



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2021 – 12:11 PM EDT

PDB ID : 6PFZ  
Title : Structure of a NAD-Dependent Persulfide Reductase from *A. fulgidus*  
Authors : Sazinsky, M.H.; Shabdar, S.; Garcia-Constineiras, A.; Crane III, E.J.  
Deposited on : 2019-06-23  
Resolution : 3.10 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.18  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.18

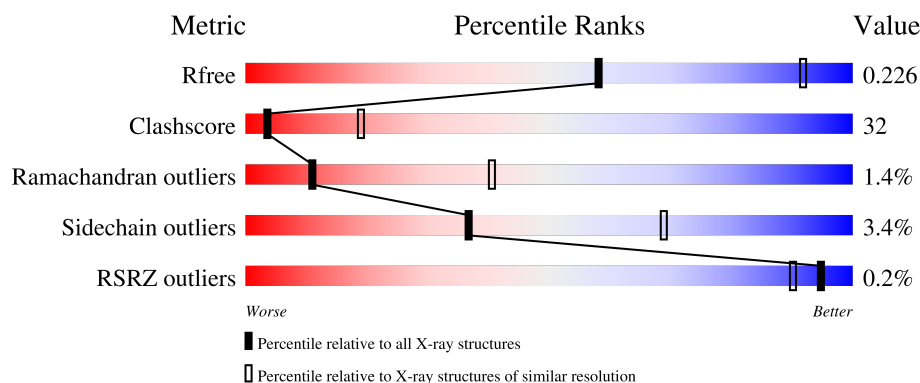
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	551	<div> <div style="width: 60%;"></div> <div style="width: 36%;"></div> <div style="width: 4%;"></div> <div style="width: 2%;"></div> </div> 60% 36% ..
1	B	551	<div> <div style="width: 56%;"></div> <div style="width: 40%;"></div> <div style="width: 4%;"></div> <div style="width: 2%;"></div> </div> 56% 40% ..
1	C	551	<div> <div style="width: 51%;"></div> <div style="width: 42%;"></div> <div style="width: 4%;"></div> <div style="width: 2%;"></div> <div style="width: 1%;"></div> </div> 51% 42% ...
1	D	551	<div> <div style="width: 55%;"></div> <div style="width: 40%;"></div> <div style="width: 4%;"></div> <div style="width: 2%;"></div> <div style="width: 1%;"></div> </div> 55% 40% ...

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CA	A	903	-	-	-	X

2 Entry composition ⓘ

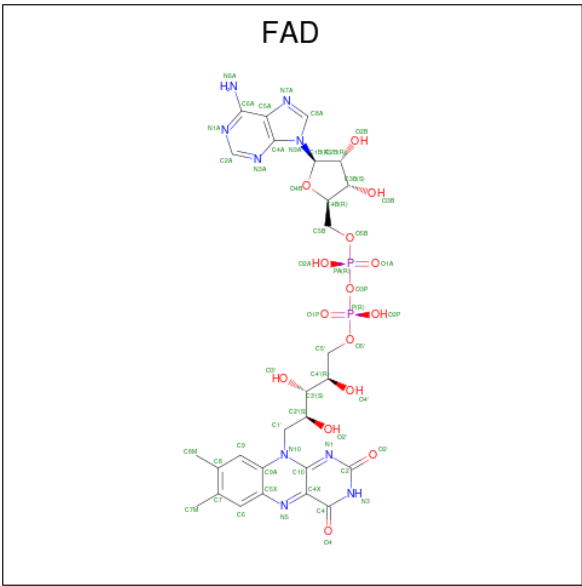
There are 5 unique types of molecules in this entry. The entry contains 16676 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 NADH oxidase (NoxA-3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	536	Total	C	N	O	S	0	0	0
			4044	2560	685	782	17			
1	A	541	Total	C	N	O	S	0	0	0
			4081	2585	691	788	17			
1	B	541	Total	C	N	O	S	0	0	0
			4106	2599	703	787	17			
1	C	535	Total	C	N	O	S	0	0	0
			4023	2551	682	773	17			

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: C<sub>27</sub>H<sub>33</sub>N<sub>9</sub>O<sub>15</sub>P<sub>2</sub>).



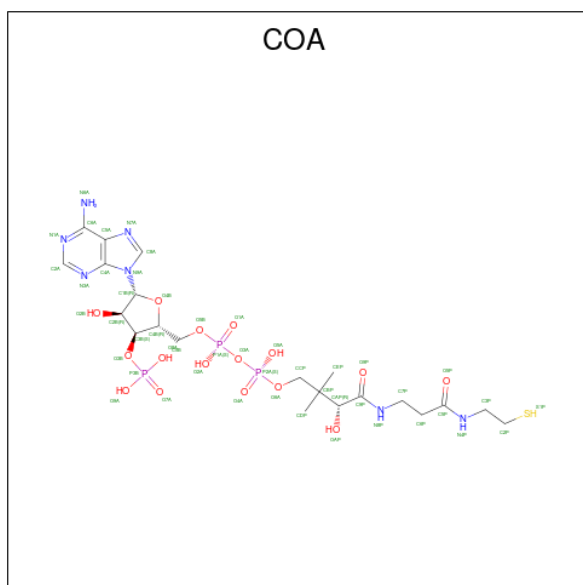
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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

- Molecule 3 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	D	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	C	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		
4	C	2	Total	Ca	0	0
			2	2		

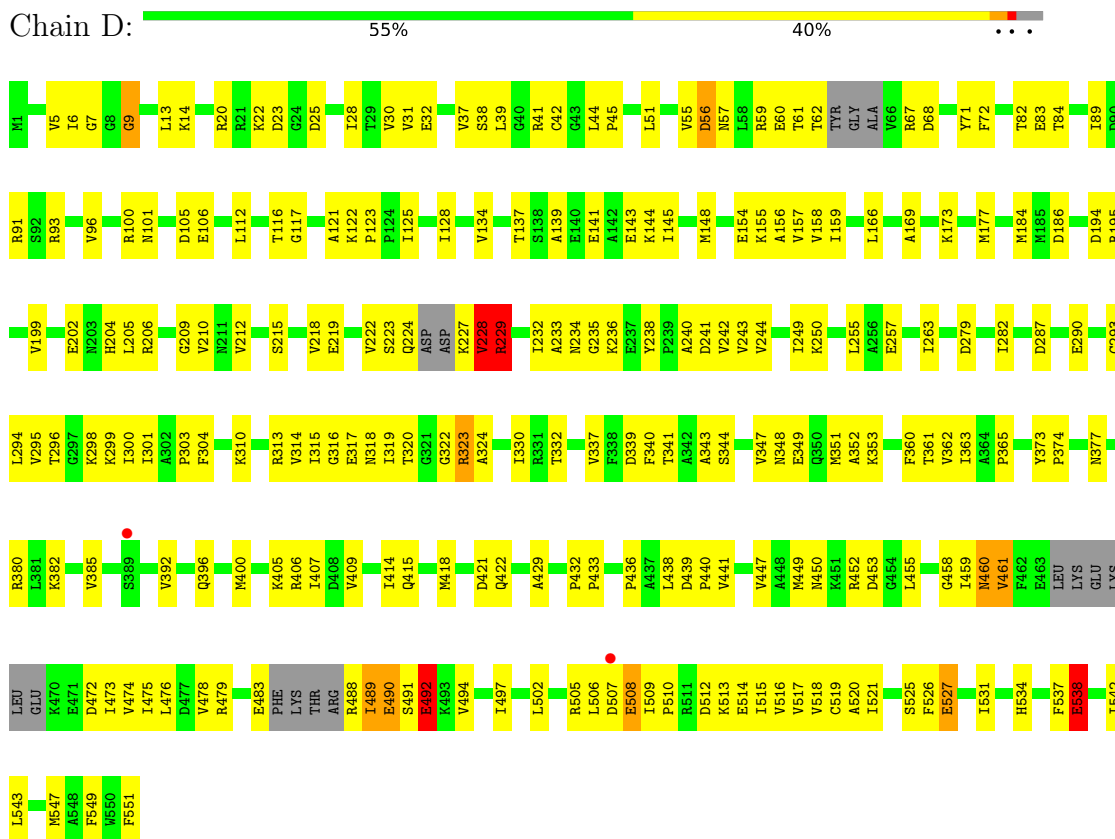
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	3	Total 3	O 3	0	0
5	B	11	Total 11	O 11	0	0

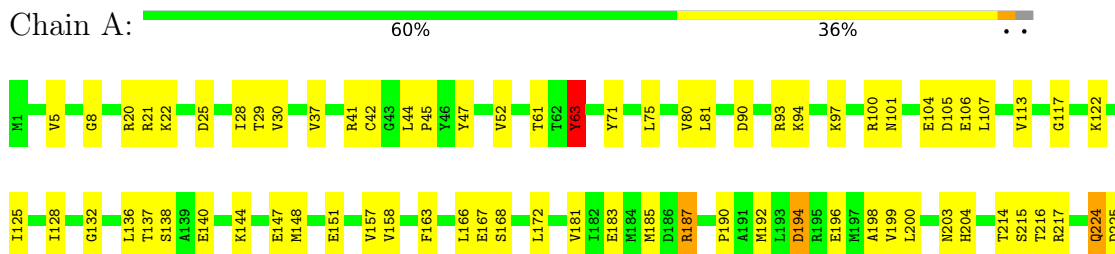
### 3 Residue-property plots

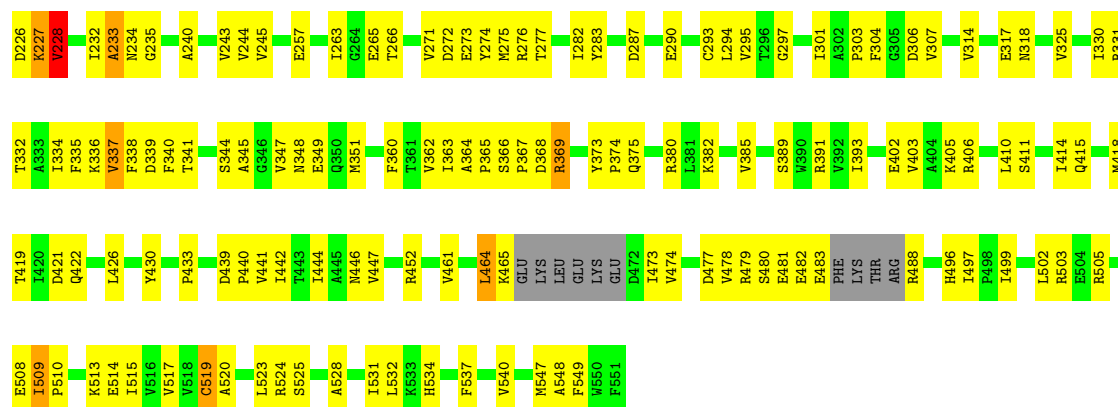
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: NADH oxidase (NoxA-3)



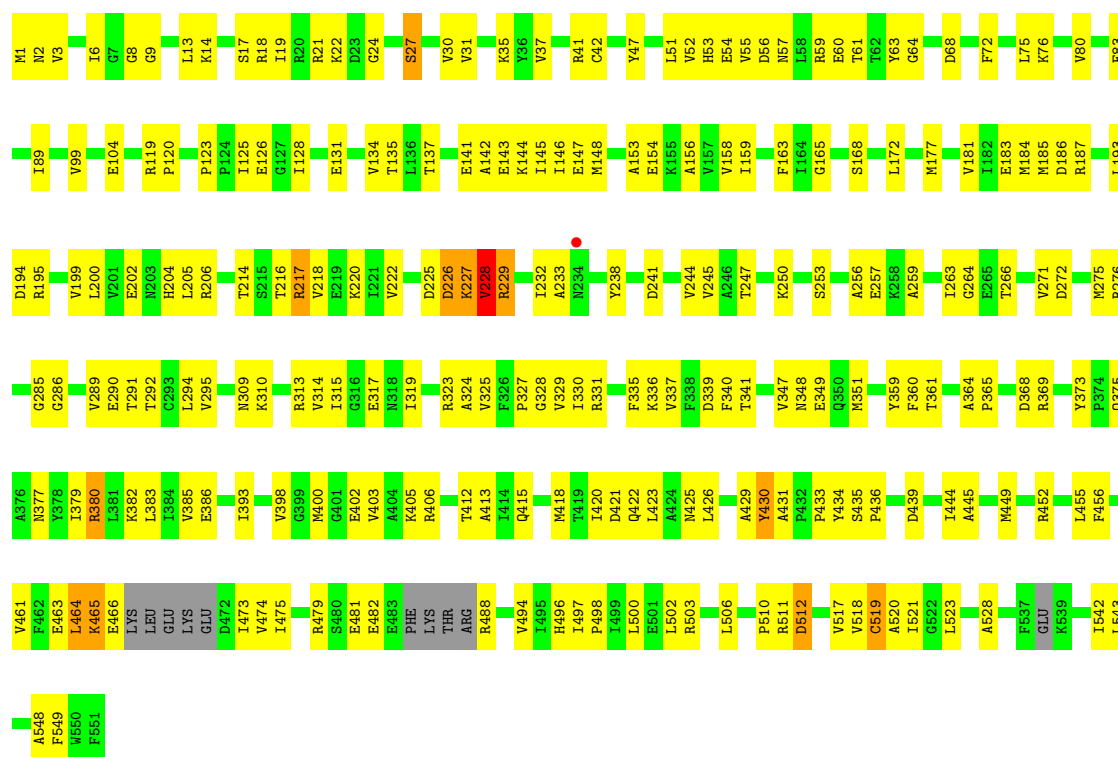
#### • Molecule 1: NADH oxidase (NoxA-3)





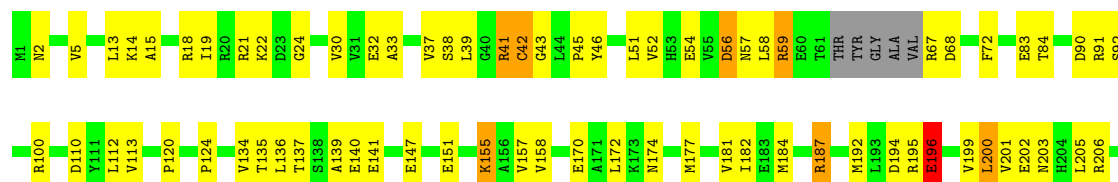
• Molecule 1: NADH oxidase (NoxA-3)

Chain B: 56% 40%



• Molecule 1: NADH oxidase (NoxA-3)

Chain C: 51% 42%



G522	R456	Y378	I301	V210
L523	E457	I379	A302	N211
R524	G458	R380	P303	V212
S525	I459	L381		V213
F526	N460	K382	R313	T214
E527	V461		V314	
A528	F462	K387	I315	R217
S529	E463		G316	V218
R530	L464	W390	E317	E219
I531	R465	R391	N318	K220
L532	E466	V392	I319	I221
K533	LYS		T320	I222
H534	LEU	M400		S223
A535	GLU	G401	A324	Q224
G536	LYS	E402	V325	D225
F537	GLU	V403	F326	D226
E538	ASP	A404	P327	K227
K539	1473	K405	G328	V228
W540	V474	R406	V329	R229
K541	I475	I407	I330	A230
I542	L476	D408	R331	V231
L543	V478		T332	I232
O545	R479	T412	A333	ALA
G546	S480	I413	I334	N234
R547	E481	I414	F335	
A548	E482	Q415	K336	Y238
F549		A416	V337	P239
W550		G417	F338	A240
F551		M418	D339	D241
		T419	F340	
		I420	T341	V244
		D421	A342	
		Q422	A343	A256
		L423	S344	
		A424	A345	L261
		N425	G346	
		L426	V347	T266
			R348	
		P433	E349	I269
		Y434	Q350	
		S435	M351	E273
		P436	A352	Y274
		A437	K353	M275
		L438	E354	R276
		D439		T277
			Y359	S278
		I442	F360	D279
		T443	T361	
		I444	V362	I282
		A445	I363	Y283
		R446	A364	
		V447	P365	D287
		A448		C288
		M449		V289
		N450	D368	E290
		R451		
		R452	Y373	C293
		D453	P374	L294
		G454	Q375	
		A520	A376	L300
		I521	N377	

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.98Å 100.36Å 136.20Å 90.00° 91.89° 90.00°	Depositor
Resolution (Å)	39.48 – 3.10 84.93 – 2.77	Depositor EDS
% Data completeness (in resolution range)	97.9 (39.48-3.10) 96.3 (84.93-2.77)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.09 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, $R_{free}$	0.202 , 0.229 0.203 , 0.226	Depositor DCC
$R_{free}$ test set	2829 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.6	Xtriage
Anisotropy	0.038	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 53.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	16676	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.75% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: FAD, CA, COA

