Full wwPDB X-ray Structure Validation Report (i)

Sep 26, 2023 – 06:45 AM EDT

PDB ID	:	6AWF
Title	:	Escherichia coli quinol:fumarate reductase crystallized without dicarboxylate
Authors	:	Iverson, T.M.
Deposited on	:	2017-09-05
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 (i) 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 (i)) were used in the production of this report:

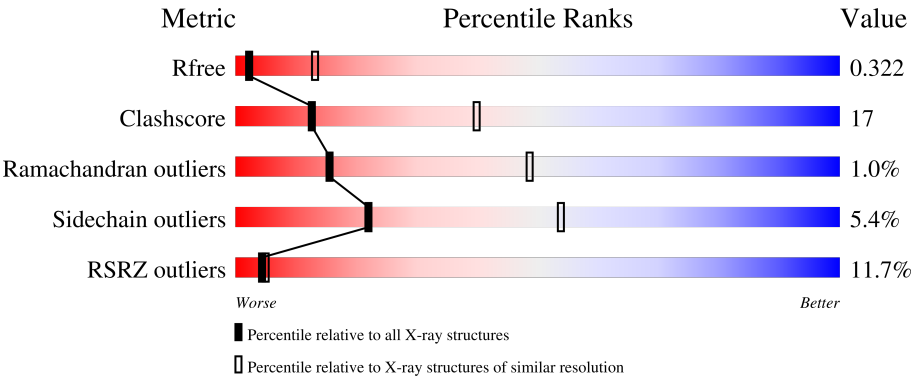
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	602	13% 67% 26% • 5%
1	E	602	8% 59% 19% • 19%
2	B	243	11% 60% 35% • •
2	F	243	16% 68% 28% • •
3	C	130	12% 57% 39% •

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Mol	Chain	Length	Quality of chain
3	G	130	9% 72% 25%
4	D	119	6% 75% 23%
4	H	119	6% 76% 22%

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
6	PO4	E	702	-	-	X	X
7	FES	F	301	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 15831 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	573	Total	C	N	O	S	0	0	0
			4391	2741	786	833	31			
1	E	487	Total	C	N	O	S	0	0	0
			3642	2264	648	702	28			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	241	Total	C	N	O	S	0	0	0
			1865	1176	318	352	19			
2	F	238	Total	C	N	O	S	0	0	0
			1842	1162	314	347	19			

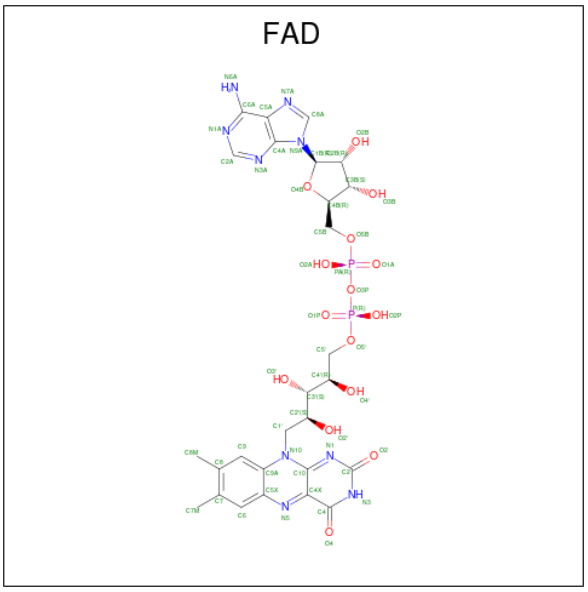
- Molecule 3 is a protein called Fumarate reductase subunit C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	130	Total	C	N	O	S	0	0	0
			1054	717	165	169	3			
3	G	130	Total	C	N	O	S	0	0	0
			1058	720	166	169	3			

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

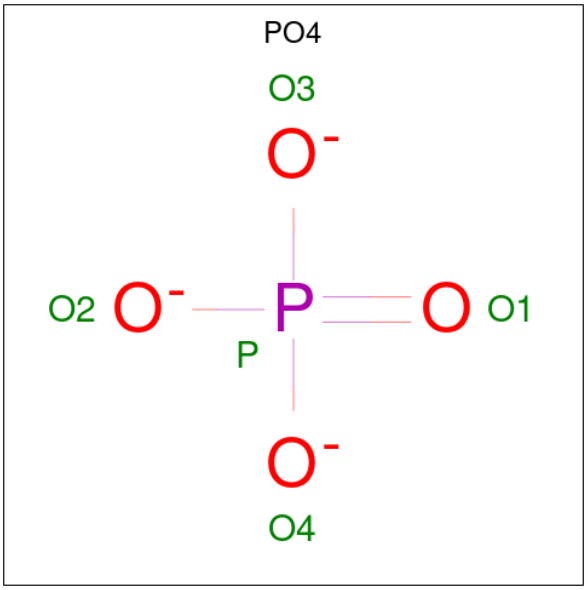
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	119	Total	C	N	O	S	0	0	0
			908	614	145	142	7			
4	H	118	Total	C	N	O	S	0	0	0
			917	620	150	140	7			

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



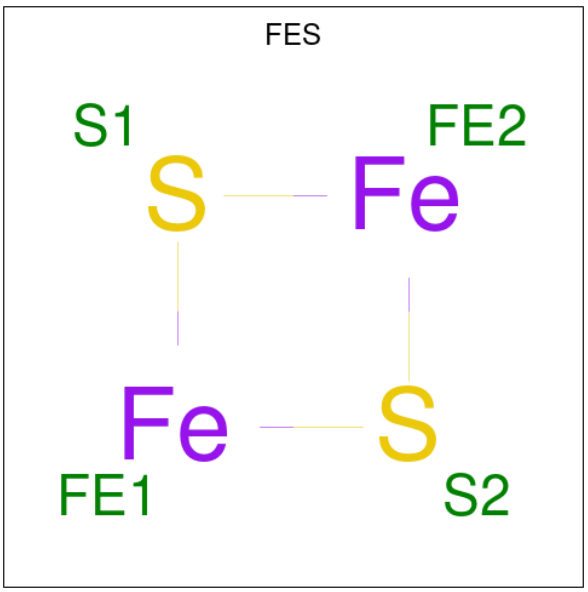
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	E	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



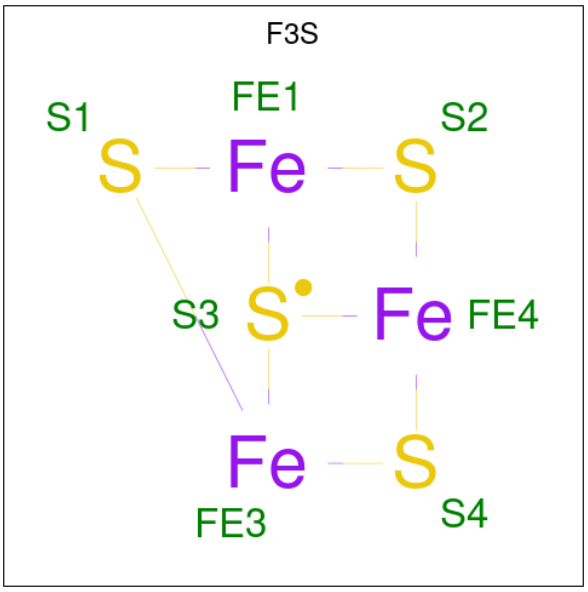
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	O	P		0	0
			5	4	1			
6	E	1	Total	O	P		0	0
			5	4	1			

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



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

- Molecule 8 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



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

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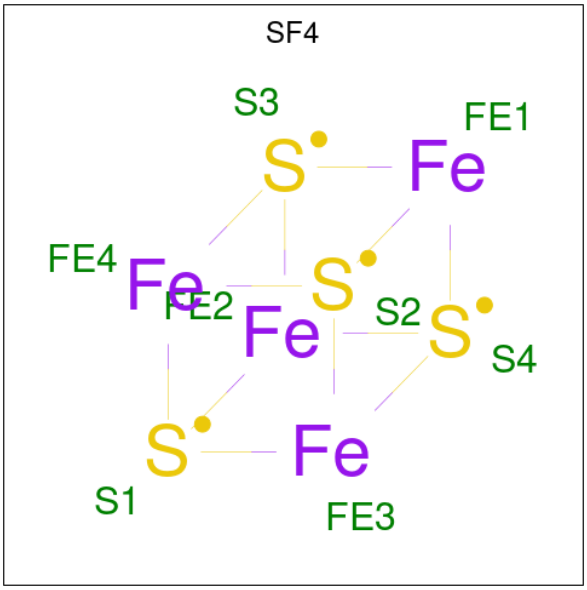
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	F	1	Total Fe S 7 3 4	0	0

- Molecule 9 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



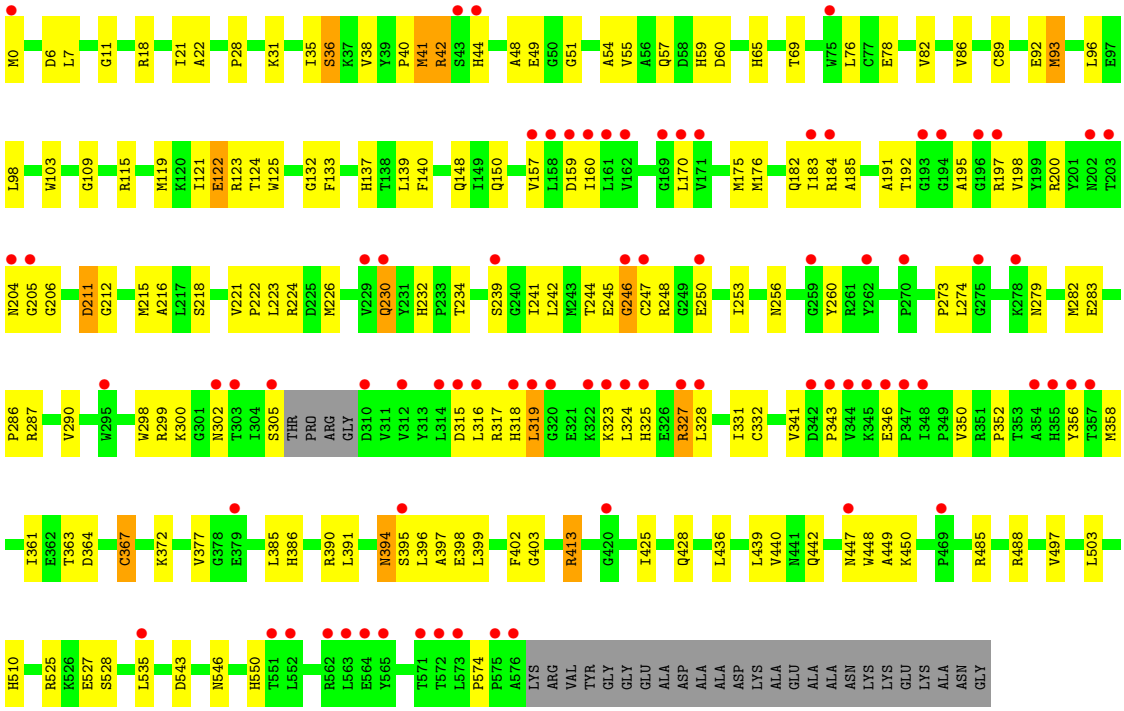
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total Fe S 8 4 4	0	0
9	F	1	Total Fe S 8 4 4	0	0

3 Residue-property plots (i)

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.

