



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 02:52 PM EDT

PDB ID : 3P4Q / pdb_00003p4q
Title : Crystal structure of Menaquinol:oxidoreductase in complex with oxaloacetate
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 : 2010-10-06
Resolution : 3.35 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	:	9.0.015 (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

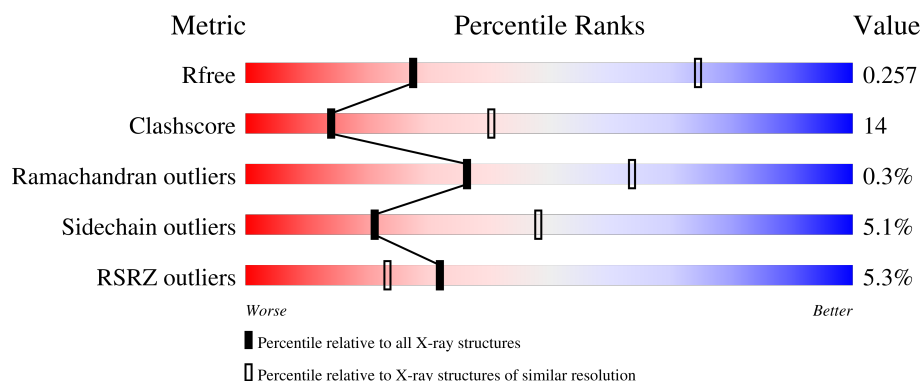
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1099 (3.40-3.32)
Clashscore	190562	1116 (3.40-3.32)
Ramachandran outliers	187476	1101 (3.40-3.32)
Sidechain outliers	187428	1101 (3.40-3.32)
RSRZ outliers	180081	1099 (3.40-3.32)

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	
1	M	577	
2	B	243	
2	N	243	

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Mol	Chain	Length	Quality of chain
3	C	130	
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	246	-	-	X	-
9	SF4	B	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 protein.

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			

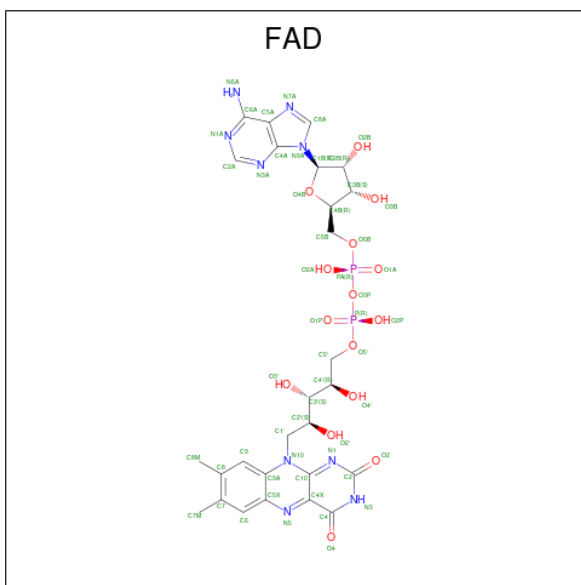
- Molecule 3 is a protein called Fumarate reductase subunit C.

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.

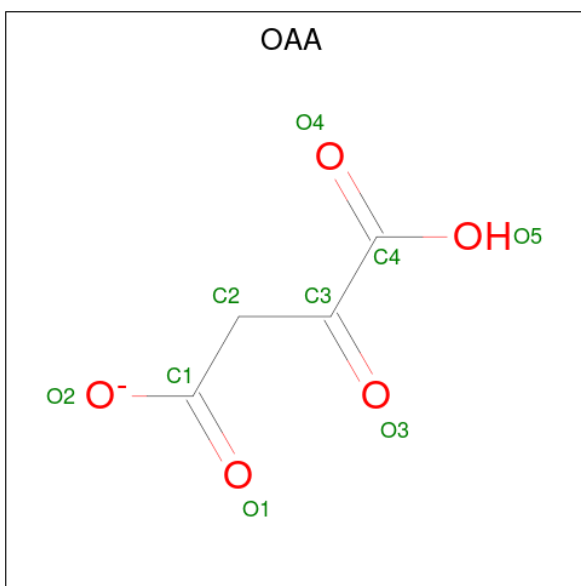
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			
4	P	119	Total	C	N	O	S	0	0	0
			926	626	151	142	7			

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



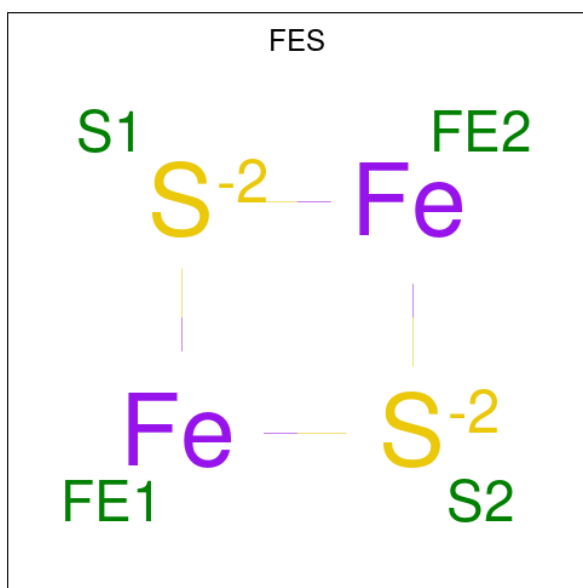
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
5	M	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 6 is OXALOACETATE ION (CCD ID: OAA) (formula: $\text{C}_4\text{H}_3\text{O}_5$).



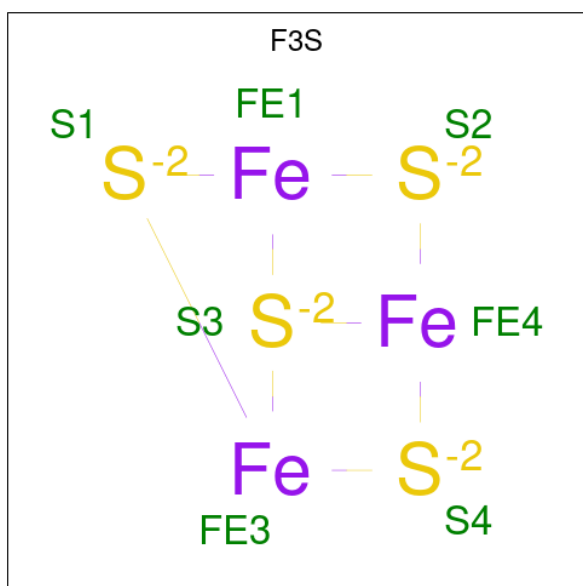
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total 9	C 4	O 5	0	0
6	M	1	Total 9	C 4	O 5	0	0

- 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).



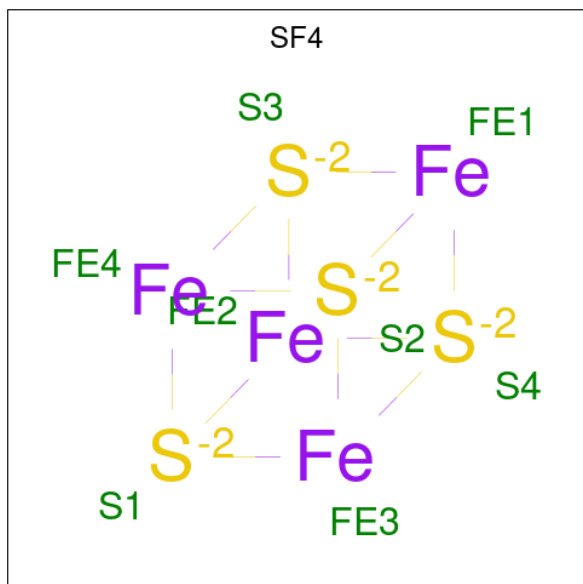
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		

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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).

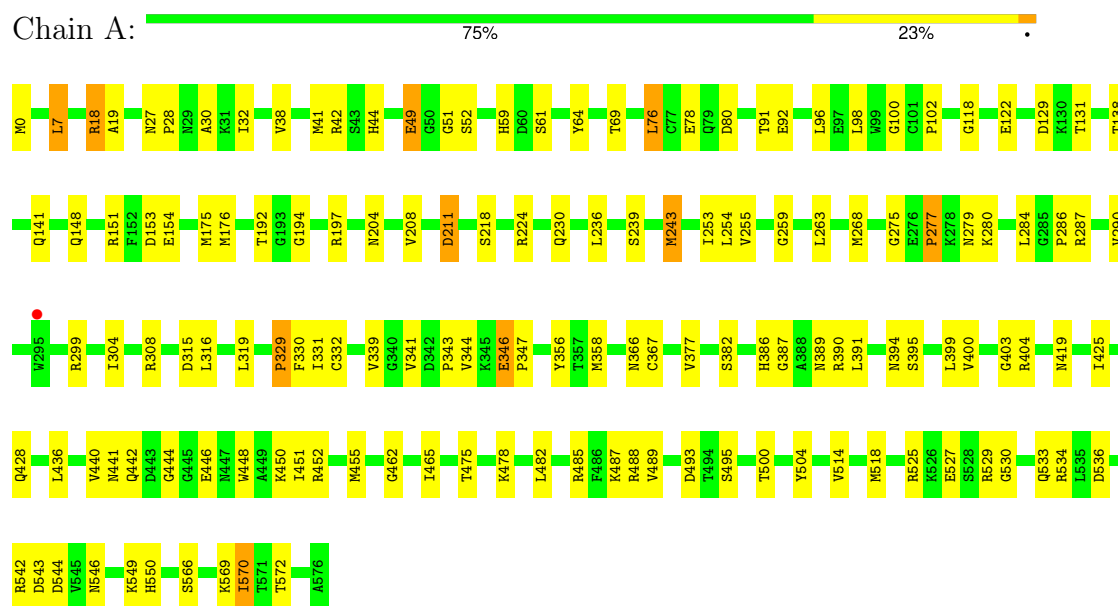


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		
9	N	1	Total	Fe	S	0	0
			8	4	4		

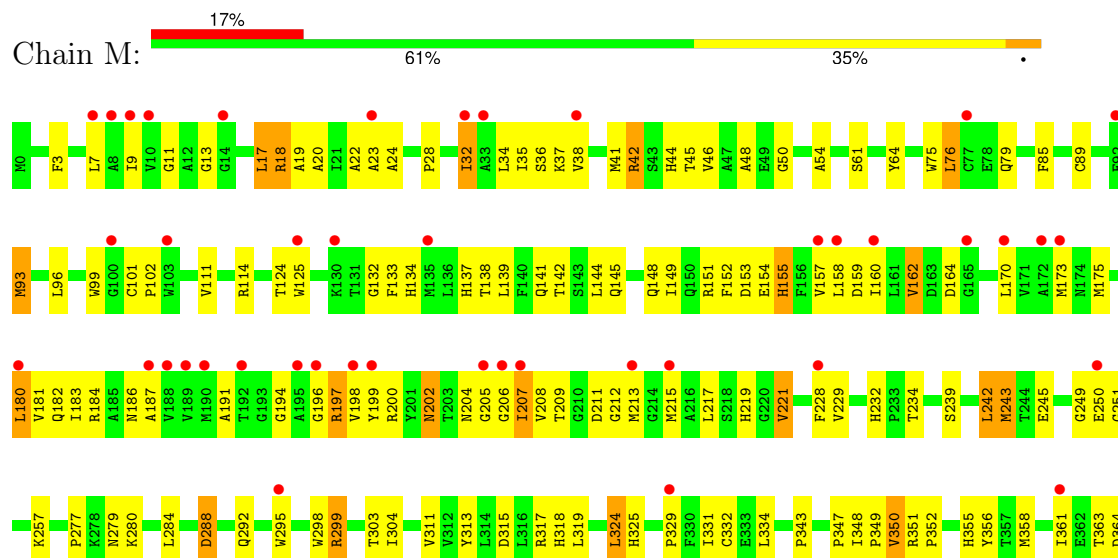
3 Residue-property plots

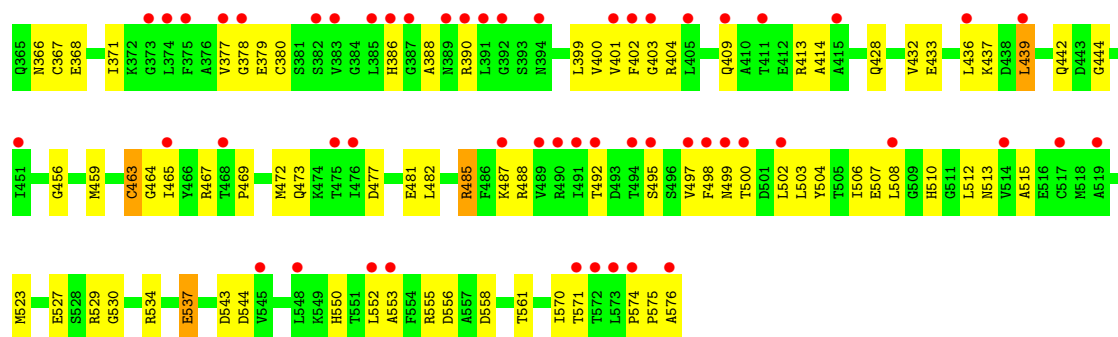
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

