



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:59 AM UTC

PDB ID : 6AWF / pdb_00006awf
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

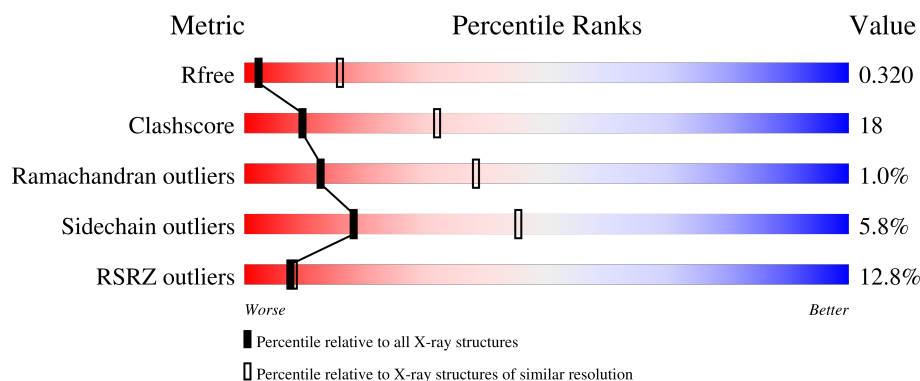
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	602	15% 65% 27% 5%
1	E	602	10% 58% 20% 19%
2	B	243	14% 59% 34% 6%
2	F	243	18% 69% 26% 5%
3	C	130	4% 55% 40% 5%

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Mol	Chain	Length	Quality of chain
3	G	130	
4	D	119	
4	H	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
6	PO4	E	702	-	-	X	-
7	FES	F	301	-	-	X	-

2 Entry composition

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.

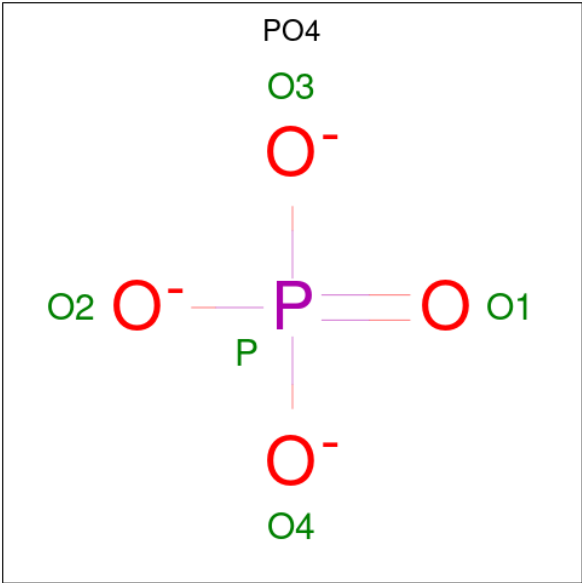
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	119	Total	C	N	O	S	0	0	0
			908	614	145	142	7			
4	H	118	Total	C	N	O	S	0	0	0
			917	620	150	140	7			

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



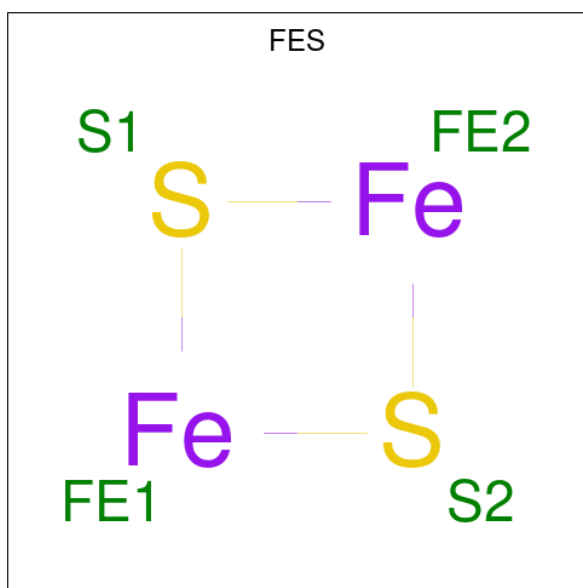
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
5	E	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



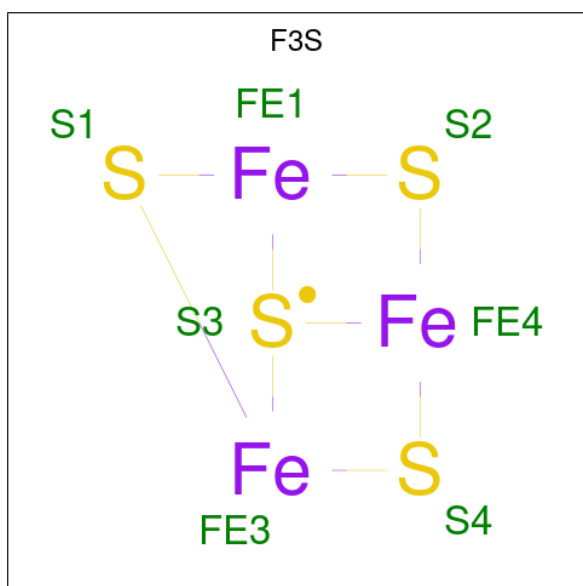
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 7 is FE2/S2 (INORGANIC) CLUSTER (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	F	1	Total	Fe	S	0	0
			4	2	2		

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



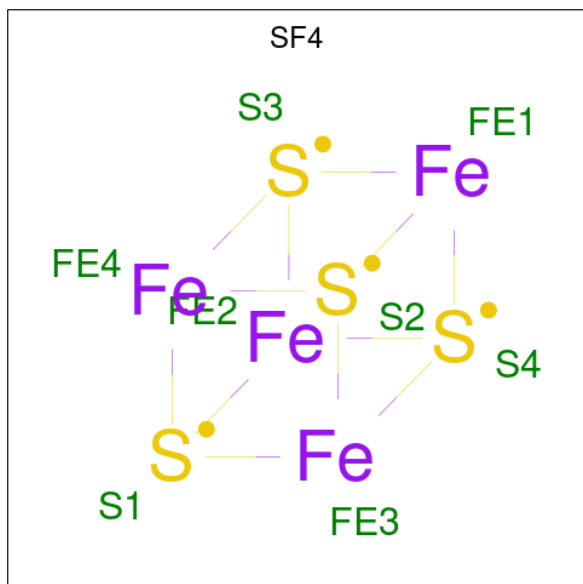
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	B	1	Total	Fe	S	0	0
			7	3	4		