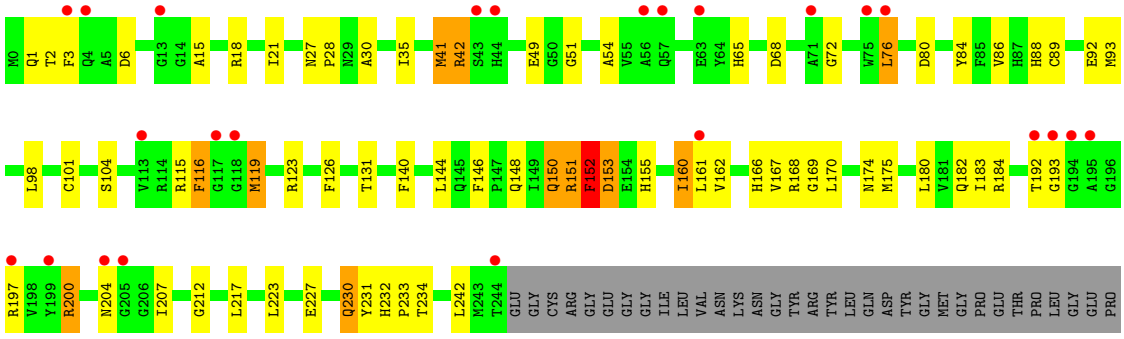
• Molecule 1: Fumarate reductase flavoprotein subunit

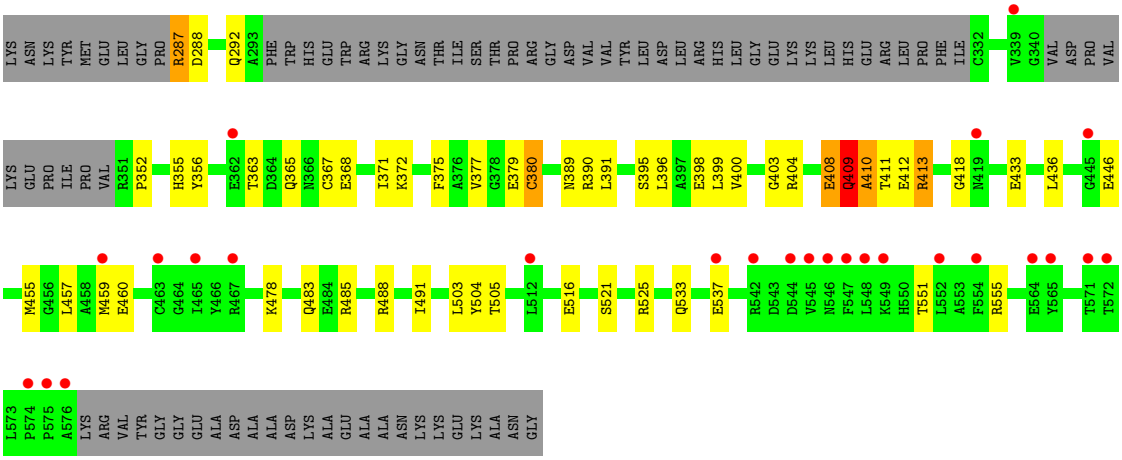
Chain A:



• Molecule 1: Fumarate reductase flavoprotein subunit

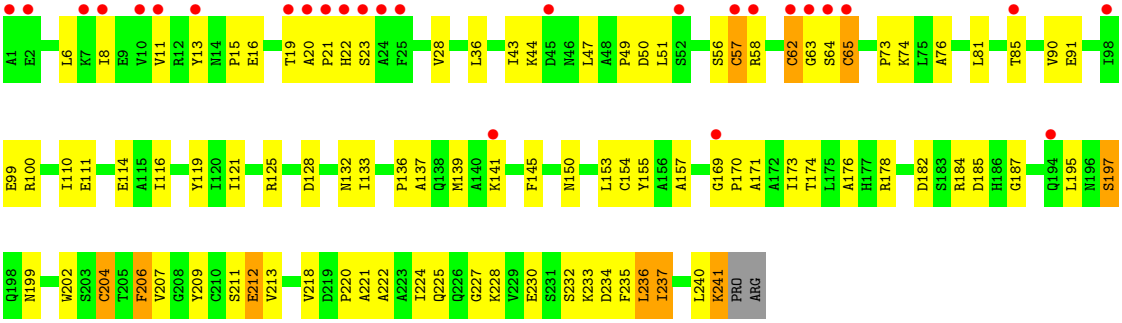
Chain E:





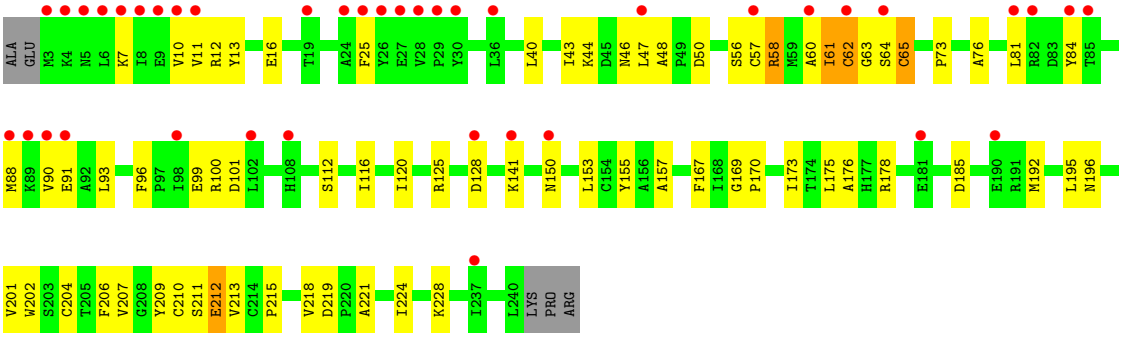
• Molecule 2: Fumarate reductase iron-sulfur subunit

Chain B:



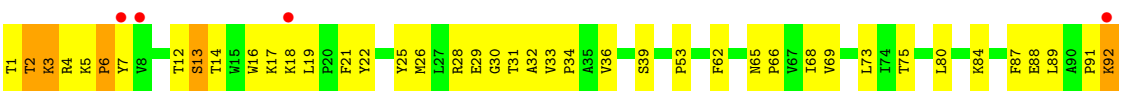
• Molecule 2: Fumarate reductase iron-sulfur subunit

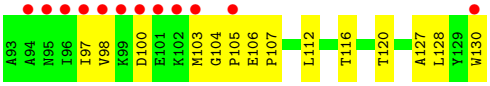
Chain F:



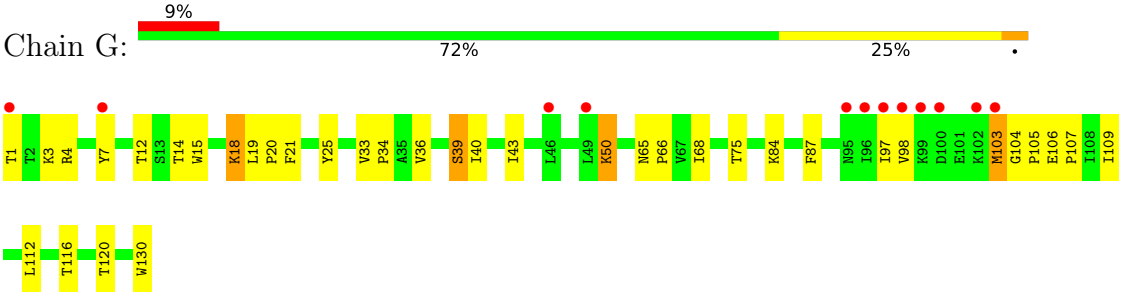
• Molecule 3: Fumarate reductase subunit C

Chain C:

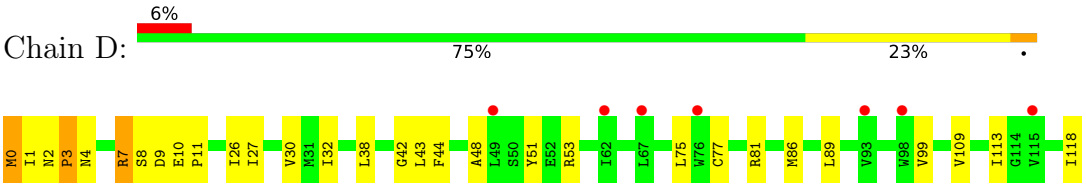




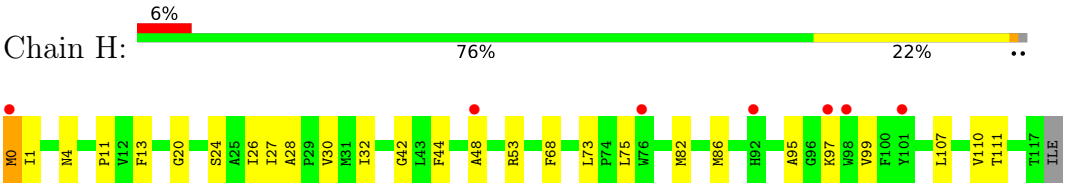
• Molecule 3: Fumarate reductase subunit C



• Molecule 4: Fumarate reductase subunit D



• Molecule 4: Fumarate reductase subunit D



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	113.32Å 117.99Å 125.29Å 90.00° 98.80° 90.00°	Depositor
Resolution (Å)	46.91 – 3.35 48.32 – 3.35	Depositor EDS
% Data completeness (in resolution range)	76.4 (46.91-3.35) 60.3 (48.32-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.27 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.285 , 0.318 0.287 , 0.322	Depositor DCC
R_{free} test set	1730 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å^2)	59.1	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 19.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	15831	wwPDB-VP
Average B, all atoms (Å^2)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.82% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: PO4, FES, F3S, SF4, FAD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.59	2/4480 (0.0%)	0.75	1/6060 (0.0%)
1	E	0.53	0/3708	0.74	3/5023 (0.1%)
2	B	0.62	1/1907 (0.1%)	0.76	0/2586
2	F	0.52	1/1884 (0.1%)	0.66	0/2556
3	C	0.48	0/1090	0.66	0/1492
3	G	0.47	0/1094	0.64	0/1496
4	D	0.46	0/938	0.65	0/1284
4	H	0.40	0/947	0.61	0/1292
All	All	0.54	4/16048 (0.0%)	0.71	4/21789 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	367	CYS	CB-SG	-6.96	1.70	1.82
2	F	65	CYS	CB-SG	-5.95	1.72	1.81
1	A	574	PRO	N-CD	5.58	1.55	1.47
2	B	65	CYS	CB-SG	-5.07	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	115	ARG	N-CA-C	9.07	135.49	111.00
1	A	574	PRO	N-CA-CB	6.08	110.60	103.30
1	E	409	GLN	C-N-CA	-5.93	106.86	121.70
1	E	119	MET	C-N-CA	-5.22	108.65	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4391	0	4260	139	0
1	E	3642	0	3466	152	0
2	B	1865	0	1817	98	0
2	F	1842	0	1790	62	0
3	C	1054	0	1097	70	0
3	G	1058	0	1108	31	0
4	D	908	0	927	29	0
4	H	917	0	960	22	0
5	A	53	0	29	3	0
5	E	53	0	29	3	0
6	A	5	0	0	0	0
6	E	5	0	0	2	0
7	B	4	0	0	0	0
7	F	4	0	0	2	0
8	B	7	0	0	0	0
8	F	7	0	0	0	0
9	B	8	0	0	0	0
9	F	8	0	0	0	0
All	All	15831	0	15483	523	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 17.