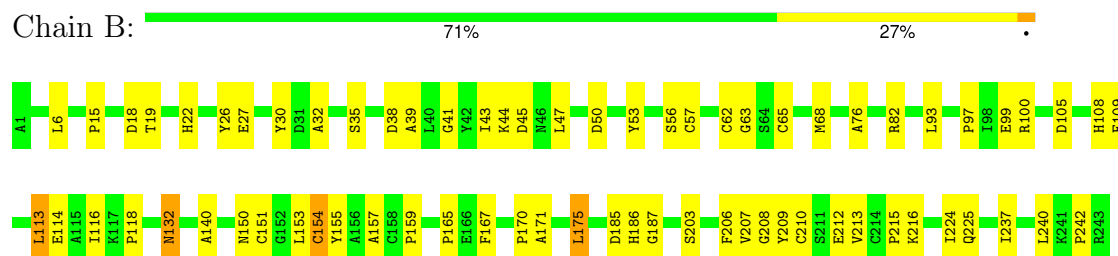


• Molecule 1: Fumarate reductase flavoprotein subunit

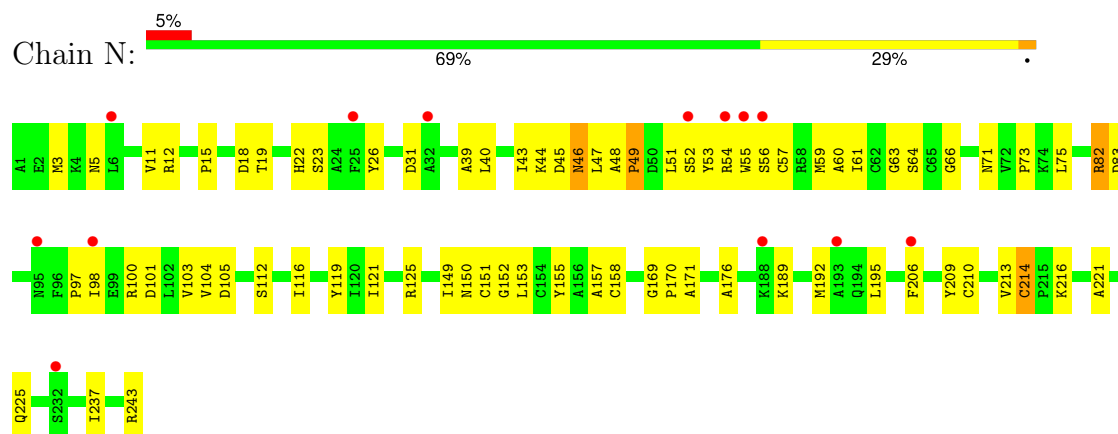




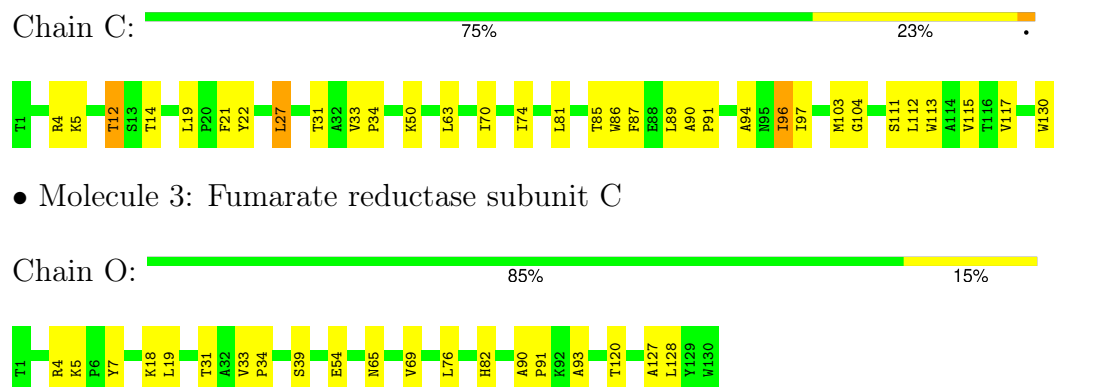
• Molecule 2: Fumarate reductase iron-sulfur protein



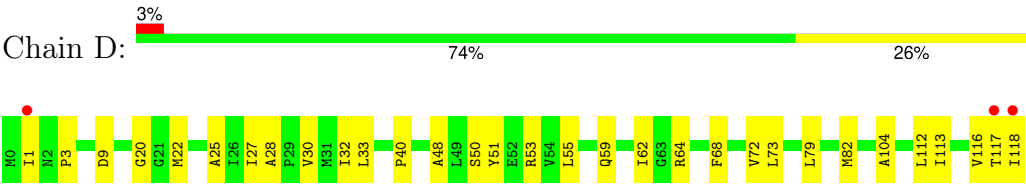
• Molecule 2: Fumarate reductase iron-sulfur protein



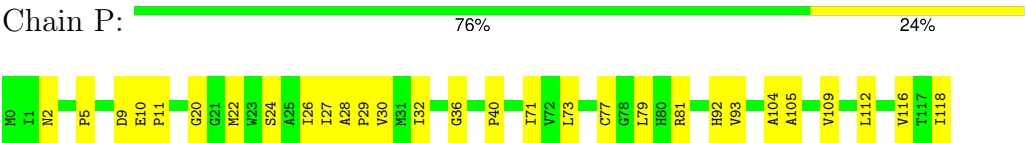
• Molecule 3: Fumarate reductase subunit C



• 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	96.64Å 137.96Å 272.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.57 – 3.35 47.57 – 3.35	Depositor EDS
% Data completeness (in resolution range)	89.2 (47.57-3.35) 88.9 (47.57-3.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.72 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.220 , 0.261 0.219 , 0.257	Depositor DCC
R_{free} test set	1036 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å ²)	66.7	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 41.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	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 2.58% 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: F3S, FAD, OAA, SF4, FES

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	0.46	0/4541	0.84	1/6139 (0.0%)
1	M	0.46	0/4541	0.88	4/6139 (0.1%)
2	B	0.45	0/1931	0.83	0/2617
2	N	0.46	0/1931	0.84	0/2617
3	C	0.43	0/1094	0.83	0/1496
3	O	0.46	0/1094	0.84	3/1496 (0.2%)
4	D	0.48	0/956	0.92	0/1303
4	P	0.45	0/956	0.85	0/1303
All	All	0.46	0/17044	0.85	8/23110 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	495	SER	N-CA-C	-6.95	98.46	109.23
3	O	19	LEU	CA-C-N	6.01	127.36	119.84
3	O	19	LEU	C-N-CA	6.01	127.36	119.84
1	M	355	HIS	N-CA-C	5.91	120.04	112.12
1	M	239	SER	N-CA-C	-5.32	107.44	114.04
3	O	19	LEU	N-CA-C	5.26	114.36	108.25
1	A	239	SER	N-CA-C	-5.24	107.44	113.88
1	M	209	THR	N-CA-C	-5.11	106.73	113.17

