



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:35 PM UTC

PDB ID : 1DZN / pdb_00001dzn
Title : Asp170Ser mutant of vanillyl-alcohol oxidase
Authors : Van Den heuvel, R.H.H.; Fraaije, M.W.; Van Berkel, W.J.H.; Mattevi, A.
Deposited on : 2000-03-05
Resolution : 2.80 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

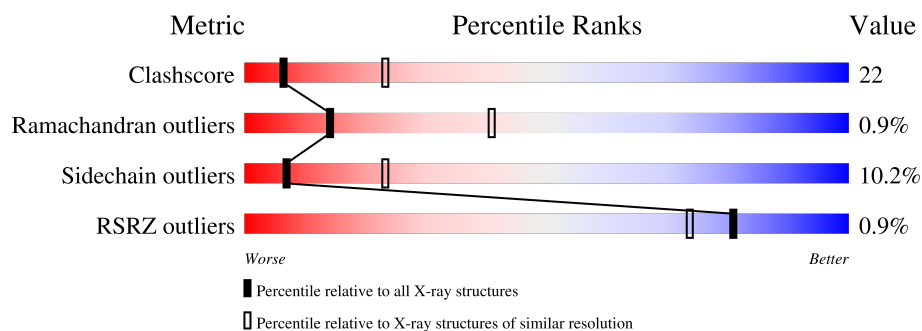
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	560	
1	B	560	

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 8821 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.

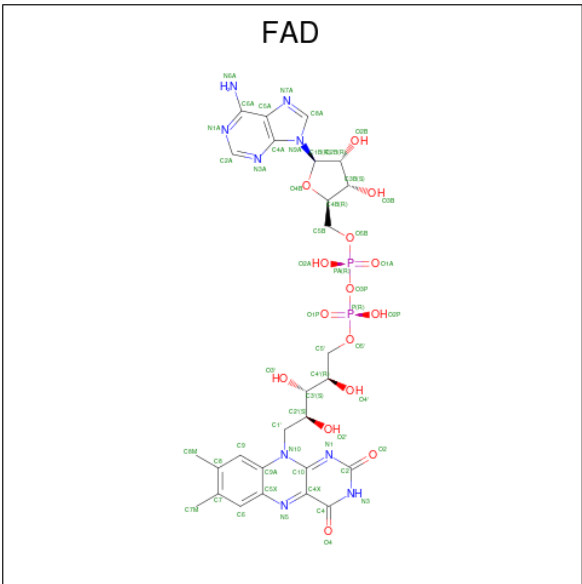
- Molecule 1 is a protein called VANILLYL-ALCOHOL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	0	0
			4315	2774	731	787	23			
1	B	550	Total	C	N	O	S	0	0	0
			4316	2775	731	787	23			

There are 5 discrepancies between the modelled and reference sequences:

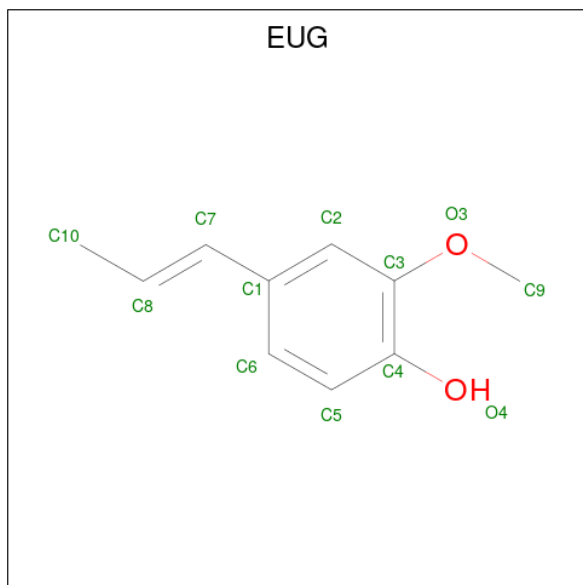
Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ALA	GLU	conflict	UNP P56216
B	6	ALA	GLU	conflict	UNP P56216
A	274	GLY	ARG	conflict	UNP P56216
B	274	GLY	ARG	conflict	UNP P56216
B	170	SER	ASP	engineered mutation	UNP P56216

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

- Molecule 3 is 2-methoxy-4-[(1E)-prop-1-en-1-yl]phenol (CCD ID: EUG) (formula: C₁₀H₁₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	9	2		
3	B	1	Total	C	O	0	0
			11	9	2		

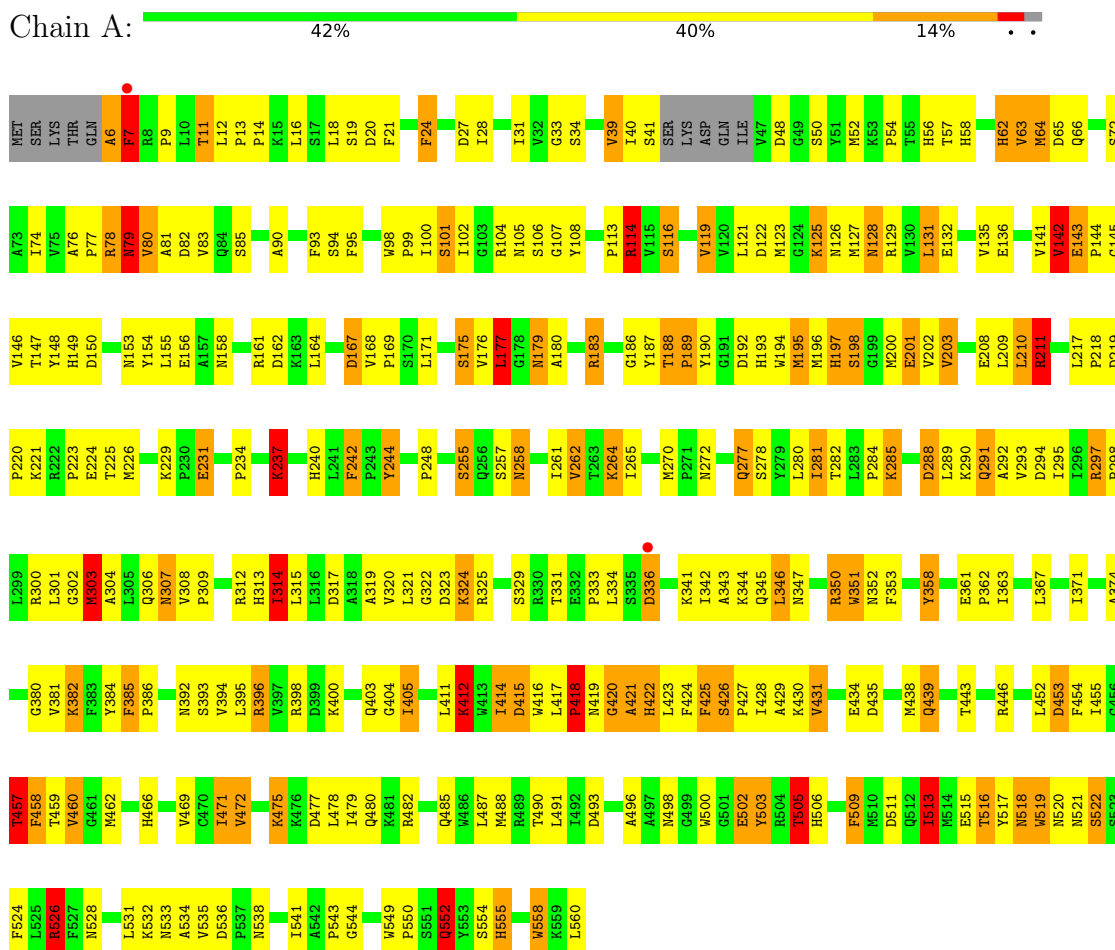
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	30	Total	O	0	0
			30	30		
4	B	32	Total	O	0	0
			32	32		

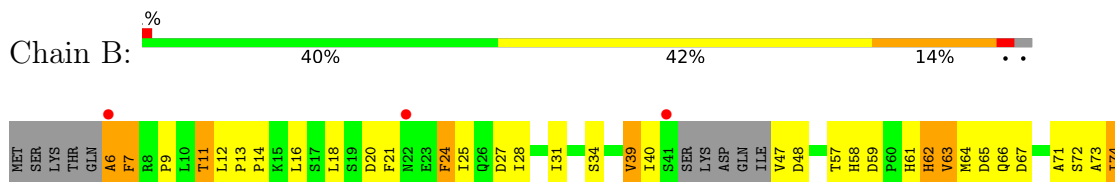
3 Residue-property plots

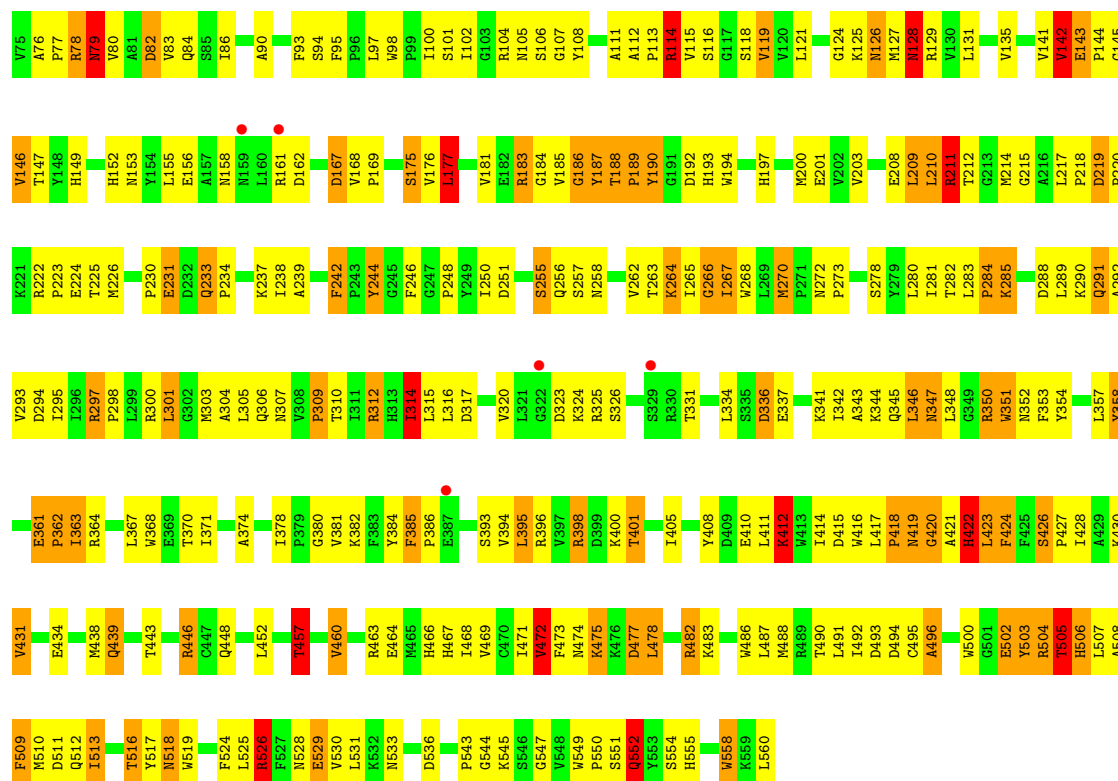
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



• Molecule 1: VANILLYL-ALCOHOL OXIDASE





4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	131.33Å 131.33Å 134.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 20.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	83.7 (20.00-2.80) 82.7 (20.00-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.09 (at 2.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.227 , 0.291 0.221 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	37.2	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.025 for l,-k,h 0.038 for -l,-k,-h 0.031 for -h,-l,-k 0.024 for -h,l,k 0.056 for -h,k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	8821	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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: FAD, EUG

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	0.87	2/4434 (0.0%)	2.35	251/6032 (4.2%)
1	B	0.87	3/4435 (0.1%)	2.31	243/6034 (4.0%)
All	All	0.87	5/8869 (0.1%)	2.33	494/12066 (4.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	422	HIS	CE1-NE2	7.20	1.39	1.32
1	B	422	HIS	CD2-NE2	7.03	1.45	1.37
1	A	422	HIS	CD2-NE2	6.47	1.45	1.37
1	B	422	HIS	CE1-NE2	5.12	1.37	1.32
1	B	128	ASN	CA-CB	5.12	1.61	1.53