All (523) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:GLU:CB	4:D:0:MET:HE1	1.48	1.42
1:A:232:HIS:CE1	1:A:242:LEU:HD11	1.61	1.34
1:E:155:HIS:CE1	1:E:174:ASN:CG	2.00	1.34
1:E:155:HIS:CE1	1:E:174:ASN:ND2	1.96	1.30
1:E:155:HIS:HE1	1:E:174:ASN:ND2	1.28	1.26
1:A:197:ARG:HD2	1:A:205:GLY:O	1.24	1.25
1:A:245:GLU:O	1:A:247:CYS:N	1.73	1.19
2:B:99:GLU:CD	3:C:4:ARG:NH1	1.97	1.17
2:B:99:GLU:OE2	3:C:4:ARG:NH1	1.78	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:PHE:O	1:E:155:HIS:CD2	1.99	1.16
4:D:2:ASN:OD1	4:D:4:ASN:N	1.80	1.15
1:E:1:GLN:NE2	1:E:3:PHE:CZ	2.17	1.13
1:E:155:HIS:ND1	1:E:174:ASN:OD1	1.83	1.10
1:E:152:PHE:O	1:E:155:HIS:HD2	1.34	1.06
1:E:160:ILE:CD1	1:E:162:VAL:HG23	1.86	1.06
1:A:195:ALA:O	1:A:198:VAL:HG13	1.54	1.05
1:E:409:GLN:O	1:E:410:ALA:C	1.90	1.05
2:B:111:GLU:CB	4:D:0:MET:CE	2.35	1.04
2:B:99:GLU:OE1	3:C:4:ARG:NH1	1.90	1.03
2:B:20:ALA:HB1	2:B:21:PRO:HD2	1.41	1.03
1:A:197:ARG:HH11	1:A:197:ARG:HB3	1.25	1.01
1:E:155:HIS:ND1	1:E:174:ASN:CG	2.12	1.01
1:A:232:HIS:CE1	1:A:242:LEU:CD1	2.44	0.99
1:E:144:LEU:HD21	1:E:151:ARG:NH2	1.79	0.97
2:B:16:GLU:OE2	3:C:3:LYS:HD2	1.63	0.97
1:E:160:ILE:HG12	1:E:161:LEU:H	1.24	0.96
1:E:119:MET:CE	1:E:391:LEU:HD23	1.96	0.95
2:F:57:CYS:HB3	2:F:62:CYS:HB3	1.49	0.94
1:E:160:ILE:HG12	1:E:161:LEU:N	1.82	0.91
1:A:197:ARG:CD	1:A:205:GLY:O	2.16	0.91
1:A:197:ARG:HB3	1:A:197:ARG:NH1	1.88	0.88
1:E:230:GLN:HE21	1:E:355:HIS:HD2	1.21	0.88
1:A:356:TYR:CD2	1:A:390:ARG:HD3	2.09	0.87
1:E:119:MET:HE2	1:E:391:LEU:HD23	1.54	0.86
1:A:115:ARG:NE	1:A:279:ASN:HB2	1.91	0.85
2:B:236:LEU:HD12	2:B:240:LEU:HD13	1.57	0.85
2:B:236:LEU:HD12	2:B:240:LEU:CD1	2.05	0.85
1:E:144:LEU:HD21	1:E:151:ARG:HH22	1.41	0.85
1:E:144:LEU:CD2	1:E:151:ARG:NH2	2.38	0.85
1:E:390:ARG:HD2	1:E:395:SER:HB2	1.59	0.84
3:G:12:THR:HG22	3:G:14:THR:H	1.42	0.84
1:E:155:HIS:CE1	1:E:174:ASN:OD1	2.28	0.83
1:E:287:ARG:NH2	1:E:390:ARG:O	2.11	0.83
1:E:160:ILE:HD11	1:E:167:VAL:HG23	1.60	0.83
1:A:119:MET:SD	1:A:123:ARG:NH1	2.52	0.82
2:B:236:LEU:O	2:B:240:LEU:HD13	1.80	0.81
1:E:160:ILE:CD1	1:E:162:VAL:CG2	2.59	0.81
1:A:82:VAL:HG22	1:A:385:LEU:HD12	1.64	0.80
2:F:73:PRO:HG2	2:F:213:VAL:HG11	1.61	0.80
1:E:160:ILE:CG1	1:E:161:LEU:N	2.45	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:PHE:C	1:E:155:HIS:HD2	1.86	0.79
2:B:13:TYR:OH	3:C:5:LYS:CG	2.30	0.78
2:B:99:GLU:CD	3:C:4:ARG:HH11	1.67	0.78
1:E:409:GLN:O	1:E:411:THR:N	2.18	0.76
1:E:160:ILE:CD1	1:E:167:VAL:HG23	2.15	0.76
1:E:42:ARG:NH2	2:F:63:GLY:O	2.19	0.76
1:E:160:ILE:CG1	1:E:167:VAL:HG23	2.16	0.76
2:B:99:GLU:CD	3:C:4:ARG:HH12	1.77	0.75
1:A:6:ASP:OD2	4:H:4:ASN:ND2	2.19	0.75
1:E:1:GLN:NE2	1:E:3:PHE:HZ	1.83	0.74
1:A:230:GLN:OE1	1:A:390:ARG:HG2	1.88	0.74
2:F:65:CYS:SG	2:F:76:ALA:N	2.60	0.74
2:F:170:PRO:HA	2:F:224:ILE:HD11	1.68	0.74
2:B:15:PRO:CB	3:C:5:LYS:HB3	2.18	0.73
1:E:119:MET:CE	1:E:391:LEU:CD2	2.66	0.73
2:B:20:ALA:HB1	2:B:21:PRO:CD	2.17	0.73
1:A:35:ILE:HD11	1:A:183:ILE:HD12	1.69	0.72
2:F:11:VAL:HG21	2:F:91:GLU:HG2	1.71	0.72
2:F:99:GLU:OE2	3:G:4:ARG:NH1	2.22	0.72
2:F:57:CYS:SG	2:F:58:ARG:N	2.62	0.72
1:E:51:GLY:HA2	1:E:131:THR:HG21	1.70	0.72
4:D:2:ASN:OD1	4:D:3:PRO:N	2.23	0.71
1:E:144:LEU:CD2	1:E:151:ARG:HH22	2.00	0.71
1:E:160:ILE:HG13	1:E:167:VAL:CG2	2.20	0.71
1:A:245:GLU:C	1:A:247:CYS:H	1.92	0.71
1:E:155:HIS:CE1	1:E:174:ASN:HD21	2.05	0.71
1:E:152:PHE:C	1:E:155:HIS:CD2	2.64	0.71
1:A:44:HIS:CE1	1:A:204:ASN:HA	2.26	0.71
1:E:160:ILE:HD13	1:E:162:VAL:HG23	1.72	0.70
1:A:182:GLN:OE1	1:A:184:ARG:NH1	2.20	0.70
3:G:104:GLY:HA2	3:G:107:PRO:HD2	1.74	0.70
4:D:8:SER:OG	4:D:9:ASP:N	2.21	0.69
1:A:245:GLU:C	1:A:247:CYS:N	2.46	0.69
2:B:241:LYS:HG3	2:B:241:LYS:O	1.92	0.69
4:D:7:ARG:O	4:D:7:ARG:HG2	1.91	0.69
1:E:160:ILE:HD11	1:E:162:VAL:CG2	2.23	0.69
1:E:119:MET:HE3	1:E:391:LEU:CD2	2.23	0.69
1:E:160:ILE:HD11	1:E:162:VAL:HG23	1.75	0.69
1:E:182:GLN:OE1	1:E:184:ARG:NH1	2.25	0.68
1:A:197:ARG:NE	1:A:206:GLY:HA2	2.07	0.68
1:E:15:ALA:HB2	1:E:399:LEU:HD22	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:PRO:HB3	3:C:5:LYS:HB3	1.75	0.68
4:D:4:ASN:ND2	1:E:6:ASP:OD2	2.27	0.68
1:E:18:ARG:HG2	1:E:400:VAL:HA	1.74	0.68
2:B:235:PHE:CD1	4:D:11:PRO:HG2	2.29	0.67
2:F:57:CYS:O	2:F:58:ARG:HB2	1.95	0.67
2:B:182:ASP:OD2	2:B:184:ARG:NH2	2.21	0.67
1:A:543:ASP:OD2	1:A:546:ASN:HB2	1.94	0.67
1:A:232:HIS:ND1	1:A:242:LEU:CD1	2.59	0.66
2:F:57:CYS:O	2:F:58:ARG:CB	2.42	0.66
1:E:150:GLN:HG3	1:E:150:GLN:O	1.96	0.66
2:B:13:TYR:OH	3:C:5:LYS:HG3	1.95	0.66
2:B:57:CYS:HB3	2:B:62:CYS:HB3	1.77	0.66
3:C:75:THR:HG22	4:D:32:ILE:HD13	1.78	0.66
1:E:160:ILE:HG13	1:E:167:VAL:HG23	1.78	0.66
1:E:227:GLU:OE1	1:E:525:ARG:NE	2.27	0.66
4:H:0:MET:HG2	4:H:1:ILE:H	1.61	0.66
1:A:0:MET:HB3	1:A:182:GLN:HE21	1.61	0.66
1:E:42:ARG:HG2	2:F:64:SER:HB3	1.77	0.66
1:E:180:LEU:HD11	1:E:436:LEU:HD23	1.79	0.65
1:E:150:GLN:O	1:E:151:ARG:O	2.14	0.64
1:E:153:ASP:N	1:E:153:ASP:OD1	2.30	0.64
1:A:195:ALA:O	1:A:198:VAL:CG1	2.40	0.64
1:E:152:PHE:CE2	1:E:183:ILE:HD11	2.32	0.64
2:B:157:ALA:O	3:C:22:TYR:OH	2.12	0.64
1:A:232:HIS:HD2	1:A:234:THR:H	1.44	0.64
1:A:234:THR:HG22	1:A:350:VAL:HG21	1.79	0.64
2:B:155:TYR:CZ	2:B:169:GLY:HA3	2.33	0.64
2:B:224:ILE:O	2:B:227:GLY:N	2.31	0.63
2:B:16:GLU:OE2	3:C:3:LYS:CD	2.44	0.63
1:E:119:MET:HE2	1:E:391:LEU:CD2	2.27	0.63
3:C:33:VAL:HB	3:C:34:PRO:HD3	1.80	0.63
3:G:75:THR:HG22	4:H:32:ILE:HD13	1.81	0.63
2:B:136:PRO:HB2	3:C:100:ASP:HB3	1.80	0.63
2:B:207:VAL:HG22	3:C:25:TYR:CZ	2.34	0.63
1:A:436:LEU:O	1:A:440:VAL:HG23	1.99	0.62
2:B:233:LYS:O	2:B:237:ILE:CG1	2.48	0.62
3:C:28:ARG:NH1	3:C:29:GLU:OE2	2.32	0.62
1:E:28:PRO:HA	1:E:148:GLN:HE21	1.62	0.62
2:B:13:TYR:OH	3:C:5:LYS:HG2	1.99	0.62
2:F:12:ARG:NE	2:F:101:ASP:OD1	2.24	0.62
3:C:12:THR:HG22	3:C:14:THR:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:PHE:HB3	1:E:155:HIS:HD2	1.65	0.62
1:A:230:GLN:OE1	1:A:390:ARG:NE	2.30	0.62
2:F:57:CYS:HB3	2:F:62:CYS:CB	2.25	0.62
1:E:355:HIS:NE2	6:E:702:PO4:O3	2.30	0.62
1:E:230:GLN:HE21	1:E:355:HIS:CD2	2.11	0.61
1:A:157:VAL:HG22	1:A:170:LEU:HD13	1.82	0.61
2:B:236:LEU:HD12	2:B:240:LEU:HD11	1.82	0.61
1:A:42:ARG:HG2	2:B:64:SER:HB3	1.82	0.61
4:D:9:ASP:N	4:D:9:ASP:OD1	2.34	0.61
1:A:54:ALA:HB2	1:A:89:CYS:HB3	1.83	0.60
3:G:98:VAL:HG22	3:G:103:MET:HB3	1.82	0.60
1:A:232:HIS:O	1:A:352:PRO:HA	2.01	0.60
3:G:15:TRP:O	3:G:18:LYS:HG2	2.00	0.60
2:B:154:CYS:SG	2:B:170:PRO:HG2	2.42	0.60
2:B:173:ILE:HD13	2:B:224:ILE:HG23	1.82	0.60
1:A:245:GLU:O	1:A:248:ARG:N	2.31	0.60
1:A:197:ARG:HH11	1:A:197:ARG:CB	2.09	0.60
3:G:120:THR:HG23	4:H:30:VAL:HB	1.84	0.59
2:B:233:LYS:O	2:B:237:ILE:HG12	2.03	0.59
1:A:11:GLY:HA3	1:A:191:ALA:O	2.02	0.59
1:A:57:GLN:NE2	1:A:122:GLU:HG2	2.18	0.58
1:E:160:ILE:HD13	1:E:160:ILE:C	2.23	0.58
2:F:202:TRP:CE2	4:H:11:PRO:HD3	2.38	0.58
1:A:42:ARG:HD2	1:A:42:ARG:N	2.19	0.58
1:A:247:CYS:SG	1:A:331:ILE:HG21	2.44	0.58
2:B:155:TYR:OH	2:B:169:GLY:HA3	2.03	0.58
4:D:42:GLY:HA2	4:D:44:PHE:CE1	2.39	0.57
4:H:20:GLY:HA2	4:H:73:LEU:HB3	1.85	0.57
1:A:332:CYS:HA	1:A:343:PRO:HG2	1.87	0.57
3:C:5:LYS:HG3	3:C:5:LYS:O	2.03	0.57
1:E:193:GLY:H	1:E:380:CYS:HB3	1.69	0.57
1:A:93:MET:HB3	1:A:125:TRP:CZ3	2.39	0.57
1:A:211:ASP:O	1:A:215:MET:HG3	2.03	0.57
1:E:152:PHE:HB3	1:E:155:HIS:CD2	2.40	0.57
2:B:212:GLU:HG3	3:C:21:PHE:CE2	2.40	0.57
1:E:1:GLN:NE2	1:E:3:PHE:CE2	2.70	0.57
1:A:232:HIS:ND1	1:A:242:LEU:HD13	2.20	0.56
2:B:50:ASP:O	2:B:100:ARG:NH2	2.34	0.56
2:B:185:ASP:OD1	2:B:187:GLY:N	2.30	0.56
3:G:130:TRP:O	4:H:53:ARG:NE	2.34	0.56
2:B:11:VAL:HG21	2:B:91:GLU:HG3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:169:GLY:O	2:B:173:ILE:HG13	2.05	0.56