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	4449	0	4335	107	0
1	M	4449	0	4333	187	0
2	B	1888	0	1840	66	0
2	N	1888	0	1838	67	0
3	C	1058	0	1108	35	0
3	O	1058	0	1108	17	0
4	D	926	0	971	23	0
4	P	926	0	971	19	0
5	A	53	0	31	9	0
5	M	53	0	31	20	0
6	A	9	0	2	0	0
6	M	9	0	2	2	0
7	B	4	0	0	0	0
7	N	4	0	0	1	0
8	B	7	0	0	2	0
8	N	7	0	0	3	0
9	B	8	0	0	7	0
9	N	8	0	0	1	0
All	All	16804	0	16570	475	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 (475) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:HIS:NE2	5:A:601:FAD:HM82	1.22	1.46
2:N:11:VAL:HA	2:N:23:SER:OG	1.20	1.24
1:M:37:LYS:HE3	5:M:601:FAD:C8A	1.75	1.17
2:N:54:ARG:HH21	2:N:103:VAL:HG12	1.06	1.15
1:A:44:HIS:NE2	5:A:601:FAD:C8M	2.17	1.06
1:M:37:LYS:CE	5:M:601:FAD:C8A	2.34	1.05
2:B:154:CYS:SG	9:B:246:SF4:FE3	1.51	1.00
1:M:37:LYS:HE2	5:M:601:FAD:N7A	1.77	1.00
1:M:48:ALA:HB3	1:M:132:GLY:HA3	1.43	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:197:ARG:HD2	1:M:197:ARG:C	1.88	0.94
2:N:11:VAL:CA	2:N:23:SER:OG	2.15	0.93
2:N:54:ARG:HH21	2:N:103:VAL:CG1	1.83	0.91
4:D:55:LEU:HG	4:D:59:GLN:HE21	1.36	0.91
2:N:54:ARG:NH2	2:N:103:VAL:HG12	1.86	0.89
2:N:11:VAL:HA	2:N:23:SER:HG	1.33	0.88
1:M:37:LYS:CE	5:M:601:FAD:N7A	2.36	0.87
2:B:154:CYS:HG	9:B:246:SF4:FE3	0.87	0.87
1:M:250:GLU:O	1:M:319:LEU:HD11	1.73	0.87
2:B:154:CYS:SG	9:B:246:SF4:S2	2.74	0.86
1:M:527:GLU:OE2	1:M:529:ARG:NH1	2.08	0.86
1:A:49:GLU:HA	1:A:129:ASP:O	1.76	0.85
2:N:18:ASP:CG	2:N:22:HIS:HE2	1.86	0.84
3:O:31:THR:HG21	3:O:82:HIS:HB2	1.59	0.84
1:M:377:VAL:HG21	1:M:403:GLY:HA2	1.59	0.84
2:N:26:TYR:HB3	2:N:47:LEU:HD13	1.58	0.84
1:A:500:THR:HB	1:A:504:TYR:CE1	2.15	0.82
1:M:497:VAL:HG21	3:O:4:ARG:HB3	1.61	0.82
2:B:242:PRO:HB2	4:P:92:HIS:HB3	1.62	0.82
3:C:33:VAL:HA	4:D:82:MET:HE2	1.59	0.81
2:B:212:GLU:HG3	3:C:21:PHE:HE2	1.46	0.81
1:M:36:SER:HA	5:M:601:FAD:N3A	1.94	0.81
1:M:61:SER:HB3	1:M:64:TYR:HD1	1.43	0.80
1:M:197:ARG:HD2	1:M:197:ARG:O	1.82	0.80
2:N:43:ILE:HD13	2:N:47:LEU:HD12	1.64	0.77
3:C:103:MET:HG2	3:C:104:GLY:H	1.50	0.77
1:M:199:TYR:CD2	1:M:459:MET:HB3	2.19	0.77
1:A:44:HIS:CD2	5:A:601:FAD:HM82	2.17	0.76
2:N:116:ILE:CG2	2:N:176:ALA:HB2	2.15	0.76
1:M:570:ILE:HG21	1:M:575:PRO:HD3	1.66	0.75
2:B:154:CYS:HB2	2:B:170:PRO:HG2	1.68	0.75
2:B:151:CYS:SG	9:B:246:SF4:FE1	1.80	0.74
1:M:215:MET:HB3	1:M:510:HIS:CE1	2.23	0.74
2:N:116:ILE:HG21	2:N:176:ALA:HB2	1.69	0.73
1:A:197:ARG:HB2	1:A:208:VAL:O	1.89	0.73
1:A:546:ASN:O	1:A:549:LYS:HE2	1.88	0.73
3:C:50:LYS:HZ1	4:D:64:ARG:HH12	1.34	0.72
1:M:377:VAL:HG23	1:M:402:PHE:O	1.89	0.72
2:B:15:PRO:HB3	3:C:5:LYS:H	1.54	0.71
1:A:41:MET:HE2	2:B:150:ASN:HD22	1.56	0.71
1:A:243:MET:HA	1:A:243:MET:HE2	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:37:LYS:HE3	5:M:601:FAD:H8A	1.68	0.71
1:A:49:GLU:CA	1:A:129:ASP:O	2.38	0.70
1:M:251:GLY:HA2	1:M:277:PRO:HG2	1.72	0.70
1:M:556:ASP:HB2	1:M:558:ASP:OD1	1.91	0.70
2:B:57:CYS:HB3	2:B:62:CYS:HB3	1.73	0.70
1:M:194:GLY:O	1:M:208:VAL:HG12	1.91	0.70
2:N:51:LEU:HD23	2:N:52:SER:N	2.07	0.70
1:M:213:MET:HE2	1:M:380:CYS:HA	1.74	0.70
1:A:341:VAL:HG13	1:A:346:GLU:HB3	1.74	0.70
2:B:151:CYS:HG	9:B:246:SF4:FE1	1.07	0.70
2:N:210:CYS:SG	2:N:221:ALA:HB2	2.32	0.69
2:B:155:TYR:HE1	2:B:171:ALA:HB3	1.58	0.69
1:M:152:PHE:HB3	1:M:155:HIS:NE2	2.07	0.69
2:B:132:ASN:HD22	2:B:132:ASN:H	1.40	0.69
4:D:55:LEU:HG	4:D:59:GLN:NE2	2.07	0.69
2:B:18:ASP:OD2	2:B:22:HIS:CD2	2.46	0.69
1:A:346:GLU:HG3	1:A:347:PRO:HD2	1.75	0.68
3:C:103:MET:HG2	3:C:104:GLY:N	2.08	0.68
1:A:570:ILE:HD13	1:A:570:ILE:H	1.58	0.68
1:M:24:ALA:HB2	1:M:32:ILE:HD11	1.76	0.68
1:M:245:GLU:HB2	6:M:802:OAA:O5	1.94	0.68
1:A:98:LEU:HD23	2:B:132:ASN:HD21	1.58	0.67
2:N:40:LEU:HB3	2:N:53:TYR:CE2	2.30	0.66
1:M:211:ASP:OD2	1:M:507:GLU:HG2	1.95	0.66
2:B:65:CYS:HB3	2:B:76:ALA:H	1.60	0.66
4:P:10:GLU:N	4:P:11:PRO:HD2	2.10	0.66
3:C:19:LEU:HB2	3:C:22:TYR:CD2	2.31	0.65
1:M:205:GLY:HA3	2:N:56:SER:O	1.95	0.65
2:B:206:PHE:HE2	3:C:89:LEU:HD22	1.62	0.65
2:B:18:ASP:OD2	2:B:22:HIS:NE2	2.29	0.65
1:A:275:GLY:O	1:A:277:PRO:HD3	1.97	0.65
3:O:33:VAL:HB	3:O:34:PRO:HD3	1.79	0.64
1:M:137:HIS:HD2	1:M:141:GLN:HE21	1.45	0.64
3:C:33:VAL:HA	4:D:82:MET:CE	2.28	0.64
1:M:299:ARG:HE	1:M:299:ARG:HA	1.63	0.64
1:M:197:ARG:O	1:M:197:ARG:CD	2.46	0.63
1:M:292:GLN:HG2	1:M:465:ILE:HG21	1.80	0.63
1:M:444:GLY:HA3	1:M:488:ARG:O	1.98	0.63
9:B:246:SF4:FE3	9:B:246:SF4:S2	1.90	0.63
4:P:79:LEU:HD12	4:P:104:ALA:HB2	1.80	0.62
2:N:54:ARG:HE	2:N:103:VAL:HG13	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:467:ARG:HB3	1:M:472:MET:HE3	1.82	0.62
2:N:151:CYS:SG	2:N:153:LEU:HD12	2.40	0.62
1:M:215:MET:HB3	1:M:510:HIS:HE1	1.64	0.62
1:A:308:ARG:HH12	1:A:339:VAL:HA	1.64	0.62
2:N:51:LEU:HD23	2:N:52:SER:H	1.63	0.62
2:B:97:PRO:HG2	2:B:105:ASP:HB3	1.82	0.61
1:A:49:GLU:CB	1:A:129:ASP:O	2.49	0.61
2:B:212:GLU:HG3	3:C:21:PHE:CE2	2.33	0.61
1:A:514:VAL:HG12	1:A:518:MET:HE3	1.82	0.61
2:N:192:MET:HA	2:N:195:LEU:HD22	1.82	0.61
4:P:105:ALA:O	4:P:109:VAL:HG23	2.01	0.61
2:N:60:ALA:HA	7:N:245:FES:S1	2.40	0.61
1:M:433:GLU:O	1:M:437:LYS:HB2	2.01	0.61
1:A:69:THR:HA	1:A:391:LEU:HD22	1.82	0.61
1:M:211:ASP:OD1	1:M:507:GLU:HA	2.00	0.61
1:M:304:ILE:HG21	1:M:313:TYR:CE1	2.35	0.60
1:M:28:PRO:O	1:M:148:GLN:HG2	2.01	0.60
1:M:37:LYS:HE2	5:M:601:FAD:C5A	2.30	0.60
4:P:22:MET:HE3	4:P:22:MET:HA	1.83	0.60
1:M:37:LYS:HE2	5:M:601:FAD:C8A	2.16	0.60
1:M:217:LEU:HD23	1:M:555:ARG:N	2.17	0.60
1:M:18:ARG:NH1	1:M:404:ARG:HA	2.17	0.59
2:B:167:PHE:CD1	2:B:203:SER:HB2	2.37	0.59
2:N:71:ASN:HB3	3:O:18:LYS:HE2	1.85	0.59
1:M:137:HIS:HD2	1:M:141:GLN:NE2	2.01	0.59
1:A:386:HIS:ND1	1:A:390:ARG:HG3	2.17	0.59
3:C:86:TRP:HE1	4:D:22:MET:HE2	1.67	0.59
1:M:35:ILE:HG13	1:M:155:HIS:HB2	1.84	0.59
1:A:462:GLY:HA3	1:A:475:THR:OG1	2.03	0.58
1:A:197:ARG:HG3	1:A:208:VAL:O	2.03	0.58
1:M:20:ALA:HB2	1:M:34:LEU:HD12	1.85	0.58
1:M:114:ARG:O	1:M:124:THR:HB	2.02	0.58
1:M:234:THR:HG22	1:M:350:VAL:HG11	1.85	0.58
1:A:390:ARG:HD2	1:A:395:SER:HB2	1.84	0.58
1:M:48:ALA:HB3	1:M:132:GLY:CA	2.26	0.58
1:M:50:GLY:HA3	5:M:601:FAD:O4	2.03	0.58
1:M:61:SER:HB3	1:M:64:TYR:CD1	2.33	0.58
1:A:263:LEU:O	1:A:268:MET:HB2	2.04	0.57
1:M:44:HIS:CE1	1:M:204:ASN:HA	2.40	0.57
1:M:298:TRP:HA	1:M:303:THR:HG23	1.85	0.57
2:N:97:PRO:HA	3:O:7:TYR:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:358:MET:HG2	1:M:390:ARG:HB2	1.87	0.57
1:M:180:LEU:H	1:M:180:LEU:HD22	1.69	0.57
1:M:158:LEU:HD13	1:M:436:LEU:HG	1.85	0.57
1:M:219:HIS:NE2	1:M:371:ILE:HG12	2.20	0.56
3:C:113:TRP:O	3:C:117:VAL:HG23	2.05	0.56
1:M:162:VAL:HG21	1:M:219:HIS:HE1	1.69	0.56
2:N:54:ARG:NH2	2:N:103:VAL:CG1	2.58	0.56
2:N:155:TYR:HE1	2:N:171:ALA:HB3	1.69	0.56
1:A:356:TYR:HE1	5:A:601:FAD:O3'	1.89	0.56
2:B:185:ASP:C	2:B:185:ASP:OD1	2.49	0.56
4:D:20:GLY:HA2	4:D:73:LEU:HB3	1.88	0.56
2:N:151:CYS:SG	2:N:152:GLY:N	2.78	0.56
2:B:170:PRO:HA	2:B:224:ILE:HD11	1.88	0.56
4:D:1:ILE:O	4:D:3:PRO:HD3	2.05	0.56
1:M:41:MET:HB2	1:M:137:HIS:CE1	2.41	0.56
2:N:225:GLN:HE21	3:O:93:ALA:HB2	1.71	0.56
2:B:108:HIS:CE1	2:B:165:PRO:O	2.60	0.55
1:A:51:GLY:HA2	1:A:131:THR:HG21	1.87	0.55
4:P:2:ASN:O	4:P:5:PRO:HD3	2.05	0.55
1:A:386:HIS:CE1	1:A:390:ARG:HG3	2.42	0.55
1:M:212:GLY:HA2	1:M:215:MET:HE2	1.89	0.55
1:M:217:LEU:HD23	1:M:555:ARG:H	1.71	0.55