All (494) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	398	ARG	CD-NE-CZ	37.80	177.31	124.40
1	B	398	ARG	CD-NE-CZ	30.43	167.00	124.40
1	B	211	ARG	CD-NE-CZ	19.36	151.50	124.40
1	A	211	ARG	CD-NE-CZ	19.11	151.16	124.40
1	A	526	ARG	CD-NE-CZ	18.35	150.10	124.40
1	B	526	ARG	CD-NE-CZ	14.49	144.69	124.40
1	A	6	ALA	CA-C-N	12.61	145.62	121.54
1	A	6	ALA	C-N-CA	12.61	145.62	121.54
1	B	6	ALA	CA-C-N	12.40	145.22	121.54
1	B	6	ALA	C-N-CA	12.40	145.22	121.54
1	A	422	HIS	CE1-NE2-CD2	-12.30	96.69	109.00
1	A	129	ARG	N-CA-C	12.18	127.49	109.59
1	B	336	ASP	CA-CB-CG	-11.58	101.02	112.60
1	A	543	PRO	CA-C-O	-11.37	109.33	121.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	129	ARG	N-CA-C	10.99	125.74	109.59
1	A	526	ARG	NE-CZ-NH2	10.95	129.05	119.20
1	A	351	TRP	CA-C-O	-10.79	108.92	121.11
1	B	297	ARG	CD-NE-CZ	10.78	139.49	124.40
1	B	422	HIS	CE1-NE2-CD2	-10.75	98.25	109.00
1	A	477	ASP	CA-CB-CG	10.57	123.17	112.60
1	A	536	ASP	CA-CB-CG	10.24	122.84	112.60
1	B	536	ASP	CA-CB-CG	9.98	122.58	112.60
1	B	128	ASN	N-CA-C	9.70	125.25	113.41
1	A	520	ASN	OD1-CG-ND2	9.55	132.16	122.60
1	A	153	ASN	CA-CB-CG	9.52	122.12	112.60
1	A	180	ALA	CA-C-O	-9.44	110.55	120.55
1	A	528	ASN	CA-CB-CG	-9.33	103.27	112.60
1	A	336	ASP	CA-CB-CG	-9.30	103.30	112.60
1	B	72	SER	N-CA-C	-9.30	102.06	113.41
1	B	114	ARG	N-CA-CB	9.29	123.78	110.12
1	B	127	MET	CA-C-O	9.23	132.56	122.13
1	B	526	ARG	NE-CZ-NH2	9.09	127.39	119.20
1	B	24	PHE	CA-CB-CG	9.08	122.88	113.80
1	B	293	VAL	CA-C-O	-9.04	111.65	121.05
1	A	128	ASN	N-CA-C	8.96	124.52	113.50
1	A	211	ARG	NE-CZ-NH2	8.94	127.25	119.20
1	B	167	ASP	CA-C-O	-8.94	110.40	120.32
1	A	24	PHE	CA-CB-CG	8.94	122.73	113.80
1	B	112	ALA	N-CA-C	8.89	119.83	109.60
1	A	72	SER	N-CA-C	-8.77	102.71	113.41
1	A	304	ALA	N-CA-C	-8.71	102.78	113.41
1	B	526	ARG	NE-CZ-NH1	-8.70	112.80	121.50
1	A	27	ASP	CA-CB-CG	8.69	121.29	112.60
1	B	6	ALA	CA-C-O	8.69	135.57	120.80
1	B	304	ALA	N-CA-C	-8.68	102.86	113.97
1	B	107	GLY	N-CA-C	-8.63	104.42	114.69
1	B	186	GLY	O-C-N	-8.62	115.72	123.65
1	A	480	GLN	OE1-CD-NE2	-8.58	114.02	122.60
1	B	457	THR	CB-CA-C	-8.58	91.96	109.38
1	A	183	ARG	CA-C-N	8.54	130.19	120.53
1	A	183	ARG	C-N-CA	8.54	130.19	120.53
1	B	325	ARG	NE-CZ-NH2	8.51	126.86	119.20
1	B	104	ARG	CD-NE-CZ	8.44	136.22	124.40
1	B	446	ARG	NE-CZ-NH1	8.44	129.94	121.50
1	A	218	PRO	CA-C-O	-8.37	111.26	121.31
1	A	167	ASP	CA-C-O	-8.35	111.39	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	256	GLN	OE1-CD-NE2	-8.32	114.28	122.60
1	A	446	ARG	CD-NE-CZ	8.32	136.04	124.40
1	A	63	VAL	N-CA-CB	8.25	123.26	112.12
1	A	297	ARG	CD-NE-CZ	8.18	135.85	124.40
1	B	405	ILE	CA-C-O	8.17	123.97	119.15
1	B	114	ARG	CA-C-O	-8.16	111.90	120.55
1	A	303	MET	CA-C-O	8.12	131.05	120.98
1	A	64	MET	CA-C-O	-8.10	112.02	121.82
1	A	211	ARG	N-CA-CB	8.06	124.74	110.80
1	B	153	ASN	CA-CB-CG	8.05	120.65	112.60
1	B	58	HIS	CA-CB-CG	-8.05	105.75	113.80
1	A	313	HIS	CA-C-O	-8.04	112.32	121.81
1	B	114	ARG	CD-NE-CZ	7.97	135.56	124.40
1	B	536	ASP	CA-C-O	7.96	131.58	120.83
1	A	434	GLU	CB-CG-CD	-7.90	99.17	112.60
1	B	101	SER	CA-C-O	7.88	128.73	119.67
1	A	183	ARG	CD-NE-CZ	7.85	135.39	124.40
1	B	185	VAL	CA-C-N	7.83	129.78	121.48
1	B	185	VAL	C-N-CA	7.83	129.78	121.48
1	A	63	VAL	N-CA-C	-7.80	105.88	113.53
1	B	560	LEU	CA-C-O	-7.75	107.63	120.80
1	A	323	ASP	CA-CB-CG	7.72	120.32	112.60
1	B	536	ASP	O-C-N	-7.72	114.42	121.37
1	B	211	ARG	NE-CZ-NH1	-7.72	113.78	121.50
1	A	193	HIS	CA-CB-CG	-7.71	106.08	113.80
1	B	218	PRO	CA-C-O	-7.69	112.57	121.34
1	B	457	THR	N-CA-CB	7.69	124.89	111.13
1	A	107	GLY	N-CA-C	-7.67	104.27	114.25
1	B	304	ALA	CA-C-O	7.67	127.18	118.97
1	B	31	ILE	N-CA-C	7.57	118.16	110.82
1	B	439	GLN	CA-C-O	-7.55	112.89	120.82
1	B	217	LEU	O-C-N	7.55	127.35	121.23
1	A	127	MET	CA-C-O	7.55	130.94	121.58
1	A	145	GLY	N-CA-C	7.52	122.94	114.67
1	A	218	PRO	O-C-N	7.48	132.08	123.10
1	A	127	MET	CA-C-N	7.48	134.86	121.92
1	A	127	MET	C-N-CA	7.48	134.86	121.92
1	A	466	HIS	CA-CB-CG	7.46	121.26	113.80
1	A	415	ASP	CA-CB-CG	-7.46	105.14	112.60
1	A	533	ASN	CA-C-O	-7.45	111.85	120.20
1	B	552	GLN	CA-CB-CG	7.44	128.97	114.10
1	B	351	TRP	CA-C-O	-7.41	112.44	121.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	422	HIS	ND1-CE1-NE2	7.37	115.77	108.40
1	A	114	ARG	CD-NE-CZ	7.36	134.70	124.40
1	A	325	ARG	NE-CZ-NH2	7.35	125.81	119.20
1	B	505	THR	CB-CA-C	-7.34	96.78	111.17
1	B	18	LEU	CA-C-N	7.30	130.66	120.29
1	B	18	LEU	C-N-CA	7.30	130.66	120.29
1	A	104	ARG	CD-NE-CZ	7.29	134.61	124.40
1	A	208	GLU	CA-C-O	7.27	129.83	121.47
1	A	114	ARG	N-CA-CB	7.26	120.79	110.12
1	A	125	LYS	CA-C-O	-7.26	112.53	121.02
1	A	524	PHE	CA-C-O	-7.25	113.14	120.90
1	B	381	VAL	CA-C-O	-7.21	113.43	121.36
1	B	162	ASP	N-CA-C	-7.20	104.53	113.38
1	B	477	ASP	CA-CB-CG	7.17	119.77	112.60
1	A	294	ASP	CA-CB-CG	7.17	119.77	112.60
1	B	63	VAL	N-CA-CB	7.16	123.04	111.23
1	A	435	ASP	CA-C-N	7.14	129.72	120.44
1	A	435	ASP	C-N-CA	7.14	129.72	120.44
1	A	217	LEU	O-C-N	7.12	127.89	121.19
1	A	381	VAL	CA-C-O	-7.10	113.55	121.36
1	A	552	GLN	CB-CG-CD	7.09	124.65	112.60
1	B	27	ASP	CA-CB-CG	7.08	119.69	112.60
1	B	127	MET	CA-C-N	7.04	134.70	122.09
1	B	127	MET	C-N-CA	7.04	134.70	122.09
1	B	323	ASP	CA-CB-CG	7.03	119.63	112.60
1	B	463	ARG	O-C-N	7.01	130.48	122.20
1	B	258	ASN	CA-CB-CG	7.00	119.61	112.60
1	B	145	GLY	N-CA-C	7.00	122.63	114.16
1	A	121	LEU	CA-C-O	6.96	128.16	120.92
1	A	425	PHE	CA-C-O	6.94	127.79	120.36
1	A	211	ARG	CA-CB-CG	6.92	127.94	114.10
1	A	208	GLU	O-C-N	-6.92	115.14	122.96
1	B	529	GLU	O-C-N	-6.91	114.79	122.12
1	B	74	ILE	O-C-N	-6.88	115.06	123.10
1	A	422	HIS	CG-CD2-NE2	6.87	114.07	107.20
1	A	101	SER	CA-C-O	6.85	127.55	119.67
1	B	446	ARG	CD-NE-CZ	6.83	133.97	124.40
1	B	246	PHE	O-C-N	-6.82	114.33	123.19
1	A	63	VAL	CB-CA-C	-6.82	103.97	110.65
1	B	543	PRO	CA-C-O	-6.82	113.94	121.23
1	B	48	ASP	CA-CB-CG	6.81	119.41	112.60
1	A	244	TYR	N-CA-C	6.81	118.36	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	ARG	CA-CB-CG	6.81	127.72	114.10
1	A	422	HIS	ND1-CE1-NE2	6.81	115.21	108.40
1	A	6	ALA	CA-C-O	6.80	132.37	120.80
1	A	304	ALA	CA-C-O	6.77	127.06	119.41
1	A	422	HIS	N-CA-CB	6.73	121.21	110.85
1	B	114	ARG	CA-C-N	-6.72	114.30	122.90
1	B	114	ARG	C-N-CA	-6.72	114.30	122.90
1	A	136	GLU	CA-C-O	-6.71	112.25	119.97
1	A	128	ASN	N-CA-CB	-6.70	100.67	110.53
1	B	270	MET	CA-C-O	6.70	124.62	119.46
1	A	18	LEU	CA-C-N	6.70	129.26	120.28
1	A	18	LEU	C-N-CA	6.70	129.26	120.28
1	B	303	MET	O-C-N	-6.70	115.10	122.67
1	B	175	SER	CA-C-O	6.69	127.72	120.43
1	B	448	GLN	OE1-CD-NE2	-6.68	115.92	122.60
1	A	114	ARG	CA-C-N	-6.68	114.35	122.90
1	A	114	ARG	C-N-CA	-6.68	114.35	122.90
1	A	515	GLU	CA-C-O	6.68	127.66	119.11
1	B	460	VAL	CB-CA-C	-6.68	104.72	111.80
1	A	518	ASN	N-CA-C	6.65	120.86	113.21
1	B	419	ASN	OD1-CG-ND2	6.63	129.23	122.60
1	A	154	TYR	O-C-N	6.63	128.90	122.07
1	A	264	LYS	CA-C-O	-6.58	114.41	121.45