1:A:42:ARG:NH2	2:B:63:GLY:O	2.38	0.56
4:D:48:ALA:O	4:D:53:ARG:HD3	2.06	0.56
1:E:160:ILE:CD1	1:E:161:LEU:N	2.68	0.56
1:A:413:ARG:HH11	1:A:413:ARG:HB2	1.70	0.56
1:A:372:LYS:HE3	1:A:413:ARG:HE	1.71	0.56
4:D:2:ASN:CG	4:D:3:PRO:N	2.59	0.56
1:E:227:GLU:OE1	1:E:551:THR:OG1	2.19	0.56
1:A:282:MET:HB3	1:A:283:GLU:OE1	2.06	0.55
1:E:408:GLU:O	1:E:411:THR:HB	2.06	0.55
1:A:48:ALA:HB3	1:A:132:GLY:HA3	1.86	0.55
2:F:116:ILE:HD13	2:F:176:ALA:HB2	1.87	0.55
3:G:130:TRP:HB2	4:H:53:ARG:HH21	1.70	0.55
2:B:119:TYR:O	2:B:121:ILE:HG13	2.07	0.55
3:C:5:LYS:N	3:C:6:PRO:HD3	2.22	0.55
3:C:116:THR:OG1	4:D:26:ILE:HA	2.06	0.55
1:E:356:TYR:CZ	1:E:390:ARG:HD3	2.41	0.55
1:E:356:TYR:CE1	1:E:390:ARG:HD3	2.41	0.55
3:G:116:THR:HA	4:H:26:ILE:HG23	1.90	0.55
2:B:44:LYS:NZ	2:B:51:LEU:O	2.32	0.54
2:F:167:PHE:CE2	2:F:169:GLY:HA2	2.42	0.54
3:C:29:GLU:OE1	4:D:81:ARG:HG2	2.07	0.54
3:C:65:ASN:HB3	3:C:68:ILE:H	1.73	0.54
2:B:209:TYR:CZ	3:C:19:LEU:HD21	2.43	0.54
1:E:409:GLN:C	1:E:411:THR:N	2.61	0.54
1:A:447:ASN:ND2	1:A:450:LYS:HG2	2.21	0.54
1:E:152:PHE:CB	1:E:155:HIS:HD2	2.20	0.54
1:E:232:HIS:HE1	6:E:702:PO4:O4	1.90	0.54
3:G:65:ASN:HB3	3:G:68:ILE:H	1.73	0.54
2:F:11:VAL:CG2	2:F:91:GLU:HG2	2.37	0.54
1:E:155:HIS:ND1	1:E:174:ASN:HA	2.22	0.54
1:E:175:MET:HG2	1:E:503:LEU:HD11	1.89	0.54
1:A:48:ALA:HB1	1:A:396:LEU:HD11	1.91	0.53
1:A:300:LYS:HB2	1:A:302:ASN:OD1	2.08	0.53
2:B:197:SER:OG	2:B:199:ASN:N	2.40	0.53
2:B:16:GLU:HG2	3:C:3:LYS:CG	2.38	0.53
2:B:116:ILE:HB	2:B:176:ALA:HB2	1.90	0.53
1:A:250:GLU:HB3	1:A:319:LEU:HD11	1.91	0.53
1:A:55:VAL:HG13	1:A:60:ASP:HB3	1.89	0.53
1:A:96:LEU:HD21	1:A:139:LEU:HD21	1.89	0.53
1:A:239:SER:HB2	1:A:241:ILE:HG13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:144:LEU:HD21	1:E:151:ARG:HH21	1.69	0.53
1:E:152:PHE:CA	1:E:155:HIS:HD2	2.22	0.53
1:A:40:PRO:HB2	1:A:140:PHE:CD1	2.44	0.53
2:B:145:PHE:HA	2:B:218:VAL:HG13	1.91	0.53
1:E:140:PHE:CE1	1:E:151:ARG:NH2	2.77	0.53
1:E:504:TYR:CE2	2:F:44:LYS:HE2	2.44	0.53
2:B:73:PRO:HG2	2:B:213:VAL:HG11	1.90	0.53
2:B:204:CYS:O	2:B:228:LYS:NZ	2.32	0.53
1:E:166:HIS:CD2	1:E:372:LYS:HB3	2.44	0.52
4:H:42:GLY:HA2	4:H:44:PHE:CE1	2.43	0.52
1:E:140:PHE:CZ	1:E:151:ARG:NH2	2.77	0.52
1:A:54:ALA:CB	1:A:89:CYS:HB3	2.39	0.52
2:B:207:VAL:HG22	3:C:25:TYR:CE1	2.45	0.52
1:E:35:ILE:HD11	1:E:183:ILE:HD12	1.91	0.52
1:E:483:GLN:NE2	1:E:555:ARG:HH22	2.06	0.52
1:E:292:GLN:OE1	1:E:533:GLN:HG3	2.10	0.52
1:E:399:LEU:HD11	5:E:701:FAD:O4'	2.09	0.52
2:F:65:CYS:HB2	7:F:301:FES:S2	2.49	0.52
2:F:155:TYR:CE1	2:F:170:PRO:HD2	2.45	0.52
4:H:68:PHE:HD1	4:H:111:THR:HG22	1.75	0.52
1:A:246:GLY:O	1:A:328:LEU:HD21	2.10	0.52
2:B:206:PHE:CE2	3:C:89:LEU:HB3	2.43	0.52
2:F:57:CYS:C	2:F:58:ARG:CG	2.76	0.52
2:B:170:PRO:HA	2:B:224:ILE:HD11	1.90	0.52
3:C:5:LYS:N	3:C:6:PRO:CD	2.71	0.52
1:A:18:ARG:NH1	1:A:92:GLU:OE1	2.41	0.52
2:B:20:ALA:CB	2:B:21:PRO:CD	2.84	0.52
1:A:230:GLN:OE1	1:A:390:ARG:CG	2.58	0.52
2:F:116:ILE:HD13	2:F:176:ALA:N	2.25	0.52
2:B:137:ALA:HA	3:C:100:ASP:HA	1.92	0.51
1:E:150:GLN:C	1:E:151:ARG:O	2.47	0.51
2:F:60:ALA:HA	7:F:301:FES:S1	2.50	0.51
3:G:50:LYS:HE2	3:G:50:LYS:HA	1.92	0.51
1:E:42:ARG:HD2	1:E:42:ARG:N	2.25	0.51
1:E:356:TYR:HE2	1:E:395:SER:HG	1.59	0.51
3:G:33:VAL:HB	3:G:34:PRO:HD3	1.91	0.51
1:A:256:ASN:HD21	1:A:260:TYR:HB3	1.76	0.51
1:A:76:LEU:O	1:A:550:HIS:HE1	1.94	0.50
1:A:244:THR:H	1:A:331:ILE:HD11	1.76	0.50
2:B:171:ALA:O	2:B:174:THR:N	2.44	0.50
1:E:230:GLN:NE2	1:E:355:HIS:HD2	2.01	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:130:TRP:O	4:D:53:ARG:NE	2.40	0.50
3:G:106:GLU:CD	3:G:106:GLU:H	2.15	0.50
3:C:19:LEU:HB3	3:C:22:TYR:CD2	2.47	0.50
2:F:155:TYR:CZ	2:F:169:GLY:HA3	2.47	0.50
1:A:148:GLN:OE1	1:A:148:GLN:N	2.29	0.50
3:G:33:VAL:HA	4:H:82:MET:CE	2.42	0.50
1:A:41:MET:HE1	1:A:140:PHE:CE2	2.47	0.50
3:C:105:PRO:HD2	3:C:106:GLU:OE2	2.12	0.50
2:F:173:ILE:HG23	2:F:195:LEU:CD2	2.41	0.50
1:A:55:VAL:HG22	1:A:60:ASP:OD2	2.12	0.49
1:E:150:GLN:C	1:E:150:GLN:HE21	2.15	0.49
1:A:159:ASP:OD1	1:A:160:ILE:N	2.45	0.49
1:A:89:CYS:SG	1:A:397:ALA:HB1	2.52	0.49
2:F:157:ALA:HB1	2:F:209:TYR:CD2	2.47	0.49
1:A:372:LYS:HE3	1:A:413:ARG:NE	2.27	0.49
2:B:221:ALA:O	2:B:225:GLN:HG2	2.12	0.49
2:B:233:LYS:O	2:B:237:ILE:HG13	2.12	0.49
1:A:192:THR:OG1	1:A:212:GLY:HA3	2.12	0.49
2:B:240:LEU:N	2:B:240:LEU:HD12	2.27	0.49
3:C:2:THR:OG1	3:C:3:LYS:N	2.43	0.49
1:E:160:ILE:CG1	1:E:167:VAL:CG2	2.83	0.49
1:A:57:GLN:HE22	1:A:122:GLU:HG2	1.78	0.49
1:A:286:PRO:O	1:A:290:VAL:HG23	2.13	0.49
2:B:234:ASP:HA	2:B:237:ILE:HG13	1.95	0.49
1:E:54:ALA:CB	1:E:89:CYS:HB3	2.43	0.49
3:G:19:LEU:HD12	3:G:20:PRO:HD2	1.94	0.49
1:A:42:ARG:NH2	2:B:150:ASN:O	2.46	0.49
1:A:51:GLY:HA3	1:A:124:THR:CG2	2.43	0.49
1:A:93:MET:HB3	1:A:125:TRP:CE3	2.47	0.49
1:A:98:LEU:HD21	2:B:125:ARG:HD3	1.95	0.49
2:F:212:GLU:HG3	3:G:21:PHE:CE2	2.48	0.48
4:D:2:ASN:OD1	4:D:3:PRO:C	2.46	0.48
1:E:230:GLN:HE22	1:E:390:ARG:HH21	1.61	0.48
1:A:211:ASP:HA	1:A:510:HIS:CD2	2.48	0.48
1:E:491:ILE:HD11	1:E:505:THR:HG21	1.94	0.48
2:B:232:SER:O	2:B:235:PHE:N	2.46	0.48
1:E:160:ILE:HD13	1:E:161:LEU:N	2.26	0.48
2:B:13:TYR:HH	3:C:5:LYS:HG3	1.79	0.48
3:C:127:ALA:O	3:C:128:LEU:HD23	2.13	0.48
1:E:160:ILE:HD11	1:E:162:VAL:HG22	1.94	0.48
1:A:204:ASN:HD22	5:A:701:FAD:HM83	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:227:GLU:OE2	1:E:521:SER:HB3	2.13	0.48
1:E:446:GLU:HB2	1:E:488:ARG:O	2.14	0.48
2:F:202:TRP:NE1	4:H:11:PRO:HD3	2.29	0.48
2:F:207:VAL:HG22	3:G:25:TYR:CE1	2.49	0.48
2:B:6:LEU:HD11	2:B:85:THR:HA	1.96	0.48
1:A:176:MET:O	1:A:497:VAL:HA	2.14	0.47
4:H:27:ILE:O	4:H:30:VAL:HG12	2.14	0.47
3:G:130:TRP:HB2	4:H:53:ARG:NH2	2.29	0.47
1:A:36:SER:OG	1:A:38:VAL:O	2.23	0.47
1:A:224:ARG:HD2	1:A:550:HIS:CG	2.50	0.47
3:G:105:PRO:O	3:G:109:ILE:HG13	2.14	0.47
2:B:20:ALA:CB	2:B:21:PRO:HD2	2.28	0.47
1:A:76:LEU:HD23	1:A:76:LEU:HA	1.64	0.47
2:F:116:ILE:HD13	2:F:176:ALA:CA	2.45	0.47
3:C:62:PHE:CZ	3:C:68:ILE:HG13	2.50	0.47
3:C:116:THR:O	3:C:120:THR:OG1	2.26	0.47
2:F:99:GLU:OE1	3:G:4:ARG:HD2	2.14	0.47
2:B:222:ALA:HB2	3:C:92:LYS:HE3	1.96	0.47
1:A:448:TRP:CG	1:A:449:ALA:N	2.83	0.47
1:E:200:ARG:HG3	1:E:457:LEU:HD23	1.97	0.47
2:F:173:ILE:HG21	2:F:201:VAL:HG12	1.97	0.47
3:G:36:VAL:O	3:G:40:ILE:HG12	2.15	0.47
2:B:36:LEU:HD11	2:B:90:VAL:HG21	1.98	0.46
2:B:110:ILE:O	2:B:114:GLU:HG3	2.15	0.46
2:B:43:ILE:HG23	2:B:47:LEU:HB2	1.97	0.46
1:E:98:LEU:HD21	2:F:125:ARG:HD3	1.97	0.46
1:A:175:MET:HG2	1:A:503:LEU:HD11	1.96	0.46
1:A:395:SER:HB3	5:A:701:FAD:N1	2.30	0.46
1:E:152:PHE:CB	1:E:155:HIS:CD2	2.98	0.46
2:F:192:MET:HB3	2:F:196:ASN:HD21	1.80	0.46
4:H:48:ALA:O	4:H:53:ARG:HD3	2.15	0.46
1:A:485:ARG:HG2	1:A:488:ARG:NH2	2.31	0.46
2:B:65:CYS:SG	2:B:76:ALA:N	2.89	0.46
1:E:390:ARG:CD	1:E:395:SER:HB2	2.39	0.46
1:E:409:GLN:O	1:E:412:GLU:N	2.48	0.46
2:F:46:ASN:O	2:F:47:LEU:HD23	2.14	0.46
3:C:80:LEU:HD23	3:C:80:LEU:HA	1.54	0.46
2:B:57:CYS:O	2:B:58:ARG:HB2	2.15	0.46
2:B:62:CYS:SG	2:B:63:GLY:N	2.88	0.46
1:E:119:MET:HE3	1:E:391:LEU:HG	1.97	0.46
4:H:95:ALA:O	4:H:99:VAL:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:THR:HA	1:A:391:LEU:HD22	1.96	0.46
1:E:65:HIS:ND1	1:E:86:VAL:HG12	2.31	0.46
1:E:180:LEU:HD12	1:E:433:GLU:HG3	1.97	0.46
2:F:81:LEU:HD22	2:F:88:MET:SD	2.56	0.46
1:E:119:MET:HE3	1:E:391:LEU:CG	2.46	0.46
1:E:230:GLN:OE1	1:E:390:ARG:HB3	2.16	0.46
3:C:98:VAL:HG23	3:C:98:VAL:O	2.15	0.46
2:F:57:CYS:CB	2:F:62:CYS:HB3	2.34	0.46
2:F:173:ILE:HD13	2:F:201:VAL:HG12	1.97	0.46
2:F:210:CYS:SG	2:F:221:ALA:HB2	2.56	0.46
3:C:120:THR:HG23	4:D:30:VAL:HB	1.98	0.45
1:E:231:TYR:O	1:E:233:PRO:HD3	2.15	0.45
1:A:98:LEU:HD23	2:B:132:ASN:ND2	2.30	0.45
1:A:51:GLY:O	1:A:396:LEU:HD12	2.17	0.45