1:M:18:ARG:HH12	1:M:22:ALA:HB2	1.70	0.55
1:M:37:LYS:HD2	1:M:207:ILE:HB	1.88	0.55
1:M:245:GLU:CB	6:M:802:OAA:O5	2.55	0.55
2:N:51:LEU:HD22	2:N:53:TYR:CD2	2.42	0.55
1:A:61:SER:HB3	1:A:64:TYR:CD2	2.42	0.54
2:B:35:SER:O	2:B:38:ASP:HB2	2.08	0.54
3:C:87:PHE:HE2	4:D:25:ALA:HB1	1.72	0.54
1:M:23:ALA:HB1	1:M:32:ILE:HG21	1.89	0.54
1:M:41:MET:HG2	1:M:42:ARG:HE	1.71	0.54
3:C:87:PHE:CE1	3:C:112:LEU:HB3	2.43	0.54
1:M:50:GLY:CA	5:M:601:FAD:O4	2.56	0.54
1:M:157:VAL:HG21	1:M:215:MET:HE1	1.89	0.54
2:N:98:ILE:HB	3:O:7:TYR:HB3	1.90	0.54
1:M:199:TYR:CE2	1:M:459:MET:HB3	2.43	0.54
3:C:33:VAL:HB	3:C:34:PRO:HD3	1.90	0.53
1:M:54:ALA:HB3	1:M:125:TRP:NE1	2.24	0.53
1:M:537:GLU:H	1:M:537:GLU:CD	2.16	0.53
1:M:221:VAL:HG22	1:M:371:ILE:HD13	1.90	0.53
2:N:3:MET:HE2	2:N:31:ASP:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:130:TRP:HB2	4:D:53:ARG:HH21	1.74	0.53
1:M:36:SER:HA	5:M:601:FAD:C2A	2.39	0.53
2:N:63:GLY:O	2:N:151:CYS:HA	2.09	0.53
2:N:73:PRO:HG2	2:N:213:VAL:HG11	1.91	0.53
1:A:192:THR:HA	5:A:601:FAD:O4B	2.09	0.53
1:A:446:GLU:HB2	1:A:488:ARG:O	2.09	0.53
1:M:331:ILE:HD12	1:M:331:ILE:H	1.73	0.53
1:A:204:ASN:N	1:A:204:ASN:HD22	2.05	0.53
2:B:154:CYS:SG	9:B:246:SF4:S4	3.06	0.53
1:M:152:PHE:HB3	1:M:155:HIS:CD2	2.44	0.53
3:O:90:ALA:N	3:O:91:PRO:HD2	2.24	0.52
2:B:185:ASP:OD1	2:B:187:GLY:N	2.31	0.52
2:B:159:PRO:HG3	3:C:22:TYR:CE1	2.45	0.52
3:C:27:LEU:HD13	3:C:81:LEU:HD21	1.92	0.52
2:N:18:ASP:CG	2:N:22:HIS:NE2	2.62	0.52
1:A:243:MET:HA	1:A:243:MET:CE	2.37	0.52
2:B:39:ALA:O	2:B:43:ILE:HG12	2.10	0.52
1:M:151:ARG:NH1	1:M:153:ASP:OD1	2.35	0.52
2:N:44:LYS:HA	2:N:48:ALA:O	2.10	0.52
1:A:129:ASP:OD2	1:A:329:PRO:HD2	2.10	0.52
1:M:37:LYS:HG3	1:M:38:VAL:H	1.75	0.52
1:A:18:ARG:HG2	1:A:400:VAL:HA	1.91	0.52
1:M:288:ASP:O	1:M:292:GLN:HG3	2.10	0.52
1:A:18:ARG:NH1	1:A:92:GLU:OE2	2.42	0.51
1:A:118:GLY:HA2	1:A:279:ASN:HD21	1.75	0.51
1:A:332:CYS:HA	1:A:343:PRO:HG3	1.91	0.51
1:A:230:GLN:HB2	1:A:358:MET:HE1	1.92	0.51
1:A:446:GLU:HB2	1:A:489:VAL:HA	1.93	0.51
1:M:17:LEU:C	1:M:17:LEU:HD22	2.35	0.51
4:D:27:ILE:O	4:D:27:ILE:HG22	2.10	0.51
1:M:199:TYR:CE1	1:M:229:VAL:HG11	2.46	0.51
1:M:101:CYS:HB2	1:M:138:THR:HG21	1.93	0.50
1:A:80:ASP:OD2	1:A:569:LYS:HG2	2.12	0.50
2:B:65:CYS:CB	2:B:76:ALA:H	2.25	0.50
1:M:45:THR:HG23	5:M:601:FAD:H5'1	1.92	0.50
1:A:425:ILE:O	1:A:428:GLN:HB2	2.11	0.50
1:M:7:LEU:HB2	1:M:32:ILE:HG22	1.92	0.50
1:M:377:VAL:CG2	1:M:402:PHE:O	2.59	0.50
1:M:378:GLY:HA2	1:M:399:LEU:HD23	1.93	0.50
2:N:43:ILE:CD1	2:N:47:LEU:HD12	2.37	0.50
1:A:534:ARG:HH21	1:A:536:ASP:CG	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:46:VAL:CG2	1:M:133:PHE:HD1	2.25	0.50
1:M:553:ALA:HB1	1:M:561:THR:HG21	1.94	0.50
1:M:304:ILE:N	1:M:304:ILE:HD12	2.27	0.50
2:B:57:CYS:HB3	2:B:62:CYS:CB	2.40	0.50
1:A:448:TRP:CH2	1:A:504:TYR:HB3	2.46	0.50
1:M:35:ILE:HG12	5:M:601:FAD:H2A	1.93	0.50
1:A:525:ARG:NH1	1:A:527:GLU:OE2	2.44	0.49
1:M:481:GLU:HG2	1:M:485:ARG:HD3	1.93	0.49
2:N:54:ARG:NH2	2:N:104:VAL:O	2.45	0.49
1:A:27:ASN:OD1	1:A:30:ALA:N	2.43	0.49
3:C:19:LEU:HB2	3:C:22:TYR:HD2	1.77	0.49
1:M:311:VAL:HG12	1:M:351:ARG:HB3	1.93	0.49
1:M:481:GLU:O	1:M:485:ARG:HD3	2.12	0.49
1:A:197:ARG:CB	1:A:208:VAL:O	2.60	0.49
2:B:185:ASP:OD1	2:B:186:HIS:N	2.46	0.49
1:M:211:ASP:O	1:M:510:HIS:ND1	2.43	0.49
3:O:7:TYR:CD1	3:O:7:TYR:C	2.90	0.49
4:P:112:LEU:O	4:P:116:VAL:HG22	2.12	0.49
1:A:230:GLN:HB3	1:A:356:TYR:HB3	1.95	0.49
1:M:219:HIS:C	1:M:219:HIS:CD2	2.90	0.49
1:M:553:ALA:HB1	1:M:561:THR:CG2	2.42	0.49
1:A:98:LEU:CD2	2:B:132:ASN:HD21	2.25	0.49
1:A:253:ILE:HG13	1:A:315:ASP:HB3	1.94	0.49
1:M:199:TYR:HE2	1:M:459:MET:O	1.96	0.49
2:N:19:THR:HA	3:O:5:LYS:NZ	2.28	0.49
1:A:395:SER:HB3	5:A:601:FAD:N1	2.27	0.49
1:A:504:TYR:CE1	2:B:44:LYS:HE2	2.48	0.49
2:N:82:ARG:HD2	2:N:83:ASP:OD1	2.13	0.49
1:A:504:TYR:CD1	2:B:44:LYS:HE2	2.48	0.49
1:M:469:PRO:HG3	1:M:534:ARG:HH21	1.78	0.49
1:M:194:GLY:HA2	1:M:213:MET:HE3	1.94	0.48
3:C:85:THR:O	3:C:89:LEU:HG	2.13	0.48
3:O:39:SER:OG	4:P:71:ILE:O	2.31	0.48
4:D:48:ALA:O	4:D:53:ARG:HD3	2.14	0.48
1:A:49:GLU:HB3	1:A:129:ASP:O	2.12	0.48
2:N:18:ASP:OD2	2:N:22:HIS:NE2	2.41	0.48
2:B:206:PHE:CD1	2:B:225:GLN:HG3	2.48	0.48
1:M:197:ARG:O	1:M:197:ARG:CG	2.61	0.48
1:M:459:MET:O	1:M:463:CYS:O	2.32	0.48
1:M:37:LYS:O	1:M:154:GLU:HA	2.13	0.48
1:M:11:GLY:HA3	1:M:191:ALA:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:36:GLY:O	4:P:40:PRO:HG3	2.14	0.48
2:B:65:CYS:HB3	2:B:76:ALA:HB3	1.95	0.48
1:M:299:ARG:HE	1:M:299:ARG:CA	2.27	0.48
2:B:113:LEU:HD23	2:B:175:LEU:HD23	1.96	0.48
1:M:295:TRP:CD1	1:M:295:TRP:C	2.91	0.48
1:A:550:HIS:HB2	1:A:566:SER:OG	2.14	0.47
4:D:68:PHE:CE1	4:D:72:VAL:HG21	2.50	0.47
1:M:37:LYS:O	1:M:175:MET:SD	2.72	0.47
1:M:363:THR:HB	1:M:367:CYS:HA	1.95	0.47
1:A:304:ILE:HD12	1:A:304:ILE:H	1.79	0.47
4:D:79:LEU:HD12	4:D:104:ALA:HB2	1.96	0.47
1:M:157:VAL:H	5:M:601:FAD:H62A	1.62	0.47
1:M:279:ASN:O	1:M:280:LYS:HB2	2.14	0.47
2:B:132:ASN:HD22	2:B:132:ASN:N	2.11	0.47
1:M:377:VAL:HG22	1:M:378:GLY:N	2.29	0.47
1:A:243:MET:HE2	1:A:331:ILE:HD12	1.95	0.47
2:N:26:TYR:HB3	2:N:47:LEU:CD1	2.37	0.47
1:A:197:ARG:CG	1:A:208:VAL:O	2.62	0.47
1:M:93:MET:HE3	1:M:93:MET:HA	1.95	0.47
2:N:158:CYS:CA	8:N:246:F3S:S4	3.03	0.47
1:A:7:LEU:CD2	1:A:32:ILE:HG12	2.45	0.47
1:A:391:LEU:O	1:A:394:ASN:HB2	2.14	0.47
1:M:313:TYR:HD2	1:M:347:PRO:HG2	1.78	0.47
1:A:452:ARG:NH2	2:B:45:ASP:OD2	2.48	0.47
3:C:130:TRP:OXT	4:D:53:ARG:NE	2.48	0.47
1:M:500:THR:HB	1:M:504:TYR:CE1	2.49	0.47
2:N:19:THR:HA	3:O:5:LYS:HZ2	1.79	0.47
2:N:158:CYS:HA	8:N:246:F3S:S4	2.55	0.47
1:A:176:MET:CG	3:C:4:ARG:HH11	2.27	0.47
1:M:196:GLY:HA3	1:M:204:ASN:HD22	1.79	0.47
1:M:204:ASN:OD1	5:M:601:FAD:HM83	2.15	0.47
1:M:334:LEU:HD21	2:N:59:MET:HE3	1.97	0.47
1:A:436:LEU:O	1:A:440:VAL:HG23	2.14	0.47
1:M:469:PRO:HB3	1:M:523:MET:HE1	1.97	0.47
1:M:18:ARG:HH12	1:M:404:ARG:HA	1.81	0.46
1:M:537:GLU:CD	1:M:537:GLU:N	2.73	0.46
2:N:214:CYS:HG	9:N:244:SF4:FE3	1.32	0.46
2:B:63:GLY:O	2:B:151:CYS:HA	2.16	0.46
4:D:112:LEU:O	4:D:116:VAL:HG22	2.15	0.46
1:M:243:MET:HE2	1:M:331:ILE:HG23	1.97	0.46
1:A:330:PHE:HE1	2:B:216:LYS:HZ2	1.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:LEU:HD12	2:B:175:LEU:HA	1.60	0.46
1:A:96:LEU:HD11	1:A:400:VAL:HG11	1.97	0.46
1:M:158:LEU:HD21	1:M:506:ILE:HD13	1.96	0.46
1:M:503:LEU:HA	1:M:506:ILE:HD12	1.97	0.46
1:A:286:PRO:O	1:A:290:VAL:HG23	2.16	0.46
1:A:451:ILE:HG23	1:A:482:LEU:HD22	1.97	0.46
1:M:79:GLN:HB2	1:M:571:THR:HG23	1.97	0.46
3:O:76:LEU:HD13	4:P:32:ILE:HB	1.97	0.46
1:A:442:GLN:NE2	1:A:487:LYS:C	2.74	0.46
2:B:207:VAL:HG23	8:B:245:F3S:S2	2.55	0.46
1:M:473:GLN:NE2	1:M:477:ASP:OD1	2.48	0.46
1:M:217:LEU:HD12	1:M:221:VAL:O	2.15	0.46
1:M:311:VAL:HG21	1:M:349:PRO:HB3	1.98	0.46
3:C:111:SER:O	3:C:115:VAL:HG23	2.16	0.46
1:M:17:LEU:HA	1:M:34:LEU:HD11	1.97	0.46
1:M:213:MET:CE	1:M:380:CYS:HA	2.42	0.46
1:A:194:GLY:O	1:A:208:VAL:HG13	2.16	0.46
1:M:162:VAL:CG2	1:M:219:HIS:HE1	2.29	0.46
1:M:388:ALA:HB1	1:M:530:GLY:HA3	1.97	0.46
1:M:506:ILE:O	1:M:510:HIS:HD2	1.99	0.46
2:B:210:CYS:O	2:B:213:VAL:HG22	2.16	0.46
1:M:85:PHE:HD1	1:M:402:PHE:CE2	2.33	0.46
1:M:464:GLY:O	1:M:465:ILE:C	2.58	0.46
1:A:527:GLU:OE2	1:A:529:ARG:NH1	2.49	0.45
