85	0.58
1:B:3306:ARG:C	1:B:3307:GLU:HG2	2.28	0.58
1:A:1266:ASP:HB3	1:A:1272:MET:HG3	1.86	0.58
1:B:3262:GLN:O	1:B:3266:ASP:OD2	2.22	0.57
1:A:779:HIS:ND1	1:A:951:GLU:OE2	2.37	0.57
1:A:876:ASN:O	1:A:876:ASN:ND2	2.27	0.57
1:B:3158:MET:HE1	1:B:3162:LEU:HG	1.85	0.57
1:A:775:GLU:CD	1:A:961:ASP:HB2	2.29	0.57
1:A:964:TRP:CG	1:A:1162:LEU:HD13	2.39	0.57
1:B:2788:MET:HE2	1:B:2821:PHE:HB3	1.85	0.57
1:B:3337:ARG:HG3	1:B:3341:GLU:OE1	2.05	0.57
1:B:3052:GLU:HB3	1:B:3158:MET:O	2.04	0.57
1:A:765:LYS:HZ3	1:A:919:GLU:HG3	1.69	0.57
1:A:1367:THR:HG23	1:A:1372:LEU:O	2.04	0.57
1:B:2981:THR:HG21	1:B:2994:ALA:HB2	1.86	0.57
1:B:2793:ILE:O	1:B:2793:ILE:HG13	2.04	0.57
1:B:3360:LYS:CB	1:B:3364:ARG:NH1	2.64	0.57
1:A:971:LEU:CD2	1:A:1063:VAL:HG22	2.35	0.57
1:B:3287:LYS:NZ	1:B:3315:GLU:OE1	2.36	0.57
1:B:3363:GLN:HE21	1:B:3378:GLY:HA3	1.68	0.57
1:A:767:GLN:O	1:A:771:LYS:HG2	2.05	0.57
1:A:887:ARG:CG	1:A:918:ASP:OD2	2.53	0.57
1:A:1257:ARG:NE	1:A:1295:GLU:OE1	2.38	0.57
1:B:2821:PHE:HE1	1:B:2825:LEU:HD11	1.68	0.57
1:A:775:GLU:HG2	1:A:961:ASP:HB2	1.83	0.56
1:B:2912:LEU:HD21	1:B:2915:ARG:HH12	1.68	0.56
1:A:1057:ALA:HA	1:A:1090:ILE:CG1	2.35	0.56
1:B:2976:GLU:O	1:B:2976:GLU:HG2	2.05	0.56
1:A:760:ALA:HB2	1:A:788:MET:HE3	1.87	0.56
1:B:2895:PHE:O	1:B:2899:VAL:HG23	2.05	0.56
1:B:2939:CYS:HA	6:B:6058:HOH:O	2.05	0.56
1:B:3133:GLN:O	1:B:3137:GLU:HG3	2.05	0.56
1:B:3158:MET:HE2	1:B:3163:LEU:HG	1.87	0.56
1:B:3180:SER:H	1:B:3261:GLN:NE2	2.03	0.56
1:A:1410:SER:O	1:A:1412:SER:N	2.39	0.56
1:B:2930:TRP:NE1	1:B:2934:VAL:HG21	2.21	0.56
1:B:2964:TRP:CZ2	1:B:2966:ARG:HD2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2766:SER:OG	1:B:2884:LEU:HD22	2.05	0.56
1:A:981:THR:HG21	1:A:994:ALA:HB2	1.86	0.56
1:A:1158:MET:HE1	1:A:1162:LEU:CG	2.36	0.56
1:A:1322:TYR:HB3	1:A:1324:GLN:HE22	1.71	0.56
1:B:2794:VAL:HG13	1:B:2795:HIS:CD2	2.39	0.56
1:B:2979:ASP:OD1	1:B:2980:LEU:N	2.38	0.56
1:B:3158:MET:HE3	1:B:3159:PRO:CD	2.31	0.56
1:B:3257:ARG:O	1:B:3261:GLN:HG3	2.05	0.56
1:B:3330:GLN:C	1:B:3331:LEU:HD12	2.31	0.56
1:B:3353:THR:CG2	5:B:2453:NAP:H62A	2.18	0.56
1:B:3366:MET:HE2	1:B:3380:PHE:CE1	2.41	0.56
1:A:965:LYS:HG3	1:A:968:LYS:CB	2.36	0.55
1:B:3000:ARG:HA	1:B:3014:PHE:O	2.07	0.55
1:A:961:ASP:C	1:A:963:SER:N	2.65	0.55
1:A:1333:GLU:HA	1:A:1369:GLN:NE2	2.21	0.55
1:B:2773:LEU:O	1:B:2776:ILE:HG22	2.06	0.55
1:B:2846:ASN:O	1:B:3385:ARG:NH2	2.40	0.55
1:B:3110:GLN:HG3	1:B:3111:GLN:N	2.22	0.55
1:A:799:GLU:HG2	1:A:802:VAL:CG2	2.36	0.55
1:A:1371:LYS:CG	1:A:1371:LYS:O	2.55	0.55
1:A:1346:ILE:HD13	1:A:1362:ILE:CD1	2.37	0.55
1:B:2760:ALA:HB1	1:B:2815:PRO:CG	2.37	0.55
1:A:1057:ALA:HA	1:A:1090:ILE:HG12	1.89	0.55
1:A:1194:ILE:O	5:A:1453:NAP:H5N	2.07	0.55
1:A:1316:PRO:HG2	1:A:1317:ASP:OD1	2.05	0.55
1:B:2757:ILE:HG12	1:B:2803:LEU:HB2	1.89	0.55
1:B:3110:GLN:O	1:B:3113:ALA:HB3	2.07	0.55
1:A:1051:LEU:HD21	1:A:1163:LEU:HD12	1.89	0.54
1:A:1193:ALA:HB1	5:A:1453:NAP:H51N	1.89	0.54
1:B:2877:VAL:HG12	1:B:2878:ARG:O	2.06	0.54
1:A:1239:ASN:C	1:A:1239:ASN:ND2	2.64	0.54
1:A:1239:ASN:ND2	1:A:1241:GLN:H	2.06	0.54
1:A:762:GLU:HB2	1:A:809:PHE:CE1	2.43	0.54
1:A:959:SER:O	1:A:960:ASN:CB	2.54	0.54
1:B:3325:ASP:O	1:B:3329:GLU:HB2	2.08	0.54
1:A:1056:PRO:O	1:A:1058:ASN:N	2.38	0.54
1:A:1318:ARG:CB	1:A:1319:PRO:HD2	2.38	0.54
1:B:3112:PHE:HZ	1:B:3146:MET:HE1	1.73	0.54
1:A:756:THR:OG1	1:A:799:GLU:OE2	2.25	0.54
1:A:1036:PHE:CE1	1:A:1172:PRO:HB3	2.43	0.54
1:B:2970:ARG:HB3	1:B:3079:TRP:CZ3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:THR:HG1	1:A:799:GLU:CD	2.16	0.53
1:B:2964:TRP:HZ2	1:B:2966:ARG:NH1	2.06	0.53
1:B:2843:VAL:HG22	1:B:3382:SER:OG	2.09	0.53
1:B:3351:ASP:OD1	1:B:3353:THR:HB	2.07	0.53
1:A:1048:ILE:HD13	1:A:1057:ALA:HB2	1.91	0.53
1:A:1057:ALA:HA	1:A:1090:ILE:CD1	2.38	0.53
1:A:1373:SER:C	1:A:1375:GLU:N	2.63	0.53
1:B:2787:SER:HB2	1:B:2789:GLU:HG2	1.90	0.53
1:B:2802:VAL:O	1:B:2879:PHE:HA	2.08	0.53
1:B:3010:ARG:HE	5:B:2453:NAP:C5N	2.22	0.53
1:B:3132:LEU:O	1:B:3134:GLU:N	2.41	0.53
1:A:912:LEU:HD22	1:A:915:ARG:NH1	2.16	0.53
1:A:979:ASP:OD1	1:A:979:ASP:C	2.50	0.53
1:A:1346:ILE:HD13	1:A:1362:ILE:HD13	1.89	0.53
1:B:3408:LEU:HA	1:B:3411:GLU:HB2	1.91	0.53
1:A:1004:GLN:NE2	1:A:1008:SER:OG	2.42	0.53
1:B:3345:HIS:ND1	1:B:3389:ARG:HA	2.23	0.53
1:A:1394:ILE:HG22	1:A:1396:GLY:H	1.73	0.52
1:B:3054:ALA:O	1:B:3056:PRO:HD3	2.09	0.52
1:A:846:ASN:O	1:A:1385:ARG:NH2	2.42	0.52
1:A:1127:VAL:HA	1:A:1130:LYS:CE	2.38	0.52
1:A:1410:SER:O	1:A:1413:ILE:HG22	2.08	0.52
1:B:2752:ARG:HD2	1:B:2782:ASP:HB2	1.91	0.52
1:B:3146:MET:HE2	1:B:3167:LEU:CD2	2.39	0.52
1:B:3309:TYR:CD2	1:B:3331:LEU:HD11	2.45	0.52
1:B:2840:SER:O	1:B:2843:VAL:HB	2.09	0.52
1:B:3019:THR:HG21	1:B:3025:LEU:HB2	1.89	0.52
1:A:1158:MET:HE1	1:A:1162:LEU:CB	2.38	0.52
1:B:2966:ARG:O	1:B:2966:ARG:CG	2.57	0.52
1:A:1328:GLN:HE22	1:A:1364:ARG:NH1	2.08	0.52
1:B:3245:ILE:HD13	1:B:3335:VAL:HG22	1.91	0.52
1:B:3363:GLN:HA	1:B:3381:ILE:HD11	1.92	0.52
1:A:970:ARG:HB3	1:A:1079:TRP:CZ3	2.44	0.52
1:A:1286:SER:HA	1:A:1312:TYR:CE2	2.44	0.52
1:B:3162:LEU:HD12	1:B:3166:GLN:HG3	1.90	0.52
1:B:3242:VAL:CG1	1:B:3344:GLY:HA2	2.38	0.52
1:A:1162:LEU:HD12	1:A:1166:GLN:CG	2.40	0.51
1:B:3313:SER:O	1:B:3320:LYS:HE3	2.10	0.51
1:A:974:VAL:HG12	1:A:976:GLU:H	1.76	0.51
1:B:3034:GLY:O	1:B:3226:CYS:HA	2.10	0.51
1:B:2972:THR:HG21	1:B:3064:GLU:OE2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1087:PRO:O	1:A:1088:CYS:HB3	2.10	0.51
1:A:1143:ASN:O	1:A:1207:HIS:HE1	1.94	0.51
1:B:3019:THR:HG23	1:B:3025:LEU:HB2	1.93	0.51
1:B:3162:LEU:CD1	1:B:3166:GLN:HG3	2.41	0.51
1:B:3309:TYR:HB3	1:B:3326:VAL:HG11	1.92	0.51
1:A:775:GLU:CG	1:A:961:ASP:HB2	2.41	0.51
1:A:1360:LYS:O	1:A:1364:ARG:HG3	2.11	0.51
1:A:1064:GLU:HA	1:A:1080:LYS:O	2.11	0.51
1:A:1318:ARG:HB2	1:A:1319:PRO:HD2	1.92	0.51
1:B:2821:PHE:CE1	1:B:2825:LEU:HD11	2.45	0.51
1:A:1058:ASN:HA	1:A:1089:THR:HB	1.93	0.50
1:A:1157:GLN:O	1:A:1159:PRO:HD3	2.10	0.50
1:B:3180:SER:H	1:B:3261:GLN:HE21	1.58	0.50
1:A:964:TRP:CH2	1:A:966:ARG:HG3	2.46	0.50
1:A:1071:THR:CG2	1:A:1072:ALA:N	2.59	0.50
1:A:1195:VAL:HA	5:A:1453:NAP:C5N	2.41	0.50
1:A:904:GLU:OE2	1:A:910:ARG:NH1	2.42	0.50
1:B:3015:VAL:O	1:B:3189:HIS:HA	2.12	0.50
1:A:1239:ASN:HD22	1:A:1240:PRO:N	2.08	0.50
1:A:1268:GLN:NE2	1:A:1302:LYS:HE2	2.26	0.50
1:B:3351:ASP:OD1	1:B:3353:THR:N	2.43	0.50
1:B:3076:ILE:HG23	1:B:3076:ILE:O	2.11	0.50
1:B:3360:LYS:HE2	1:B:3360:LYS:HA	1.94	0.50
1:B:3113:ALA:C	1:B:3115:LEU:H	2.19	0.50
1:B:3240:PRO:HG2	1:B:3241:GLN:NE2	2.26	0.50
1:A:1055:PRO:O	1:A:1056:PRO:C	2.55	0.49
1:A:898:ALA:O	1:A:902:LEU:HG	2.12	0.49
1:B:3132:LEU:O	1:B:3133:GLN:C	2.55	0.49
1:B:3380:PHE:C	1:B:3380:PHE:CD1	2.90	0.49
1:A:1140:TRP:CD1	1:A:1409:ARG:HD2	2.47	0.49
1:B:2790:GLU:HG2	1:B:2790:GLU:O	2.12	0.49
1:B:3004:GLN:NE2	1:B:3008:SER:OG	2.46	0.49
1:B:3145:THR:O	1:B:3149:VAL:HG23	2.12	0.49
1:A:910:ARG:HD3	1:A:913:LYS:HA	1.95	0.49
1:A:971:LEU:HD23	1:A:1063:VAL:HG22	1.95	0.49
1:A:1022:ASN:ND2	1:A:1024:GLU:CG	2.73	0.49
1:A:1198:HIS:NE2	1:A:1206:VAL:CG2	2.75	0.49
1:B:2879:PHE:CD1	1:B:2903:LEU:HD13	2.47	0.49
1:B:2959:SER:HA	1:B:3110:GLN:NE2	2.24	0.49
1:A:837:GLU:O	1:A:838:ARG:CB	2.61	0.49
1:A:1309:TYR:HB3	1:A:1326:VAL:HG11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2968:LYS:O	1:B:3065:MET:HA	2.13	0.49
1:A:912:LEU:CD1	1:A:934:VAL:HA	2.42	0.49
1:B:2961:ASP:C	1:B:2963:SER:H	2.21	0.49
1:B:3140:TRP:HA	1:B:3140:TRP:CE3	2.47	0.49
1:B:3069:ARG:HG2	6:B:6069:HOH:O	2.12	0.48
1:B:3010:ARG:NH2	5:B:2453:NAP:H51N	2.28	0.48
1:B:3123:GLN:NE2	1:B:3126:LEU:HD12	2.28	0.48
1:B:2759:TYR:HA	1:B:2805:VAL:O	2.12	0.48
1:B:3359:LEU:HD23	1:B:3359:LEU:C	2.38	0.48
1:B:3144:PRO:HA	1:B:3148:GLU:OE1	2.13	0.48
1:A:1331:LEU:O	1:A:1332:ALA:C	2.56	0.48
1:A:1346:ILE:CD1	1:A:1362:ILE:HD11	2.43	0.48
1:B:2964:TRP:HZ2	1:B:2966:ARG:HH11	1.59	0.48
1:A:1142:LYS:O	1:A:1143:ASN:C	2.56	0.48
1:A:843:VAL:O	1:A:847:SER:HB2	2.14	0.48
1:B:3122:LYS:O	1:B:3126:LEU:HG	2.13	0.48
1:B:3089:THR:OG1	1:B:3092:GLN:HG3	2.13	0.48
1:A:761:THR:HB	1:A:766:SER:HB2	1.95	0.48
1:A:977:ALA:HB2	1:A:1060:VAL:CG2	2.44	0.48
1:A:1328:GLN:HE22	1:A:1364:ARG:HH11	1.61	0.48
1:A:784:LYS:HD2	1:A:784:LYS:HA	1.59	0.48
1:A:996:ARG:O	1:A:1017:LEU:HA	2.14	0.48
1:B:3299:ALA:O	1:B:3304:VAL:HB	2.13	0.48
1:B:3247:VAL:HG11	1:B:3327:LEU:HD21	1.96	0.47
1:B:3324:GLN:HE22	5:B:2453:NAP:H2A	1.79	0.47
1:A:961:ASP:CG	1:A:962:ARG:N	2.72	0.47
1:A:1105:THR:OG1	1:A:1108:GLN:HG3	2.13	0.47
1:B:3053:ASP:HB3	1:B:3160:ALA:CB	2.45	0.47
1:A:1110:GLN:HE21	1:A:1110:GLN:HA	1.78	0.47
1:A:1056:PRO:C	1:A:1058:ASN:N	2.72	0.47
1:B:3057:ALA:HA	1:B:3090:ILE:HG22	1.96	0.47
1:B:3140:TRP:HA	1:B:3140:TRP:HE3	1.80	0.47
1:B:3377:ALA:O	1:B:3381:ILE:HG13	2.15	0.47
1:A:1224:VAL:O	1:A:1224:VAL:HG12	2.14	0.47