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	0.76	0/4139	0.90	3/5609 (0.1%)
1	B	0.77	0/4163	0.89	1/5634 (0.0%)
1	C	0.79	0/4079	0.83	1/5527 (0.0%)
1	D	0.73	0/4099	0.91	2/5552 (0.0%)
All	All	0.76	0/16480	0.88	7/22322 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	228	VAL	N-CA-C	8.67	134.42	111.00
1	A	509	ILE	C-N-CD	-8.46	101.98	120.60
1	B	227	LYS	N-CA-C	-6.96	92.20	111.00
1	D	228	VAL	N-CA-C	6.30	128.02	111.00
1	D	9	GLY	N-CA-C	-5.73	98.77	113.10
1	C	229	ARG	N-CA-C	-5.62	95.83	111.00
1	A	63	TYR	N-CA-C	-5.25	96.83	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4081	0	4098	206	0
1	B	4106	0	4152	257	0
1	C	4023	0	4026	356	0
1	D	4044	0	4057	266	0
2	A	53	0	31	3	0
2	B	53	0	31	3	0
2	C	53	0	31	7	0
2	D	53	0	31	4	0
3	A	48	0	32	9	0
3	B	48	0	32	8	0
3	C	48	0	32	12	0
3	D	48	0	32	8	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	2	0	0	0	0
5	A	3	0	0	0	0
5	B	11	0	0	0	0
All	All	16676	0	16585	1054	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (1054) 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:C:495:ILE:CD1	1:C:508:GLU:HG2	1.37	1.54
1:C:495:ILE:HD11	1:C:508:GLU:CG	1.37	1.53
1:C:509:ILE:HG21	1:C:537:PHE:CE2	1.53	1.42
1:C:509:ILE:HG21	1:C:537:PHE:CZ	1.54	1.41
1:C:529:SER:CB	1:C:542:ILE:HD11	1.54	1.36
1:C:509:ILE:CG2	1:C:537:PHE:CE2	2.07	1.36
1:D:223:SER:HB2	1:D:227:LYS:N	1.39	1.35
1:C:529:SER:HB3	1:C:542:ILE:CD1	1.57	1.34
1:A:421:ASP:OD1	1:A:452:ARG:NH2	1.66	1.24
1:C:476:LEU:CD2	1:C:478:VAL:HG23	1.68	1.22
1:C:331:ARG:NH1	1:C:351:MET:SD	2.12	1.21
1:C:509:ILE:CG2	1:C:537:PHE:HE2	1.43	1.21
1:B:47:TYR:CZ	1:B:55:VAL:CG2	2.30	1.14
1:B:380:ARG:HH12	1:B:548:ALA:HB1	1.00	1.14
1:B:380:ARG:NH1	1:B:548:ALA:HB1	1.61	1.13
1:B:47:TYR:CZ	1:B:55:VAL:HG22	1.83	1.13
1:A:194:ASP:OD2	1:A:382:LYS:NZ	1.83	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:275:MET:CG	1:C:315:ILE:HD11	1.81	1.11
1:A:483:GLU:O	1:A:488:ARG:N	1.81	1.11
1:B:47:TYR:CE1	1:B:55:VAL:HG22	1.86	1.09
1:C:84:THR:HG22	1:C:100:ARG:HG2	1.27	1.09
1:D:314:VAL:HB	1:D:324:ALA:HB1	1.27	1.09
1:A:232:ILE:O	1:A:235:GLY:N	1.88	1.07
1:D:472:ASP:O	1:D:473:ILE:HG23	1.53	1.06
1:D:41:ARG:NH2	1:D:137:THR:HG23	1.70	1.06
1:A:473:ILE:HG23	1:A:514:GLU:O	1.53	1.06
1:C:275:MET:HG2	1:C:315:ILE:CD1	1.86	1.06
1:C:84:THR:HG21	1:C:100:ARG:HD3	1.41	1.03
1:A:421:ASP:CG	1:A:452:ARG:HH22	1.61	1.02
1:B:47:TYR:CE1	1:B:55:VAL:CG2	2.44	1.01
1:B:184:MET:HE1	1:B:217:ARG:NH2	1.76	1.01
1:C:42:CYS:HB2	3:C:902:COA:H21	1.38	1.01
1:B:461:VAL:HG21	1:B:549:PHE:O	1.60	1.00
1:B:1:MET:CE	1:B:3:VAL:CG2	2.39	1.00
1:C:232:ILE:CB	1:C:238:TYR:HE1	1.74	1.00
1:D:497:ILE:HD12	1:D:509:ILE:HD11	1.42	1.00
1:D:25:ASP:OD1	1:C:534:HIS:HE1	1.45	0.99
1:D:461:VAL:HG11	1:D:549:PHE:O	1.63	0.99
1:C:187:ARG:HH22	1:C:350:GLN:HE21	1.00	0.99
1:D:461:VAL:HG21	1:D:549:PHE:HB3	1.45	0.98
1:A:430:TYR:OH	3:B:902:COA:S1P	2.20	0.97
1:C:419:THR:HG22	1:C:421:ASP:H	1.23	0.97
1:C:42:CYS:HB2	3:C:902:COA:C2P	1.93	0.97
1:C:509:ILE:CG2	1:C:537:PHE:CZ	2.37	0.97
1:C:476:LEU:CD2	1:C:478:VAL:CG2	2.41	0.97
1:C:275:MET:HG2	1:C:315:ILE:HD11	1.41	0.96
1:C:5:VAL:CG2	1:C:30:VAL:HG22	1.94	0.96
1:D:223:SER:CB	1:D:227:LYS:N	2.29	0.95
1:C:32:GLU:OE2	2:C:901:FAD:O2B	1.85	0.95
1:D:439:ASP:OD1	1:D:440:PRO:HD2	1.66	0.95
1:D:224:GLN:H	1:D:227:LYS:N	1.64	0.95
1:C:438:LEU:CD2	1:C:442:ILE:HG21	1.97	0.94
1:C:476:LEU:HD21	1:C:478:VAL:CG2	1.98	0.94
1:C:438:LEU:HD23	1:C:442:ILE:HG21	1.49	0.93
1:C:400:MET:HE3	1:C:400:MET:HA	1.48	0.93
1:B:449:MET:HE3	1:B:452:ARG:NH2	1.84	0.93
1:C:222:VAL:CG2	1:C:229:ARG:CB	2.48	0.92
1:A:481:GLU:N	1:A:481:GLU:OE1	2.01	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:ASP:OD1	1:A:106:GLU:N	2.00	0.92
1:B:184:MET:CE	1:B:217:ARG:NH2	2.32	0.92
1:C:84:THR:HG22	1:C:100:ARG:CG	1.99	0.92
1:B:217:ARG:HG3	1:B:217:ARG:HH11	1.33	0.92
1:A:505:ARG:NH1	1:A:508:GLU:OE2	2.02	0.91
1:D:41:ARG:HH21	1:D:137:THR:HG23	1.28	0.91
1:B:463:GLU:HG3	1:B:464:LEU:N	1.84	0.91
1:B:222:VAL:HG11	1:B:229:ARG:HH11	1.36	0.91
1:A:216:THR:HB	1:A:233:ALA:HB3	1.50	0.91
1:B:463:GLU:O	1:B:465:LYS:N	2.04	0.90
1:C:509:ILE:HG23	1:C:537:PHE:HE2	1.35	0.90
1:C:42:CYS:SG	3:C:902:COA:H32	2.11	0.90
1:D:222:VAL:CG2	1:D:229:ARG:HB2	2.02	0.90
1:B:184:MET:CE	1:B:217:ARG:HH21	1.85	0.89
1:D:100:ARG:NH2	1:D:105:ASP:OD2	2.05	0.89
1:D:472:ASP:O	1:D:473:ILE:CG2	2.21	0.89
1:B:158:VAL:HG22	1:B:244:VAL:CG2	2.03	0.89
1:D:439:ASP:OD1	1:D:440:PRO:CD	2.22	0.88
1:B:463:GLU:CG	1:B:464:LEU:H	1.85	0.88
1:C:509:ILE:HG21	1:C:537:PHE:HZ	1.38	0.87
1:C:457:GLU:HB3	1:C:541:LYS:NZ	1.88	0.87
1:D:330:ILE:HG13	1:D:415:GLN:HG2	1.53	0.87
1:D:57:ASN:O	1:D:60:GLU:HG2	1.75	0.86
1:C:187:ARG:NH2	1:C:350:GLN:HE21	1.72	0.86
1:B:463:GLU:HG3	1:B:464:LEU:H	1.37	0.86
1:C:84:THR:CG2	1:C:100:ARG:HG2	2.05	0.85
1:A:217:ARG:H	1:A:233:ALA:HB2	1.42	0.85
1:D:461:VAL:HG21	1:D:549:PHE:CB	2.07	0.85
1:D:534:HIS:ND1	1:C:24:GLY:HA3	1.91	0.84
1:C:497:ILE:HG23	1:C:505:ARG:HD3	1.58	0.84
1:D:61:THR:O	1:D:62:THR:OG1	1.94	0.84
1:A:508:GLU:OE1	1:A:508:GLU:N	2.11	0.84
1:D:25:ASP:OD1	1:C:534:HIS:CE1	2.30	0.84
1:C:22:LYS:HB2	1:C:320:THR:HG21	1.61	0.83
1:C:222:VAL:HG22	1:C:229:ARG:O	1.79	0.83
1:B:380:ARG:HH12	1:B:548:ALA:CB	1.88	0.83
1:C:516:VAL:HG22	1:C:541:LYS:HB2	1.58	0.83
1:D:155:LYS:HD2	1:D:241:ASP:OD2	1.79	0.82
1:C:52:VAL:HG11	1:C:58:LEU:HD11	1.61	0.82
1:C:476:LEU:HD23	1:C:478:VAL:HG23	1.61	0.82
1:D:222:VAL:HG22	1:D:229:ARG:HB2	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LEU:HD12	1:A:335:PHE:CE1	2.14	0.82
1:B:232:ILE:CB	1:B:238:TYR:HE1	1.93	0.82
1:C:157:VAL:HG23	1:C:240:ALA:HB2	1.60	0.82
1:D:507:ASP:O	1:D:508:GLU:HG2	1.79	0.82
1:C:277:THR:OG1	1:C:282:ILE:O	1.98	0.81
1:D:497:ILE:CD1	1:D:509:ILE:HD11	2.09	0.81
1:B:1:MET:CE	1:B:3:VAL:HG23	2.07	0.81
1:B:142:ALA:O	1:B:145:ILE:HG22	1.79	0.81
1:D:518:VAL:HG23	1:D:543:LEU:HD23	1.61	0.81
1:A:365:PRO:HB3	1:A:380:ARG:HG3	1.63	0.81
1:D:409:VAL:HG13	1:C:412:THR:HG21	1.61	0.81
1:D:20:ARG:HE	1:D:20:ARG:HA	1.43	0.81
1:A:47:TYR:HA	1:A:52:VAL:HG22	1.62	0.81
1:C:275:MET:CB	1:C:315:ILE:HD11	2.11	0.81
1:D:32:GLU:OE1	2:D:901:FAD:O2B	1.99	0.81
1:C:455:LEU:HD23	1:C:526:PHE:HZ	1.46	0.81
1:C:459:ILE:HD12	1:C:460:ASN:O	1.81	0.81
1:C:21:ARG:NE	3:C:902:COA:O9A	2.15	0.80
1:C:457:GLU:HB3	1:C:541:LYS:HZ2	1.46	0.80
1:D:491:SER:OG	1:D:492:GLU:N	2.14	0.80
1:C:275:MET:CG	1:C:315:ILE:CD1	2.53	0.80
1:A:232:ILE:O	1:A:234:ASN:N	2.15	0.80
1:D:154:GLU:HA	1:D:177:MET:HG2	1.63	0.80
1:C:187:ARG:HH22	1:C:350:GLN:NE2	1.80	0.79
1:B:125:ILE:HG22	1:B:128:ILE:HB	1.65	0.79
1:B:463:GLU:C	1:B:465:LYS:H	1.85	0.79
1:D:348:ASN:HB3	1:D:351:MET:HE2	1.65	0.78
1:A:502:LEU:CD2	1:A:531:ILE:HD11	2.12	0.78
1:C:84:THR:CG2	1:C:100:ARG:CD	2.60	0.78
1:C:84:THR:CG2	1:C:100:ARG:HD3	2.12	0.78
1:A:502:LEU:HD22	1:A:531:ILE:HD11	1.64	0.78
1:C:525:SER:HB3	1:C:542:ILE:HG23	1.66	0.78
1:C:232:ILE:CB	1:C:238:TYR:CE1	2.65	0.78
1:C:187:ARG:HH12	1:C:350:GLN:NE2	1.82	0.77
1:D:432:PRO:HG3	1:C:42:CYS:O	1.84	0.77
1:C:155:LYS:HD2	1:C:241:ASP:OD2	1.84	0.77
1:D:84:THR:HG23	1:D:100:ARG:HB3	1.65	0.77
1:B:474:VAL:HG21	1:B:510:PRO:HD2	1.67	0.77
1:B:421:ASP:OD1	1:B:452:ARG:NH1	2.17	0.77
1:D:255:LEU:HD12	1:D:255:LEU:H	1.49	0.77
1:D:526:PHE:CD2	3:C:902:COA:H8A	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:ILE:CG2	1:D:116:THR:CG2	2.63	0.76
1:C:476:LEU:HD21	1:C:478:VAL:HG22	1.64	0.76
1:D:158:VAL:HG22	1:D:244:VAL:HG22	1.67	0.76
1:D:194:ASP:OD2	1:D:349:GLU:HG3	1.85	0.76
1:C:339:ASP:HB3	1:C:400:MET:HE1	1.68	0.76
1:D:313:ARG:NH1	3:D:902:COA:O7A	2.19	0.75
1:C:283:TYR:CD1	1:C:319:ILE:HD11	2.21	0.75
1:D:186:ASP:OD2	1:D:195:ARG:HD2	1.86	0.75
1:B:463:GLU:CG	1:B:464:LEU:N	2.44	0.75
1:B:465:LYS:CD	1:B:473:ILE:CD1	2.65	0.75
1:C:5:VAL:HG22	1:C:30:VAL:HG22	1.67	0.75
1:C:42:CYS:CB	3:C:902:COA:H21	2.17	0.75
1:B:21:ARG:NH2	3:B:902:COA:O5A	2.20	0.75
1:C:335:PHE:HE1	1:C:337:VAL:HG13	1.52	0.75
1:D:392:VAL:HG12	1:D:414:ILE:HG12	1.69	0.75
1:C:84:THR:HG21	1:C:100:ARG:CD	2.16	0.75
1:B:42:CYS:SG	3:B:902:COA:H32	2.25	0.75
1:B:449:MET:CE	1:B:452:ARG:NH2	2.50	0.74
1:D:41:ARG:HH21	1:D:137:THR:CG2	1.97	0.74
1:A:418:MET:HA	1:A:422:GLN:HE21	1.50	0.74
1:D:526:PHE:HD2	3:C:902:COA:H8A	1.51	0.74
1:B:158:VAL:HG22	1:B:244:VAL:HG21	1.70	0.74
1:C:529:SER:CB	1:C:542:ILE:CD1	2.35	0.74
1:C:227:LYS:HG3	1:C:228:VAL:N	2.02	0.74
1:A:293:CYS:SG	1:A:331:ARG:NH2	2.60	0.74
1:C:275:MET:HB3	1:C:315:ILE:CD1	2.18	0.74
1:B:1:MET:HE1	1:B:3:VAL:CG2	2.17	0.74
1:C:545:GLY:HA3	1:C:549:PHE:CE1	2.23	0.74
1:C:275:MET:HB3	1:C:315:ILE:HD11	1.70	0.73
1:D:294:LEU:HB2	1:D:330:ILE:HD11	1.70	0.73
1:D:483:GLU:O	1:D:488:ARG:N	2.21	0.73
1:B:418:MET:HA	1:B:422:GLN:HE21	1.53	0.73
1:C:172:LEU:HD22	1:C:177:MET:CE	2.18	0.73
1:C:419:THR:HG22	1:C:421:ASP:N	2.03	0.73
1:B:465:LYS:HD3	1:B:473:ILE:HD11	1.70	0.73
3:A:902:COA:HS1	1:B:430:TYR:HH	1.36	0.73
1:A:464:LEU:HG	1:A:464:LEU:O	1.89	0.73
1:B:496:HIS:CD2	1:B:498:PRO:HD3	2.23	0.73
1:C:84:THR:CG2	1:C:100:ARG:CG	2.64	0.73
1:B:481:GLU:O	1:B:482:GLU:HB2	1.89	0.73
1:A:464:LEU:H	1:A:464:LEU:HD23	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:373:TYR:CZ	1:D:433:PRO:HB3	2.23	0.72
1:D:439:ASP:OD1	1:D:440:PRO:N	2.22	0.72
1:B:47:TYR:CE1	1:B:55:VAL:HG23	2.23	0.72
1:A:277:THR:HG22	1:A:282:ILE:O	1.90	0.72
1:B:465:LYS:CD	1:B:473:ILE:HD11	2.20	0.72
1:D:365:PRO:HG2	1:D:521:ILE:HG23	1.72	0.72
1:D:199:VAL:HG21	1:D:551:PHE:HZ	1.54	0.72
1:A:21:ARG:NH1	3:A:902:COA:O9A	2.23	0.71
1:A:158:VAL:HG22	1:A:244:VAL:HG22	1.73	0.71
1:D:405:LYS:HA	1:C:405:LYS:HG3	1.72	0.71
3:A:902:COA:S1P	1:B:430:TYR:OH	2.49	0.71
1:A:21:ARG:NH2	3:A:902:COA:O4A	2.23	0.71
1:B:348:ASN:H	1:B:351:MET:HE3	1.56	0.71
1:B:313:ARG:NH1	3:B:902:COA:O7A	2.24	0.71
1:C:495:ILE:HD13	1:C:508:GLU:HG2	1.67	0.71
1:D:304:PHE:C	2:D:901:FAD:O3'	2.29	0.70
1:D:6:ILE:HG22	1:D:116:THR:CG2	2.22	0.70
1:A:196:GLU:O	1:A:199:VAL:HG12	1.91	0.70
1:A:217:ARG:N	1:A:233:ALA:HB2	2.06	0.70
1:C:275:MET:CB	1:C:315:ILE:CD1	2.69	0.70
1:D:42:CYS:SG	3:D:902:COA:H32	2.31	0.70
1:B:222:VAL:HG11	1:B:229:ARG:NH1	2.07	0.70
1:D:418:MET:HA	1:D:422:GLN:HE21	1.57	0.70
1:A:369:ARG:HH12	1:A:375:GLN:HB2	1.57	0.70
1:D:5:VAL:HB	1:D:30:VAL:HG22	1.72	0.69
1:D:432:PRO:CG	1:C:42:CYS:O	2.40	0.69
1:C:519:CYS:SG	1:C:522:GLY:N	2.63	0.69
1:D:534:HIS:CE1	1:C:24:GLY:C	2.65	0.69
1:A:166:LEU:CD1	1:A:335:PHE:CE1	2.74	0.69
1:B:143:GLU:HA	1:B:146:ILE:HG22	1.74	0.69
1:C:332:THR:HA	1:C:344:SER:O	1.92	0.69
1:C:504:GLU:O	1:C:505:ARG:O	2.09	0.69
1:A:63:TYR:HD1	1:A:63:TYR:H	1.41	0.69
1:B:47:TYR:CZ	1:B:55:VAL:HG23	2.24	0.69
1:D:20:ARG:NH2	1:D:28:ILE:CD1	2.56	0.69
1:B:123:PRO:HD3	1:B:247:THR:HG21	1.75	0.69
1:B:421:ASP:CG	1:B:452:ARG:HH12	1.96	0.69
1:C:517:VAL:N	1:C:541:LYS:O	2.25	0.68
1:D:348:ASN:OD1	1:D:349:GLU:N	2.26	0.68
1:A:166:LEU:HD12	1:A:335:PHE:CZ	2.29	0.68
1:C:335:PHE:CE1	1:C:337:VAL:HG13	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:ILE:CG2	1:D:116:THR:HG22	2.23	0.68
1:D:491:SER:O	1:D:492:GLU:HB2	1.92	0.68
1:B:204:HIS:HE1	1:B:339:ASP:H	1.39	0.68
1:B:276:ARG:NH1	1:B:323:ARG:HH12	1.92	0.68
1:C:509:ILE:HG22	1:C:537:PHE:CE2	2.21	0.68
1:A:479:ARG:O	1:A:496:HIS:CE1	2.47	0.67
1:C:476:LEU:HD23	1:C:476:LEU:C	2.15	0.67
1:B:276:ARG:HH12	1:B:323:ARG:HH12	1.43	0.67
1:B:214:THR:O	1:B:216:THR:HG23	1.95	0.67
1:C:182:ILE:HD13	1:C:213:VAL:CG2	2.25	0.67
1:D:141:GLU:O	1:D:145:ILE:HD12	1.95	0.67
1:A:497:ILE:CD1	1:A:509:ILE:HD11	2.25	0.67
1:C:200:LEU:HD22	1:C:340:PHE:HE2	1.58	0.67
1:C:337:VAL:CG2	1:C:340:PHE:HB2	2.25	0.67
1:C:351:MET:HA	1:C:354:GLU:HG2	1.77	0.67
1:D:125:ILE:HG23	1:D:128:ILE:HB	1.77	0.66
1:C:158:VAL:HB	1:C:181:VAL:HG23	1.77	0.66
1:D:459:ILE:C	1:D:459:ILE:HD12	2.16	0.66
1:A:528:ALA:O	1:A:532:LEU:HD12	1.96	0.66
1:B:347:VAL:HG23	1:B:351:MET:HB2	1.77	0.66
1:C:227:LYS:O	1:C:228:VAL:HG13	1.96	0.66
1:C:227:LYS:C	1:C:228:VAL:HG22	2.15	0.66
1:C:499:ILE:HG23	1:C:500:LEU:N	2.10	0.66
1:C:337:VAL:HG21	1:C:340:PHE:HB2	1.76	0.66
1:B:512:ASP:OD2	1:B:512:ASP:N	2.28	0.66
1:C:147:GLU:O	1:C:151:GLU:HG3	1.96	0.66
1:C:476:LEU:HD22	1:C:478:VAL:HG23	1.70	0.66
1:D:478:VAL:O	1:D:479:ARG:HG3	1.96	0.66
1:A:330:ILE:HG13	1:A:415:GLN:HG2	1.78	0.66
1:B:184:MET:HE3	1:B:217:ARG:HH21	1.61	0.66
1:D:20:ARG:HA	1:D:20:ARG:NE	2.11	0.65
1:C:84:THR:HG22	1:C:100:ARG:CD	2.25	0.65
1:C:335:PHE:HE1	1:C:337:VAL:CG1	2.09	0.65
1:C:546:GLY:C	1:C:548:ALA:H	1.97	0.65
1:C:275:MET:CE	1:C:326:PHE:HB3	2.26	0.65
1:B:135:THR:HG22	1:B:245:VAL:HG22	1.77	0.65
1:B:294:LEU:HD13	1:B:329:VAL:N	2.12	0.65
1:A:20:ARG:NH2	1:A:28:ILE:HD12	2.11	0.65
1:B:1:MET:HE3	1:B:3:VAL:CG2	2.24	0.65
1:B:135:THR:O	1:B:141:GLU:HG2	1.96	0.65
1:C:313:ARG:NH1	3:C:902:COA:O7A	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:ALA:HB2	1:D:177:MET:CE	2.27	0.65
1:B:184:MET:HE3	1:B:217:ARG:NH2	2.12	0.65
1:B:217:ARG:HG3	1:B:217:ARG:NH1	2.08	0.65
1:C:477:ASP:OD1	1:C:479:ARG:HB2	1.97	0.65
1:D:14:LYS:NZ	3:D:902:COA:O3A	2.30	0.64
1:D:222:VAL:HG22	1:D:229:ARG:CB	2.27	0.64
1:B:186:ASP:OD2	1:B:195:ARG:HD2	1.96	0.64
1:D:134:VAL:HG21	1:D:145:ILE:HD11	1.78	0.64
1:A:42:CYS:SG	3:A:902:COA:H32	2.38	0.64
1:A:519:CYS:SG	1:A:520:ALA:N	2.70	0.64
1:A:194:ASP:CG	1:A:382:LYS:HZ3	1.95	0.64
1:B:232:ILE:CB	1:B:238:TYR:CE1	2.80	0.64
1:B:314:VAL:HG23	1:B:324:ALA:HB3	1.79	0.64
1:A:30:VAL:CG1	1:A:80:VAL:HG22	2.28	0.64
1:A:224:GLN:HB3	1:A:228:VAL:HG13	1.79	0.64
1:B:518:VAL:HG22	1:B:543:LEU:HD22	1.79	0.64
1:B:227:LYS:O	1:B:228:VAL:HG13	1.97	0.64
1:D:310:LYS:HD3	1:C:425:ASN:HA	1.79	0.64
1:D:222:VAL:O	1:D:228:VAL:HA	1.97	0.64
1:B:275:MET:CB	1:B:315:ILE:HD11	2.28	0.64
1:C:476:LEU:HD23	1:C:476:LEU:O	1.98	0.64
1:B:227:LYS:O	1:B:228:VAL:HG22	1.98	0.64
1:C:363:ILE:HG22	1:C:382:LYS:HG3	1.80	0.64
1:C:5:VAL:HG21	1:C:30:VAL:HG22	1.80	0.63
1:C:497:ILE:CG2	1:C:505:ARG:HD3	2.28	0.63
1:C:42:CYS:HB2	3:C:902:COA:S1P	2.38	0.63
1:D:194:ASP:H	1:D:396:GLN:HE22	1.44	0.63
1:A:341:THR:HG23	1:A:403:VAL:CG2	2.28	0.63
1:B:383:LEU:HB2	1:B:444:ILE:HG12	1.80	0.63
1:B:195:ARG:O	1:B:199:VAL:HG13	1.98	0.63
1:B:227:LYS:C	1:B:228:VAL:HG22	2.17	0.63
1:C:438:LEU:HD22	1:C:442:ILE:CG2	2.28	0.63
1:B:465:LYS:HD2	1:B:473:ILE:CD1	2.28	0.63
1:B:17:SER:OG	1:B:76:LYS:NZ	2.31	0.63
1:C:479:ARG:O	1:C:480:SER:HB3	1.99	0.63
1:D:51:LEU:HD22	1:C:374:PRO:HG3	1.80	0.63
1:D:139:ALA:O	1:D:143:GLU:HG2	1.98	0.63
1:D:363:ILE:HG12	1:D:382:LYS:HG3	1.80	0.62
1:C:408:ASP:O	1:C:412:THR:HG23	1.98	0.62
1:A:47:TYR:CA	1:A:52:VAL:HG22	2.28	0.62
1:A:138:SER:HB2	1:A:140:GLU:OE1	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:VAL:HG23	1:C:240:ALA:CB	2.30	0.62
1:A:71:TYR:CZ	1:A:75:LEU:HD22	2.35	0.62
1:C:519:CYS:N	1:C:525:SER:OG	2.33	0.62
1:A:364:ALA:HB3	1:A:444:ILE:HD12	1.82	0.62
1:B:463:GLU:C	1:B:465:LYS:N	2.47	0.62
1:B:461:VAL:CG2	1:B:549:PHE:O	2.43	0.62
1:B:464:LEU:C	1:B:466:GLU:H	2.03	0.62
1:B:154:GLU:O	1:B:177:MET:HB3	2.00	0.62
1:C:228:VAL:HG23	1:C:240:ALA:O	1.99	0.62
1:C:438:LEU:CD2	1:C:442:ILE:CG2	2.76	0.62
1:C:438:LEU:HD22	1:C:442:ILE:HG21	1.79	0.62
1:C:201:VAL:O	1:C:205:LEU:HD12	2.00	0.61
1:D:20:ARG:NH2	1:D:28:ILE:HD12	2.15	0.61
1:A:406:ARG:NH1	1:A:439:ASP:OD2	2.33	0.61
1:A:482:GLU:C	1:A:483:GLU:HG3	2.21	0.61
1:B:47:TYR:CE1	1:B:53:HIS:O	2.53	0.61
1:C:330:ILE:HD13	1:C:415:GLN:HG3	1.82	0.61
1:C:545:GLY:CA	1:C:549:PHE:CE1	2.83	0.61
1:C:526:PHE:HA	1:C:542:ILE:HD13	1.82	0.61
1:D:91:ARG:HH11	1:D:279:ASP:HB2	1.66	0.61
1:B:1:MET:HE1	1:B:3:VAL:HG21	1.83	0.61
1:C:222:VAL:HG21	1:C:229:ARG:CB	2.30	0.61
1:D:159:ILE:HG12	1:D:218:VAL:HG21	1.81	0.61
1:B:325:VAL:HG12	1:B:327:PRO:HD3	1.83	0.61
1:D:6:ILE:HG22	1:D:116:THR:HG22	1.83	0.61
1:D:59:ARG:HA	1:D:67:ARG:HH21	1.64	0.61
1:C:222:VAL:HG23	1:C:229:ARG:CB	2.28	0.61
1:D:290:GLU:OE1	1:D:299:LYS:HD3	2.01	0.61
1:B:120:PRO:HD3	1:B:137:THR:HG21	1.83	0.61
1:B:360:PHE:CZ	1:B:385:VAL:HG21	2.36	0.61