1:M:37:LYS:HG2	5:M:601:FAD:O2B	2.16	0.45
1:M:366:ASN:HB3	1:M:409:GLN:HG3	1.98	0.45
4:P:77:CYS:O	4:P:81:ARG:HG3	2.16	0.45
1:A:76:LEU:O	1:A:387:GLY:HA2	2.15	0.45
1:A:450:LYS:HA	1:A:450:LYS:HD3	1.75	0.45
2:B:154:CYS:HB2	2:B:170:PRO:CG	2.42	0.45
2:B:50:ASP:O	2:B:100:ARG:NH2	2.49	0.45
3:C:90:ALA:N	3:C:91:PRO:CD	2.80	0.45
2:B:32:ALA:O	2:B:82:ARG:NH1	2.49	0.45
1:M:257:LYS:HA	1:M:304:ILE:HD11	1.98	0.45
1:M:232:HIS:O	1:M:352:PRO:HA	2.16	0.45
4:P:9:ASP:OD1	4:P:9:ASP:N	2.50	0.45
1:M:99:TRP:CD1	1:M:142:THR:HG21	2.52	0.45
1:M:436:LEU:HA	1:M:439:LEU:HB2	1.99	0.45
2:N:112:SER:O	2:N:116:ILE:HG12	2.17	0.45
3:C:50:LYS:NZ	4:D:117:THR:HG22	2.32	0.45
2:B:109:PHE:C	2:B:109:PHE:CD2	2.93	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:153:LEU:HD12	2:B:215:PRO:HD3	1.98	0.44
2:B:6:LEU:HB2	2:B:30:TYR:CE2	2.51	0.44
1:M:159:ASP:OD2	1:M:160:ILE:N	2.50	0.44
2:N:75:LEU:HG	2:N:153:LEU:HD11	1.98	0.44
1:A:211:ASP:CB	5:A:601:FAD:H61A	2.30	0.44
1:M:298:TRP:HA	1:M:303:THR:CG2	2.47	0.44
4:P:28:ALA:N	4:P:29:PRO:HD2	2.32	0.44
1:M:508:LEU:O	1:M:512:LEU:HG	2.17	0.44
1:A:478:LYS:HA	1:A:478:LYS:HD2	1.86	0.44
1:M:356:TYR:CZ	1:M:379:GLU:HG3	2.52	0.44
1:A:28:PRO:HA	1:A:148:GLN:HE21	1.83	0.44
1:A:255:VAL:HB	1:A:259:GLY:HA2	2.00	0.44
1:A:570:ILE:HD13	1:A:570:ILE:N	2.30	0.44
1:A:358:MET:HE3	1:A:389:ASN:HA	1.99	0.44
2:N:15:PRO:HD3	2:N:100:ARG:HG2	1.99	0.44
1:M:498:PHE:O	2:N:100:ARG:NH2	2.50	0.44
1:M:206:GLY:N	2:N:55:TRP:CZ3	2.86	0.43
1:A:377:VAL:HG21	1:A:403:GLY:HA2	2.00	0.43
1:A:543:ASP:OD2	1:A:546:ASN:ND2	2.51	0.43
2:B:157:ALA:HB1	2:B:209:TYR:CD2	2.53	0.43
1:M:79:GLN:NE2	1:M:571:THR:H	2.15	0.43
1:A:366:ASN:O	1:A:367:CYS:HB2	2.18	0.43
1:M:46:VAL:HG23	1:M:133:PHE:HD1	1.82	0.43
2:B:68:MET:HG2	2:B:93:LEU:HA	1.99	0.43
2:B:132:ASN:H	2:B:132:ASN:ND2	2.13	0.43
1:M:492:THR:CG2	2:N:49:PRO:HG2	2.49	0.43
1:A:399:LEU:HD11	5:A:601:FAD:H4'	2.00	0.43
1:M:315:ASP:OD1	1:M:317:ARG:HG2	2.19	0.43
1:M:428:GLN:O	1:M:432:VAL:HG23	2.17	0.43
4:P:10:GLU:N	4:P:11:PRO:CD	2.80	0.43
1:A:356:TYR:CE2	1:A:390:ARG:HD3	2.54	0.43
1:M:200:ARG:HB2	1:M:456:GLY:HA3	2.01	0.43
1:M:364:ASP:OD1	1:M:368:GLU:N	2.52	0.43
2:N:12:ARG:NE	2:N:101:ASP:OD2	2.48	0.43
1:A:154:GLU:O	1:A:175:MET:HB2	2.18	0.43
1:A:230:GLN:NE2	1:A:287:ARG:NH1	2.67	0.43
4:D:30:VAL:O	4:D:33:LEU:HB3	2.18	0.43
1:M:186:ASN:CB	1:M:414:ALA:HA	2.49	0.43
1:M:228:PHE:CZ	1:M:388:ALA:HA	2.53	0.43
4:P:26:ILE:HB	4:P:27:ILE:HD12	2.01	0.43
3:C:87:PHE:CE2	4:D:25:ALA:HB1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:42:ARG:NH2	2:N:150:ASN:O	2.52	0.43
1:M:75:TRP:CD1	1:M:575:PRO:HA	2.54	0.43
1:M:292:GLN:HG2	1:M:465:ILE:CG2	2.46	0.43
2:N:45:ASP:C	2:N:46:ASN:HD22	2.26	0.43
1:A:441:ASN:O	1:A:442:GLN:C	2.62	0.43
1:M:7:LEU:CD2	1:M:187:ALA:HB3	2.49	0.43
2:N:157:ALA:HB1	2:N:209:TYR:CD2	2.54	0.43
1:M:442:GLN:NE2	1:M:487:LYS:HD3	2.34	0.42
2:B:242:PRO:HB3	4:P:93:VAL:C	2.44	0.42
3:C:33:VAL:CA	4:D:82:MET:HE2	2.41	0.42
1:M:324:LEU:HG	1:M:325:HIS:CE1	2.54	0.42
1:A:236:LEU:HD21	1:A:243:MET:SD	2.59	0.42
2:N:149:ILE:HG23	2:N:216:LYS:HG3	1.99	0.42
3:O:65:ASN:O	3:O:69:VAL:HG23	2.19	0.42
1:A:204:ASN:N	1:A:204:ASN:ND2	2.67	0.42
1:A:493:ASP:OD1	1:A:495:SER:OG	2.32	0.42
1:M:32:ILE:HG13	1:M:149:ILE:HA	2.01	0.42
1:A:279:ASN:O	1:A:280:LYS:HB2	2.20	0.42
1:A:542:ARG:HH21	1:A:544:ASP:CG	2.26	0.42
1:M:242:LEU:HD22	5:M:601:FAD:H6	2.02	0.42
1:M:249:GLY:HA2	1:M:284:LEU:HD11	2.01	0.42
2:N:149:ILE:CG2	2:N:216:LYS:HG3	2.50	0.42
1:M:196:GLY:HA3	1:M:204:ASN:ND2	2.34	0.42
3:O:127:ALA:C	3:O:128:LEU:HD23	2.44	0.42
1:A:529:ARG:HB2	1:A:542:ARG:HG3	2.02	0.42
2:B:109:PHE:C	2:B:109:PHE:HD2	2.27	0.42
1:M:9:ILE:HG21	1:M:19:ALA:HB3	2.00	0.42
2:N:46:ASN:HD22	2:N:46:ASN:N	2.17	0.42
1:A:18:ARG:HH12	1:A:404:ARG:HH11	1.68	0.42
1:A:100:GLY:O	1:A:102:PRO:HD3	2.18	0.42
1:A:224:ARG:NH2	1:A:382:SER:O	2.53	0.42
1:A:254:LEU:HD12	1:A:263:LEU:HD11	2.02	0.42
3:C:31:THR:O	3:C:34:PRO:HD2	2.20	0.42
1:M:17:LEU:HD11	1:M:139:LEU:CB	2.49	0.42
1:M:76:LEU:O	1:M:550:HIS:NE2	2.53	0.42
1:M:17:LEU:HD21	1:M:139:LEU:HB3	2.02	0.42
1:A:92:GLU:OE1	1:A:404:ARG:HD2	2.20	0.41
1:A:151:ARG:NH1	1:A:153:ASP:OD2	2.54	0.41
1:A:316:LEU:O	1:A:319:LEU:HB2	2.20	0.41
1:M:492:THR:HG23	2:N:49:PRO:HG2	2.01	0.41
1:M:513:ASN:HB3	1:M:555:ARG:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:51:LEU:HD22	2:N:53:TYR:HD2	1.82	0.41
2:B:57:CYS:HB3	2:B:62:CYS:SG	2.58	0.41
3:C:94:ALA:HB1	3:C:96:ILE:HD11	2.02	0.41
1:M:428:GLN:O	1:M:432:VAL:N	2.54	0.41
1:A:19:ALA:HA	1:A:403:GLY:O	2.20	0.41
1:A:49:GLU:H	1:A:49:GLU:HG2	1.75	0.41
3:C:12:THR:C	3:C:14:THR:H	2.28	0.41
1:M:332:CYS:SG	1:M:343:PRO:HG3	2.61	0.41
1:A:455:MET:HE2	1:A:455:MET:HB3	1.98	0.41
2:B:240:LEU:O	2:B:242:PRO:HD3	2.20	0.41
1:M:102:PRO:HG2	1:M:134:HIS:CD2	2.56	0.41
2:N:206:PHE:HA	8:N:246:F3S:S1	2.60	0.41
1:A:59:HIS:CD2	1:A:59:HIS:H	2.37	0.41
2:B:208:GLY:N	8:B:245:F3S:S1	2.90	0.41
1:M:3:PHE:HB3	1:M:183:ILE:HG23	2.02	0.41
1:M:37:LYS:N	5:M:601:FAD:N3A	2.69	0.41
1:M:183:ILE:HG22	1:M:184:ARG:N	2.35	0.41
1:A:141:GLN:HB3	2:B:118:PRO:O	2.21	0.41
3:C:87:PHE:O	3:C:91:PRO:HD3	2.20	0.41
1:M:76:LEU:HD22	1:M:76:LEU:HA	1.91	0.41
1:M:85:PHE:HB2	1:M:402:PHE:HE2	1.86	0.41
1:M:499:ASN:HA	2:N:100:ARG:HH22	1.85	0.41
2:B:15:PRO:HG3	2:B:99:GLU:O	2.21	0.41
1:M:13:GLY:HA3	5:M:601:FAD:O1P	2.20	0.41
1:M:79:GLN:OE1	1:M:570:ILE:HG23	2.21	0.41
1:A:151:ARG:NH2	2:B:114:GLU:OE2	2.54	0.41
1:M:145:GLN:HE21	2:N:119:TYR:HB2	1.85	0.41
1:M:181:VAL:HG12	1:M:182:GLN:N	2.36	0.41
1:M:198:VAL:HG11	1:M:515:ALA:HB2	2.03	0.41
5:M:601:FAD:H9	5:M:601:FAD:H1'1	1.81	0.41
2:N:39:ALA:O	2:N:43:ILE:HG12	2.21	0.41
4:P:20:GLY:HA2	4:P:73:LEU:HB3	2.03	0.41
4:P:24:SER:O	4:P:28:ALA:HB3	2.21	0.41
2:B:41:GLY:HA2	2:B:53:TYR:OH	2.21	0.41
2:N:57:CYS:SG	2:N:61:ILE:HG22	2.61	0.41
2:N:97:PRO:HG2	2:N:105:ASP:HB3	2.02	0.41
1:A:530:GLY:O	1:A:533:GLN:NE2	2.53	0.40
2:B:26:TYR:HD2	2:B:47:LEU:HD12	1.85	0.40
1:M:400:VAL:HG23	1:M:401:VAL:HG23	2.02	0.40
2:N:64:SER:C	2:N:66:GLY:H	2.29	0.40
1:A:78:GLU:OE1	1:A:569:LYS:HB3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:601:FAD:H9	5:A:601:FAD:H1'1	1.88	0.40
4:D:50:SER:O	4:D:51:TYR:C	2.64	0.40
4:D:28:ALA:O	4:D:32:ILE:HG13	2.21	0.40
1:M:42:ARG:HA	1:M:42:ARG:HD3	1.72	0.40
1:M:324:LEU:HG	1:M:325:HIS:ND1	2.37	0.40
1:M:574:PRO:C	1:M:576:ALA:H	2.29	0.40
2:N:155:TYR:CE2	2:N:169:GLY:HA3	2.56	0.40
1:A:176:MET:HG2	3:C:4:ARG:HH11	1.85	0.40
2:B:140:ALA:HB1	3:C:97:ILE:HD12	2.04	0.40
2:B:206:PHE:CE1	2:B:225:GLN:HG3	2.57	0.40
1:M:202:ASN:HD22	1:M:202:ASN:N	2.18	0.40
3:O:90:ALA:N	3:O:91:PRO:CD	2.84	0.40
3:C:63:LEU:HB2	4:D:40:PRO:HB3	2.03	0.40
3:C:70:ILE:O	3:C:74:ILE:HG13	2.22	0.40
3:O:120:THR:HG23	4:P:30:VAL:HB	2.04	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	575/577 (100%)	551 (96%)	21 (4%)	3 (0%)	24	52
1	M	575/577 (100%)	541 (94%)	33 (6%)	1 (0%)	43	70
2	B	241/243 (99%)	231 (96%)	9 (4%)	1 (0%)	30	58
2	N	241/243 (99%)	228 (95%)	11 (5%)	2 (1%)	16	44
3	C	128/130 (98%)	122 (95%)	6 (5%)	0	100	100
3	O	128/130 (98%)	123 (96%)	5 (4%)	0	100	100
4	D	117/119 (98%)	109 (93%)	8 (7%)	0	100	100
4	P	117/119 (98%)	115 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2122/2138 (99%)	2020 (95%)	95 (4%)	7 (0%)	36	63