1	A	31	ILE	N-CA-C	6.58	117.20	110.82
1	B	146	VAL	CA-C-O	-6.58	112.56	120.78
1	B	177	LEU	CA-CB-CG	6.57	139.30	116.30
1	A	85	SER	O-C-N	6.57	129.18	122.09
1	B	460	VAL	N-CA-C	6.56	116.68	107.37
1	B	415	ASP	CA-CB-CG	-6.54	106.06	112.60
1	B	258	ASN	O-C-N	-6.53	113.15	121.97
1	B	426	SER	N-CA-C	6.52	120.22	109.79
1	B	39	VAL	N-CA-C	6.51	117.49	107.99
1	B	79	ASN	N-CA-CB	-6.50	100.02	110.55
1	B	6	ALA	O-C-N	-6.50	112.60	123.00
1	B	82	ASP	CA-CB-CG	-6.48	106.12	112.60
1	B	183	ARG	CD-NE-CZ	6.47	133.46	124.40
1	B	424	PHE	N-CA-C	6.47	120.05	109.76
1	A	143	GLU	O-C-N	-6.45	116.50	121.14
1	B	126	ASN	OD1-CG-ND2	6.45	129.05	122.60
1	B	181	VAL	CA-C-O	-6.44	113.52	120.47
1	A	211	ARG	NE-CZ-NH1	-6.44	115.06	121.50
1	B	347	ASN	OD1-CG-ND2	6.44	129.04	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	558	TRP	N-CA-C	6.42	121.12	113.28
1	B	7	PHE	CA-CB-CG	6.42	120.22	113.80
1	B	312	ARG	CD-NE-CZ	-6.40	115.44	124.40
1	A	281	ILE	CA-C-O	-6.38	113.63	120.59
1	A	255	SER	N-CA-CB	6.37	120.94	110.69
1	A	490	THR	N-CA-C	-6.36	104.27	111.14
1	A	149	HIS	CA-CB-CG	-6.35	107.45	113.80
1	B	524	PHE	CA-C-O	-6.35	114.10	120.90
1	B	242	PHE	CA-CB-CG	6.34	120.14	113.80
1	B	431	VAL	N-CA-CB	6.33	121.67	111.23
1	B	67	ASP	CA-C-O	6.29	127.56	119.95
1	B	518	ASN	OD1-CG-ND2	6.29	128.89	122.60
1	A	421	ALA	CA-C-O	-6.28	113.44	120.66
1	A	426	SER	N-CA-C	6.28	119.83	109.79
1	A	142	VAL	N-CA-CB	-6.26	101.92	112.44
1	A	7	PHE	N-CA-C	6.26	124.13	110.80
1	A	168	VAL	CB-CA-C	-6.26	101.82	111.89
1	A	490	THR	CA-C-O	-6.25	114.26	120.70
1	A	552	GLN	CA-CB-CG	6.24	126.57	114.10
1	B	446	ARG	NE-CZ-NH2	-6.23	113.59	119.20
1	A	431	VAL	N-CA-CB	6.23	121.51	111.23
1	B	71	ALA	CA-C-O	-6.22	114.65	121.87
1	B	509	PHE	CA-CB-CG	-6.22	107.58	113.80
1	B	218	PRO	O-C-N	6.22	130.55	123.03
1	A	135	VAL	N-CA-C	6.21	116.37	110.53
1	A	392	ASN	OD1-CG-ND2	-6.21	116.39	122.60
1	B	505	THR	N-CA-C	6.20	117.65	108.60
1	A	560	LEU	CA-C-O	-6.19	110.28	120.80
1	A	505	THR	CB-CA-C	-6.18	97.06	111.09
1	A	54	PRO	N-CA-C	6.17	120.12	110.80
1	A	439	GLN	OE1-CD-NE2	6.16	128.76	122.60
1	B	547	GLY	CA-C-N	-6.15	114.68	122.43
1	B	547	GLY	C-N-CA	-6.15	114.68	122.43
1	A	526	ARG	NE-CZ-NH1	-6.14	115.36	121.50
1	B	512	GLN	CB-CG-CD	6.14	123.03	112.60
1	A	244	TYR	CA-C-O	-6.12	114.39	120.82
1	B	530	VAL	CA-C-O	-6.11	114.69	121.17
1	A	385	PHE	CA-CB-CG	6.11	119.91	113.80
1	B	528	ASN	CA-CB-CG	-6.09	106.51	112.60
1	B	62	HIS	N-CA-C	6.09	118.83	110.24
1	A	58	HIS	CA-CB-CG	-6.08	107.72	113.80
1	B	142	VAL	N-CA-CB	-6.07	102.25	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	544	GLY	N-CA-C	6.07	120.07	113.58
1	B	303	MET	CA-C-O	6.05	128.60	121.40
1	A	164	LEU	N-CA-C	6.05	119.26	109.40
1	A	438	MET	O-C-N	6.04	128.31	122.03
1	A	425	PHE	O-C-N	-6.04	116.33	123.22
1	A	320	VAL	N-CA-CB	6.04	117.61	110.55
1	B	7	PHE	N-CA-C	6.04	123.66	110.80
1	A	314	ILE	CB-CG1-CD1	6.03	126.47	113.80
1	A	192	ASP	CA-CB-CG	6.03	118.63	112.60
1	A	162	ASP	CA-CB-CG	6.03	118.63	112.60
1	B	300	ARG	CA-C-O	6.02	126.92	120.24
1	A	162	ASP	N-CA-C	-6.01	105.99	113.38
1	B	244	TYR	N-CA-C	5.99	118.30	111.11
1	A	458	PHE	CA-C-N	-5.99	114.74	123.00
1	A	458	PHE	C-N-CA	-5.99	114.74	123.00
1	B	294	ASP	CA-CB-CG	5.99	118.59	112.60
1	A	197	HIS	N-CA-C	5.98	118.25	110.53
1	A	34	SER	CA-C-N	5.96	128.54	120.38
1	A	34	SER	C-N-CA	5.96	128.54	120.38
1	A	505	THR	N-CA-C	5.95	117.83	108.96
1	B	467	HIS	CA-C-O	-5.95	114.73	120.92
1	B	264	LYS	CA-C-O	-5.94	114.92	121.33
1	A	333	PRO	CA-C-O	-5.91	114.81	121.43
1	A	175	SER	CA-C-O	5.90	126.86	120.43
1	A	485	GLN	OE1-CD-NE2	5.90	128.50	122.60
1	B	256	GLN	CG-CD-NE2	5.90	125.25	116.40
1	A	122	ASP	CA-CB-CG	5.88	118.48	112.60
1	B	200	MET	CA-C-N	-5.88	114.81	123.05
1	B	200	MET	C-N-CA	-5.88	114.81	123.05
1	A	179	ASN	O-C-N	-5.88	115.98	122.09
1	B	438	MET	N-CA-C	-5.87	104.80	111.14
1	B	439	GLN	O-C-N	5.86	128.11	122.07
1	A	6	ALA	O-C-N	-5.85	113.64	123.00
1	A	460	VAL	CB-CA-C	-5.85	105.60	111.80
1	B	78	ARG	CD-NE-CZ	5.84	132.58	124.40
1	A	114	ARG	CB-CG-CD	5.83	124.71	111.30
1	B	422	HIS	N-CA-CB	5.83	120.17	110.85
1	B	314	ILE	CB-CG1-CD1	5.82	126.03	113.80
1	A	62	HIS	N-CA-C	5.81	118.66	110.23
1	A	255	SER	N-CA-C	-5.78	100.29	109.59
1	B	326	SER	CA-C-O	-5.78	112.28	119.38
1	B	533	ASN	CA-C-O	-5.78	113.73	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	509	PHE	CA-CB-CG	-5.77	108.03	113.80
1	A	457	THR	N-CA-CB	5.77	122.26	111.53
1	A	429	ALA	CA-C-O	-5.77	114.89	121.58
1	B	147	THR	CA-C-O	-5.75	115.33	121.94
1	A	187	TYR	CA-CB-CG	-5.75	103.56	113.90
1	B	434	GLU	CB-CG-CD	-5.75	102.83	112.60
1	A	149	HIS	CB-CG-CD2	5.74	138.67	131.20
1	B	211	ARG	N-CA-CB	5.73	120.72	110.80
1	A	471	ILE	N-CA-CB	-5.73	105.33	111.46
1	A	78	ARG	CD-NE-CZ	5.71	132.39	124.40
1	A	471	ILE	CA-C-N	-5.71	115.74	123.10
1	A	471	ILE	C-N-CA	-5.71	115.74	123.10
1	B	131	LEU	N-CA-C	5.71	118.44	111.82
1	B	336	ASP	CA-C-N	5.71	127.92	120.28
1	B	336	ASP	C-N-CA	5.71	127.92	120.28
1	A	380	GLY	N-CA-C	5.70	122.93	115.47
1	A	534	ALA	N-CA-C	5.69	117.16	111.07
1	B	309	PRO	CA-C-O	-5.68	114.50	121.31
1	A	513	ILE	O-C-N	-5.68	115.98	121.83
1	B	119	VAL	CB-CA-C	-5.67	104.44	111.08
1	B	187	TYR	CA-CB-CG	-5.67	103.69	113.90
1	A	520	ASN	CB-CG-OD1	-5.67	109.46	120.80
1	B	233	GLN	CB-CG-CD	5.67	122.24	112.60
1	A	56	HIS	CA-CB-CG	5.67	119.47	113.80
1	A	229	LYS	N-CA-C	-5.67	102.91	109.93
1	B	472	VAL	N-CA-CB	5.67	121.69	111.21
1	B	364	ARG	CA-C-N	5.66	128.18	120.54
1	B	364	ARG	C-N-CA	5.66	128.18	120.54
1	B	558	TRP	N-CA-C	5.65	120.33	113.38
1	B	358	TYR	N-CA-C	5.65	118.11	108.90
1	B	39	VAL	N-CA-CB	-5.64	104.61	111.21
1	A	538	ASN	OD1-CG-ND2	-5.64	116.96	122.60
1	A	384	TYR	CA-C-O	-5.64	114.17	120.66
1	A	404	GLY	CA-C-O	5.64	125.27	119.01
1	B	401	THR	CA-CB-OG1	5.64	118.06	109.60
1	B	135	VAL	N-CA-C	5.62	115.81	110.53
1	B	412	LYS	N-CA-C	5.62	118.17	111.71
1	A	19	SER	N-CA-CB	-5.62	101.86	110.12
1	A	421	ALA	N-CA-C	-5.61	99.88	109.24
1	A	396	ARG	CA-C-O	-5.60	114.61	120.55
1	A	218	PRO	N-CA-CB	5.59	108.54	103.34
1	B	168	VAL	CB-CA-C	-5.59	103.03	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	HIS	CB-CG-ND1	-5.59	114.31	122.70
1	B	316	LEU	N-CA-CB	5.59	118.34	110.12
1	B	84	GLN	O-C-N	5.59	128.52	122.15
1	B	128	ASN	N-CA-CB	-5.59	102.31	110.47
1	A	119	VAL	CA-C-N	-5.58	113.98	121.80
1	A	119	VAL	C-N-CA	-5.58	113.98	121.80
1	A	438	MET	N-CA-C	-5.58	104.88	110.97
1	A	405	ILE	CA-C-O	5.57	127.42	119.95
1	B	181	VAL	N-CA-CB	5.56	120.84	110.77
1	B	464	GLU	CA-C-O	5.56	127.68	121.40
1	A	424	PHE	N-CA-C	5.55	118.68	109.46
1	B	31	ILE	CB-CA-C	-5.55	104.77	112.04
1	A	119	VAL	CB-CA-C	-5.55	104.25	110.96
1	A	300	ARG	CA-C-O	5.54	126.41	120.70
1	A	457	THR	CB-CA-C	-5.53	97.28	109.56
1	B	128	ASN	CB-CA-C	-5.53	99.57	109.24
1	B	190	TYR	O-C-N	-5.53	115.55	122.35
1	A	131	LEU	N-CA-C	5.53	119.19	112.23
1	A	201	GLU	CA-C-O	5.52	126.39	120.38
1	B	208	GLU	CB-CA-C	5.52	118.94	109.51