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

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

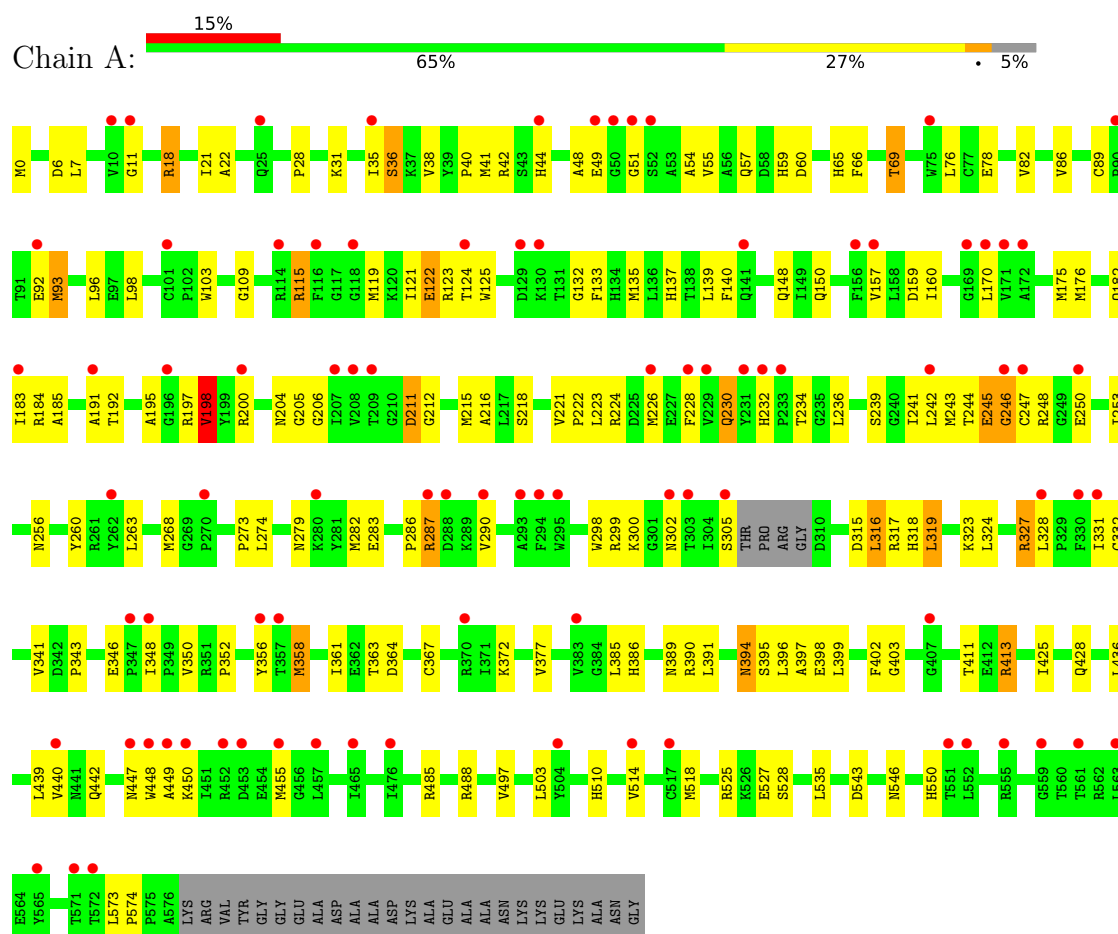


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	Fe	S	0	0
			8	4	4		
9	F	1	Total	Fe	S	0	0
			8	4	4		

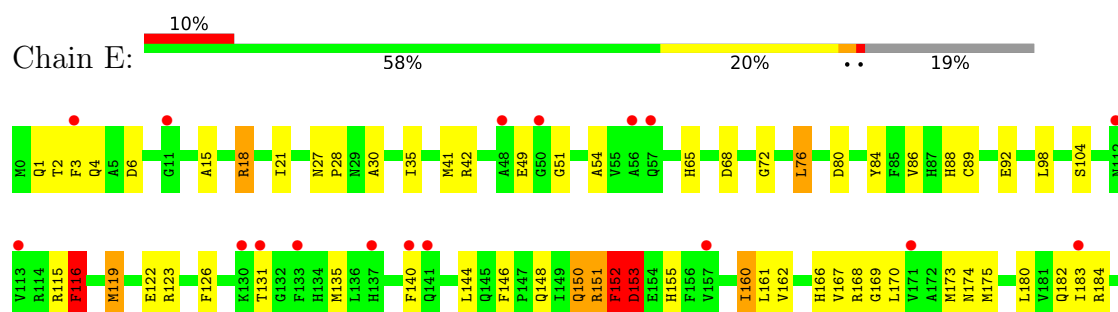
3 Residue-property plots

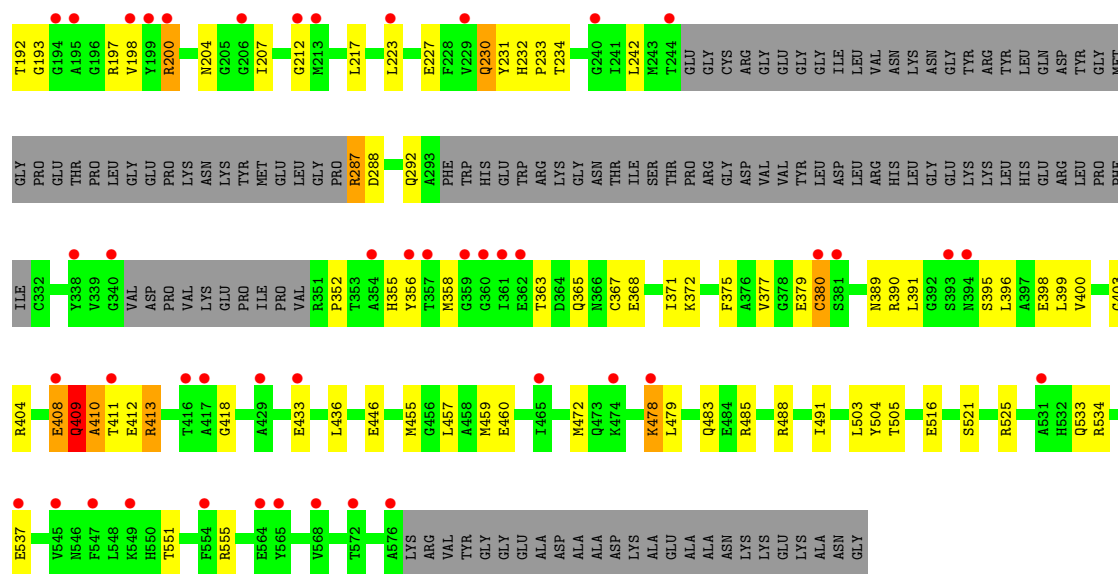
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