1:A:245:GLU:O	1:A:246:GLY:C	2.41	0.45
1:A:363:THR:HB	1:A:367:CYS:HA	1.97	0.45
2:B:235:PHE:CD1	4:D:11:PRO:CG	2.98	0.45
1:E:54:ALA:HB2	1:E:89:CYS:HB3	1.99	0.45
1:E:232:HIS:O	1:E:352:PRO:HA	2.16	0.45
1:A:133:PHE:CE1	1:A:137:HIS:CD2	3.04	0.45
1:E:363:THR:HA	1:E:368:GLU:O	2.17	0.45
1:E:483:GLN:HG3	1:E:516:GLU:OE2	2.17	0.45
2:F:10:VAL:HG22	2:F:90:VAL:HB	1.99	0.45
2:F:153:LEU:HD12	2:F:215:PRO:HD3	1.98	0.45
2:B:74:LYS:HA	2:B:153:LEU:HD13	1.99	0.45
3:C:104:GLY:HA2	3:C:107:PRO:HD2	1.98	0.45
2:B:236:LEU:CD1	2:B:240:LEU:HD11	2.47	0.45
3:C:36:VAL:HG12	4:D:75:LEU:HD23	1.99	0.45
3:C:87:PHE:CD1	3:C:112:LEU:HD13	2.52	0.45
2:F:210:CYS:SG	2:F:211:SER:N	2.88	0.45
1:A:244:THR:HG22	1:A:331:ILE:HG13	1.99	0.45
3:C:26:MET:O	3:C:30:GLY:N	2.48	0.45
3:C:62:PHE:CE2	3:C:68:ILE:HG21	2.52	0.45
1:E:160:ILE:HG12	1:E:169:GLY:O	2.17	0.45
2:F:116:ILE:HB	2:F:176:ALA:HB2	1.98	0.45
2:F:202:TRP:CZ3	2:F:228:LYS:HD3	2.51	0.45
1:A:28:PRO:HA	1:A:148:GLN:HE21	1.81	0.45
2:B:44:LYS:NZ	2:B:49:PRO:O	2.40	0.45
1:E:98:LEU:CD2	2:F:125:ARG:HD3	2.47	0.45
1:A:399:LEU:HD11	5:A:701:FAD:O4'	2.17	0.44
1:E:377:VAL:HG21	1:E:403:GLY:HA2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:120:ILE:HD13	2:F:185:ASP:HB2	1.99	0.44
1:A:317:ARG:C	1:A:319:LEU:H	2.21	0.44
1:A:341:VAL:O	1:A:343:PRO:HD3	2.17	0.44
3:G:98:VAL:HG23	3:G:98:VAL:O	2.17	0.44
1:A:31:LYS:NZ	1:A:150:GLN:HB2	2.32	0.44
4:H:13:PHE:HE2	4:H:97:LYS:HE2	1.82	0.44
1:A:119:MET:H	1:A:279:ASN:HD21	1.64	0.44
1:A:341:VAL:HG13	1:A:346:GLU:HB2	1.99	0.44
1:A:398:GLU:HG3	1:A:402:PHE:HD2	1.82	0.44
1:E:41:MET:HE3	1:E:140:PHE:CE2	2.52	0.44
2:F:141:LYS:HA	3:G:97:ILE:HD11	1.98	0.44
1:A:316:LEU:O	1:A:319:LEU:HB2	2.18	0.44
2:B:157:ALA:HB2	2:B:213:VAL:HG21	1.99	0.44
3:C:87:PHE:CE1	3:C:112:LEU:HB3	2.53	0.44
1:E:21:ILE:HG23	1:E:146:PHE:CE2	2.52	0.44
1:E:148:GLN:OE1	1:E:148:GLN:N	2.37	0.44
2:B:8:ILE:HD11	2:B:81:LEU:HD11	2.00	0.44
1:E:152:PHE:CE2	1:E:183:ILE:CD1	3.01	0.44
2:F:7:LYS:HE2	2:F:25:PHE:CD2	2.53	0.44
3:C:12:THR:HG22	3:C:14:THR:N	2.33	0.44
1:E:217:LEU:HD21	1:E:223:LEU:HG	2.00	0.44
1:E:396:LEU:HG	5:E:701:FAD:C2	2.48	0.44
2:F:50:ASP:O	2:F:100:ARG:NH2	2.35	0.44
2:F:192:MET:HB3	2:F:196:ASN:ND2	2.33	0.44
1:A:273:PRO:O	1:A:274:LEU:C	2.55	0.44
1:A:35:ILE:CD1	1:A:183:ILE:HD12	2.45	0.43
1:A:223:LEU:HB3	1:A:226:MET:CG	2.48	0.43
1:A:413:ARG:HH11	1:A:413:ARG:CB	2.31	0.43
4:D:0:MET:HE2	4:D:0:MET:HB2	1.80	0.43
1:A:535:LEU:HA	1:A:535:LEU:HD23	1.73	0.43
1:E:204:ASN:HD22	1:E:204:ASN:N	2.15	0.43
1:A:197:ARG:CD	1:A:206:GLY:HA2	2.48	0.43
1:E:162:VAL:HG21	1:E:371:ILE:HD13	2.00	0.43
1:A:103:TRP:O	2:B:139:MET:HE1	2.18	0.43
1:A:425:ILE:O	1:A:428:GLN:HB2	2.18	0.43
1:E:18:ARG:NH1	1:E:92:GLU:OE1	2.50	0.43
1:A:413:ARG:HD3	1:A:413:ARG:HA	1.67	0.43
1:E:413:ARG:HD3	1:E:413:ARG:HA	1.67	0.43
1:A:65:HIS:ND1	1:A:86:VAL:HG12	2.33	0.43
3:C:5:LYS:O	3:C:7:TYR:N	2.52	0.43
1:E:379:GLU:OE2	5:E:701:FAD:O3'	2.28	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:87:PHE:CZ	3:G:112:LEU:HB3	2.53	0.43
1:A:497:VAL:CG2	3:C:3:LYS:O	2.66	0.43
3:C:2:THR:OG1	3:C:4:ARG:HG3	2.18	0.43
1:E:367:CYS:O	1:E:375:PHE:HD2	2.02	0.43
2:F:13:TYR:CZ	3:G:7:TYR:HB2	2.54	0.43
2:F:44:LYS:HA	2:F:48:ALA:O	2.18	0.43
1:A:439:LEU:HD12	1:A:442:GLN:NE2	2.34	0.43
1:A:497:VAL:HG21	3:C:3:LYS:O	2.19	0.43
2:B:202:TRP:CE2	4:D:11:PRO:HD3	2.54	0.43
1:E:42:ARG:NH2	2:F:150:ASN:O	2.50	0.43
2:F:207:VAL:HG22	3:G:25:TYR:CZ	2.54	0.43
1:A:327:ARG:O	1:A:328:LEU:HD23	2.19	0.43
1:A:109:GLY:HA3	2:B:133:ILE:CG2	2.49	0.42
2:F:57:CYS:O	2:F:58:ARG:CG	2.67	0.42
1:A:98:LEU:HD13	2:B:125:ARG:O	2.20	0.42
1:A:395:SER:O	1:A:398:GLU:HB3	2.19	0.42
2:B:206:PHE:CE2	2:B:225:GLN:HG3	2.54	0.42
1:E:363:THR:HB	1:E:367:CYS:HA	2.01	0.42
1:E:395:SER:O	1:E:398:GLU:HB3	2.19	0.42
2:F:93:LEU:HD23	2:F:96:PHE:CE2	2.54	0.42
2:B:16:GLU:HG2	3:C:3:LYS:HG3	2.01	0.42
2:B:207:VAL:O	3:C:21:PHE:HE1	2.02	0.42
4:D:27:ILE:O	4:D:30:VAL:HG12	2.19	0.42
3:G:21:PHE:CD1	3:G:21:PHE:O	2.73	0.42
1:A:21:ILE:O	1:A:22:ALA:C	2.57	0.42
1:E:80:ASP:OD2	1:E:365:GLN:HG2	2.19	0.42
1:A:386:HIS:HB3	1:A:390:ARG:HA	2.01	0.42
2:B:116:ILE:H	2:B:116:ILE:HG13	1.73	0.42
3:C:3:LYS:HB2	3:C:3:LYS:HE3	1.21	0.42
1:E:18:ARG:CZ	1:E:404:ARG:HG3	2.50	0.42
1:E:72:GLY:O	1:E:389:ASN:HB3	2.20	0.42
1:E:92:GLU:OE2	1:E:404:ARG:HD2	2.19	0.42
1:E:483:GLN:NE2	1:E:555:ARG:NH2	2.67	0.42
1:A:324:LEU:HD23	1:A:328:LEU:HD12	2.02	0.42
2:B:224:ILE:H	2:B:224:ILE:HG13	1.47	0.42
1:E:160:ILE:HD12	1:E:162:VAL:HG23	1.89	0.42
1:A:60:ASP:HB2	1:A:121:ILE:HG21	2.02	0.42
1:E:140:PHE:HE1	1:E:151:ARG:NE	2.18	0.42
1:A:230:GLN:OE1	1:A:390:ARG:CD	2.68	0.42
2:B:15:PRO:HB2	3:C:5:LYS:HB3	1.99	0.42
2:B:211:SER:HA	2:B:220:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:192:THR:OG1	1:E:212:GLY:HA3	2.20	0.42
1:A:377:VAL:HG21	1:A:403:GLY:HA2	2.01	0.42
2:B:16:GLU:CG	3:C:3:LYS:HG2	2.49	0.42
3:C:16:TRP:CZ3	3:C:17:LYS:HG2	2.54	0.42
1:E:76:LEU:HD23	1:E:76:LEU:HA	1.81	0.42
1:A:253:ILE:CG1	1:A:315:ASP:HB3	2.50	0.42
1:E:84:TYR:CE1	1:E:88:HIS:CE1	3.08	0.42
1:E:193:GLY:N	1:E:380:CYS:HB3	2.35	0.42
2:B:13:TYR:HH	3:C:5:LYS:CG	2.30	0.41
2:B:99:GLU:OE1	3:C:4:ARG:HD2	2.20	0.41
1:E:27:ASN:ND2	1:E:30:ALA:HB2	2.34	0.41
1:E:161:LEU:O	1:E:168:ARG:N	2.37	0.41
1:A:250:GLU:CB	1:A:319:LEU:HD11	2.51	0.41
2:F:16:GLU:OE2	3:G:3:LYS:HD2	2.20	0.41
2:B:141:LYS:HA	3:C:97:ILE:HD11	2.02	0.41
3:C:88:GLU:O	3:C:91:PRO:HD2	2.20	0.41
4:D:38:LEU:HD22	4:D:43:LEU:HB2	2.02	0.41
1:A:221:VAL:HG11	1:A:361:ILE:HG23	2.03	0.41
1:E:152:PHE:CA	1:E:155:HIS:CD2	3.03	0.41
1:E:232:HIS:HB2	1:E:355:HIS:CG	2.55	0.41
1:A:115:ARG:HE	1:A:279:ASN:HB2	1.75	0.41
1:A:133:PHE:CE1	1:A:137:HIS:NE2	2.89	0.41
3:C:30:GLY:C	3:C:32:ALA:H	2.24	0.41
1:E:54:ALA:O	1:E:123:ARG:HB2	2.20	0.41
1:E:207:ILE:H	1:E:207:ILE:HG12	1.65	0.41
1:E:232:HIS:HD2	1:E:234:THR:H	1.68	0.41
2:F:218:VAL:O	2:F:219:ASP:HB3	2.21	0.41
4:D:109:VAL:O	4:D:113:ILE:HG13	2.21	0.41
2:B:8:ILE:HD12	2:B:28:VAL:HG21	2.02	0.41
3:G:98:VAL:CG2	3:G:103:MET:HB3	2.47	0.41
3:C:69:VAL:O	3:C:73:LEU:HG	2.20	0.41
4:D:10:GLU:N	4:D:11:PRO:HD2	2.36	0.41
2:F:84:TYR:HB3	2:F:88:MET:HB2	2.02	0.41
1:A:256:ASN:ND2	1:A:260:TYR:HB3	2.36	0.41
1:A:391:LEU:O	1:A:394:ASN:HB2	2.21	0.41
1:E:68:ASP:HB3	1:E:391:LEU:HD21	2.03	0.41
1:A:41:MET:CE	1:A:140:PHE:CE2	3.04	0.40
3:C:53:PRO:HB3	4:D:51:TYR:CD2	2.56	0.40
1:E:455:MET:O	1:E:459:MET:HG2	2.21	0.40
4:H:24:SER:O	4:H:28:ALA:HB3	2.21	0.40
1:A:59:HIS:H	1:A:59:HIS:CD2	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:ARG:HG2	1:A:527:GLU:HG3	2.02	0.40
3:C:130:TRP:HB2	4:D:53:ARG:HH21	1.87	0.40
1:E:460:GLU:O	1:E:460:GLU:HG3	2.21	0.40
1:A:216:ALA:HB1	1:A:221:VAL:HB	2.03	0.40
1:A:298:TRP:HZ3	1:A:299:ARG:CZ	2.34	0.40
2:F:40:LEU:HA	2:F:43:ILE:HD12	2.03	0.40
2:F:93:LEU:HD12	2:F:93:LEU:HA	1.85	0.40
1:A:250:GLU:HB3	1:A:323:LYS:HE2	2.03	0.40
1:A:398:GLU:HG3	1:A:402:PHE:CD2	2.57	0.40
2:B:173:ILE:HG23	2:B:195:LEU:CD2	2.52	0.40
3:C:13:SER:HB2	4:D:89:LEU:O	2.20	0.40
1:E:104:SER:N	1:E:126:PHE:O	2.47	0.40
1:E:232:HIS:CG	1:E:242:LEU:HD11	2.56	0.40
2:F:175:LEU:HA	2:F:175:LEU:HD12	1.90	0.40
4:H:13:PHE:CE2	4:H:97:LYS:HE2	2.56	0.40
4:H:107:LEU:HA	4:H:110:VAL:HB	2.02	0.40
1:A:7:LEU:HA	1:A:185:ALA:HB1	2.03	0.40
2:B:207:VAL:HG22	3:C:25:TYR:CE2	2.56	0.40
1:E:155:HIS:HE1	1:E:174:ASN:CG	1.66	0.40
1:E:288:ASP:OD2	1:E:389:ASN:ND2	2.54	0.40
3:G:39:SER:O	3:G:43:ILE:HG13	2.21	0.40
4:H:75:LEU:HD23	4:H:75:LEU:HA	1.98	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	569/602 (94%)	526 (92%)	37 (6%)	6 (1%)	14	46
1	E	479/602 (80%)	445 (93%)	29 (6%)	5 (1%)	15	49
2	B	239/243 (98%)	210 (88%)	28 (12%)	1 (0%)	34	68