1	B	312	ARG	O-C-N	-5.51	116.88	123.06
1	A	533	ASN	OD1-CG-ND2	-5.51	117.09	122.60
1	B	158	ASN	O-C-N	-5.51	115.69	122.25
1	B	467	HIS	CA-C-N	-5.51	115.59	122.48
1	B	467	HIS	C-N-CA	-5.51	115.59	122.48
1	A	99	PRO	CA-C-O	-5.51	115.33	121.23
1	B	121	LEU	CA-C-O	5.51	126.79	120.84
1	B	336	ASP	OD1-CG-OD2	5.51	136.12	122.90
1	B	363	ILE	N-CA-C	5.49	115.69	110.42
1	B	452	LEU	CA-C-O	-5.49	114.77	120.70
1	B	466	HIS	CA-CB-CG	5.48	119.28	113.80
1	B	209	LEU	CA-C-O	-5.47	114.46	120.43
1	A	303	MET	O-C-N	-5.47	115.25	122.47
1	A	522	SER	CB-CA-C	-5.47	103.96	111.73
1	B	141	VAL	N-CA-CB	5.47	118.75	111.64
1	A	307	ASN	CB-CG-ND2	5.47	124.60	116.40
1	B	486	TRP	N-CA-C	-5.46	105.41	111.36
1	B	385	PHE	CA-CB-CG	5.45	119.25	113.80
1	A	39	VAL	N-CA-C	5.45	116.15	108.36
1	B	551	SER	CA-CB-OG	-5.45	100.20	111.10
1	B	490	THR	N-CA-C	-5.45	104.99	111.69
1	B	47	VAL	CA-C-N	5.44	127.58	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	VAL	C-N-CA	5.44	127.58	120.28
1	A	412	LYS	N-CA-C	5.44	117.97	111.71
1	A	453	ASP	CA-C-O	-5.44	115.78	121.55
1	A	158	ASN	OD1-CG-ND2	-5.44	117.16	122.60
1	B	239	ALA	CA-C-O	5.43	127.00	120.92
1	B	219	ASP	N-CA-C	-5.43	102.81	109.65
1	B	482	ARG	CD-NE-CZ	5.43	132.00	124.40
1	A	177	LEU	CA-CB-CG	5.42	135.29	116.30
1	B	265	ILE	CA-C-N	-5.42	117.05	122.20
1	B	265	ILE	C-N-CA	-5.42	117.05	122.20
1	A	132	GLU	CA-C-N	-5.42	115.72	123.10
1	A	132	GLU	C-N-CA	-5.42	115.72	123.10
1	A	329	SER	CA-C-O	5.42	125.33	119.15
1	B	184	GLY	N-CA-C	5.41	119.47	112.54
1	A	498	ASN	CA-CB-CG	-5.41	107.19	112.60
1	A	277	GLN	CA-CB-CG	5.40	124.91	114.10
1	A	128	ASN	CB-CA-C	-5.39	99.47	109.29
1	B	214	MET	CB-CA-C	5.39	120.68	109.95
1	B	552	GLN	CB-CG-CD	5.38	121.75	112.60
1	A	272	ASN	O-C-N	5.38	125.79	121.38
1	A	424	PHE	CB-CA-C	-5.38	100.98	109.80
1	A	459	THR	N-CA-CB	5.38	119.01	110.57
1	A	479	ILE	O-C-N	5.37	127.17	121.91
1	A	195	MET	CA-C-O	-5.37	112.34	119.10
1	B	362	PRO	CA-C-O	-5.36	110.85	120.60
1	B	114	ARG	O-C-N	5.35	127.79	122.12
1	B	297	ARG	CA-C-N	5.35	124.86	119.19
1	B	297	ARG	C-N-CA	5.35	124.86	119.19
1	B	518	ASN	N-CA-C	5.35	118.92	112.93
1	A	505	THR	O-C-N	5.34	129.24	123.10
1	A	80	VAL	CA-C-O	-5.34	115.19	120.85
1	B	111	ALA	CA-C-O	-5.32	113.28	119.14
1	A	168	VAL	O-C-N	5.32	125.82	121.40
1	A	218	PRO	CA-C-N	-5.32	113.54	120.67
1	A	218	PRO	C-N-CA	-5.32	113.54	120.67
1	B	209	LEU	O-C-N	5.32	129.28	123.27
1	B	410	GLU	N-CA-C	5.32	119.52	113.19
1	A	502	GLU	N-CA-CB	-5.32	102.51	110.17
1	A	7	PHE	CA-CB-CG	5.32	119.12	113.80
1	B	34	SER	CA-C-N	5.31	127.39	120.28
1	B	34	SER	C-N-CA	5.31	127.39	120.28
1	B	192	ASP	CA-CB-CG	5.30	117.90	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	462	MET	N-CA-C	5.30	116.74	111.07
1	B	73	ALA	CA-C-O	-5.30	115.56	121.23
1	A	435	ASP	CA-CB-CG	-5.29	107.31	112.60
1	B	266	GLY	CA-C-N	-5.28	116.22	123.14
1	B	266	GLY	C-N-CA	-5.28	116.22	123.14
1	B	268	TRP	CA-C-N	-5.28	115.27	122.93
1	B	268	TRP	C-N-CA	-5.28	115.27	122.93
1	B	370	THR	O-C-N	5.28	127.50	122.07
1	B	158	ASN	CA-C-O	5.27	125.81	119.59
1	A	79	ASN	N-CA-CB	-5.27	101.38	110.76
1	A	221	LYS	CA-C-N	5.27	131.72	122.08
1	A	221	LYS	C-N-CA	5.27	131.72	122.08
1	B	504	ARG	NE-CZ-NH1	-5.26	116.24	121.50
1	A	261	ILE	O-C-N	5.26	129.26	123.10
1	A	414	ILE	CA-CB-CG2	5.26	119.44	110.50
1	A	460	VAL	N-CA-C	5.25	114.83	107.37
1	B	438	MET	O-C-N	5.25	127.76	122.09
1	B	193	HIS	CA-CB-CG	-5.25	108.55	113.80
1	B	472	VAL	O-C-N	5.25	128.49	123.14
1	B	189	PRO	CB-CA-C	5.25	119.30	111.85
1	B	312	ARG	NH1-CZ-NH2	5.25	126.12	119.30
1	B	316	LEU	O-C-N	5.24	127.68	122.12
1	A	33	GLY	O-C-N	-5.24	117.60	122.47
1	A	211	ARG	N-CA-C	-5.24	99.91	108.76
1	B	215	GLY	O-C-N	-5.24	116.86	122.73
1	B	143	GLU	N-CA-CB	5.23	117.36	109.82
1	A	150	ASP	O-C-N	5.23	127.45	122.07
1	B	378	ILE	CA-C-O	-5.23	114.60	119.62
1	A	258	ASN	CA-CB-CG	5.22	117.82	112.60
1	A	48	ASP	N-CA-C	5.21	117.70	111.71
1	A	336	ASP	CA-C-N	5.21	127.68	120.29
1	A	336	ASP	C-N-CA	5.21	127.68	120.29
1	A	72	SER	N-CA-CB	5.20	118.06	110.47
1	A	147	THR	N-CA-CB	5.20	117.88	110.44
1	B	203	VAL	N-CA-CB	5.19	117.28	111.21
1	A	382	LYS	CA-C-O	-5.19	114.56	120.32
1	A	291	GLN	OE1-CD-NE2	5.19	127.79	122.60
1	B	25	ILE	CA-C-O	-5.19	115.66	121.05
1	B	219	ASP	CB-CA-C	5.19	117.81	109.41
1	A	99	PRO	N-CA-C	5.18	119.01	111.03
1	A	555	HIS	O-C-N	-5.18	116.63	122.12
1	B	291	GLN	OE1-CD-NE2	5.18	127.78	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	529	GLU	CA-C-N	5.17	127.08	120.56
1	B	529	GLU	C-N-CA	5.17	127.08	120.56
1	A	203	VAL	O-C-N	5.17	129.14	123.10
1	B	320	VAL	N-CA-CB	5.16	116.59	110.55
1	A	419	ASN	OD1-CG-ND2	5.16	127.76	122.60
1	A	358	TYR	N-CA-C	5.16	116.79	108.34
1	A	321	LEU	CA-C-O	-5.15	115.09	120.55
1	A	262	VAL	N-CA-CB	-5.15	105.13	111.00
1	B	263	THR	CA-C-O	-5.14	113.47	118.97
1	B	208	GLU	CA-C-O	5.14	127.53	121.36
1	A	64	MET	N-CA-C	-5.14	102.40	110.36
1	B	496	ALA	O-C-N	-5.14	115.98	122.20
1	A	515	GLU	O-C-N	-5.13	114.94	122.43
1	B	127	MET	O-C-N	-5.13	116.76	122.55
1	A	288	ASP	CA-C-N	5.12	127.41	120.44
1	A	288	ASP	C-N-CA	5.12	127.41	120.44
1	B	211	ARG	NE-CZ-NH2	5.12	123.81	119.20
1	B	152	HIS	CA-C-O	5.12	126.38	120.90
1	A	242	PHE	CA-C-N	5.12	124.43	118.85
1	A	242	PHE	C-N-CA	5.12	124.43	118.85
1	B	176	VAL	CA-C-N	5.11	127.58	120.63
1	B	176	VAL	C-N-CA	5.11	127.58	120.63
1	A	293	VAL	CA-C-O	-5.11	115.73	121.05
1	B	384	TYR	CA-C-O	-5.11	114.65	120.32
1	B	212	THR	N-CA-C	5.11	116.69	110.41
1	A	479	ILE	CA-C-O	-5.10	115.76	121.17
1	A	521	ASN	CA-CB-CG	-5.10	107.50	112.60
1	A	237	LYS	CA-CB-CG	5.09	124.28	114.10
1	A	452	LEU	N-CA-C	5.09	117.69	109.40
1	A	425	PHE	CA-CB-CG	-5.09	108.71	113.80
1	A	320	VAL	N-CA-C	-5.08	105.54	110.42
1	B	285	LYS	N-CA-C	5.08	118.23	110.20
1	A	52	MET	CB-CA-C	5.08	120.61	109.99
1	B	72	SER	N-CA-CB	5.07	117.87	110.47
1	B	59	ASP	CA-C-N	5.07	124.68	119.56
1	B	59	ASP	C-N-CA	5.07	124.68	119.56
1	A	277	GLN	OE1-CD-NE2	-5.07	117.53	122.60
1	A	148	TYR	CA-C-N	5.06	127.38	120.54
1	A	148	TYR	C-N-CA	5.06	127.38	120.54
1	A	272	ASN	N-CA-C	-5.06	103.34	109.57
1	A	324	LYS	O-C-N	-5.06	116.75	122.12
1	A	189	PRO	CB-CA-C	5.06	120.10	112.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	536	ASP	CA-C-O	5.06	127.09	121.22
1	B	361	GLU	O-C-N	5.06	124.98	120.48
1	B	422	HIS	CG-CD2-NE2	5.06	112.26	107.20
1	B	312	ARG	N-CA-C	5.05	118.36	110.32
1	B	508	ALA	N-CA-C	5.05	119.20	113.19
1	A	336	ASP	OD1-CG-OD2	5.05	135.02	122.90
1	B	438	MET	CA-C-O	-5.04	115.51	120.70
1	A	285	LYS	N-CA-C	5.04	118.16	110.20
1	B	380	GLY	N-CA-C	5.04	122.06	115.36
1	A	164	LEU	CA-C-O	-5.03	115.27	120.70
1	A	422	HIS	CB-CG-CD2	5.03	137.73	131.20
1	A	136	GLU	O-C-N	5.02	128.44	122.27
1	A	403	GLN	OE1-CD-NE2	5.02	127.62	122.60
1	B	129	ARG	CB-CA-C	-5.02	102.73	110.26
1	B	506	HIS	CA-CB-CG	-5.02	108.78	113.80
1	A	453	ASP	O-C-N	5.02	128.98	122.81
1	B	544	GLY	N-CA-C	5.01	120.69	114.37
1	B	267	ILE	CA-C-O	-5.01	115.13	120.39

