



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 12:05 PM EDT

PDB ID : 3P4R / pdb_00003p4r
Title : Crystal structure of Menaquinol:fumarate oxidoreductase in complex with glutarate
Authors : Tomasiak, T.M.; Archuleta, T.L.; Andrell, J.; Luna-Chavez, C.; Davis, T.A.; Sarwar, M.; Ham, A.J.; McDonald, W.H.; Yankowskaya, V.; Stern, H.A.; Johnston, J.N.; Maklashina, E.; Cecchini, G.; Iverson, T.M.
Deposited on : 2010-10-07
Resolution : 3.05 Å(reported)

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<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>.

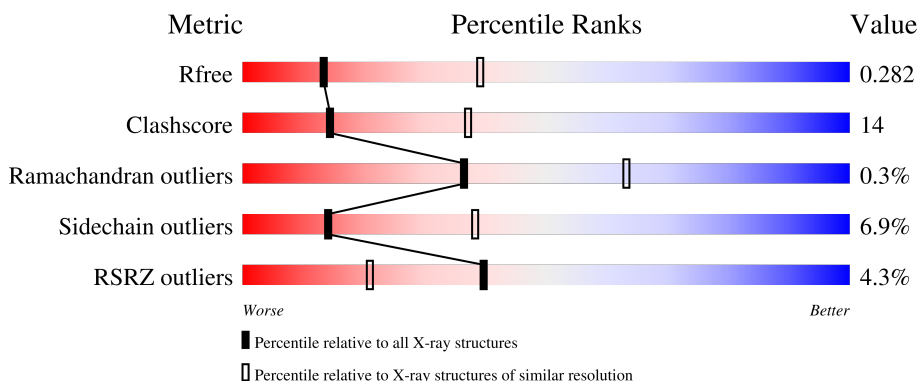
The following versions of software and data (see [references](#) ①) were used in the production of this report:

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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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X-RAY DIFFRACTION

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	577	77% 21%
1	M	577	61% 35%
2	B	243	81% 16%
2	N	243	66% 33%
3	C	130	75% 22%

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Mol	Chain	Length	Quality of chain
3	O	130	
4	D	119	
4	P	119	

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
8	F3S	B	245	-	-	X	-
8	F3S	N	245	-	-	X	-
9	SF4	N	246	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 16804 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 Fumarate reductase flavoprotein subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	577	Total	C	N	O	S	0	0	0
			4449	2775	802	841	31			
1	M	577	Total	C	N	O	S	0	0	0
			4449	2775	802	841	31			

- Molecule 2 is a protein called Fumarate reductase iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	243	Total	C	N	O	S	0	0	0
			1888	1189	323	357	19			
2	N	243	Total	C	N	O	S	0	0	0
			1888	1189	323	357	19			

- Molecule 3 is a protein called Fumarate reductase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	130	Total	C	N	O	S	0	0	0
			1058	720	166	169	3			
3	O	130	Total	C	N	O	S	0	0	0
			1058	720	166	169	3			

- Molecule 4 is a protein called Fumarate reductase subunit D.

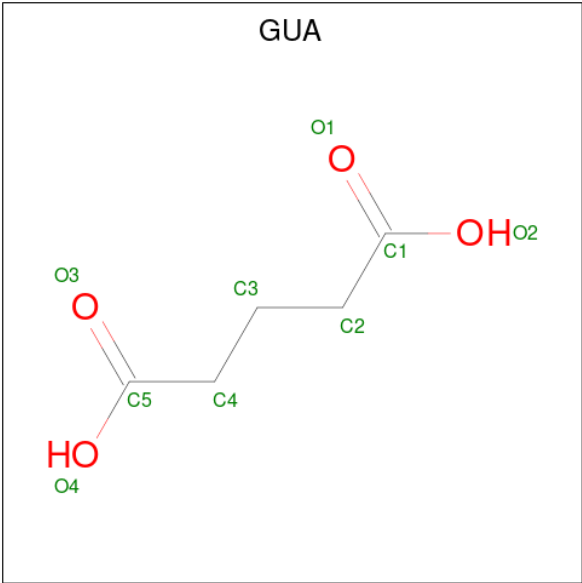
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			
4	P	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



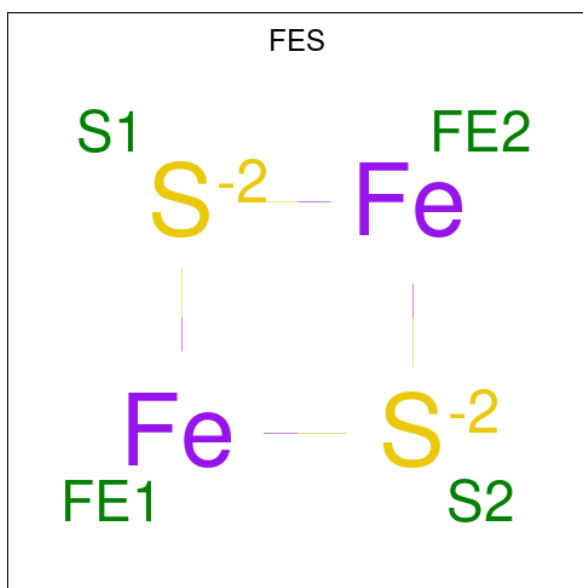
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
5	M	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 6 is GLUTARIC ACID (CCD ID: GUA) (formula: C₅H₈O₄).



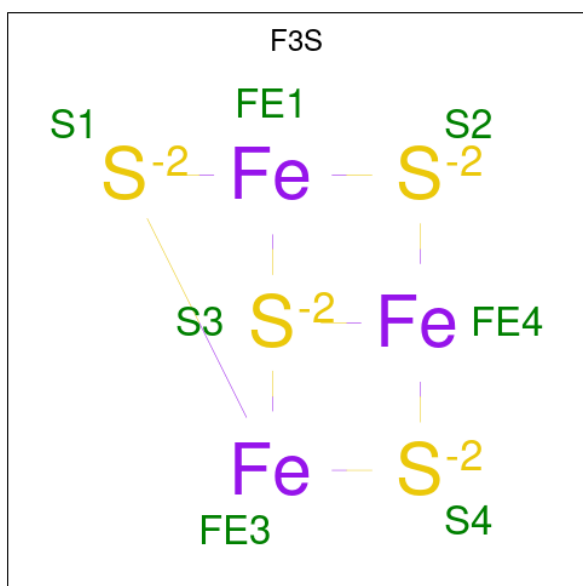
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			9	5	4		
6	M	1	Total	C	O	0	0
			9	5	4		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Fe	S	0	0
			4	2	2		
7	N	1	Total	Fe	S	0	0
			4	2	2		

- Molecule 8 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



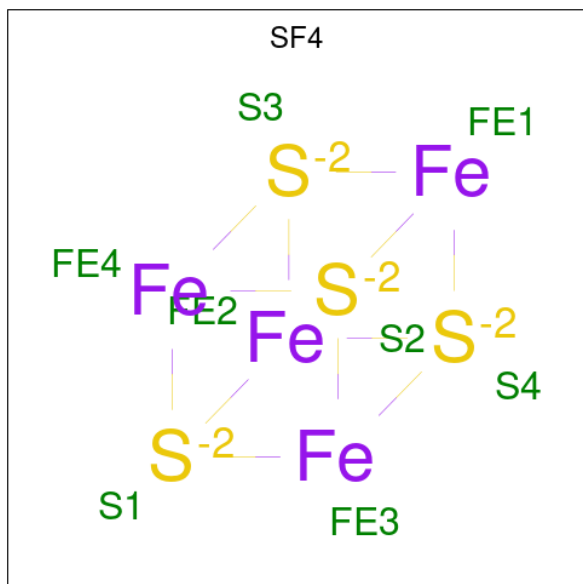
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		

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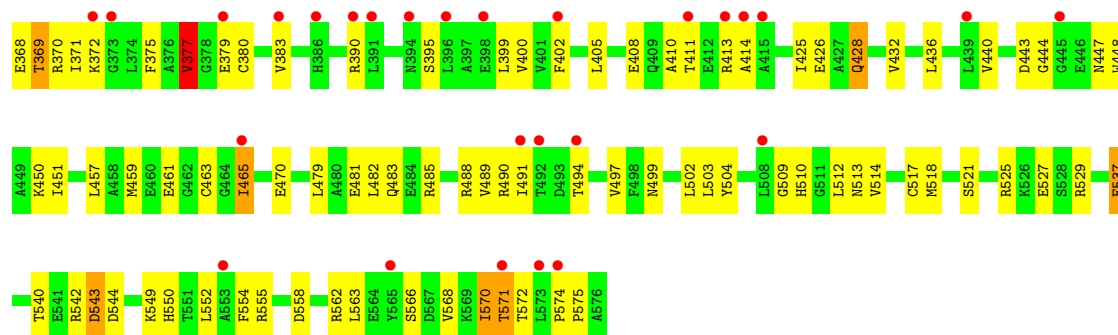
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	N	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 9 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).

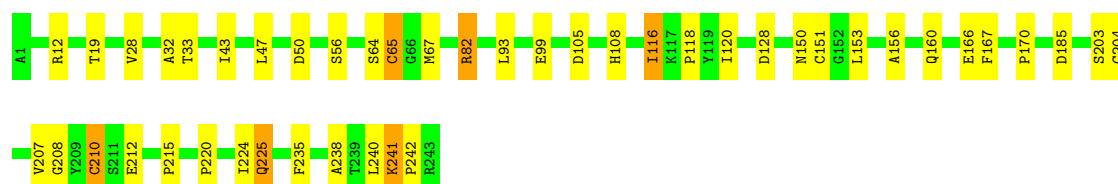


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		
9	N	1	Total	Fe	S	0	0
			8	4	4		



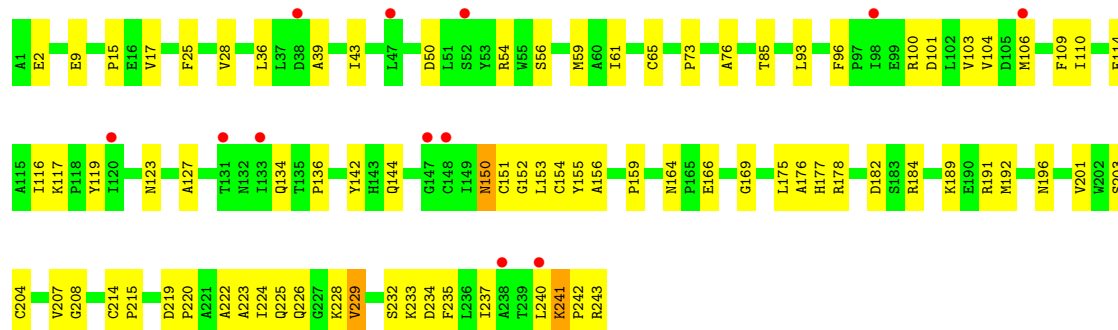
• Molecule 2: Fumarate reductase iron-sulfur subunit

Chain B: 81% 16%



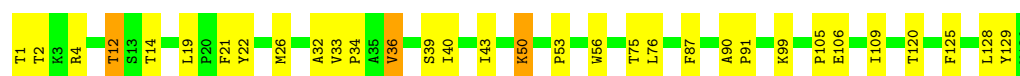
• Molecule 2: Fumarate reductase iron-sulfur subunit