1:A:1268:GLN:HE22	1:A:1302:LYS:HE2	1.80	0.47
1:B:2789:GLU:C	1:B:2791:TYR:H	2.23	0.47
1:B:3158:MET:HE1	1:B:3162:LEU:HB3	1.97	0.47
1:B:3351:ASP:CB	1:B:3399:LEU:HG	2.44	0.47
1:A:947:ASP:OD1	1:A:947:ASP:N	2.48	0.47
1:A:1049:GLU:HG3	1:A:1049:GLU:O	2.15	0.47
1:A:1113:ALA:C	1:A:1115:LEU:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1333:GLU:HA	1:A:1369:GLN:HE21	1.78	0.47
1:B:2970:ARG:HD2	1:B:3079:TRP:CE3	2.49	0.46
1:B:3379:VAL:O	1:B:3382:SER:HB3	2.15	0.46
1:B:2760:ALA:HB2	1:B:2788:MET:SD	2.55	0.46
1:A:964:TRP:CB	1:A:1162:LEU:HD13	2.45	0.46
1:B:3362:ILE:O	1:B:3366:MET:HG2	2.15	0.46
1:B:3405:THR:O	1:B:3409:ARG:HG3	2.15	0.46
1:A:772:THR:O	1:A:776:ILE:HG13	2.15	0.46
1:A:1027:TYR:CE2	1:A:1188:VAL:HG22	2.49	0.46
1:B:3400:ARG:O	1:B:3404:VAL:HB	2.16	0.46
1:A:1062:LYS:CG	1:A:1087:PRO:HG3	2.42	0.46
1:A:1133:GLN:O	1:A:1134:GLU:C	2.57	0.46
1:B:2842:LYS:HA	1:B:2846:ASN:HD22	1.80	0.46
1:A:780:ALA:CB	1:A:948:VAL:HG21	2.42	0.46
1:A:1059:HIS:O	1:A:1061:VAL:HG13	2.16	0.46
1:B:2902:LEU:HD23	1:B:2905:GLU:OE1	2.16	0.46
1:A:1134:GLU:H	1:A:1134:GLU:CD	2.23	0.46
1:B:2971:LEU:HD12	1:B:3055:PRO:CG	2.44	0.46
1:A:1049:GLU:O	1:A:1049:GLU:CG	2.64	0.46
1:B:2787:SER:CB	1:B:2789:GLU:HG2	2.46	0.46
1:B:2884:LEU:N	1:B:2884:LEU:CD1	2.77	0.46
1:B:2889:TYR:CD1	1:B:3352:VAL:HG21	2.50	0.46
1:A:799:GLU:O	1:A:877:VAL:HG22	2.16	0.46
1:A:1362:ILE:O	1:A:1366:MET:HG2	2.16	0.46
1:B:2846:ASN:O	1:B:2891:HIS:CE1	2.69	0.46
1:B:3281:PHE:CG	1:B:3282:GLY:N	2.84	0.46
1:A:1080:LYS:NZ	1:B:3079:TRP:O	2.48	0.45
1:B:3104:PRO:HG3	1:B:3146:MET:SD	2.56	0.45
1:A:1317:ASP:OD1	1:A:1317:ASP:N	2.46	0.45
1:B:2775:GLU:OE1	1:B:2775:GLU:HA	2.17	0.45
1:A:961:ASP:O	1:A:963:SER:N	2.48	0.45
1:A:1309:TYR:CE1	1:A:1331:LEU:HD21	2.51	0.45
1:B:2776:ILE:HG23	1:B:2777:PHE:N	2.32	0.45
1:B:2788:MET:HE2	1:B:2821:PHE:CB	2.47	0.45
1:B:2904:GLU:OE1	1:B:2910:ARG:NH2	2.49	0.45
1:B:3312:TYR:H	1:B:3321:LYS:HG3	1.82	0.45
1:A:762:GLU:HG3	1:A:809:PHE:CG	2.51	0.45
1:B:3109:LEU:O	1:B:3110:GLN:C	2.60	0.45
1:B:3158:MET:HE1	1:B:3162:LEU:HD23	1.97	0.45
1:A:946:ASP:OD1	1:A:946:ASP:C	2.60	0.45
1:B:2755:ALA:HB2	1:B:2801:LEU:HD23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1317:ASP:C	1:A:1318:ARG:HG2	2.42	0.45
1:A:1372:LEU:HB3	1:A:1376:ASP:CB	2.41	0.45
1:B:2786:MET:SD	1:B:2791:TYR:HB2	2.57	0.45
1:A:840:SER:O	1:A:844:ARG:HG3	2.17	0.45
1:B:3249:PRO:CD	1:B:3354:MET:HE2	2.44	0.45
1:B:3055:PRO:O	1:B:3056:PRO:C	2.60	0.45
1:B:3062:LYS:HD2	1:B:3081:ASP:CG	2.42	0.45
1:B:3247:VAL:CG2	1:B:3348:VAL:HG22	2.47	0.45
1:B:3338:ALA:HA	1:B:3342:GLN:HB2	1.99	0.45
1:A:787:SER:OG	1:A:789:GLU:HG2	2.16	0.45
1:B:3026:GLN:HA	1:B:3026:GLN:OE1	2.17	0.45
1:A:875:ALA:HA	1:A:907:GLY:O	2.16	0.44
1:B:2806:THR:O	1:B:2883:GLY:HA2	2.18	0.44
1:B:3306:ARG:O	1:B:3307:GLU:HG2	2.18	0.44
1:A:841:TYR:HE2	1:A:846:ASN:ND2	2.16	0.44
1:B:3019:THR:HG22	1:B:3022:ASN:HB2	1.99	0.44
1:B:3067:GLU:OE1	1:B:3080:LYS:HG3	2.16	0.44
1:A:1050:ARG:HD2	1:A:1050:ARG:O	2.17	0.44
1:A:1061:VAL:HG23	1:A:1061:VAL:O	2.18	0.44
1:A:1251:THR:C	1:A:1253:ILE:H	2.25	0.44
1:A:1351:ASP:CB	1:A:1399:LEU:HG	2.47	0.44
5:A:1453:NAP:O3D	5:A:1453:NAP:PA	2.70	0.44
1:B:2769:TYR:CD2	1:B:2884:LEU:HD21	2.52	0.44
1:B:2971:LEU:CD2	1:B:3063:VAL:HG22	2.48	0.44
1:B:3062:LYS:HD2	1:B:3081:ASP:OD1	2.18	0.44
1:B:3360:LYS:HB3	1:B:3364:ARG:CZ	2.44	0.44
1:A:830:HIS:NE2	1:A:838:ARG:O	2.34	0.44
1:A:1080:LYS:NZ	1:B:3080:LYS:HA	2.33	0.44
1:B:3053:ASP:HB3	1:B:3160:ALA:HB2	1.99	0.44
1:B:3134:GLU:OE1	1:B:3134:GLU:HA	2.18	0.44
1:B:3201:ASP:HB2	1:B:3402:TYR:OH	2.18	0.44
1:B:3330:GLN:HB2	1:B:3331:LEU:HD12	1.98	0.44
1:B:3115:LEU:HD22	1:B:3157:GLN:O	2.18	0.44
1:B:3132:LEU:O	1:B:3135:TYR:N	2.50	0.44
1:A:841:TYR:CE2	1:A:846:ASN:ND2	2.86	0.43
1:A:1089:THR:HG23	1:A:1092:GLN:OE1	2.18	0.43
1:A:1249:PRO:HG3	1:A:1354:MET:HG3	2.00	0.43
1:B:2928:ARG:HH12	1:B:3130:LYS:HA	1.82	0.43
1:B:3193:ALA:CB	5:B:2453:NAP:C5D	2.95	0.43
1:A:1027:TYR:CE1	1:A:1177:ILE:HG21	2.53	0.43
1:A:1158:MET:CE	1:A:1159:PRO:HD2	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3110:GLN:CG	1:B:3111:GLN:N	2.81	0.43
1:B:3078:ASN:HB2	1:B:3080:LYS:HZ3	1.82	0.43
1:A:889:TYR:CD1	1:A:1352:VAL:HG21	2.54	0.43
1:A:1132:LEU:O	1:A:1136:GLU:HG2	2.18	0.43
1:B:2882:PHE:CD1	1:B:2915:ARG:HB3	2.53	0.43
1:A:813:ASP:HB3	1:A:814:PRO:CD	2.49	0.43
1:B:3242:VAL:CG1	1:B:3343:GLY:O	2.65	0.43
1:B:3250:GLY:O	1:B:3253:ILE:HG22	2.18	0.43
1:B:3364:ARG:C	1:B:3366:MET:N	2.73	0.43
1:A:1054:ALA:O	1:A:1055:PRO:C	2.59	0.43
1:B:2845:PHE:CE2	1:B:2898:ALA:HA	2.54	0.43
1:A:1158:MET:HA	1:A:1159:PRO:HD3	1.81	0.43
1:A:1242:VAL:HG22	1:A:1243:PRO:HD2	2.00	0.43
1:A:779:HIS:HB3	1:A:948:VAL:HG22	2.01	0.43
1:A:814:PRO:C	1:A:815:PRO:O	2.59	0.43
1:B:3103:PRO:HA	1:B:3104:PRO:HD3	1.93	0.43
1:B:2788:MET:HE1	1:B:2895:PHE:CZ	2.54	0.43
1:B:2816:GLU:C	1:B:2818:GLY:H	2.27	0.43
1:B:3112:PHE:CZ	1:B:3146:MET:HE1	2.53	0.43
1:B:2787:SER:C	1:B:2789:GLU:H	2.26	0.42
1:B:3220:ALA:O	1:B:3221:ASP:HB2	2.19	0.42
1:A:1385:ARG:HG2	1:A:1390:TYR:HB3	2.00	0.42
1:B:2912:LEU:HD23	1:B:2930:TRP:CD1	2.55	0.42
1:A:1039:ASN:O	1:A:1095:LYS:HD2	2.19	0.42
1:B:3019:THR:HG22	1:B:3022:ASN:CB	2.48	0.42
1:A:1143:ASN:N	1:A:1144:PRO:CD	2.82	0.42
1:B:3003:LEU:HD21	1:B:3014:PHE:HB2	2.02	0.42
1:A:1158:MET:HE1	1:A:1162:LEU:HD23	2.02	0.42
1:A:1343:GLY:HA2	1:A:1389:ARG:NH2	2.34	0.42
1:B:2912:LEU:HD23	1:B:2934:VAL:CG2	2.47	0.42
1:B:3158:MET:HE1	1:B:3162:LEU:CD2	2.48	0.42
1:B:3214:TRP:O	1:B:3218:ILE:HG23	2.18	0.42
1:A:762:GLU:HG3	1:A:809:PHE:CD1	2.55	0.42
1:A:936:LYS:HA	1:A:936:LYS:HD2	1.86	0.42
1:B:2823:CYS:HA	1:B:2826:MET:HB2	2.02	0.42
1:B:2877:VAL:HG12	1:B:2878:ARG:N	2.34	0.42
1:B:3050:ARG:O	1:B:3050:ARG:HG3	2.18	0.42
1:B:3130:LYS:O	1:B:3132:LEU:HG	2.19	0.42
1:A:1195:VAL:HA	5:A:1453:NAP:H5N	2.01	0.42
1:A:1408:LEU:O	1:A:1409:ARG:C	2.63	0.42
1:B:3121:GLU:O	1:B:3125:LEU:HG	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3401:THR:O	1:B:3405:THR:HB	2.20	0.42
1:A:904:GLU:OE2	1:A:910:ARG:NH2	2.50	0.42
1:A:985:SER:HA	1:A:990:LYS:O	2.19	0.42
1:B:3309:TYR:CE1	1:B:3331:LEU:HD21	2.55	0.42
1:B:3409:ARG:O	1:B:3413:ILE:HG13	2.19	0.42
1:A:965:LYS:CD	1:A:968:LYS:HD2	2.43	0.42
1:B:2788:MET:HE2	1:B:2821:PHE:CG	2.55	0.42
1:B:3244:CYS:HA	1:B:3345:HIS:O	2.19	0.42
1:A:970:ARG:HD2	1:A:1079:TRP:CE3	2.55	0.41
1:A:784:LYS:HG2	1:B:2976:GLU:OE1	2.21	0.41
1:A:901:THR:O	1:A:905:GLU:HG3	2.20	0.41
1:B:2779:HIS:HB2	1:B:2935:PHE:HZ	1.86	0.41
1:B:2879:PHE:CD1	1:B:2879:PHE:C	2.98	0.41
1:B:3257:ARG:HA	1:B:3260:TRP:CD2	2.55	0.41
1:A:970:ARG:HD3	1:A:972:THR:CG2	2.50	0.41
1:A:1062:LYS:CE	1:A:1087:PRO:HG3	2.42	0.41
1:B:2936:LYS:HE3	1:B:2940:ASP:OD2	2.21	0.41
1:B:2964:TRP:CG	1:B:3162:LEU:HD13	2.55	0.41
1:B:3162:LEU:O	1:B:3166:GLN:HG2	2.19	0.41
1:A:998:LEU:HD21	1:A:1018:HIS:HB2	2.01	0.41
1:A:1318:ARG:CB	1:A:1319:PRO:CD	2.98	0.41
1:A:962:ARG:C	1:A:963:SER:O	2.64	0.41
1:A:996:ARG:HG3	6:A:5035:HOH:O	2.19	0.41
1:A:1054:ALA:HB2	1:A:1160:ALA:HB2	2.01	0.41
1:B:3040:HIS:O	1:B:3044:VAL:HG23	2.20	0.41
1:B:3109:LEU:O	1:B:3112:PHE:N	2.54	0.41
1:B:3371:LYS:HA	1:B:3371:LYS:HD3	1.62	0.41
1:A:810:GLY:HA2	6:A:5051:HOH:O	2.20	0.41
1:A:1251:THR:C	1:A:1253:ILE:N	2.79	0.41
1:B:2912:LEU:CD2	1:B:2934:VAL:CG2	2.94	0.41
1:A:1198:HIS:CE1	1:A:1206:VAL:HG22	2.54	0.41
1:A:1268:GLN:NE2	1:A:1302:LYS:CD	2.84	0.41
1:A:1324:GLN:CG	1:A:1357:ASP:HB3	2.45	0.41
1:B:2828:MET:HG2	1:B:2906:LEU:HD22	2.01	0.41
1:A:780:ALA:N	1:A:948:VAL:HG21	2.35	0.41
1:A:935:PHE:CE2	1:A:948:VAL:HG11	2.56	0.41
1:A:979:ASP:OD1	1:A:980:LEU:N	2.54	0.41
1:A:1158:MET:HE3	1:A:1159:PRO:N	2.35	0.41
1:A:1263:ARG:HA	1:A:1263:ARG:HD3	1.81	0.41
1:B:2793:ILE:HD13	1:B:2824:ALA:CB	2.51	0.41
1:B:3353:THR:CG2	5:B:2453:NAP:N6A	2.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2773:LEU:O	1:B:2776:ILE:CG2	2.69	0.41
1:B:3158:MET:HA	1:B:3159:PRO:HD3	1.85	0.41
1:B:3347:TYR:CZ	1:B:3391:HIS:CD2	3.09	0.41
1:A:762:GLU:HG2	1:A:815:PRO:HB3	2.04	0.40
1:A:1013:ILE:HD13	1:A:1194:ILE:HD11	2.04	0.40
1:B:2928:ARG:O	1:B:2931:ALA:HB3	2.21	0.40
1:B:2961:ASP:C	1:B:2963:SER:N	2.78	0.40
1:A:982:GLN:HA	1:A:982:GLN:OE1	2.20	0.40
1:A:1081:ASP:O	1:A:1082:GLU:C	2.63	0.40
1:A:1183:MET:HG2	1:A:1184:TYR:CE2	2.56	0.40
1:B:3266:ASP:HB3	1:B:3272:MET:HG3	2.02	0.40
1:B:3332:ALA:HB1	1:B:3365:ILE:HG23	2.02	0.40
1:A:1024:GLU:OE1	1:A:1024:GLU:HA	2.22	0.40
1:A:1328:GLN:HE21	1:A:1361:ALA:CB	2.31	0.40
1:A:1399:LEU:O	1:A:1400:ARG:C	2.64	0.40
1:B:2843:VAL:HG12	1:B:2844:ARG:N	2.36	0.40
1:B:2998:LEU:HD23	1:B:2998:LEU:HA	1.90	0.40
1:A:935:PHE:CZ	1:A:948:VAL:HG11	2.57	0.40
1:B:3354:MET:SD	1:B:3354:MET:C	3.04	0.40
1:A:983:GLY:O	1:A:987:VAL:HG23	2.22	0.40
1:B:2756:THR:HG22	1:B:2758:LEU:HG	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1133:GLN:OE1	1:B:3364:ARG:NE[1_654]	2.08	0.12