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	4315	0	4224	186	0
1	B	4316	0	4228	193	0
2	A	53	0	30	10	0
2	B	53	0	30	8	0
3	A	11	0	7	0	0
3	B	11	0	7	2	0
4	A	30	0	0	3	0
4	B	32	0	0	2	0
All	All	8821	0	8526	379	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 22.

All (379) 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)
2:B:600:FAD:H8A	2:B:600:FAD:C5B	1.74	1.16
2:A:600:FAD:H8A	2:A:600:FAD:H51A	1.17	1.15
2:A:600:FAD:H8A	2:A:600:FAD:C5B	1.85	1.06
2:B:600:FAD:H8A	2:B:600:FAD:H51A	1.08	1.05
2:B:600:FAD:H51A	2:B:600:FAD:C8A	1.99	0.93
1:B:312:ARG:HG2	1:B:457:THR:HG23	1.54	0.86
2:A:600:FAD:H51A	2:A:600:FAD:C8A	2.05	0.85
1:A:385:PHE:HB3	1:A:386:PRO:HD2	1.60	0.82
1:B:14:PRO:HG3	1:B:558:TRP:CZ2	2.17	0.80
1:A:14:PRO:HG3	1:A:558:TRP:CZ2	2.19	0.78
1:B:14:PRO:HG3	1:B:558:TRP:HZ2	1.47	0.77
1:B:79:ASN:ND2	1:B:82:ASP:H	1.84	0.76
2:B:600:FAD:N1	2:B:600:FAD:O3'	2.19	0.76
1:B:385:PHE:HB3	1:B:386:PRO:HD2	1.68	0.76
1:A:6:ALA:HB3	1:A:39:VAL:HG21	1.68	0.75
1:A:79:ASN:ND2	1:A:82:ASP:H	1.85	0.74
1:A:312:ARG:HG2	1:A:457:THR:HG23	1.67	0.74
1:A:14:PRO:HG3	1:A:558:TRP:HZ2	1.52	0.74
1:A:57:THR:HG22	1:A:74:ILE:HD11	1.71	0.73
1:B:478:LEU:HD12	1:B:478:LEU:H	1.54	0.73
1:B:177:LEU:HD21	1:B:262:VAL:HG12	1.71	0.73
1:B:143:GLU:HB3	1:B:144:PRO:HD2	1.69	0.73
1:A:79:ASN:C	1:A:79:ASN:HD22	1.97	0.72
1:B:443:THR:HG21	1:B:469:VAL:HG21	1.70	0.72
1:A:367:LEU:HD21	1:B:363:ILE:HD11	1.73	0.70
1:B:6:ALA:HB3	1:B:39:VAL:HG21	1.72	0.70
1:B:385:PHE:HB3	1:B:386:PRO:CD	2.21	0.70
1:A:417:LEU:HB3	1:A:418:PRO:HD2	1.71	0.70
1:B:417:LEU:HB3	1:B:418:PRO:HD2	1.72	0.70
1:B:416:TRP:HB3	1:B:472:VAL:HG21	1.74	0.70
1:A:478:LEU:HD12	1:A:478:LEU:H	1.58	0.69
1:A:297:ARG:HB3	1:A:298:PRO:CD	2.23	0.68
1:A:428:ILE:HD11	1:A:503:TYR:HB3	1.76	0.68
1:B:11:THR:HG21	1:B:116:SER:HB3	1.75	0.68
1:A:443:THR:HG21	1:A:469:VAL:HG21	1.76	0.68
1:B:282:THR:HG22	1:B:352:ASN:HD22	1.59	0.68
1:A:385:PHE:HB3	1:A:386:PRO:CD	2.24	0.68
1:A:416:TRP:HB3	1:A:472:VAL:HG21	1.74	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:428:ILE:HD11	1:B:503:TYR:HB3	1.77	0.67
2:B:600:FAD:C5B	2:B:600:FAD:C8A	2.64	0.67
1:A:341:LYS:O	1:A:345:GLN:HG3	1.95	0.67
1:A:297:ARG:HG3	1:A:431:VAL:O	1.95	0.67
1:A:282:THR:HG22	1:A:352:ASN:HD22	1.59	0.66
1:B:341:LYS:O	1:B:345:GLN:HG3	1.95	0.66
1:A:177:LEU:HD21	1:A:262:VAL:HG12	1.79	0.65
1:A:190:TYR:CE1	1:A:270:MET:HG3	2.32	0.65
1:B:66:GLN:O	1:B:66:GLN:HG2	1.96	0.65
2:A:600:FAD:N1	2:A:600:FAD:O3'	2.29	0.65
1:A:12:LEU:HB3	1:A:13:PRO:HD2	1.79	0.64
1:B:167:ASP:OD1	1:B:186:GLY:HA3	1.97	0.64
1:A:93:PHE:O	1:A:94:SER:HB2	1.98	0.64
1:A:9:PRO:HG3	1:A:21:PHE:CE2	2.33	0.64
1:A:209:LEU:HD11	1:A:231:GLU:HG3	1.78	0.64
1:A:161:ARG:HH21	1:A:405:ILE:HD11	1.63	0.64
1:B:12:LEU:HB3	1:B:13:PRO:HD2	1.79	0.64
1:B:297:ARG:HG3	1:B:431:VAL:O	1.97	0.64
1:B:242:PHE:CE2	1:B:244:TYR:HB2	2.34	0.63
1:A:361:GLU:N	1:A:362:PRO:HD2	2.14	0.63
1:A:179:ASN:ND2	2:A:600:FAD:O3'	2.31	0.62
1:B:93:PHE:O	1:B:94:SER:HB2	2.00	0.62
1:B:297:ARG:HB3	1:B:298:PRO:CD	2.29	0.62
1:A:6:ALA:HB3	1:A:39:VAL:CG2	2.29	0.61
1:A:242:PHE:CE2	1:A:244:TYR:HB2	2.35	0.61
1:A:189:PRO:HG2	1:A:270:MET:HE1	1.82	0.61
1:A:411:LEU:O	1:A:414:ILE:HD12	2.00	0.61
1:B:189:PRO:HG2	1:B:270:MET:HE1	1.83	0.61
1:A:430:LYS:HD2	1:B:237:LYS:HB3	1.83	0.61
1:A:80:VAL:HB	1:A:231:GLU:HG2	1.82	0.60
1:A:516:THR:HG22	1:A:517:TYR:CD1	2.36	0.60
1:B:314:ILE:HG13	1:B:343:ALA:HB2	1.83	0.60
1:A:66:GLN:O	1:A:66:GLN:HG2	1.99	0.60
1:A:98:TRP:CD2	1:A:113:PRO:HA	2.37	0.60
1:B:297:ARG:HB3	1:B:298:PRO:HD3	1.83	0.60
1:B:393:SER:OG	1:B:396:ARG:HG3	2.01	0.60
1:A:278:SER:OG	1:A:386:PRO:HG3	2.02	0.59
1:B:443:THR:HA	1:B:491:LEU:CD2	2.33	0.59
1:B:284:PRO:O	1:B:350:ARG:HB2	2.03	0.59
1:A:280:LEU:CB	1:A:395:LEU:HD22	2.33	0.59
1:B:142:VAL:HG22	1:B:146:VAL:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:ASP:OD1	1:B:394:VAL:HG21	2.03	0.58
1:A:11:THR:HG21	1:A:116:SER:HB3	1.85	0.58
1:A:237:LYS:HB3	1:B:430:LYS:HD2	1.84	0.58
1:A:505:THR:HG23	4:A:2021:HOH:O	2.03	0.58
1:B:513:ILE:O	1:B:516:THR:HB	2.03	0.58
1:B:341:LYS:O	1:B:344:LYS:HG2	2.02	0.58
1:A:280:LEU:HB3	1:A:395:LEU:HD22	1.85	0.58
1:A:478:LEU:HB3	1:A:482:ARG:NH2	2.18	0.58
1:A:142:VAL:HG22	1:A:146:VAL:HG21	1.86	0.57
1:B:80:VAL:HB	1:B:231:GLU:HG2	1.85	0.57
1:A:297:ARG:HB3	1:A:298:PRO:HD3	1.86	0.57
1:A:169:PRO:HB2	4:A:2009:HOH:O	2.04	0.57
1:B:9:PRO:HG2	1:B:12:LEU:CD2	2.35	0.57
1:B:312:ARG:HG2	1:B:457:THR:CG2	2.32	0.57
1:B:285:LYS:HB2	1:B:288:ASP:OD2	2.05	0.57
1:A:341:LYS:O	1:A:344:LYS:HG2	2.05	0.56
1:B:427:PRO:HA	1:B:502:GLU:HA	1.86	0.56
1:B:79:ASN:C	1:B:79:ASN:HD22	2.12	0.56
1:A:342:ILE:O	1:A:346:LEU:HG	2.06	0.56
1:A:550:PRO:HB2	1:A:552:GLN:NE2	2.19	0.56
1:A:425:PHE:CE2	1:A:427:PRO:HG3	2.41	0.56
1:B:6:ALA:HB3	1:B:39:VAL:CG2	2.35	0.56
1:B:125:LYS:HG2	1:B:126:ASN:OD1	2.04	0.56
1:A:411:LEU:HD23	1:A:414:ILE:CD1	2.36	0.56
1:A:282:THR:HG22	1:A:352:ASN:ND2	2.20	0.56
1:B:9:PRO:HG3	1:B:21:PHE:CE2	2.40	0.56
1:B:361:GLU:N	1:B:362:PRO:HD2	2.21	0.56
1:A:167:ASP:OD1	1:A:186:GLY:HA3	2.06	0.56
1:B:77:PRO:O	1:B:126:ASN:HB2	2.06	0.55
1:B:209:LEU:HD11	1:B:231:GLU:HG3	1.87	0.55
1:B:225:THR:HG21	1:B:234:PRO:HG3	1.89	0.55
1:A:314:ILE:HD11	1:A:343:ALA:HA	1.89	0.55
1:A:518:ASN:O	1:A:519:TRP:C	2.48	0.55
1:A:9:PRO:HG3	1:A:21:PHE:CZ	2.42	0.55
2:A:600:FAD:C5B	2:A:600:FAD:C8A	2.73	0.54
1:A:363:ILE:HD11	1:B:367:LEU:HD21	1.88	0.54
1:A:194:TRP:O	1:A:197:HIS:HD2	1.90	0.54
1:A:439:GLN:HA	1:A:500:TRP:CH2	2.42	0.54
1:A:443:THR:HA	1:A:491:LEU:CD2	2.38	0.54
1:A:79:ASN:HD21	1:A:82:ASP:H	1.53	0.54
1:A:13:PRO:HG2	1:A:16:LEU:HD22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:GLU:O	1:A:144:PRO:C	2.49	0.54
1:B:187:TYR:O	1:B:307:ASN:HB2	2.08	0.54
1:B:411:LEU:HD23	1:B:414:ILE:CD1	2.38	0.54
1:A:552:GLN:H	1:A:552:GLN:HE21	1.54	0.54
1:B:98:TRP:CD2	1:B:113:PRO:HA	2.43	0.53
1:B:493:ASP:O	1:B:496:ALA:HB3	2.08	0.53
1:B:230:PRO:O	1:B:231:GLU:C	2.51	0.53
1:A:79:ASN:ND2	1:A:79:ASN:C	2.66	0.53
1:B:12:LEU:HB3	1:B:13:PRO:CD	2.38	0.53
1:A:314:ILE:HG13	1:A:343:ALA:HB2	1.90	0.53
1:B:210:LEU:HD23	1:B:211:ARG:N	2.24	0.53
1:B:57:THR:HG22	1:B:74:ILE:HD11	1.91	0.53
1:B:315:LEU:HD21	1:B:334:LEU:HD12	1.90	0.53
1:B:550:PRO:HB2	1:B:552:GLN:NE2	2.24	0.53
1:A:315:LEU:HD21	1:A:334:LEU:HD12	1.90	0.53
1:B:143:GLU:HB3	1:B:144:PRO:CD	2.39	0.53
1:A:312:ARG:HG2	1:A:457:THR:CG2	2.36	0.52
1:A:289:LEU:HD22	1:A:351:TRP:CZ2	2.43	0.52
1:A:367:LEU:O	1:A:371:ILE:HG13	2.10	0.52
1:B:289:LEU:HD22	1:B:351:TRP:CZ2	2.45	0.52
1:B:414:ILE:O	1:B:420:GLY:HA3	2.09	0.52
1:A:9:PRO:HG2	1:A:12:LEU:CD2	2.40	0.52
1:A:248:PRO:HG3	1:B:257:SER:HB2	1.92	0.52
1:B:478:LEU:HB3	1:B:482:ARG:NH2	2.24	0.52
1:B:24:PHE:O	1:B:28:ILE:HG12	2.09	0.52
1:B:282:THR:HG22	1:B:352:ASN:ND2	2.25	0.52
1:B:224:GLU:CD	1:B:224:GLU:H	2.18	0.52
1:B:483:LYS:O	1:B:487:LEU:N	2.37	0.52
1:B:95:PHE:CE1	1:B:119:VAL:HG23	2.45	0.51
1:B:143:GLU:O	1:B:144:PRO:C	2.53	0.51
1:A:519:TRP:CZ3	1:B:211:ARG:HG2	2.45	0.51
1:A:317:ASP:OD1	1:A:394:VAL:HG21	2.11	0.51
1:B:219:ASP:OD1	1:B:220:PRO:HD2	2.10	0.51
1:B:266:GLY:O	1:B:267:ILE:HD13	2.10	0.51
1:B:312:ARG:CG	1:B:457:THR:HG23	2.33	0.51
1:B:361:GLU:O	1:B:362:PRO:C	2.53	0.51
1:B:367:LEU:O	1:B:371:ILE:HG13	2.11	0.51
1:B:280:LEU:HB3	1:B:395:LEU:HD22	1.93	0.51
1:A:114:ARG:NH1	1:A:511:ASP:OD2	2.44	0.51
1:A:102:ILE:HG12	1:A:175:SER:HB2	1.93	0.51
1:A:219:ASP:OD1	1:A:220:PRO:HD2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:ASP:O	1:B:86:ILE:HG13	2.12	0.50
1:B:398:ARG:HA	1:B:401:THR:HB	1.94	0.50
1:B:421:ALA:HB2	1:B:475:LYS:HG2	1.94	0.50
1:B:421:ALA:HB3	1:B:473:PHE:CZ	2.47	0.50
1:A:393:SER:OG	1:A:396:ARG:HG3	2.11	0.50
1:B:545:LYS:HE2	2:B:600:FAD:O2B	2.11	0.50
1:A:161:ARG:NH2	1:A:405:ILE:HD11	2.26	0.50
1:A:421:ALA:HB2	1:A:475:LYS:HG2	1.94	0.50
1:B:9:PRO:HG3	1:B:21:PHE:CZ	2.47	0.50
1:B:183:ARG:O	1:B:503:TYR:HE2	1.95	0.50
1:B:443:THR:HG21	1:B:469:VAL:CG2	2.40	0.50
1:B:518:ASN:O	1:B:519:TRP:C	2.55	0.50
1:A:77:PRO:O	1:A:126:ASN:HB2	2.12	0.50
1:A:302:GLY:O	1:A:303:MET:HB2	2.12	0.50
1:A:242:PHE:CZ	1:A:244:TYR:HB2	2.47	0.49
1:B:169:PRO:HB2	4:B:2015:HOH:O	2.12	0.49
1:A:12:LEU:HB3	1:A:13:PRO:CD	2.42	0.49
1:B:13:PRO:HG2	1:B:16:LEU:HD22	1.94	0.49
1:A:90:ALA:O	1:A:94:SER:N	2.45	0.49
1:A:439:GLN:HA	1:A:500:TRP:CZ3	2.47	0.49
1:B:357:LEU:HD13	1:B:368:TRP:HB2	1.93	0.49
1:A:531:LEU:HD22	1:B:531:LEU:HD22	1.94	0.49
1:B:108:TYR:O	1:B:506:HIS:HA	2.13	0.49
1:B:155:LEU:O	1:B:156:GLU:C	2.55	0.49
1:B:64:MET:HB2	4:B:2007:HOH:O	2.12	0.49
1:A:248:PRO:HG3	1:B:257:SER:CB	2.43	0.49