Chain N: 5% 66% 33%



• Molecule 3: Fumarate reductase subunit C

Chain C: 75% 22%

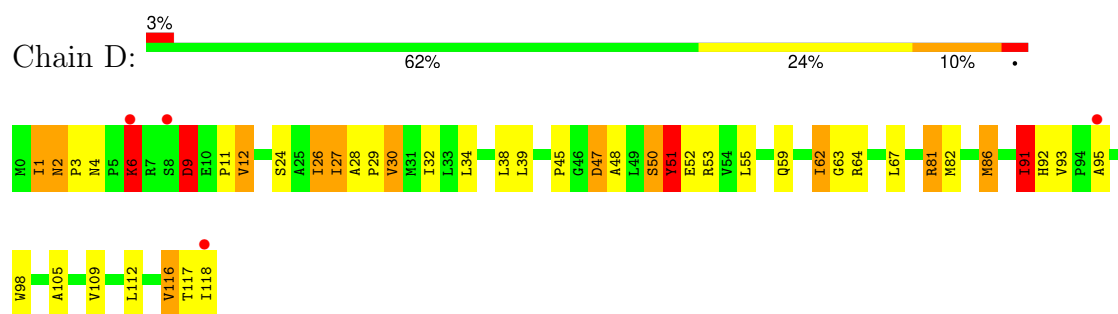


• Molecule 3: Fumarate reductase subunit C

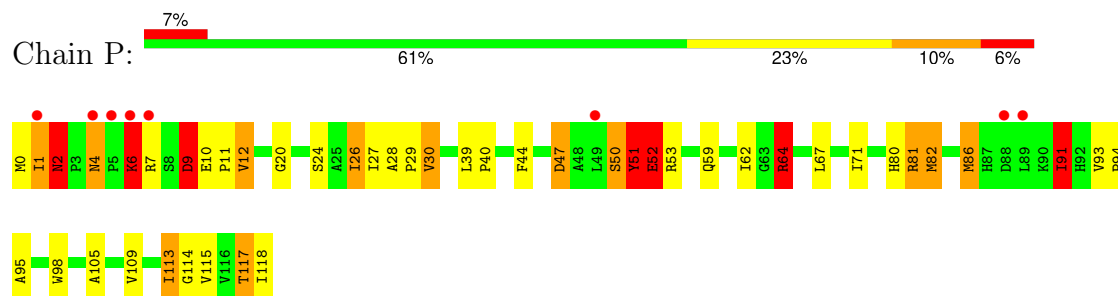
Chain O: 4% 78% 19%



• Molecule 4: Fumarate reductase subunit D



• Molecule 4: Fumarate reductase subunit D



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.68Å 138.02Å 269.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.05 40.00 – 3.05	Depositor EDS
% Data completeness (in resolution range)	95.3 (40.00-3.05) 94.6 (40.00-3.05)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.05 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.248 , 0.284 0.247 , 0.282	Depositor DCC
R_{free} test set	1254 reflections (1.82%)	wwPDB-VP
Wilson B-factor (Å ²)	78.8	Xtriage
Anisotropy	0.452	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16804	wwPDB-VP
Average B, all atoms (Å ²)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% 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, FES, SF4, F3S, GUA

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	0.50	0/4541	0.87	4/6139 (0.1%)
1	M	0.44	0/4541	0.88	5/6139 (0.1%)
2	B	0.47	0/1931	0.84	1/2617 (0.0%)
2	N	0.45	0/1931	0.84	0/2617
3	C	0.49	0/1094	0.88	0/1496
3	O	0.46	0/1094	0.90	2/1496 (0.1%)
4	D	1.28	17/956 (1.8%)	1.40	14/1303 (1.1%)
4	P	1.51	15/956 (1.6%)	1.41	15/1303 (1.2%)
All	All	0.64	32/17044 (0.2%)	0.94	41/23110 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	D	0	2
4	P	0	2
All	All	0	4

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	9	ASP	CG-OD1	18.39	1.60	1.25
4	P	47	ASP	CG-OD2	13.00	1.50	1.25
4	P	51	TYR	CZ-OH	12.18	1.63	1.38
4	P	47	ASP	CA-CB	11.71	1.68	1.53
4	P	4	ASN	CB-CG	11.11	1.79	1.52
4	D	51	TYR	CE1-CZ	-11.03	1.11	1.38
4	P	51	TYR	CE2-CZ	-10.39	1.13	1.38
4	D	51	TYR	CG-CD1	-9.91	1.18	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	P	4	ASN	CG-ND2	9.68	1.53	1.33
4	P	81	ARG	CZ-NH1	9.67	1.46	1.32
4	D	51	TYR	CE2-CZ	-9.65	1.15	1.38
4	D	47	ASP	CG-OD1	9.29	1.43	1.25
4	D	6	LYS	CD-CE	8.60	1.78	1.52
4	D	51	TYR	CZ-OH	7.75	1.54	1.38
4	D	51	TYR	N-CA	-7.73	1.36	1.46
4	P	51	TYR	CB-CG	-7.68	1.34	1.51
4	P	64	ARG	CZ-NH1	7.28	1.43	1.32
4	D	51	TYR	CG-CD2	-7.09	1.24	1.39
4	D	4	ASN	CB-CG	6.81	1.69	1.52
4	P	80	HIS	CE1-NE2	6.78	1.39	1.32
4	D	91	ILE	CB-CG1	6.65	1.66	1.53
4	D	81	ARG	CZ-NH1	6.58	1.42	1.32
4	D	91	ILE	CG1-CD1	6.22	1.75	1.51
4	D	4	ASN	CG-OD1	5.98	1.34	1.23
4	D	62	ILE	CB-CG1	5.84	1.65	1.53
4	P	62	ILE	CB-CG1	5.72	1.64	1.53
4	D	47	ASP	CG-OD2	-5.71	1.14	1.25
4	P	6	LYS	CD-CE	5.61	1.69	1.52
4	D	51	TYR	CA-C	5.61	1.60	1.52
4	D	81	ARG	CZ-NH2	5.35	1.40	1.33
4	P	62	ILE	CG1-CD1	5.17	1.72	1.51
4	P	82	MET	SD-CE	5.01	1.92	1.79

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	47	ASP	CA-CB-CG	-14.98	97.61	112.60
4	D	4	ASN	OD1-CG-ND2	-12.47	110.12	122.60
4	P	4	ASN	OD1-CG-ND2	-11.68	110.92	122.60
4	D	51	TYR	CD1-CG-CD2	-11.63	100.66	118.10
4	D	47	ASP	CA-CB-CG	-11.49	101.11	112.60
4	D	51	TYR	CB-CG-CD2	11.37	137.85	120.80
4	P	51	TYR	CD1-CG-CD2	-11.01	101.58	118.10
4	P	91	ILE	CB-CG1-CD1	10.59	136.04	113.80
4	D	51	TYR	CE1-CZ-CE2	-10.39	99.52	120.30
4	D	51	TYR	N-CA-CB	-9.55	94.34	110.49
4	P	47	ASP	CB-CG-OD2	8.66	138.33	118.40
4	P	51	TYR	CG-CD2-CE2	7.61	132.61	121.20
4	P	4	ASN	CB-CG-ND2	7.28	127.32	116.40
4	D	51	TYR	CD1-CE1-CZ	7.23	132.62	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	2	ASN	CA-C-N	7.20	126.70	118.85
4	P	2	ASN	C-N-CA	7.20	126.70	118.85
3	O	52	GLY	CA-C-N	7.15	127.14	119.28
3	O	52	GLY	C-N-CA	7.15	127.14	119.28
4	D	51	TYR	CZ-CE2-CD2	7.01	132.21	119.60
1	M	39	TYR	CA-C-N	6.77	128.31	119.84
1	M	39	TYR	C-N-CA	6.77	128.31	119.84
4	P	51	TYR	CD1-CE1-CZ	6.68	131.62	119.60
4	P	81	ARG	CD-NE-CZ	-6.24	115.67	124.40
1	M	221	VAL	CA-C-N	6.06	126.26	119.90
1	M	221	VAL	C-N-CA	6.06	126.26	119.90
4	P	47	ASP	CB-CG-OD1	-5.98	104.64	118.40
4	D	47	ASP	N-CA-C	5.88	118.41	110.88
4	D	116	VAL	N-CA-C	-5.71	105.84	112.98
4	D	51	TYR	CB-CA-C	5.70	121.76	110.42
2	B	65	CYS	N-CA-C	5.60	119.38	112.54
4	D	30	VAL	CB-CA-C	-5.35	105.03	111.88
1	A	342	ASP	CA-C-N	5.34	125.06	119.82
1	A	342	ASP	C-N-CA	5.34	125.06	119.82
4	P	51	TYR	CB-CG-CD1	5.31	128.77	120.80
4	P	81	ARG	NE-CZ-NH2	-5.27	114.46	119.20
1	M	377	VAL	N-CA-C	5.24	114.92	108.53
4	D	27	ILE	N-CA-C	5.16	118.12	112.96
1	A	27	ASN	CA-C-N	5.09	124.75	119.56
1	A	27	ASN	C-N-CA	5.09	124.75	119.56
4	P	52	GLU	CG-CD-OE2	-5.06	106.77	118.40
4	D	52	GLU	CG-CD-OE1	5.04	129.99	118.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	D	51	TYR	Sidechain
4	D	9	ASP	Sidechain
4	P	51	TYR	Sidechain
4	P	9	ASP	Sidechain

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	4449	0	4335	97	0
1	M	4449	0	4335	170	0
2	B	1888	0	1841	39	0
2	N	1888	0	1838	65	0
3	C	1058	0	1108	26	0
3	O	1058	0	1108	32	0
4	D	926	0	971	44	0
4	P	926	0	971	51	0
5	A	53	0	31	8	0
5	M	53	0	30	14	0
6	A	9	0	0	1	0
6	M	9	0	0	2	0
7	B	4	0	0	0	0
7	N	4	0	0	0	0
8	B	7	0	0	6	0
8	N	7	0	0	3	0
9	B	8	0	0	1	0
9	N	8	0	0	6	0
All	All	16804	0	16568	468	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 14.