1:C:495:ILE:HD11	1:C:508:GLU:HG3	1.69	0.61
1:D:224:GLN:N	1:D:227:LYS:N	2.44	0.60
1:B:464:LEU:N	1:B:464:LEU:HD12	2.16	0.60
1:D:67:ARG:HG3	1:D:71:TYR:CD1	2.36	0.60
1:C:211:ASN:OD1	1:C:212:VAL:N	2.34	0.60
1:B:1:MET:HE3	1:B:3:VAL:HG23	1.80	0.60
1:B:519:CYS:SG	1:B:520:ALA:N	2.74	0.60
1:C:546:GLY:C	1:C:548:ALA:N	2.53	0.60
1:D:295:VAL:HG23	1:D:296:THR:HG23	1.84	0.60
1:D:360:PHE:CE2	1:D:385:VAL:CG1	2.85	0.60
1:D:195:ARG:O	1:D:199:VAL:HG13	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:361:THR:HG23	1:D:382:LYS:HE3	1.84	0.60
1:C:200:LEU:HD22	1:C:340:PHE:CE2	2.35	0.60
1:A:373:TYR:CZ	1:A:433:PRO:HB3	2.36	0.60
1:C:172:LEU:HD22	1:C:177:MET:HE1	1.83	0.60
1:C:187:ARG:HH12	1:C:350:GLN:HE22	1.50	0.60
1:C:224:GLN:O	1:C:225:ASP:HB2	2.02	0.60
1:D:236:LYS:HD3	1:D:238:TYR:OH	2.02	0.60
1:A:410:LEU:O	1:A:414:ILE:HG13	2.02	0.59
1:D:508:GLU:O	1:D:510:PRO:HD3	2.01	0.59
1:D:219:GLU:OE2	1:D:233:ALA:HA	2.02	0.59
1:B:226:ASP:OD1	1:B:226:ASP:N	2.33	0.59
1:D:295:VAL:CG2	1:D:347:VAL:HG23	2.32	0.59
1:C:172:LEU:HD22	1:C:177:MET:HE3	1.84	0.59
1:C:227:LYS:O	1:C:228:VAL:HG22	2.01	0.59
1:C:275:MET:HE3	1:C:326:PHE:HB3	1.84	0.59
1:D:472:ASP:C	1:D:473:ILE:HG23	2.22	0.59
1:A:136:LEU:HD12	1:A:168:SER:OG	2.03	0.59
1:D:22:LYS:HD3	1:D:320:THR:HG21	1.85	0.59
1:D:337:VAL:HG23	1:D:337:VAL:O	2.02	0.59
1:D:32:GLU:O	1:D:83:GLU:N	2.36	0.59
1:D:436:PRO:HG2	1:D:438:LEU:O	2.03	0.59
1:A:42:CYS:HB2	3:A:902:COA:S1P	2.42	0.59
1:B:294:LEU:CD1	1:B:329:VAL:N	2.65	0.59
1:D:489:ILE:O	1:D:490:GLU:HB2	2.03	0.59
1:B:244:VAL:HG23	1:B:244:VAL:O	2.03	0.59
1:C:287:ASP:OD2	2:C:901:FAD:H5'1	2.03	0.59
1:A:474:VAL:CG2	1:A:513:LYS:HE3	2.33	0.59
1:B:47:TYR:OH	1:B:55:VAL:CG2	2.50	0.59
1:C:222:VAL:HG22	1:C:229:ARG:C	2.22	0.59
1:C:332:THR:HG22	1:C:345:ALA:CB	2.33	0.59
1:D:461:VAL:CG1	1:D:549:PHE:O	2.45	0.59
1:A:97:LYS:HE2	1:A:104:GLU:OE1	2.03	0.59
1:B:365:PRO:HG2	1:B:521:ILE:HB	1.84	0.59
1:C:475:ILE:HD11	1:C:494:VAL:HG22	1.85	0.59
1:D:144:LYS:O	1:D:148:MET:HG3	2.03	0.58
1:B:30:VAL:HG13	1:B:80:VAL:HA	1.85	0.58
1:C:275:MET:HG2	1:C:315:ILE:HD13	1.81	0.58
1:D:227:LYS:C	1:D:228:VAL:HG22	2.23	0.58
1:B:6:ILE:HA	1:B:31:VAL:HG22	1.83	0.58
1:B:449:MET:CE	1:B:452:ARG:HH22	2.16	0.58
1:C:231:VAL:O	1:C:231:VAL:HG23	2.01	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:314:VAL:HB	1:D:324:ALA:CB	2.19	0.58
1:D:525:SER:CB	1:D:542:ILE:HD11	2.33	0.58
1:B:228:VAL:O	1:B:229:ARG:HD2	2.03	0.58
1:D:360:PHE:CE2	1:D:385:VAL:HG11	2.39	0.58
1:C:365:PRO:HB3	1:C:380:ARG:HG2	1.85	0.58
1:A:331:ARG:NH1	1:A:351:MET:SD	2.77	0.58
1:B:1:MET:HE2	1:B:3:VAL:HG23	1.86	0.58
1:D:233:ALA:O	1:D:234:ASN:HB3	2.02	0.58
1:B:337:VAL:O	1:B:337:VAL:HG13	2.02	0.58
1:C:330:ILE:HG13	1:C:332:THR:HG23	1.85	0.58
1:B:295:VAL:HG23	1:B:330:ILE:HD12	1.84	0.58
1:D:37:VAL:HG13	1:D:37:VAL:O	2.03	0.58
1:B:369:ARG:HH12	1:B:375:GLN:HB2	1.69	0.58
1:C:181:VAL:HG12	1:C:212:VAL:HA	1.86	0.58
1:D:295:VAL:HG21	1:D:347:VAL:HG23	1.86	0.58
1:A:128:ILE:HD11	1:A:245:VAL:HG21	1.85	0.58
1:C:41:ARG:C	1:C:43:GLY:H	2.07	0.58
1:C:509:ILE:H	1:C:509:ILE:CD1	2.17	0.58
1:D:55:VAL:HG13	1:D:56:ASP:N	2.18	0.57
1:A:337:VAL:HG21	1:A:340:PHE:HB2	1.86	0.57
1:C:283:TYR:CD1	1:C:319:ILE:CD1	2.86	0.57
1:C:283:TYR:HB3	1:C:315:ILE:HG13	1.85	0.57
1:D:173:LYS:HD2	1:D:177:MET:O	2.04	0.57
1:D:494:VAL:O	1:D:494:VAL:HG13	2.03	0.57
1:C:349:GLU:OE1	1:C:359:TYR:OH	2.17	0.57
1:C:461:VAL:HG22	1:C:461:VAL:O	2.04	0.57
1:D:232:ILE:CB	1:D:238:TYR:HE1	2.17	0.57
1:D:13:LEU:HD22	1:D:72:PHE:CE1	2.39	0.57
1:D:257:GLU:HB2	1:D:263:ILE:CG1	2.34	0.57
1:C:18:ARG:NH1	3:C:902:COA:O7A	2.38	0.57
1:A:369:ARG:NH1	1:A:375:GLN:HB2	2.20	0.57
1:D:205:LEU:HB3	1:D:210:VAL:HG13	1.85	0.57
1:D:476:LEU:HD21	1:D:502:LEU:HD11	1.85	0.57
1:D:490:GLU:OE2	1:D:490:GLU:HA	2.04	0.57
1:A:515:ILE:O	1:A:540:VAL:HA	2.05	0.57
1:B:373:TYR:CZ	1:B:433:PRO:HB3	2.39	0.57
1:C:400:MET:HA	1:C:400:MET:CE	2.29	0.57
1:D:6:ILE:HG21	1:D:116:THR:CG2	2.33	0.57
1:D:257:GLU:HB2	1:D:263:ILE:HG13	1.87	0.57
1:C:459:ILE:HG23	1:C:541:LYS:HD2	1.86	0.57
1:D:360:PHE:CZ	1:D:385:VAL:HG11	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1:MET:CE	1:B:3:VAL:HG21	2.30	0.57
1:A:295:VAL:HG23	1:A:330:ILE:HD12	1.85	0.57
2:B:901:FAD:O2'	2:B:901:FAD:O4'	2.19	0.57
1:C:339:ASP:HB3	1:C:400:MET:CE	2.34	0.57
1:C:515:ILE:HG22	1:C:539:LYS:O	2.04	0.57
1:C:545:GLY:HA3	1:C:549:PHE:CD1	2.40	0.57
1:A:194:ASP:OD1	1:A:349:GLU:HG3	2.05	0.57
1:D:6:ILE:HG22	1:D:116:THR:HG23	1.86	0.56
1:D:405:LYS:HG3	1:C:405:LYS:HG3	1.86	0.56
1:A:528:ALA:O	1:A:531:ILE:HG12	2.05	0.56
1:B:156:ALA:HB1	1:B:172:LEU:HD21	1.86	0.56
1:C:525:SER:O	1:C:542:ILE:CD1	2.53	0.56
1:A:224:GLN:O	1:A:225:ASP:HB3	2.05	0.56
1:A:426:LEU:O	1:B:310:LYS:NZ	2.38	0.56
1:B:61:THR:OG1	1:B:64:GLY:HA3	2.04	0.56
1:B:272:ASP:OD2	1:B:276:ARG:NH2	2.38	0.56
1:B:275:MET:HB2	1:B:315:ILE:CD1	2.35	0.56
1:B:464:LEU:C	1:B:466:GLU:N	2.57	0.56
1:C:275:MET:HE3	1:C:326:PHE:CB	2.35	0.56
1:C:497:ILE:HD12	1:C:509:ILE:HD11	1.87	0.56
1:A:265:GLU:O	1:A:265:GLU:HG3	2.06	0.56
1:B:18:ARG:NH1	3:B:902:COA:O7A	2.38	0.56
1:D:123:PRO:O	1:D:125:ILE:HG22	2.04	0.56
1:B:128:ILE:HD11	1:B:245:VAL:HG11	1.86	0.56
1:C:15:ALA:O	1:C:19:ILE:HG13	2.06	0.56
1:C:140:GLU:OE2	1:C:140:GLU:N	2.31	0.56
1:C:519:CYS:SG	1:C:522:GLY:CA	2.94	0.56
1:D:22:LYS:NZ	1:D:317:GLU:OE2	2.39	0.56
1:C:337:VAL:HG22	1:C:340:PHE:O	2.05	0.56
1:D:23:ASP:OD1	1:D:25:ASP:N	2.38	0.55
1:A:90:ASP:OD1	1:A:93:ARG:N	2.33	0.55
1:A:461:VAL:HG22	1:A:461:VAL:O	2.04	0.55
1:B:153:ALA:HB1	1:B:241:ASP:HB2	1.88	0.55
1:A:474:VAL:HG23	1:A:513:LYS:HE3	1.87	0.55
1:B:228:VAL:O	1:B:229:ARG:HG3	2.06	0.55
1:A:341:THR:CG2	1:A:403:VAL:HG22	2.37	0.55
1:D:518:VAL:CG2	1:D:543:LEU:HD23	2.32	0.55
1:A:481:GLU:H	1:A:481:GLU:CD	2.07	0.55
1:B:47:TYR:CE2	1:B:55:VAL:HG22	2.40	0.55
1:C:220:LYS:H	1:C:231:VAL:CG2	2.19	0.55
1:C:332:THR:HG22	1:C:345:ALA:HA	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:THR:HA	1:D:344:SER:O	2.07	0.55
1:A:337:VAL:CG2	1:A:340:PHE:HB2	2.36	0.55
1:B:158:VAL:HG13	1:B:244:VAL:HG23	1.89	0.55
1:C:379:ILE:HD12	1:C:406:ARG:HG3	1.87	0.55
1:C:457:GLU:HB3	1:C:541:LYS:HZ3	1.70	0.55
1:A:194:ASP:CG	1:A:382:LYS:NZ	2.58	0.55
1:C:158:VAL:HG22	1:C:244:VAL:HG22	1.89	0.55
1:D:475:ILE:HG12	1:D:516:VAL:CG1	2.36	0.54
1:D:93:ARG:HG3	1:D:93:ARG:HH11	1.73	0.54
1:A:369:ARG:HH12	1:A:375:GLN:CB	2.20	0.54
1:B:481:GLU:O	1:B:482:GLU:CB	2.55	0.54
1:A:301:ILE:O	1:A:303:PRO:HD3	2.07	0.54
1:D:293:CYS:HB2	1:D:300:ILE:HD13	1.90	0.54
1:A:523:LEU:HD12	3:B:902:COA:C2A	2.38	0.54
1:B:156:ALA:HB1	1:B:172:LEU:CD2	2.37	0.54
1:D:534:HIS:ND1	1:C:24:GLY:CA	2.66	0.54
1:A:332:THR:HG23	1:A:345:ALA:HB2	1.90	0.54
1:C:511:ARG:O	1:C:512:ASP:HB2	2.06	0.54
1:A:348:ASN:H	1:A:351:MET:HE3	1.72	0.54
1:A:479:ARG:O	1:A:496:HIS:HE1	1.89	0.54
1:B:253:SER:O	1:B:256:ALA:HB3	2.07	0.54
1:C:421:ASP:OD2	1:C:452:ARG:NH1	2.26	0.54
1:D:51:LEU:HD13	1:C:373:TYR:CE1	2.43	0.54
1:D:525:SER:HB3	1:D:542:ILE:HD11	1.90	0.54
1:C:368:ASP:OD1	1:C:402:GLU:HB3	2.08	0.54
1:C:495:ILE:HD11	1:C:508:GLU:HG2	0.59	0.54
1:D:348:ASN:HB3	1:D:351:MET:CE	2.36	0.54
1:D:490:GLU:O	1:D:491:SER:HB2	2.07	0.54
1:D:478:VAL:O	1:D:478:VAL:HG23	2.08	0.53
1:B:222:VAL:O	1:B:228:VAL:HA	2.08	0.53
1:C:13:LEU:HD13	1:C:38:SER:HB2	1.90	0.53
1:C:184:MET:HE1	1:C:217:ARG:HG2	1.90	0.53
1:D:362:VAL:HG21	1:D:447:VAL:HG12	1.90	0.53
1:A:29:THR:HG21	1:A:107:LEU:HD11	1.90	0.53
1:A:158:VAL:HB	1:A:181:VAL:HG22	1.90	0.53
1:B:184:MET:HE1	1:B:217:ARG:HH21	1.46	0.53
1:B:291:THR:HG22	1:B:292:THR:H	1.74	0.53
1:C:293:CYS:HB2	1:C:300:ILE:HD13	1.90	0.53
1:A:405:LYS:HG3	1:B:405:LYS:HG3	1.89	0.53
1:A:523:LEU:HD12	3:B:902:COA:H2A	1.90	0.53
1:B:368:ASP:HB3	1:B:377:ASN:H	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:MET:HG2	1:A:344:SER:HB3	1.89	0.53
1:C:457:GLU:CB	1:C:541:LYS:NZ	2.68	0.53
1:C:443:THR:O	1:C:447:VAL:HG23	2.09	0.53
1:A:157:VAL:HG23	1:A:240:ALA:HB2	1.90	0.53
1:D:318:ASN:ND2	1:D:324:ALA:HB3	2.24	0.53
1:B:134:VAL:HG23	1:B:244:VAL:HG12	1.91	0.53
1:B:496:HIS:CD2	1:B:496:HIS:C	2.81	0.53
1:C:509:ILE:CG2	1:C:537:PHE:HZ	2.07	0.53
1:D:169:ALA:HB1	1:D:210:VAL:HG21	1.90	0.53
1:D:314:VAL:CB	1:D:324:ALA:HB1	2.19	0.53
1:D:406:ARG:NH1	1:D:440:PRO:HD2	2.24	0.53
1:A:341:THR:HG23	1:A:403:VAL:HG22	1.90	0.53
1:A:534:HIS:CG	1:B:24:GLY:HA3	2.43	0.53
1:C:135:THR:H	1:C:141:GLU:HG2	1.72	0.53
1:C:187:ARG:NH1	1:C:350:GLN:NE2	2.55	0.53
1:D:458:GLY:HA2	1:D:542:ILE:HG22	1.91	0.53
1:A:71:TYR:CZ	1:A:75:LEU:CD2	2.92	0.53
1:A:347:VAL:HG12	1:A:393:ILE:O	2.09	0.53
1:B:347:VAL:HG12	1:B:393:ILE:O	2.08	0.53
1:D:37:VAL:O	1:D:38:SER:HB3	2.09	0.52
1:D:323:ARG:HD3	1:D:323:ARG:C	2.29	0.52
1:C:14:LYS:HE3	3:C:902:COA:H121	1.91	0.52
1:C:400:MET:HE3	1:C:400:MET:CA	2.32	0.52
1:C:508:GLU:O	1:C:509:ILE:C	2.47	0.52
1:B:406:ARG:NH1	1:B:439:ASP:OD2	2.42	0.52
1:B:465:LYS:HD2	1:B:473:ILE:HD13	1.92	0.52
1:A:464:LEU:O	1:A:465:LYS:C	2.47	0.52
1:C:532:LEU:O	1:C:535:ALA:HB3	2.10	0.52
1:B:42:CYS:HB2	3:B:902:COA:H21	1.92	0.52
2:D:901:FAD:O2'	2:D:901:FAD:O4'	2.16	0.52
1:B:464:LEU:O	1:B:466:GLU:N	2.42	0.52
1:C:525:SER:O	1:C:542:ILE:HD13	2.10	0.52
1:D:9:GLY:HA3	2:D:901:FAD:O1P	2.09	0.52
1:C:187:ARG:N	1:C:187:ARG:CD	2.73	0.52
1:C:301:ILE:O	1:C:303:PRO:HD3	2.09	0.52
1:C:339:ASP:CB	1:C:400:MET:HE1	2.38	0.52
1:C:497:ILE:HG23	1:C:505:ARG:CD	2.35	0.52
1:D:6:ILE:CG2	1:D:116:THR:HG23	2.37	0.52
1:A:314:VAL:O	1:A:318:ASN:ND2	2.39	0.52
1:D:14:LYS:HZ3	3:D:902:COA:H121	1.72	0.52
1:D:39:LEU:HA	1:D:59:ARG:HG2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:349:GLU:O	1:D:353:LYS:HG2	2.10	0.52
1:A:22:LYS:HE2	1:A:317:GLU:OE2	2.10	0.52
1:B:52:VAL:HG12	1:B:52:VAL:O	2.10	0.52
1:B:275:MET:HB2	1:B:315:ILE:HD11	1.92	0.52
1:B:364:ALA:HB3	1:B:444:ILE:HD12	1.92	0.52
1:C:509:ILE:CD1	1:C:509:ILE:N	2.73	0.52
1:C:545:GLY:CA	1:C:549:PHE:HE1	2.23	0.52
1:D:20:ARG:O	1:D:20:ARG:HD3	2.09	0.52
1:D:117:GLY:HA2	1:D:287:ASP:HB2	1.90	0.52
1:D:343:ALA:HB3	1:D:407:ILE:HG13	1.92	0.52
1:A:20:ARG:CZ	1:A:28:ILE:HD12	2.39	0.52
1:B:47:TYR:CD1	1:B:55:VAL:HG22	2.42	0.52
1:C:2:ASN:OD1	1:C:2:ASN:N	2.40	0.52
1:C:423:LEU:HD23	1:C:445:ALA:HB2	1.90	0.52
1:C:22:LYS:HD3	1:C:320:THR:OG1	2.10	0.52
1:B:294:LEU:CD1	1:B:328:GLY:C	2.79	0.51
1:B:349:GLU:OE2	1:B:359:TYR:CE2	2.63	0.51
1:C:196:GLU:OE2	1:C:196:GLU:HA	2.09	0.51
1:A:187:ARG:HB2	1:A:198:ALA:HB1	1.91	0.51
1:B:430:TYR:CD1	1:B:436:PRO:O	2.63	0.51
1:C:41:ARG:NH2	2:C:901:FAD:HM81	2.25	0.51
1:C:546:GLY:O	1:C:548:ALA:N	2.43	0.51
1:C:5:VAL:HB	1:C:113:VAL:HB	1.92	0.51
1:C:452:ARG:C	1:C:454:GLY:H	2.14	0.51
1:D:112:LEU:HD23	1:D:282:ILE:HG12	1.91	0.51
1:B:57:ASN:HA	1:B:60:GLU:HG2	1.93	0.51
1:B:341:THR:O	1:B:398:VAL:HA	2.11	0.51
1:C:455:LEU:HD23	1:C:526:PHE:CZ	2.36	0.51
1:C:457:GLU:CB	1:C:541:LYS:HZ3	2.22	0.51
1:D:527:GLU:O	1:D:531:ILE:HG13	2.11	0.51
1:A:75:LEU:HG	1:A:75:LEU:O	2.11	0.51
1:C:462:PHE:O	1:C:464:LEU:N	2.44	0.51
1:A:274:TYR:O	1:A:275:MET:HB2	2.10	0.51
1:A:406:ARG:HH11	1:A:439:ASP:CG	2.14	0.51
1:C:275:MET:HE1	1:C:326:PHE:HB3	1.91	0.51
2:C:901:FAD:O2'	2:C:901:FAD:O4'	2.21	0.51
1:D:134:VAL:CG2	1:D:244:VAL:HG12	2.41	0.51
1:B:200:LEU:HD13	1:B:380:ARG:HD3	1.92	0.51
1:A:25:ASP:OD1	1:A:25:ASP:O	2.29	0.51
1:B:119:ARG:NH2	1:B:250:LYS:HD2	2.26	0.51
1:B:294:LEU:HD11	1:B:328:GLY:C	2.31	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:463:GLU:HG2	1:B:464:LEU:H	1.71	0.51
1:A:168:SER:O	1:A:172:LEU:HB2	2.11	0.51
1:B:380:ARG:HB3	1:B:549:PHE:HZ	1.75	0.51
1:A:71:TYR:CE1	1:A:75:LEU:HD22	2.46	0.51
1:B:518:VAL:HG22	1:B:543:LEU:CD2	2.40	0.51
1:D:234:ASN:O	1:D:235:GLY:C	2.48	0.50
1:D:61:THR:C	1:D:62:THR:HG1	2.02	0.50
1:D:301:ILE:O	1:D:303:PRO:HD3	2.11	0.50
1:A:214:THR:O	1:A:216:THR:HG23	2.10	0.50
1:A:61:THR:HB	1:A:63:TYR:CE1	2.46	0.50
1:A:157:VAL:O	1:A:243:VAL:HA	2.12	0.50
1:B:2:ASN:HB3	1:B:27:SER:HB3	1.94	0.50
1:C:363:ILE:HG12	1:C:544:GLU:HB3	1.92	0.50
1:D:505:ARG:O	1:D:506:LEU:HD23	2.11	0.50
1:B:380:ARG:NH1	1:B:548:ALA:CB	2.52	0.50
1:C:273:GLU:OE2	1:C:273:GLU:HA	2.10	0.50
1:C:509:ILE:N	1:C:509:ILE:HD12	2.25	0.50
1:C:419:THR:H	1:C:422:GLN:HG2	1.75	0.50
1:D:148:MET:HE2	1:D:242:VAL:HG12	1.93	0.50
1:A:224:GLN:HB3	1:A:228:VAL:CG1	2.41	0.50
1:A:266:THR:HG23	1:A:290:GLU:OE2	2.11	0.50
1:A:272:ASP:OD1	1:A:274:TYR:N	2.45	0.50
1:C:196:GLU:OE1	1:C:460:ASN:HB2	2.11	0.50
1:D:20:ARG:HH21	1:D:28:ILE:CD1	2.23	0.50
1:D:222:VAL:CG2	1:D:229:ARG:CB	2.84	0.50
1:D:318:ASN:HD21	1:D:324:ALA:HB3	1.76	0.50
1:A:360:PHE:CE2	1:A:385:VAL:CG1	2.94	0.50
1:A:368:ASP:OD1	1:A:402:GLU:HB3	2.12	0.50
1:A:200:LEU:HD11	1:A:549:PHE:CE2	2.47	0.49
1:A:391:ARG:HA	1:A:419:THR:HA	1.94	0.49
1:A:497:ILE:HD12	1:A:509:ILE:HD11	1.94	0.49
1:B:479:ARG:HH22	1:B:488:ARG:N	2.10	0.49
1:C:199:VAL:HG22	1:C:203:ASN:OD1	2.12	0.49
1:A:100:ARG:O	1:A:101:ASN:HB2	2.11	0.49
1:C:33:ALA:O	1:C:83:GLU:HA	2.12	0.49
1:B:47:TYR:OH	1:B:55:VAL:HG23	2.11	0.49
1:B:217:ARG:NH1	1:B:217:ARG:CG	2.72	0.49
1:C:337:VAL:O	1:C:338:PHE:C	2.50	0.49
1:C:337:VAL:HG23	1:C:340:PHE:H	1.76	0.49
1:C:477:ASP:OD1	1:C:479:ARG:CB	2.60	0.49
1:B:285:GLY:HA2	1:B:289:VAL:HG21	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:ARG:HG3	1:C:283:TYR:CE2	2.48	0.49
1:C:436:PRO:HG2	1:C:438:LEU:O	2.12	0.49
1:A:373:TYR:CG	1:A:374:PRO:HD2	2.47	0.49
1:B:360:PHE:CE2	1:B:385:VAL:CG2	2.96	0.49
1:C:455:LEU:CD2	1:C:526:PHE:HZ	2.22	0.49
1:D:100:ARG:O	1:D:101:ASN:HB2	2.11	0.49
1:D:488:ARG:O	1:D:490:GLU:N	2.45	0.49
1:A:330:ILE:HG13	1:A:415:GLN:CG	2.41	0.49
1:D:68:ASP:O	1:D:71:TYR:HB3	2.13	0.49
1:B:143:GLU:HA	1:B:146:ILE:CG2	2.40	0.49
1:C:157:VAL:CG2	1:C:240:ALA:HB2	2.35	0.49
1:C:184:MET:SD	1:C:217:ARG:HG2	2.52	0.49
1:C:361:THR:HG23	1:C:382:LYS:HE3	1.94	0.49
1:D:41:ARG:HH22	1:D:137:THR:HG23	1.68	0.49
1:D:406:ARG:NH1	1:D:439:ASP:OD1	2.37	0.49
1:B:295:VAL:HG23	1:B:330:ILE:CD1	2.42	0.49
1:B:369:ARG:NH1	1:B:375:GLN:HB2	2.28	0.49
1:C:317:GLU:O	1:C:320:THR:OG1	2.23	0.49
1:D:121:ALA:HA	1:D:250:LYS:HE3	1.95	0.48
1:B:47:TYR:HE1	1:B:53:HIS:O	1.96	0.48
1:B:340:PHE:CE1	1:B:400:MET:HG3	2.47	0.48
1:C:206:ARG:HA	1:C:210:VAL:O	2.13	0.48
1:C:294:LEU:HD21	1:C:328:GLY:HA3	1.95	0.48
1:C:335:PHE:CE2	1:C:342:ALA:HB3	2.48	0.48
1:B:41:ARG:NH2	2:B:901:FAD:HM81	2.28	0.48
1:C:227:LYS:HG3	1:C:228:VAL:H	1.74	0.48
1:B:456:PHE:CD1	1:B:542:ILE:HG21	2.48	0.48
1:C:187:ARG:N	1:C:187:ARG:HD2	2.27	0.48
1:D:156:ALA:HB2	1:D:177:MET:HE1	1.96	0.48
1:D:228:VAL:HG23	1:D:240:ALA:O	2.13	0.48
1:B:158:VAL:HG22	1:B:244:VAL:HG22	1.89	0.48
1:C:199:VAL:O	1:C:202:GLU:HB3	2.13	0.48
1:C:474:VAL:CG1	1:C:515:ILE:HD12	2.44	0.48
1:A:199:VAL:O	1:A:203:ASN:OD1	2.32	0.48
1:A:341:THR:HG23	1:A:403:VAL:HG21	1.95	0.48
1:C:349:GLU:O	1:C:353:LYS:HG3	2.14	0.48
1:D:347:VAL:CG1	1:D:352:ALA:HB2	2.44	0.48
1:A:132:GLY:HA2	1:A:148:MET:SD	2.54	0.48
1:B:502:LEU:O	1:B:503:ARG:C	2.51	0.48
1:C:266:THR:OG1	1:C:290:GLU:HG3	2.14	0.48
1:A:503:ARG:NH1	1:B:75:LEU:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:ASP:OD1	1:C:303:PRO:HA	2.14	0.48
1:D:91:ARG:HD2	1:D:279:ASP:HB2	1.95	0.47
1:D:228:VAL:O	1:D:229:ARG:HD3	2.14	0.47
1:A:5:VAL:HG13	1:A:113:VAL:HB	1.96	0.47
1:A:505:ARG:HG3	1:A:505:ARG:O	2.13	0.47
1:B:431:ALA:HB3	1:B:434:TYR:HD2	1.79	0.47
1:C:45:PRO:HD3	2:C:901:FAD:HM72	1.95	0.47
1:C:495:ILE:CD1	1:C:508:GLU:CG	2.29	0.47
1:D:125:ILE:CG2	1:D:128:ILE:HB	2.43	0.47
1:D:155:LYS:HD2	1:D:241:ASP:CG	2.34	0.47
1:A:257:GLU:HB2	1:A:263:ILE:HG13	1.96	0.47
3:A:902:COA:C2A	1:B:523:LEU:HD12	2.44	0.47
1:C:13:LEU:HD22	1:C:72:PHE:CE2	2.50	0.47
1:A:185:MET:HG3	1:A:190:PRO:HG3	1.96	0.47
1:A:389:SER:OG	1:A:391:ARG:HG2	2.15	0.47
1:C:275:MET:HB3	1:C:315:ILE:HD12	1.95	0.47
1:C:341:THR:CG2	1:C:403:VAL:HG22	2.43	0.47
1:A:63:TYR:CD1	1:A:63:TYR:N	2.73	0.47
1:C:220:LYS:N	1:C:231:VAL:CG2	2.77	0.47
1:B:360:PHE:CZ	1:B:385:VAL:CG2	2.97	0.47
1:B:488:ARG:O	1:B:488:ARG:HG2	2.15	0.47