1:A:224:GLU:CD	1:A:224:GLU:H	2.19	0.49
1:A:361:GLU:O	1:A:362:PRO:C	2.55	0.49
1:B:79:ASN:ND2	1:B:82:ASP:N	2.57	0.49
1:B:491:LEU:O	1:B:492:ILE:C	2.55	0.49
1:A:258:ASN:HB2	1:A:541:ILE:O	2.12	0.49
1:B:278:SER:OG	1:B:386:PRO:HG3	2.13	0.49
1:A:488:MET:HG2	1:A:509:PHE:CE2	2.48	0.48
1:A:549:TRP:HB2	1:A:555:HIS:HE1	1.78	0.48
1:B:341:LYS:HG2	1:B:344:LYS:NZ	2.28	0.48
1:B:423:LEU:O	1:B:471:ILE:HB	2.13	0.48
1:B:280:LEU:CB	1:B:395:LEU:HD22	2.43	0.48
1:B:315:LEU:HD22	1:B:416:TRP:CZ2	2.48	0.48
1:A:505:THR:HG21	1:A:513:ILE:CD1	2.43	0.48
1:A:155:LEU:O	1:A:156:GLU:C	2.54	0.48
1:B:194:TRP:O	1:B:197:HIS:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:GLN:HE21	1:B:500:TRP:CG	2.31	0.48
1:A:307:ASN:O	1:A:309:PRO:HD3	2.13	0.48
1:A:493:ASP:O	1:A:496:ALA:HB3	2.13	0.48
1:B:341:LYS:HA	1:B:344:LYS:HD3	1.94	0.48
1:B:411:LEU:O	1:B:414:ILE:HD12	2.14	0.48
1:B:342:ILE:O	1:B:346:LEU:HG	2.14	0.48
1:B:115:VAL:HG13	1:B:558:TRP:CH2	2.48	0.47
1:A:257:SER:HB2	1:B:248:PRO:HG3	1.96	0.47
1:B:516:THR:HG22	1:B:517:TYR:CD1	2.49	0.47
1:A:62:HIS:H	1:A:62:HIS:CD2	2.30	0.47
1:B:446:ARG:HH21	1:B:494:ASP:CG	2.22	0.47
1:A:95:PHE:CE1	1:A:119:VAL:HG23	2.49	0.47
1:B:354:TYR:CE2	1:B:394:VAL:HG12	2.49	0.47
1:A:171:LEU:HD11	2:A:600:FAD:HM72	1.97	0.47
1:A:277:GLN:HE21	1:A:278:SER:N	2.13	0.47
1:A:423:LEU:O	1:A:471:ILE:HB	2.14	0.47
1:A:513:ILE:O	1:A:516:THR:HB	2.15	0.47
1:B:314:ILE:HD11	1:B:343:ALA:HA	1.97	0.47
1:A:24:PHE:O	1:A:28:ILE:HG12	2.15	0.47
1:A:79:ASN:HD21	1:A:82:ASP:N	2.12	0.47
1:A:143:GLU:HB3	1:A:144:PRO:HD2	1.96	0.47
1:B:90:ALA:HB1	1:B:95:PHE:O	2.15	0.47
1:B:238:ILE:HG22	1:B:238:ILE:O	2.15	0.47
1:B:190:TYR:CE1	1:B:270:MET:HG3	2.51	0.46
1:B:506:HIS:O	1:B:507:LEU:C	2.58	0.46
1:B:549:TRP:CH2	1:B:558:TRP:HB3	2.50	0.46
1:B:525:LEU:O	1:B:529:GLU:HG3	2.14	0.46
1:A:455:ILE:HG13	4:A:2025:HOH:O	2.15	0.46
1:A:427:PRO:HA	1:A:502:GLU:HA	1.97	0.46
1:A:195:MET:HG2	1:B:244:TYR:OH	2.16	0.46
1:A:285:LYS:HB2	1:A:288:ASP:OD2	2.16	0.46
1:A:341:LYS:HG2	1:A:344:LYS:NZ	2.31	0.46
1:B:346:LEU:O	1:B:347:ASN:HB2	2.15	0.46
1:B:526:ARG:HA	1:B:526:ARG:HD3	1.55	0.46
1:B:149:HIS:CE1	1:B:408:TYR:HE1	2.34	0.46
1:A:210:LEU:HD23	1:A:211:ARG:N	2.31	0.45
1:B:233:GLN:HB3	1:B:234:PRO:HD2	1.97	0.45
1:B:314:ILE:HD13	1:B:314:ILE:O	2.16	0.45
1:A:281:ILE:HD12	1:A:353:PHE:HD2	1.80	0.45
1:A:346:LEU:O	1:A:347:ASN:HB2	2.17	0.45
1:B:90:ALA:O	1:B:94:SER:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:TYR:O	1:A:506:HIS:HA	2.17	0.45
1:A:552:GLN:NE2	1:A:552:GLN:H	2.14	0.45
1:A:177:LEU:HD22	1:A:265:ILE:HB	1.98	0.45
1:B:305:LEU:HD23	1:B:305:LEU:HA	1.79	0.45
1:B:549:TRP:HB2	1:B:555:HIS:HE1	1.82	0.45
1:A:211:ARG:HG2	1:B:519:TRP:CZ3	2.52	0.45
1:B:102:ILE:HD13	1:B:102:ILE:HA	1.87	0.45
1:B:443:THR:HA	1:B:491:LEU:HD21	1.98	0.45
1:B:77:PRO:HG3	1:B:83:VAL:HG22	1.99	0.45
1:A:183:ARG:O	1:A:503:TYR:HE2	2.00	0.45
1:B:188:THR:CB	1:B:189:PRO:CD	2.95	0.45
1:B:348:LEU:HB3	1:B:352:ASN:HD21	1.82	0.45
1:B:310:THR:HB	1:B:457:THR:HG21	1.99	0.45
1:B:505:THR:HG21	1:B:513:ILE:CD1	2.47	0.44
1:A:78:ARG:HB2	1:A:82:ASP:OD2	2.17	0.44
1:A:439:GLN:HE21	1:A:500:TRP:CG	2.35	0.44
1:B:13:PRO:HG3	1:B:95:PHE:CE1	2.52	0.44
1:B:419:ASN:O	1:B:420:GLY:C	2.61	0.44
1:A:64:MET:O	1:A:65:ASP:C	2.60	0.44
1:A:295:ILE:HG23	1:A:374:ALA:HB1	1.99	0.44
1:B:64:MET:O	1:B:65:ASP:C	2.59	0.44
1:A:161:ARG:O	1:A:161:ARG:HG2	2.18	0.44
1:A:175:SER:O	1:A:176:VAL:C	2.58	0.44
1:B:62:HIS:CD2	1:B:62:HIS:H	2.35	0.44
1:B:79:ASN:HD22	1:B:82:ASP:H	1.60	0.44
1:B:324:LYS:HB2	1:B:416:TRP:CD2	2.53	0.44
1:B:223:PRO:O	1:B:226:MET:HG2	2.17	0.44
1:B:309:PRO:HD2	1:B:460:VAL:HB	1.99	0.44
1:A:201:GLU:CD	1:A:264:LYS:HD2	2.43	0.44
1:A:289:LEU:HD11	1:A:458:PHE:CE2	2.53	0.44
1:B:439:GLN:HA	1:B:500:TRP:CH2	2.52	0.44
1:A:291:GLN:O	1:A:292:ALA:C	2.60	0.44
1:A:361:GLU:N	1:A:362:PRO:CD	2.80	0.44
1:A:262:VAL:O	2:A:600:FAD:N6A	2.43	0.44
1:A:280:LEU:HB2	1:A:395:LEU:HD22	2.00	0.44
1:B:102:ILE:HG12	1:B:175:SER:HB2	1.98	0.44
1:B:210:LEU:HD23	1:B:210:LEU:C	2.42	0.44
1:A:20:ASP:O	1:A:21:PHE:C	2.61	0.43
1:A:79:ASN:ND2	1:A:82:ASP:N	2.62	0.43
1:B:443:THR:HA	1:B:491:LEU:HD22	2.00	0.43
1:A:284:PRO:O	1:A:350:ARG:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ILE:O	1:A:420:GLY:HA3	2.17	0.43
1:A:443:THR:HG21	1:A:469:VAL:CG2	2.46	0.43
1:A:13:PRO:HG2	1:A:16:LEU:CD2	2.48	0.43
1:A:98:TRP:CB	1:A:113:PRO:HB3	2.48	0.43
1:A:297:ARG:CB	1:A:298:PRO:CD	2.90	0.43
1:B:90:ALA:HB2	1:B:97:LEU:HD21	2.00	0.43
2:B:600:FAD:H2'	2:B:600:FAD:H5'2	1.38	0.43
1:B:446:ARG:HB2	1:B:491:LEU:HD21	2.00	0.43
1:A:315:LEU:HD22	1:A:416:TRP:CZ2	2.54	0.43
1:B:230:PRO:O	1:B:233:GLN:HG3	2.19	0.43
1:A:13:PRO:HG3	1:A:95:PHE:CE1	2.54	0.43
1:A:225:THR:HG21	1:A:234:PRO:HG3	2.01	0.43
1:A:526:ARG:HA	1:A:526:ARG:HD3	1.67	0.43
1:B:416:TRP:HB3	1:B:472:VAL:CG2	2.47	0.43
1:B:9:PRO:HG2	1:B:12:LEU:HD23	2.00	0.43
1:B:295:ILE:HG23	1:B:374:ALA:HB1	2.01	0.43
1:B:76:ALA:HA	1:B:77:PRO:HD2	1.85	0.43
1:B:504:ARG:HH11	1:B:504:ARG:HD3	1.61	0.43
1:A:324:LYS:HG3	1:A:416:TRP:CZ2	2.54	0.43
1:B:474:ASN:ND2	1:B:477:ASP:HB2	2.34	0.43
1:B:297:ARG:O	1:B:301:LEU:HB2	2.19	0.42
1:A:141:VAL:HG21	1:A:240:HIS:CE1	2.54	0.42
1:A:188:THR:O	1:A:189:PRO:C	2.60	0.42
1:A:202:VAL:HG12	1:A:203:VAL:N	2.35	0.42
1:A:258:ASN:HB2	1:A:532:LYS:NZ	2.34	0.42
1:B:272:ASN:OD1	1:B:273:PRO:HD2	2.19	0.42
1:B:414:ILE:HD11	2:B:600:FAD:HM71	2.01	0.42
1:A:80:VAL:CB	1:A:231:GLU:HG2	2.49	0.42
1:B:307:ASN:HB3	1:B:358:TYR:CE1	2.54	0.42
1:A:280:LEU:HD11	1:A:352:ASN:HD22	1.85	0.42
1:A:439:GLN:CA	1:A:500:TRP:CH2	3.02	0.42
1:A:77:PRO:HG3	1:A:83:VAL:HG22	2.01	0.42
1:A:324:LYS:HB2	1:A:416:TRP:CD2	2.54	0.42
1:A:518:ASN:HA	1:A:522:SER:HA	2.01	0.42
1:B:79:ASN:HD21	1:B:82:ASP:N	2.17	0.42
1:B:412:LYS:O	1:B:412:LYS:HD3	2.20	0.42
1:B:446:ARG:HB3	1:B:487:LEU:HD12	2.01	0.42
1:B:478:LEU:H	1:B:478:LEU:CD1	2.27	0.42
1:A:308:VAL:HG13	1:A:460:VAL:O	2.19	0.42
1:A:454:PHE:CD1	1:A:454:PHE:C	2.98	0.42
1:B:183:ARG:HG3	1:B:255:SER:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:LEU:CD2	1:B:363:ILE:HD11	2.47	0.42
1:A:412:LYS:O	1:A:415:ASP:HB2	2.20	0.42
1:A:417:LEU:HB3	1:A:418:PRO:CD	2.46	0.42
1:A:443:THR:HA	1:A:491:LEU:HD21	2.02	0.42
1:B:291:GLN:O	1:B:292:ALA:C	2.63	0.42
1:A:189:PRO:HB2	1:A:270:MET:HE3	2.01	0.41
1:A:549:TRP:HB2	1:A:555:HIS:CE1	2.55	0.41
1:B:281:ILE:HD12	1:B:353:PHE:HD2	1.84	0.41
1:A:76:ALA:HA	1:A:77:PRO:HD2	1.85	0.41
1:A:425:PHE:CD2	1:A:427:PRO:HD3	2.55	0.41
1:B:114:ARG:NH1	1:B:511:ASP:OD2	2.53	0.41
1:B:161:ARG:HG2	1:B:161:ARG:O	2.20	0.41
1:A:307:ASN:HB3	1:A:358:TYR:CE1	2.55	0.41
1:A:312:ARG:CG	1:A:457:THR:HG23	2.43	0.41
1:A:549:TRP:CH2	1:A:558:TRP:HB3	2.55	0.41
1:B:280:LEU:HD11	1:B:282:THR:HG22	2.03	0.41
1:A:131:LEU:HB2	1:A:141:VAL:O	2.19	0.41
1:B:337:GLU:H	1:B:337:GLU:CD	2.28	0.41
1:A:196:MET:HE2	1:A:196:MET:HA	2.02	0.41
2:A:600:FAD:HO3'	2:A:600:FAD:C10	2.29	0.41
1:B:250:ILE:O	1:B:251:ASP:C	2.62	0.41
1:A:471:ILE:HD13	1:A:487:LEU:HD23	2.02	0.41
1:B:79:ASN:ND2	1:B:79:ASN:C	2.78	0.41
1:A:280:LEU:HD11	1:A:282:THR:HG22	2.03	0.41
1:A:315:LEU:CD1	1:A:453:ASP:HB3	2.51	0.41
1:A:9:PRO:HG2	1:A:12:LEU:HD23	2.03	0.41
1:A:79:ASN:ND2	1:A:81:ALA:N	2.69	0.41
1:A:123:MET:HB3	1:A:123:MET:HE3	1.85	0.41
1:A:125:LYS:HG2	1:A:126:ASN:OD1	2.20	0.41
1:A:317:ASP:OD1	1:A:394:VAL:HG11	2.20	0.41
1:A:505:THR:HG21	1:A:513:ILE:HD13	2.03	0.41
1:B:128:ASN:HD22	1:B:128:ASN:HA	1.55	0.41
1:B:468:ILE:HD11	3:B:601:EUG:H93	2.03	0.41
1:B:488:MET:HG2	1:B:509:PHE:CE2	2.56	0.41
1:A:223:PRO:O	1:A:226:MET:HG2	2.20	0.41
1:A:319:ALA:HA	1:A:322:GLY:O	2.20	0.41
1:B:20:ASP:O	1:B:21:PHE:C	2.63	0.41
1:B:201:GLU:CD	1:B:264:LYS:HD2	2.46	0.41
1:B:398:ARG:O	1:B:401:THR:N	2.54	0.41
1:A:519:TRP:CE3	1:B:211:ARG:HG2	2.56	0.40
1:B:124:GLY:O	1:B:125:LYS:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ARG:HG3	1:B:224:GLU:OE1	2.21	0.40
1:B:368:TRP:HA	1:B:368:TRP:CE3	2.56	0.40
1:B:315:LEU:HD22	1:B:416:TRP:CH2	2.56	0.40
1:B:494:ASP:O	1:B:495:CYS:C	2.64	0.40
1:B:505:THR:HG21	1:B:513:ILE:HD13	2.03	0.40
1:A:80:VAL:CG1	1:A:231:GLU:HG2	2.51	0.40
1:A:90:ALA:HB1	1:A:95:PHE:O	2.22	0.40
1:B:424:PHE:CZ	3:B:601:EUG:H6	2.57	0.40
1:B:142:VAL:HG22	1:B:146:VAL:CB	2.51	0.40
1:A:531:LEU:O	1:A:535:VAL:HG22	2.22	0.40
2:A:600:FAD:H2'	2:A:600:FAD:H5'2	1.35	0.40
1:B:61:HIS:ND1	1:B:422:HIS:ND1	2.70	0.40
1:B:510:MET:O	1:B:511:ASP:C	2.63	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	546/560 (98%)	496 (91%)	44 (8%)	6 (1%)	11	36
1	B	546/560 (98%)	491 (90%)	51 (9%)	4 (1%)	18	47
All	All	1092/1120 (98%)	987 (90%)	95 (9%)	10 (1%)	14	41