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	56	SER
1	A	329	PRO
1	A	444	GLY
2	N	170	PRO
1	A	277	PRO
1	M	329	PRO
2	N	49	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	460/460 (100%)	437 (95%)	23 (5%)	22	49
1	M	460/460 (100%)	420 (91%)	40 (9%)	9	32
2	B	205/205 (100%)	197 (96%)	8 (4%)	28	54
2	N	205/205 (100%)	196 (96%)	9 (4%)	25	51
3	C	111/111 (100%)	108 (97%)	3 (3%)	39	60
3	O	111/111 (100%)	110 (99%)	1 (1%)	70	75
4	D	97/97 (100%)	93 (96%)	4 (4%)	27	53
4	P	97/97 (100%)	96 (99%)	1 (1%)	68	74
All	All	1746/1746 (100%)	1657 (95%)	89 (5%)	21	48

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	MET
1	A	7	LEU
1	A	18	ARG

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Mol	Chain	Res	Type
1	A	38	VAL
1	A	42	ARG
1	A	49	GLU
1	A	52	SER
1	A	76	LEU
1	A	91	THR
1	A	122	GLU
1	A	138	THR
1	A	211	ASP
1	A	218	SER
1	A	243	MET
1	A	284	LEU
1	A	299	ARG
1	A	344	VAL
1	A	346	GLU
1	A	419	ASN
1	A	465	ILE
1	A	485	ARG
1	A	570	ILE
1	A	572	THR
2	B	19	THR
2	B	27	GLU
2	B	113	LEU
2	B	116	ILE
2	B	132	ASN
2	B	154	CYS
2	B	175	LEU
2	B	237	ILE
3	C	12	THR
3	C	27	LEU
3	C	96	ILE
4	D	9	ASP
4	D	62	ILE
4	D	113	ILE
4	D	118	ILE
1	M	17	LEU
1	M	18	ARG
1	M	32	ILE
1	M	42	ARG
1	M	76	LEU
1	M	89	CYS
1	M	93	MET

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Mol	Chain	Res	Type
1	M	96	LEU
1	M	111	VAL
1	M	144	LEU
1	M	155	HIS
1	M	162	VAL
1	M	164	ASP
1	M	170	LEU
1	M	173	MET
1	M	180	LEU
1	M	197	ARG
1	M	202	ASN
1	M	207	ILE
1	M	221	VAL
1	M	242	LEU
1	M	243	MET
1	M	288	ASP
1	M	299	ARG
1	M	318	HIS
1	M	324	LEU
1	M	348	ILE
1	M	350	VAL
1	M	361	ILE
1	M	386	HIS
1	M	413	ARG
1	M	439	LEU
1	M	463	CYS
1	M	482	LEU
1	M	485	ARG
1	M	502	LEU
1	M	537	GLU
1	M	543	ASP
1	M	544	ASP
1	M	552	LEU
2	N	5	ASN
2	N	46	ASN
2	N	82	ARG
2	N	121	ILE
2	N	125	ARG
2	N	189	LYS
2	N	214	CYS
2	N	237	ILE
2	N	243	ARG

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Mol	Chain	Res	Type
3	O	54	GLU
4	P	118	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	87	HIS
1	A	95	GLN
1	A	141	GLN
1	A	182	GLN
1	A	279	ASN
1	A	292	GLN
1	A	296	HIS
1	A	428	GLN
1	A	520	HIS
1	A	546	ASN
2	B	5	ASN
2	B	108	HIS
2	B	123	ASN
2	B	132	ASN
2	B	143	HIS
2	B	150	ASN
2	B	194	GLN
3	C	51	ASN
3	C	72	ASN
4	D	59	GLN
4	D	92	HIS
1	M	44	HIS
1	M	134	HIS
1	M	137	HIS
1	M	145	GLN
1	M	202	ASN
1	M	219	HIS
1	M	292	GLN
1	M	394	ASN
1	M	428	GLN
1	M	434	GLN
1	M	442	GLN
1	M	546	ASN
2	N	5	ASN
2	N	46	ASN
2	N	95	ASN

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Mol	Chain	Res	Type
2	N	150	ASN
2	N	225	GLN
3	O	72	ASN
3	O	95	ASN

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](#)

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	$\# Z > 2$
5	FAD	M	601	-	58,58,58	1.88	10 (17%)	85,89,89	1.79	20 (23%)
9	SF4	B	246	2	0,12,12	-	-	-		
7	FES	B	244	2	0,4,4	-	-	-		
5	FAD	A	601	-	58,58,58	1.18	7 (12%)	85,89,89	1.75	25 (29%)
6	OAA	A	702	-	8,8,8	2.25	3 (37%)	8,10,10	1.29	0
6	OAA	M	802	-	8,8,8	2.27	4 (50%)	8,10,10	1.42	1 (12%)
8	F3S	N	246	2	0,9,9	-	-	-		
7	FES	N	245	2	0,4,4	-	-	-		
9	SF4	N	244	2	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	F3S	B	245	2	0,9,9	-	-	-		

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FAD	M	601	-	-	20/34/50/50	0/6/6/6
9	SF4	B	246	2	-	-	0/6/5/5
7	FES	B	244	2	-	-	0/1/1/1
5	FAD	A	601	-	-	4/34/50/50	0/6/6/6
6	OAA	A	702	-	-	4/8/8/8	-
6	OAA	M	802	-	-	1/8/8/8	-
8	F3S	N	246	2	-	-	0/3/3/3
7	FES	N	245	2	-	-	0/1/1/1
9	SF4	N	244	2	-	-	0/6/5/5
8	F3S	B	245	2	-	-	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	601	FAD	C2A-N3A	-5.86	1.23	1.33
5	M	601	FAD	C4A-N3A	5.53	1.44	1.34
5	M	601	FAD	C2A-N1A	5.04	1.42	1.33
5	M	601	FAD	O4B-C1B	4.52	1.52	1.42
5	M	601	FAD	C8A-N9A	-4.04	1.30	1.37
6	A	702	OAA	O3-C3	3.98	1.31	1.23
6	M	802	OAA	O3-C3	3.96	1.31	1.23
6	A	702	OAA	O4-C4	3.68	1.31	1.22
6	M	802	OAA	O4-C4	3.55	1.31	1.22
5	M	601	FAD	P-O3P	3.13	1.62	1.59
6	A	702	OAA	O1-C1	3.03	1.32	1.22
6	M	802	OAA	O1-C1	2.84	1.31	1.22
5	M	601	FAD	C4X-N5	2.81	1.36	1.30
5	A	601	FAD	C2B-C1B	-2.70	1.45	1.53
5	A	601	FAD	C4X-N5	2.61	1.36	1.30
5	M	601	FAD	PA-O3P	2.61	1.62	1.59
5	M	601	FAD	C1B-N9A	2.53	1.53	1.46
5	A	601	FAD	C10-N10	2.49	1.42	1.37
5	A	601	FAD	O2B-C2B	-2.43	1.36	1.43
5	A	601	FAD	C4A-N9A	-2.37	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	FAD	O3B-C3B	-2.30	1.37	1.43
5	A	601	FAD	C8A-N7A	2.28	1.36	1.31
6	M	802	OAA	C3-C4	-2.19	1.50	1.53
5	M	601	FAD	C4A-N9A	2.10	1.42	1.37

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	601	FAD	N3A-C2A-N1A	-5.84	119.74	128.58
5	M	601	FAD	N3A-C4A-N9A	5.56	136.62	127.17
5	A	601	FAD	N3A-C2A-N1A	-5.35	120.48	128.58
5	M	601	FAD	C5A-C4A-N9A	-4.26	101.17	105.81
5	A	601	FAD	C5A-C4A-N3A	-4.10	121.06	126.72
5	M	601	FAD	C2A-N1A-C6A	4.05	125.38	118.73
5	A	601	FAD	O2B-C2B-C1B	3.96	123.74	110.10
5	A	601	FAD	N9A-C8A-N7A	-3.83	108.50	113.94
5	A	601	FAD	C2A-N3A-C4A	3.50	120.38	111.83
5	M	601	FAD	C5A-C4A-N3A	-3.32	122.15	126.72
5	M	601	FAD	C4A-N9A-C1B	-3.29	118.94	126.63
5	A	601	FAD	C4A-C5A-N7A	-3.26	106.86	110.58
5	A	601	FAD	C4A-N9A-C8A	3.14	109.04	105.74
5	M	601	FAD	C2A-N3A-C4A	3.07	119.33	111.83
5	A	601	FAD	C4-N3-C2	-3.05	120.23	125.64
5	M	601	FAD	O4B-C1B-N9A	3.01	113.87	108.09
5	M	601	FAD	C4X-C4-N3	2.90	120.63	113.25
5	M	601	FAD	C4-C4X-N5	2.83	122.11	118.21
5	M	601	FAD	C4-N3-C2	-2.83	120.62	125.64
5	A	601	FAD	C5X-N5-C4X	2.82	122.65	118.09
5	A	601	FAD	C4X-C4-N3	2.82	120.44	113.25
5	M	601	FAD	O4B-C4B-C5B	-2.71	100.67	109.33
5	A	601	FAD	O4B-C1B-N9A	2.69	113.26	108.09
6	M	802	OAA	O4-C4-C3	-2.65	118.52	121.81
5	A	601	FAD	O2B-C2B-C3B	-2.64	103.34	111.82
5	A	601	FAD	C5A-N7A-C8A	2.61	107.55	103.45
5	M	601	FAD	C9A-C5X-N5	-2.48	119.82	122.45
5	A	601	FAD	C4X-C10-N1	-2.44	118.60	124.59
5	A	601	FAD	C4A-N9A-C1B	-2.39	121.04	126.63
5	M	601	FAD	C1B-N9A-C8A	2.37	132.35	127.09
5	A	601	FAD	C3B-C2B-C1B	2.33	105.88	101.46
5	A	601	FAD	O4-C4-C4X	-2.33	120.38	126.53
5	A	601	FAD	C9A-C5X-N5	-2.30	120.01	122.45
5	M	601	FAD	O2B-C2B-C1B	2.28	117.94	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	M	601	FAD	O4-C4-C4X	-2.27	120.53	126.53
5	A	601	FAD	C10-C4X-N5	-2.26	120.19	124.81
5	A	601	FAD	C10-N1-C2	2.24	121.70	116.85
5	M	601	FAD	C4B-O4B-C1B	-2.23	104.54	109.47
5	M	601	FAD	C4A-N9A-C8A	2.22	108.07	105.74
5	A	601	FAD	N3A-C4A-N9A	2.19	130.90	127.17
5	A	601	FAD	C4-C4X-N5	2.17	121.20	118.21
5	M	601	FAD	C10-C4X-N5	-2.15	120.42	124.81
5	M	601	FAD	C5X-N5-C4X	2.10	121.49	118.09
5	A	601	FAD	O3P-P-O1P	-2.10	104.39	110.70
5	A	601	FAD	C6A-C5A-N7A	2.05	136.04	132.09
5	A	601	FAD	C5A-C4A-N9A	2.04	108.03	105.81