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	622/688 (90%)	569 (92%)	40 (6%)	13 (2%)	5	4
1	B	608/688 (88%)	548 (90%)	51 (8%)	9 (2%)	8	8
All	All	1230/1376 (89%)	1117 (91%)	91 (7%)	22 (2%)	6	6

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	839	LYS
1	A	848	VAL
1	A	960	ASN
1	A	963	SER
1	A	1411	GLU
1	B	2948	VAL
1	B	3131	GLY
1	B	3133	GLN
1	A	838	ARG
1	A	962	ARG
1	A	1410	SER
1	B	2843	VAL
1	A	1370	GLY
1	B	3053	ASP
1	B	3114	SER
1	B	3286	SER
1	B	3374	GLU
1	A	1057	ALA
1	A	1069	ARG
1	B	3317	ASP
1	A	1055	PRO
1	A	978	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	543/601 (90%)	509 (94%)	34 (6%)	16	23

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	531/601 (88%)	494 (93%)	37 (7%)	14	19
All	All	1074/1202 (89%)	1003 (93%)	71 (7%)	15	21

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	751	LYS
1	A	752	ARG
1	A	787	SER
1	A	809	PHE
1	A	820	LYS
1	A	830	HIS
1	A	844	ARG
1	A	847	SER
1	A	876	ASN
1	A	890	PRO
1	A	912	LEU
1	A	915	ARG
1	A	946	ASP
1	A	949	ASN
1	A	950	ILE
1	A	970	ARG
1	A	979	ASP
1	A	991	ARG
1	A	1022	ASN
1	A	1055	PRO
1	A	1056	PRO
1	A	1058	ASN
1	A	1078	ASN
1	A	1161	THR
1	A	1165	THR
1	A	1218	ILE
1	A	1242	VAL
1	A	1297	LEU
1	A	1317	ASP
1	A	1324	GLN
1	A	1333	GLU
1	A	1371	LYS
1	A	1405	THR
1	A	1413	ILE
1	B	2756	THR
1	B	2762	GLU

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Mol	Chain	Res	Type
1	B	2792	ASP
1	B	2793	ILE
1	B	2840	SER
1	B	2890	PRO
1	B	2914	MET
1	B	2915	ARG
1	B	2919	GLU
1	B	2946	ASP
1	B	2965	LYS
1	B	2970	ARG
1	B	3020	ASN
1	B	3022	ASN
1	B	3049	GLU
1	B	3055	PRO
1	B	3056	PRO
1	B	3068	GLU
1	B	3070	ASN
1	B	3078	ASN
1	B	3090	ILE
1	B	3124	ARG
1	B	3171	GLN
1	B	3221	ASP
1	B	3238	ARG
1	B	3266	ASP
1	B	3272	MET
1	B	3287	LYS
1	B	3324	GLN
1	B	3346	ILE
1	B	3367	THR
1	B	3369	GLN
1	B	3380	PHE
1	B	3399	LEU
1	B	3405	THR
1	B	3406	ASN
1	B	3411	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	798	HIS
1	A	876	ASN
1	A	949	ASN

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Mol	Chain	Res	Type
1	A	986	ASN
1	A	988	HIS
1	A	1001	GLN
1	A	1002	ASN
1	A	1004	GLN
1	A	1022	ASN
1	A	1070	ASN
1	A	1078	ASN
1	A	1110	GLN
1	A	1111	GLN
1	A	1143	ASN
1	A	1166	GLN
1	A	1216	ASN
1	A	1239	ASN
1	A	1241	GLN
1	A	1262	GLN
1	A	1264	GLN
1	A	1268	GLN
1	A	1290	HIS
1	A	1324	GLN
1	A	1328	GLN
1	A	1342	GLN
1	B	2795	HIS
1	B	2798	HIS
1	B	2846	ASN
1	B	2967	ASN
1	B	2982	GLN
1	B	2986	ASN
1	B	2988	HIS
1	B	3004	GLN
1	B	3020	ASN
1	B	3078	ASN
1	B	3110	GLN
1	B	3111	GLN
1	B	3123	GLN
1	B	3166	GLN
1	B	3216	ASN
1	B	3241	GLN
1	B	3261	GLN
1	B	3262	GLN
1	B	3285	GLN
1	B	3324	GLN

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Mol	Chain	Res	Type
1	B	3342	GLN
1	B	3363	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	A	1452	-	58,58,58	5.98	44 (75%)	85,89,89	3.46	31 (36%)
4	FAD	B	2452	-	58,58,58	5.81	40 (68%)	85,89,89	3.47	31 (36%)
5	NAP	A	1453	-	50,52,52	2.02	10 (20%)	71,80,80	2.26	17 (23%)
5	NAP	B	2453	-	50,52,52	2.60	11 (22%)	71,80,80	2.51	24 (33%)
2	SO3	A	1500	-	1,3,3	2.49	1 (100%)	0,3,3	-	-
2	SO3	B	2500	-	1,3,3	2.46	1 (100%)	0,3,3	-	-
3	FMN	A	1451	-	33,33,33	4.06	19 (57%)	48,50,50	2.54	19 (39%)
3	FMN	B	2451	-	33,33,33	4.17	19 (57%)	48,50,50	2.46	17 (35%)

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	A	1452	-	-	5/34/50/50	0/6/6/6
4	FAD	B	2452	-	-	5/34/50/50	0/6/6/6
5	NAP	A	1453	-	-	18/35/67/67	0/5/5/5
5	NAP	B	2453	-	-	16/35/67/67	0/5/5/5
3	FMN	A	1451	-	-	0/18/18/18	0/3/3/3
3	FMN	B	2451	-	-	0/18/18/18	0/3/3/3

