Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 04:50 AM EDT

PDB ID	:	3P4Q
Title	:	Crystal structure of Menaquinol:oxidoreductase in complex with oxaloacetate
Authors	:	Tomasiak, T.M.; Archuleta, T.L.; Andrell, J.; Luna-Chavez, C.; Davis, T.A.; Sarwar, M.; Ham, A.J.; McDonald, W.H.; Yankowskaya, V.; Stern, H.A.; Johnston, J.N.; Maklashina, E.; Cecchini, G.; Iverson, T.M.
Deposited on	:	2010-10-06
Resolution	:	3.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (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:

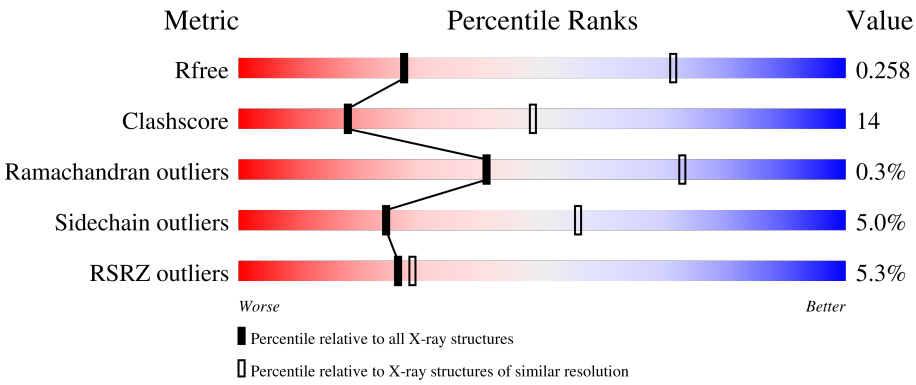
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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	577	77% 22% •
1	M	577	15% 63% 34% •
2	B	243	71% 28% •
2	N	243	8% 72% 27% •

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Mol	Chain	Length	Quality of chain
3	C	130	75% 23%
3	O	130	2% 85% 14%
4	D	119	% 76% 24%
4	P	119	77% 23%

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	OAA	M	802	-	-	-	X
8	F3S	B	245	-	-	X	-
8	F3S	N	246	-	-	X	-
9	SF4	B	246	-	-	X	-
9	SF4	N	244	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 16804 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fumarate reductase flavoprotein subunit.

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

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

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

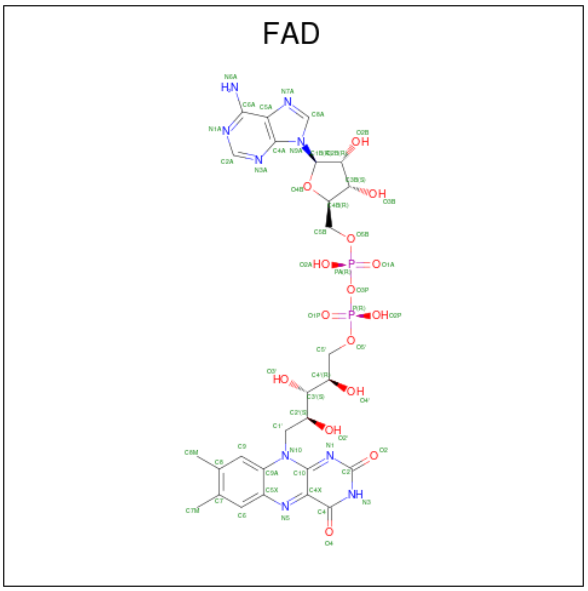
- Molecule 3 is a protein called Fumarate reductase subunit C.

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

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

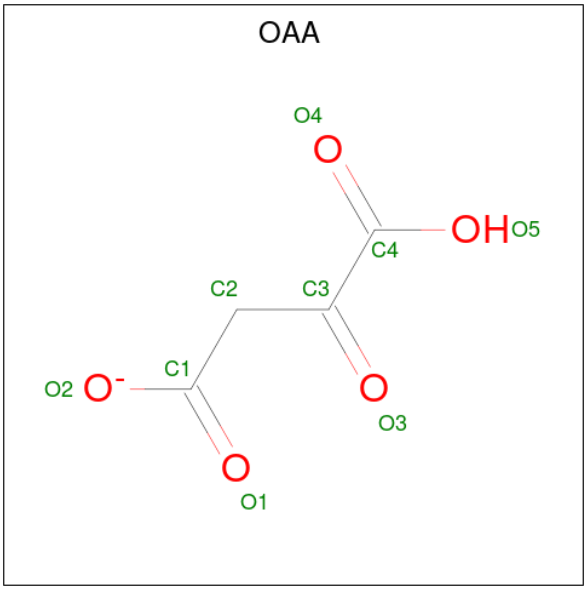
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	119	926	626	151	142	7	0	0	0
4	P	119	926	626	151	142	7	0	0	0

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



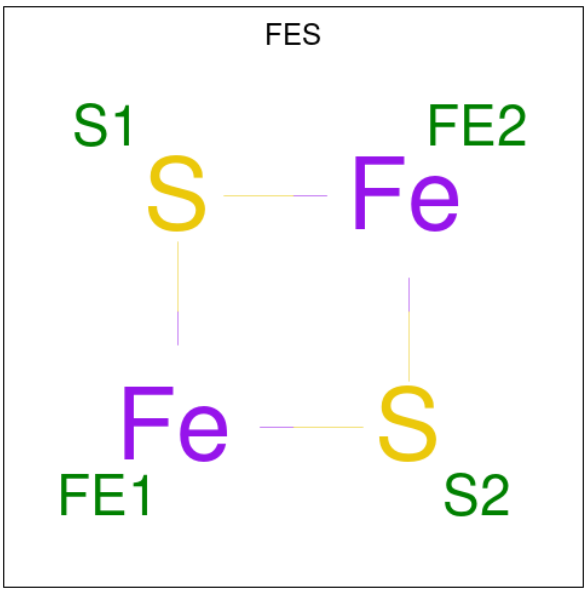
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
5	A	1	53	27	9	15	2	0	0
			Total	C	N	O	P		
5	M	1	53	27	9	15	2	0	0

- Molecule 6 is OXALOACETATE ION (three-letter code: OAA) (formula: $C_4H_3O_5$).



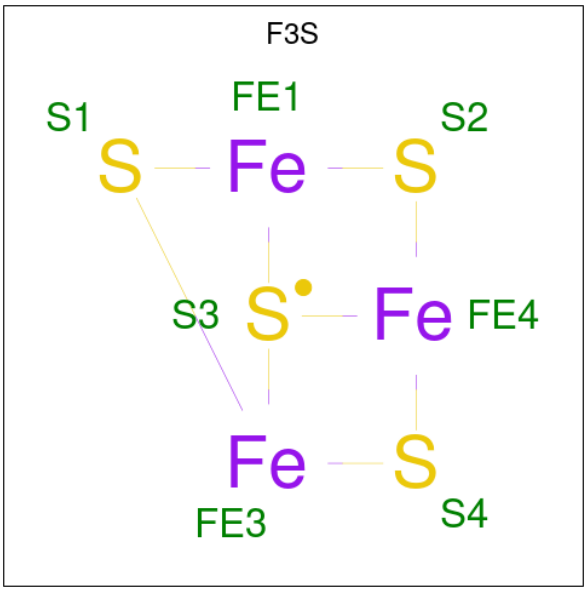
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
6	A	1	9	4	5	0	0
			Total	C	O		
6	M	1	9	4	5	0	0