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	601	FAD	N10-C1'-C2'-O2'
5	A	601	FAD	C5'-O5'-P-O2P
5	M	601	FAD	C5B-O5B-PA-O2A
5	M	601	FAD	C5B-O5B-PA-O3P
5	M	601	FAD	P-O3P-PA-O5B
5	M	601	FAD	N10-C1'-C2'-O2'
5	M	601	FAD	N10-C1'-C2'-C3'
5	M	601	FAD	C1'-C2'-C3'-O3'
5	M	601	FAD	C1'-C2'-C3'-C4'
5	M	601	FAD	O2'-C2'-C3'-O3'
5	M	601	FAD	O2'-C2'-C3'-C4'
5	M	601	FAD	C2'-C3'-C4'-O4'
5	M	601	FAD	C2'-C3'-C4'-C5'
5	M	601	FAD	O3'-C3'-C4'-O4'
5	M	601	FAD	O3'-C3'-C4'-C5'
5	M	601	FAD	C5'-O5'-P-O2P
6	A	702	OAA	C2-C3-C4-O5
5	M	601	FAD	O4B-C4B-C5B-O5B
5	M	601	FAD	C3B-C4B-C5B-O5B
5	A	601	FAD	PA-O3P-P-O5'
6	A	702	OAA	C1-C2-C3-O3
6	A	702	OAA	O3-C3-C4-O4
6	A	702	OAA	C2-C3-C4-O4
5	M	601	FAD	C5'-O5'-P-O1P
5	M	601	FAD	C5'-O5'-P-O3P

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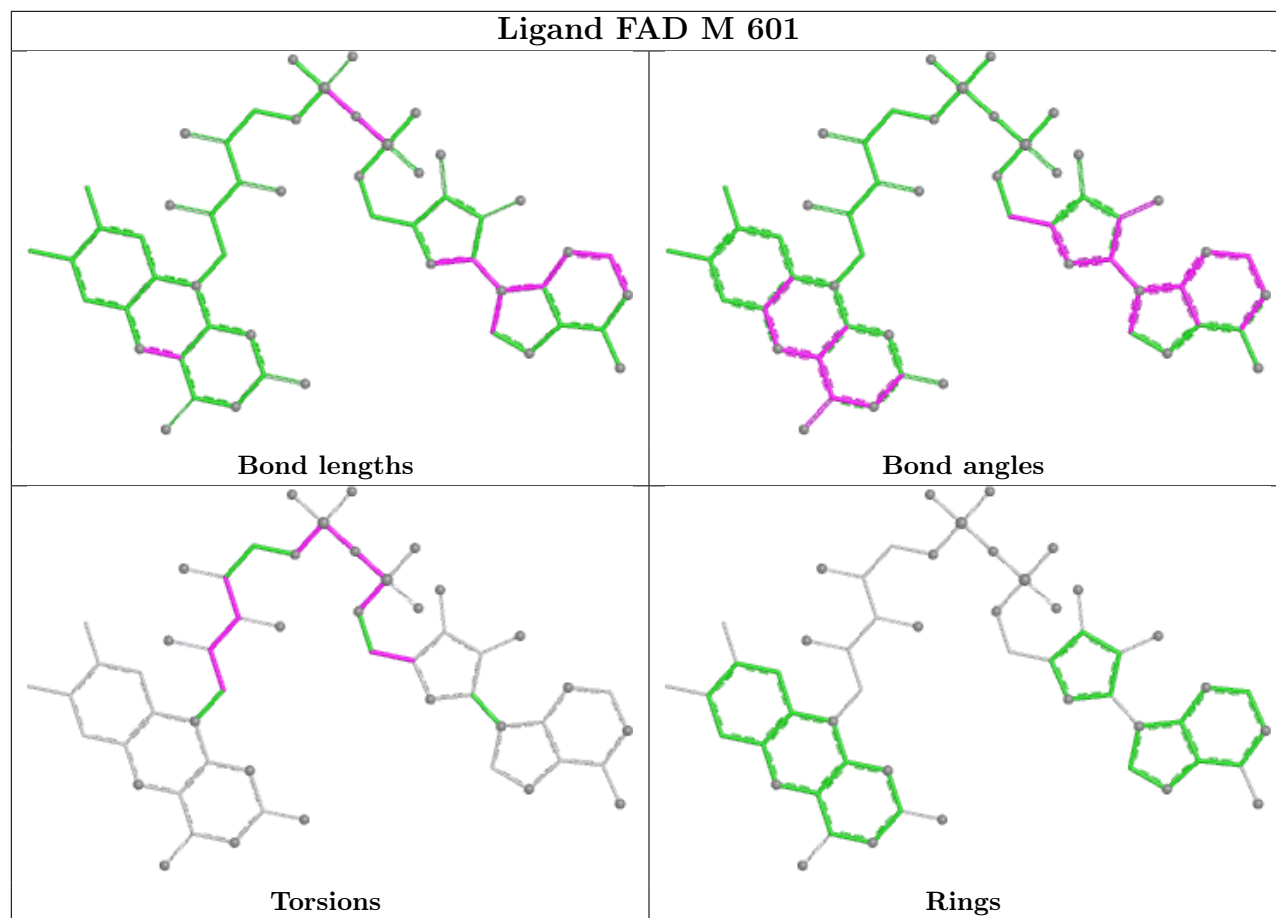
Mol	Chain	Res	Type	Atoms
5	M	601	FAD	PA-O3P-P-O1P
6	M	802	OAA	O1-C1-C2-C3
5	M	601	FAD	PA-O3P-P-O2P
5	A	601	FAD	PA-O3P-P-O2P

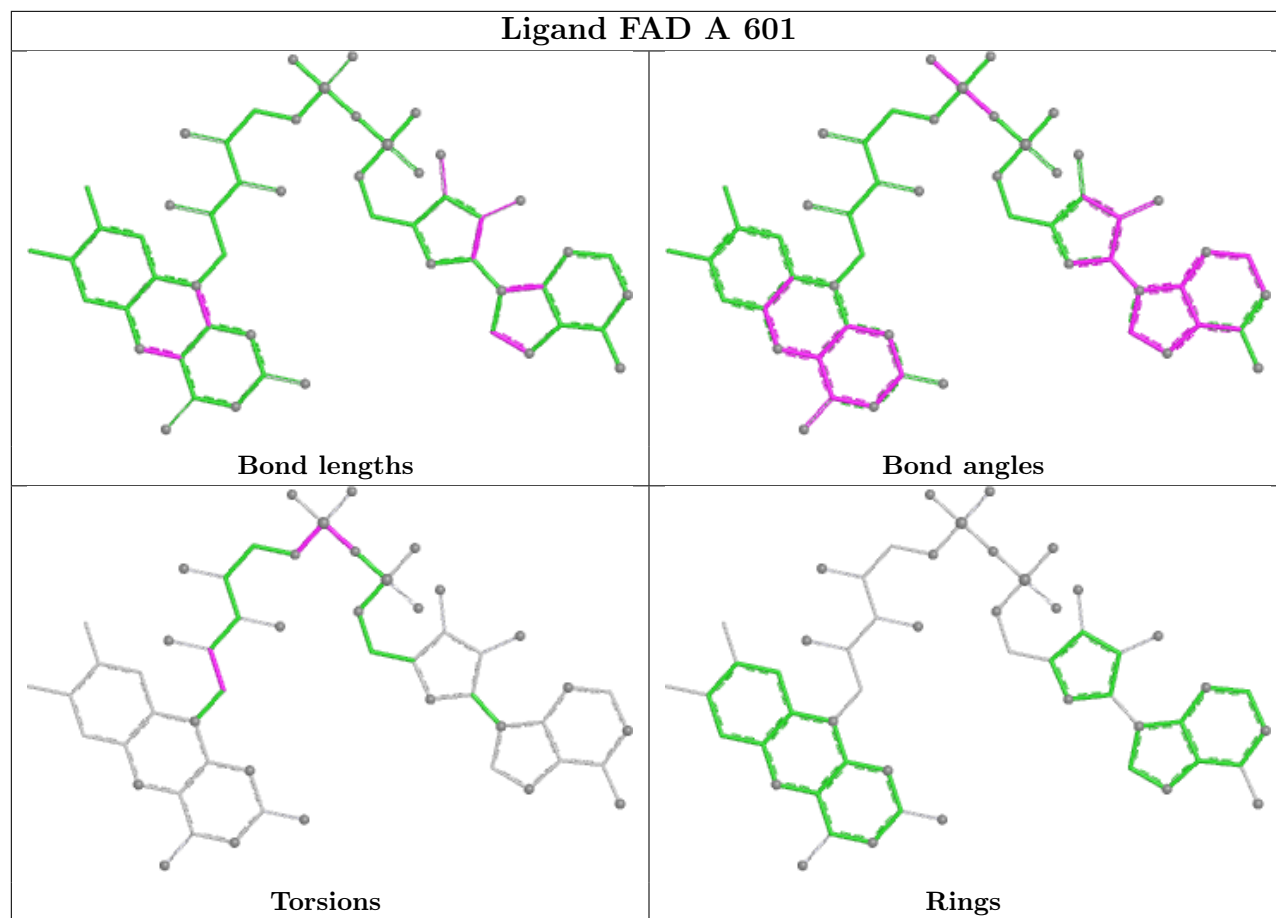
There are no ring outliers.