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	F	236/243 (97%)	217 (92%)	17 (7%)	2 (1%)	19 53
3	C	128/130 (98%)	116 (91%)	8 (6%)	4 (3%)	4 25
3	G	128/130 (98%)	119 (93%)	8 (6%)	1 (1%)	19 53
4	D	117/119 (98%)	101 (86%)	14 (12%)	2 (2%)	9 36
4	H	116/119 (98%)	104 (90%)	12 (10%)	0	100 100
All	All	2012/2188 (92%)	1838 (91%)	153 (8%)	21 (1%)	15 49

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	GLY
1	A	318	HIS
1	E	151	ARG
1	A	78	GLU
2	B	56	SER
3	C	6	PRO
3	C	18	LYS
2	F	56	SER
2	F	61	ILE
1	A	287	ARG
3	C	13	SER
4	D	3	PRO
3	G	18	LYS
1	A	222	PRO
1	A	364	ASP
1	E	152	PHE
3	C	31	THR
4	D	99	VAL
1	E	116	PHE
1	E	410	ALA
1	E	418	GLY

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	452/475 (95%)	434 (96%)	18 (4%)	31	62
1	E	366/475 (77%)	342 (93%)	24 (7%)	16	47
2	B	202/205 (98%)	187 (93%)	15 (7%)	13	42
2	F	200/205 (98%)	191 (96%)	9 (4%)	27	59
3	C	110/111 (99%)	102 (93%)	8 (7%)	14	43
3	G	111/111 (100%)	105 (95%)	6 (5%)	22	54
4	D	93/97 (96%)	87 (94%)	6 (6%)	17	48
4	H	96/97 (99%)	94 (98%)	2 (2%)	53	77
All	All	1630/1776 (92%)	1542 (95%)	88 (5%)	22	54

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	SER
1	A	41	MET
1	A	42	ARG
1	A	49	GLU
1	A	93	MET
1	A	122	GLU
1	A	200	ARG
1	A	211	ASP
1	A	218	SER
1	A	230	GLN
1	A	305	SER
1	A	319	LEU
1	A	325	HIS
1	A	327	ARG
1	A	358	MET
1	A	394	ASN
1	A	413	ARG
1	A	528	SER
2	B	19	THR
2	B	22	HIS
2	B	23	SER
2	B	57	CYS
2	B	62	CYS
2	B	128	ASP
2	B	178	ARG
2	B	197	SER
2	B	204	CYS

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Mol	Chain	Res	Type
2	B	206	PHE
2	B	212	GLU
2	B	230	GLU
2	B	236	LEU
2	B	237	ILE
2	B	241	LYS
3	C	1	THR
3	C	2	THR
3	C	3	LYS
3	C	39	SER
3	C	66	PRO
3	C	84	LYS
3	C	92	LYS
3	C	103	MET
4	D	0	MET
4	D	1	ILE
4	D	7	ARG
4	D	77	CYS
4	D	86	MET
4	D	118	ILE
1	E	2	THR
1	E	41	MET
1	E	42	ARG
1	E	49	GLU
1	E	76	LEU
1	E	93	MET
1	E	101	CYS
1	E	116	PHE
1	E	150	GLN
1	E	152	PHE
1	E	153	ASP
1	E	160	ILE
1	E	170	LEU
1	E	197	ARG
1	E	200	ARG
1	E	230	GLN
1	E	287	ARG
1	E	380	CYS
1	E	408	GLU
1	E	409	GLN
1	E	413	ARG
1	E	478	LYS

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Mol	Chain	Res	Type
1	E	485	ARG
1	E	537	GLU
2	F	58	ARG
2	F	61	ILE
2	F	62	CYS
2	F	112	SER
2	F	128	ASP
2	F	178	ARG
2	F	204	CYS
2	F	206	PHE
2	F	212	GLU
3	G	1	THR
3	G	39	SER
3	G	50	LYS
3	G	66	PRO
3	G	84	LYS
3	G	103	MET
4	H	0	MET
4	H	86	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	204	ASN
1	A	232	HIS
1	A	292	GLN
1	A	366	ASN
1	A	394	ASN
1	A	510	HIS
1	A	520	HIS
4	D	87	HIS
1	E	1	GLN
1	E	150	GLN
1	E	155	HIS
1	E	166	HIS
1	E	174	ASN
1	E	204	ASN
1	E	230	GLN
1	E	232	HIS
1	E	409	GLN
1	E	442	GLN
1	E	483	GLN

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Mol	Chain	Res	Type
4	H	59	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides 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	B	302	2	0,9,9	-	-	-		
6	PO4	E	702	-	4,4,4	1.30	0	6,6,6	0.64	0
9	SF4	B	303	2	0,12,12	-	-	-		
8	F3S	F	302	2	0,9,9	-	-	-		
5	FAD	A	701	1	53,58,58	0.54	0	68,89,89	0.89	3 (4%)
7	FES	F	301	-	0,4,4	-	-	-		
9	SF4	F	303	2	0,12,12	-	-	-		
5	FAD	E	701	1	53,58,58	0.52	0	68,89,89	0.83	2 (2%)
6	PO4	A	702	-	4,4,4	1.38	0	6,6,6	0.43	0
7	FES	B	301	2	0,4,4	-	-	-		