1:C:187:ARG:HA	1:C:214:THR:HG21	1.95	0.47
1:D:14:LYS:HZ2	3:D:902:COA:P2A	2.37	0.47
1:D:409:VAL:HG21	1:C:408:ASP:HB3	1.97	0.47
1:B:276:ARG:HH12	1:B:323:ARG:NH1	2.10	0.47
1:B:291:THR:HG22	1:B:328:GLY:HA2	1.96	0.47
1:C:56:ASP:OD2	1:C:59:ARG:NH1	2.47	0.47
1:C:222:VAL:O	1:C:228:VAL:HA	2.15	0.47
1:D:489:ILE:O	1:D:489:ILE:HG22	2.13	0.47
1:B:154:GLU:HG3	1:B:177:MET:HA	1.96	0.47
1:B:194:ASP:OD2	1:B:349:GLU:HG3	2.15	0.47
1:B:286:GLY:O	1:B:289:VAL:HB	2.14	0.47
1:D:450:ASN:ND2	1:D:526:PHE:HE2	2.12	0.47
1:D:461:VAL:HG21	1:D:549:PHE:HB2	1.93	0.47
1:B:291:THR:CG2	1:B:328:GLY:HA2	2.44	0.47
1:A:287:ASP:OD2	2:A:901:FAD:O3'	2.27	0.47
1:A:341:THR:HB	1:B:434:TYR:OH	2.14	0.47
1:A:519:CYS:HB3	1:A:525:SER:OG	2.15	0.47
1:D:89:ILE:HG23	1:D:96:VAL:HG22	1.95	0.47
1:D:488:ARG:HA	1:D:547:MET:CE	2.45	0.47
1:B:47:TYR:CD1	1:B:53:HIS:O	2.68	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:461:VAL:O	1:B:461:VAL:HG22	2.14	0.47
1:C:495:ILE:HD11	1:C:508:GLU:CD	2.24	0.47
1:C:499:ILE:CG2	1:C:500:LEU:N	2.78	0.47
1:A:360:PHE:CE2	1:A:385:VAL:HG13	2.51	0.46
1:A:439:ASP:O	1:A:442:ILE:N	2.48	0.46
1:B:502:LEU:CD2	1:B:506:LEU:HD21	2.46	0.46
1:B:549:PHE:CD1	1:B:549:PHE:N	2.82	0.46
1:C:362:VAL:HG21	1:C:447:VAL:HG12	1.96	0.46
3:D:902:COA:H8A	1:C:526:PHE:CD2	2.49	0.46
1:A:419:THR:H	1:A:422:GLN:HG2	1.80	0.46
1:A:480:SER:OG	1:A:481:GLU:OE1	2.25	0.46
1:C:505:ARG:C	1:C:507:ASP:H	2.18	0.46
1:C:526:PHE:HA	1:C:542:ILE:CD1	2.46	0.46
1:A:304:PHE:HB3	2:A:901:FAD:O2	2.16	0.46
1:B:125:ILE:CG2	1:B:128:ILE:HB	2.41	0.46
1:B:347:VAL:HG23	1:B:351:MET:CB	2.44	0.46
1:C:112:LEU:CD2	1:C:282:ILE:HG23	2.45	0.46
1:C:199:VAL:HG13	1:C:200:LEU:N	2.31	0.46
1:C:387:LYS:HA	1:C:390:TRP:CZ3	2.50	0.46
1:D:125:ILE:CD1	1:D:218:VAL:HG12	2.46	0.46
1:B:542:ILE:HG21	1:B:542:ILE:HD13	1.65	0.46
1:C:58:LEU:N	1:C:58:LEU:HD12	2.30	0.46
1:C:368:ASP:HB3	1:C:377:ASN:H	1.81	0.46
1:C:421:ASP:HA	1:C:449:MET:HE1	1.98	0.46
1:C:464:LEU:HD23	1:C:464:LEU:HA	1.63	0.46
1:D:93:ARG:HG3	1:D:93:ARG:NH1	2.30	0.46
1:A:272:ASP:OD1	1:A:275:MET:N	2.48	0.46
1:A:362:VAL:HG21	1:A:447:VAL:HG12	1.98	0.46
1:C:283:TYR:CE1	1:C:319:ILE:CD1	2.98	0.46
1:C:373:TYR:CG	1:C:374:PRO:HD2	2.51	0.46
1:A:363:ILE:HG12	1:A:382:LYS:HG3	1.97	0.46
1:C:475:ILE:HD12	1:C:475:ILE:O	2.16	0.46
1:C:498:PRO:HB2	1:C:501:GLU:HG3	1.98	0.46
1:D:67:ARG:HG3	1:D:71:TYR:CE1	2.51	0.46
1:D:134:VAL:HG23	1:D:244:VAL:HG12	1.97	0.46
1:D:475:ILE:HG12	1:D:516:VAL:HG12	1.97	0.46
1:A:47:TYR:HA	1:A:52:VAL:CG2	2.39	0.46
1:C:39:LEU:HD11	1:C:139:ALA:HB2	1.98	0.46
1:D:537:PHE:C	1:D:538:GLU:CG	2.85	0.46
1:A:477:ASP:OD1	1:A:479:ARG:HB3	2.16	0.46
1:A:509:ILE:CG2	1:A:515:ILE:HD13	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:LYS:O	1:B:148:MET:HG3	2.16	0.46
1:B:402:GLU:OE2	1:B:402:GLU:HA	2.15	0.46
1:B:475:ILE:HG22	1:B:494:VAL:HG23	1.97	0.46
1:B:497:ILE:HG13	1:B:497:ILE:O	2.16	0.46
1:D:158:VAL:HG22	1:D:244:VAL:CG2	2.41	0.46
1:A:187:ARG:HB2	1:A:198:ALA:CB	2.44	0.46
1:B:154:GLU:O	1:B:154:GLU:HG3	2.16	0.46
1:B:202:GLU:HG2	1:B:206:ARG:NH2	2.31	0.46
1:C:5:VAL:HG12	1:C:113:VAL:HB	1.97	0.46
1:C:287:ASP:OD2	2:C:901:FAD:H3'	2.16	0.46
1:A:93:ARG:NH2	1:A:106:GLU:OE2	2.49	0.46
1:A:439:ASP:O	1:A:440:PRO:C	2.52	0.46
1:A:478:VAL:HA	1:A:497:ILE:O	2.15	0.46
1:B:216:THR:HB	1:B:233:ALA:HB3	1.98	0.46
1:C:196:GLU:OE2	1:C:196:GLU:CA	2.63	0.46
1:C:256:ALA:O	1:C:261:LEU:HB2	2.16	0.46
1:C:275:MET:CB	1:C:315:ILE:HD12	2.46	0.46
1:C:416:ALA:HB3	1:C:418:MET:HG3	1.98	0.46
1:D:476:LEU:HD23	1:D:517:VAL:HG22	1.98	0.45
1:B:131:GLU:HB2	1:B:226:ASP:HB3	1.98	0.45
1:B:205:LEU:HD21	1:B:337:VAL:CG2	2.46	0.45
1:C:302:ALA:HB2	1:C:329:VAL:HG21	1.98	0.45
1:C:474:VAL:HG11	1:C:515:ILE:HD12	1.98	0.45
1:D:202:GLU:HG3	1:D:212:VAL:HG11	1.97	0.45
1:B:423:LEU:HD12	1:B:426:LEU:HD22	1.96	0.45
1:C:219:GLU:HB2	1:C:231:VAL:HG23	1.98	0.45
1:D:318:ASN:HA	1:D:322:GLY:H	1.80	0.45
1:B:163:PHE:HB2	1:B:335:PHE:HB3	1.99	0.45
1:C:38:SER:O	1:C:38:SER:OG	2.32	0.45
1:C:373:TYR:CZ	1:C:433:PRO:HB3	2.51	0.45
1:A:45:PRO:HD3	2:A:901:FAD:HM72	1.98	0.45
1:A:502:LEU:CD2	1:A:531:ILE:CD1	2.91	0.45
1:C:37:VAL:O	1:C:38:SER:HB3	2.16	0.45
1:C:134:VAL:HG23	1:C:244:VAL:HG12	1.98	0.45
1:C:545:GLY:O	1:C:548:ALA:HB3	2.17	0.45
1:B:204:HIS:HE1	1:B:339:ASP:N	2.12	0.45
1:C:202:GLU:HG2	1:C:206:ARG:NH2	2.31	0.45
1:C:336:LYS:NZ	1:C:338:PHE:O	2.49	0.45
1:A:8:GLY:O	1:A:37:VAL:HG23	2.17	0.45
1:A:21:ARG:NH2	3:A:902:COA:O5A	2.50	0.45
1:A:293:CYS:O	1:A:297:GLY:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:GLU:OE1	1:C:460:ASN:OD1	2.34	0.45
1:D:510:PRO:O	1:D:512:ASP:N	2.48	0.45
1:A:163:PHE:O	1:A:167:GLU:HG3	2.17	0.45
1:B:8:GLY:HA3	1:B:37:VAL:HG23	1.99	0.45
1:C:275:MET:HG3	1:C:315:ILE:HD11	1.89	0.45
1:C:450:ASN:O	1:C:455:LEU:HB3	2.17	0.45
1:D:234:ASN:O	1:D:236:LYS:N	2.50	0.45
1:D:421:ASP:OD2	1:D:449:MET:HE3	2.17	0.45
1:D:534:HIS:CE1	1:C:24:GLY:O	2.70	0.45
1:A:75:LEU:HB2	1:B:500:LEU:HD23	1.98	0.45
1:D:14:LYS:NZ	3:D:902:COA:P2A	2.90	0.45
1:D:157:VAL:O	1:D:243:VAL:HA	2.17	0.45
1:D:295:VAL:HG13	1:D:330:ILE:HD12	1.98	0.45
1:C:5:VAL:CB	1:C:113:VAL:HB	2.47	0.45
1:C:192:MET:HE3	1:C:192:MET:HB3	1.85	0.45
1:C:529:SER:HB3	1:C:542:ILE:HD11	0.63	0.45
1:D:473:ILE:HG22	1:D:514:GLU:HB3	1.98	0.45
1:B:158:VAL:HB	1:B:181:VAL:HG22	1.99	0.45
1:B:217:ARG:H	1:B:233:ALA:HB2	1.82	0.45
1:B:379:ILE:CG2	1:B:403:VAL:HG12	2.46	0.45
1:D:341:THR:HG23	1:C:434:TYR:OH	2.17	0.44
1:D:449:MET:HE3	1:D:452:ARG:HH12	1.83	0.44
1:A:360:PHE:CZ	1:A:385:VAL:HG11	2.52	0.44
1:B:135:THR:HG22	1:B:245:VAL:CG2	2.47	0.44
1:B:294:LEU:HD11	1:B:328:GLY:CA	2.47	0.44
1:B:331:ARG:CZ	1:B:351:MET:SD	3.04	0.44
1:C:515:ILE:HG23	1:C:515:ILE:O	2.17	0.44
1:D:315:ILE:O	1:D:319:ILE:HG12	2.18	0.44
1:D:360:PHE:CE2	1:D:385:VAL:HG13	2.52	0.44
1:D:507:ASP:C	1:D:508:GLU:HG2	2.36	0.44
1:A:61:THR:O	1:A:63:TYR:O	2.34	0.44
1:A:273:GLU:HB3	1:A:325:VAL:CG2	2.47	0.44
1:A:330:ILE:HA	1:A:330:ILE:HD13	1.59	0.44
1:B:22:LYS:NZ	1:B:22:LYS:HB3	2.33	0.44
1:B:418:MET:HA	1:B:422:GLN:NE2	2.29	0.44
1:A:464:LEU:H	1:A:464:LEU:CD2	2.23	0.44
1:D:82:THR:HG22	1:D:83:GLU:HG3	1.99	0.44
1:B:183:GLU:HG3	1:B:185:MET:H	1.83	0.44
1:D:361:THR:CG2	1:D:382:LYS:HE3	2.46	0.44
1:D:520:ALA:O	1:D:521:ILE:HD12	2.17	0.44
1:A:366:SER:OG	1:A:367:PRO:HD2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:ASP:O	1:A:441:VAL:N	2.50	0.44
1:B:217:ARG:O	1:B:233:ALA:HB2	2.17	0.44
1:C:5:VAL:CG1	1:C:113:VAL:HB	2.48	0.44
1:A:44:LEU:N	1:A:45:PRO:HD2	2.33	0.44
1:A:295:VAL:HG23	1:A:330:ILE:CD1	2.48	0.44
1:A:509:ILE:HA	1:A:510:PRO:HD2	1.66	0.44
1:A:547:MET:O	1:A:548:ALA:C	2.51	0.44
1:B:373:TYR:CE2	1:B:433:PRO:HB3	2.52	0.44
1:C:22:LYS:CB	1:C:320:THR:HG21	2.42	0.44
1:D:353:LYS:HB3	1:D:353:LYS:HE2	1.62	0.44
1:D:406:ARG:HB3	1:D:441:VAL:HG23	2.00	0.44
1:A:232:ILE:C	1:A:234:ASN:N	2.70	0.44
1:B:380:ARG:HB3	1:B:549:PHE:CZ	2.53	0.44
1:C:187:ARG:CZ	1:C:350:GLN:HE21	2.29	0.44
1:C:200:LEU:CD1	1:C:380:ARG:HD2	2.48	0.44
1:D:227:LYS:C	1:D:228:VAL:CG2	2.85	0.44
1:D:316:GLY:O	1:D:320:THR:HG22	2.18	0.44
1:D:360:PHE:CD2	1:D:385:VAL:HG13	2.53	0.44
1:B:13:LEU:HD12	1:B:72:PHE:CE1	2.53	0.44
1:C:91:ARG:HH11	1:C:279:ASP:HB2	1.83	0.44
1:D:6:ILE:HG22	1:D:6:ILE:O	2.17	0.44
1:D:7:GLY:N	1:D:31:VAL:O	2.47	0.44
1:D:173:LYS:NZ	1:D:209:GLY:O	2.47	0.44
1:D:453:ASP:HB2	1:D:455:LEU:CD1	2.48	0.44
1:A:406:ARG:HB3	1:A:441:VAL:HG23	1.99	0.44
1:A:517:VAL:HG23	1:A:540:VAL:CG2	2.47	0.44
1:B:349:GLU:OE2	1:B:359:TYR:OH	2.18	0.44
1:B:479:ARG:NH2	1:B:488:ARG:N	2.65	0.44
1:B:496:HIS:NE2	1:B:498:PRO:HD3	2.33	0.44
1:C:419:THR:HG22	1:C:421:ASP:HB2	2.00	0.44
1:D:121:ALA:H	1:D:249:ILE:HA	1.83	0.43
1:D:330:ILE:HG13	1:D:415:GLN:CG	2.38	0.43
1:B:285:GLY:CA	1:B:289:VAL:HG21	2.48	0.43
1:B:465:LYS:HD3	1:B:473:ILE:CD1	2.37	0.43
1:C:68:ASP:OD1	1:C:68:ASP:N	2.40	0.43
1:D:20:ARG:CZ	1:D:28:ILE:HD12	2.48	0.43
1:D:55:VAL:CG1	1:D:56:ASP:N	2.80	0.43
1:D:537:PHE:C	1:D:538:GLU:HG2	2.39	0.43
1:A:336:LYS:HG2	1:A:337:VAL:O	2.18	0.43
1:B:61:THR:OG1	1:B:64:GLY:CA	2.66	0.43
1:B:413:ALA:CB	1:B:418:MET:HE3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:ARG:HH21	3:C:902:COA:H131	1.83	0.43
1:C:182:ILE:HD13	1:C:213:VAL:HG22	1.96	0.43
1:D:105:ASP:OD1	1:D:106:GLU:N	2.44	0.43
1:D:542:ILE:HG21	1:D:542:ILE:HD13	1.65	0.43
1:B:351:MET:HE3	1:B:351:MET:HB2	1.89	0.43
1:C:170:GLU:O	1:C:174:ASN:OD1	2.36	0.43
1:C:499:ILE:HG23	1:C:500:LEU:H	1.78	0.43
1:D:377:ASN:HB3	1:D:400:MET:O	2.18	0.43
1:A:41:ARG:NH1	1:A:137:THR:O	2.51	0.43
1:A:360:PHE:CD2	1:A:385:VAL:HG13	2.52	0.43
1:A:497:ILE:HD11	1:A:509:ILE:HD11	2.01	0.43
1:B:14:LYS:HD2	1:B:309:ASN:HB3	1.99	0.43
1:B:385:VAL:HG11	1:B:420:ILE:HG21	2.00	0.43
1:B:385:VAL:HG11	1:B:420:ILE:CG2	2.48	0.43
1:C:269:ILE:CG2	1:C:277:THR:CG2	2.95	0.43
1:D:405:LYS:HG3	1:C:405:LYS:HA	2.00	0.43
1:B:51:LEU:HD23	1:B:51:LEU:HA	1.84	0.43
1:C:476:LEU:HD22	1:C:478:VAL:CG2	2.37	0.43
1:D:202:GLU:O	1:D:205:LEU:HB2	2.19	0.43
1:D:409:VAL:CG2	1:C:408:ASP:HB3	2.49	0.43
1:A:306:ASP:OD1	1:A:307:VAL:N	2.51	0.43
1:D:41:ARG:NH2	1:D:137:THR:CG2	2.58	0.43
1:D:184:MET:O	1:D:215:SER:HA	2.19	0.43
1:A:22:LYS:HD3	1:B:455:LEU:HD11	2.01	0.43
1:A:276:ARG:HG2	1:A:283:TYR:CZ	2.54	0.43
1:A:360:PHE:CE2	1:A:385:VAL:HG11	2.53	0.43
1:B:52:VAL:O	1:B:53:HIS:HB2	2.19	0.43
1:C:438:LEU:HD22	1:C:442:ILE:HG22	1.99	0.43
1:A:204:HIS:CE1	1:A:339:ASP:HB2	2.54	0.43
1:B:134:VAL:CG2	1:B:244:VAL:HG12	2.48	0.43
1:C:341:THR:HB	1:C:403:VAL:HG22	2.00	0.43
1:C:378:TYR:CE2	1:C:521:ILE:HD13	2.54	0.43
1:C:528:ALA:O	1:C:531:ILE:HB	2.18	0.43
1:D:374:PRO:HG3	1:C:51:LEU:HD22	2.01	0.43
1:B:9:GLY:HA3	2:B:901:FAD:O1P	2.18	0.43
1:C:57:ASN:N	1:C:57:ASN:OD1	2.51	0.43
1:C:120:PRO:HD3	1:C:137:THR:HG21	2.01	0.43
1:C:227:LYS:C	1:C:228:VAL:CG2	2.83	0.43
1:C:361:THR:CG2	1:C:382:LYS:HE3	2.49	0.43
1:D:438:LEU:HA	1:D:438:LEU:HD23	1.80	0.43
1:B:228:VAL:O	1:B:229:ARG:CG	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:517:VAL:HG11	1:B:528:ALA:HB3	1.99	0.43
1:C:135:THR:O	1:C:141:GLU:HG2	2.18	0.43
1:C:347:VAL:HG12	1:C:352:ALA:HB2	2.01	0.43
1:C:482:GLU:OE1	1:C:496:HIS:HD2	2.02	0.43
1:D:549:PHE:N	1:D:549:PHE:CD1	2.87	0.42
1:A:338:PHE:CD1	1:A:338:PHE:N	2.81	0.42
1:A:426:LEU:HD12	1:B:415:GLN:OE1	2.19	0.42
1:A:446:ASN:HB3	1:B:313:ARG:NH1	2.34	0.42
1:B:496:HIS:HD2	1:B:498:PRO:HD3	1.78	0.42
1:C:220:LYS:HB3	1:C:231:VAL:HG21	2.01	0.42
1:C:224:GLN:C	1:C:226:ASP:N	2.73	0.42
1:D:461:VAL:CG2	1:D:549:PHE:HB2	2.49	0.42
1:A:183:GLU:HG3	1:A:185:MET:H	1.83	0.42
1:C:194:ASP:OD2	1:C:349:GLU:HG3	2.19	0.42
1:C:288:CYS:SG	1:C:289:VAL:HG23	2.59	0.42
1:A:166:LEU:CD1	1:A:335:PHE:CZ	3.00	0.42
1:A:406:ARG:HB3	1:A:441:VAL:CG2	2.50	0.42
1:C:225:ASP:O	1:C:226:ASP:HB2	2.19	0.42
1:C:545:GLY:HA2	1:C:549:PHE:HE1	1.83	0.42
1:D:20:ARG:HH21	1:D:28:ILE:HD11	1.83	0.42
1:D:459:ILE:HD12	1:D:459:ILE:O	2.19	0.42
1:B:330:ILE:HD13	1:B:330:ILE:HA	1.70	0.42
1:D:67:ARG:HG3	1:D:71:TYR:CG	2.55	0.42
1:B:159:ILE:HD13	1:B:218:VAL:HG21	2.01	0.42
1:B:349:GLU:OE2	1:B:359:TYR:HE2	2.03	0.42
1:D:166:LEU:HD23	1:D:166:LEU:HA	1.86	0.42
1:C:374:PRO:O	1:C:375:GLN:HB2	2.19	0.42
1:A:473:ILE:CG2	1:A:474:VAL:N	2.82	0.42
1:B:165:GLY:O	1:B:168:SER:HB2	2.20	0.42
1:C:343:ALA:HB3	1:C:407:ILE:HG13	2.02	0.42
1:B:465:LYS:HD2	1:B:473:ILE:HD11	1.95	0.42
1:A:61:THR:C	1:A:63:TYR:O	2.58	0.42
1:C:54:GLU:OE2	1:C:54:GLU:HA	2.19	0.42
1:C:90:ASP:OD1	1:C:92:SER:OG	2.30	0.42
1:C:439:ASP:O	1:C:443:THR:HG23	2.20	0.42
1:D:233:ALA:C	1:D:235:GLY:N	2.73	0.42
1:B:99:VAL:HA	1:B:104:GLU:HA	2.01	0.42
1:B:379:ILE:HB	1:B:403:VAL:HG12	2.02	0.42
1:A:117:GLY:HA2	1:A:287:ASP:HB2	2.02	0.41
1:B:275:MET:HB3	1:B:315:ILE:HD11	2.00	0.41
1:C:136:LEU:HA	1:C:136:LEU:HD22	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:VAL:HB	1:A:275:MET:HA	2.03	0.41
1:A:508:GLU:O	1:A:510:PRO:CD	2.68	0.41
1:B:126:GLU:CD	1:B:220:LYS:HE3	2.40	0.41
1:C:32:GLU:CD	2:C:901:FAD:O2B	2.56	0.41
1:C:41:ARG:C	1:C:43:GLY:N	2.73	0.41
1:C:195:ARG:O	1:C:196:GLU:C	2.59	0.41
1:C:497:ILE:HD12	1:C:509:ILE:CD1	2.48	0.41
1:D:22:LYS:HE2	1:D:22:LYS:HB3	1.80	0.41
1:D:148:MET:CE	1:D:242:VAL:HG12	2.49	0.41
1:D:228:VAL:O	1:D:229:ARG:CD	2.68	0.41
1:D:474:VAL:HG13	1:D:515:ILE:HG12	2.02	0.41
1:D:510:PRO:C	1:D:512:ASP:H	2.24	0.41
1:A:369:ARG:NH1	1:A:375:GLN:CB	2.81	0.41
1:B:22:LYS:HD2	1:B:317:GLU:OE2	2.20	0.41
1:B:271:VAL:HB	1:B:275:MET:HA	2.01	0.41
1:B:361:THR:HG21	1:B:382:LYS:HE3	2.02	0.41
1:A:90:ASP:O	1:A:94:LYS:N	2.54	0.41
1:A:166:LEU:HD13	1:A:335:PHE:CE1	2.54	0.41
1:A:226:ASP:O	1:A:227:LYS:CB	2.68	0.41
1:A:325:VAL:O	1:B:425:ASN:ND2	2.47	0.41
1:A:499:ILE:HD12	1:A:524:ARG:HB3	2.02	0.41
1:B:445:ALA:O	1:B:449:MET:HG3	2.20	0.41
1:C:509:ILE:HG23	1:C:537:PHE:CE2	2.21	0.41
1:C:517:VAL:HB	1:C:542:ILE:HG12	2.02	0.41
1:D:204:HIS:CE1	1:D:339:ASP:HB2	2.55	0.41
1:A:158:VAL:HG22	1:A:244:VAL:CG2	2.46	0.41
1:A:479:ARG:HB3	1:A:479:ARG:HE	1.78	0.41
1:C:332:THR:HG22	1:C:345:ALA:CA	2.51	0.41
1:C:473:ILE:HD12	1:C:473:ILE:N	2.35	0.41
1:D:459:ILE:HD12	1:D:460:ASN:O	2.20	0.41
1:D:537:PHE:O	1:D:538:GLU:HG3	2.21	0.41
1:A:509:ILE:HG22	1:A:537:PHE:CE1	2.56	0.41
1:C:419:THR:CG2	1:C:421:ASP:HB2	2.51	0.41
1:C:475:ILE:HD12	1:C:475:ILE:C	2.41	0.41
1:A:144:LYS:O	1:A:148:MET:HG3	2.21	0.41
1:A:271:VAL:HA	1:A:276:ARG:O	2.21	0.41
1:A:426:LEU:HD21	1:B:412:THR:HG23	2.02	0.41
1:C:5:VAL:HG12	1:C:113:VAL:CG2	2.51	0.41
1:C:525:SER:HB3	1:C:542:ILE:CG2	2.44	0.41
1:D:298:LYS:HG2	1:D:299:LYS:N	2.35	0.41
1:B:35:LYS:HE2	1:B:83:GLU:OE2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ASP:HA	1:B:59:ARG:CG	2.51	0.41
1:D:20:ARG:NE	1:D:20:ARG:CA	2.76	0.41
1:D:154:GLU:CA	1:D:177:MET:HG2	2.42	0.41
1:D:206:ARG:NH1	1:D:212:VAL:HG13	2.36	0.41
1:D:330:ILE:HA	1:D:330:ILE:HD13	1.72	0.41
1:D:406:ARG:HH11	1:D:439:ASP:CG	2.20	0.41
1:D:432:PRO:HG2	1:C:42:CYS:O	2.20	0.41
1:D:506:LEU:HD23	1:D:506:LEU:HA	1.84	0.41
1:D:506:LEU:O	1:D:508:GLU:N	2.53	0.41
1:A:81:LEU:HD12	1:A:81:LEU:N	2.36	0.41
1:A:125:ILE:HD13	1:A:125:ILE:HG21	1.88	0.41
1:A:232:ILE:C	1:A:234:ASN:H	2.24	0.41
1:A:294:LEU:HB2	1:A:330:ILE:HD11	2.02	0.41
1:A:345:ALA:CB	1:A:411:SER:HB3	2.51	0.41
1:A:477:ASP:OD1	1:A:477:ASP:C	2.58	0.41
1:B:59:ARG:HH22	1:B:68:ASP:HB3	1.86	0.41
1:B:264:GLY:HA3	1:B:290:GLU:OE2	2.20	0.41
1:B:456:PHE:CD1	1:B:542:ILE:CG2	3.04	0.41
1:C:43:GLY:O	1:C:46:TYR:N	2.54	0.41
1:C:52:VAL:HG13	1:C:57:ASN:HB2	2.02	0.41
1:D:194:ASP:OD1	1:D:348:ASN:OD1	2.38	0.41
1:A:21:ARG:NH2	3:A:902:COA:H52A	2.35	0.41
1:A:334:ILE:HB	1:B:429:ALA:HB1	2.03	0.41
1:B:19:ILE:HD11	1:B:319:ILE:HD12	2.02	0.41
1:B:89:ILE:HB	1:B:259:ALA:HB2	2.02	0.41
3:D:902:COA:O5B	1:C:523:LEU:HD21	2.21	0.40
1:B:30:VAL:CG1	1:B:80:VAL:HG22	2.51	0.40
1:B:474:VAL:HG21	1:B:510:PRO:CD	2.43	0.40
1:C:225:ASP:O	1:C:226:ASP:CB	2.69	0.40
1:C:317:GLU:HG2	1:C:324:ALA:HB2	2.03	0.40
1:C:392:VAL:HG23	1:C:414:ILE:CG1	2.52	0.40
1:D:228:VAL:O	1:D:229:ARG:CG	2.69	0.40
1:D:429:ALA:HB1	1:C:334:ILE:HB	2.03	0.40
1:D:534:HIS:ND1	1:C:24:GLY:C	2.74	0.40
1:B:1:MET:HE2	1:B:3:VAL:CG2	2.38	0.40
1:B:8:GLY:HA2	1:B:13:LEU:CD2	2.51	0.40
1:C:269:ILE:H	1:C:269:ILE:HG13	1.71	0.40
1:D:44:LEU:N	1:D:45:PRO:HD2	2.36	0.40
1:D:494:VAL:O	1:D:494:VAL:CG1	2.69	0.40
1:A:473:ILE:HG22	1:A:474:VAL:N	2.36	0.40
1:B:257:GLU:HB2	1:B:263:ILE:HG13	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:TYR:O	1:C:275:MET:CB	2.69	0.40
1:C:275:MET:CE	1:C:326:PHE:CB	2.93	0.40
1:C:508:GLU:C	1:C:509:ILE:O	2.58	0.40
1:C:510:PRO:O	1:C:511:ARG:CB	2.70	0.40
1:D:234:ASN:C	1:D:236:LYS:N	2.74	0.40
1:D:520:ALA:HA	1:D:547:MET:HB2	2.04	0.40
1:C:41:ARG:O	1:C:43:GLY:N	2.55	0.40
1:C:477:ASP:C	1:C:479:ARG:H	2.25	0.40
1:C:479:ARG:HB3	1:C:480:SER:H	1.70	0.40
1:A:147:GLU:O	1:A:151:GLU:HG3	2.21	0.40
1:B:225:ASP:C	1:B:226:ASP:OD1	2.60	0.40
1:B:266:THR:OG1	1:B:290:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