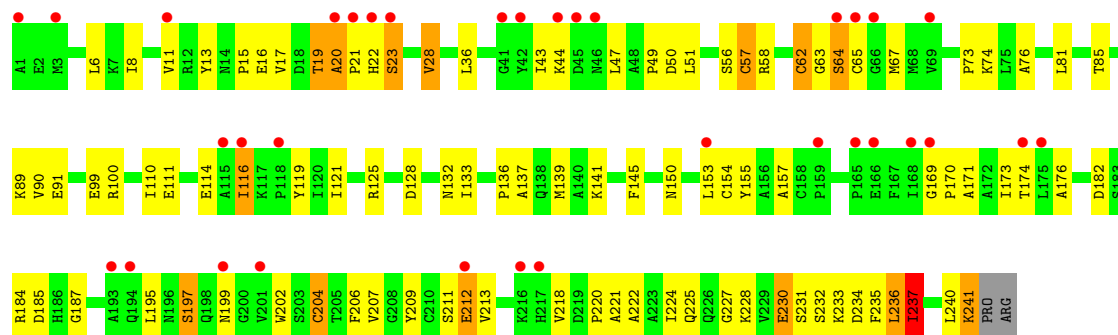


• Molecule 1: Fumarate reductase flavoprotein subunit

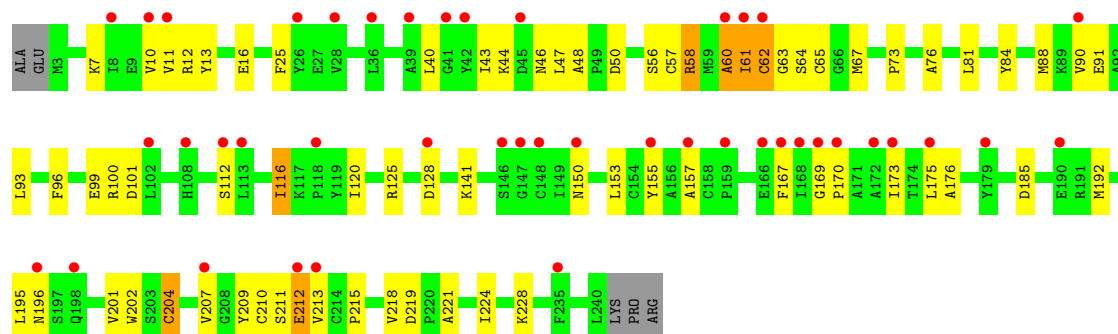




• Molecule 2: Fumarate reductase iron-sulfur subunit

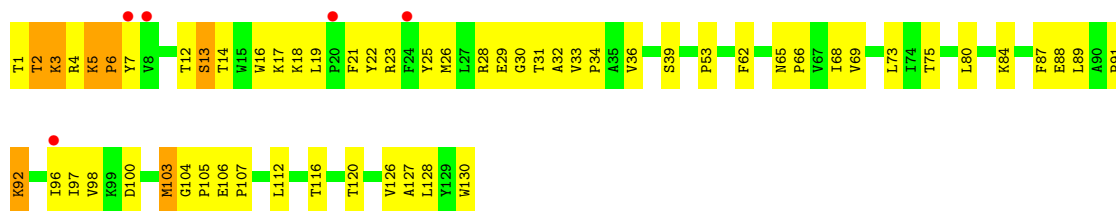


• Molecule 2: Fumarate reductase iron-sulfur subunit

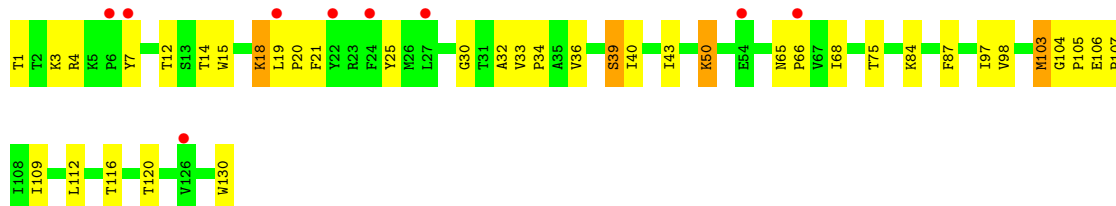


• Molecule 3: Fumarate reductase subunit C

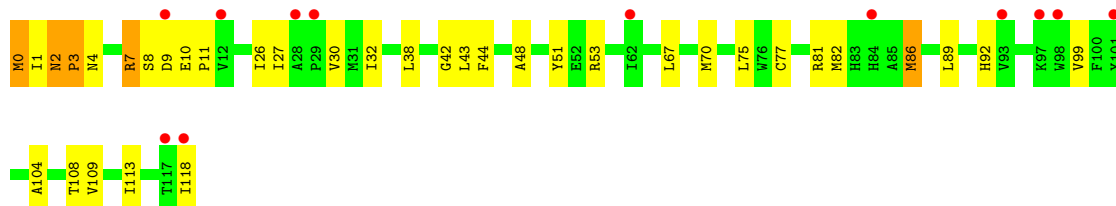




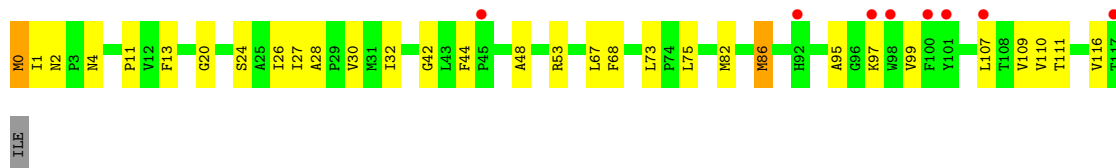
● Molecule 3: Fumarate reductase subunit C



● Molecule 4: Fumarate reductase subunit D



● Molecule 4: Fumarate reductase subunit D



ILE

4 Data and refinement statistics

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 46.91 – 3.35	Depositor EDS
% Data completeness (in resolution range)	76.4 (46.91-3.35) 60.3 (46.91-3.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.27 (at 3.33Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.285 , 0.318 0.289 , 0.320	Depositor DCC
R_{free} test set	2000 reflections (4.25%)	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 , 14.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.80	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FAD, FES, F3S, SF4, PO4

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	3/4480 (0.1%)	0.83	6/6060 (0.1%)
1	E	0.54	0/3708	0.88	8/5023 (0.2%)
2	B	0.66	1/1907 (0.1%)	0.89	8/2586 (0.3%)
2	F	0.49	1/1884 (0.1%)	0.71	0/2556
3	C	0.50	0/1090	0.76	2/1492 (0.1%)
3	G	0.43	0/1094	0.70	0/1496
4	D	0.53	0/938	0.84	3/1284 (0.2%)
4	H	0.37	0/947	0.70	1/1292 (0.1%)
All	All	0.55	5/16048 (0.0%)	0.82	28/21789 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	348	ILE	CA-C	7.66	1.59	1.53
1	A	573	LEU	C-N	-6.30	1.25	1.33
2	B	28	VAL	CA-C	5.96	1.56	1.52
2	F	60	ALA	CA-C	-5.94	1.48	1.53
1	A	574	PRO	N-CD	5.66	1.55	1.47

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	115	ARG	N-CA-C	20.14	135.49	112.93
1	A	245	GLU	N-CA-C	-11.11	99.14	111.14
4	D	2	ASN	CA-C-N	-8.94	108.67	119.84
4	D	2	ASN	C-N-CA	-8.94	108.67	119.84
1	E	119	MET	CA-C-N	-8.67	108.65	120.44
1	E	119	MET	C-N-CA	-8.67	108.65	120.44
1	A	573	LEU	CA-C-N	8.50	129.13	120.38
1	A	573	LEU	C-N-CA	8.50	129.13	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	574	PRO	N-CA-CB	7.75	110.60	103.08
1	E	409	GLN	CA-C-N	-7.68	106.86	121.54
1	E	409	GLN	C-N-CA	-7.68	106.86	121.54
2	B	237	ILE	CB-CA-C	-7.55	102.03	111.70
4	H	116	VAL	N-CA-C	-7.47	105.07	112.17
2	B	19	THR	N-CA-C	-7.29	104.42	113.38
2	B	23	SER	N-CA-C	6.91	119.48	110.43
1	A	198	VAL	N-CA-C	-6.62	104.00	113.07
1	E	4	GLN	N-CA-C	6.12	118.20	110.24
1	E	116	PHE	N-CA-C	6.07	123.72	110.80
2	B	20	ALA	CA-C-N	5.99	127.32	119.84
2	B	20	ALA	C-N-CA	5.99	127.32	119.84
4	D	92	HIS	N-CA-C	5.86	117.75	108.67
2	B	17	VAL	N-CA-C	5.75	121.29	109.34
3	C	5	LYS	CA-C-N	5.67	126.93	119.84
3	C	5	LYS	C-N-CA	5.67	126.93	119.84
2	B	64	SER	CA-C-N	5.50	129.48	120.63
2	B	64	SER	C-N-CA	5.50	129.48	120.63
1	A	348	ILE	O-C-N	5.18	125.50	121.46
1	E	153	ASP	N-CA-C	5.05	117.42	110.35