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



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
7	B	1	4	2	2	0	0
7	N	1	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
			Total	Fe	S		
8	B	1	7	3	4	0	0

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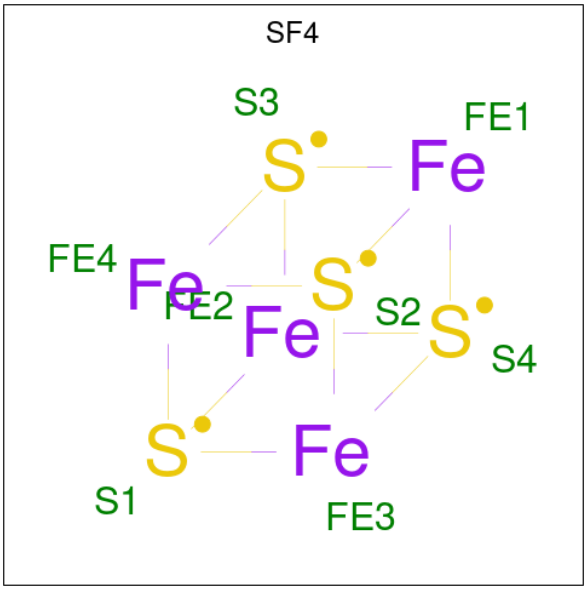
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
8	N	1	7	3	4	0	0

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



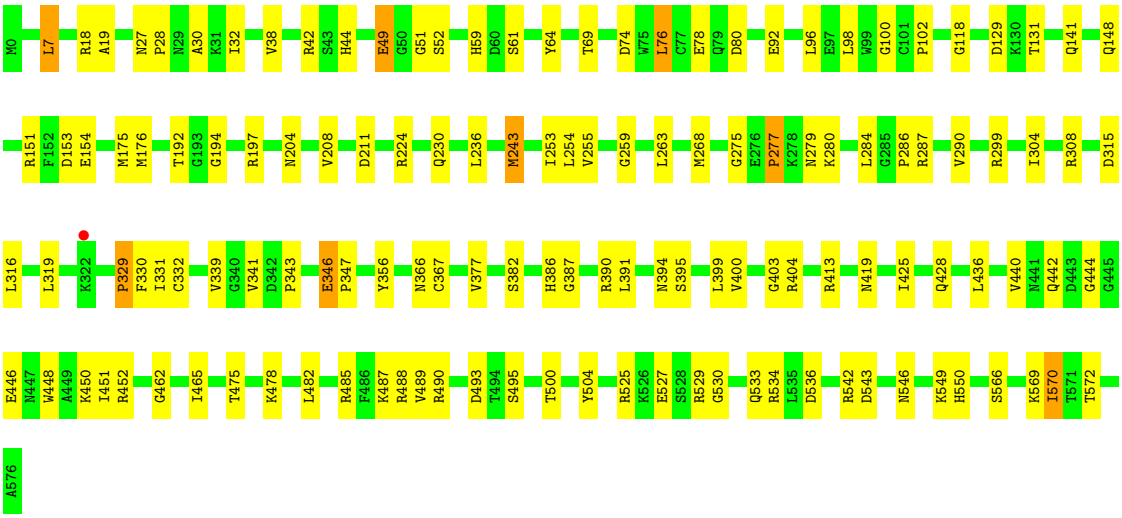
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Fe	S		
9	B	1	8	4	4	0	0
9	N	1	8	4	4	0	0

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.

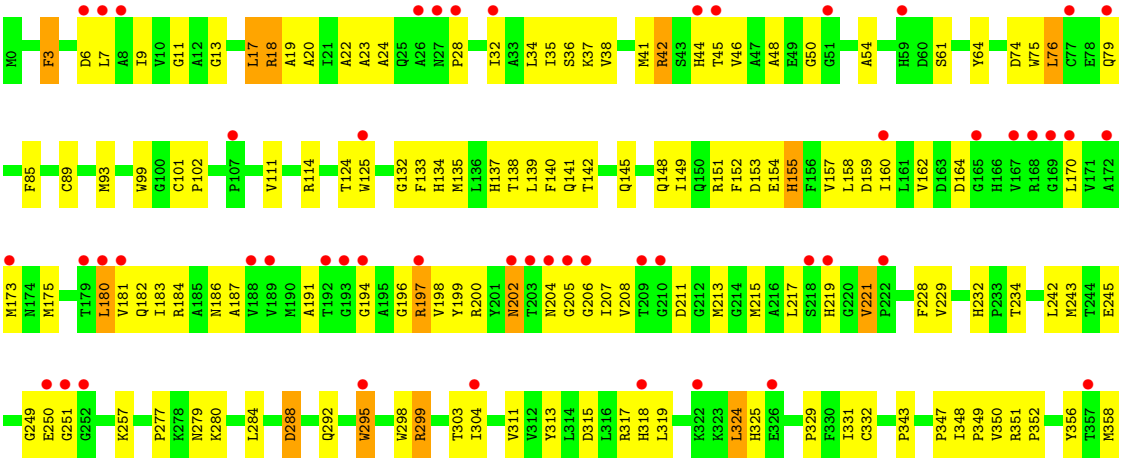
• Molecule 1: Fumarate reductase flavoprotein subunit

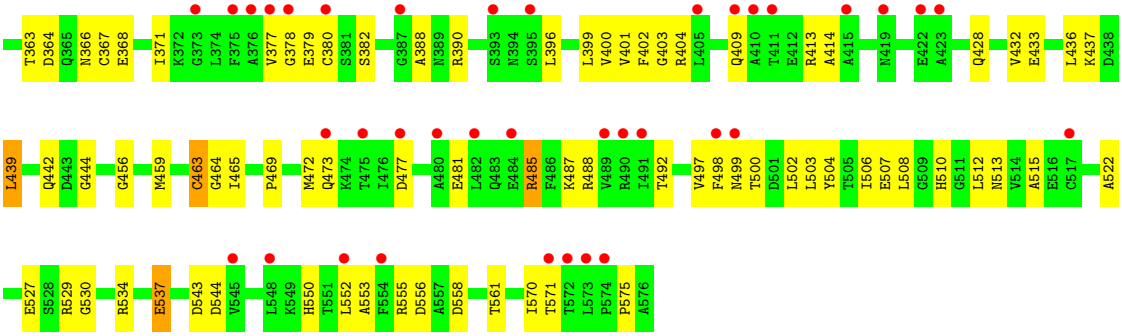
Chain A:



• Molecule 1: Fumarate reductase flavoprotein subunit

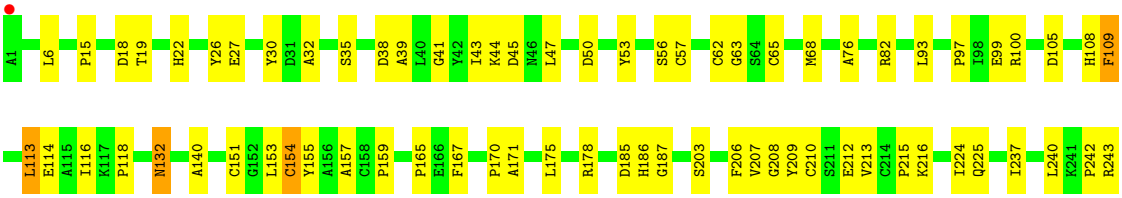
Chain M:





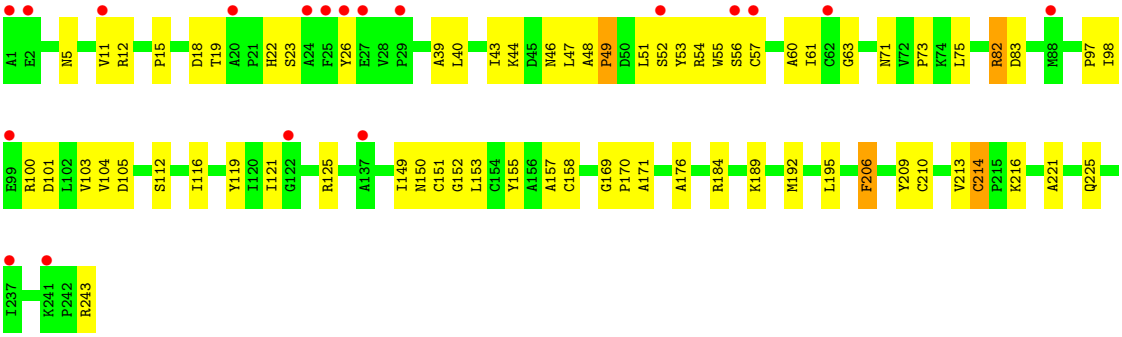
- Molecule 2: Fumarate reductase iron-sulfur protein

Chain B:



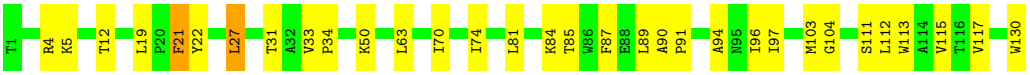
- Molecule 2: Fumarate reductase iron-sulfur protein

Chain N:



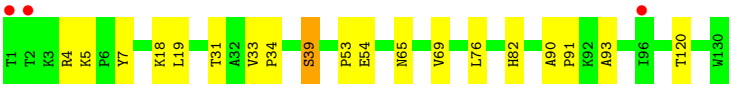
- Molecule 3: Fumarate reductase subunit C

Chain C:



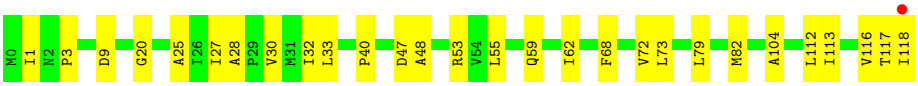
- Molecule 3: Fumarate reductase subunit C

Chain O:



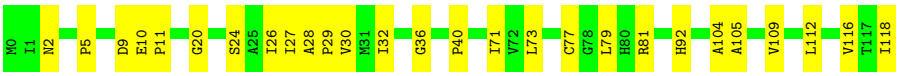
• Molecule 4: Fumarate reductase subunit D

Chain D:



• Molecule 4: Fumarate reductase subunit D

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	96.64Å 137.96Å 272.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.57 – 3.35 47.58 – 3.35	Depositor EDS
% Data completeness (in resolution range)	89.2 (47.57-3.35) 89.0 (47.58-3.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.72 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.220 , 0.261 0.219 , 0.258	Depositor DCC
R_{free} test set	1036 reflections (1.95%)	wwPDB-VP
Wilson B-factor (Å^2)	66.7	Xtriage
Anisotropy	0.365	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 33.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	16804	wwPDB-VP
Average B, all atoms (Å^2)	95.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

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

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	0.37	0/4541	0.52	0/6139
1	M	0.34	0/4541	0.56	0/6139
2	B	0.36	0/1931	0.53	0/2617
2	N	0.33	0/1931	0.51	0/2617
3	C	0.34	0/1094	0.49	0/1496
3	O	0.35	0/1094	0.45	0/1496
4	D	0.38	0/956	0.53	0/1303
4	P	0.34	0/956	0.48	0/1303
All	All	0.35	0/17044	0.52	0/23110

There are no bond length outliers.

There are no bond angle outliers.

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	4449	0	4335	101	0
1	M	4449	0	4333	180	0
2	B	1888	0	1840	63	0
2	N	1888	0	1838	64	0
3	C	1058	0	1108	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	O	1058	0	1108	16	0
4	D	926	0	971	19	0
4	P	926	0	971	17	0
5	A	53	0	31	10	0
5	M	53	0	31	20	0
6	A	9	0	2	0	0
6	M	9	0	2	2	0
7	B	4	0	0	0	0
7	N	4	0	0	1	0
8	B	7	0	0	2	0
8	N	7	0	0	3	0
9	B	8	0	0	7	0
9	N	8	0	0	2	0
All	All	16804	0	16570	451	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 14.