8 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	M	601	FAD	20	0
9	B	246	SF4	7	0
5	A	601	FAD	9	0
6	M	802	OAA	2	0
8	N	246	F3S	3	0
7	N	245	FES	1	0
9	N	244	SF4	1	0
8	B	245	F3S	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 ⓘ

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%)	-0.54	1 (0%) 91 87	29, 46, 91, 117	0
1	M	577/577 (100%)	1.07	97 (16%) 4 5	88, 155, 184, 215	0
2	B	243/243 (100%)	-0.55	0 100 100	29, 51, 75, 133	0
2	N	243/243 (100%)	0.65	13 (5%) 32 23	76, 129, 206, 230	0
3	C	130/130 (100%)	-0.45	0 100 100	53, 69, 98, 108	0
3	O	130/130 (100%)	0.02	0 100 100	60, 93, 153, 194	0
4	D	119/119 (100%)	-0.27	3 (2%) 58 43	49, 65, 91, 108	0
4	P	119/119 (100%)	-0.15	0 100 100	57, 81, 139, 168	0
All	All	2138/2138 (100%)	0.10	114 (5%) 32 23	29, 80, 179, 230	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	188	VAL	7.1
1	M	189	VAL	6.0
1	M	387	GLY	5.5
1	M	394	ASN	5.1
2	N	52	SER	5.1
1	M	386	HIS	5.1
1	M	8	ALA	4.7
1	M	385	LEU	4.5
1	M	517	CYS	4.3
1	M	498	PHE	4.2
1	M	502	LEU	4.1
1	M	405	LEU	4.1
1	M	465	ILE	4.1
1	M	14	GLY	4.0
1	M	295	TRP	4.0
1	M	170	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	M	499	ASN	3.7
1	M	378	GLY	3.6
1	M	377	VAL	3.5
1	M	411	THR	3.4
1	M	33	ALA	3.4
1	M	160	ILE	3.3
1	M	196	GLY	3.2
1	M	573	LEU	3.1
1	M	489	VAL	3.1
1	M	491	ILE	3.1
4	D	118	ILE	3.1
1	M	409	GLN	3.1
1	M	514	VAL	3.0
1	M	10	VAL	3.0
1	M	402	PHE	3.0
1	M	195	ALA	2.9
1	M	439	LEU	2.9
1	M	165	GLY	2.9
1	M	215	MET	2.9
1	M	373	GLY	2.8
1	M	574	PRO	2.8
1	M	572	THR	2.8
1	M	476	ILE	2.8
1	M	77	CYS	2.8
1	M	475	THR	2.8
1	M	375	PHE	2.8
1	M	576	ALA	2.8
1	M	228	PHE	2.7
1	M	125	TRP	2.7
1	M	198	VAL	2.7
1	M	23	ALA	2.7
1	M	7	LEU	2.7
1	M	180	LEU	2.6
1	M	495	SER	2.6
1	M	497	VAL	2.6
1	M	571	THR	2.6
1	M	9	ILE	2.6
1	M	206	GLY	2.6
1	M	374	LEU	2.6
1	M	383	VAL	2.6
1	M	100	GLY	2.5
1	M	158	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	M	389	ASN	2.5
1	M	415	ALA	2.5
2	N	95	ASN	2.5
1	M	401	VAL	2.5
1	M	361	ILE	2.4
2	N	206	PHE	2.4
1	M	552	LEU	2.4
1	M	392	GLY	2.4
2	N	98	ILE	2.4
1	M	382	SER	2.4
4	D	117	THR	2.4
1	M	187	ALA	2.4
1	M	172	ALA	2.3
1	M	519	ALA	2.3
1	M	390	ARG	2.3
1	M	329	PRO	2.3
1	M	32	ILE	2.3
1	M	205	GLY	2.3
2	N	56	SER	2.3
2	N	25	PHE	2.3
1	M	173	MET	2.3
1	M	500	THR	2.3
1	M	38	VAL	2.3
1	M	490	ARG	2.3
1	M	92	GLU	2.2
1	M	190	MET	2.2
1	M	135	MET	2.2
1	M	553	ALA	2.2
2	N	6	LEU	2.2
1	M	494	THR	2.2
1	M	103	TRP	2.2
4	D	1	ILE	2.2
2	N	55	TRP	2.2
1	M	548	LEU	2.1
1	M	213	MET	2.1
1	A	295	TRP	2.1
1	M	192	THR	2.1
1	M	130	LYS	2.1
1	M	508	LEU	2.1
2	N	54	ARG	2.1
1	M	207	ILE	2.1
2	N	193	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	M	250	GLU	2.1
1	M	545	VAL	2.1
1	M	468	THR	2.1
1	M	492	THR	2.1
1	M	403	GLY	2.1
2	N	188	LYS	2.0
2	N	232	SER	2.0
1	M	391	LEU	2.0
1	M	451	ILE	2.0
1	M	199	TYR	2.0
1	M	487	LYS	2.0
1	M	157	VAL	2.0
1	M	436	LEU	2.0
2	N	32	ALA	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.

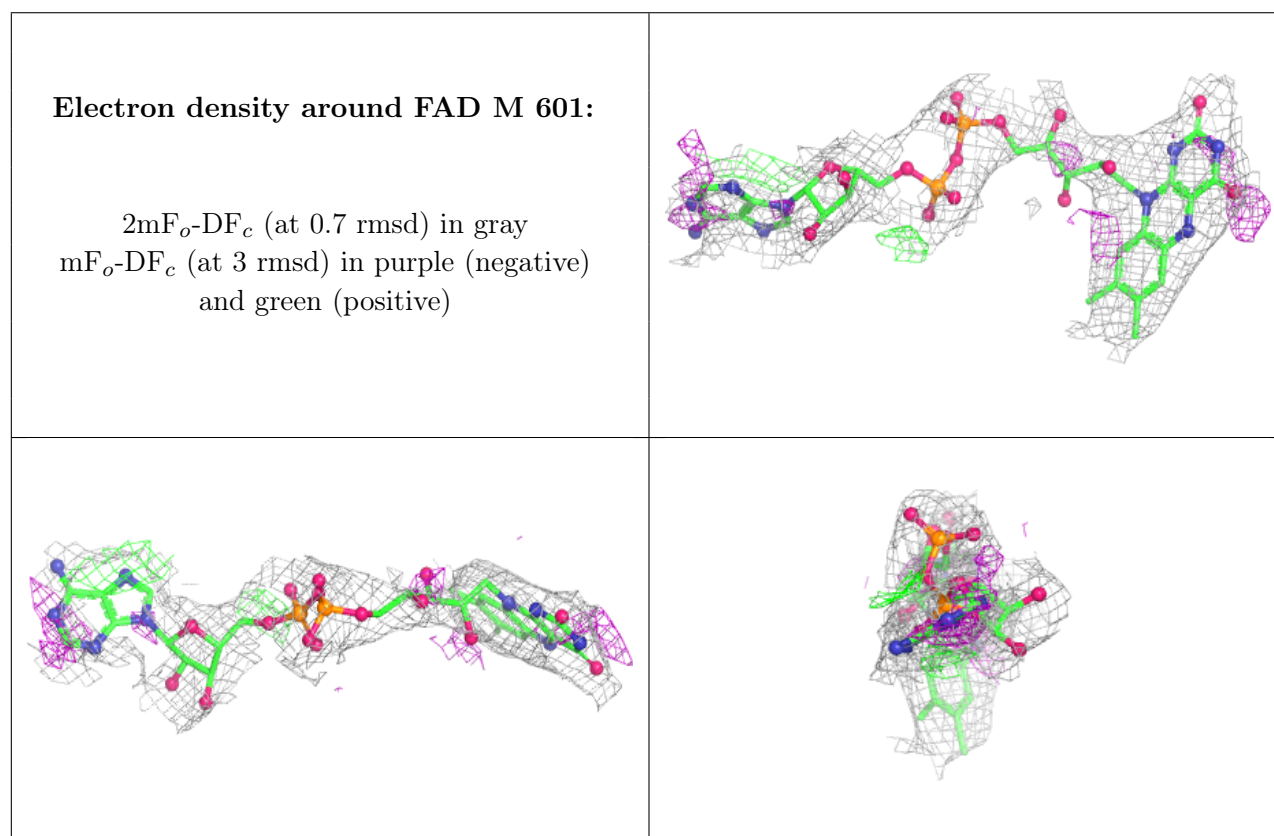
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	OAA	M	802	9/9	0.56	0.19	114,114,115,115	0
6	OAA	A	702	9/9	0.82	0.20	45,48,49,50	0
5	FAD	M	601	53/53	0.82	0.14	95,109,125,126	0
5	FAD	A	601	53/53	0.94	0.11	43,47,57,61	0
8	F3S	N	246	7/7	0.97	0.06	75,75,76,76	0
9	SF4	N	244	8/8	0.97	0.06	82,82,83,83	0
7	FES	N	245	4/4	0.98	0.05	88,88,89,90	0
9	SF4	B	246	8/8	0.99	0.06	63,65,66,66	0
8	F3S	B	245	7/7	0.99	0.04	45,47,47,47	0

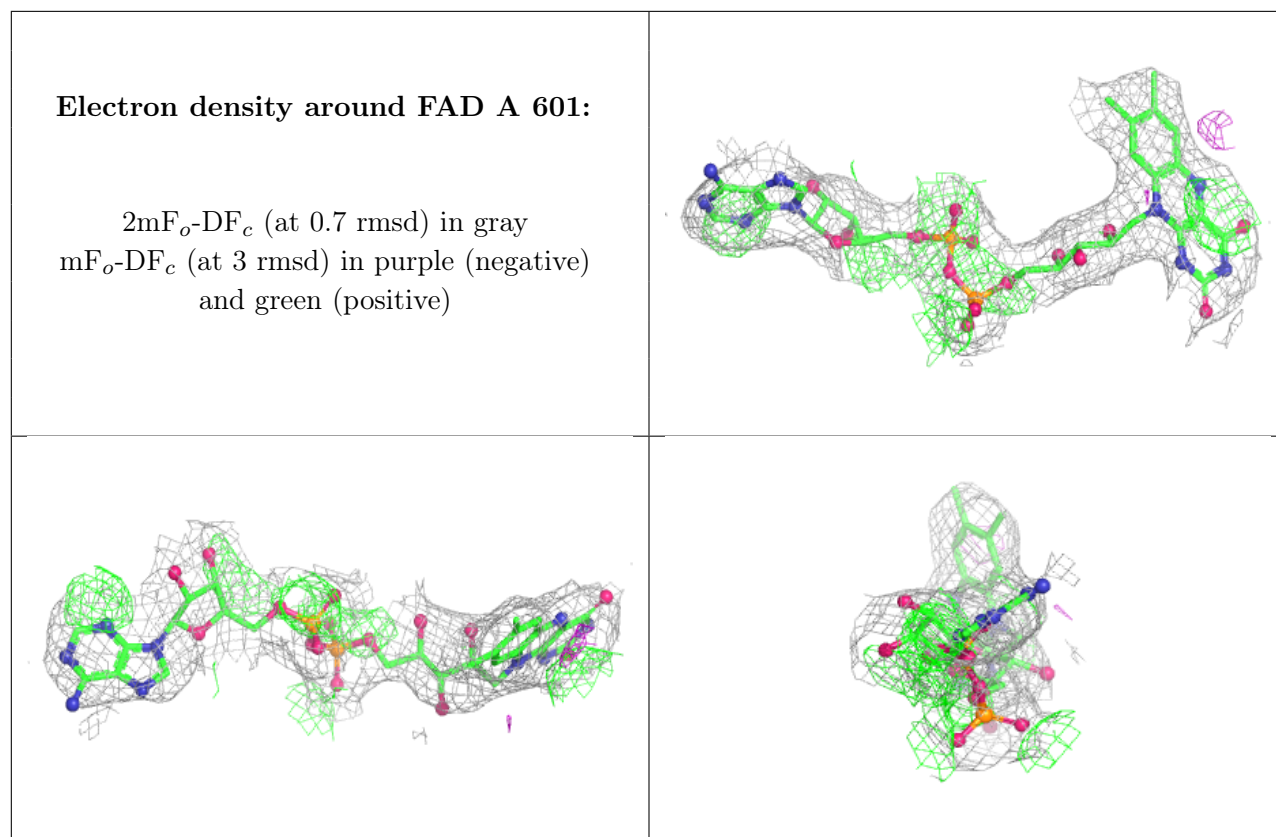
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	FES	B	244	4/4	1.00	0.02	32,34,34,35	0

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.