## 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	535/551 (97%)	506 (95%)	24 (4%)	5 (1%)	17	52
1	B	533/551 (97%)	494 (93%)	36 (7%)	3 (1%)	25	59
1	C	525/551 (95%)	476 (91%)	36 (7%)	13 (2%)	5	27
1	D	526/551 (96%)	492 (94%)	26 (5%)	8 (2%)	10	39
All	All	2119/2204 (96%)	1968 (93%)	122 (6%)	29 (1%)	11	40

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	228	VAL
1	D	489	ILE
1	D	492	GLU

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Mol	Chain	Res	Type
1	A	227	LYS
1	A	233	ALA
1	B	464	LEU
1	C	229	ARG
1	C	479	ARG
1	C	480	SER
1	C	505	ARG
1	C	510	PRO
1	D	229	ARG
1	A	194	ASP
1	A	228	VAL
1	C	196	GLU
1	C	226	ASP
1	C	228	VAL
1	C	463	GLU
1	D	538	GLU
1	B	465	LYS
1	C	42	CYS
1	D	490	GLU
1	D	508	GLU
1	B	228	VAL
1	C	338	PHE
1	C	453	ASP
1	D	461	VAL
1	A	337	VAL
1	C	124	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	423/446 (95%)	414 (98%)	9 (2%)	53	79
1	B	428/446 (96%)	410 (96%)	18 (4%)	30	62
1	C	415/446 (93%)	397 (96%)	18 (4%)	29	62
1	D	420/446 (94%)	408 (97%)	12 (3%)	42	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1686/1784 (94%)	1629 (97%)	57 (3%)	37 69