All (468) 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)
4:D:6:LYS:CD	4:D:6:LYS:CE	1.78	1.58
4:D:91:ILE:CD1	4:D:91:ILE:CG1	1.76	1.57
4:P:4:ASN:CG	4:P:4:ASN:CB	1.79	1.55
4:P:51:TYR:OH	4:P:51:TYR:CZ	1.63	1.50
1:A:44:HIS:NE2	5:A:601:FAD:HM82	1.31	1.37
1:M:11:GLY:HA2	5:M:601:FAD:H1B	1.25	1.18
2:N:214:CYS:SG	9:N:246:SF4:S1	2.43	1.17
4:D:92:HIS:HB3	2:N:243:ARG:HB3	1.28	1.15
1:M:44:HIS:NE2	5:M:601:FAD:C8M	2.19	1.05
4:D:86:MET:HE3	4:D:91:ILE:HG21	1.37	1.05
1:A:44:HIS:NE2	5:A:601:FAD:C8M	2.20	1.05
4:P:86:MET:HE3	4:P:91:ILE:HG21	1.32	1.02
1:A:372:LYS:HE3	1:A:413:ARG:HH12	1.25	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:CYS:HG	8:B:245:F3S:FE1	0.79	0.97
4:D:55:LEU:HG	4:D:59:GLN:HE21	1.31	0.94
2:N:116:ILE:HG21	2:N:176:ALA:HB2	1.47	0.94
4:D:55:LEU:HG	4:D:59:GLN:NE2	1.83	0.94
1:M:44:HIS:NE2	5:M:601:FAD:HM83	1.81	0.92
2:N:214:CYS:SG	9:N:246:SF4:FE4	1.61	0.92
1:A:44:HIS:CE1	5:A:601:FAD:HM82	2.04	0.92
1:M:537:GLU:H	1:M:537:GLU:CD	1.80	0.90
3:O:120:THR:HG23	4:P:30:VAL:HG23	1.51	0.90
1:M:44:HIS:NE2	5:M:601:FAD:HM81	1.87	0.89
2:B:151:CYS:HG	9:B:246:SF4:FE1	0.83	0.88
1:M:11:GLY:HA2	5:M:601:FAD:C1B	2.05	0.86
1:M:158:LEU:HD13	1:M:436:LEU:HD11	1.57	0.85
4:P:26:ILE:HG22	4:P:27:ILE:HG13	1.56	0.85
4:P:47:ASP:HB2	4:P:50:SER:OG	1.76	0.84
2:B:32:ALA:O	2:B:82:ARG:NH1	2.10	0.83
4:D:26:ILE:HG22	4:D:27:ILE:HG13	1.60	0.83
9:N:246:SF4:FE3	9:N:246:SF4:S2	1.69	0.83
1:A:92:GLU:HA	1:A:92:GLU:OE1	1.79	0.82
2:B:210:CYS:SG	8:B:245:F3S:FE3	1.71	0.82
4:P:47:ASP:OD1	4:P:47:ASP:N	2.07	0.81
2:N:214:CYS:HG	9:N:246:SF4:FE4	0.96	0.81
1:A:208:VAL:HG12	1:A:208:VAL:O	1.81	0.80
2:N:116:ILE:CG2	2:N:176:ALA:HB2	2.10	0.80
1:M:390:ARG:HD2	1:M:395:SER:HB2	1.64	0.80
1:A:390:ARG:HH22	6:A:577:GUA:C1	1.95	0.79
2:N:222:ALA:O	2:N:226:GLN:HG3	1.82	0.78
4:D:6:LYS:CE	4:D:6:LYS:CG	2.62	0.78
1:M:213:MET:HE2	1:M:360:GLY:HA2	1.65	0.78
1:M:217:LEU:HG	1:M:555:ARG:HB3	1.65	0.77
4:D:64:ARG:HG2	4:D:64:ARG:HH11	1.49	0.77
3:O:5:LYS:O	3:O:5:LYS:HG3	1.85	0.76
1:M:1:GLN:HE21	1:M:2:THR:H	1.34	0.76
2:B:204:CYS:SG	8:B:245:F3S:FE1	1.76	0.75
4:P:51:TYR:HE1	4:P:52:GLU:OE1	1.69	0.75
2:N:196:ASN:ND2	2:N:234:ASP:OD2	2.20	0.75
3:O:28:ARG:O	3:O:31:THR:HB	1.87	0.75
9:N:246:SF4:S1	9:N:246:SF4:FE4	1.77	0.75
1:M:217:LEU:HG	1:M:555:ARG:CB	2.17	0.74
2:N:154:CYS:SG	9:N:246:SF4:S2	2.85	0.74
1:A:232:HIS:CG	1:A:242:LEU:HD11	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:56:TRP:CD1	4:P:51:TYR:HB3	2.23	0.74
1:A:321:GLU:OE1	1:A:344:VAL:HG21	1.89	0.73
1:M:2:THR:HA	1:M:182:GLN:O	1.88	0.72
3:O:40:ILE:HA	3:O:43:ILE:HD12	1.71	0.72
1:M:322:LYS:O	1:M:326:GLU:HB2	1.89	0.72
3:O:31:THR:HG21	3:O:82:HIS:HB2	1.71	0.72
3:O:33:VAL:HB	3:O:34:PRO:HD3	1.71	0.72
1:A:269:GLY:HA2	1:A:282:MET:HE1	1.72	0.72
1:A:324:LEU:HD23	1:A:328:LEU:HD12	1.71	0.71
4:P:51:TYR:CE1	4:P:52:GLU:HG2	2.25	0.71
2:B:225:GLN:HA	2:B:225:GLN:HE21	1.55	0.71
2:B:210:CYS:HG	8:B:245:F3S:FE3	1.07	0.70
2:N:204:CYS:SG	2:N:224:ILE:HG21	2.31	0.70
1:A:197:ARG:HD2	1:A:206:GLY:HA2	1.73	0.69
2:N:54:ARG:HE	2:N:103:VAL:HG13	1.57	0.69
1:A:324:LEU:HD13	1:A:344:VAL:HG22	1.74	0.69
2:N:28:VAL:HG22	2:N:43:ILE:HD11	1.74	0.69
4:D:92:HIS:HB3	2:N:243:ARG:CB	2.17	0.69
1:M:48:ALA:HB3	1:M:132:GLY:HA3	1.75	0.68
1:M:152:PHE:HB3	1:M:155:HIS:ND1	2.08	0.68
3:C:2:THR:OG1	3:C:4:ARG:HG2	1.92	0.68
1:A:356:TYR:CE1	1:A:379:GLU:HG3	2.28	0.68
1:M:7:LEU:HD21	1:M:411:THR:HA	1.75	0.68
1:M:224:ARG:NH2	1:M:363:THR:O	2.26	0.67
1:A:18:ARG:HG2	1:A:400:VAL:HA	1.77	0.67
1:M:152:PHE:HD2	1:M:155:HIS:CE1	2.12	0.67
2:N:225:GLN:HE21	3:O:93:ALA:HB2	1.58	0.67
1:A:253:ILE:HG13	1:A:315:ASP:HB3	1.76	0.67
2:N:164:ASN:OD1	2:N:166:GLU:HG2	1.95	0.67
1:A:514:VAL:HG12	1:A:518:MET:HE3	1.77	0.67
1:M:162:VAL:HG21	1:M:371:ILE:HD13	1.76	0.67
1:A:204:ASN:N	1:A:204:ASN:HD22	1.93	0.66
1:M:155:HIS:CD2	1:M:174:ASN:HA	2.31	0.66
2:B:28:VAL:HG22	2:B:43:ILE:HD11	1.77	0.66
3:C:12:THR:HG22	3:C:14:THR:H	1.60	0.66
1:M:525:ARG:HD2	1:M:527:GLU:HG2	1.78	0.66
4:P:44:PHE:HE1	4:P:47:ASP:HA	1.61	0.66
1:M:315:ASP:OD1	1:M:317:ARG:HG3	1.95	0.66
1:A:11:GLY:HA2	5:A:601:FAD:H1B	1.77	0.65
3:C:50:LYS:HB3	4:D:118:ILE:CG2	2.26	0.65
3:C:33:VAL:HB	3:C:34:PRO:HD3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:ASN:HD22	1:A:174:ASN:C	2.05	0.65
1:M:42:ARG:NH2	2:N:150:ASN:O	2.30	0.65
1:A:46:VAL:HG23	1:A:133:PHE:HA	1.78	0.65
4:D:86:MET:HG3	4:D:93:VAL:HG21	1.78	0.65
1:A:41:MET:HE2	2:B:150:ASN:HD22	1.62	0.64
1:M:116:PHE:CE2	1:M:245:GLU:HB3	2.32	0.64
1:M:529:ARG:HH21	1:M:542:ARG:HE	1.44	0.64
1:A:0:MET:HE1	1:A:429:ALA:HB1	1.79	0.64
1:M:92:GLU:HB3	1:M:400:VAL:HB	1.78	0.64
4:D:92:HIS:CB	2:N:243:ARG:HB3	2.17	0.64
2:B:238:ALA:HA	2:B:241:LYS:HD2	1.79	0.64
3:C:50:LYS:CB	4:D:118:ILE:HG22	2.29	0.63
1:M:224:ARG:HH21	1:M:363:THR:H	1.46	0.63
1:A:372:LYS:HE3	1:A:413:ARG:NH1	2.06	0.63
3:C:50:LYS:HB3	4:D:118:ILE:HG22	1.81	0.63
1:M:35:ILE:HD13	1:M:157:VAL:HG23	1.81	0.63
2:N:65:CYS:HB2	2:N:76:ALA:HB3	1.80	0.63
4:P:86:MET:HE3	4:P:91:ILE:CG2	2.19	0.62
1:M:232:HIS:HD2	1:M:234:THR:O	1.83	0.62
1:A:390:ARG:HD2	1:A:395:SER:HB2	1.82	0.62
1:A:398:GLU:HG2	1:A:402:PHE:HD1	1.64	0.62
1:A:208:VAL:O	1:A:208:VAL:CG1	2.48	0.62
1:M:316:LEU:HB3	1:M:319:LEU:HD12	1.82	0.61
1:M:331:ILE:HA	1:M:334:LEU:HD12	1.83	0.61
1:A:546:ASN:O	1:A:549:LYS:HE2	2.00	0.61
1:M:233:PRO:HG2	1:M:248:ARG:HH22	1.64	0.61
1:A:61:SER:HB3	1:A:64:TYR:CD2	2.36	0.61
2:B:242:PRO:HB3	4:P:93:VAL:C	2.26	0.61
3:C:120:THR:HA	4:D:30:VAL:HG21	1.83	0.61
3:C:105:PRO:O	3:C:109:ILE:HG12	2.00	0.60
3:O:50:LYS:HG3	4:P:118:ILE:HA	1.83	0.60
1:A:232:HIS:CD2	1:A:242:LEU:HD11	2.36	0.60
1:M:105:ARG:HD3	2:N:134:GLN:O	2.00	0.60
1:M:222:PRO:HG2	1:M:362:GLU:HB3	1.82	0.60
3:C:120:THR:HG23	4:D:30:VAL:HG22	1.84	0.60
1:M:158:LEU:HD22	1:M:436:LEU:HD21	1.83	0.60
1:A:176:MET:HE3	1:A:176:MET:HA	1.84	0.60
1:M:6:ASP:OD2	1:M:30:ALA:HA	2.03	0.59
3:O:28:ARG:HD2	4:P:81:ARG:NH2	2.18	0.59
1:M:155:HIS:HD2	1:M:174:ASN:HA	1.68	0.59
3:C:120:THR:HA	4:D:30:VAL:CG2	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:GLU:HB2	1:A:347:PRO:CD	2.33	0.59
1:A:462:GLY:HA3	1:A:475:THR:OG1	2.03	0.59
2:B:153:LEU:HD12	2:B:215:PRO:HD3	1.83	0.58
1:M:197:ARG:HD2	1:M:206:GLY:HA2	1.83	0.58
1:A:65:HIS:HA	1:A:123:ARG:NH1	2.18	0.58
1:M:18:ARG:NH1	1:M:92:GLU:OE1	2.36	0.58
1:M:84:TYR:OH	1:M:405:LEU:HD11	2.03	0.58
1:A:321:GLU:OE1	1:A:321:GLU:HA	2.03	0.58
1:M:95:GLN:HE21	2:N:127:ALA:HB2	1.69	0.58
1:M:180:LEU:HD12	1:M:180:LEU:H	1.69	0.57
1:A:174:ASN:ND2	1:A:177:GLU:H	2.01	0.57
2:B:120:ILE:CD1	2:B:185:ASP:HB2	2.34	0.57
4:D:86:MET:HE3	4:D:91:ILE:CG2	2.21	0.57
1:M:44:HIS:CE1	1:M:204:ASN:HA	2.39	0.57
1:M:510:HIS:O	1:M:514:VAL:HG23	2.04	0.57
3:O:31:THR:CG2	3:O:82:HIS:HB2	2.34	0.57
1:A:7:LEU:HD21	1:A:32:ILE:HG12	1.86	0.57
1:M:46:VAL:HG23	1:M:133:PHE:HA	1.87	0.57
3:O:90:ALA:N	3:O:91:PRO:HD2	2.19	0.57
4:P:4:ASN:CG	4:P:4:ASN:CA	2.72	0.57
1:M:399:LEU:HD21	5:M:601:FAD:O2P	2.05	0.56
2:N:134:GLN:NE2	2:N:142:TYR:HE2	2.03	0.56