All (451) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:HIS:NE2	5:A:601:FAD:HM82	1.42	1.34
2:N:11:VAL:HA	2:N:23:SER:OG	1.20	1.24
1:M:37:LYS:HE3	5:M:601:FAD:C8A	1.75	1.17
2:N:54:ARG:HH21	2:N:103:VAL:HG12	1.06	1.15
1:A:44:HIS:NE2	5:A:601:FAD:C8M	2.17	1.06
1:M:37:LYS:CE	5:M:601:FAD:C8A	2.34	1.05
2:B:154:CYS:SG	9:B:246:SF4:FE3	1.51	1.00
1:M:37:LYS:HE2	5:M:601:FAD:N7A	1.77	1.00
1:M:48:ALA:HB3	1:M:132:GLY:HA3	1.43	0.96
2:N:11:VAL:CA	2:N:23:SER:OG	2.15	0.93
2:N:54:ARG:HH21	2:N:103:VAL:CG1	1.83	0.91
4:D:55:LEU:HG	4:D:59:GLN:HE21	1.36	0.91
1:M:197:ARG:HD2	1:M:197:ARG:C	1.88	0.91
2:N:11:VAL:HA	2:N:23:SER:HG	1.35	0.90
2:N:54:ARG:NH2	2:N:103:VAL:HG12	1.86	0.89
1:M:37:LYS:CE	5:M:601:FAD:N7A	2.36	0.87
2:B:154:CYS:HG	9:B:246:SF4:FE3	0.87	0.87
1:M:250:GLU:O	1:M:319:LEU:HD11	1.73	0.87
2:B:154:CYS:SG	9:B:246:SF4:S2	2.74	0.86
1:M:527:GLU:OE2	1:M:529:ARG:NH1	2.08	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:GLU:HA	1:A:129:ASP:O	1.76	0.85
3:O:31:THR:HG21	3:O:82:HIS:HB2	1.59	0.84
1:M:377:VAL:HG21	1:M:403:GLY:HA2	1.59	0.84
2:N:26:TYR:HB3	2:N:47:LEU:HD13	1.58	0.84
1:A:500:THR:HB	1:A:504:TYR:CE1	2.15	0.82
1:M:497:VAL:HG21	3:O:4:ARG:HB3	1.61	0.82
2:B:242:PRO:HB2	4:P:92:HIS:HB3	1.62	0.82
2:B:212:GLU:HG3	3:C:21:PHE:HE2	1.46	0.81
1:M:36:SER:HA	5:M:601:FAD:N3A	1.94	0.81
1:M:61:SER:HB3	1:M:64:TYR:HD1	1.43	0.80
1:M:197:ARG:HD2	1:M:197:ARG:O	1.82	0.80
2:N:18:ASP:CG	2:N:22:HIS:HE2	1.86	0.79
2:N:43:ILE:HD13	2:N:47:LEU:HD12	1.64	0.77
3:C:103:MET:HG2	3:C:104:GLY:H	1.50	0.77
1:M:199:TYR:CD2	1:M:459:MET:HB3	2.19	0.77
2:N:116:ILE:CG2	2:N:176:ALA:HB2	2.15	0.76
3:C:50:LYS:HZ2	4:D:117:THR:HG22	1.51	0.75
1:M:570:ILE:HG21	1:M:575:PRO:HD3	1.66	0.75
2:B:154:CYS:HB2	2:B:170:PRO:HG2	1.68	0.75
2:B:151:CYS:SG	9:B:246:SF4:FE1	1.80	0.74
1:M:215:MET:HB3	1:M:510:HIS:CE1	2.23	0.74
2:N:116:ILE:HG21	2:N:176:ALA:HB2	1.69	0.73
1:A:197:ARG:HB2	1:A:208:VAL:O	1.89	0.73
1:A:546:ASN:O	1:A:549:LYS:HE2	1.88	0.73
1:M:377:VAL:HG23	1:M:402:PHE:O	1.89	0.72
2:B:15:PRO:HB3	3:C:5:LYS:H	1.54	0.71
1:M:37:LYS:HE3	5:M:601:FAD:H8A	1.68	0.71
1:A:49:GLU:CA	1:A:129:ASP:O	2.38	0.70
1:M:251:GLY:HA2	1:M:277:PRO:HG2	1.72	0.70
1:M:556:ASP:HB2	1:M:558:ASP:OD1	1.91	0.70
2:B:57:CYS:HB3	2:B:62:CYS:HB3	1.73	0.70
1:M:194:GLY:O	1:M:208:VAL:HG12	1.91	0.70
3:C:33:VAL:HA	4:D:82:MET:HE2	1.74	0.70
2:N:51:LEU:HD23	2:N:52:SER:N	2.07	0.70
1:A:341:VAL:HG13	1:A:346:GLU:HB3	1.74	0.70
2:B:151:CYS:HG	9:B:246:SF4:FE1	1.07	0.70
2:N:210:CYS:SG	2:N:221:ALA:HB2	2.32	0.69
2:B:155:TYR:HE1	2:B:171:ALA:HB3	1.58	0.69
1:M:152:PHE:HB3	1:M:155:HIS:NE2	2.07	0.69
2:B:132:ASN:HD22	2:B:132:ASN:H	1.40	0.69
4:D:55:LEU:HG	4:D:59:GLN:NE2	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:18:ASP:OD2	2:B:22:HIS:CD2	2.46	0.69
2:N:214:CYS:SG	9:N:244:SF4:FE3	1.85	0.69
1:A:346:GLU:HG3	1:A:347:PRO:HD2	1.75	0.68
3:C:103:MET:HG2	3:C:104:GLY:N	2.08	0.68
1:A:570:ILE:HD13	1:A:570:ILE:H	1.58	0.68
1:M:24:ALA:HB2	1:M:32:ILE:HD11	1.76	0.68
1:M:245:GLU:HB2	6:M:802:OAA:O5	1.94	0.68
1:A:98:LEU:HD23	2:B:132:ASN:HD21	1.58	0.67
2:N:40:LEU:HB3	2:N:53:TYR:CE2	2.30	0.66
1:M:211:ASP:OD2	1:M:507:GLU:HG2	1.95	0.66
2:B:65:CYS:HB3	2:B:76:ALA:H	1.60	0.66
4:P:10:GLU:N	4:P:11:PRO:HD2	2.10	0.66
3:C:19:LEU:HB2	3:C:22:TYR:CD2	2.31	0.65
1:M:205:GLY:HA3	2:N:56:SER:O	1.95	0.65
2:B:206:PHE:HE2	3:C:89:LEU:HD22	1.62	0.65
2:B:18:ASP:OD2	2:B:22:HIS:NE2	2.29	0.65
1:A:275:GLY:O	1:A:277:PRO:HD3	1.97	0.65
3:O:33:VAL:HB	3:O:34:PRO:HD3	1.79	0.64
1:M:137:HIS:HD2	1:M:141:GLN:HE21	1.45	0.64
3:C:33:VAL:HA	4:D:82:MET:CE	2.28	0.64
1:M:299:ARG:HE	1:M:299:ARG:HA	1.63	0.64
1:M:197:ARG:O	1:M:197:ARG:CD	2.46	0.63
1:A:243:MET:HA	1:A:243:MET:HE2	1.79	0.63
1:M:292:GLN:HG2	1:M:465:ILE:HG21	1.80	0.63
1:M:472:MET:HE1	1:M:522:ALA:HB1	1.81	0.63
1:M:444:GLY:HA3	1:M:488:ARG:O	1.98	0.63
9:B:246:SF4:FE3	9:B:246:SF4:S2	1.90	0.63
4:P:79:LEU:HD12	4:P:104:ALA:HB2	1.80	0.62
2:N:54:ARG:HE	2:N:103:VAL:HG13	1.63	0.62
2:N:151:CYS:SG	2:N:153:LEU:HD12	2.40	0.62
1:M:215:MET:HB3	1:M:510:HIS:HE1	1.64	0.62
1:A:308:ARG:HH12	1:A:339:VAL:HA	1.64	0.62