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	4391	0	4260	150	0
1	E	3642	0	3466	158	0
2	B	1865	0	1817	100	0
2	F	1842	0	1790	67	0
3	C	1054	0	1097	74	0
3	G	1058	0	1108	36	0
4	D	908	0	927	32	0
4	H	917	0	960	26	0
5	A	53	0	29	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	558	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 18.

All (558) 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	1.45	1.44
1:E:155:HIS:CE1	1:E:174:ASN:CG	2.00	1.39
1:A:232:HIS:CE1	1:A:242:LEU:HD11	1.61	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
2:B:99:GLU:CD	3:C:4:ARG:NH1	1.97	1.22
1:A:245:GLU:O	1:A:247:CYS:N	1.73	1.19
2:B:99:GLU:OE2	3:C:4:ARG:NH1	1.78	1.17
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:409:GLN:O	1:E:410:ALA:C	1.90	1.09
1:E:155:HIS:ND1	1:E:174:ASN:CG	2.12	1.07
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:GLU:OE2	3:C:3:LYS:HD2	1.63	0.97
1:E:119:MET:HE2	1:E:391:LEU:HD23	1.45	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	0.94
2:F:57:CYS:HB3	2:F:62:CYS:HB3	1.49	0.94
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
2:B:99:GLU:CD	3:C:4:ARG:HH11	1.67	0.88
1:E:230:GLN:HE21	1:E:355:HIS:HD2	1.21	0.88
1:E:160:ILE:HG12	1:E:161:LEU:N	1.82	0.88
1:A:356:TYR:CD2	1:A:390:ARG:HD3	2.09	0.87
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:152:PHE:C	1:E:155:HIS:HD2	1.86	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
2:B:99:GLU:CD	3:C:4:ARG:HH12	1.77	0.80
1:E:160:ILE:CG1	1:E:161:LEU:N	2.45	0.79
1:E:119:MET:HE2	1:E:391:LEU:CD2	2.12	0.79
2:B:13:TYR:OH	3:C:5:LYS:CG	2.30	0.78
1:E:409:GLN:O	1:E:411:THR:N	2.18	0.76
1:A:245:GLU:C	1:A:247:CYS:H	1.92	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
1:E:152:PHE:C	1:E:155:HIS:CD2	2.64	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
1:A:245:GLU:C	1:A:247:CYS:N	2.46	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:155:HIS:CE1	1:E:174:ASN:HD21	2.05	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
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:160:ILE:HD11	1:E:162:VAL:HG23	1.75	0.69
1:A:358:MET:HE3	1:A:389:ASN:HA	1.75	0.68
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
2:B:241:LYS:HG3	2:B:241:LYS:O	1.92	0.68
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
4:H:86:MET:HE3	4:H:86:MET:HA	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:157:ALA:O	3:C:22:TYR:OH	2.12	0.65
3:C:96:ILE:HD12	3:C:103:MET:HE2	1.79	0.65
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
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:160:ILE:HD13	1:E:160:ILE:C	2.23	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
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:E:358:MET:HE3	1:E:389:ASN:HA	1.82	0.61
1:A:245:GLU:O	1:A:246:GLY:C	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:2:ASN:CG	4:D:3:PRO:N	2.59	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
4:D:2:ASN:OD1	4:D:3:PRO:C	2.46	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
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:41:MET:HE3	1:A:140:PHE:CE2	2.39	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
2:F:57:CYS:C	2:F:58:ARG:CG	2.76	0.57
1:A:232:HIS:ND1	1:A:242:LEU:HD13	2.20	0.56
1:A:263:LEU:HD22	1:A:268:MET:HE1	1.87	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
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:150:GLN:C	1:E:151:ARG:O	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:LYS:HE3	1:A:413:ARG:HE	1.71	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
3:G:106:GLU:CD	3:G:106:GLU:H	2.15	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
1:E:150:GLN:C	1:E:150:GLN:HE21	2.15	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:A:197:ARG:HD2	1:A:205:GLY:C	2.23	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:13:TYR:HH	3:C:5:LYS:HG3	1.72	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:E:41:MET:HE2	2:F:150:ASN:OD1	2.09	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
1:E:144:LEU:HD21	1:E:151:ARG:HH21	1.69	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:155:HIS:HE1	1:E:174:ASN:CG	1.66	0.53
3:G:33:VAL:HG22	4:H:82:MET:HE2	1.90	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:119:MET:HE3	1:E:391:LEU:CD2	2.39	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: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:E:41:MET:HE3	1:E:140:PHE:CE2	2.45	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
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:472:MET:HE1	1:E:534:ARG:CZ	2.40	0.51
1:A:236:LEU:HD11	1:A:243:MET:HE3	1.92	0.51
1:E:42:ARG:HD2	1:E:42:ARG:N	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:130:TRP:O	4:D:53:ARG:NE	2.40	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
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: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
1:A:317:ARG:C	1:A:319:LEU:H	2.21	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
4:D:104:ALA:O	4:D:108:THR:OG1	2.24	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
1:A:273:PRO:O	1:A:274:LEU:C	2.55	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
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:E:227:GLU:OE2	1:E:521:SER:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:21:ILE:O	1:A:22:ALA:C	2.57	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
3:C:36:VAL:HG21	4:D:82:MET:HE1	1.96	0.47
2:F:116:ILE:HD13	2:F:176:ALA:CA	2.45	0.47
3:G:33:VAL:HA	4:H:82:MET:HE3	1.96	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
1:A:103:TRP:O	2:B:139:MET:HE1	2.16	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
1:E:198:VAL:HA	1:E:455:MET:HE3	1.97	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
2:F:204:CYS:O	2:F:228:LYS:NZ	2.42	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
4:H:95:ALA:O	4:H:99:VAL:HG23	2.15	0.46
2:F:67:MET:HE2	2:F:67:MET:HB3	1.79	0.46
1:A:69:THR:HA	1:A:391:LEU:HD22	1.96	0.46
3:C:30:GLY:C	3:C:32:ALA:H	2.24	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: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: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
4:D:86:MET:HE3	4:D:86:MET:HA	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:F:120:ILE:HD13	2:F:185:ASP:HB2	1.99	0.44
1:A:230:GLN:HB2	1:A:358:MET:HE1	1.99	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
3:C:30:GLY:C	3:C:32:ALA:N	2.75	0.44
3:G:30:GLY:C	3:G:32:ALA:N	2.75	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
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
1:A:514:VAL:HG12	1:A:518:MET:HE3	2.00	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
4:H:1:ILE:O	4:H:2:ASN:C	2.61	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: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
1:A:535:LEU:HA	1:A:535:LEU:HD23	1.73	0.43
3:C:106:GLU:CD	3:C:106:GLU:H	2.26	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:425:ILE:O	1:A:428:GLN:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:ARG:NH1	1:E:92:GLU:OE1	2.50	0.43
1:E:478:LYS:O	1:E:479:LEU:C	2.59	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:41:MET:HE2	2:B:150:ASN:OD1	2.19	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
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:228:PHE:HB3	1:A:358:MET:HE2	1.99	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:E:459:MET:HE3	1:E:459:MET:HB3	1.77	0.43
1:A:109:GLY:HA3	2:B:133:ILE:CG2	2.49	0.42
1:E:135:MET:HE2	1:E:135:MET:HB3	1.85	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
2:B:230:GLU:O	2:B:231:SER:C	2.62	0.42
3:C:12:THR:C	3:C:14:THR:H	2.26	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:135:MET:HE2	1:A:135:MET:HB3	1.82	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
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
2:B:65:CYS:O	2:B:67:MET:HE3	2.20	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:A:286:PRO:O	1:A:287:ARG:C	2.62	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
1:E:287:ARG:HH21	1:E:389:ASN:CG	2.27	0.42
2:F:12:ARG:HE	2:F:101:ASP:CG	2.20	0.42
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:E:119:MET:HE3	1:E:391:LEU:HG	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:232:HIS:HD2	1:E:234:THR:H	1.68	0.41
2:F:99:GLU:CD	3:G:4:ARG:HH11	2.29	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
4:D:70:MET:O	4:D:70:MET:HE3	2.21	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:65:HIS:O	1:A:66:PHE:C	2.64	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
1:A:455:MET:HE2	1:A:455:MET:HB3	1.83	0.40
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
3:G:30:GLY:C	3:G:32:ALA:H	2.29	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	11	36
1	E	479/602 (80%)	445 (93%)	29 (6%)	5 (1%)	12	38
2	B	239/243 (98%)	210 (88%)	28 (12%)	1 (0%)	30	58
2	F	236/243 (97%)	217 (92%)	17 (7%)	2 (1%)	16	44
3	C	128/130 (98%)	116 (91%)	8 (6%)	4 (3%)	3	17
3	G	128/130 (98%)	119 (93%)	8 (6%)	1 (1%)	16	44
4	D	117/119 (98%)	101 (86%)	14 (12%)	2 (2%)	7	27
4	H	116/119 (98%)	104 (90%)	12 (10%)	0	100	100
All	All	2012/2188 (92%)	1838 (91%)	153 (8%)	21 (1%)	12	38