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	56	ASP
1	D	122	LYS
1	D	229	ARG
1	D	323	ARG
1	D	340	PHE
1	D	380	ARG
1	D	460	ASN
1	D	492	GLU
1	D	513	LYS
1	D	519	CYS
1	D	527	GLU
1	D	538	GLU
1	A	63	TYR
1	A	122	LYS
1	A	187	ARG
1	A	215	SER
1	A	224	GLN
1	A	228	VAL
1	A	369	ARG
1	A	464	LEU
1	A	519	CYS
1	B	27	SER
1	B	54	GLU
1	B	63	TYR
1	B	147	GLU
1	B	187	ARG
1	B	193	LEU
1	B	217	ARG
1	B	226	ASP
1	B	228	VAL
1	B	229	ARG
1	B	336	LYS
1	B	380	ARG
1	B	386	GLU
1	B	430	TYR
1	B	435	SER
1	B	511	ARG

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Mol	Chain	Res	Type
1	B	512	ASP
1	B	519	CYS
1	C	41	ARG
1	C	56	ASP
1	C	59	ARG
1	C	110	ASP
1	C	155	LYS
1	C	187	ARG
1	C	196	GLU
1	C	200	LEU
1	C	227	LYS
1	C	228	VAL
1	C	239	PRO
1	C	277	THR
1	C	287	ASP
1	C	406	ARG
1	C	426	LEU
1	C	479	ARG
1	C	481	GLU
1	C	496	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	57	ASN
1	D	101	ASN
1	D	309	ASN
1	D	396	GLN
1	D	422	GLN
1	D	496	HIS
1	A	57	ASN
1	A	375	GLN
1	A	422	GLN
1	A	496	HIS
1	B	204	HIS
1	C	350	GLN
1	C	425	ASN
1	C	534	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	COA	B	902	-	41,50,50	2.37	8 (19%)	52,75,75	1.87	13 (25%)
2	FAD	B	901	-	51,58,58	1.95	15 (29%)	60,89,89	1.98	17 (28%)
2	FAD	D	901	-	51,58,58	1.81	13 (25%)	60,89,89	1.92	15 (25%)
2	FAD	C	901	-	51,58,58	1.85	14 (27%)	60,89,89	1.93	18 (30%)
2	FAD	A	901	-	51,58,58	1.90	13 (25%)	60,89,89	2.06	20 (33%)
3	COA	D	902	-	41,50,50	2.26	8 (19%)	52,75,75	1.79	12 (23%)
3	COA	A	902	-	41,50,50	2.34	10 (24%)	52,75,75	2.14	14 (26%)
3	COA	C	902	-	41,50,50	2.30	10 (24%)	52,75,75	2.22	19 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COA	B	902	-	-	11/44/64/64	0/3/3/3
2	FAD	B	901	-	-	4/30/50/50	0/6/6/6
2	FAD	D	901	-	-	5/30/50/50	0/6/6/6
2	FAD	C	901	-	-	10/30/50/50	0/6/6/6
2	FAD	A	901	-	-	10/30/50/50	0/6/6/6
3	COA	D	902	-	-	6/44/64/64	0/3/3/3
3	COA	A	902	-	-	17/44/64/64	0/3/3/3
3	COA	C	902	-	-	12/44/64/64	0/3/3/3

All (91) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	902	COA	O4B-C1B	8.48	1.52	1.41
3	D	902	COA	O4B-C1B	7.12	1.51	1.41
3	C	902	COA	O4B-C1B	7.04	1.50	1.41
2	B	901	FAD	C4X-C10	6.81	1.45	1.38
3	B	902	COA	O4B-C1B	6.80	1.50	1.41
2	D	901	FAD	C4X-C10	6.45	1.45	1.38
2	A	901	FAD	C4X-C10	6.44	1.45	1.38
3	B	902	COA	C9P-N8P	6.27	1.47	1.33
3	C	902	COA	C9P-N8P	6.17	1.47	1.33
2	C	901	FAD	C4X-C10	5.94	1.44	1.38
3	B	902	COA	C5P-N4P	5.93	1.46	1.33
3	A	902	COA	C9P-N8P	5.82	1.46	1.33
3	D	902	COA	C5P-N4P	5.75	1.46	1.33
3	D	902	COA	C9P-N8P	5.53	1.45	1.33
3	C	902	COA	C5P-N4P	5.12	1.45	1.33
3	A	902	COA	C5P-N4P	4.79	1.44	1.33
3	B	902	COA	C2B-C1B	-4.16	1.47	1.53
2	C	901	FAD	C2-N3	-4.16	1.29	1.38
2	B	901	FAD	C2B-C1B	-4.00	1.47	1.53
3	C	902	COA	C2B-C3B	-3.94	1.44	1.52
2	A	901	FAD	C2-N3	-3.88	1.30	1.38
2	D	901	FAD	C2-N3	-3.82	1.30	1.38
2	A	901	FAD	C6-C5X	-3.69	1.36	1.41
3	D	902	COA	C2B-C3B	-3.62	1.44	1.52
3	B	902	COA	C6A-N6A	3.52	1.46	1.34
3	B	902	COA	C2B-C3B	-3.49	1.45	1.52
2	B	901	FAD	C6-C5X	-3.48	1.36	1.41
2	C	901	FAD	C6-C5X	-3.47	1.36	1.41
2	C	901	FAD	C2B-C1B	-3.39	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	901	FAD	C6-C5X	-3.21	1.36	1.41
3	A	902	COA	C2B-C3B	-3.19	1.45	1.52
3	C	902	COA	C6A-N6A	3.17	1.45	1.34
3	D	902	COA	C2B-C1B	-3.16	1.49	1.53
3	B	902	COA	C4A-N3A	-3.14	1.31	1.35
3	A	902	COA	C6A-N6A	3.13	1.45	1.34
2	B	901	FAD	C1'-N10	-3.10	1.45	1.48
2	B	901	FAD	C2-N3	-3.09	1.32	1.38
3	C	902	COA	C2B-C1B	-3.08	1.49	1.53
2	A	901	FAD	C2B-C1B	-3.05	1.49	1.53
3	D	902	COA	C6A-N6A	3.01	1.45	1.34
2	D	901	FAD	C1'-N10	-2.98	1.45	1.48
2	A	901	FAD	C4'-C3'	-2.97	1.47	1.53
3	A	902	COA	O4B-C4B	2.89	1.51	1.45
2	D	901	FAD	C2B-C1B	-2.85	1.49	1.53
2	C	901	FAD	C2-N1	-2.80	1.32	1.38
3	D	902	COA	O4B-C4B	2.67	1.51	1.45
2	B	901	FAD	C4-C4X	2.65	1.45	1.41
2	D	901	FAD	C2-N1	-2.65	1.32	1.38
3	C	902	COA	P3B-O9A	-2.61	1.44	1.54
2	B	901	FAD	C2-N1	-2.60	1.33	1.38
2	A	901	FAD	C2-N1	-2.59	1.33	1.38
2	C	901	FAD	C4-C4X	2.56	1.45	1.41
3	C	902	COA	O4B-C4B	2.53	1.50	1.45
2	D	901	FAD	O4B-C4B	-2.46	1.39	1.45
2	B	901	FAD	P-O2P	-2.43	1.43	1.55
2	A	901	FAD	C2'-C3'	-2.39	1.49	1.53
2	A	901	FAD	P-O2P	-2.38	1.44	1.55
2	B	901	FAD	P-O1P	-2.38	1.42	1.50
3	A	902	COA	C5A-N7A	2.37	1.48	1.39
2	B	901	FAD	C4'-C3'	-2.34	1.49	1.53
2	C	901	FAD	C1'-N10	-2.33	1.45	1.48
2	C	901	FAD	O4B-C4B	-2.31	1.39	1.45
2	C	901	FAD	PA-O2A	-2.30	1.44	1.55
2	D	901	FAD	C2B-C3B	-2.29	1.47	1.53
3	B	902	COA	O4B-C4B	2.28	1.50	1.45
2	C	901	FAD	C9A-C5X	2.28	1.47	1.42
3	A	902	COA	P1A-O5B	2.27	1.68	1.59
3	C	902	COA	P3B-O3B	2.24	1.63	1.59
3	A	902	COA	C5A-C4A	2.19	1.46	1.40
3	D	902	COA	C2A-N3A	2.19	1.35	1.32
2	B	901	FAD	C2B-C3B	-2.19	1.47	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	FAD	C9A-C5X	2.17	1.46	1.42
2	B	901	FAD	C4A-N3A	-2.16	1.32	1.35
2	A	901	FAD	PA-O2A	-2.12	1.45	1.55
2	D	901	FAD	PA-O2A	-2.10	1.45	1.55
3	A	902	COA	C2B-C1B	-2.10	1.50	1.53
2	D	901	FAD	C5A-N7A	-2.09	1.32	1.39
2	C	901	FAD	C5A-N7A	-2.08	1.32	1.39
2	A	901	FAD	P-O1P	-2.07	1.43	1.50
2	B	901	FAD	O4B-C4B	-2.07	1.40	1.45
2	A	901	FAD	C5A-N7A	-2.06	1.32	1.39
2	D	901	FAD	C4-C4X	2.06	1.44	1.41
2	D	901	FAD	P-O2P	-2.06	1.45	1.55
2	C	901	FAD	P-O2P	-2.05	1.45	1.55
2	C	901	FAD	C2B-C3B	-2.05	1.47	1.53
2	B	901	FAD	PA-O2A	-2.05	1.45	1.55
2	B	901	FAD	C5A-N7A	-2.05	1.32	1.39
3	C	902	COA	P3B-O8A	-2.02	1.47	1.54
2	A	901	FAD	C4-C4X	2.02	1.44	1.41
2	D	901	FAD	C9A-C5X	2.01	1.46	1.42
2	C	901	FAD	C8-C7	2.01	1.45	1.40

All (128) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	901	FAD	C4-N3-C2	8.19	122.06	115.14
3	A	902	COA	C2P-C3P-N4P	-7.48	95.22	112.31
2	D	901	FAD	C4-N3-C2	7.02	121.06	115.14
2	A	901	FAD	C4-N3-C2	6.13	120.32	115.14
2	C	901	FAD	C4-N3-C2	5.67	119.93	115.14
3	C	902	COA	CEP-CBP-CCP	-5.52	99.22	108.23
3	A	902	COA	CEP-CBP-CAP	5.29	117.99	108.82
2	A	901	FAD	C4'-C3'-C2'	-5.19	102.56	113.36
3	D	902	COA	C6P-C7P-N8P	-4.94	101.93	111.90
3	A	902	COA	O4B-C1B-C2B	-4.66	100.12	106.93
2	A	901	FAD	C1'-N10-C10	4.62	122.54	118.41
2	D	901	FAD	C4X-N5-C5X	4.51	121.28	116.77
3	C	902	COA	O6A-CCP-CBP	-4.36	103.53	110.55
3	A	902	COA	C6P-C7P-N8P	-4.31	103.20	111.90
2	D	901	FAD	C4-C4X-C10	-4.19	117.17	119.95
3	B	902	COA	C5B-C4B-C3B	-4.17	100.58	114.40
2	A	901	FAD	N3A-C2A-N1A	-4.12	122.25	128.68
3	B	902	COA	CEP-CBP-CAP	4.08	115.90	108.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	902	COA	N3A-C2A-N1A	-4.08	122.31	128.68
3	C	902	COA	CDP-CBP-CCP	-3.98	101.74	108.23
2	D	901	FAD	O3B-C3B-C2B	-3.98	98.96	111.82
2	C	901	FAD	C9A-N10-C10	-3.96	116.72	121.91
2	A	901	FAD	C9A-N10-C10	-3.92	116.77	121.91
2	C	901	FAD	C1'-N10-C10	3.91	121.91	118.41
2	B	901	FAD	C4X-C4-N3	-3.89	118.12	123.43
2	B	901	FAD	C1'-N10-C9A	3.88	121.34	118.29
2	B	901	FAD	C4-C4X-C10	-3.85	117.40	119.95
3	A	902	COA	N3A-C2A-N1A	-3.84	122.68	128.68
2	C	901	FAD	N3A-C2A-N1A	-3.82	122.70	128.68
3	C	902	COA	C2P-C3P-N4P	-3.78	103.68	112.31
3	B	902	COA	C7P-C6P-C5P	-3.77	106.07	112.36
3	C	902	COA	C6P-C7P-N8P	-3.77	104.29	111.90
2	B	901	FAD	C4X-N5-C5X	3.72	120.49	116.77
2	C	901	FAD	O3B-C3B-C2B	-3.68	99.91	111.82
3	D	902	COA	N3A-C2A-N1A	-3.68	122.93	128.68
3	B	902	COA	C3P-N4P-C5P	-3.65	116.05	122.84
2	D	901	FAD	N3A-C2A-N1A	-3.64	122.99	128.68
2	C	901	FAD	C1'-N10-C9A	3.61	121.14	118.29
2	A	901	FAD	O3B-C3B-C2B	-3.60	100.18	111.82
2	D	901	FAD	O2B-C2B-C3B	-3.57	100.27	111.82
3	D	902	COA	C5B-C4B-C3B	-3.56	102.60	114.40
3	C	902	COA	O9P-C9P-N8P	-3.56	115.36	122.99
3	B	902	COA	P2A-O3A-P1A	-3.52	120.74	132.83
2	B	901	FAD	N3A-C2A-N1A	-3.39	123.38	128.68
2	C	901	FAD	O2B-C2B-C3B	-3.38	100.88	111.82
2	A	901	FAD	C4A-C5A-N7A	-3.38	105.88	109.40
2	C	901	FAD	C4-C4X-C10	-3.35	117.73	119.95
2	A	901	FAD	C4X-C4-N3	-3.33	118.87	123.43
3	C	902	COA	CEP-CBP-CDP	3.27	115.82	109.17
3	D	902	COA	C7P-C6P-C5P	-3.22	107.00	112.36
2	C	901	FAD	C4'-C3'-C2'	-3.14	106.82	113.36
2	C	901	FAD	C4X-C4-N3	-3.12	119.16	123.43
3	C	902	COA	CAP-C9P-N8P	3.11	122.76	116.58
2	C	901	FAD	C4X-N5-C5X	3.10	119.86	116.77
3	C	902	COA	O3B-C3B-C2B	-3.05	100.63	111.68
3	C	902	COA	P2A-O3A-P1A	-3.00	122.54	132.83
2	B	901	FAD	O3B-C3B-C2B	-2.99	102.16	111.82
3	B	902	COA	C6P-C5P-N4P	2.95	121.40	116.42
3	D	902	COA	P2A-O3A-P1A	-2.95	122.69	132.83
3	B	902	COA	N3A-C2A-N1A	-2.90	124.14	128.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	902	COA	C7P-N8P-C9P	-2.90	117.42	122.59
2	D	901	FAD	C1'-N10-C9A	2.87	120.55	118.29
2	A	901	FAD	O2'-C2'-C3'	-2.86	102.13	109.10
2	B	901	FAD	C4-C4X-N5	2.86	121.86	118.60
2	A	901	FAD	C1'-N10-C9A	2.84	120.53	118.29
2	D	901	FAD	C4-C4X-N5	2.83	121.83	118.60
2	D	901	FAD	C4X-C4-N3	-2.83	119.56	123.43
2	B	901	FAD	C9A-N10-C10	-2.83	118.21	121.91
3	B	902	COA	O4B-C1B-C2B	-2.83	102.80	106.93
3	C	902	COA	CDP-CBP-CAP	2.74	113.57	108.82
3	D	902	COA	C5A-C6A-N6A	-2.72	116.22	120.35
3	A	902	COA	CAP-C9P-N8P	2.71	121.97	116.58
2	B	901	FAD	O2B-C2B-C3B	-2.69	103.11	111.82
3	A	902	COA	O9P-C9P-N8P	-2.67	117.27	122.99
2	B	901	FAD	O4B-C1B-C2B	-2.64	103.08	106.93
3	A	902	COA	C7P-C6P-C5P	-2.63	107.98	112.36
2	A	901	FAD	C4-C4X-C10	-2.62	118.21	119.95
3	D	902	COA	N6A-C6A-N1A	2.56	123.89	118.57
3	C	902	COA	O5B-C5B-C4B	2.56	117.79	108.99
2	A	901	FAD	O2A-PA-O1A	2.54	124.80	112.24
3	A	902	COA	C1B-N9A-C4A	-2.54	122.18	126.64
2	A	901	FAD	O2B-C2B-C3B	-2.53	103.64	111.82
3	D	902	COA	O4B-C1B-C2B	-2.53	103.23	106.93
3	D	902	COA	C2P-C3P-N4P	-2.51	106.58	112.31
2	C	901	FAD	C4A-C5A-N7A	-2.50	106.80	109.40
3	C	902	COA	O2B-C2B-C3B	-2.47	104.14	111.17
2	C	901	FAD	C2A-N1A-C6A	2.46	122.96	118.75
2	C	901	FAD	P-O3P-PA	-2.45	124.43	132.83
2	A	901	FAD	C4X-N5-C5X	2.44	119.21	116.77
2	A	901	FAD	C5X-C9A-N10	2.41	119.46	117.72
2	A	901	FAD	C2A-N1A-C6A	2.40	122.85	118.75
3	C	902	COA	C5B-C4B-C3B	-2.39	106.46	114.40
3	A	902	COA	O5B-C5B-C4B	2.37	117.14	108.99
2	D	901	FAD	C4A-C5A-N7A	-2.36	106.94	109.40
3	A	902	COA	CDP-CBP-CCP	2.33	112.04	108.23
2	C	901	FAD	O2'-C2'-C3'	-2.33	103.44	109.10
2	D	901	FAD	C1'-N10-C10	2.32	120.49	118.41
3	C	902	COA	O8A-P3B-O3B	2.32	116.37	105.99
2	C	901	FAD	C5X-C9A-N10	2.32	119.39	117.72
2	C	901	FAD	C2B-C3B-C4B	2.31	107.13	102.64
2	B	901	FAD	C4A-C5A-N7A	-2.30	107.00	109.40
2	A	901	FAD	O4B-C1B-C2B	-2.30	103.57	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	901	FAD	C9A-N10-C10	-2.29	118.90	121.91
2	D	901	FAD	C4'-C3'-C2'	-2.29	108.61	113.36
2	B	901	FAD	C5X-C9A-N10	2.27	119.36	117.72
3	B	902	COA	C2A-N1A-C6A	2.26	122.62	118.75
2	D	901	FAD	P-O3P-PA	-2.25	125.09	132.83
2	A	901	FAD	C2B-C3B-C4B	2.24	106.99	102.64
3	B	902	COA	O9A-P3B-O7A	-2.23	101.95	110.68
3	D	902	COA	O8A-P3B-O7A	-2.23	101.96	110.68
3	D	902	COA	P1A-O5B-C5B	-2.22	108.66	121.68
3	B	902	COA	CAP-C9P-N8P	2.22	121.00	116.58
2	A	901	FAD	O4'-C4'-C3'	-2.21	103.73	109.10
3	B	902	COA	O5P-C5P-C6P	-2.20	118.00	122.02
3	C	902	COA	O2A-P1A-O1A	-2.19	101.42	112.24
3	A	902	COA	C5B-C4B-C3B	-2.19	107.15	114.40
2	B	901	FAD	O4'-C4'-C3'	-2.18	103.80	109.10
2	D	901	FAD	C2B-C3B-C4B	2.17	106.86	102.64
2	B	901	FAD	C1'-N10-C10	2.16	120.35	118.41
2	C	901	FAD	C5B-C4B-C3B	-2.15	107.14	115.18
3	C	902	COA	C2B-C3B-C4B	2.14	107.02	103.22
2	B	901	FAD	O2'-C2'-C3'	-2.13	103.91	109.10
3	A	902	COA	O2B-C2B-C1B	2.11	118.63	110.85
3	C	902	COA	O5A-P2A-O4A	-2.09	101.92	112.24
3	A	902	COA	O5A-P2A-O4A	-2.08	101.93	112.24
3	B	902	COA	O5A-P2A-O4A	-2.06	102.05	112.24
2	A	901	FAD	C6-C5X-N5	-2.04	116.80	119.05
2	B	901	FAD	C4'-C3'-C2'	-2.00	109.19	113.36