All (145) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1452	FAD	P-O3P	17.75	1.78	1.59
4	B	2452	FAD	P-O3P	16.14	1.76	1.59
4	A	1452	FAD	PA-O3P	-12.78	1.45	1.59
5	B	2453	NAP	C2N-N1N	12.30	1.48	1.35
4	B	2452	FAD	C2A-N1A	12.20	1.55	1.33
4	B	2452	FAD	C4A-N3A	11.96	1.56	1.34
4	B	2452	FAD	PA-O3P	-11.94	1.46	1.59
4	A	1452	FAD	C2A-N1A	11.84	1.55	1.33
4	A	1452	FAD	C9A-C5X	11.81	1.60	1.41
4	B	2452	FAD	C1'-C2'	11.38	1.68	1.52
3	B	2451	FMN	C9-C9A	11.29	1.57	1.39
4	A	1452	FAD	C4A-N3A	11.21	1.55	1.34
3	A	1451	FMN	C9-C9A	11.21	1.57	1.39
4	B	2452	FAD	C9A-C5X	10.89	1.58	1.41
4	A	1452	FAD	C1'-C2'	10.29	1.67	1.52
4	B	2452	FAD	C2A-N3A	9.03	1.50	1.33
4	A	1452	FAD	C2A-N3A	8.80	1.49	1.33
4	A	1452	FAD	C8A-N9A	8.55	1.52	1.37
4	B	2452	FAD	C8A-N9A	8.27	1.51	1.37
4	A	1452	FAD	C8-C7	8.24	1.60	1.40
5	A	1453	NAP	C2N-N1N	8.11	1.43	1.35
4	B	2452	FAD	C4'-C3'	-8.01	1.39	1.53
3	B	2451	FMN	C9A-C5A	7.90	1.53	1.41
3	A	1451	FMN	C6-C7	7.76	1.50	1.39
4	A	1452	FAD	O4'-C4'	7.50	1.59	1.43
4	B	2452	FAD	C8-C7	7.36	1.58	1.40
4	A	1452	FAD	C4'-C3'	-7.14	1.40	1.53
3	B	2451	FMN	C6-C7	7.13	1.49	1.39
4	B	2452	FAD	C2B-C1B	-7.05	1.31	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1452	FAD	C2B-C1B	-6.88	1.31	1.53
3	A	1451	FMN	C9A-C5A	6.85	1.52	1.41
3	B	2451	FMN	C4-N3	6.83	1.51	1.38
4	B	2452	FAD	C8A-N7A	-6.83	1.18	1.31
4	A	1452	FAD	C1B-N9A	6.80	1.65	1.46
4	B	2452	FAD	C1B-N9A	6.65	1.64	1.46
4	A	1452	FAD	C8A-N7A	-6.61	1.19	1.31
4	B	2452	FAD	O4'-C4'	6.60	1.57	1.43
4	B	2452	FAD	C10-N10	6.42	1.51	1.37
3	B	2451	FMN	C2'-C3'	-6.36	1.42	1.53
4	B	2452	FAD	C9-C9A	6.35	1.49	1.39
4	A	1452	FAD	C3B-C4B	-6.35	1.36	1.53
5	B	2453	NAP	O4D-C1D	6.35	1.49	1.40
3	A	1451	FMN	C2'-C3'	-6.34	1.42	1.53
4	A	1452	FAD	C9-C9A	6.32	1.49	1.39
4	A	1452	FAD	C2'-C3'	6.28	1.64	1.53
4	A	1452	FAD	P-O2P	-6.25	1.26	1.55
3	B	2451	FMN	C4A-C10	6.03	1.61	1.44
4	B	2452	FAD	P-O2P	-5.95	1.27	1.55
4	A	1452	FAD	PA-O2A	-5.95	1.27	1.55
4	B	2452	FAD	C3B-C4B	-5.80	1.38	1.53
4	B	2452	FAD	PA-O2A	-5.79	1.28	1.55
4	B	2452	FAD	C5A-C6A	5.76	1.57	1.41
3	A	1451	FMN	C4-N3	5.69	1.49	1.38
4	A	1452	FAD	C5A-C6A	5.64	1.56	1.41
4	A	1452	FAD	C5A-N7A	-5.58	1.28	1.39
3	A	1451	FMN	C5A-N5	5.57	1.49	1.39
4	A	1452	FAD	O4-C4	-5.47	1.13	1.23
4	A	1452	FAD	C8M-C8	-5.32	1.41	1.51
4	B	2452	FAD	O2'-C2'	-5.30	1.32	1.43
4	A	1452	FAD	C4X-N5	5.30	1.42	1.30
5	A	1453	NAP	P2B-O2B	5.28	1.68	1.59
3	B	2451	FMN	C5A-N5	5.25	1.49	1.39
4	B	2452	FAD	C5A-N7A	-5.18	1.29	1.39
3	A	1451	FMN	C4A-C10	5.10	1.59	1.44
3	A	1451	FMN	C8-C7	4.99	1.53	1.40
3	B	2451	FMN	C8-C7	4.97	1.52	1.40
4	A	1452	FAD	O2'-C2'	-4.88	1.33	1.43
4	A	1452	FAD	C10-N10	4.80	1.47	1.37
3	B	2451	FMN	C2-N3	4.73	1.49	1.39
4	B	2452	FAD	O4-C4	-4.68	1.14	1.23
4	A	1452	FAD	O5'-C5'	-4.65	1.27	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2452	FAD	C2'-C3'	4.62	1.61	1.53
4	B	2452	FAD	P-O1P	-4.59	1.34	1.50
4	B	2452	FAD	C4X-N5	4.57	1.40	1.30
5	B	2453	NAP	P2B-O2B	4.57	1.67	1.59
5	B	2453	NAP	C6N-N1N	4.55	1.45	1.35
3	B	2451	FMN	C9A-N10	4.54	1.49	1.41
4	B	2452	FAD	C8M-C8	-4.49	1.42	1.51
4	B	2452	FAD	C10-N1	4.42	1.42	1.33
3	B	2451	FMN	C10-N10	4.37	1.46	1.37
4	A	1452	FAD	C5B-C4B	4.32	1.64	1.51
4	A	1452	FAD	C1'-N10	4.28	1.58	1.47
3	A	1451	FMN	O3'-C3'	4.25	1.53	1.43
3	A	1451	FMN	C6-C5A	4.23	1.46	1.40
4	A	1452	FAD	P-O1P	-4.22	1.36	1.50
4	A	1452	FAD	C10-N1	4.20	1.41	1.33
3	A	1451	FMN	C10-N10	4.19	1.46	1.37
5	A	1453	NAP	PA-O3	4.17	1.64	1.59
4	B	2452	FAD	C6A-N6A	4.12	1.44	1.34
3	B	2451	FMN	C6-C5A	4.07	1.46	1.40
3	A	1451	FMN	C2-N3	4.06	1.47	1.39
5	A	1453	NAP	C6N-N1N	4.02	1.44	1.35
4	B	2452	FAD	C4A-N9A	3.98	1.46	1.37
3	B	2451	FMN	O3'-C3'	3.92	1.52	1.43
3	A	1451	FMN	C5'-C4'	3.81	1.57	1.51
5	B	2453	NAP	C4N-C3N	3.80	1.45	1.39
4	A	1452	FAD	O2-C2	-3.80	1.16	1.24
4	B	2452	FAD	O5'-C5'	-3.79	1.30	1.44
4	B	2452	FAD	PA-O1A	-3.74	1.37	1.50
3	B	2451	FMN	O2'-C2'	-3.73	1.35	1.43
4	A	1452	FAD	C5A-C4A	3.73	1.45	1.39
3	A	1451	FMN	O2'-C2'	-3.73	1.35	1.43
4	A	1452	FAD	O3B-C3B	-3.73	1.33	1.43
4	B	2452	FAD	C1'-N10	3.71	1.56	1.47
4	B	2452	FAD	O3'-C3'	3.71	1.52	1.43
5	A	1453	NAP	O4D-C1D	3.66	1.45	1.40
3	B	2451	FMN	C5'-C4'	3.57	1.56	1.51
3	A	1451	FMN	C9A-N10	3.56	1.47	1.41
4	B	2452	FAD	O3B-C3B	-3.53	1.34	1.43
4	A	1452	FAD	C6A-N6A	3.52	1.43	1.34
5	B	2453	NAP	PA-O3	-3.41	1.55	1.59
4	B	2452	FAD	C5A-C4A	3.39	1.45	1.39
4	B	2452	FAD	C5B-C4B	3.39	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1452	FAD	PA-O1A	-3.34	1.39	1.50
4	A	1452	FAD	C4A-N9A	3.22	1.44	1.37
5	B	2453	NAP	C5A-N7A	-3.20	1.33	1.39
4	A	1452	FAD	C6-C5X	-3.12	1.35	1.40
5	A	1453	NAP	C5A-N7A	-2.94	1.33	1.39
4	B	2452	FAD	C9-C8	-2.94	1.35	1.39
3	A	1451	FMN	C4A-C4	-2.90	1.33	1.44
3	A	1451	FMN	P-O1P	-2.71	1.42	1.50
5	B	2453	NAP	C2N-C3N	-2.67	1.34	1.39
5	A	1453	NAP	C4N-C3N	2.62	1.43	1.39
4	A	1452	FAD	C4-N3	2.57	1.43	1.38
5	A	1453	NAP	C3N-C7N	2.56	1.54	1.50
5	A	1453	NAP	C2D-C3D	-2.53	1.46	1.53
4	A	1452	FAD	C9-C8	-2.52	1.36	1.39
2	A	1500	SO3	O1-S	2.49	1.55	1.44
3	B	2451	FMN	P-O3P	-2.47	1.45	1.54
2	B	2500	SO3	O1-S	2.46	1.54	1.44
3	B	2451	FMN	C4A-C4	-2.45	1.35	1.44
4	A	1452	FAD	C6-C7	-2.44	1.36	1.39
5	B	2453	NAP	O3D-C3D	2.43	1.49	1.43
3	B	2451	FMN	P-O1P	-2.34	1.43	1.50
3	A	1451	FMN	C7M-C7	-2.34	1.46	1.51
4	A	1452	FAD	O3'-C3'	2.29	1.48	1.43
4	B	2452	FAD	O4B-C1B	2.28	1.47	1.42
5	B	2453	NAP	C4A-N9A	-2.24	1.33	1.37
3	A	1451	FMN	P-O3P	-2.18	1.46	1.54
5	A	1453	NAP	PN-O3	2.12	1.61	1.59
5	B	2453	NAP	C3D-C4D	-2.10	1.47	1.53
4	A	1452	FAD	C2B-C3B	-2.08	1.47	1.53
4	B	2452	FAD	C4-N3	2.08	1.42	1.38
4	A	1452	FAD	C4X-C10	-2.02	1.38	1.44
3	B	2451	FMN	C10-N1	2.01	1.37	1.33