2:N:51:LEU:HD23	2:N:52:SER:H	1.63	0.62
1:M:204:ASN:OD1	5:M:601:FAD:HM83	1.99	0.62
2:B:97:PRO:HG2	2:B:105:ASP:HB3	1.82	0.61
1:A:49:GLU:CB	1:A:129:ASP:O	2.49	0.61
2:B:212:GLU:HG3	3:C:21:PHE:CE2	2.33	0.61
2:N:192:MET:HA	2:N:195:LEU:HD22	1.82	0.61
4:P:105:ALA:O	4:P:109:VAL:HG23	2.01	0.61
2:N:60:ALA:HA	7:N:245:FES:S1	2.40	0.61
1:M:433:GLU:O	1:M:437:LYS:HB2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:THR:HA	1:A:391:LEU:HD22	1.82	0.61
1:M:211:ASP:OD1	1:M:507:GLU:HA	2.00	0.61
1:M:304:ILE:HG21	1:M:313:TYR:CE1	2.35	0.60
1:M:28:PRO:O	1:M:148:GLN:HG2	2.01	0.60
1:M:37:LYS:HE2	5:M:601:FAD:C5A	2.30	0.60
1:A:44:HIS:CE1	5:A:601:FAD:HM82	2.31	0.60
1:M:37:LYS:HE2	5:M:601:FAD:C8A	2.16	0.60
1:M:217:LEU:HD23	1:M:555:ARG:N	2.17	0.60
1:M:18:ARG:NH1	1:M:404:ARG:HA	2.17	0.59
2:B:167:PHE:CD1	2:B:203:SER:HB2	2.37	0.59
2:N:71:ASN:HB3	3:O:18:LYS:HE2	1.85	0.59
1:M:137:HIS:HD2	1:M:141:GLN:NE2	2.01	0.59
1:A:386:HIS:ND1	1:A:390:ARG:HG3	2.17	0.59
1:M:35:ILE:HG13	1:M:155:HIS:HB2	1.84	0.59
1:A:462:GLY:HA3	1:A:475:THR:OG1	2.03	0.58
1:A:197:ARG:HG3	1:A:208:VAL:O	2.03	0.58
1:M:20:ALA:HB2	1:M:34:LEU:HD12	1.85	0.58
1:M:114:ARG:O	1:M:124:THR:HB	2.02	0.58
1:M:234:THR:HG22	1:M:350:VAL:HG11	1.85	0.58
1:A:390:ARG:HD2	1:A:395:SER:HB2	1.84	0.58
1:M:48:ALA:HB3	1:M:132:GLY:CA	2.26	0.58
1:M:50:GLY:HA3	5:M:601:FAD:O4	2.03	0.58
1:M:61:SER:HB3	1:M:64:TYR:CD1	2.33	0.58
1:A:263:LEU:O	1:A:268:MET:HB2	2.04	0.57
1:M:44:HIS:CE1	1:M:204:ASN:HA	2.40	0.57
1:M:298:TRP:HA	1:M:303:THR:HG23	1.85	0.57
2:N:97:PRO:HA	3:O:7:TYR:O	2.04	0.57
1:M:358:MET:HG2	1:M:390:ARG:HB2	1.87	0.57
1:M:180:LEU:H	1:M:180:LEU:HD22	1.69	0.57
1:M:158:LEU:HD13	1:M:436:LEU:HG	1.85	0.57
1:M:219:HIS:NE2	1:M:371:ILE:HG12	2.20	0.56
3:C:113:TRP:O	3:C:117:VAL:HG23	2.05	0.56
1:M:162:VAL:HG21	1:M:219:HIS:HE1	1.69	0.56
2:N:54:ARG:NH2	2:N:103:VAL:CG1	2.58	0.56
2:N:155:TYR:HE1	2:N:171:ALA:HB3	1.69	0.56
1:A:356:TYR:HE1	5:A:601:FAD:O3'	1.89	0.56
4:D:20:GLY:HA2	4:D:73:LEU:HB3	1.88	0.56
2:N:151:CYS:SG	2:N:152:GLY:N	2.78	0.56
2:B:170:PRO:HA	2:B:224:ILE:HD11	1.88	0.56
4:D:1:ILE:O	4:D:3:PRO:HD3	2.05	0.56
1:M:41:MET:HB2	1:M:137:HIS:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:225:GLN:HE21	3:O:93:ALA:HB2	1.71	0.56
2:B:108:HIS:CE1	2:B:165:PRO:O	2.60	0.55
1:A:51:GLY:HA2	1:A:131:THR:HG21	1.87	0.55
4:P:2:ASN:O	4:P:5:PRO:HD3	2.05	0.55
1:A:386:HIS:CE1	1:A:390:ARG:HG3	2.42	0.55
1:M:217:LEU:HD23	1:M:555:ARG:H	1.71	0.55
1:M:18:ARG:HH12	1:M:22:ALA:HB2	1.70	0.55
1:M:37:LYS:HD2	1:M:207:ILE:HB	1.88	0.55
1:M:245:GLU:CB	6:M:802:OAA:O5	2.55	0.55
2:N:51:LEU:HD22	2:N:53:TYR:CD2	2.42	0.55
1:A:61:SER:HB3	1:A:64:TYR:CD2	2.42	0.54
2:B:35:SER:O	2:B:38:ASP:HB2	2.08	0.54
3:C:87:PHE:HE2	4:D:25:ALA:HB1	1.72	0.54
1:M:23:ALA:HB1	1:M:32:ILE:HG21	1.89	0.54
1:M:41:MET:HG2	1:M:42:ARG:HE	1.71	0.54
1:A:243:MET:HA	1:A:243:MET:CE	2.37	0.54
3:C:87:PHE:CE1	3:C:112:LEU:HB3	2.43	0.54
1:M:50:GLY:CA	5:M:601:FAD:O4	2.56	0.54
2:N:98:ILE:HB	3:O:7:TYR:HB3	1.90	0.54
1:M:199:TYR:CE2	1:M:459:MET:HB3	2.43	0.54
3:C:33:VAL:HB	3:C:34:PRO:HD3	1.90	0.53
1:M:54:ALA:HB3	1:M:125:TRP:NE1	2.24	0.53
1:M:221:VAL:HG22	1:M:371:ILE:HD13	1.90	0.53
3:C:130:TRP:HB2	4:D:53:ARG:HH21	1.74	0.53
1:M:36:SER:HA	5:M:601:FAD:C2A	2.39	0.53
2:N:63:GLY:O	2:N:151:CYS:HA	2.09	0.53
2:N:73:PRO:HG2	2:N:213:VAL:HG11	1.91	0.53
1:A:192:THR:HA	5:A:601:FAD:O4B	2.09	0.53
1:A:446:GLU:HB2	1:A:488:ARG:O	2.09	0.53
1:M:331:ILE:HD12	1:M:331:ILE:H	1.73	0.53
1:A:204:ASN:N	1:A:204:ASN:HD22	2.05	0.53
2:B:154:CYS:SG	9:B:246:SF4:S4	3.06	0.53
1:M:152:PHE:HB3	1:M:155:HIS:CD2	2.44	0.53
3:O:90:ALA:N	3:O:91:PRO:HD2	2.24	0.52
2:B:185:ASP:OD1	2:B:187:GLY:N	2.31	0.52
2:B:159:PRO:HG3	3:C:22:TYR:CE1	2.45	0.52
3:C:27:LEU:HD13	3:C:81:LEU:HD21	1.92	0.52
2:B:39:ALA:O	2:B:43:ILE:HG12	2.10	0.52
1:M:151:ARG:NH1	1:M:153:ASP:OD1	2.35	0.52
2:N:44:LYS:HA	2:N:48:ALA:O	2.10	0.52
1:A:129:ASP:OD2	1:A:329:PRO:HD2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:37:LYS:HG3	1:M:38:VAL:H	1.75	0.52
1:A:18:ARG:HG2	1:A:400:VAL:HA	1.91	0.52
1:M:288:ASP:O	1:M:292:GLN:HG3	2.10	0.52
1:A:18:ARG:NH1	1:A:92:GLU:OE2	2.42	0.51