2:N:36:LEU:HD23	2:N:76:ALA:HA	1.88	0.56
1:A:232:HIS:HD2	1:A:234:THR:H	1.52	0.56
4:P:51:TYR:CD1	4:P:52:GLU:N	2.74	0.56
2:N:207:VAL:HG23	8:N:245:F3S:S2	2.46	0.56
2:B:210:CYS:HB2	2:B:220:PRO:HG2	1.87	0.56
3:C:75:THR:HG22	4:D:32:ILE:HD13	1.88	0.56
3:O:33:VAL:HA	4:P:82:MET:HE2	1.88	0.56
4:P:47:ASP:CB	4:P:50:SER:OG	2.49	0.56
1:A:246:GLY:O	1:A:250:GLU:HG2	2.06	0.55
2:N:93:LEU:HG	2:N:156:ALA:HB2	1.88	0.55
1:M:44:HIS:CE1	5:M:601:FAD:HM81	2.41	0.55
1:M:214:GLY:HA3	1:M:510:HIS:CD2	2.41	0.55
2:B:212:GLU:HG3	3:C:21:PHE:CE2	2.42	0.55
3:C:53:PRO:HA	4:D:51:TYR:CE1	2.42	0.55
3:O:65:ASN:HB3	3:O:68:ILE:HG12	1.87	0.55
1:M:35:ILE:HG12	5:M:601:FAD:H2A	1.87	0.54
4:P:105:ALA:O	4:P:109:VAL:HG23	2.08	0.54
1:M:405:LEU:HA	1:M:408:GLU:HB2	1.89	0.54
1:A:197:ARG:HB2	1:A:208:VAL:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:87:PHE:O	3:C:109:ILE:HD13	2.07	0.54
1:M:5:ALA:HA	1:M:31:LYS:HB3	1.89	0.54
1:A:42:ARG:HG2	2:B:64:SER:HB3	1.89	0.54
1:A:61:SER:HB3	1:A:64:TYR:CE2	2.42	0.54
1:A:279:ASN:O	1:A:280:LYS:HB2	2.07	0.54
1:M:46:VAL:CG2	1:M:133:PHE:HA	2.38	0.54
1:M:375:PHE:CZ	1:M:410:ALA:HA	2.42	0.54
1:A:46:VAL:HB	1:A:136:LEU:HD23	1.88	0.54
3:C:125:PHE:O	3:C:129:TYR:HB2	2.07	0.54
1:M:166:HIS:CD2	1:M:372:LYS:HB3	2.43	0.54
1:A:314:LEU:HD23	1:A:348:ILE:HD11	1.89	0.54
1:M:529:ARG:NH2	1:M:544:ASP:OD1	2.41	0.54
1:M:175:MET:HE3	1:M:503:LEU:HD13	1.90	0.54
4:D:105:ALA:O	4:D:109:VAL:HG23	2.08	0.54
1:M:377:VAL:HG11	1:M:402:PHE:O	2.08	0.54
2:N:116:ILE:HG22	2:N:191:ARG:HD3	1.89	0.54
3:O:39:SER:OG	4:P:71:ILE:O	2.25	0.54
3:O:120:THR:HA	4:P:30:VAL:HG21	1.90	0.53
1:M:18:ARG:HG2	1:M:400:VAL:HA	1.89	0.53
1:M:571:THR:HG22	1:M:572:THR:N	2.23	0.53
2:B:225:GLN:HA	2:B:225:GLN:NE2	2.23	0.53
1:M:214:GLY:HA3	1:M:510:HIS:HD2	1.73	0.53
1:M:157:VAL:HG22	1:M:170:LEU:HD13	1.91	0.53
1:M:1:GLN:HE21	1:M:2:THR:N	2.02	0.53
1:M:358:MET:SD	1:M:390:ARG:N	2.82	0.53
1:M:451:ILE:HG23	1:M:482:LEU:HD22	1.91	0.53
2:N:116:ILE:HG21	2:N:176:ALA:CB	2.31	0.52
4:P:44:PHE:CE1	4:P:47:ASP:HA	2.42	0.52
1:A:10:VAL:HG21	1:A:190:MET:HE1	1.91	0.52
2:B:240:LEU:O	2:B:242:PRO:HD3	2.09	0.52
1:M:168:ARG:HD3	1:M:425:ILE:HD11	1.89	0.52
3:O:32:ALA:HB2	4:P:81:ARG:HD3	1.91	0.52
1:M:35:ILE:HD13	1:M:157:VAL:CG2	2.39	0.52
1:A:51:GLY:HA2	1:A:131:THR:HG21	1.92	0.52
1:M:44:HIS:HE1	1:M:204:ASN:HA	1.74	0.52
1:A:390:ARG:HH11	1:A:395:SER:HB3	1.74	0.52
2:N:159:PRO:HG2	2:N:207:VAL:HG21	1.91	0.52
3:O:50:LYS:HD2	4:P:117:THR:HB	1.92	0.52
4:D:62:ILE:CG2	4:D:63:GLY:N	2.73	0.52
1:A:466:TYR:CD2	1:A:535:LEU:HD21	2.44	0.52
1:M:213:MET:HE3	1:M:380:CYS:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:224:ARG:HH21	1:M:363:THR:N	2.08	0.52
2:N:155:TYR:CE2	2:N:169:GLY:HA3	2.44	0.52
1:M:79:GLN:HB2	1:M:571:THR:HB	1.91	0.51
1:M:330:PHE:HZ	2:N:61:ILE:HB	1.75	0.51
2:N:106:MET:O	2:N:110:ILE:HG12	2.11	0.51
2:N:225:GLN:NE2	3:O:93:ALA:HB2	2.23	0.51
2:B:170:PRO:HA	2:B:224:ILE:HD11	1.93	0.51
1:M:35:ILE:CD1	1:M:157:VAL:HG23	2.41	0.51
1:M:217:LEU:HD21	1:M:517:CYS:SG	2.51	0.51
2:N:153:LEU:HD12	2:N:215:PRO:HD3	1.92	0.51
1:A:326:GLU:OE2	1:A:327:ARG:NH1	2.44	0.51
1:M:226:MET:HB3	1:M:518:MET:HA	1.92	0.51
1:A:7:LEU:CD2	1:A:32:ILE:HG12	2.40	0.50
1:M:217:LEU:HG	1:M:555:ARG:HB2	1.90	0.50
1:M:369:THR:HG22	1:M:370:ARG:H	1.77	0.50
3:C:56:TRP:CD1	4:D:51:TYR:HB2	2.46	0.50
4:P:10:GLU:N	4:P:11:PRO:HD2	2.26	0.50
1:M:46:VAL:HB	1:M:136:LEU:HD23	1.94	0.50
1:M:168:ARG:HD3	1:M:425:ILE:CD1	2.42	0.50
1:A:159:ASP:HA	1:A:215:MET:HE3	1.93	0.50
1:M:152:PHE:CD2	1:M:155:HIS:CE1	2.97	0.50
1:M:103:TRP:CZ3	1:M:125:TRP:HB3	2.46	0.49
1:A:13:GLY:H	5:A:601:FAD:H4B	1.76	0.49
4:D:6:LYS:HB3	4:P:6:LYS:HG2	1.94	0.49
1:M:79:GLN:HG3	1:M:570:ILE:HA	1.95	0.49
1:M:326:GLU:HB3	1:M:327:ARG:HD3	1.94	0.49
1:A:287:ARG:NH2	1:A:390:ARG:O	2.46	0.49
1:A:308:ARG:HD2	2:B:33:THR:HG21	1.94	0.49
4:D:112:LEU:O	4:D:116:VAL:HG23	2.11	0.49
4:D:28:ALA:N	4:D:29:PRO:HD2	2.28	0.49
1:M:358:MET:HG2	1:M:390:ARG:HB2	1.93	0.49
1:M:517:CYS:O	1:M:521:SER:OG	2.27	0.49
1:A:97:GLU:OE1	1:A:105:ARG:NH2	2.37	0.49
1:M:99:TRP:CD2	1:M:142:THR:HG21	2.48	0.49
1:M:161:LEU:O	1:M:167:VAL:HA	2.13	0.49
1:M:549:LYS:HA	1:M:568:VAL:HG23	1.94	0.49
3:O:40:ILE:O	3:O:43:ILE:HB	2.12	0.49
2:N:151:CYS:SG	2:N:152:GLY:N	2.85	0.49
1:A:256:ASN:HD21	1:A:260:TYR:HB3	1.77	0.49
2:B:120:ILE:HD12	2:B:185:ASP:HB2	1.95	0.49
2:N:208:GLY:N	8:N:245:F3S:S1	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLN:HB3	2:B:118:PRO:O	2.13	0.49
3:C:125:PHE:CE1	3:C:129:TYR:HD1	2.31	0.49
1:M:11:GLY:CA	5:M:601:FAD:C1B	2.86	0.49
4:P:86:MET:HG3	4:P:93:VAL:HG21	1.93	0.49
1:M:144:LEU:HD13	2:N:114:GLU:HG2	1.94	0.48
3:O:130:TRP:HB3	4:P:53:ARG:HH21	1.78	0.48
1:A:48:ALA:HA	5:A:601:FAD:C6	2.43	0.48
1:A:174:ASN:C	1:A:174:ASN:ND2	2.71	0.48
4:P:9:ASP:C	4:P:11:PRO:HD2	2.38	0.48
1:A:390:ARG:NH1	1:A:395:SER:HB3	2.27	0.48
3:C:90:ALA:N	3:C:91:PRO:HD2	2.27	0.48
1:A:448:TRP:HE3	1:A:508:LEU:HD22	1.79	0.48
1:M:48:ALA:HB3	1:M:132:GLY:CA	2.43	0.48
1:M:491:ILE:HD13	1:M:502:LEU:HD12	1.94	0.48
1:M:549:LYS:HB2	1:M:566:SER:O	2.12	0.48
1:A:68:ASP:HB3	1:A:391:LEU:HD21	1.96	0.48
1:A:435:ARG:O	1:A:438:ASP:HB2	2.14	0.48
4:D:62:ILE:HG22	4:D:63:GLY:N	2.29	0.48
2:B:167:PHE:CD1	2:B:203:SER:HB2	2.49	0.48
1:M:497:VAL:HG21	2:N:15:PRO:HG2	1.96	0.48
2:N:201:VAL:O	2:N:228:LYS:HE3	2.14	0.48
2:N:225:GLN:HG3	3:O:93:ALA:HA	1.96	0.48
1:A:366:ASN:O	1:A:367:CYS:HB2	2.13	0.48
4:D:95:ALA:HB1	4:D:98:TRP:HB2	1.95	0.48
1:M:157:VAL:HB	5:M:601:FAD:N1A	2.28	0.48
2:N:225:GLN:HE21	3:O:93:ALA:CB	2.24	0.48
4:P:51:TYR:CD1	4:P:51:TYR:C	2.89	0.48
1:A:271:GLU:HA	1:A:282:MET:HE3	1.95	0.48
2:N:155:TYR:CZ	2:N:169:GLY:HA3	2.49	0.48
1:M:116:PHE:HE2	6:M:577:GUA:O3	1.96	0.47
1:M:273:PRO:HG2	1:M:276:GLU:HG3	1.96	0.47
4:P:51:TYR:CD2	4:P:51:TYR:N	2.81	0.47
1:M:58:ASP:C	1:M:60:ASP:H	2.21	0.47
2:N:134:GLN:NE2	2:N:142:TYR:CE2	2.83	0.47
1:M:483:GLN:NE2	1:M:555:ARG:HH12	2.12	0.47
3:C:125:PHE:CD1	3:C:129:TYR:CD1	3.02	0.47
1:M:21:ILE:O	1:M:25:GLN:HG3	2.14	0.47
1:M:133:PHE:HE2	1:M:134:HIS:CE1	2.31	0.47
2:N:50:ASP:O	2:N:100:ARG:NH1	2.46	0.47
1:A:365:GLN:H	1:A:365:GLN:CD	2.23	0.47
1:M:230:GLN:HB2	1:M:358:MET:HE2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:328:LEU:N	1:M:329:PRO:CD	2.77	0.47
3:O:64:GLN:NE2	4:P:40:PRO:O	2.43	0.47
4:P:9:ASP:O	4:P:12:VAL:HG23	2.15	0.47
3:O:25:TYR:HD1	3:O:28:ARG:NH2	2.12	0.47
1:A:346:GLU:HB2	1:A:347:PRO:HD3	1.96	0.47
2:B:225:GLN:HE21	2:B:225:GLN:CA	2.24	0.46
1:M:116:PHE:CE2	6:M:577:GUA:O3	2.68	0.46
1:M:253:ILE:HG12	1:M:318:HIS:CE1	2.50	0.46
1:M:550:HIS:HB2	1:M:566:SER:OG	2.15	0.46
2:N:39:ALA:O	2:N:43:ILE:HG12	2.15	0.46
3:C:32:ALA:HB2	4:D:81:ARG:HD3	1.97	0.46
1:M:256:ASN:HB2	1:M:302:ASN:O	2.15	0.46
2:N:106:MET:HE3	2:N:109:PHE:CD2	2.51	0.46
1:A:114:ARG:O	1:A:124:THR:HB	2.16	0.46
1:A:328:LEU:N	1:A:329:PRO:CD	2.78	0.46
3:C:36:VAL:HG21	4:D:82:MET:HE1	1.98	0.46
2:N:9:GLU:HG3	2:N:25:PHE:CE2	2.51	0.46
3:O:36:VAL:HG21	4:P:82:MET:HE1	1.98	0.46
1:A:304:ILE:HD12	1:A:304:ILE:H	1.81	0.46