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	901	FAD	C5B-O5B-PA-O1A
2	D	901	FAD	C3B-C4B-C5B-O5B
2	A	901	FAD	C5B-O5B-PA-O3P
2	A	901	FAD	C3'-C4'-C5'-O5'
2	A	901	FAD	O4'-C4'-C5'-O5'
2	A	901	FAD	C5'-O5'-P-O3P
2	A	901	FAD	PA-O3P-P-O5'
2	C	901	FAD	O4B-C4B-C5B-O5B
2	C	901	FAD	C3B-C4B-C5B-O5B
2	C	901	FAD	C3'-C4'-C5'-O5'
2	C	901	FAD	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	C	901	FAD	C5'-O5'-P-O1P
2	C	901	FAD	C5'-O5'-P-O2P
3	D	902	COA	P2A-O3A-P1A-O5B
3	D	902	COA	CCP-O6A-P2A-O4A
3	D	902	COA	S1P-C2P-C3P-N4P
3	A	902	COA	C3B-O3B-P3B-O7A
3	A	902	COA	C5B-O5B-P1A-O1A
3	A	902	COA	C5B-O5B-P1A-O2A
3	A	902	COA	C5B-O5B-P1A-O3A
3	A	902	COA	CAP-CBP-CCP-O6A
3	A	902	COA	OAP-CAP-CBP-CCP
3	A	902	COA	OAP-CAP-CBP-CEP
3	A	902	COA	N8P-C9P-CAP-OAP
3	B	902	COA	C3B-O3B-P3B-O7A
3	B	902	COA	N8P-C9P-CAP-OAP
3	C	902	COA	C3B-O3B-P3B-O9A
3	C	902	COA	C3B-C4B-C5B-O5B
3	C	902	COA	O4B-C4B-C5B-O5B
3	C	902	COA	C5B-O5B-P1A-O1A
3	C	902	COA	C9P-CAP-CBP-CEP
3	C	902	COA	S1P-C2P-C3P-N4P
2	D	901	FAD	O4B-C4B-C5B-O5B
3	A	902	COA	O4B-C4B-C5B-O5B
3	B	902	COA	C4B-C3B-O3B-P3B
3	C	902	COA	C4B-C3B-O3B-P3B
3	B	902	COA	C2B-C3B-O3B-P3B
3	C	902	COA	C2B-C3B-O3B-P3B
3	A	902	COA	C3B-C4B-C5B-O5B
3	A	902	COA	O9P-C9P-CAP-OAP
3	B	902	COA	O9P-C9P-CAP-OAP
3	A	902	COA	OAP-CAP-CBP-CDP
2	C	901	FAD	P-O3P-PA-O1A
2	C	901	FAD	PA-O3P-P-O5'
3	C	902	COA	P2A-O3A-P1A-O5B
2	D	901	FAD	C5B-O5B-PA-O3P
2	B	901	FAD	C5'-O5'-P-O3P
2	A	901	FAD	O4B-C4B-C5B-O5B
3	D	902	COA	P1A-O3A-P2A-O5A
2	D	901	FAD	C5B-O5B-PA-O2A
2	A	901	FAD	C5B-O5B-PA-O1A
2	A	901	FAD	C5B-O5B-PA-O2A
2	A	901	FAD	C5'-O5'-P-O1P

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Mol	Chain	Res	Type	Atoms
3	B	902	COA	C3B-C4B-C5B-O5B
3	A	902	COA	CDP-CBP-CCP-O6A
3	B	902	COA	CEP-CBP-CCP-O6A
3	C	902	COA	OAP-CAP-CBP-CEP
2	C	901	FAD	P-O3P-PA-O2A
3	A	902	COA	P1A-O3A-P2A-O5A
2	B	901	FAD	O4B-C4B-C5B-O5B
3	B	902	COA	CDP-CBP-CCP-O6A
2	A	901	FAD	PA-O3P-P-O1P
3	B	902	COA	P1A-O3A-P2A-O4A
2	B	901	FAD	C3B-C4B-C5B-O5B
3	A	902	COA	CEP-CBP-CCP-O6A
2	C	901	FAD	C5'-O5'-P-O3P
3	D	902	COA	CCP-O6A-P2A-O3A
3	D	902	COA	P1A-O3A-P2A-O4A
3	C	902	COA	P1A-O3A-P2A-O4A
3	C	902	COA	P1A-O3A-P2A-O5A
2	B	901	FAD	C5'-O5'-P-O1P
3	A	902	COA	CCP-O6A-P2A-O4A
3	B	902	COA	C5B-O5B-P1A-O1A
3	A	902	COA	O9P-C9P-CAP-CBP
3	B	902	COA	O9P-C9P-CAP-CBP

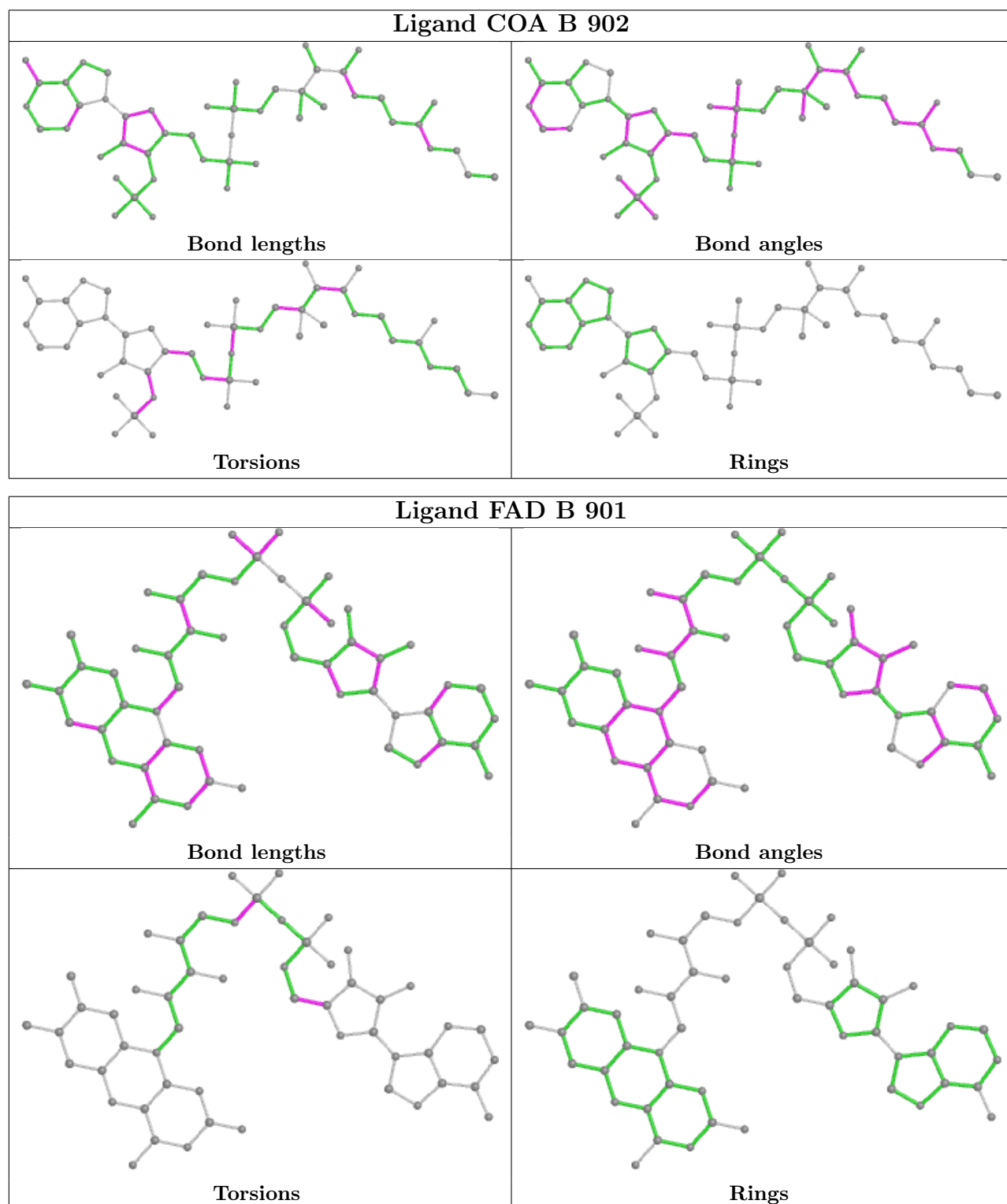
There are no ring outliers.

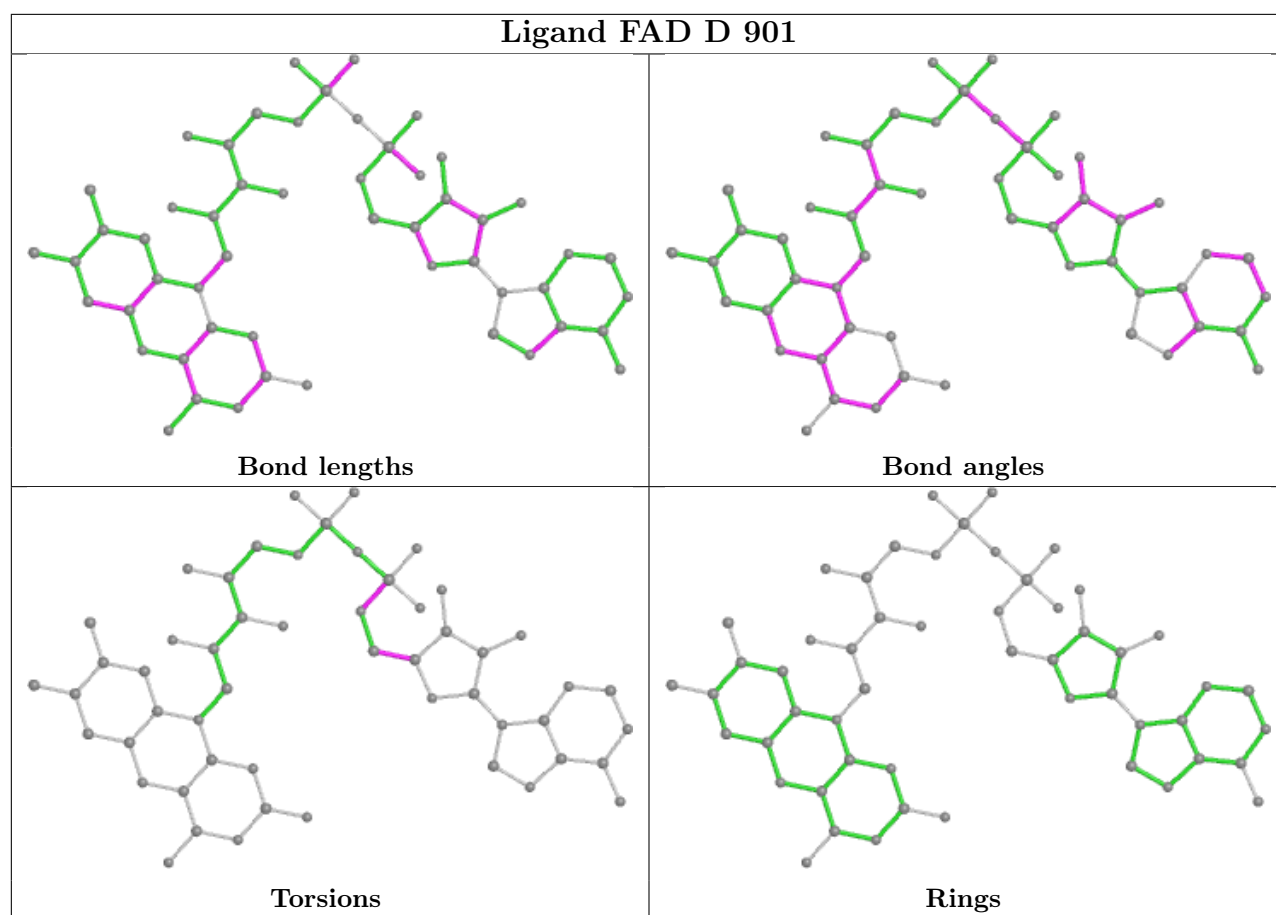
8 monomers are involved in 54 short contacts:

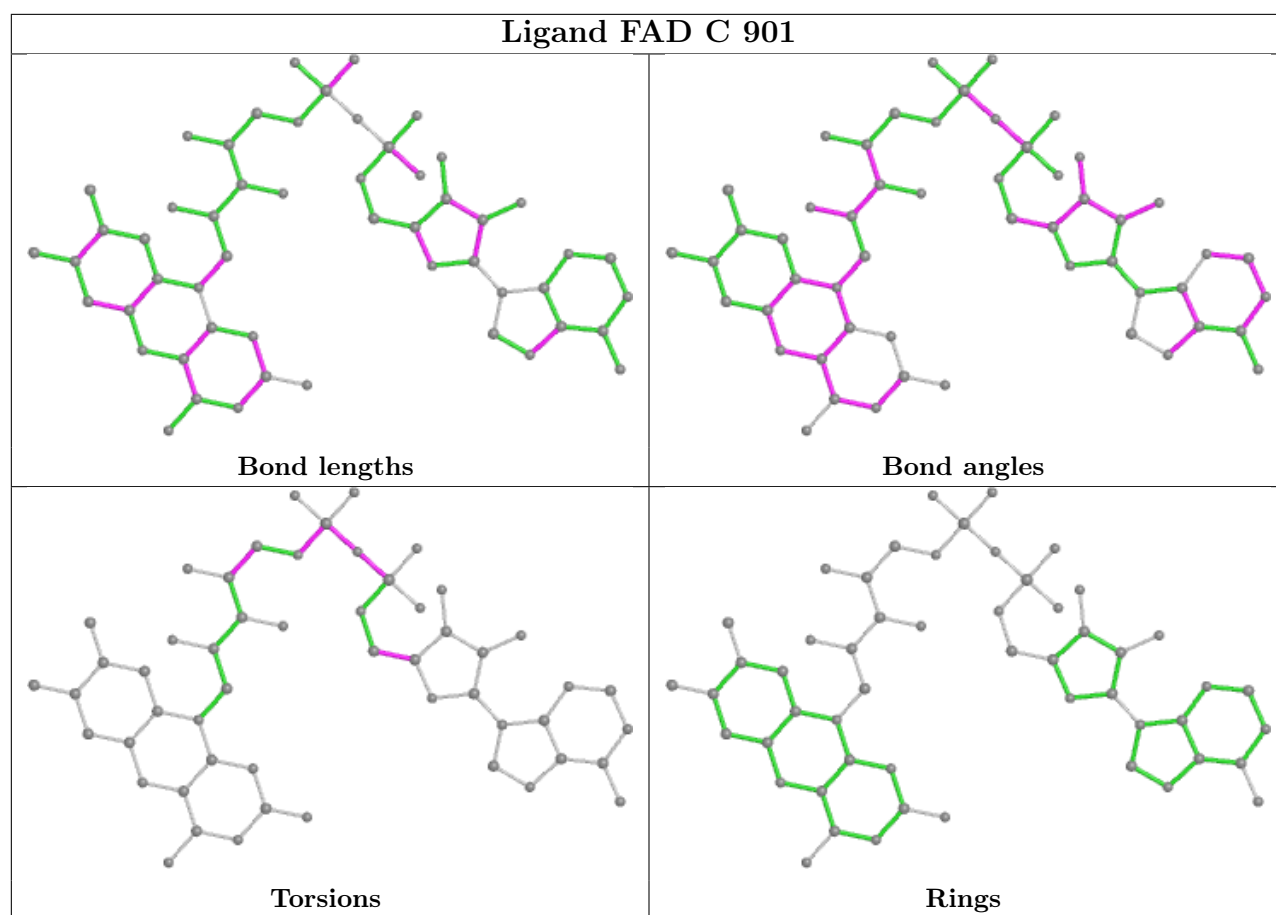
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	902	COA	8	0
2	B	901	FAD	3	0
2	D	901	FAD	4	0
2	C	901	FAD	7	0
2	A	901	FAD	3	0
3	D	902	COA	8	0
3	A	902	COA	9	0
3	C	902	COA	12	0

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

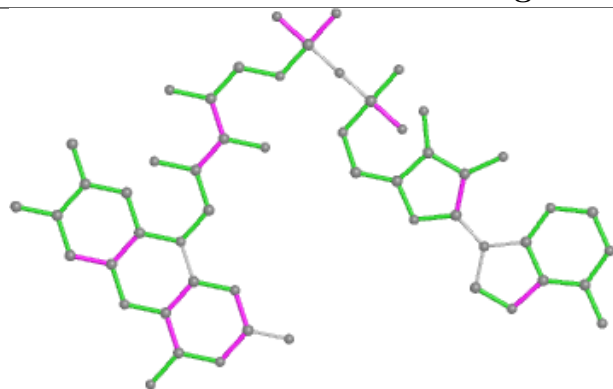
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