1:A:118:GLY:HA2	1:A:279:ASN:HD21	1.75	0.51
2:B:185:ASP:OD1	2:B:185:ASP:C	2.49	0.51
1:A:332:CYS:HA	1:A:343:PRO:HG3	1.91	0.51
4:D:27:ILE:O	4:D:27:ILE:HG22	2.10	0.51
1:A:446:GLU:HB2	1:A:489:VAL:HA	1.93	0.51
1:M:199:TYR:CE1	1:M:229:VAL:HG11	2.46	0.51
1:M:101:CYS:HB2	1:M:138:THR:HG21	1.93	0.50
1:A:80:ASP:OD2	1:A:569:LYS:HG2	2.12	0.50
2:B:65:CYS:CB	2:B:76:ALA:H	2.25	0.50
1:M:45:THR:HG23	5:M:601:FAD:H5'1	1.92	0.50
1:A:425:ILE:O	1:A:428:GLN:HB2	2.11	0.50
1:M:7:LEU:HB2	1:M:32:ILE:HG22	1.92	0.50
1:M:377:VAL:CG2	1:M:402:PHE:O	2.59	0.50
1:M:378:GLY:HA2	1:M:399:LEU:HD23	1.93	0.50
2:N:43:ILE:CD1	2:N:47:LEU:HD12	2.37	0.50
1:A:243:MET:HE2	1:A:331:ILE:HD12	1.93	0.50
1:M:46:VAL:CG2	1:M:133:PHE:HD1	2.25	0.50
1:M:553:ALA:HB1	1:M:561:THR:HG21	1.94	0.50
1:M:304:ILE:N	1:M:304:ILE:HD12	2.27	0.50
2:B:57:CYS:HB3	2:B:62:CYS:CB	2.40	0.50
1:A:448:TRP:CH2	1:A:504:TYR:HB3	2.46	0.50
1:M:35:ILE:HG12	5:M:601:FAD:H2A	1.93	0.50
1:A:525:ARG:NH1	1:A:527:GLU:OE2	2.44	0.49
1:M:481:GLU:HG2	1:M:485:ARG:HD3	1.93	0.49
2:N:54:ARG:NH2	2:N:104:VAL:O	2.45	0.49
1:A:27:ASN:OD1	1:A:30:ALA:N	2.43	0.49
3:C:19:LEU:HB2	3:C:22:TYR:HD2	1.77	0.49
1:M:213:MET:CE	1:M:380:CYS:HA	2.42	0.49
1:M:311:VAL:HG12	1:M:351:ARG:HB3	1.93	0.49
1:M:481:GLU:O	1:M:485:ARG:HD3	2.12	0.49
1:A:197:ARG:CB	1:A:208:VAL:O	2.60	0.49
2:B:185:ASP:OD1	2:B:186:HIS:N	2.46	0.49
1:M:211:ASP:O	1:M:510:HIS:ND1	2.43	0.49
4:P:112:LEU:O	4:P:116:VAL:HG22	2.12	0.49
1:A:230:GLN:HB3	1:A:356:TYR:HB3	1.95	0.49
1:M:553:ALA:HB1	1:M:561:THR:CG2	2.42	0.49
1:A:98:LEU:CD2	2:B:132:ASN:HD21	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ILE:HG13	1:A:315:ASP:HB3	1.94	0.49
1:M:199:TYR:HE2	1:M:459:MET:O	1.96	0.49
2:N:19:THR:HA	3:O:5:LYS:NZ	2.28	0.49
1:A:395:SER:HB3	5:A:601:FAD:N1	2.27	0.49
1:A:504:TYR:CE1	2:B:44:LYS:HE2	2.48	0.49
2:N:82:ARG:HD2	2:N:83:ASP:OD1	2.13	0.49
1:A:504:TYR:CD1	2:B:44:LYS:HE2	2.48	0.49
1:M:469:PRO:HG3	1:M:534:ARG:HH21	1.78	0.49
1:M:537:GLU:H	1:M:537:GLU:CD	2.16	0.49
3:C:85:THR:O	3:C:89:LEU:HG	2.13	0.48
3:O:39:SER:OG	4:P:71:ILE:O	2.31	0.48
4:D:48:ALA:O	4:D:53:ARG:HD3	2.14	0.48
1:A:49:GLU:HB3	1:A:129:ASP:O	2.12	0.48
2:N:18:ASP:OD2	2:N:22:HIS:NE2	2.41	0.48
2:B:206:PHE:CD1	2:B:225:GLN:HG3	2.48	0.48
1:M:197:ARG:O	1:M:197:ARG:CG	2.61	0.48
1:M:459:MET:O	1:M:463:CYS:O	2.32	0.48
1:M:37:LYS:O	1:M:154:GLU:HA	2.13	0.48
1:M:11:GLY:HA3	1:M:191:ALA:O	2.14	0.48
4:P:36:GLY:O	4:P:40:PRO:HG3	2.14	0.48
2:B:65:CYS:HB3	2:B:76:ALA:HB3	1.95	0.48
1:M:299:ARG:HE	1:M:299:ARG:CA	2.27	0.48
2:B:113:LEU:HD23	2:B:175:LEU:HD23	1.96	0.48
2:N:18:ASP:CG	2:N:22:HIS:NE2	2.62	0.48
1:A:550:HIS:HB2	1:A:566:SER:OG	2.14	0.47
4:D:68:PHE:CE1	4:D:72:VAL:HG21	2.50	0.47
1:M:37:LYS:O	1:M:175:MET:SD	2.72	0.47
1:M:363:THR:HB	1:M:367:CYS:HA	1.95	0.47
1:A:304:ILE:HD12	1:A:304:ILE:H	1.79	0.47
4:D:79:LEU:HD12	4:D:104:ALA:HB2	1.96	0.47
1:M:157:VAL:H	5:M:601:FAD:H62A	1.62	0.47
1:M:279:ASN:O	1:M:280:LYS:HB2	2.14	0.47
2:B:132:ASN:HD22	2:B:132:ASN:N	2.11	0.47
1:M:377:VAL:HG22	1:M:378:GLY:N	2.29	0.47
2:N:26:TYR:HB3	2:N:47:LEU:CD1	2.37	0.47
1:A:197:ARG:CG	1:A:208:VAL:O	2.62	0.47
2:N:158:CYS:CA	8:N:246:F3S:S4	3.03	0.47
1:A:7:LEU:CD2	1:A:32:ILE:HG12	2.45	0.47
1:A:391:LEU:O	1:A:394:ASN:HB2	2.14	0.47
1:M:313:TYR:HD2	1:M:347:PRO:HG2	1.78	0.47
1:A:452:ARG:NH2	2:B:45:ASP:OD2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:130:TRP:OXT	4:D:53:ARG:NE	2.48	0.47
1:M:500:THR:HB	1:M:504:TYR:CE1	2.49	0.47
2:N:158:CYS:HA	8:N:246:F3S:S4	2.55	0.47
1:A:176:MET:CG	3:C:4:ARG:HH11	2.27	0.47
1:M:196:GLY:HA3	1:M:204:ASN:HD22	1.79	0.47
1:A:436:LEU:O	1:A:440:VAL:HG23	2.14	0.47
1:M:18:ARG:HH12	1:M:404:ARG:HA	1.81	0.46
2:N:214:CYS:HG	9:N:244:SF4:FE3	1.32	0.46
2:B:63:GLY:O	2:B:151:CYS:HA	2.16	0.46
4:D:112:LEU:O	4:D:116:VAL:HG22	2.15	0.46
2:B:175:LEU:HD12	2:B:175:LEU:HA	1.60	0.46
1:A:96:LEU:HD11	1:A:400:VAL:HG11	1.97	0.46
1:M:17:LEU:C	1:M:17:LEU:HD22	2.35	0.46
1:M:158:LEU:HD21	1:M:506:ILE:HD13	1.96	0.46
1:M:503:LEU:HA	1:M:506:ILE:HD12	1.97	0.46
1:A:286:PRO:O	1:A:290:VAL:HG23	2.16	0.46
1:A:451:ILE:HG23	1:A:482:LEU:HD22	1.97	0.46