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	B	302	2	-	-	0/3/3/3
9	SF4	B	303	2	-	-	0/6/5/5
8	F3S	F	302	2	-	-	0/3/3/3
5	FAD	A	701	1	-	9/30/50/50	0/6/6/6
7	FES	F	301	-	-	-	0/1/1/1
9	SF4	F	303	2	-	-	0/6/5/5
5	FAD	E	701	1	-	10/30/50/50	0/6/6/6
7	FES	B	301	2	-	-	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	701	FAD	P-O3P-PA	-3.86	119.58	132.83
5	E	701	FAD	C5A-C6A-N6A	3.02	124.95	120.35
5	A	701	FAD	C5A-C6A-N6A	2.98	124.89	120.35
5	A	701	FAD	O5B-PA-O1A	2.85	120.20	109.07
5	A	701	FAD	O5'-P-O1P	2.30	118.04	109.07

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	701	FAD	N10-C1'-C2'-O2'
5	A	701	FAD	N10-C1'-C2'-C3'
5	A	701	FAD	O4'-C4'-C5'-O5'
5	A	701	FAD	PA-O3P-P-O5'
5	E	701	FAD	N10-C1'-C2'-O2'
5	E	701	FAD	N10-C1'-C2'-C3'
5	E	701	FAD	C3'-C4'-C5'-O5'
5	E	701	FAD	O4'-C4'-C5'-O5'
5	E	701	FAD	C5'-O5'-P-O1P
5	E	701	FAD	C5'-O5'-P-O2P
5	E	701	FAD	PA-O3P-P-O5'
5	A	701	FAD	C5'-O5'-P-O3P
5	A	701	FAD	C5'-O5'-P-O1P
5	A	701	FAD	C3'-C4'-C5'-O5'
5	A	701	FAD	O4B-C4B-C5B-O5B

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Mol	Chain	Res	Type	Atoms
5	E	701	FAD	C4'-C5'-O5'-P
5	E	701	FAD	C5'-O5'-P-O3P
5	A	701	FAD	PA-O3P-P-O1P
5	E	701	FAD	O4B-C4B-C5B-O5B

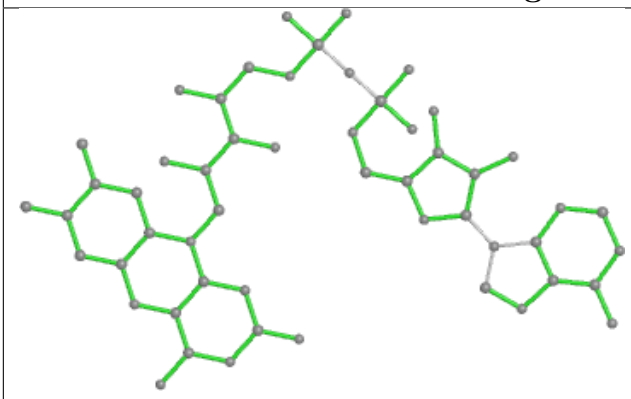
There are no ring outliers.

4 monomers are involved in 10 short contacts:

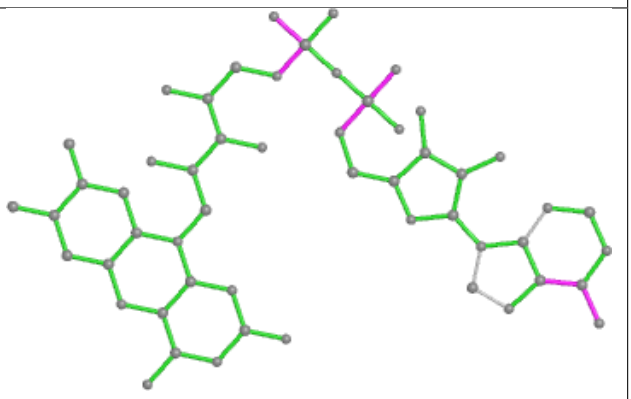
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	702	PO4	2	0
5	A	701	FAD	3	0
7	F	301	FES	2	0
5	E	701	FAD	3	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

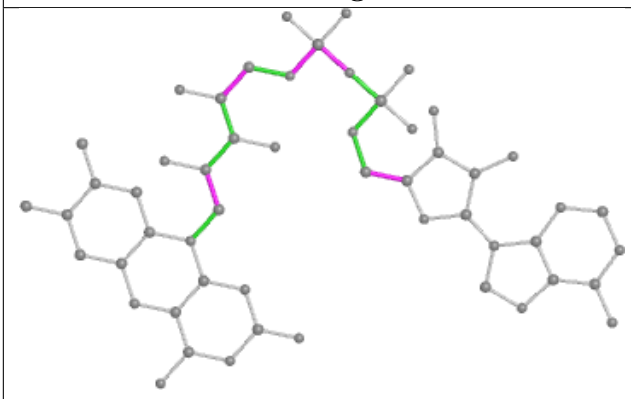
Ligand FAD A 701



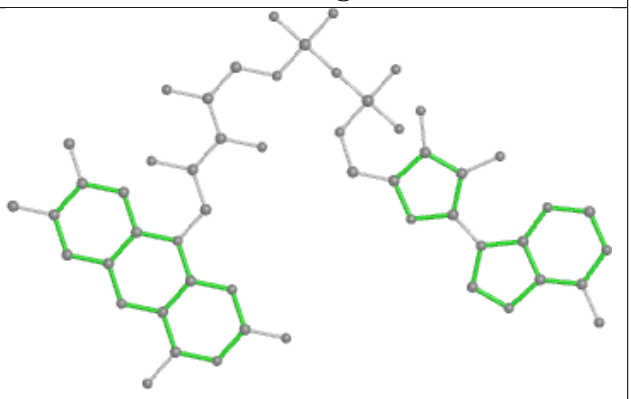
Bond lengths



Bond angles

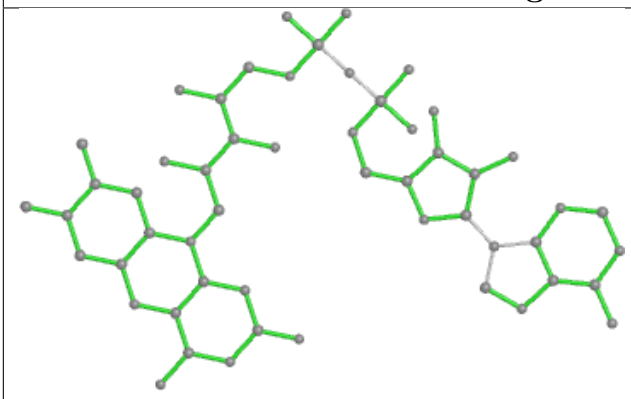


Torsions

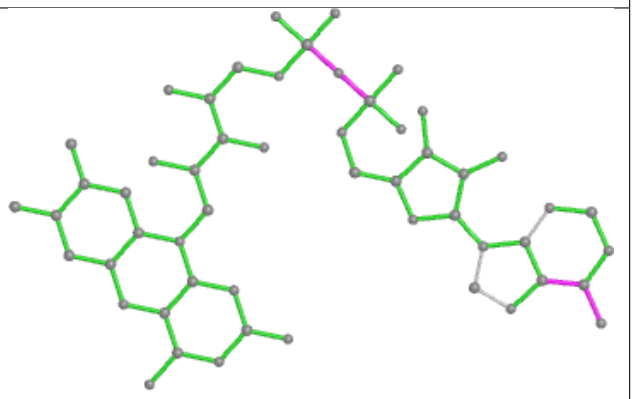


Rings

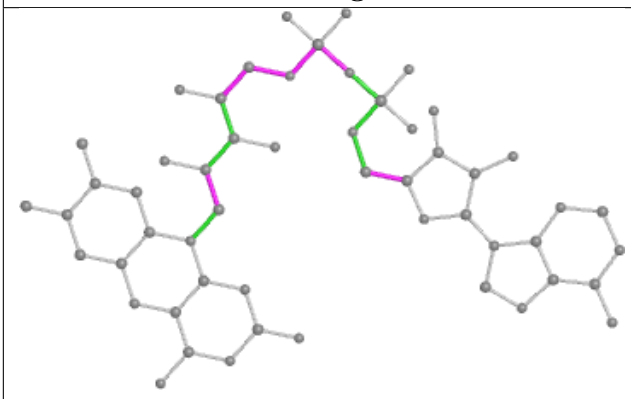
Ligand FAD E 701



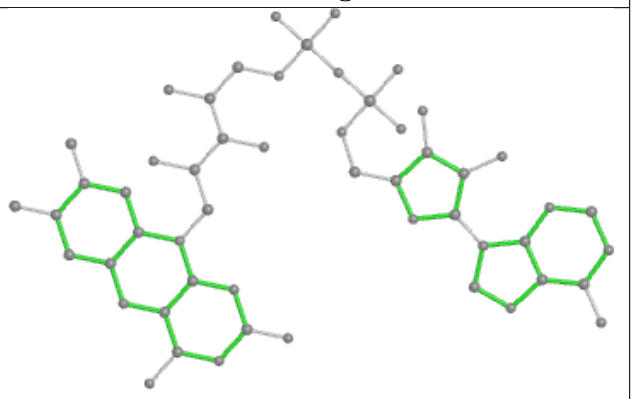
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	573/602 (95%)	0.74	80 (13%) 2 3	56, 104, 167, 214	0
1	E	487/602 (80%)	0.56	50 (10%) 6 7	57, 116, 156, 208	0
2	B	241/243 (99%)	0.36	27 (11%) 5 6	64, 93, 128, 183	0
2	F	238/243 (97%)	0.78	40 (16%) 1 1	62, 96, 127, 163	0
3	C	130/130 (100%)	0.42	16 (12%) 4 4	79, 107, 155, 209	0
3	G	130/130 (100%)	0.44	12 (9%) 9 11	78, 112, 164, 215	0
4	D	119/119 (100%)	0.20	7 (5%) 22 25	70, 116, 161, 183	0
4	H	118/119 (99%)	0.24	7 (5%) 22 25	89, 115, 172, 211	0
All	All	2036/2188 (93%)	0.56	239 (11%) 4 5	56, 107, 159, 215	0