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	420	GLY
1	B	420	GLY
1	B	105	ASN
1	A	198	SER
1	A	519	TRP

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Mol	Chain	Res	Type
1	B	418	PRO
1	A	7	PHE
1	A	105	ASN
1	A	418	PRO
1	B	284	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	462/480 (96%)	414 (90%)	48 (10%)	7	22
1	B	463/480 (96%)	417 (90%)	46 (10%)	7	24
All	All	925/960 (96%)	831 (90%)	94 (10%)	7	23

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	11	THR
1	A	40	ILE
1	A	41	SER
1	A	50	SER
1	A	63	VAL
1	A	79	ASN
1	A	100	ILE
1	A	101	SER
1	A	106	SER
1	A	114	ARG
1	A	116	SER
1	A	128	ASN
1	A	142	VAL
1	A	177	LEU
1	A	188	THR
1	A	198	SER
1	A	200	MET

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Mol	Chain	Res	Type
1	A	210	LEU
1	A	211	ARG
1	A	231	GLU
1	A	237	LYS
1	A	255	SER
1	A	290	LYS
1	A	301	LEU
1	A	303	MET
1	A	306	GLN
1	A	314	ILE
1	A	331	THR
1	A	336	ASP
1	A	346	LEU
1	A	350	ARG
1	A	382	LYS
1	A	400	LYS
1	A	412	LYS
1	A	418	PRO
1	A	422	HIS
1	A	426	SER
1	A	457	THR
1	A	472	VAL
1	A	475	LYS
1	A	503	TYR
1	A	505	THR
1	A	513	ILE
1	A	516	THR
1	A	526	ARG
1	A	552	GLN
1	A	554	SER
1	B	7	PHE
1	B	11	THR
1	B	40	ILE
1	B	63	VAL
1	B	78	ARG
1	B	79	ASN
1	B	100	ILE
1	B	106	SER
1	B	114	ARG
1	B	118	SER
1	B	128	ASN
1	B	142	VAL

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Mol	Chain	Res	Type
1	B	177	LEU
1	B	188	THR
1	B	210	LEU
1	B	211	ARG
1	B	231	GLU
1	B	255	SER
1	B	283	LEU
1	B	290	LYS
1	B	301	LEU
1	B	306	GLN
1	B	314	ILE
1	B	331	THR
1	B	336	ASP
1	B	346	LEU
1	B	350	ARG
1	B	382	LYS
1	B	395	LEU
1	B	400	LYS
1	B	412	LYS
1	B	422	HIS
1	B	423	LEU
1	B	426	SER
1	B	457	THR
1	B	472	VAL
1	B	475	LYS
1	B	478	LEU
1	B	502	GLU
1	B	503	TYR
1	B	505	THR
1	B	513	ILE
1	B	516	THR
1	B	526	ARG
1	B	552	GLN
1	B	554	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	79	ASN
1	A	128	ASN
1	A	179	ASN
1	A	197	HIS

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Mol	Chain	Res	Type
1	A	233	GLN
1	A	240	HIS
1	A	277	GLN
1	A	291	GLN
1	A	352	ASN
1	A	392	ASN
1	A	485	GLN
1	A	520	ASN
1	A	552	GLN
1	A	555	HIS
1	B	79	ASN
1	B	128	ASN
1	B	197	HIS
1	B	233	GLN
1	B	291	GLN
1	B	352	ASN
1	B	485	GLN
1	B	520	ASN
1	B	552	GLN
1	B	555	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	EUG	A	601	-	11,11,12	0.70	0	14,14,15	3.37	6 (42%)
2	FAD	B	600	1	58,58,58	2.35	11 (18%)	85,89,89	1.85	23 (27%)
2	FAD	A	600	1	58,58,58	2.45	9 (15%)	85,89,89	1.84	25 (29%)
3	EUG	B	601	-	11,11,12	0.60	0	14,14,15	2.70	7 (50%)

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	EUG	A	601	-	-	4/4/4/5	0/1/1/1
2	FAD	B	600	1	-	13/34/50/50	0/6/6/6
2	FAD	A	600	1	-	15/34/50/50	0/6/6/6
3	EUG	B	601	-	-	4/4/4/5	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	FAD	P-O3P	-14.32	1.44	1.59
2	B	600	FAD	P-O3P	-13.40	1.45	1.59
2	B	600	FAD	PA-O3P	-4.64	1.54	1.59
2	B	600	FAD	PA-O2A	-4.56	1.34	1.55
2	A	600	FAD	PA-O3P	-4.34	1.54	1.59
2	A	600	FAD	PA-O2A	-4.05	1.36	1.55
2	A	600	FAD	P-O2P	-3.54	1.38	1.55
2	B	600	FAD	P-O2P	-3.37	1.39	1.55
2	A	600	FAD	C6-C7	-3.29	1.35	1.39
2	A	600	FAD	O5'-C5'	3.07	1.56	1.44
2	B	600	FAD	O5'-C5'	2.99	1.55	1.44
2	A	600	FAD	O4B-C1B	2.93	1.48	1.42
2	A	600	FAD	O2-C2	-2.88	1.18	1.24
2	B	600	FAD	P-O5'	-2.59	1.49	1.59
2	A	600	FAD	P-O5'	-2.50	1.49	1.59
2	B	600	FAD	C6-C7	-2.35	1.36	1.39
2	B	600	FAD	O2-C2	-2.32	1.19	1.24
2	B	600	FAD	C10-N10	-2.06	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	FAD	C5A-C6A	2.03	1.46	1.41
2	B	600	FAD	O4B-C1B	2.00	1.46	1.42

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	601	EUG	O3-C3-C4	7.75	126.18	114.55
3	A	601	EUG	O3-C3-C2	-6.76	112.43	124.08
2	B	600	FAD	O4B-C1B-N9A	-5.96	96.65	108.09
2	A	600	FAD	C2B-C1B-N9A	5.56	127.12	113.30
3	B	601	EUG	O3-C3-C4	5.05	122.13	114.55
3	A	601	EUG	C9-O3-C3	4.64	124.32	117.51
2	A	600	FAD	C9A-C5X-N5	4.33	127.05	122.45
3	B	601	EUG	C9-O3-C3	4.32	123.86	117.51
2	B	600	FAD	C9A-C5X-N5	4.23	126.94	122.45
3	B	601	EUG	O3-C3-C2	-4.21	116.82	124.08
2	B	600	FAD	C2B-C1B-N9A	4.18	123.68	113.30
2	B	600	FAD	O5B-PA-O1A	-4.12	92.62	108.94
2	A	600	FAD	C5'-C4'-C3'	-4.01	104.66	112.22
2	B	600	FAD	C4'-C3'-C2'	-3.93	107.03	113.57
2	B	600	FAD	C5'-C4'-C3'	-3.84	104.97	112.22
3	A	601	EUG	O4-C4-C3	3.59	128.55	120.13
2	A	600	FAD	O3P-P-O1P	3.57	121.45	110.70
2	B	600	FAD	C5X-N5-C4X	-3.57	112.31	118.09
2	A	600	FAD	C4'-C3'-C2'	-3.53	107.70	113.57
2	B	600	FAD	O3P-P-O1P	3.49	121.22	110.70
2	A	600	FAD	O5B-PA-O1A	-3.41	95.41	108.94
2	A	600	FAD	O3B-C3B-C4B	3.36	120.72	111.08
2	B	600	FAD	O3B-C3B-C4B	3.31	120.59	111.08
2	B	600	FAD	C4X-C10-N10	3.16	121.01	116.48
3	B	601	EUG	O4-C4-C3	3.11	127.44	120.13
2	B	600	FAD	C2A-N1A-C6A	3.09	123.81	118.73
2	B	600	FAD	C6-C5X-N5	-3.05	113.38	118.44
3	B	601	EUG	C6-C5-C4	-3.03	117.46	120.50
2	A	600	FAD	C2A-N1A-C6A	2.89	123.48	118.73
2	A	600	FAD	C6-C5X-N5	-2.89	113.65	118.44
2	A	600	FAD	C5X-N5-C4X	-2.88	113.43	118.09
2	A	600	FAD	C4X-C10-N10	2.86	120.58	116.48
2	A	600	FAD	O4'-C4'-C3'	2.77	115.73	109.25
2	A	600	FAD	O3'-C3'-C2'	-2.76	102.66	108.93
3	B	601	EUG	O4-C4-C5	-2.71	112.09	119.36
2	A	600	FAD	O4B-C1B-N9A	-2.59	103.12	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	FAD	O4'-C4'-C3'	2.52	115.15	109.25
2	B	600	FAD	N3A-C2A-N1A	-2.52	124.77	128.58
2	A	600	FAD	C8M-C8-C9	2.38	123.77	119.57
2	A	600	FAD	O2'-C2'-C3'	2.37	114.80	109.25
2	A	600	FAD	O2A-PA-O1A	2.37	123.47	112.44
3	B	601	EUG	C5-C6-C1	2.35	124.25	121.22
2	B	600	FAD	O4-C4-C4X	-2.32	120.40	126.53
2	A	600	FAD	O2A-PA-O3P	-2.32	101.00	107.27
2	A	600	FAD	C4-N3-C2	-2.32	121.52	125.64
2	B	600	FAD	O4-C4-N3	2.32	124.48	120.11
2	B	600	FAD	O4B-C4B-C5B	-2.31	101.92	109.33
2	B	600	FAD	P-O5'-C5'	2.31	134.59	121.35
3	A	601	EUG	O4-C4-C5	-2.29	113.22	119.36
2	A	600	FAD	O4B-C4B-C5B	-2.21	102.24	109.33
3	A	601	EUG	C5-C6-C1	2.21	124.08	121.22
2	B	600	FAD	O2A-PA-O3P	-2.13	101.50	107.27
2	B	600	FAD	O2-C2-N1	-2.12	118.27	121.80
2	A	600	FAD	C4-C4X-C10	2.12	120.56	116.93
2	A	600	FAD	O4B-C1B-C2B	-2.11	102.11	106.62
2	A	600	FAD	C1'-C2'-C3'	-2.10	103.96	109.66
2	A	600	FAD	O2P-P-O5'	2.09	117.05	107.57
2	B	600	FAD	C9A-N10-C10	-2.07	117.59	120.75
2	B	600	FAD	C5B-C4B-C3B	2.04	122.55	115.21
2	A	600	FAD	C8M-C8-C7	-2.02	116.64	120.76
2	B	600	FAD	O2A-PA-O1A	2.00	121.77	112.44

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	FAD	C5B-O5B-PA-O1A
2	A	600	FAD	C5B-O5B-PA-O2A
2	A	600	FAD	C5B-O5B-PA-O3P
2	A	600	FAD	C4'-C5'-O5'-P
2	A	600	FAD	C5'-O5'-P-O2P
2	A	600	FAD	C5'-O5'-P-O3P
2	B	600	FAD	C5B-O5B-PA-O1A
2	B	600	FAD	C5B-O5B-PA-O2A
2	B	600	FAD	C5B-O5B-PA-O3P
2	B	600	FAD	C4'-C5'-O5'-P
2	B	600	FAD	C5'-O5'-P-O2P
2	B	600	FAD	C5'-O5'-P-O3P

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Mol	Chain	Res	Type	Atoms
3	A	601	EUG	C4-C3-O3-C9
3	B	601	EUG	C4-C3-O3-C9
3	A	601	EUG	C2-C3-O3-C9
2	A	600	FAD	O4'-C4'-C5'-O5'
2	A	600	FAD	C3'-C4'-C5'-O5'
2	B	600	FAD	C3'-C4'-C5'-O5'
3	B	601	EUG	C2-C3-O3-C9
2	A	600	FAD	P-O3P-PA-O1A
2	A	600	FAD	O2'-C2'-C3'-C4'
2	A	600	FAD	P-O3P-PA-O5B
2	B	600	FAD	P-O3P-PA-O5B
2	B	600	FAD	O4B-C4B-C5B-O5B
3	A	601	EUG	C2-C1-C7-C8
3	A	601	EUG	C6-C1-C7-C8
3	B	601	EUG	C2-C1-C7-C8
2	A	600	FAD	C3B-C4B-C5B-O5B
2	B	600	FAD	C3B-C4B-C5B-O5B
3	B	601	EUG	C6-C1-C7-C8
2	A	600	FAD	O4B-C4B-C5B-O5B
2	A	600	FAD	C2'-C3'-C4'-C5'
2	B	600	FAD	C2'-C3'-C4'-C5'
2	B	600	FAD	P-O3P-PA-O1A
2	B	600	FAD	O2'-C2'-C3'-C4'
2	A	600	FAD	N10-C1'-C2'-C3'

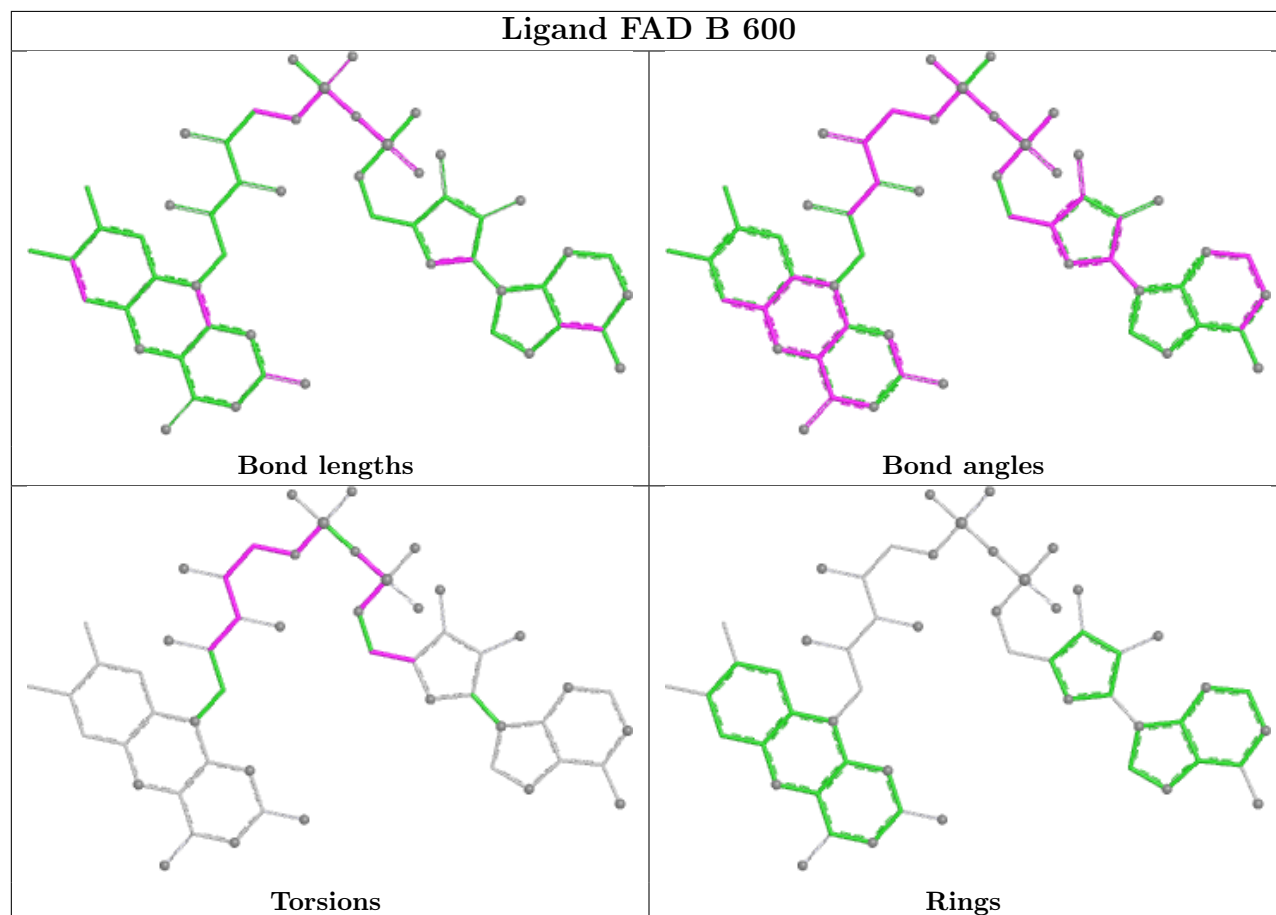
There are no ring outliers.