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2452	FAD	O4B-C1B-N9A	-15.40	78.51	108.09
4	A	1452	FAD	O4B-C1B-N9A	-15.20	78.90	108.09
4	A	1452	FAD	O2A-PA-O3P	13.52	143.82	107.27
4	B	2452	FAD	O2A-PA-O3P	13.24	143.06	107.27
5	B	2453	NAP	C4D-O4D-C1D	-9.73	101.02	109.92
4	A	1452	FAD	C4A-N9A-C8A	-9.03	96.26	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2452	FAD	C4A-N9A-C8A	-8.71	96.60	105.74
4	B	2452	FAD	C2B-C1B-N9A	8.37	134.11	113.30
5	A	1453	NAP	C4D-O4D-C1D	-8.27	102.35	109.92
4	A	1452	FAD	C2B-C1B-N9A	8.03	133.26	113.30
4	A	1452	FAD	C5X-C9A-N10	-7.39	111.29	117.97
5	A	1453	NAP	C5A-C4A-N3A	-7.27	116.70	126.72
4	B	2452	FAD	C5X-C9A-N10	-7.23	111.44	117.97
5	B	2453	NAP	C5A-C4A-N3A	-7.00	117.07	126.72
5	B	2453	NAP	N3A-C4A-N9A	6.89	138.89	127.17
4	B	2452	FAD	O3P-PA-O1A	-6.87	90.04	110.70
4	A	1452	FAD	O3P-PA-O1A	-6.86	90.07	110.70
5	A	1453	NAP	N3A-C4A-N9A	6.85	138.82	127.17
3	A	1451	FMN	C7M-C7-C6	-6.61	107.92	119.57
3	B	2451	FMN	C7M-C7-C6	-6.58	107.98	119.57
4	B	2452	FAD	O5'-P-O1P	-5.59	86.79	108.94
4	A	1452	FAD	O5'-P-O1P	-5.56	86.89	108.94
4	B	2452	FAD	N3A-C2A-N1A	-5.55	120.18	128.58
3	A	1451	FMN	C9A-C5A-N5	-5.37	116.76	122.45
4	A	1452	FAD	C4A-N9A-C1B	-5.35	114.12	126.63
3	B	2451	FMN	C5A-C9A-N10	5.23	122.69	117.97
4	B	2452	FAD	C4A-N9A-C1B	-5.20	114.48	126.63
4	A	1452	FAD	N3A-C2A-N1A	-5.16	120.77	128.58
3	A	1451	FMN	C5A-C9A-N10	5.12	122.60	117.97
5	B	2453	NAP	N3A-C2A-N1A	-5.11	120.85	128.58
3	B	2451	FMN	C9A-C5A-N5	-5.07	117.08	122.45
3	A	1451	FMN	O2-C2-N1	4.91	129.95	121.80
5	A	1453	NAP	N3A-C2A-N1A	-4.82	121.29	128.58
4	A	1452	FAD	C9-C9A-N10	4.70	128.17	121.85
3	B	2451	FMN	C7M-C7-C8	4.67	130.29	120.76
3	A	1451	FMN	C7M-C7-C8	4.60	130.15	120.76
3	B	2451	FMN	C10-N1-C2	4.47	126.54	116.85
5	A	1453	NAP	C2A-N3A-C4A	4.45	122.70	111.83
3	B	2451	FMN	O2-C2-N1	4.40	129.12	121.80
5	B	2453	NAP	C2A-N3A-C4A	4.34	122.43	111.83
4	A	1452	FAD	N9A-C8A-N7A	4.34	120.09	113.94
3	A	1451	FMN	C10-N1-C2	4.32	126.21	116.85
4	B	2452	FAD	C9-C9A-N10	4.32	127.66	121.85
5	A	1453	NAP	C6A-C5A-C4A	4.28	123.03	117.18
4	B	2452	FAD	C1B-N9A-C8A	4.24	136.51	127.09
5	A	1453	NAP	O4B-C1B-N9A	4.23	116.21	108.09
4	B	2452	FAD	O5B-PA-O1A	-4.23	92.19	108.94
5	B	2453	NAP	C5N-C4N-C3N	4.12	124.42	120.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1451	FMN	O4-C4-N3	-4.12	112.37	120.11
4	B	2452	FAD	N9A-C8A-N7A	4.11	119.77	113.94
4	A	1452	FAD	C2A-N1A-C6A	4.04	125.36	118.73
5	B	2453	NAP	O4B-C1B-N9A	4.01	115.79	108.09
4	B	2452	FAD	C3B-C2B-C1B	4.00	109.02	101.46
5	A	1453	NAP	C6A-C5A-N7A	-3.98	124.42	132.09
5	B	2453	NAP	C6A-C5A-C4A	3.97	122.59	117.18
5	B	2453	NAP	C6A-C5A-N7A	-3.93	124.51	132.09
3	B	2451	FMN	O4-C4-N3	-3.85	112.88	120.11
4	B	2452	FAD	C2A-N1A-C6A	3.84	125.04	118.73
4	A	1452	FAD	C3B-C2B-C1B	3.70	108.46	101.46
4	A	1452	FAD	O5B-PA-O1A	-3.61	94.63	108.94
4	A	1452	FAD	C1B-N9A-C8A	3.52	134.91	127.09
4	A	1452	FAD	O4B-C4B-C3B	-3.51	98.18	105.15
3	B	2451	FMN	O3P-P-O2P	3.42	120.64	107.80
4	A	1452	FAD	C4A-C5A-N7A	3.38	114.45	110.58
4	B	2452	FAD	C4A-C5A-N7A	3.37	114.43	110.58
3	B	2451	FMN	C5A-N5-C4A	3.35	123.50	118.09
3	A	1451	FMN	C5A-N5-C4A	3.32	123.47	118.09
3	A	1451	FMN	O3P-P-O2P	3.31	120.22	107.80
4	B	2452	FAD	O4B-C4B-C5B	-3.24	98.95	109.33
4	B	2452	FAD	O3'-C3'-C2'	-3.24	101.57	108.93
4	A	1452	FAD	C9A-N10-C10	3.15	125.56	120.75
4	A	1452	FAD	O3'-C3'-C2'	-3.09	101.92	108.93
4	B	2452	FAD	C9A-N10-C10	3.07	125.43	120.75
5	B	2453	NAP	N6A-C6A-N1A	3.03	125.13	118.38
4	B	2452	FAD	C1'-C2'-C3'	3.03	117.87	109.66
3	A	1451	FMN	C6-C5A-N5	3.00	123.43	118.44
4	A	1452	FAD	O4B-C4B-C5B	-3.00	99.73	109.33
4	A	1452	FAD	C7M-C7-C6	-2.98	114.32	119.57
5	B	2453	NAP	C5D-C4D-C3D	-2.89	104.80	115.21
4	A	1452	FAD	C1'-C2'-C3'	2.87	117.44	109.66
3	A	1451	FMN	O5'-C5'-C4'	-2.83	101.80	109.36
5	B	2453	NAP	O3D-C3D-C4D	2.82	119.19	111.08
3	B	2451	FMN	C9A-N10-C10	-2.82	116.45	120.75
4	B	2452	FAD	C8M-C8-C9	-2.80	114.64	119.57
5	A	1453	NAP	C5N-C4N-C3N	2.79	123.11	120.36
4	B	2452	FAD	C2B-C3B-C4B	2.78	107.98	102.61
4	B	2452	FAD	O4B-C4B-C3B	-2.76	99.67	105.15
4	A	1452	FAD	C10-N1-C2	2.74	122.78	116.85
5	A	1453	NAP	N6A-C6A-N1A	2.74	124.47	118.38
5	B	2453	NAP	O7N-C7N-C3N	-2.74	116.25	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1453	NAP	O4B-C4B-C5B	-2.70	100.69	109.33
3	A	1451	FMN	C4'-C3'-C2'	2.68	118.04	113.57
3	B	2451	FMN	C6-C5A-N5	2.67	122.87	118.44
4	A	1452	FAD	C8M-C8-C9	-2.66	114.89	119.57
4	B	2452	FAD	C7M-C7-C6	-2.64	114.93	119.57
3	B	2451	FMN	C4A-C10-N1	-2.58	118.27	124.59
5	B	2453	NAP	C4A-N9A-C8A	2.58	108.44	105.74
5	B	2453	NAP	O5B-C5B-C4B	-2.53	100.38	108.99
5	B	2453	NAP	O2N-PN-O5D	2.52	118.99	107.57
4	A	1452	FAD	C4X-C4-N3	2.49	119.60	113.25
5	A	1453	NAP	O2N-PN-O5D	2.48	118.79	107.57
3	B	2451	FMN	O5'-C5'-C4'	-2.47	102.76	109.36
3	A	1451	FMN	C9A-N10-C10	-2.46	117.00	120.75
5	B	2453	NAP	O2N-PN-O3	-2.46	100.63	107.27
3	A	1451	FMN	C4A-C10-N1	-2.44	118.60	124.59
5	B	2453	NAP	O3D-C3D-C2D	2.41	119.55	111.82
5	B	2453	NAP	O3X-P2B-O2X	2.41	116.82	107.80
5	A	1453	NAP	C5D-C4D-C3D	-2.39	106.60	115.21
4	B	2452	FAD	C10-N1-C2	2.39	122.01	116.85
5	A	1453	NAP	O5B-C5B-C4B	-2.37	100.92	108.99
5	A	1453	NAP	C4A-N9A-C8A	2.35	108.20	105.74
4	A	1452	FAD	C4-N3-C2	-2.34	121.48	125.64
5	B	2453	NAP	C2D-C3D-C4D	-2.34	98.09	102.61
3	A	1451	FMN	C5'-C4'-C3'	2.33	116.61	112.22
4	A	1452	FAD	O2P-P-O1P	2.32	123.22	112.44
3	B	2451	FMN	C4'-C3'-C2'	2.30	117.40	113.57
4	A	1452	FAD	C2B-C3B-C4B	2.30	107.05	102.61
3	A	1451	FMN	C4A-C10-N10	2.26	119.72	116.48
3	A	1451	FMN	O3'-C3'-C4'	-2.24	103.84	108.93
3	B	2451	FMN	C4A-C10-N10	2.24	119.68	116.48
4	A	1452	FAD	C7M-C7-C8	2.23	125.32	120.76
4	B	2452	FAD	O2P-P-O5'	2.23	117.67	107.57
4	B	2452	FAD	C4X-C4-N3	2.23	118.92	113.25
5	B	2453	NAP	N9A-C8A-N7A	-2.21	110.81	113.94
5	B	2453	NAP	O2A-PA-O3	-2.20	101.34	107.27
3	A	1451	FMN	N3-C2-N1	-2.17	114.89	119.50
3	A	1451	FMN	C10-C4A-N5	-2.15	120.41	124.81
5	B	2453	NAP	O5D-C5D-C4D	2.14	116.27	108.99
4	B	2452	FAD	C2'-C1'-N10	-2.13	100.11	110.20
4	A	1452	FAD	O2P-P-O5'	2.11	117.13	107.57
4	B	2452	FAD	O2P-P-O1P	2.08	122.12	112.44
3	B	2451	FMN	C10-C4A-N5	-2.07	120.59	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2452	FAD	C5A-C4A-N9A	-2.04	103.59	105.81
5	A	1453	NAP	O7N-C7N-C3N	-2.03	117.12	119.60
4	A	1452	FAD	C4X-C10-N1	-2.02	119.64	124.59
3	B	2451	FMN	C5'-C4'-C3'	2.01	116.02	112.22
5	B	2453	NAP	C4A-C5A-N7A	2.01	112.88	110.58
5	A	1453	NAP	N9A-C8A-N7A	-2.01	111.09	113.94
4	B	2452	FAD	C7M-C7-C8	2.00	124.84	120.76

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1453	NAP	C5D-O5D-PN-O3
5	A	1453	NAP	C5D-O5D-PN-O1N
5	A	1453	NAP	C5D-O5D-PN-O2N
5	A	1453	NAP	O4D-C1D-N1N-C6N
5	B	2453	NAP	C5B-O5B-PA-O1A
5	B	2453	NAP	C5B-O5B-PA-O2A
5	B	2453	NAP	C5B-O5B-PA-O3
5	B	2453	NAP	C5D-O5D-PN-O3
5	B	2453	NAP	O4D-C4D-C5D-O5D
5	A	1453	NAP	C3B-C4B-C5B-O5B
5	A	1453	NAP	O4D-C4D-C5D-O5D
5	B	2453	NAP	C3B-C4B-C5B-O5B
5	A	1453	NAP	O4B-C4B-C5B-O5B
5	A	1453	NAP	C3D-C4D-C5D-O5D
5	B	2453	NAP	O4B-C4B-C5B-O5B
5	B	2453	NAP	C3D-C4D-C5D-O5D
4	A	1452	FAD	O2'-C2'-C3'-O3'
4	B	2452	FAD	O2'-C2'-C3'-O3'
4	B	2452	FAD	O4B-C4B-C5B-O5B
5	A	1453	NAP	C2B-C1B-N9A-C8A
5	B	2453	NAP	C2B-C1B-N9A-C8A
4	A	1452	FAD	O2'-C2'-C3'-C4'
4	B	2452	FAD	O2'-C2'-C3'-C4'
5	A	1453	NAP	PA-O3-PN-O5D
5	B	2453	NAP	PA-O3-PN-O5D
4	B	2452	FAD	C3B-C4B-C5B-O5B
4	A	1452	FAD	C2B-C1B-N9A-C8A
5	A	1453	NAP	C5B-O5B-PA-O1A
5	A	1453	NAP	C5B-O5B-PA-O2A
5	A	1453	NAP	C5B-O5B-PA-O3