1:M:79:GLN:HB2	1:M:571:THR:HG23	1.97	0.46
3:O:76:LEU:HD13	4:P:32:ILE:HB	1.97	0.46
2:B:207:VAL:HG23	8:B:245:F3S:S2	2.55	0.46
1:M:473:GLN:NE2	1:M:477:ASP:OD1	2.48	0.46
1:M:217:LEU:HD12	1:M:221:VAL:O	2.15	0.46
1:M:311:VAL:HG21	1:M:349:PRO:HB3	1.98	0.46
3:C:111:SER:O	3:C:115:VAL:HG23	2.16	0.46
1:M:17:LEU:HA	1:M:34:LEU:HD11	1.97	0.46
1:A:194:GLY:O	1:A:208:VAL:HG13	2.16	0.46
1:M:162:VAL:CG2	1:M:219:HIS:HE1	2.29	0.46
1:M:388:ALA:HB1	1:M:530:GLY:HA3	1.97	0.46
1:M:506:ILE:O	1:M:510:HIS:HD2	1.99	0.46
2:B:210:CYS:O	2:B:213:VAL:HG22	2.16	0.46
1:M:85:PHE:HD1	1:M:402:PHE:CE2	2.33	0.46
1:A:534:ARG:HH21	1:A:536:ASP:CG	2.20	0.45
1:A:527:GLU:OE2	1:A:529:ARG:NH1	2.49	0.45
1:M:37:LYS:HG2	5:M:601:FAD:O2B	2.16	0.45
1:M:366:ASN:HB3	1:M:409:GLN:HG3	1.98	0.45
4:P:77:CYS:O	4:P:81:ARG:HG3	2.16	0.45
1:A:76:LEU:O	1:A:387:GLY:HA2	2.15	0.45
1:A:450:LYS:HA	1:A:450:LYS:HD3	1.75	0.45
2:B:154:CYS:HB2	2:B:170:PRO:CG	2.42	0.45
2:B:50:ASP:O	2:B:100:ARG:NH2	2.49	0.45
3:C:90:ALA:N	3:C:91:PRO:CD	2.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:ALA:O	2:B:82:ARG:NH1	2.49	0.45
1:M:257:LYS:HA	1:M:304:ILE:HD11	1.98	0.45
1:M:232:HIS:O	1:M:352:PRO:HA	2.16	0.45
4:P:9:ASP:OD1	4:P:9:ASP:N	2.50	0.45
1:A:330:PHE:HE1	2:B:216:LYS:HZ2	1.62	0.45
1:M:99:TRP:CD1	1:M:142:THR:HG21	2.52	0.45
1:M:436:LEU:HA	1:M:439:LEU:HB2	1.99	0.45
2:N:112:SER:O	2:N:116:ILE:HG12	2.17	0.45
1:A:44:HIS:NE2	5:A:601:FAD:HM81	2.21	0.45
1:M:213:MET:HE3	1:M:380:CYS:HA	1.99	0.45
3:O:7:TYR:CD1	3:O:7:TYR:C	2.90	0.45
2:B:153:LEU:HD12	2:B:215:PRO:HD3	1.98	0.44
2:B:6:LEU:HB2	2:B:30:TYR:CE2	2.51	0.44
1:M:159:ASP:OD2	1:M:160:ILE:N	2.50	0.44
2:N:75:LEU:HG	2:N:153:LEU:HD11	1.98	0.44
1:A:211:ASP:CB	5:A:601:FAD:H61A	2.30	0.44
1:M:219:HIS:CD2	1:M:219:HIS:C	2.90	0.44
1:M:298:TRP:HA	1:M:303:THR:CG2	2.47	0.44
4:P:28:ALA:N	4:P:29:PRO:HD2	2.32	0.44
1:M:508:LEU:O	1:M:512:LEU:HG	2.17	0.44
1:A:478:LYS:HA	1:A:478:LYS:HD2	1.86	0.44
1:M:356:TYR:CZ	1:M:379:GLU:HG3	2.52	0.44
1:A:28:PRO:HA	1:A:148:GLN:HE21	1.83	0.44
1:A:255:VAL:HB	1:A:259:GLY:HA2	2.00	0.44
1:A:570:ILE:HD13	1:A:570:ILE:N	2.30	0.44
2:N:15:PRO:HD3	2:N:100:ARG:HG2	1.99	0.44
1:M:498:PHE:O	2:N:100:ARG:NH2	2.50	0.44
1:M:206:GLY:N	2:N:55:TRP:CZ3	2.86	0.43
1:A:377:VAL:HG21	1:A:403:GLY:HA2	2.00	0.43
1:A:543:ASP:OD2	1:A:546:ASN:ND2	2.51	0.43
2:B:157:ALA:HB1	2:B:209:TYR:CD2	2.53	0.43
1:M:79:GLN:NE2	1:M:571:THR:H	2.15	0.43
1:A:366:ASN:O	1:A:367:CYS:HB2	2.18	0.43
1:M:46:VAL:HG23	1:M:133:PHE:HD1	1.82	0.43
2:B:68:MET:HG2	2:B:93:LEU:HA	1.99	0.43
2:B:132:ASN:H	2:B:132:ASN:ND2	2.13	0.43
1:M:492:THR:CG2	2:N:49:PRO:HG2	2.49	0.43
1:A:399:LEU:HD11	5:A:601:FAD:H4'	2.00	0.43
1:M:315:ASP:OD1	1:M:317:ARG:HG2	2.19	0.43
1:M:428:GLN:O	1:M:432:VAL:HG23	2.17	0.43
4:P:10:GLU:N	4:P:11:PRO:CD	2.80	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:TYR:CE2	1:A:390:ARG:HD3	2.54	0.43
1:M:200:ARG:HB2	1:M:456:GLY:HA3	2.01	0.43
1:M:295:TRP:CD1	1:M:295:TRP:C	2.91	0.43
1:M:364:ASP:OD1	1:M:368:GLU:N	2.52	0.43
2:N:12:ARG:NE	2:N:101:ASP:OD2	2.48	0.43
1:A:154:GLU:O	1:A:175:MET:HB2	2.18	0.43
1:A:230:GLN:NE2	1:A:287:ARG:NH1	2.67	0.43
4:D:30:VAL:O	4:D:33:LEU:HB3	2.18	0.43
1:M:186:ASN:CB	1:M:414:ALA:HA	2.49	0.43
1:M:228:PHE:CZ	1:M:388:ALA:HA	2.53	0.43
4:P:26:ILE:HB	4:P:27:ILE:HD12	2.01	0.43
3:C:87:PHE:CE2	4:D:25:ALA:HB1	2.54	0.43
1:M:42:ARG:NH2	2:N:150:ASN:O	2.52	0.43
1:M:75:TRP:CD1	1:M:575:PRO:HA	2.54	0.43
1:M:292:GLN:HG2	1:M:465:ILE:CG2	2.46	0.43
1:M:7:LEU:CD2	1:M:187:ALA:HB3	2.49	0.43
2:N:157:ALA:HB1	2:N:209:TYR:CD2	2.54	0.43
1:M:442:GLN:NE2	1:M:487:LYS:HD3	2.34	0.42
1:M:324:LEU:HG	1:M:325:HIS:CE1	2.54	0.42
1:A:236:LEU:HD21	1:A:243:MET:SD	2.59	0.42
2:N:149:ILE:HG23	2:N:216:LYS:HG3	1.99	0.42
3:O:65:ASN:O	3:O:69:VAL:HG23	2.19	0.42
1:A:204:ASN:N	1:A:204:ASN:ND2	2.67	0.42
1:A:493:ASP:OD1	1:A:495:SER:OG	2.32	0.42
1:M:32:ILE:HG13	1:M:149:ILE:HA	2.01	0.42
1:A:279:ASN:O	1:A:280:LYS:HB2	2.20	0.42
1:M:242:LEU:HD22	5:M:601:FAD:H6	2.02	0.42
1:M:249:GLY:HA2	1:M:284:LEU:HD11	2.01	0.42
2:N:149:ILE:CG2	2:N:216:LYS:HG3	2.50	0.42
1:M:135:MET:HE1	1:M:396:LEU:HB3	2.01	0.42