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

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Mol	Chain	Res	Type
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%)	431 (95%)	21 (5%)	24	50
1	E	366/475 (77%)	343 (94%)	23 (6%)	16	43
2	B	202/205 (98%)	187 (93%)	15 (7%)	13	38
2	F	200/205 (98%)	192 (96%)	8 (4%)	28	53
3	C	110/111 (99%)	100 (91%)	10 (9%)	9	30
3	G	111/111 (100%)	105 (95%)	6 (5%)	20	47
4	D	93/97 (96%)	86 (92%)	7 (8%)	12	38
4	H	96/97 (99%)	92 (96%)	4 (4%)	26	52
All	All	1630/1776 (92%)	1536 (94%)	94 (6%)	18	45

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

Mol	Chain	Res	Type
1	A	18	ARG
1	A	36	SER
1	A	49	GLU

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Mol	Chain	Res	Type
1	A	69	THR
1	A	93	MET
1	A	115	ARG
1	A	122	GLU
1	A	198	VAL
1	A	200	ARG
1	A	211	ASP
1	A	218	SER
1	A	230	GLN
1	A	305	SER
1	A	316	LEU
1	A	319	LEU
1	A	327	ARG
1	A	358	MET
1	A	394	ASN
1	A	411	THR
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	89	LYS
2	B	116	ILE
2	B	128	ASP
2	B	197	SER
2	B	204	CYS
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	23	ARG
3	C	39	SER
3	C	66	PRO
3	C	84	LYS
3	C	92	LYS
3	C	103	MET

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Mol	Chain	Res	Type
3	C	126	VAL
4	D	0	MET
4	D	1	ILE
4	D	7	ARG
4	D	67	LEU
4	D	77	CYS
4	D	86	MET
4	D	118	ILE
1	E	2	THR
1	E	18	ARG
1	E	49	GLU
1	E	76	LEU
1	E	116	PHE
1	E	122	GLU
1	E	150	GLN
1	E	152	PHE
1	E	153	ASP
1	E	160	ILE
1	E	170	LEU
1	E	173	MET
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
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	116	ILE
2	F	128	ASP
2	F	204	CYS
2	F	212	GLU
3	G	1	THR
3	G	39	SER
3	G	50	LYS

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Mol	Chain	Res	Type
3	G	66	PRO
3	G	84	LYS
3	G	103	MET
4	H	0	MET
4	H	67	LEU
4	H	86	MET
4	H	109	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	67	HIS
1	A	95	GLN
1	A	204	ASN
1	A	232	HIS
1	A	292	GLN
1	A	366	ASN
1	A	394	ASN
1	A	428	GLN
1	A	442	GLN
1	A	510	HIS
1	A	520	HIS
2	B	5	ASN
2	B	70	ASN
2	B	198	GLN
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
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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	FAD	E	701	1	58,58,58	0.73	1 (1%)	85,89,89	0.56	0
7	FES	F	301	-	0,4,4	-	-	-		
8	F3S	B	302	2	0,9,9	-	-	-		
6	PO4	E	702	-	4,4,4	1.35	0	6,6,6	0.67	0
5	FAD	A	701	1	58,58,58	0.46	0	85,89,89	0.77	3 (3%)
9	SF4	B	303	2	0,12,12	-	-	-		
9	SF4	F	303	2	0,12,12	-	-	-		
6	PO4	A	702	-	4,4,4	1.44	0	6,6,6	0.43	0
7	FES	B	301	2	0,4,4	-	-	-		
8	F3S	F	302	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
7	FES	F	301	-	-	-	0/1/1/1
8	F3S	B	302	2	-	-	0/3/3/3
5	FAD	A	701	1	-	10/34/50/50	0/6/6/6
9	SF4	B	303	2	-	-	0/6/5/5
9	SF4	F	303	2	-	-	0/6/5/5
5	FAD	E	701	1	-	11/34/50/50	0/6/6/6
7	FES	B	301	2	-	-	0/1/1/1
8	F3S	F	302	2	-	-	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	701	FAD	P-O3P	-4.59	1.54	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	701	FAD	O5B-PA-O1A	2.84	120.20	108.94
5	A	701	FAD	C4'-C3'-C2'	-2.55	109.32	113.57
5	A	701	FAD	O5'-P-O1P	2.30	118.04	108.94

There are no chirality outliers.