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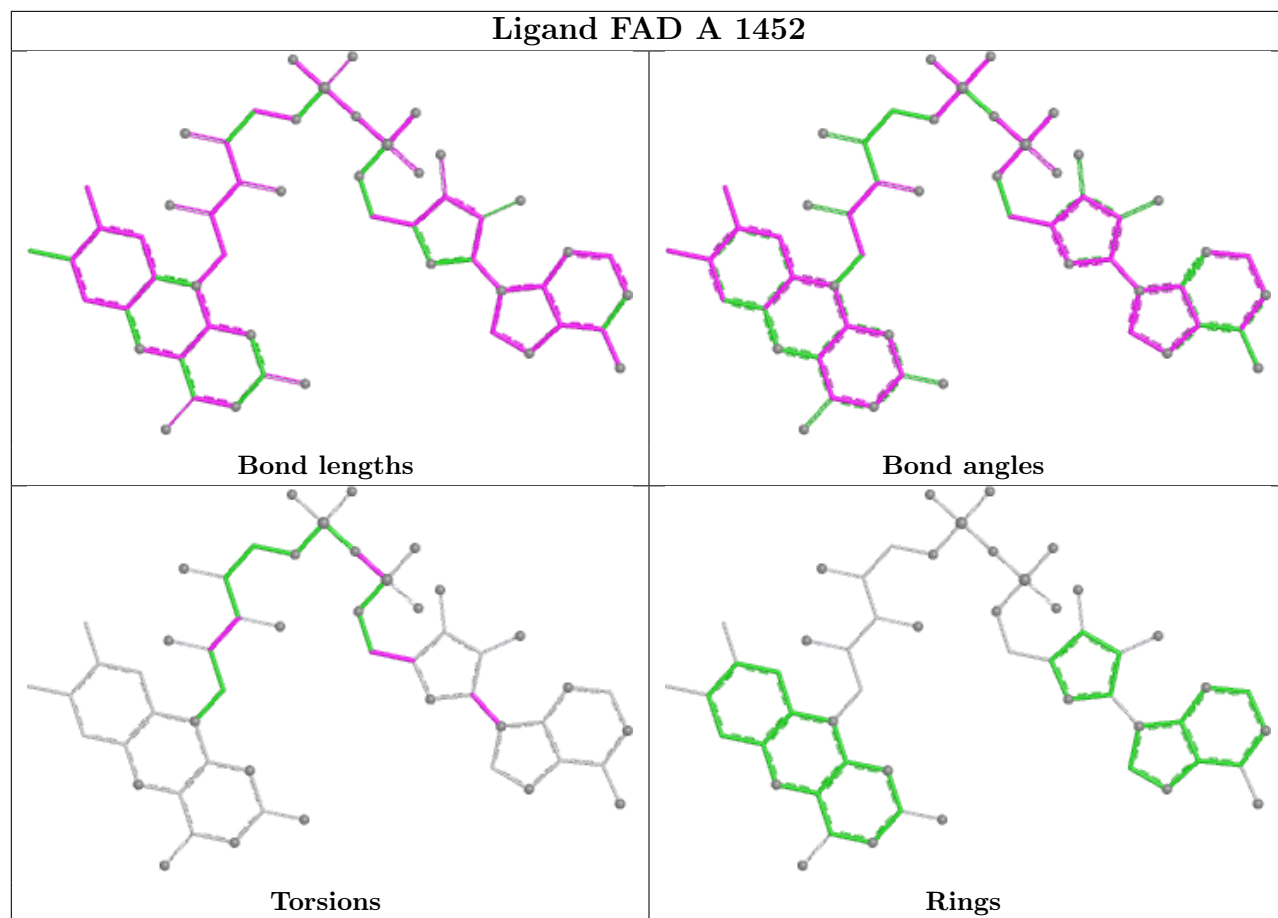
Mol	Chain	Res	Type	Atoms
5	B	2453	NAP	C5D-O5D-PN-O1N
5	A	1453	NAP	C2B-C1B-N9A-C4A
5	B	2453	NAP	C2B-C1B-N9A-C4A
5	A	1453	NAP	C2D-C1D-N1N-C2N
5	B	2453	NAP	C2D-C1D-N1N-C2N
5	A	1453	NAP	O4D-C1D-N1N-C2N
4	A	1452	FAD	P-O3P-PA-O1A
4	B	2452	FAD	C2B-C1B-N9A-C8A
5	A	1453	NAP	O4B-C1B-N9A-C8A
5	B	2453	NAP	O4B-C1B-N9A-C8A
4	A	1452	FAD	O4B-C4B-C5B-O5B
5	A	1453	NAP	C4D-C5D-O5D-PN
5	B	2453	NAP	C4D-C5D-O5D-PN
5	B	2453	NAP	PA-O3-PN-O2N

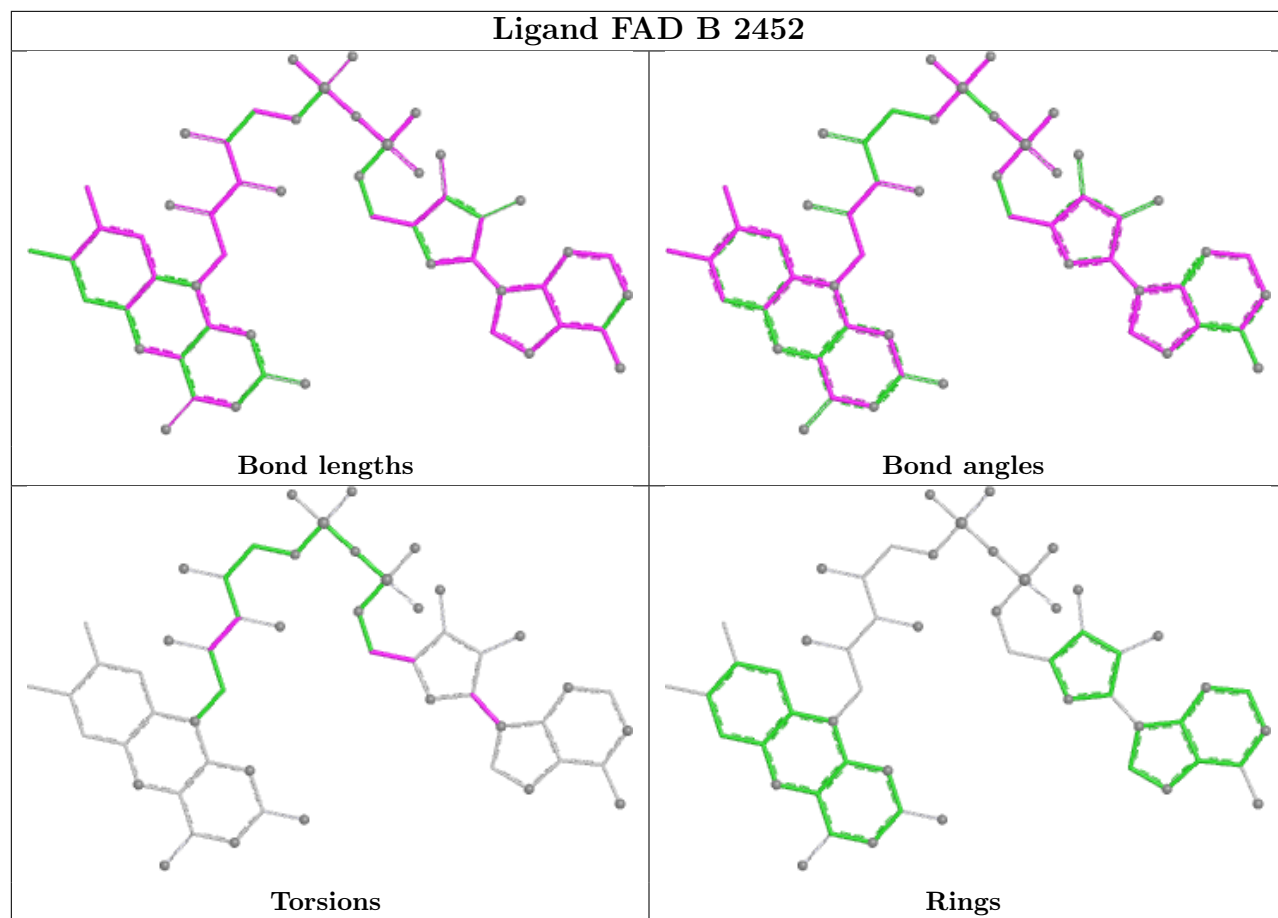
There are no ring outliers.

2 monomers are involved in 22 short contacts:

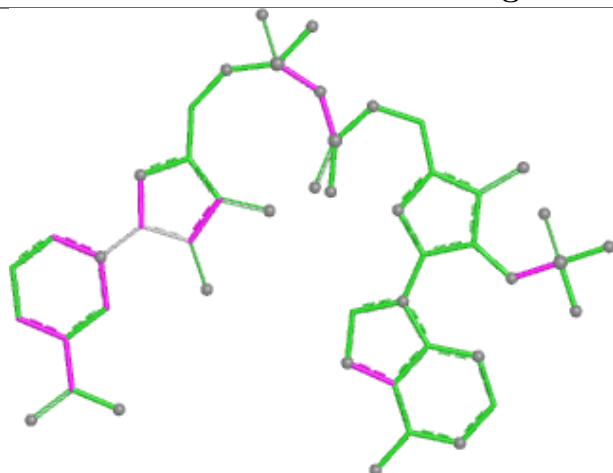
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1453	NAP	9	0
5	B	2453	NAP	13	0

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.