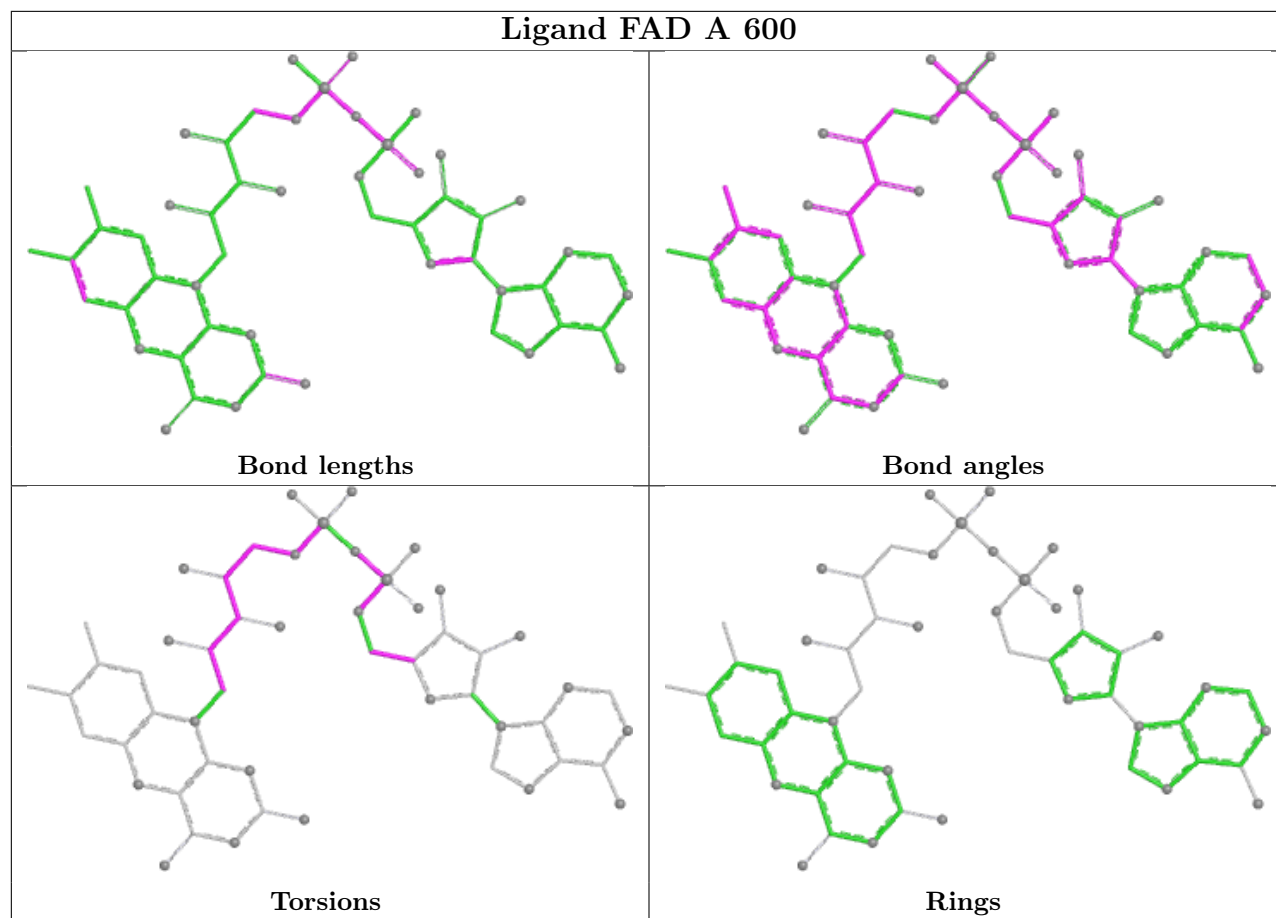
3 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	FAD	8	0
2	A	600	FAD	10	0
3	B	601	EUG	2	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.





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, 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	550/560 (98%)	-0.03	2 (0%) 88 84	16, 28, 53, 77	0
1	B	550/560 (98%)	0.02	8 (1%) 72 63	16, 28, 54, 77	0
All	All	1100/1120 (98%)	-0.00	10 (0%) 81 74	16, 28, 54, 77	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	ALA	3.9
1	B	22	ASN	3.8
1	B	161	ARG	3.4
1	B	41	SER	2.5
1	B	322	GLY	2.5
1	B	387	GLU	2.5
1	B	329	SER	2.3
1	A	7	PHE	2.2
1	B	159	ASN	2.0
1	A	336	ASP	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](#)

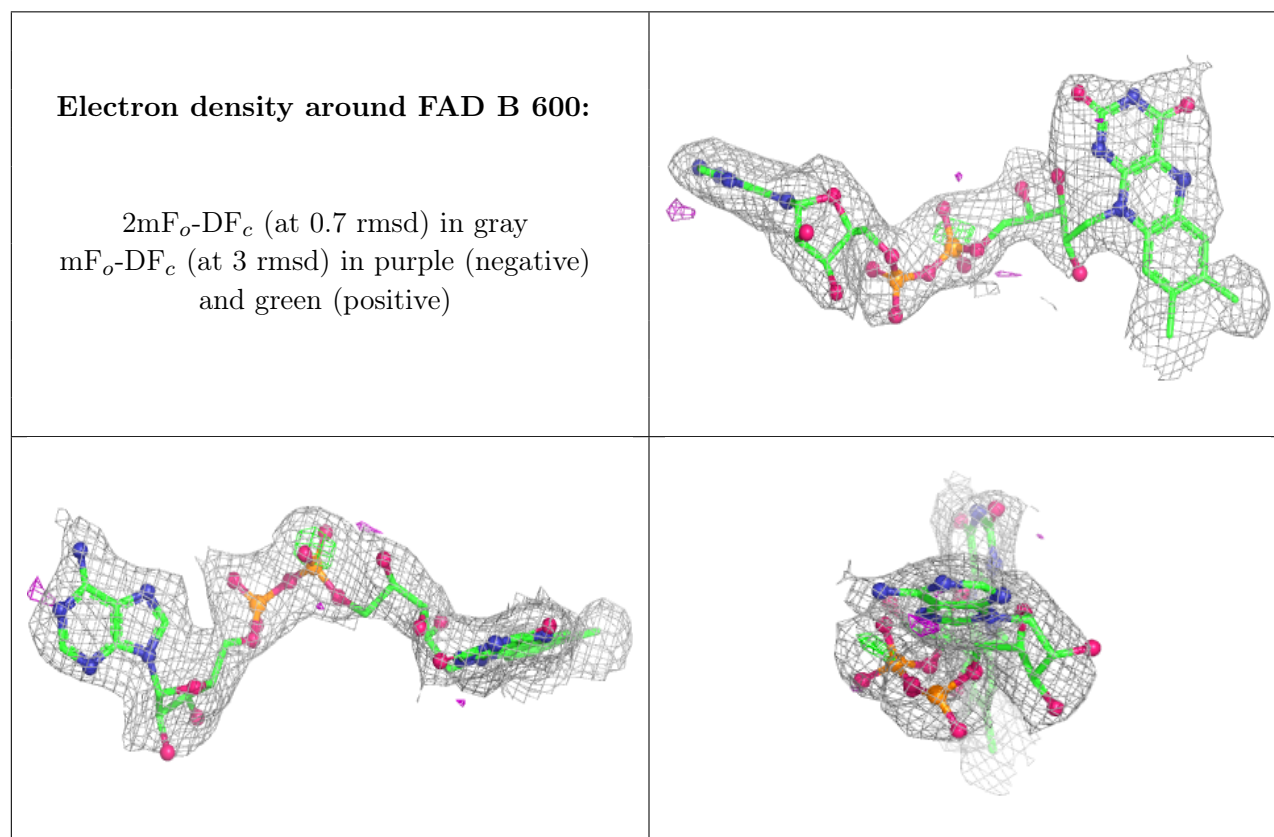
There are no oligosaccharides in this entry.

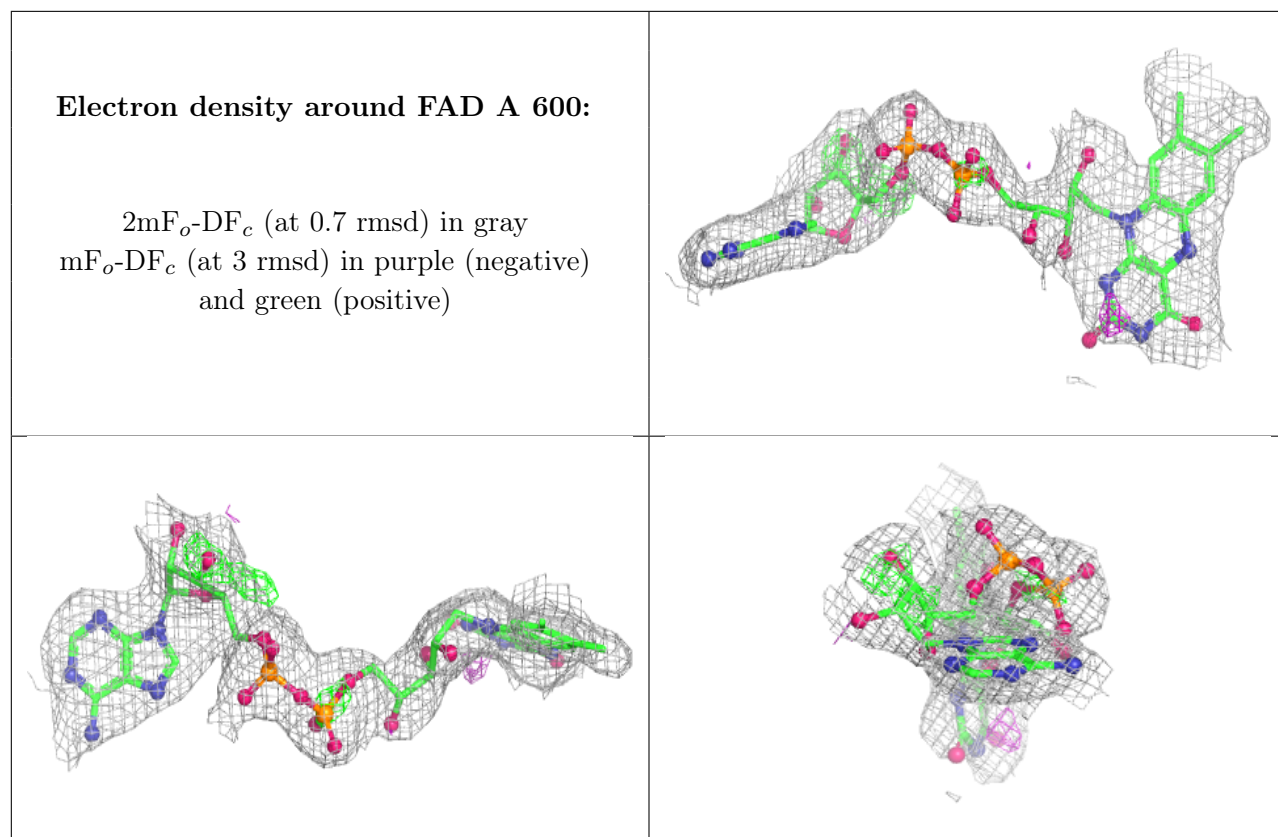
6.4 Ligands [i](#)

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
3	EUG	A	601	11/12	0.85	0.13	34,35,37,37	0
2	FAD	B	600	53/53	0.91	0.13	47,51,52,52	0
2	FAD	A	600	53/53	0.91	0.14	47,51,52,52	0
3	EUG	B	601	11/12	0.91	0.11	34,35,37,38	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.





6.5 Other polymers [i](#)

There are no such residues in this entry.