All (21) 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	C5'-O5'-P-O3P
5	E	701	FAD	PA-O3P-P-O5'
5	A	701	FAD	C5'-O5'-P-O1P
5	A	701	FAD	C5'-O5'-P-O3P
5	A	701	FAD	C3'-C4'-C5'-O5'
5	E	701	FAD	C4'-C5'-O5'-P
5	A	701	FAD	PA-O3P-P-O1P

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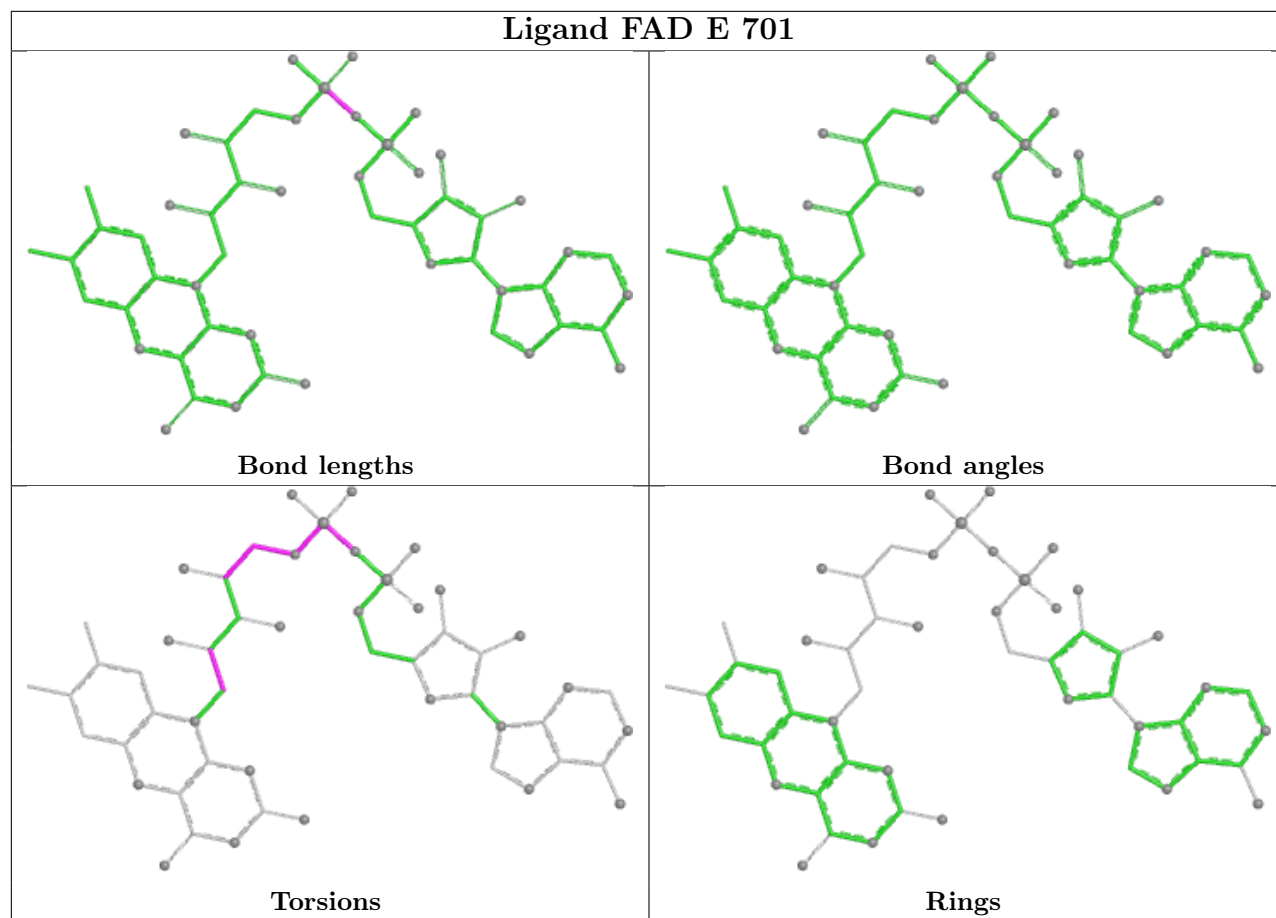
Mol	Chain	Res	Type	Atoms
5	A	701	FAD	O4B-C4B-C5B-O5B
5	A	701	FAD	PA-O3P-P-O2P
5	E	701	FAD	PA-O3P-P-O1P
5	E	701	FAD	PA-O3P-P-O2P

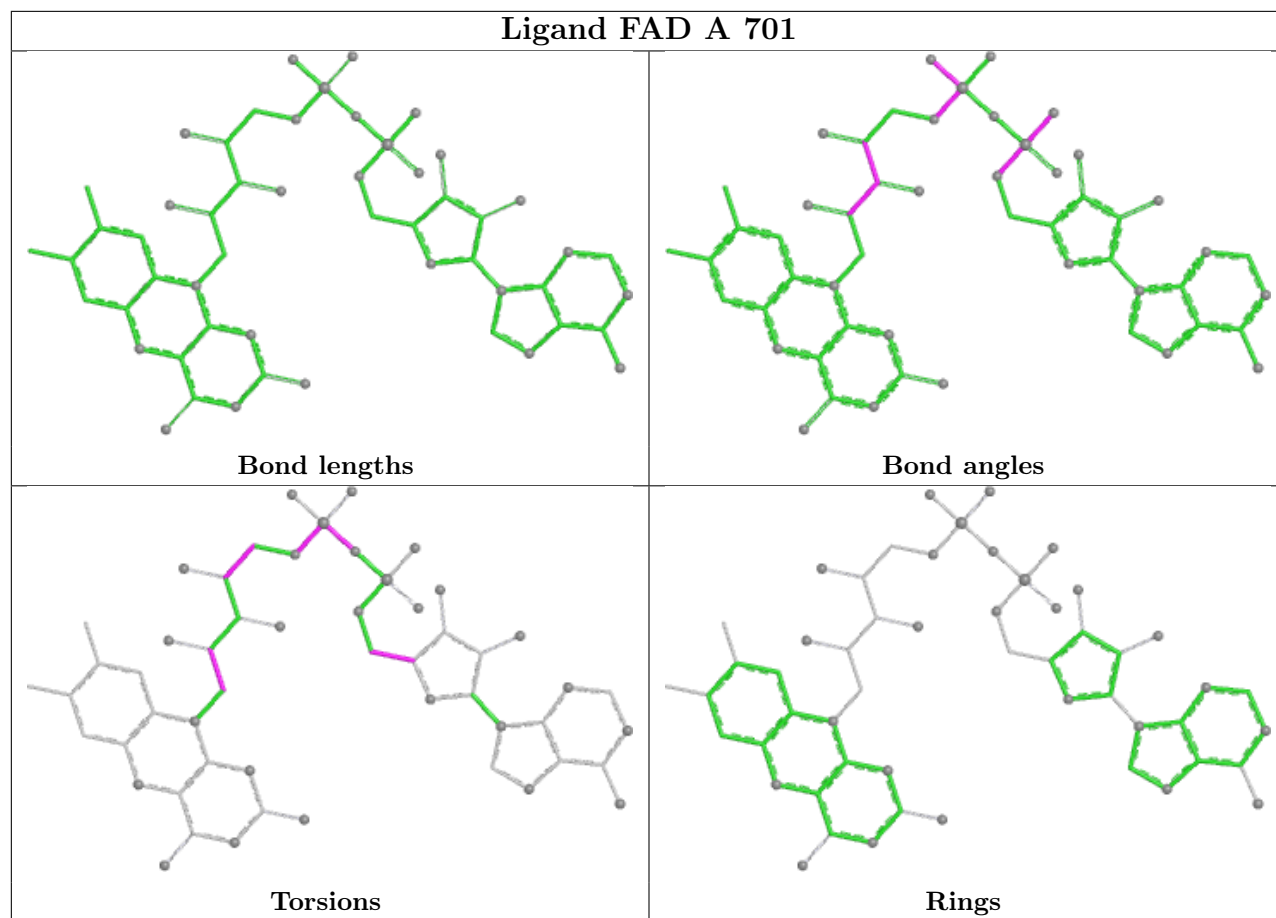
There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	701	FAD	3	0
7	F	301	FES	2	0
6	E	702	PO4	2	0
5	A	701	FAD	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	573/602 (95%)	1.03	88 (15%) 5 6	56, 104, 167, 214	0
1	E	487/602 (80%)	0.94	62 (12%) 8 8	57, 116, 156, 208	0
2	B	241/243 (99%)	1.02	34 (14%) 6 7	64, 93, 128, 183	0
2	F	238/243 (97%)	1.15	43 (18%) 3 4	62, 96, 127, 163	0
3	C	130/130 (100%)	0.62	5 (3%) 44 31	79, 107, 155, 209	0
3	G	130/130 (100%)	0.58	9 (6%) 23 18	78, 112, 164, 215	0
4	D	119/119 (100%)	0.80	12 (10%) 12 12	70, 116, 161, 183	0
4	H	118/119 (99%)	0.62	8 (6%) 23 18	89, 115, 172, 211	0
All	All	2036/2188 (93%)	0.93	261 (12%) 7 8	56, 107, 159, 215	0