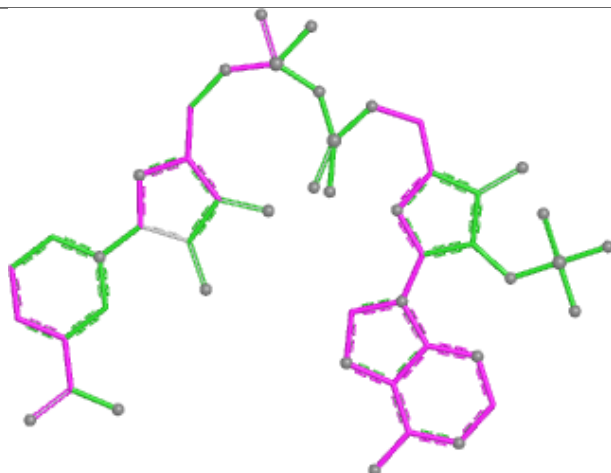




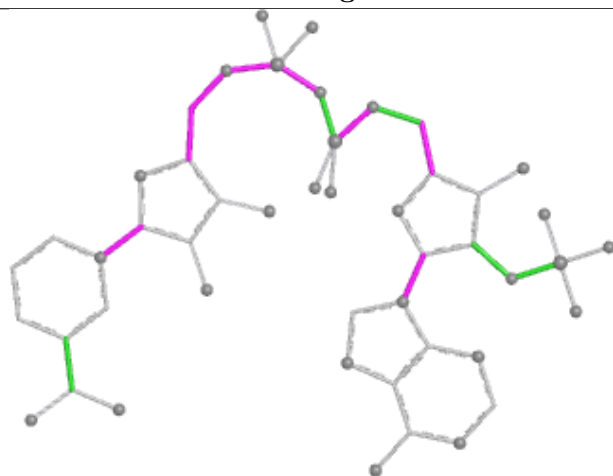
Ligand NAP A 1453



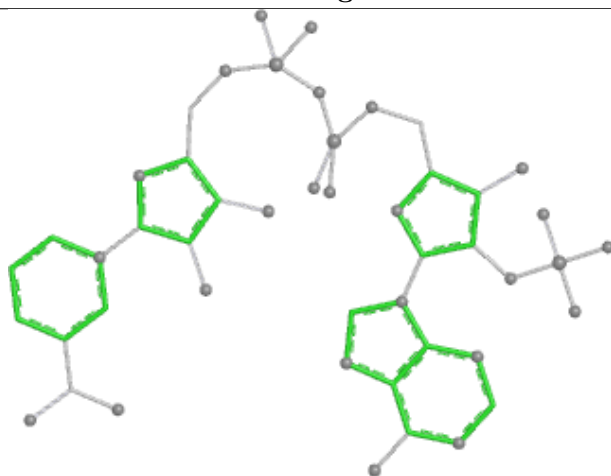
Bond lengths



Bond angles

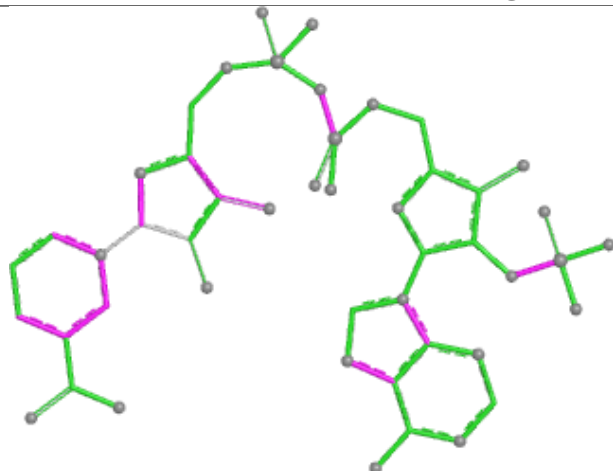


Torsions

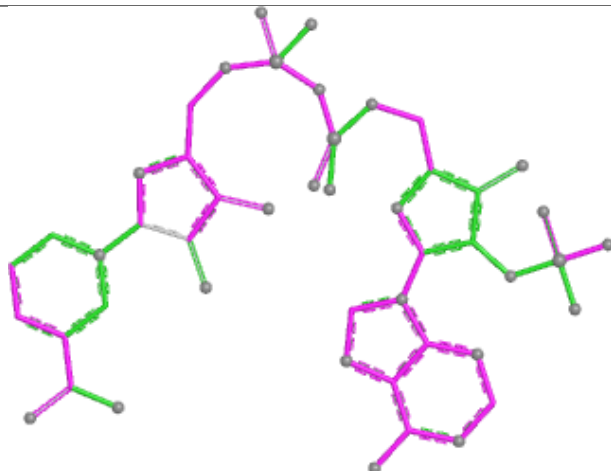


Rings

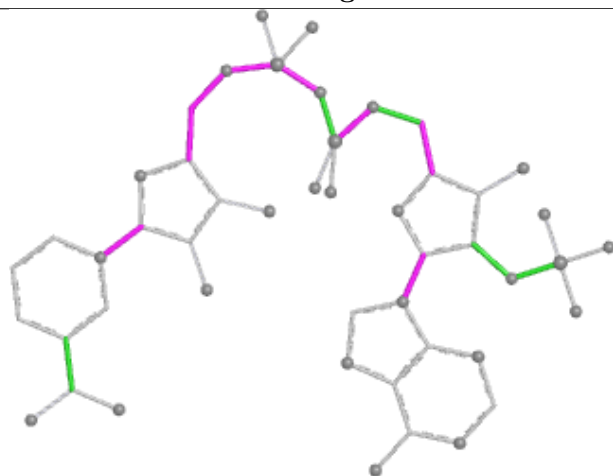
Ligand NAP B 2453



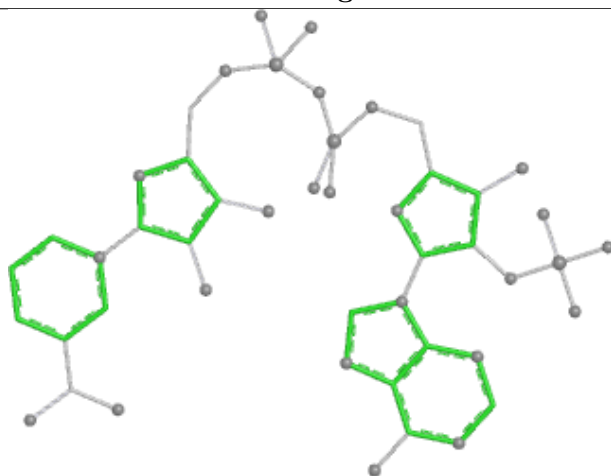
Bond lengths



Bond angles

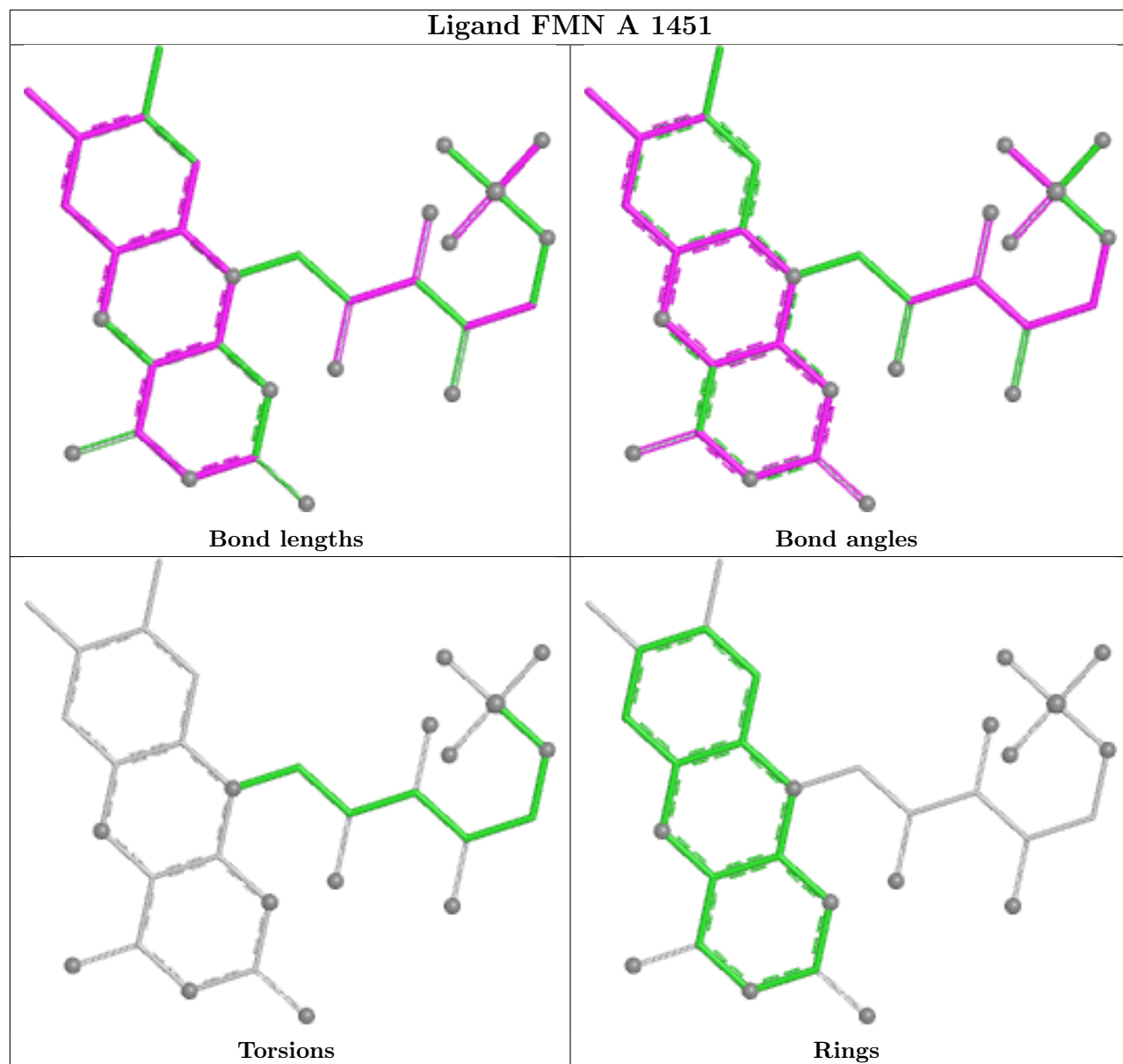


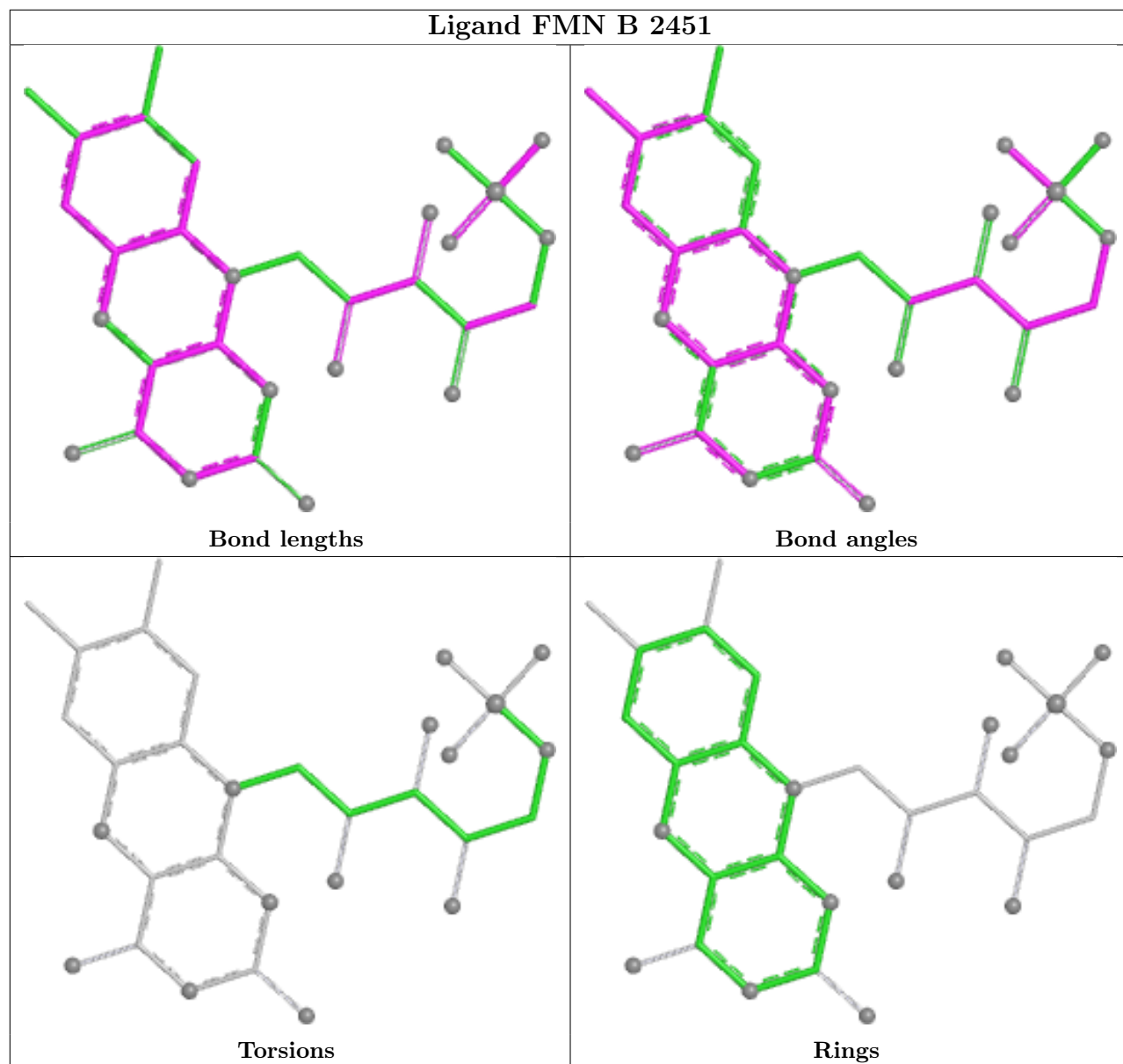
Torsions



Rings

Ligand FMN A 1451





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	630/688 (91%)	0.32	20 (3%) 50 52	28, 52, 88, 99	0
1	B	616/688 (89%)	0.45	28 (4%) 38 40	24, 61, 93, 100	0
All	All	1246/1376 (90%)	0.38	48 (3%) 43 45	24, 56, 92, 100	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1413	ILE	3.9
1	B	2902	LEU	3.9
1	A	948	VAL	3.6
1	B	3410	SER	3.4
1	A	946	ASP	3.3
1	B	2824	ALA	3.2
1	A	950	ILE	3.2
1	B	2787	SER	3.1
1	B	3316	PRO	3.1
1	A	846	ASN	3.0
1	B	2944	VAL	2.9
1	A	1057	ALA	2.8
1	A	830	HIS	2.8
1	B	3413	ILE	2.8
1	A	838	ARG	2.7
1	B	2907	GLY	2.7
1	B	3365	ILE	2.6
1	B	2948	VAL	2.6
1	A	1073	LEU	2.6
1	B	3411	GLU	2.5
1	B	2845	PHE	2.5
1	A	849	SER	2.5
1	B	2802	VAL	2.5
1	B	2791	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	836	GLU	2.5
1	B	3375	GLU	2.5
1	B	2952	LYS	2.5
1	A	971	LEU	2.4
1	A	1071	THR	2.4
1	B	2794	VAL	2.4
1	A	848	VAL	2.4
1	B	3288	ILE	2.3
1	B	2898	ALA	2.3
1	B	2825	LEU	2.3
1	B	2964	TRP	2.3
1	A	1157	GLN	2.2
1	B	2905	GLU	2.2
1	A	1059	HIS	2.2
1	A	964	TRP	2.2
1	A	962	ARG	2.2
1	A	1056	PRO	2.2
1	B	2846	ASN	2.1
1	B	2894	ALA	2.1
1	B	2818	GLY	2.1
1	B	2753	VAL	2.1
1	B	2906	LEU	2.1
1	A	1403	GLU	2.0
1	B	3073	LEU	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](#)

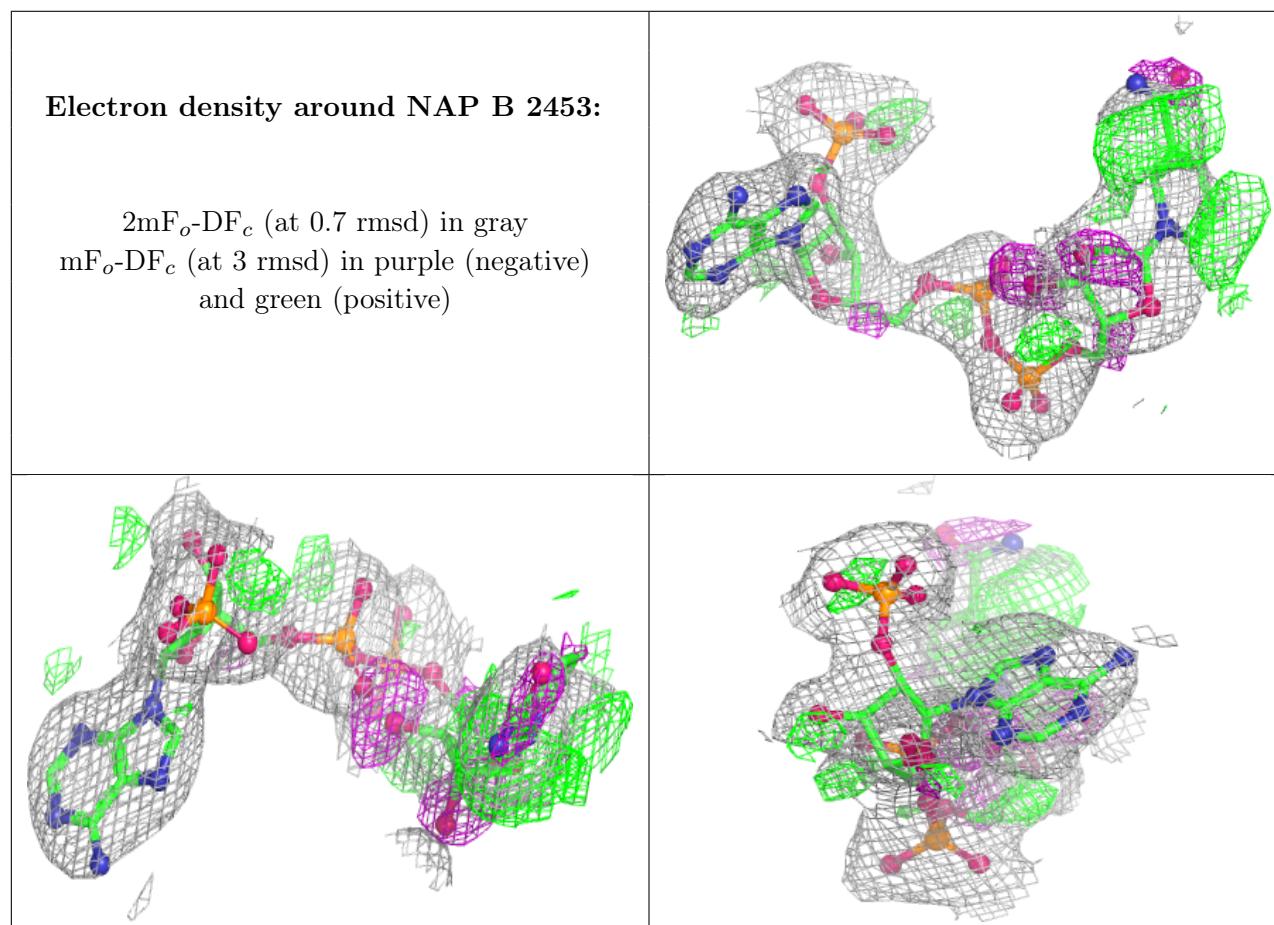
There are no oligosaccharides in this entry.