1:M:35:ILE:HD12	1:M:155:HIS:HB3	1.98	0.46
1:A:151:ARG:NH1	1:A:153:ASP:OD2	2.48	0.46
1:M:142:THR:O	1:M:145:GLN:HG2	2.16	0.46
2:N:136:PRO:HB2	3:O:100:ASP:OD1	2.16	0.46
1:M:499:ASN:O	1:M:503:LEU:HG	2.15	0.46
2:B:108:HIS:ND1	4:D:1:ILE:HD11	2.31	0.46
1:M:312:VAL:HG13	1:M:313:TYR:N	2.31	0.46
1:M:509:GLY:HA2	1:M:512:LEU:HD12	1.98	0.46
4:D:9:ASP:C	4:D:11:PRO:HD2	2.40	0.45
1:M:83:ASP:O	1:M:87:HIS:HD2	1.99	0.45
1:M:10:VAL:HG13	5:M:601:FAD:C2A	2.46	0.45
1:M:440:VAL:O	1:M:490:ARG:NH1	2.50	0.45
1:M:521:SER:HA	1:M:563:LEU:HD21	1.98	0.45
2:N:59:MET:HG3	2:N:61:ILE:HG22	1.99	0.45
4:P:95:ALA:HB1	4:P:98:TRP:HB2	1.98	0.45
1:M:10:VAL:HG22	1:M:157:VAL:HG21	1.98	0.45
1:M:428:GLN:O	1:M:432:VAL:HG23	2.17	0.45
2:N:177:HIS:CE1	2:N:226:GLN:HB2	2.52	0.45
1:M:151:ARG:NH1	1:M:153:ASP:OD2	2.50	0.45
1:M:203:THR:OG1	1:M:355:HIS:ND1	2.38	0.45
1:M:17:LEU:O	1:M:21:ILE:HG13	2.17	0.45
1:A:390:ARG:CD	1:A:395:SER:HB2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:78:GLU:O	1:M:82:VAL:HG23	2.17	0.45
2:B:67:MET:HE2	2:B:67:MET:HB3	1.86	0.45
1:M:103:TRP:O	1:M:105:ARG:HG3	2.17	0.45
1:A:41:MET:HE3	1:A:140:PHE:CE2	2.51	0.44
2:B:120:ILE:HD13	2:B:185:ASP:HB2	1.98	0.44
1:M:232:HIS:O	1:M:352:PRO:HA	2.17	0.44
1:M:211:ASP:O	1:M:215:MET:HG3	2.17	0.44
1:M:222:PRO:HB3	1:M:554:PHE:CZ	2.53	0.44
2:N:235:PHE:HA	4:P:7:ARG:NH2	2.31	0.44
2:N:241:LYS:H	2:N:242:PRO:HD2	1.83	0.44
1:A:398:GLU:HG2	1:A:402:PHE:CD1	2.48	0.44
4:D:2:ASN:ND2	4:D:3:PRO:HD2	2.32	0.44
2:N:144:GLN:NE2	2:N:219:ASP:HB2	2.33	0.44
2:N:229:VAL:O	2:N:233:LYS:HG3	2.18	0.44
2:B:12:ARG:HH22	2:B:50:ASP:CG	2.26	0.44
4:D:9:ASP:O	4:D:12:VAL:HG23	2.17	0.44
1:M:356:TYR:CZ	1:M:379:GLU:HG3	2.52	0.44
1:M:35:ILE:CD1	1:M:155:HIS:HB3	2.48	0.44
1:M:324:LEU:HD23	1:M:328:LEU:HD12	1.99	0.44
2:N:182:ASP:C	2:N:184:ARG:H	2.26	0.44
4:P:28:ALA:N	4:P:29:PRO:HD2	2.32	0.44
4:P:59:GLN:HA	4:P:64:ARG:NH1	2.33	0.44
1:A:204:ASN:N	1:A:204:ASN:ND2	2.64	0.44
1:M:66:PHE:HZ	1:M:79:GLN:HB3	1.81	0.44
1:M:231:TYR:HA	1:M:353:THR:O	2.18	0.44
1:M:233:PRO:HG2	1:M:248:ARG:NH2	2.30	0.44
1:M:364:ASP:OD1	1:M:368:GLU:N	2.46	0.44
2:N:229:VAL:HG12	2:N:233:LYS:NZ	2.33	0.44
2:B:166:GLU:OE1	2:B:166:GLU:HA	2.18	0.43
2:B:235:PHE:CD1	4:D:11:PRO:HG2	2.53	0.43
3:C:76:LEU:HD13	4:D:32:ILE:HB	1.98	0.43
2:N:224:ILE:HD13	8:N:245:F3S:S3	2.58	0.43
1:A:146:PHE:HB2	1:A:149:ILE:HD12	1.99	0.43
2:N:175:LEU:O	2:N:178:ARG:HB3	2.18	0.43
1:M:197:ARG:HB2	1:M:208:VAL:O	2.19	0.43
3:O:120:THR:CG2	4:P:30:VAL:HG23	2.37	0.43
1:M:448:TRP:CH2	1:M:504:TYR:HB3	2.52	0.43
1:M:459:MET:O	1:M:463:CYS:HB2	2.18	0.43
1:M:552:LEU:HD11	1:M:566:SER:HB3	2.00	0.43
3:O:122:VAL:O	3:O:126:VAL:HG23	2.18	0.43
1:M:399:LEU:CD2	5:M:601:FAD:O2P	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ALA:HB2	1:A:393:SER:OG	2.19	0.43
3:C:40:ILE:HA	3:C:43:ILE:HD12	2.00	0.43
1:M:479:LEU:HA	1:M:482:LEU:HD12	2.00	0.43
4:P:20:GLY:O	4:P:24:SER:HB3	2.19	0.43
1:A:230:GLN:NE2	1:A:390:ARG:HH21	2.17	0.43
1:M:11:GLY:O	1:M:16:GLY:HA3	2.19	0.43
1:M:543:ASP:OD1	1:M:543:ASP:C	2.61	0.43
1:A:230:GLN:HE22	1:A:390:ARG:HH21	1.66	0.42
1:M:485:ARG:O	1:M:489:VAL:HG23	2.19	0.42
1:A:45:THR:OG1	5:A:601:FAD:O2A	2.28	0.42
2:B:160:GLN:OE1	2:B:160:GLN:HA	2.18	0.42
1:M:51:GLY:HA2	1:M:131:THR:HG21	2.01	0.42
2:B:116:ILE:H	2:B:116:ILE:HG13	1.73	0.42
1:M:481:GLU:O	1:M:485:ARG:HG3	2.19	0.42
4:P:52:GLU:HG2	4:P:52:GLU:H	1.54	0.42
1:A:356:TYR:HE1	5:A:601:FAD:O3'	2.03	0.42
2:B:99:GLU:OE2	2:B:105:ASP:HB2	2.20	0.42
1:M:62:PHE:CE2	1:M:87:HIS:HA	2.55	0.42
4:D:34:LEU:HD23	4:D:38:LEU:HD12	2.02	0.42
1:M:76:LEU:HG	1:M:529:ARG:HD3	2.01	0.42
1:M:447:ASN:HB3	1:M:450:LYS:HG2	2.01	0.42
3:O:28:ARG:HD2	4:P:81:ARG:HH21	1.85	0.42
3:O:120:THR:HG23	4:P:30:VAL:CG2	2.35	0.42
3:O:130:TRP:HB3	4:P:53:ARG:NH2	2.34	0.42
1:A:92:GLU:OE2	1:A:404:ARG:HD2	2.20	0.42
2:B:208:GLY:N	8:B:245:F3S:S1	2.92	0.42
1:M:11:GLY:CA	5:M:601:FAD:H1B	2.19	0.42
1:M:356:TYR:CE2	1:M:390:ARG:HD3	2.54	0.42
2:N:159:PRO:CG	2:N:207:VAL:HG21	2.49	0.42
1:A:244:THR:HG22	1:A:331:ILE:HG13	2.01	0.42
1:M:1:GLN:NE2	1:M:2:THR:N	2.68	0.42
5:M:601:FAD:H1'1	5:M:601:FAD:H9	1.63	0.42
4:P:51:TYR:HE1	4:P:52:GLU:CD	2.28	0.42
1:A:446:GLU:HG2	1:A:451:ILE:HD11	2.01	0.41
1:M:217:LEU:HD23	1:M:513:ASN:HB3	2.01	0.41
1:M:465:ILE:H	1:M:465:ILE:HG12	1.62	0.41
2:B:43:ILE:HD12	2:B:47:LEU:HD12	2.01	0.41
4:D:47:ASP:HB3	4:D:50:SER:OG	2.20	0.41
1:M:574:PRO:HA	1:M:575:PRO:HD3	1.92	0.41
1:A:342:ASP:HA	1:A:343:PRO:HD2	1.92	0.41
1:A:467:ARG:O	1:A:534:ARG:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLN:OE1	1:A:184:ARG:NH2	2.50	0.41
4:P:113:ILE:HG22	4:P:114:GLY:N	2.35	0.41
4:D:48:ALA:HA	4:D:53:ARG:HD3	2.02	0.41
1:M:5:ALA:HB1	1:M:31:LYS:O	2.21	0.41
1:M:20:ALA:HB2	1:M:34:LEU:HD13	2.03	0.41
1:A:311:VAL:HG21	1:A:349:PRO:HB3	2.01	0.41
2:B:242:PRO:HB3	4:P:94:PRO:N	2.36	0.41
1:M:89:CYS:HB2	1:M:90:PRO:HD3	2.03	0.41
1:M:342:ASP:HB3	1:M:345:LYS:HB3	2.02	0.41
4:P:0:MET:SD	4:P:1:ILE:HD13	2.61	0.41
4:P:2:ASN:OD1	4:P:2:ASN:C	2.64	0.41
1:A:186:ASN:HB3	1:A:417:ALA:HB2	2.02	0.41
3:C:128:LEU:O	4:D:45:PRO:HG2	2.21	0.41
1:M:443:ASP:HA	1:M:490:ARG:HD3	2.03	0.41
1:A:356:TYR:CZ	1:A:379:GLU:HG3	2.56	0.41
1:M:146:PHE:HB3	1:M:148:GLN:OE1	2.21	0.41
1:M:485:ARG:HA	1:M:488:ARG:HG2	2.03	0.41
2:N:116:ILE:CG2	2:N:176:ALA:CB	2.89	0.41
4:P:0:MET:SD	4:P:0:MET:C	3.04	0.41
1:A:386:HIS:ND1	1:A:390:ARG:HG3	2.36	0.41
1:A:448:TRP:CH2	1:A:504:TYR:HB3	2.56	0.41
1:A:556:ASP:OD2	1:A:562:ARG:HD2	2.20	0.41
1:M:46:VAL:O	1:M:133:PHE:N	2.54	0.41
2:N:96:PHE:HB3	2:N:104:VAL:HB	2.03	0.41
3:C:19:LEU:HD23	3:C:22:TYR:CE2	2.56	0.40
1:M:116:PHE:HE2	1:M:245:GLU:HB3	1.82	0.40
1:M:131:THR:O	1:M:135:MET:HG3	2.21	0.40
1:M:145:GLN:HB3	2:N:119:TYR:CE2	2.56	0.40
1:M:187:ALA:HB2	1:M:414:ALA:HB2	2.03	0.40
1:M:554:PHE:HB2	1:M:562:ARG:HB2	2.03	0.40
1:A:240:GLY:HA2	1:A:353:THR:HG21	2.03	0.40
1:A:346:GLU:CB	1:A:347:PRO:CD	2.99	0.40
2:N:220:PRO:O	2:N:223:ALA:HB3	2.22	0.40
1:M:41:MET:HE2	2:N:150:ASN:HD22	1.85	0.40
1:M:145:GLN:HB3	2:N:119:TYR:CZ	2.57	0.40
2:N:73:PRO:HB2	2:N:153:LEU:HD22	2.03	0.40
2:N:117:LYS:O	2:N:191:ARG:NH2	2.46	0.40
1:A:76:LEU:O	1:A:550:HIS:HE1	2.04	0.40
2:B:93:LEU:HG	2:B:156:ALA:HB2	2.03	0.40
3:C:33:VAL:HA	4:D:82:MET:HE2	2.03	0.40
1:M:76:LEU:HD11	1:M:525:ARG:HH22	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:108:HIS:CE1	4:D:1:ILE:HD11	2.57	0.40
2:B:207:VAL:HG23	8:B:245:F3S:S2	2.62	0.40
4:D:55:LEU:CG	4:D:59:GLN:NE2	2.69	0.40
1:M:295:TRP:O	1:M:299:ARG:HG2	2.22	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	575/577 (100%)	551 (96%)	24 (4%)	0	100	100
1	M	575/577 (100%)	545 (95%)	28 (5%)	2 (0%)	36	63
2	B	241/243 (99%)	229 (95%)	10 (4%)	2 (1%)	16	42
2	N	241/243 (99%)	225 (93%)	13 (5%)	3 (1%)	10	32
3	C	128/130 (98%)	125 (98%)	3 (2%)	0	100	100
3	O	128/130 (98%)	123 (96%)	5 (4%)	0	100	100
4	D	117/119 (98%)	103 (88%)	14 (12%)	0	100	100
4	P	117/119 (98%)	104 (89%)	13 (11%)	0	100	100
All	All	2122/2138 (99%)	2005 (94%)	110 (5%)	7 (0%)	36	63