All (261) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	45	ASP	12.1
2	B	212	GLU	11.1
2	F	150	ASN	8.1
1	E	141	GLN	7.5
2	B	169	GLY	6.7
1	A	328	LEU	6.5
4	D	98	TRP	5.9
2	F	41	GLY	5.8
2	F	169	GLY	5.8
1	A	453	ASP	5.6
2	F	175	LEU	5.5
1	A	565	TYR	5.5
2	F	198	GLN	5.3
2	F	45	ASP	5.3
2	B	42	TYR	5.2
1	A	357	THR	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	294	PHE	5.1
1	E	229	VAL	5.0
1	E	357	THR	4.9
2	F	168	ILE	4.8
2	B	46	ASN	4.8
2	F	190	GLU	4.7
1	A	331	ILE	4.6
3	C	8	VAL	4.5
1	E	433	GLU	4.4
2	F	167	PHE	4.2
1	A	229	VAL	4.2
2	F	113	LEU	4.2
1	A	50	GLY	4.1
1	E	195	ALA	4.0
1	A	118	GLY	4.0
1	A	246	GLY	4.0
2	B	41	GLY	4.0
1	E	361	ILE	3.9
1	E	199	TYR	3.8
2	B	194	GLN	3.8
1	A	141	GLN	3.8
2	F	207	VAL	3.8
1	E	130	LYS	3.7
1	A	563	LEU	3.7
3	C	24	PHE	3.7
1	A	247	CYS	3.6
1	A	290	VAL	3.6
2	F	128	ASP	3.6
1	A	157	VAL	3.5
2	B	11	VAL	3.5
2	B	21	PRO	3.5
1	A	552	LEU	3.5
2	F	213	VAL	3.5
4	H	97	LYS	3.4
1	A	302	ASN	3.4
4	D	93	VAL	3.4
3	G	22	TYR	3.4
1	A	35	ILE	3.4
2	F	157	ALA	3.4
1	A	572	THR	3.4
2	F	170	PRO	3.4
1	A	130	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
2	F	112	SER	3.3
1	A	200	ARG	3.3
1	E	537	GLU	3.3
1	E	213	MET	3.3
1	A	561	THR	3.3
1	E	198	VAL	3.3
2	F	148	CYS	3.2
1	A	348	ILE	3.2
2	F	166	GLU	3.2
1	A	101	CYS	3.2
1	A	449	ALA	3.2
2	B	174	THR	3.2
2	B	22	HIS	3.2
2	F	61	ILE	3.2
1	A	551	THR	3.2
1	A	407	GLY	3.1
2	B	65	CYS	3.1
2	B	168	ILE	3.1
1	E	531	ALA	3.1
1	E	564	GLU	3.1
1	E	465	ILE	3.1
1	A	156	PHE	3.1
2	B	216	LYS	3.1
2	F	60	ALA	3.0
2	B	217	HIS	3.0
2	F	90	VAL	3.0
2	B	23	SER	2.9
2	F	118	PRO	2.9
2	F	108	HIS	2.9
2	B	166	GLU	2.9
1	A	233	PRO	2.9
1	A	465	ILE	2.9
1	A	10	VAL	2.9
1	A	440	VAL	2.9
1	A	44	HIS	2.8
1	E	340	GLY	2.8
2	B	116	ILE	2.8
4	H	101	TYR	2.8
1	A	124	THR	2.8
2	F	147	GLY	2.8
1	E	380	CYS	2.8
3	C	20	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	7	TYR	2.8
2	F	10	VAL	2.8
1	A	183	ILE	2.8
1	E	194	GLY	2.8
1	E	200	ARG	2.8
1	E	576	ALA	2.8
2	F	39	ALA	2.8
2	F	159	PRO	2.8
4	D	97	LYS	2.7
2	B	201	VAL	2.7
1	E	133	PHE	2.7
1	E	554	PHE	2.7
1	E	572	THR	2.7
2	F	235	PHE	2.7
1	A	11	GLY	2.7
1	A	51	GLY	2.7
2	F	42	TYR	2.7
1	A	92	GLU	2.7
1	A	52	SER	2.7
2	B	69	VAL	2.7
1	A	25	GLN	2.7
1	E	57	GLN	2.6
4	D	62	ILE	2.6
1	A	209	THR	2.6
1	A	170	LEU	2.6
1	A	242	LEU	2.6
1	E	338	TYR	2.6
1	A	517	CYS	2.6
1	E	416	THR	2.6
1	E	113	VAL	2.6
2	F	11	VAL	2.6
1	E	244	THR	2.6
1	A	232	HIS	2.6
1	E	240	GLY	2.6
1	E	417	ALA	2.6
1	A	455	MET	2.5
1	E	3	PHE	2.5
4	H	92	HIS	2.5
1	A	457	LEU	2.5
2	F	62	CYS	2.5
1	E	223	LEU	2.5
1	A	280	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
4	H	45	PRO	2.5
2	F	36	LEU	2.5
1	A	514	VAL	2.5
4	D	118	ILE	2.5
1	A	571	THR	2.5
1	E	547	PHE	2.5
2	F	146	SER	2.5
1	A	356	TYR	2.5
2	B	193	ALA	2.4
2	B	118	PRO	2.4
4	D	84	HIS	2.4
2	B	66	GLY	2.4
3	G	126	VAL	2.4
1	E	381	SER	2.4
1	E	131	THR	2.4
1	A	171	VAL	2.4
1	A	231	TYR	2.4
1	E	157	VAL	2.4
1	A	191	ALA	2.4
2	B	20	ALA	2.4
2	F	212	GLU	2.4
4	D	12	VAL	2.4
1	A	196	GLY	2.4
2	F	172	ALA	2.4
1	A	226	MET	2.4
4	H	107	LEU	2.4
4	H	98	TRP	2.4
2	B	3	MET	2.4
1	E	11	GLY	2.3
1	A	370	ARG	2.3
3	G	24	PHE	2.3
1	A	347	PRO	2.3
1	A	450	LYS	2.3
4	H	117	THR	2.3
1	A	129	ASP	2.3
1	A	208	VAL	2.3
1	A	305	SER	2.3
2	B	199	ASN	2.3
1	A	270	PRO	2.3
2	B	159	PRO	2.3
3	G	54	GLU	2.3
3	G	66	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	56	ALA	2.3
1	E	429	ALA	2.3
2	B	175	LEU	2.3
1	E	137	HIS	2.3
1	A	116	PHE	2.3
2	F	26	TYR	2.3
4	D	9	ASP	2.3
1	A	75	TRP	2.2
2	F	28	VAL	2.2
1	A	49	GLU	2.2
1	A	207	ILE	2.2
3	G	6	PRO	2.2
2	F	155	TYR	2.2
1	E	393	SER	2.2
2	B	64	SER	2.2
1	E	394	ASN	2.2
1	E	362	GLU	2.2
1	A	448	TRP	2.2
1	A	504	TYR	2.2
2	F	179	TYR	2.2
1	E	112	ASN	2.2
1	E	50	GLY	2.2
2	B	1	ALA	2.2
1	E	171	VAL	2.2
1	E	545	VAL	2.2
2	F	102	LEU	2.2
3	G	19	LEU	2.2
1	A	293	ALA	2.2
1	A	447	ASN	2.2
1	A	90	PRO	2.2
1	A	559	GLY	2.2
1	E	360	GLY	2.2
1	A	287	ARG	2.2
4	H	100	PHE	2.2
1	A	172	ALA	2.1
2	F	196	ASN	2.1
1	A	330	PHE	2.1
1	A	303	THR	2.1
3	G	7	TYR	2.1
1	E	48	ALA	2.1
1	A	228	PHE	2.1
1	E	474	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	153	LEU	2.1
2	B	165	PRO	2.1
1	E	140	PHE	2.1
1	E	568	VAL	2.1
1	A	295	TRP	2.1
1	E	478	LYS	2.1
1	E	549	LYS	2.1
2	F	173	ILE	2.1
3	C	96	ILE	2.1
1	E	212	GLY	2.1
1	A	250	GLU	2.1
2	B	44	LYS	2.1
1	A	114	ARG	2.1
1	A	262	TYR	2.1
2	B	115	ALA	2.1
1	A	476	ILE	2.0
1	A	555	ARG	2.0
1	E	354	ALA	2.0
4	D	117	THR	2.0
1	E	408	GLU	2.0
1	A	452	ARG	2.0
3	G	27	LEU	2.0
1	E	183	ILE	2.0
1	E	356	TYR	2.0
1	E	411	THR	2.0
4	D	28	ALA	2.0
1	E	565	TYR	2.0
4	D	101	TYR	2.0
1	A	288	ASP	2.0
1	A	169	GLY	2.0
1	E	206	GLY	2.0
1	E	359	GLY	2.0
4	D	29	PRO	2.0
1	A	383	VAL	2.0
2	F	8	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