All (239) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	95	ASN	7.5
2	F	8	ILE	7.4
2	F	25	PHE	7.1
1	E	575	PRO	7.1
2	F	27	GLU	5.8
3	G	102	LYS	5.8
2	F	30	TYR	5.8
2	F	6	LEU	5.8
1	A	161	LEU	5.5
2	F	90	VAL	5.4
1	E	205	GLY	5.4
1	A	169	GLY	5.4
1	A	171	VAL	5.2
1	A	270	PRO	5.2
2	F	28	VAL	5.1
1	E	537	GLU	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	575	PRO	5.0
1	A	565	TYR	5.0
2	B	1	ALA	5.0
1	A	302	ASN	4.9
3	C	95	ASN	4.8
2	F	3	MET	4.8
3	C	7	TYR	4.7
3	G	103	MET	4.7
1	E	544	ASP	4.6
1	A	202	ASN	4.6
1	A	576	ALA	4.5
2	F	88	MET	4.5
3	C	97	ILE	4.5
2	F	10	VAL	4.5
1	E	554	PHE	4.4
1	A	552	LEU	4.4
2	F	7	LYS	4.4
2	B	21	PRO	4.4
2	F	81	LEU	4.4
1	E	75	TRP	4.3
2	F	9	GLU	4.3
4	H	97	LYS	4.3
3	G	7	TYR	4.2
3	G	97	ILE	4.2
1	A	303	THR	4.2
2	B	11	VAL	4.1
2	F	5	ASN	4.1
3	G	96	ILE	4.1
1	A	322	LYS	4.1
2	F	11	VAL	4.1
3	C	96	ILE	4.1
1	A	204	ASN	4.0
3	C	98	VAL	4.0
2	F	85	THR	4.0
4	H	92	HIS	4.0
3	C	102	LYS	4.0
3	G	99	LYS	4.0
1	E	542	ARG	3.8
2	F	98	ILE	3.8
1	A	310	ASP	3.8
1	A	348	ILE	3.8
3	G	1	THR	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	328	LEU	3.7
1	A	205	GLY	3.6
2	B	64	SER	3.6
1	A	160	ILE	3.6
3	C	8	VAL	3.6
2	B	8	ILE	3.6
1	A	250	GLU	3.6
1	E	199	TYR	3.5
1	E	193	GLY	3.5
2	F	84	TYR	3.5
1	A	564	GLU	3.5
2	B	19	THR	3.5
3	C	99	LYS	3.5
3	C	103	MET	3.5
1	E	546	ASN	3.4
1	E	194	GLY	3.4
1	A	170	LEU	3.4
1	A	323	LYS	3.4
2	F	26	TYR	3.4
2	F	62	CYS	3.3
1	A	344	VAL	3.3
1	E	3	PHE	3.3
2	F	57	CYS	3.3
1	A	318	HIS	3.3
1	E	547	PHE	3.3
1	A	324	LEU	3.3
2	F	89	LYS	3.3
1	A	356	TYR	3.3
2	B	24	ALA	3.3
1	E	576	ALA	3.2
1	A	247	CYS	3.2
1	E	244	THR	3.2
2	B	194	GLN	3.2
1	A	275	GLY	3.2
3	C	100	ASP	3.2
1	E	549	LYS	3.1
2	F	4	LYS	3.1
1	E	419	ASN	3.1
1	E	118	GLY	3.1
2	F	19	THR	3.1
2	F	190	GLU	3.1
1	A	343	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
4	D	115	VAL	3.1
1	A	230	GLN	3.0
1	A	312	VAL	3.0
2	B	62	CYS	3.0
2	B	85	THR	3.0
2	B	65	CYS	3.0
1	A	325	HIS	3.0
1	E	117	GLY	3.0
1	E	465	ILE	3.0
1	A	447	ASN	3.0
1	A	571	THR	3.0
1	A	183	ILE	2.9
1	E	192	THR	2.9
4	H	98	TRP	2.9
1	A	316	LEU	2.9
1	E	197	ARG	2.9
2	B	23	SER	2.9
2	B	10	VAL	2.9
1	A	44	HIS	2.9
3	C	101	GLU	2.9
2	B	20	ALA	2.8
2	F	128	ASP	2.8
1	A	355	HIS	2.8
1	A	194	GLY	2.8
1	A	196	GLY	2.8
2	F	24	ALA	2.8
1	A	319	LEU	2.8
2	F	91	GLU	2.8
3	G	100	ASP	2.8
1	A	563	LEU	2.8
2	F	64	SER	2.8
3	C	94	ALA	2.8
2	B	98	ILE	2.7
2	F	108	HIS	2.7
3	G	98	VAL	2.7
1	E	565	TYR	2.7
2	B	57	CYS	2.7
1	A	315	ASP	2.7
1	A	193	GLY	2.7
1	E	564	GLU	2.6
4	H	101	TYR	2.6
1	A	162	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
4	H	0	MET	2.6
1	A	246	GLY	2.6
1	A	395	SER	2.6
1	A	0	MET	2.6
1	E	445	GLY	2.6
4	H	48	ALA	2.5
4	D	62	ILE	2.5
2	F	82	ARG	2.5
4	D	93	VAL	2.5
1	E	44	HIS	2.5
1	E	63	GLU	2.5
4	D	67	LEU	2.5
1	A	203	THR	2.5
1	E	13	GLY	2.5
2	B	169	GLY	2.4
2	F	141	LYS	2.4
1	E	545	VAL	2.4
1	A	562	ARG	2.4
2	B	141	LYS	2.4
1	E	467	ARG	2.4
1	E	548	LEU	2.4
4	D	98	TRP	2.4
1	E	4	GLN	2.4
1	A	314	LEU	2.4
3	G	49	LEU	2.4
3	C	130	TRP	2.4
2	B	58	ARG	2.4
1	A	159	ASP	2.4
1	A	239	SER	2.4
1	A	535	LEU	2.4
1	A	197	ARG	2.4
2	B	22	HIS	2.4
1	A	43	SER	2.4
2	B	13	TYR	2.4
4	H	76	TRP	2.4
1	E	195	ALA	2.4
1	E	572	THR	2.4
1	A	184	ARG	2.3
1	A	551	THR	2.3
1	E	362	GLU	2.3
1	A	573	LEU	2.3
1	A	342	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	60	ALA	2.3
1	A	327	ARG	2.3
1	A	347	PRO	2.3
3	C	92	LYS	2.3
1	E	552	LEU	2.3
1	A	320	GLY	2.2
1	E	574	PRO	2.2
1	A	572	THR	2.2
1	A	469	PRO	2.2
2	F	29	PRO	2.2
1	A	305	SER	2.2
1	A	262	TYR	2.2
1	E	57	GLN	2.2
1	A	345	LYS	2.2
3	C	105	PRO	2.2
3	G	46	LEU	2.2
1	E	43	SER	2.2
2	B	25	PHE	2.2
2	F	150	ASN	2.2
1	A	354	ALA	2.2
2	B	52	SER	2.2
1	A	379	GLU	2.2
1	E	204	ASN	2.2
1	A	420	GLY	2.2
1	E	339	VAL	2.1
1	E	76	LEU	2.1
2	B	63	GLY	2.1
2	F	102	LEU	2.1
1	A	158	LEU	2.1
1	A	157	VAL	2.1
3	C	18	LYS	2.1
2	F	181	GLU	2.1
2	B	45	ASP	2.1
1	A	229	VAL	2.1
2	F	237	ILE	2.1
1	E	571	THR	2.1
1	E	71	ALA	2.1
2	B	2	GLU	2.1
2	F	36	LEU	2.1
2	B	7	LYS	2.0
1	E	463	CYS	2.0
1	A	357	THR	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	56	ALA	2.0
1	A	278	LYS	2.0
1	A	75	TRP	2.0
1	E	512	LEU	2.0
2	F	47	LEU	2.0
1	A	295	TRP	2.0
1	A	259	GLY	2.0
1	E	113	VAL	2.0
1	E	459	MET	2.0
4	D	76	TRP	2.0
1	E	161	LEU	2.0
1	A	346	GLU	2.0
4	D	49	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

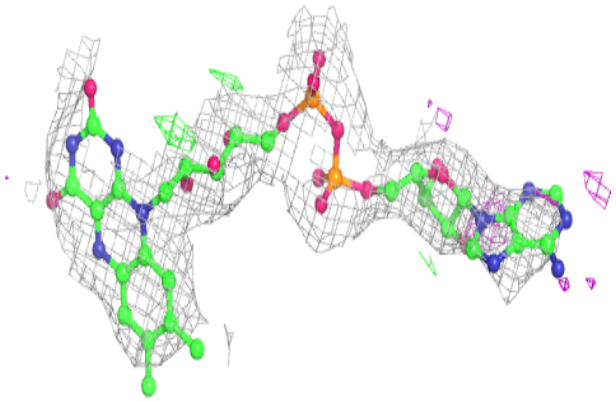
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

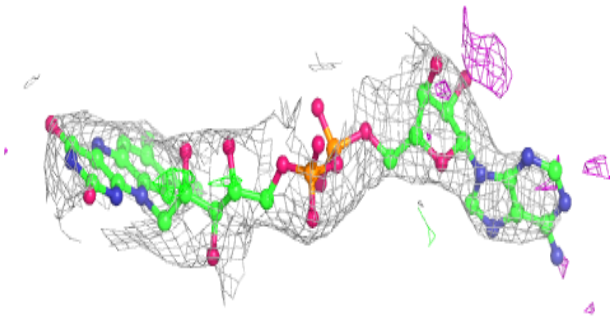
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PO4	E	702	5/5	0.50	0.44	205,205,206,207	0
6	PO4	A	702	5/5	0.70	0.40	172,173,175,176	0
5	FAD	A	701	53/53	0.82	0.43	85,91,97,104	0
5	FAD	E	701	53/53	0.89	0.33	84,97,113,119	0
7	FES	F	301	4/4	0.98	0.31	77,79,82,83	0
7	FES	B	301	4/4	0.99	0.36	68,71,76,115	0
8	F3S	B	302	7/7	0.99	0.21	56,58,93,162	0
8	F3S	F	302	7/7	0.99	0.21	55,63,100,119	0
9	SF4	B	303	8/8	0.99	0.24	56,71,88,138	0
9	SF4	F	303	8/8	0.99	0.22	60,69,91,121	0

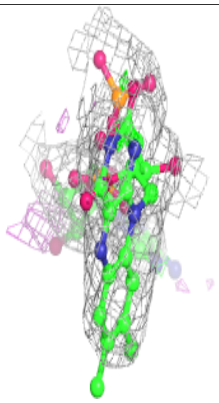
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around FAD A 701:

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

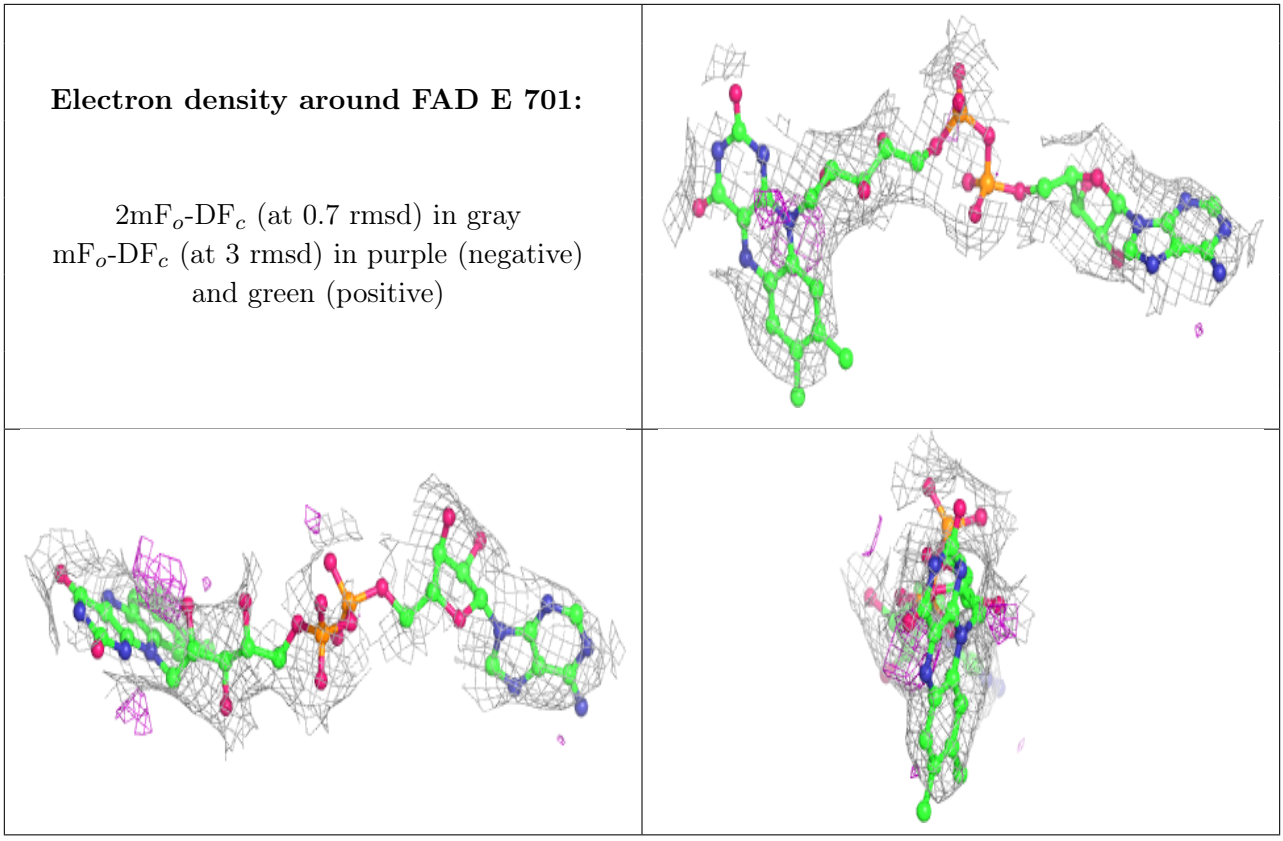






Electron density around FAD E 701:

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



6.5 Other polymers (i)

There are no such residues in this entry.