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	N	56	SER
2	B	56	SER
1	M	444	GLY
2	N	101	ASP
2	B	82	ARG
1	M	328	LEU

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Mol	Chain	Res	Type
2	N	241	LYS

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	460/460 (100%)	441 (96%)	19 (4%)	27	55
1	M	460/460 (100%)	419 (91%)	41 (9%)	9	29
2	B	205/205 (100%)	198 (97%)	7 (3%)	32	59
2	N	205/205 (100%)	193 (94%)	12 (6%)	18	44
3	C	111/111 (100%)	103 (93%)	8 (7%)	13	37
3	O	111/111 (100%)	106 (96%)	5 (4%)	24	52
4	D	97/97 (100%)	84 (87%)	13 (13%)	4	14
4	P	97/97 (100%)	81 (84%)	16 (16%)	2	9
All	All	1746/1746 (100%)	1625 (93%)	121 (7%)	14	38

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	ARG
1	A	31	LYS
1	A	49	GLU
1	A	74	ASP
1	A	92	GLU
1	A	174	ASN
1	A	182	GLN
1	A	200	ARG
1	A	204	ASN
1	A	208	VAL
1	A	276	GLU
1	A	317	ARG
1	A	321	GLU
1	A	327	ARG

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Mol	Chain	Res	Type
1	A	344	VAL
1	A	422	GLU
1	A	459	MET
1	A	489	VAL
1	A	558	ASP
2	B	19	THR
2	B	65	CYS
2	B	116	ILE
2	B	128	ASP
2	B	210	CYS
2	B	225	GLN
2	B	241	LYS
3	C	1	THR
3	C	12	THR
3	C	26	MET
3	C	36	VAL
3	C	39	SER
3	C	50	LYS
3	C	99	LYS
3	C	106	GLU
4	D	1	ILE
4	D	2	ASN
4	D	6	LYS
4	D	9	ASP
4	D	12	VAL
4	D	24	SER
4	D	26	ILE
4	D	39	LEU
4	D	50	SER
4	D	67	LEU
4	D	86	MET
4	D	91	ILE
4	D	117	THR
1	M	1	GLN
1	M	2	THR
1	M	17	LEU
1	M	18	ARG
1	M	27	ASN
1	M	35	ILE
1	M	57	GLN
1	M	76	LEU
1	M	93	MET

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Mol	Chain	Res	Type
1	M	143	SER
1	M	202	ASN
1	M	209	THR
1	M	227	GLU
1	M	243	MET
1	M	244	THR
1	M	283	GLU
1	M	295	TRP
1	M	299	ARG
1	M	312	VAL
1	M	321	GLU
1	M	322	LYS
1	M	327	ARG
1	M	344	VAL
1	M	353	THR
1	M	369	THR
1	M	377	VAL
1	M	383	VAL
1	M	413	ARG
1	M	426	GLU
1	M	428	GLN
1	M	457	LEU
1	M	461	GLU
1	M	465	ILE
1	M	470	GLU
1	M	494	THR
1	M	537	GLU
1	M	540	THR
1	M	543	ASP
1	M	558	ASP
1	M	570	ILE
1	M	571	THR
2	N	2	GLU
2	N	17	VAL
2	N	85	THR
2	N	123	ASN
2	N	150	ASN
2	N	189	LYS
2	N	192	MET
2	N	203	SER
2	N	229	VAL
2	N	232	SER

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Mol	Chain	Res	Type
2	N	237	ILE
2	N	240	LEU
3	O	5	LYS
3	O	31	THR
3	O	54	GLU
3	O	84	LYS
3	O	130	TRP
4	P	1	ILE
4	P	2	ASN
4	P	6	LYS
4	P	12	VAL
4	P	26	ILE
4	P	30	VAL
4	P	39	LEU
4	P	50	SER
4	P	52	GLU
4	P	64	ARG
4	P	67	LEU
4	P	86	MET
4	P	91	ILE
4	P	113	ILE
4	P	115	VAL
4	P	117	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	A	134	HIS
1	A	137	HIS
1	A	141	GLN
1	A	150	GLN
1	A	174	ASN
1	A	230	GLN
1	A	232	HIS
1	A	258	ASN
1	A	279	ASN
1	A	292	GLN
1	A	428	GLN
1	A	434	GLN
1	A	442	GLN
2	B	22	HIS

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Mol	Chain	Res	Type
2	B	134	GLN
2	B	150	ASN
2	B	225	GLN
3	C	72	ASN
3	C	95	ASN
4	D	59	GLN
4	D	80	HIS
4	D	83	HIS
4	D	84	HIS
4	D	92	HIS
1	M	1	GLN
1	M	4	GLN
1	M	57	GLN
1	M	59	HIS
1	M	67	HIS
1	M	87	HIS
1	M	95	GLN
1	M	137	HIS
1	M	166	HIS
1	M	232	HIS
1	M	279	ASN
1	M	296	HIS
1	M	409	GLN
1	M	428	GLN
1	M	447	ASN
1	M	483	GLN
1	M	513	ASN
1	M	532	HIS
2	N	95	ASN
2	N	123	ASN
2	N	132	ASN
2	N	138	GLN
2	N	177	HIS
2	N	225	GLN
2	N	226	GLN
3	O	72	ASN
4	P	59	GLN
4	P	80	HIS
4	P	83	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 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	$\# Z > 2$
8	F3S	N	245	2	0,9,9	-	-	-		
5	FAD	M	601	-	58,58,58	1.30	8 (13%)	85,89,89	1.75	16 (18%)
6	GUA	M	577	-	8,8,8	1.00	0	9,9,9	1.06	0
8	F3S	B	245	2	0,9,9	-	-	-		
7	FES	B	244	2	0,4,4	-	-	-		
7	FES	N	244	2	0,4,4	-	-	-		
5	FAD	A	601	-	58,58,58	0.98	4 (6%)	85,89,89	1.75	19 (22%)
6	GUA	A	577	-	8,8,8	1.06	0	9,9,9	0.99	0
9	SF4	B	246	2	0,12,12	-	-	-		
9	SF4	N	246	2	0,12,12	-	-	-		

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
8	F3S	N	245	2	-	-	0/3/3/3
5	FAD	M	601	-	-	10/34/50/50	0/6/6/6
6	GUA	M	577	-	-	6/6/6/6	-
8	F3S	B	245	2	-	-	0/3/3/3
7	FES	B	244	2	-	-	0/1/1/1
7	FES	N	244	2	-	-	0/1/1/1
5	FAD	A	601	-	-	5/34/50/50	0/6/6/6
6	GUA	A	577	-	-	3/6/6/6	-
9	SF4	B	246	2	-	-	0/6/5/5
9	SF4	N	246	2	-	-	0/6/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	601	FAD	O3B-C3B	4.30	1.53	1.43
5	M	601	FAD	O2B-C2B	-3.14	1.35	1.43
5	M	601	FAD	C10-N10	2.47	1.42	1.37
5	A	601	FAD	C4X-N5	2.46	1.36	1.30
5	A	601	FAD	C8A-N7A	2.43	1.36	1.31
5	M	601	FAD	C5X-N5	-2.38	1.35	1.39
5	M	601	FAD	P-O3P	2.24	1.61	1.59
5	M	601	FAD	C4A-N9A	-2.24	1.33	1.37
5	M	601	FAD	C4X-N5	2.21	1.35	1.30
5	M	601	FAD	C8A-N7A	2.16	1.35	1.31
5	A	601	FAD	C5X-N5	-2.06	1.35	1.39
5	A	601	FAD	C4-N3	-2.06	1.35	1.38