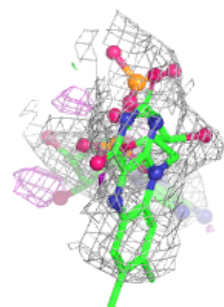
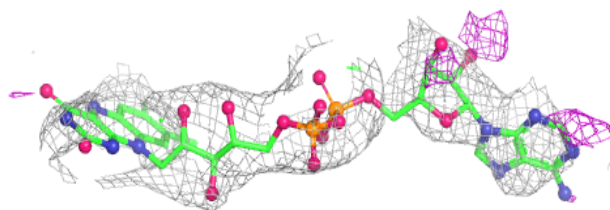
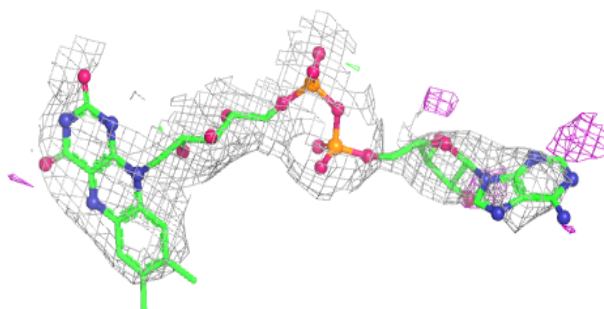
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	PO4	E	702	5/5	0.47	0.24	205,205,206,207	0
5	FAD	A	701	53/53	0.83	0.15	85,91,97,104	0
6	PO4	A	702	5/5	0.84	0.45	172,173,175,176	0
5	FAD	E	701	53/53	0.88	0.11	84,97,113,119	0
7	FES	F	301	4/4	0.96	0.08	77,79,82,83	0
9	SF4	F	303	8/8	0.97	0.05	60,69,91,121	0
8	F3S	B	302	7/7	0.98	0.07	56,58,93,162	0
8	F3S	F	302	7/7	0.98	0.06	55,63,100,119	0
9	SF4	B	303	8/8	0.98	0.06	56,71,88,138	0
7	FES	B	301	4/4	0.98	0.11	68,71,76,115	0

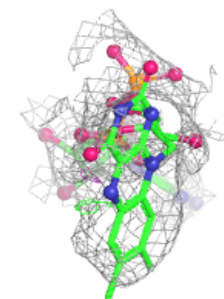
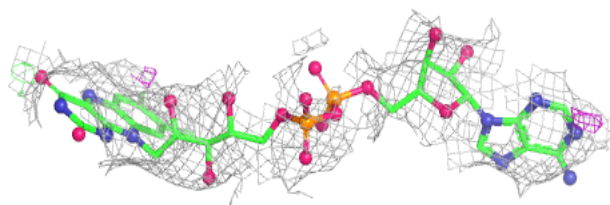
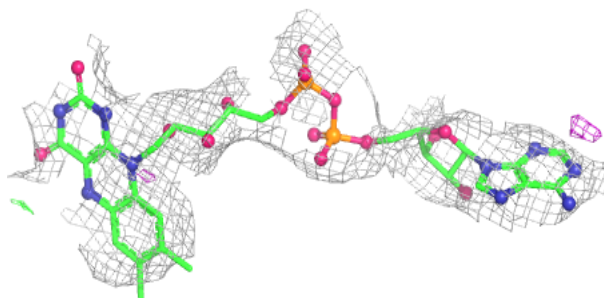
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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