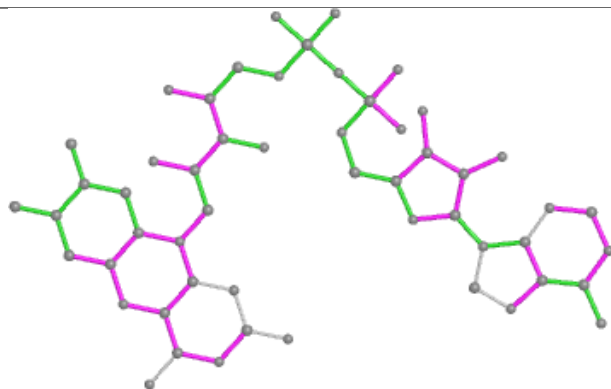




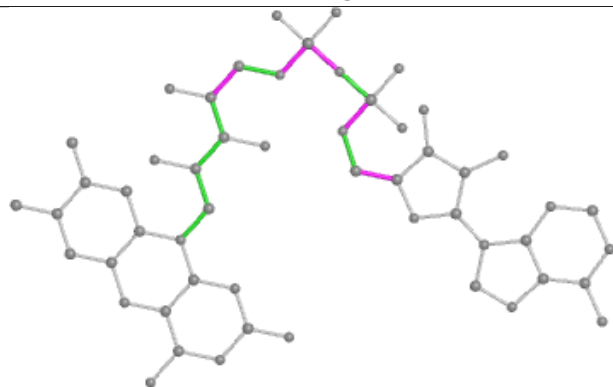
## Ligand FAD A 901



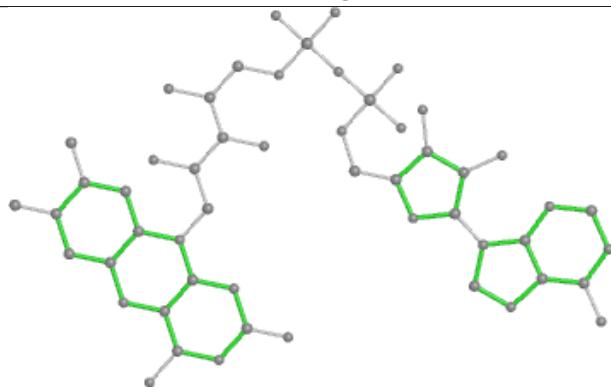
Bond lengths



Bond angles

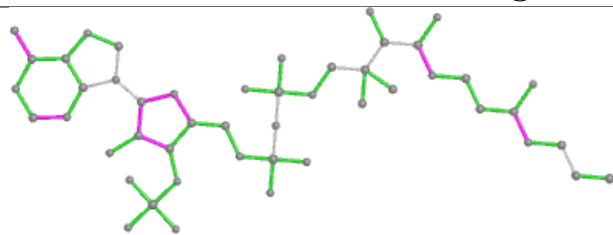


Torsions

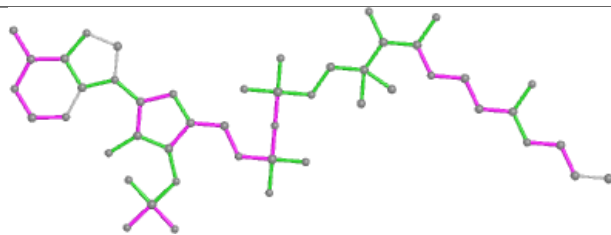


Rings

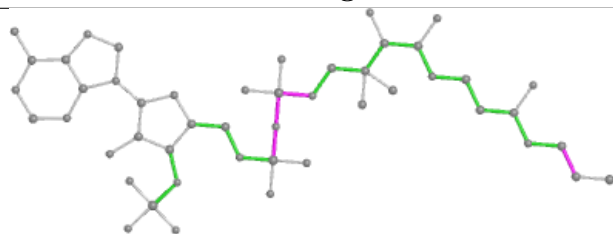
## Ligand COA D 902



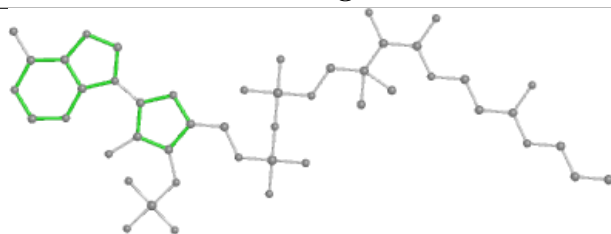
Bond lengths



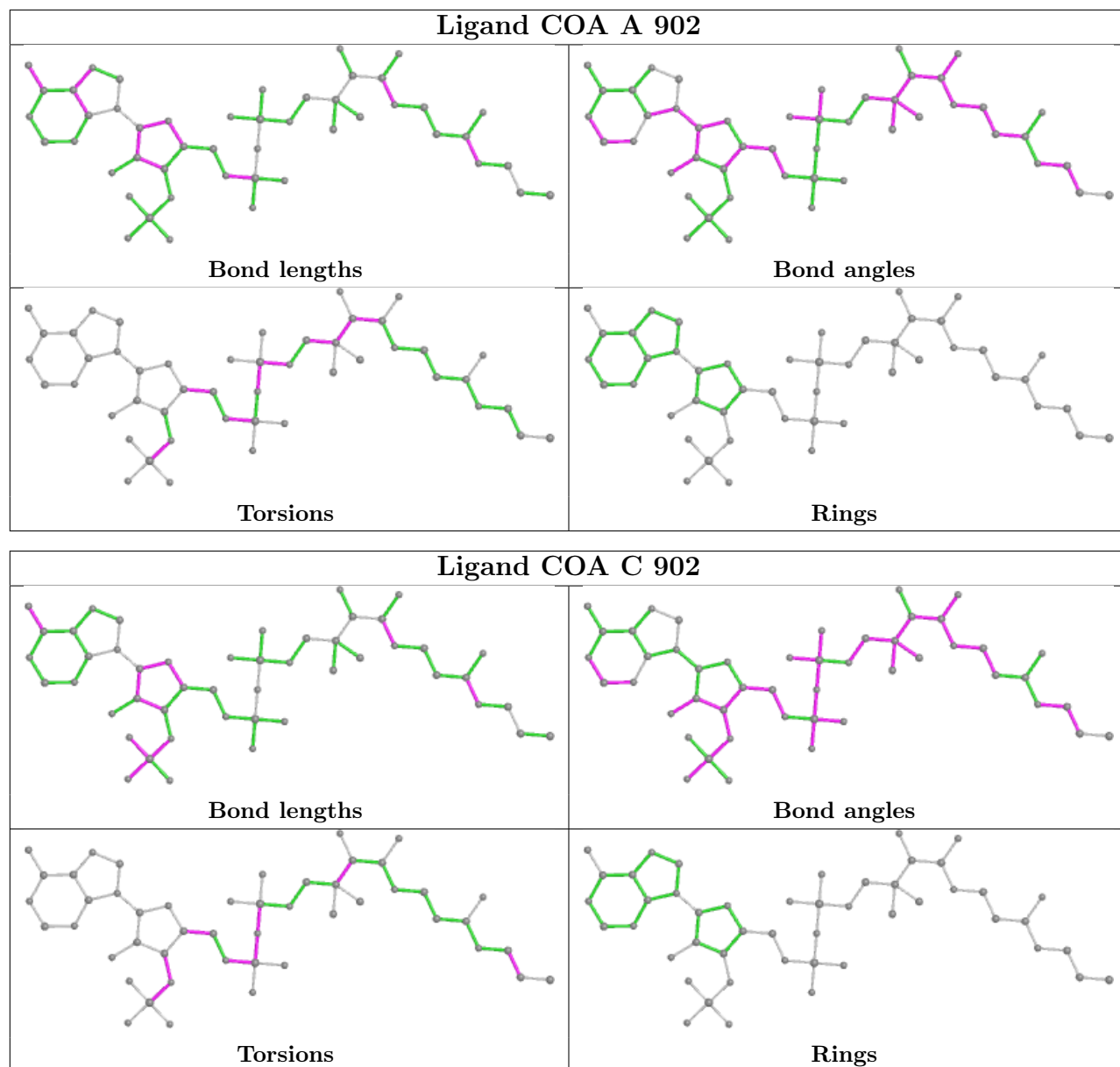
Bond angles



Torsions



Rings



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	541/551 (98%)	-0.49	0	100	100	26, 47, 71, 87	0
1	B	541/551 (98%)	-0.46	1 (0%)	95	90	23, 48, 72, 97	0
1	C	535/551 (97%)	-0.31	1 (0%)	95	90	39, 60, 84, 174	0
1	D	536/551 (97%)	-0.38	2 (0%)	92	84	33, 58, 83, 112	0
All	All	2153/2204 (97%)	-0.41	4 (0%)	95	90	23, 53, 79, 174	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	234	ASN	3.2
1	D	507	ASP	2.8
1	C	512	ASP	2.7
1	D	389	SER	2.0

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

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

### 6.3 Carbohydrates [i](#)

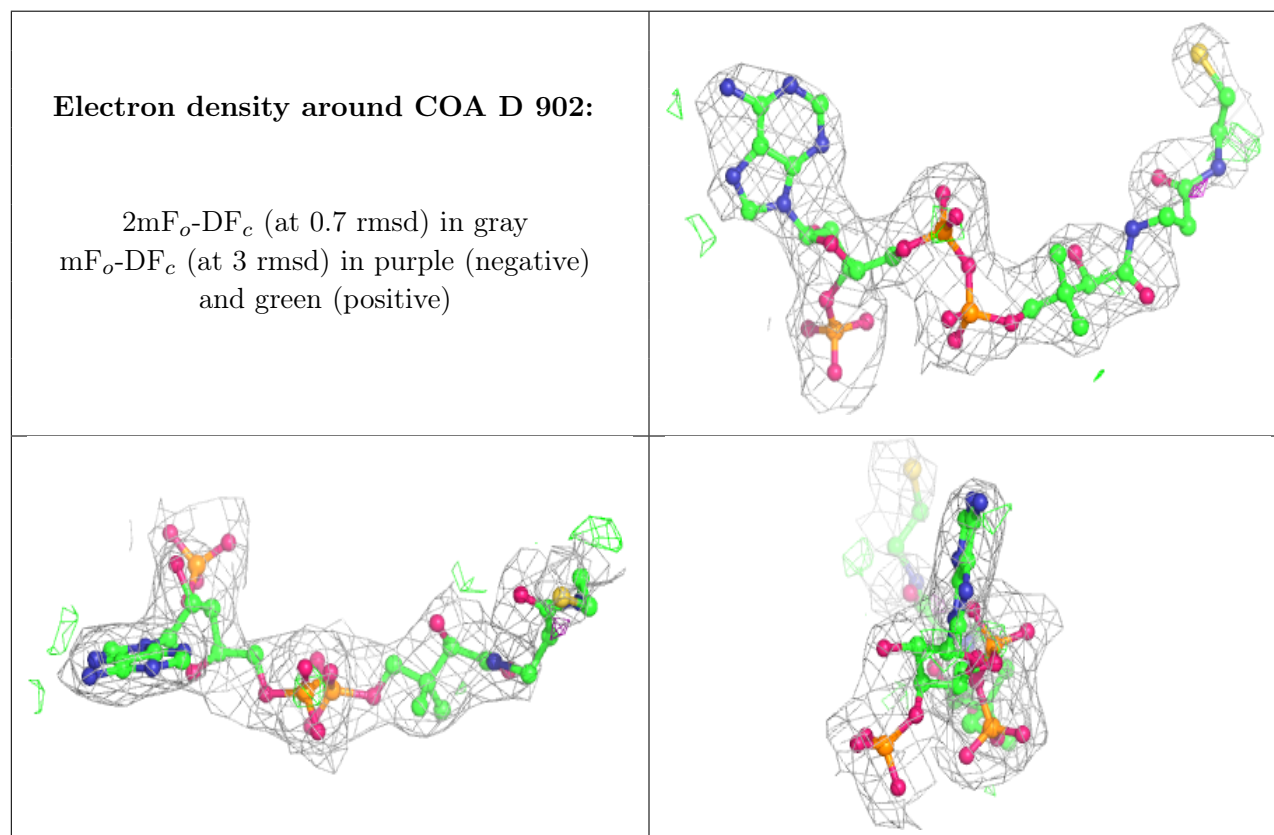
There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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

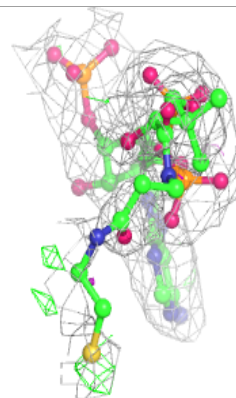
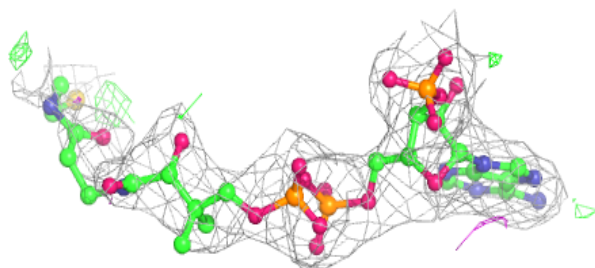
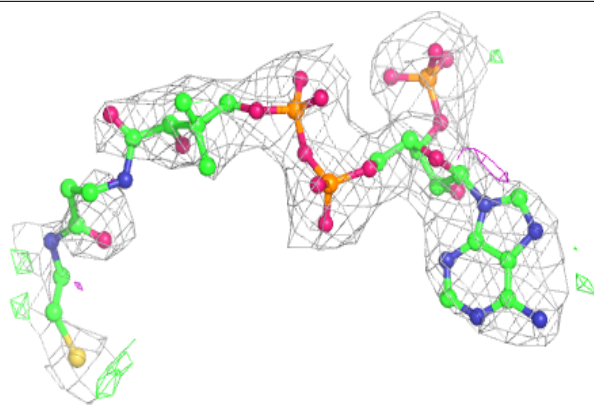
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	C	904	1/1	0.60	0.21	102,102,102,102	0
4	CA	A	903	1/1	0.78	0.48	122,122,122,122	0
4	CA	B	903	1/1	0.82	0.23	69,69,69,69	0
4	CA	C	903	1/1	0.90	0.10	62,62,62,62	0
3	COA	D	902	48/48	0.90	0.20	34,60,89,221	0
3	COA	B	902	48/48	0.93	0.22	37,62,88,91	0
3	COA	A	902	48/48	0.94	0.18	31,53,84,91	0
3	COA	C	902	48/48	0.94	0.23	41,79,121,123	0
2	FAD	B	901	53/53	0.96	0.18	39,64,80,101	0
2	FAD	C	901	53/53	0.96	0.14	27,45,61,74	0
2	FAD	D	901	53/53	0.97	0.13	28,47,63,67	0
2	FAD	A	901	53/53	0.97	0.15	29,45,56,68	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.

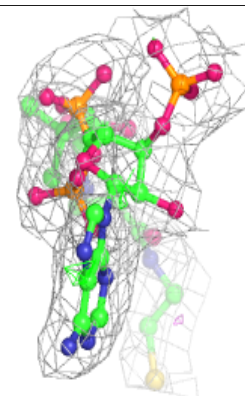
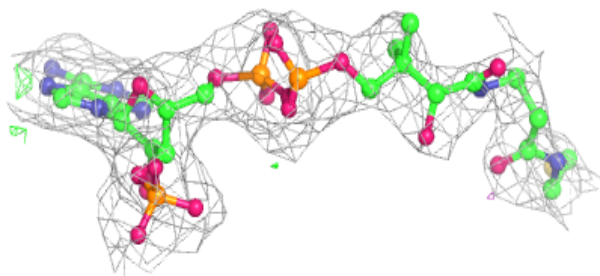
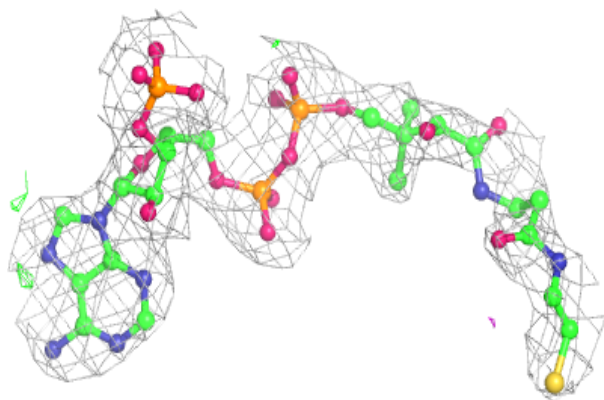


**Electron density around COA B 902:**

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

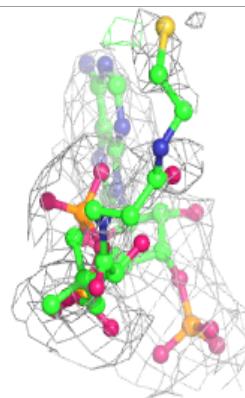
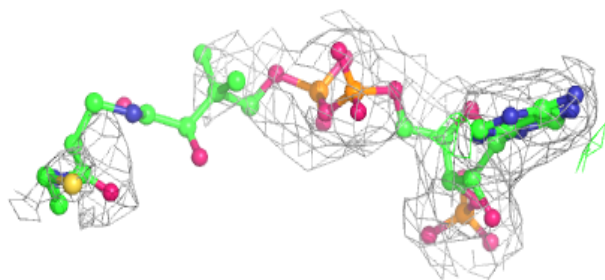
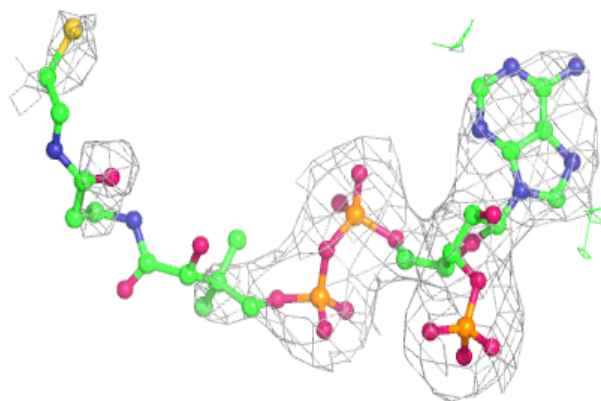
**Electron density around COA A 902:**

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

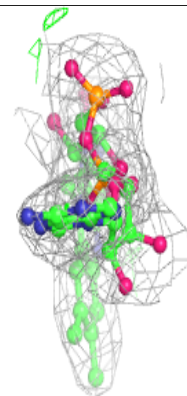
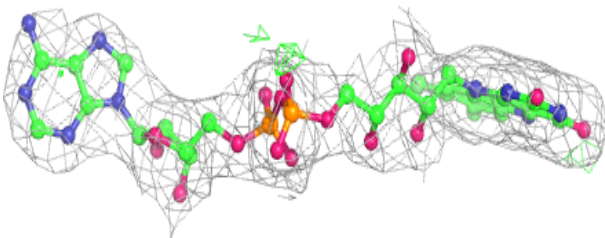
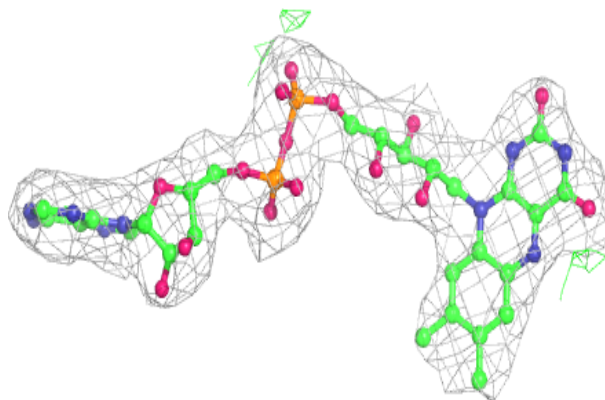


**Electron density around COA C 902:**

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

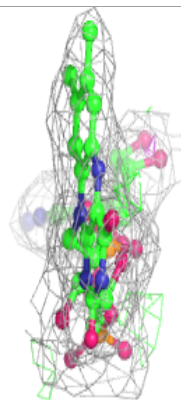
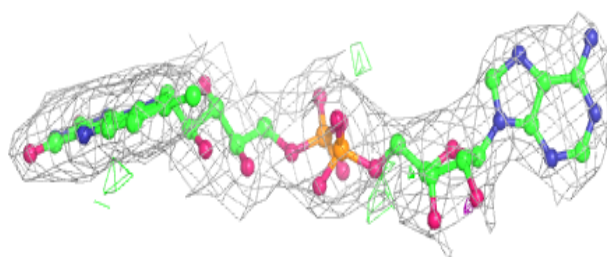
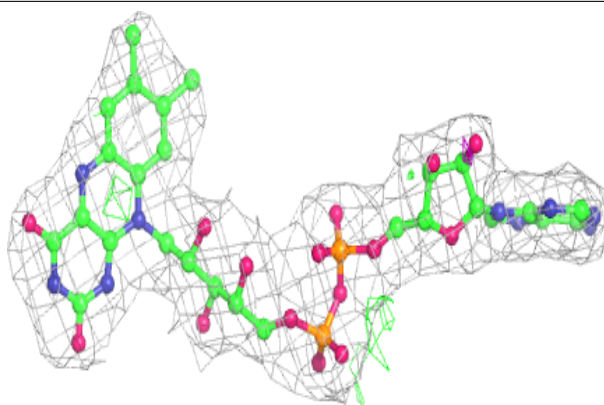
**Electron density around FAD B 901:**

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

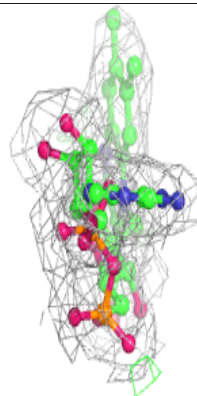
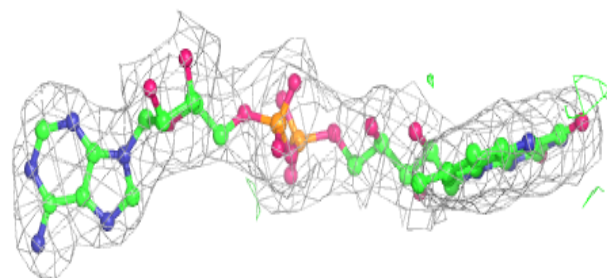
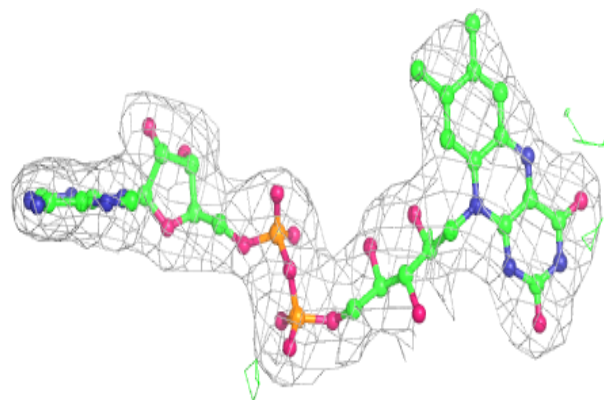


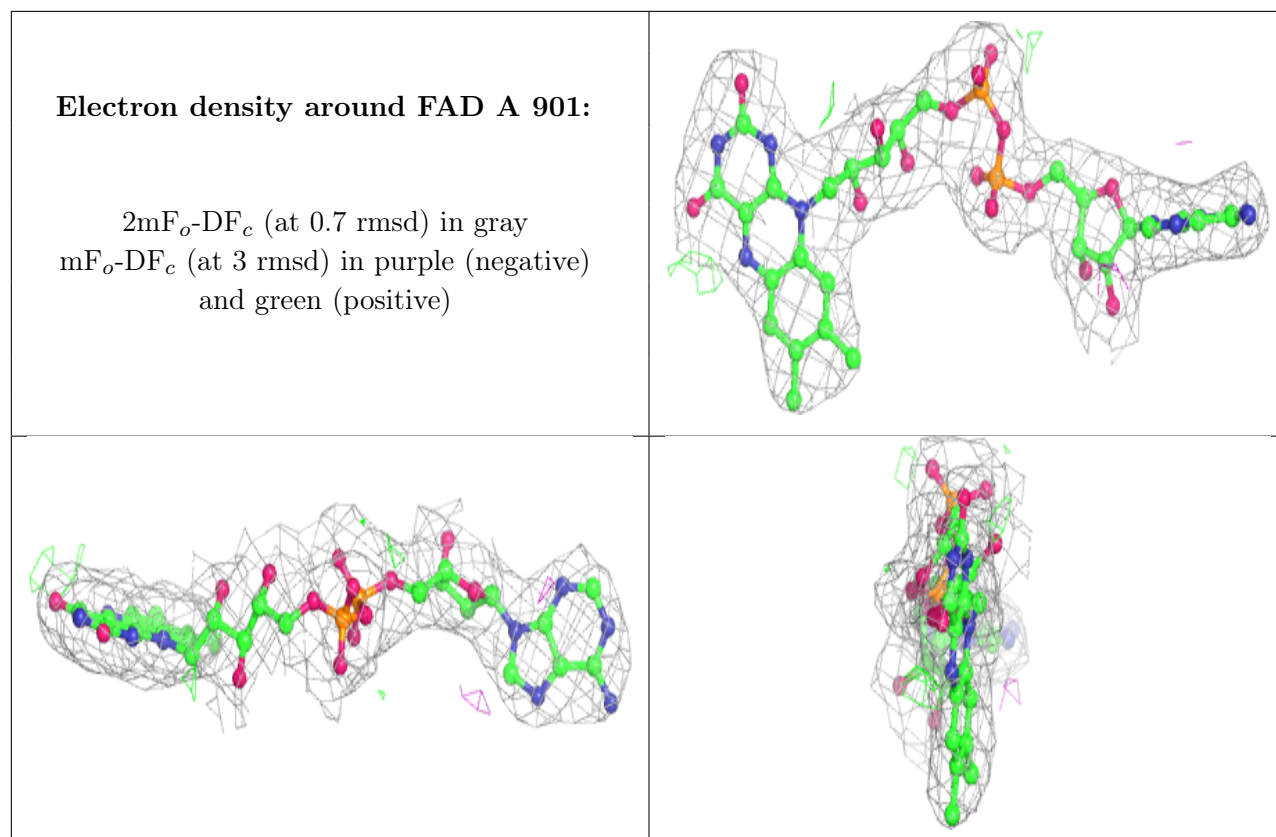
**Electron density around FAD C 901:**

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

**Electron density around FAD D 901:**

$2mF_o-DF_c$  (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.