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	601	FAD	C2B-C1B-N9A	-5.80	98.90	113.30
5	A	601	FAD	N3A-C2A-N1A	-5.63	120.06	128.58
5	M	601	FAD	N3A-C2A-N1A	-5.27	120.60	128.58
5	A	601	FAD	C5A-C4A-N3A	-4.94	119.91	126.72
5	M	601	FAD	C5A-C4A-N3A	-4.21	120.92	126.72
5	A	601	FAD	O4B-C1B-N9A	4.10	115.96	108.09
5	A	601	FAD	N9A-C8A-N7A	-3.95	108.33	113.94
5	A	601	FAD	C2A-N3A-C4A	3.84	121.20	111.83
5	M	601	FAD	N9A-C8A-N7A	-3.77	108.58	113.94
5	M	601	FAD	C2A-N3A-C4A	3.30	119.90	111.83
5	M	601	FAD	C4A-N9A-C8A	3.21	109.11	105.74
5	M	601	FAD	C4-N3-C2	-3.02	120.28	125.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	FAD	C4A-C5A-N7A	-2.97	107.19	110.58
5	A	601	FAD	N3A-C4A-N9A	2.95	132.19	127.17
5	M	601	FAD	O4B-C1B-C2B	-2.94	100.32	106.62
5	M	601	FAD	C5X-C9A-N10	2.91	120.60	117.97
5	A	601	FAD	C4A-N9A-C8A	2.90	108.79	105.74
5	A	601	FAD	C5A-N7A-C8A	2.76	107.79	103.45
5	A	601	FAD	C4-N3-C2	-2.73	120.80	125.64
5	M	601	FAD	C4A-C5A-N7A	-2.70	107.49	110.58
5	M	601	FAD	C4X-C4-N3	2.67	120.06	113.25
5	A	601	FAD	C4X-C10-N10	2.64	120.26	116.48
5	M	601	FAD	N3A-C4A-N9A	2.64	131.65	127.17
5	A	601	FAD	C4X-C4-N3	2.59	119.84	113.25
5	M	601	FAD	O4-C4-C4X	-2.58	119.72	126.53
5	A	601	FAD	C1'-C2'-C3'	2.51	116.47	109.66
5	M	601	FAD	C5A-N7A-C8A	2.51	107.39	103.45
5	A	601	FAD	C4-C4X-N5	2.36	121.46	118.21
5	M	601	FAD	C4X-C10-N1	-2.29	118.97	124.59
5	A	601	FAD	C4'-C3'-C2'	-2.26	109.81	113.57
5	A	601	FAD	O4-C4-C4X	-2.22	120.67	126.53
5	A	601	FAD	C10-C4X-N5	-2.19	120.34	124.81
5	A	601	FAD	O2-C2-N1	-2.05	118.40	121.80
5	A	601	FAD	C4X-C10-N1	-2.05	119.57	124.59
5	M	601	FAD	C9A-N10-C10	-2.05	117.63	120.75

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	FAD	C5B-O5B-PA-O2A
5	A	601	FAD	C5B-O5B-PA-O3P
5	A	601	FAD	N10-C1'-C2'-O2'
5	M	601	FAD	C5B-O5B-PA-O1A
5	M	601	FAD	C5B-O5B-PA-O2A
5	M	601	FAD	C5B-O5B-PA-O3P
5	M	601	FAD	N10-C1'-C2'-O2'
5	M	601	FAD	N10-C1'-C2'-C3'
5	M	601	FAD	C3'-C4'-C5'-O5'
5	M	601	FAD	O4'-C4'-C5'-O5'
5	A	601	FAD	C3B-C4B-C5B-O5B
6	M	577	GUA	C1-C2-C3-C4
5	M	601	FAD	O4B-C4B-C5B-O5B
6	M	577	GUA	C2-C3-C4-C5

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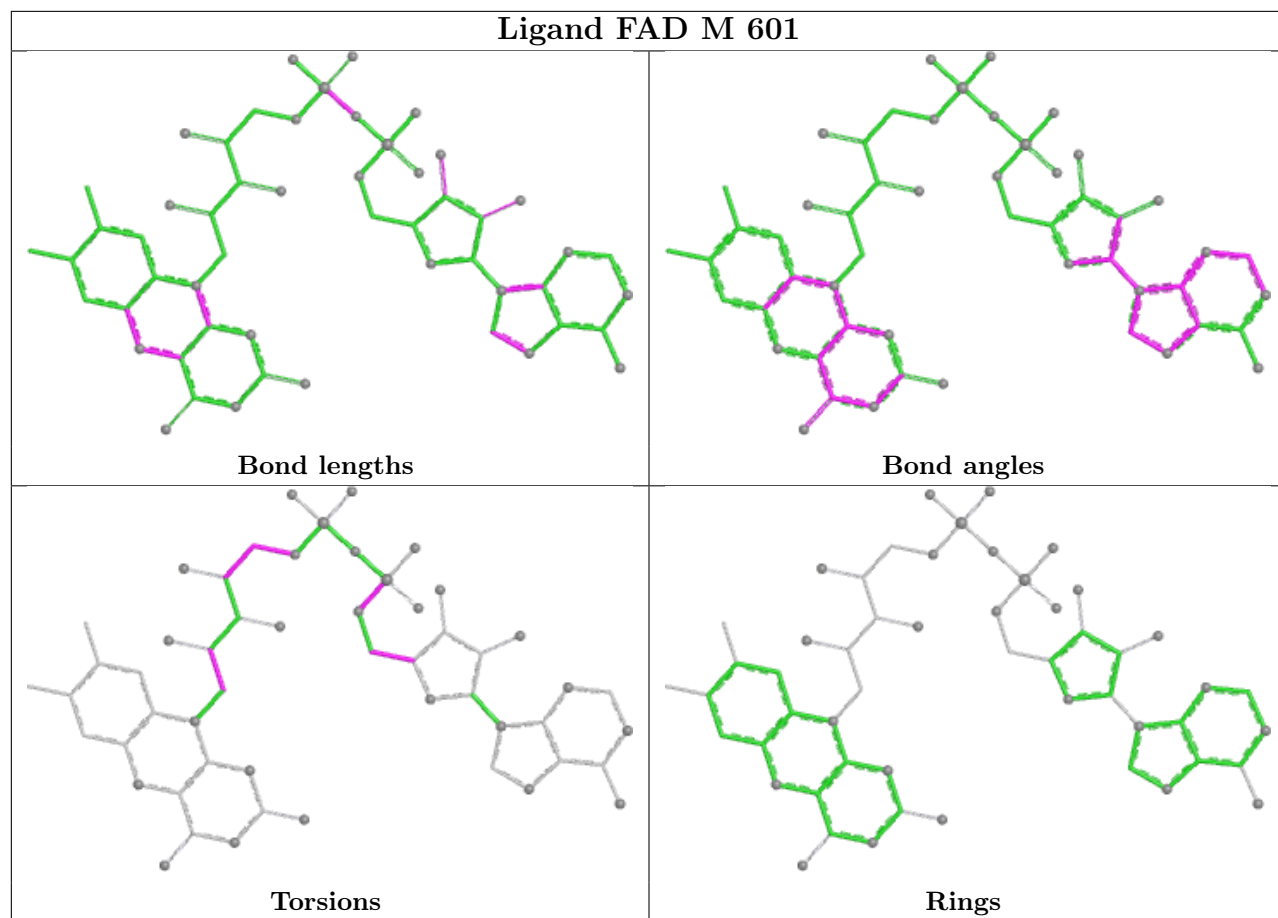
Mol	Chain	Res	Type	Atoms
5	M	601	FAD	C3B-C4B-C5B-O5B
5	A	601	FAD	O4B-C4B-C5B-O5B
5	M	601	FAD	C4'-C5'-O5'-P
6	M	577	GUA	C3-C4-C5-O4
6	M	577	GUA	C3-C4-C5-O3
6	M	577	GUA	O2-C1-C2-C3
6	M	577	GUA	O1-C1-C2-C3
6	A	577	GUA	O2-C1-C2-C3
6	A	577	GUA	O1-C1-C2-C3
6	A	577	GUA	C2-C3-C4-C5

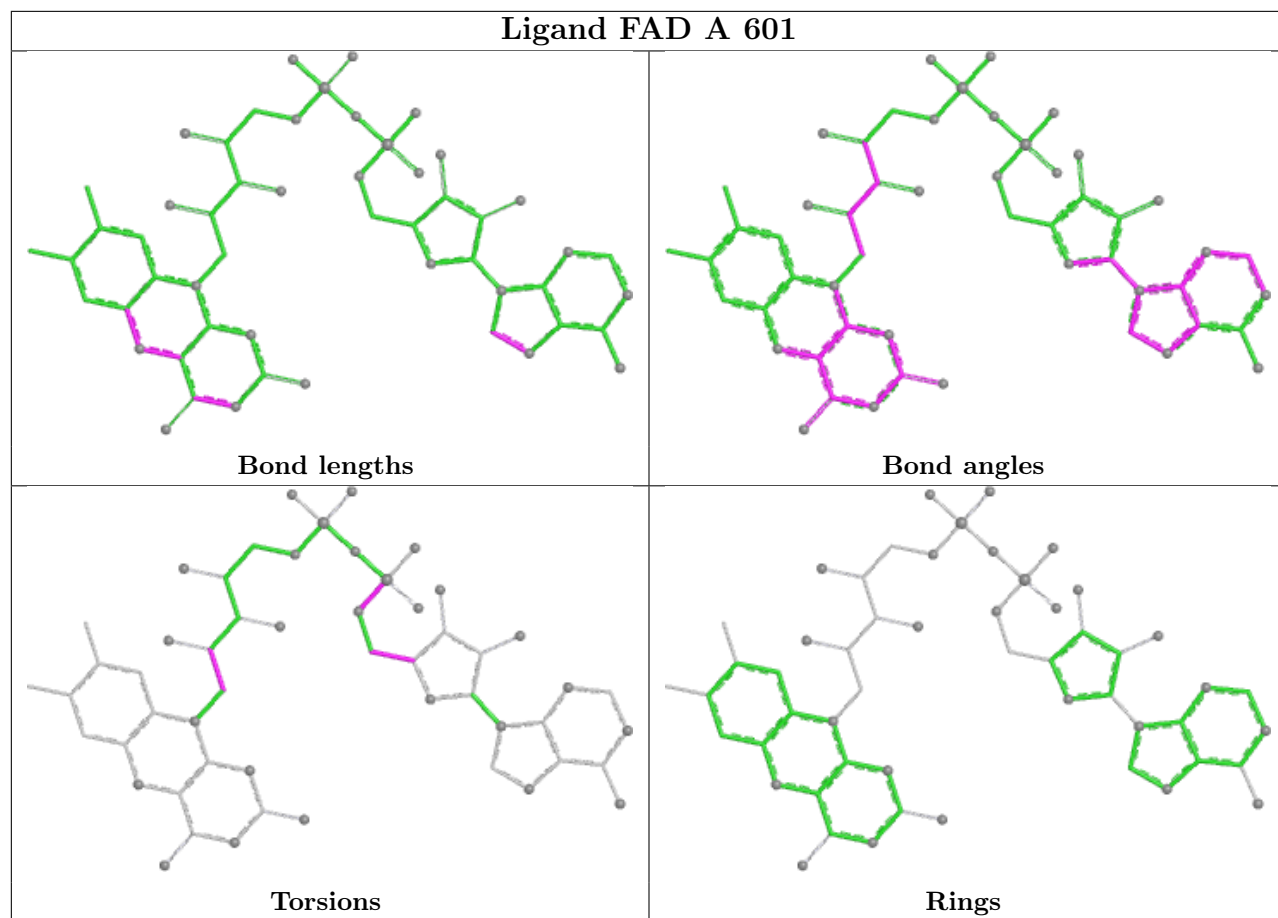
There are no ring outliers.