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.

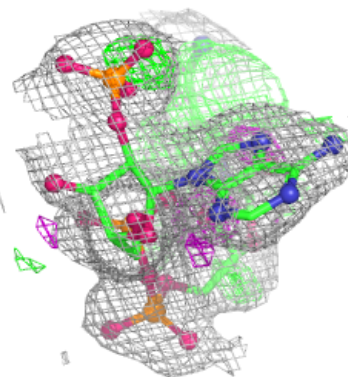
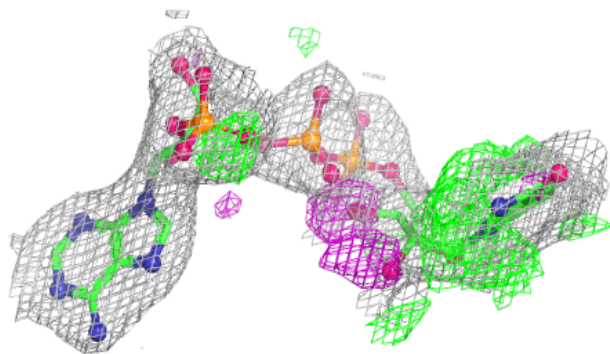
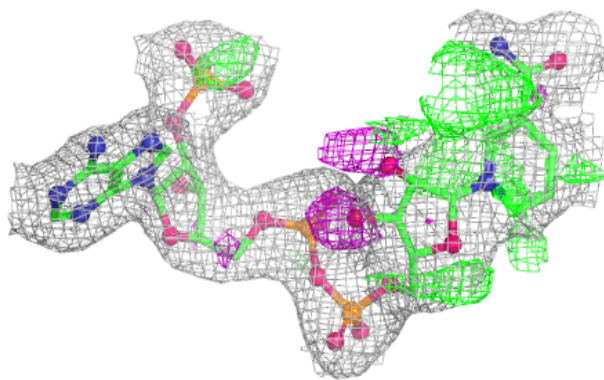
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO3	A	1500	4/4	0.81	0.12	67,68,68,68	4
2	SO3	B	2500	4/4	0.81	0.09	79,80,81,82	0
5	NAP	B	2453	48/48	0.84	0.12	40,47,59,61	0
5	NAP	A	1453	48/48	0.87	0.11	27,44,54,56	0
3	FMN	B	2451	31/31	0.94	0.09	45,49,53,54	0
3	FMN	A	1451	31/31	0.95	0.07	32,35,38,41	0
4	FAD	A	1452	53/53	0.96	0.07	17,30,51,53	0
4	FAD	B	2452	53/53	0.96	0.07	17,29,59,59	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.



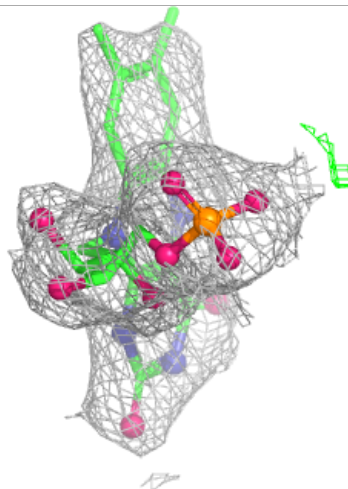
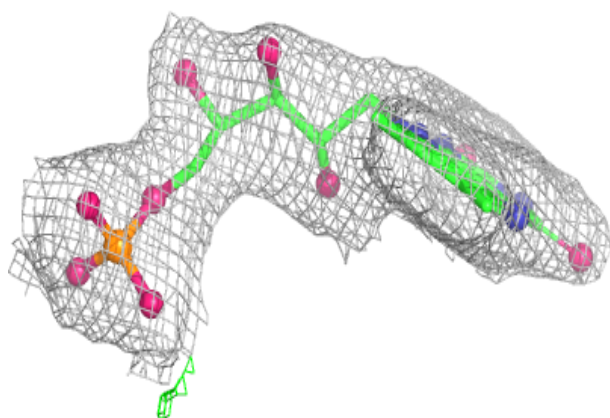
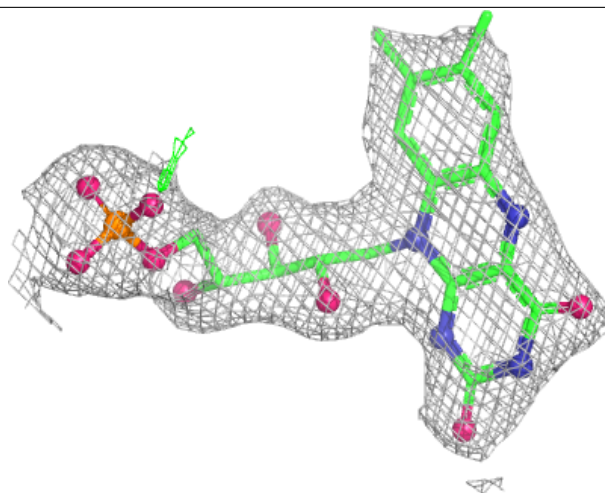
Electron density around NAP A 1453:

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



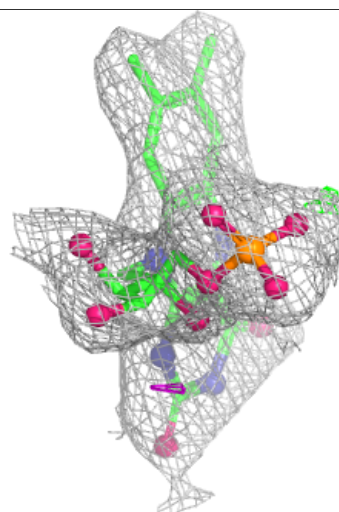
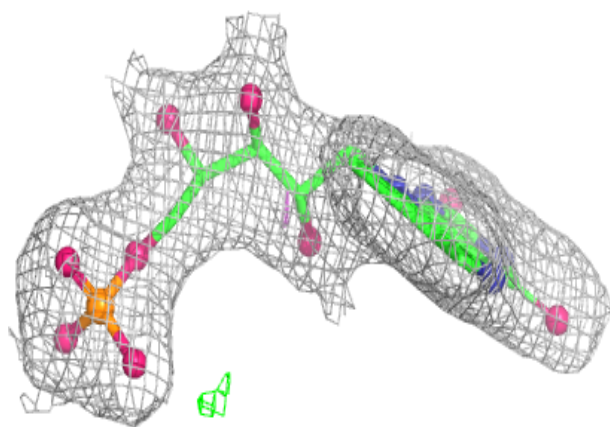
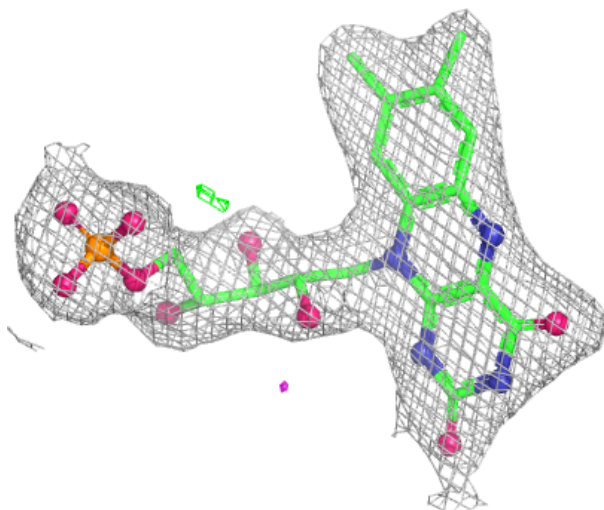
Electron density around FMN B 2451:

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



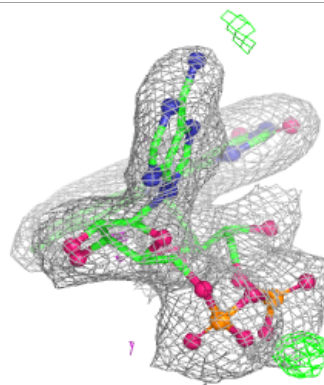
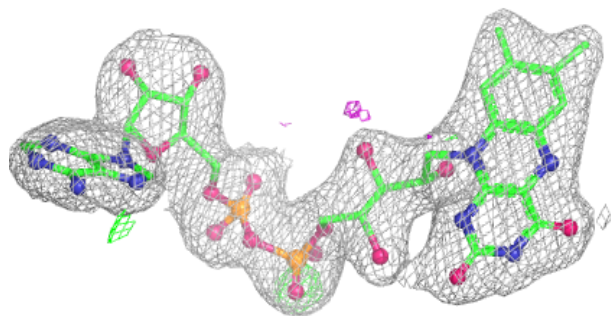
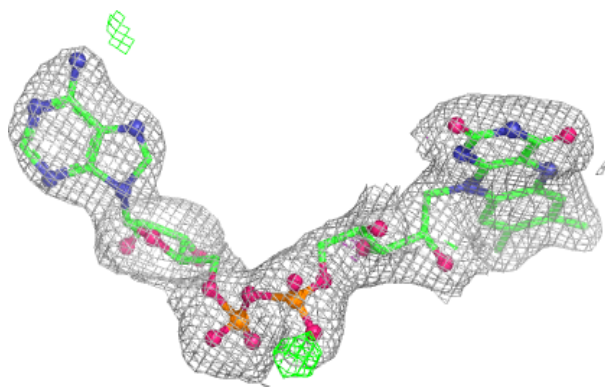
Electron density around FMN A 1451:

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

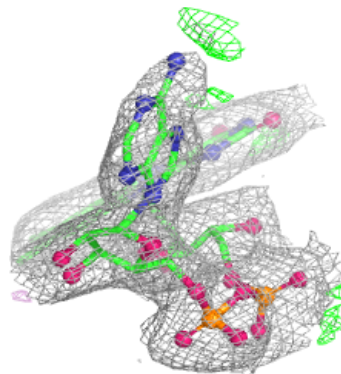
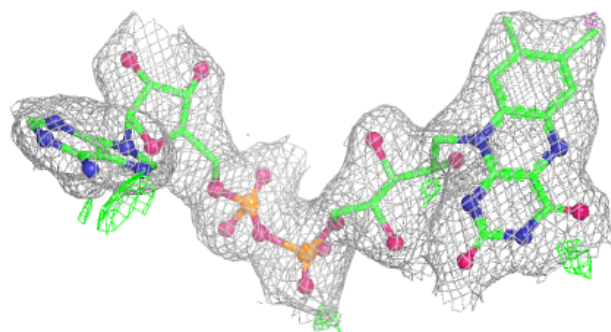
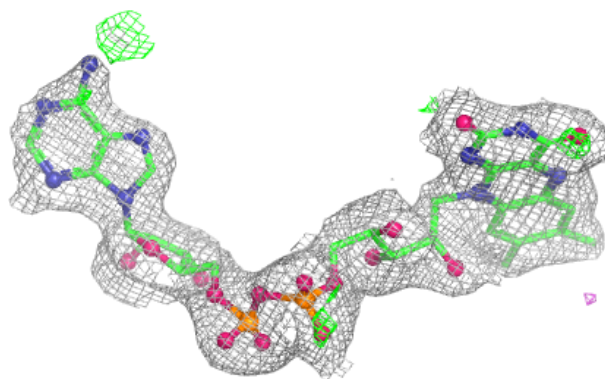


Electron density around FAD A 1452:

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

**Electron density around FAD B 2452:**

$2mF_o-DF_c$ (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.