8 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	N	245	F3S	3	0
5	M	601	FAD	14	0
6	M	577	GUA	2	0
8	B	245	F3S	6	0
5	A	601	FAD	8	0
6	A	577	GUA	1	0
9	B	246	SF4	1	0
9	N	246	SF4	6	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	577/577 (100%)	-0.20	3 (0%) 87 72	44, 61, 96, 134	0
1	M	577/577 (100%)	0.87	59 (10%) 12 6	72, 135, 169, 186	0
2	B	243/243 (100%)	-0.12	0 100 100	46, 67, 104, 154	0
2	N	243/243 (100%)	0.54	12 (4%) 35 17	65, 106, 151, 167	0
3	C	130/130 (100%)	-0.04	0 100 100	58, 80, 106, 155	0
3	O	130/130 (100%)	0.44	5 (3%) 44 24	72, 102, 147, 197	0
4	D	119/119 (100%)	0.27	4 (3%) 48 27	59, 83, 124, 158	0
4	P	119/119 (100%)	0.50	8 (6%) 24 12	72, 91, 178, 254	0
All	All	2138/2138 (100%)	0.29	91 (4%) 40 21	44, 87, 158, 254	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	8	ALA	5.5
1	M	32	ILE	4.1
4	P	1	ILE	4.0
2	N	38	ASP	3.9
4	P	7	ARG	3.8
1	M	188	VAL	3.8
4	D	118	ILE	3.7
2	N	238	ALA	3.6
1	M	415	ALA	3.6
1	M	411	THR	3.6
4	P	5	PRO	3.5
1	M	373	GLY	3.4
1	M	386	HIS	3.3
1	M	492	THR	3.3
1	M	402	PHE	3.3
2	N	148	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
4	P	88	ASP	3.1
1	M	383	VAL	3.0
1	M	553	ALA	3.0
1	M	91	THR	3.0
1	M	491	ILE	2.9
1	M	396	LEU	2.9
1	M	223	LEU	2.9
4	D	95	ALA	2.9
1	M	169	GLY	2.8
1	M	465	ILE	2.8
1	M	187	ALA	2.8
1	M	171	VAL	2.7
1	M	158	LEU	2.7
3	O	129	TYR	2.7
4	D	6	LYS	2.7
3	O	64	GLN	2.7
1	M	573	LEU	2.7
1	M	574	PRO	2.7
1	M	207	ILE	2.7
1	M	250	GLU	2.7
1	M	33	ALA	2.7
1	M	508	LEU	2.6
2	N	133	ILE	2.6
1	M	7	LEU	2.6
2	N	47	LEU	2.6
1	M	219	HIS	2.6
4	P	4	ASN	2.5
1	M	445	GLY	2.5
1	M	189	VAL	2.5
1	M	439	LEU	2.5
1	M	23	ALA	2.4
1	M	15	ALA	2.4
2	N	120	ILE	2.4
1	M	77	CYS	2.4
1	A	379	GLU	2.4
1	M	192	THR	2.3
1	M	413	ARG	2.3
1	M	414	ALA	2.3
1	M	390	ARG	2.3
1	A	477	ASP	2.3
1	M	80	ASP	2.3
1	M	159	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	M	565	TYR	2.3
3	O	8	VAL	2.3
4	P	6	LYS	2.3
1	M	44	HIS	2.3
1	M	391	LEU	2.2
2	N	240	LEU	2.2
4	P	89	LEU	2.2
3	O	9	ARG	2.2
1	A	129	ASP	2.2
1	M	129	ASP	2.2
1	M	372	LYS	2.2
2	N	131	THR	2.2
2	N	106	MET	2.2
4	P	49	LEU	2.2
1	M	379	GLU	2.2
1	M	295	TRP	2.2
4	D	8	SER	2.1
1	M	210	GLY	2.1
2	N	147	GLY	2.1
1	M	571	THR	2.1
1	M	172	ALA	2.1
2	N	52	SER	2.1
1	M	209	THR	2.1
1	M	394	ASN	2.1
1	M	398	GLU	2.1
1	M	186	ASN	2.1
2	N	98	ILE	2.1
3	O	130	TRP	2.1
1	M	494	THR	2.1
1	M	170	LEU	2.0
1	M	14	GLY	2.0
1	M	100	GLY	2.0
1	M	322	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

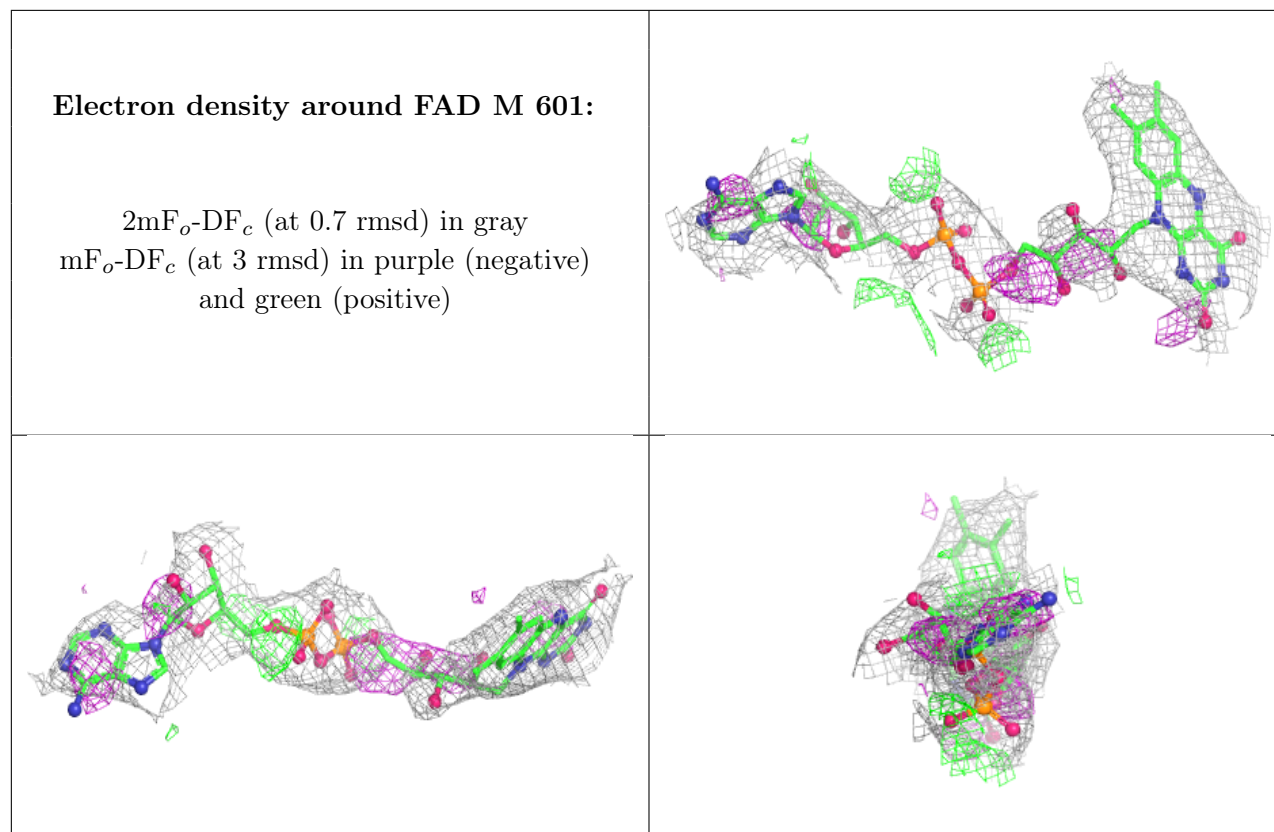
There are no oligosaccharides in this entry.

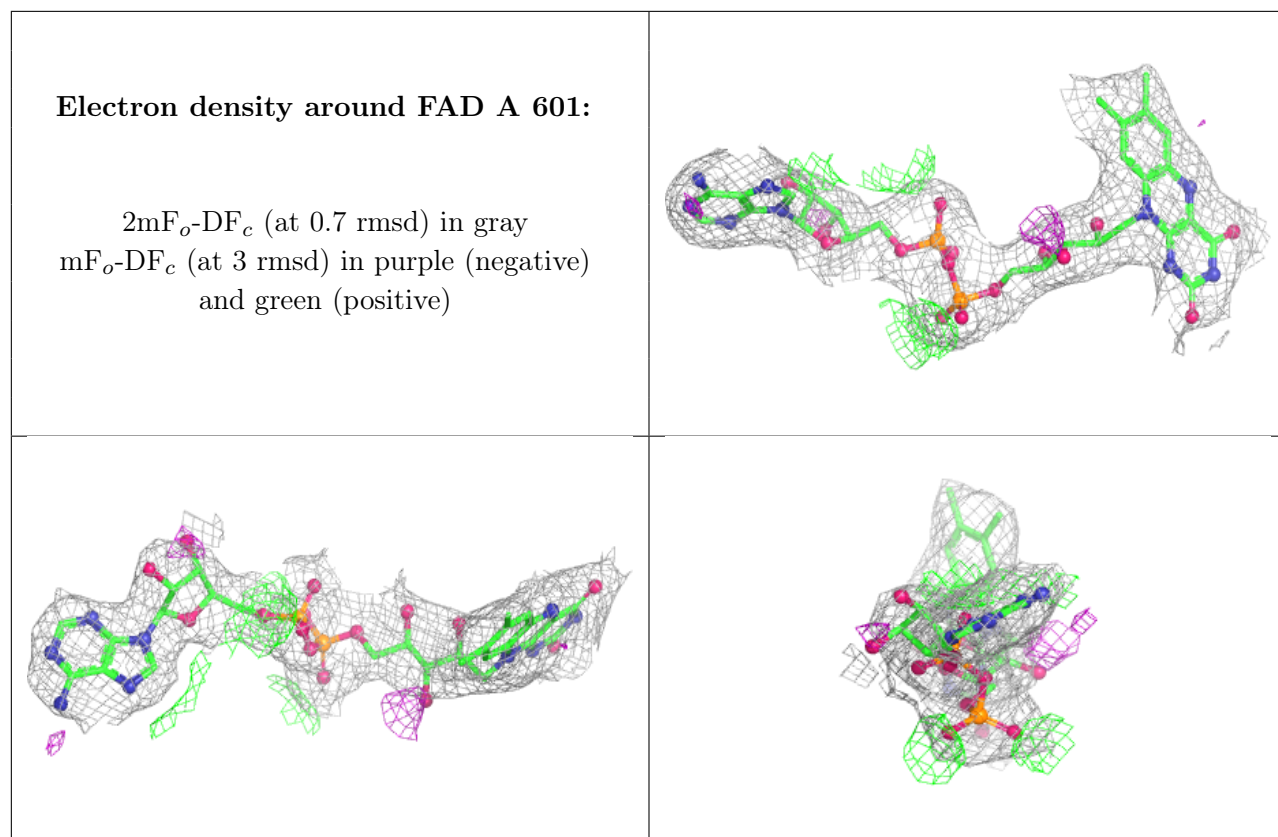
6.4 Ligands ⓘ

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(Å ²)	Q<0.9
6	GUA	M	577	9/9	0.72	0.20	86,87,88,88	0
6	GUA	A	577	9/9	0.77	0.20	61,62,65,65	0
5	FAD	M	601	53/53	0.84	0.12	65,84,96,96	0
9	SF4	N	246	8/8	0.90	0.10	88,88,89,89	0
8	F3S	N	245	7/7	0.94	0.10	93,95,96,96	0
5	FAD	A	601	53/53	0.96	0.07	35,43,47,48	0
8	F3S	B	245	7/7	0.97	0.09	75,77,79,80	0
9	SF4	B	246	8/8	0.98	0.07	71,74,76,76	0
7	FES	B	244	4/4	0.99	0.04	50,50,54,55	0
7	FES	N	244	4/4	0.99	0.04	72,73,73,74	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.