1:M:196:GLY:HA3	1:M:204:ASN:ND2	2.34	0.42
1:A:529:ARG:HB2	1:A:542:ARG:HG3	2.02	0.42
1:M:9:ILE:HG21	1:M:19:ALA:HB3	2.00	0.42
2:N:46:ASN:HD22	2:N:46:ASN:N	2.17	0.42
1:A:18:ARG:HH12	1:A:404:ARG:HH11	1.68	0.42
1:A:100:GLY:O	1:A:102:PRO:HD3	2.18	0.42
1:A:224:ARG:NH2	1:A:382:SER:O	2.53	0.42
1:A:254:LEU:HD12	1:A:263:LEU:HD11	2.02	0.42
3:C:31:THR:O	3:C:34:PRO:HD2	2.20	0.42
1:M:17:LEU:HD11	1:M:139:LEU:CB	2.49	0.42
1:M:76:LEU:O	1:M:550:HIS:NE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:464:GLY:O	1:M:465:ILE:C	2.58	0.42
1:M:537:GLU:CD	1:M:537:GLU:N	2.73	0.42
1:M:17:LEU:HD21	1:M:139:LEU:HB3	2.02	0.42
1:A:92:GLU:OE1	1:A:404:ARG:HD2	2.20	0.41
1:A:151:ARG:NH1	1:A:153:ASP:OD2	2.54	0.41
1:A:316:LEU:O	1:A:319:LEU:HB2	2.20	0.41
1:M:492:THR:HG23	2:N:49:PRO:HG2	2.01	0.41
1:M:513:ASN:HB3	1:M:555:ARG:HD2	2.02	0.41
2:N:51:LEU:HD22	2:N:53:TYR:HD2	1.82	0.41
2:B:57:CYS:HB3	2:B:62:CYS:SG	2.58	0.41
3:C:94:ALA:HB1	3:C:96:ILE:HD11	2.02	0.41
1:M:428:GLN:O	1:M:432:VAL:N	2.54	0.41
1:A:19:ALA:HA	1:A:403:GLY:O	2.20	0.41
1:A:49:GLU:H	1:A:49:GLU:HG2	1.75	0.41
1:A:442:GLN:NE2	1:A:487:LYS:C	2.74	0.41
1:M:332:CYS:SG	1:M:343:PRO:HG3	2.61	0.41
2:B:240:LEU:O	2:B:242:PRO:HD3	2.20	0.41
1:M:102:PRO:HG2	1:M:134:HIS:CD2	2.56	0.41
2:N:206:PHE:HA	8:N:246:F3S:S1	2.60	0.41
1:A:59:HIS:CD2	1:A:59:HIS:H	2.37	0.41
2:B:109:PHE:C	2:B:109:PHE:CD2	2.93	0.41
2:B:208:GLY:N	8:B:245:F3S:S1	2.90	0.41
1:M:3:PHE:HB3	1:M:183:ILE:HG23	2.02	0.41
1:M:37:LYS:N	5:M:601:FAD:N3A	2.69	0.41
1:M:183:ILE:HG22	1:M:184:ARG:N	2.35	0.41
1:A:141:GLN:HB3	2:B:118:PRO:O	2.21	0.41
3:C:87:PHE:O	3:C:91:PRO:HD3	2.20	0.41
1:M:76:LEU:HD22	1:M:76:LEU:HA	1.91	0.41
1:M:85:PHE:HB2	1:M:402:PHE:HE2	1.86	0.41
1:M:499:ASN:HA	2:N:100:ARG:HH22	1.85	0.41
2:B:15:PRO:HG3	2:B:99:GLU:O	2.21	0.41
1:M:13:GLY:HA3	5:M:601:FAD:O1P	2.20	0.41
1:M:79:GLN:OE1	1:M:570:ILE:HG23	2.21	0.41
1:A:151:ARG:NH2	2:B:114:GLU:OE2	2.54	0.41
1:M:145:GLN:HE21	2:N:119:TYR:HB2	1.85	0.41
1:M:181:VAL:HG12	1:M:182:GLN:N	2.36	0.41
1:M:198:VAL:HG11	1:M:515:ALA:HB2	2.03	0.41
5:M:601:FAD:H9	5:M:601:FAD:H1'1	1.81	0.41
2:N:39:ALA:O	2:N:43:ILE:HG12	2.21	0.41
4:P:20:GLY:HA2	4:P:73:LEU:HB3	2.03	0.41
4:P:24:SER:O	4:P:28:ALA:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:GLY:HA2	2:B:53:TYR:OH	2.21	0.41
2:N:57:CYS:SG	2:N:61:ILE:HG22	2.61	0.41
2:N:97:PRO:HG2	2:N:105:ASP:HB3	2.02	0.41
1:A:530:GLY:O	1:A:533:GLN:NE2	2.53	0.40
2:B:26:TYR:HD2	2:B:47:LEU:HD12	1.85	0.40
1:M:400:VAL:HG23	1:M:401:VAL:HG23	2.02	0.40
1:A:78:GLU:OE1	1:A:569:LYS:HB3	2.21	0.40
5:A:601:FAD:H9	5:A:601:FAD:H1'1	1.88	0.40
4:D:28:ALA:O	4:D:32:ILE:HG13	2.21	0.40
1:M:42:ARG:HA	1:M:42:ARG:HD3	1.72	0.40
1:M:324:LEU:HG	1:M:325:HIS:ND1	2.37	0.40
2:N:155:TYR:CE2	2:N:169:GLY:HA3	2.56	0.40
1:A:176:MET:HG2	3:C:4:ARG:HH11	1.85	0.40
2:B:140:ALA:HB1	3:C:97:ILE:HD12	2.04	0.40
2:B:206:PHE:CE1	2:B:225:GLN:HG3	2.57	0.40
1:M:202:ASN:HD22	1:M:202:ASN:N	2.18	0.40
3:O:90:ALA:N	3:O:91:PRO:CD	2.84	0.40
3:C:63:LEU:HB2	4:D:40:PRO:HB3	2.03	0.40
3:C:70:ILE:O	3:C:74:ILE:HG13	2.22	0.40
2:N:19:THR:HA	3:O:5:LYS:HZ3	1.86	0.40
3:O:120:THR:HG23	4:P:30:VAL:HB	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	575/577 (100%)	551 (96%)	21 (4%)	3 (0%)	29 63
1	M	575/577 (100%)	541 (94%)	33 (6%)	1 (0%)	47 78
2	B	241/243 (99%)	231 (96%)	9 (4%)	1 (0%)	34 68
2	N	241/243 (99%)	228 (95%)	11 (5%)	2 (1%)	19 53

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	128/130 (98%)	122 (95%)	6 (5%)	0	100	100
3	O	128/130 (98%)	123 (96%)	5 (4%)	0	100	100
4	D	117/119 (98%)	109 (93%)	8 (7%)	0	100	100
4	P	117/119 (98%)	115 (98%)	2 (2%)	0	100	100
All	All	2122/2138 (99%)	2020 (95%)	95 (4%)	7 (0%)	41	73

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	56	SER
1	A	329	PRO
1	A	444	GLY
2	N	170	PRO
1	A	277	PRO
1	M	329	PRO
2	N	49	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	460/460 (100%)	442 (96%)	18 (4%)	32	62
1	M	460/460 (100%)	424 (92%)	36 (8%)	12	40
2	B	205/205 (100%)	195 (95%)	10 (5%)	25	57
2	N	205/205 (100%)	196 (96%)	9 (4%)	28	59
3	C	111/111 (100%)	107 (96%)	4 (4%)	35	64
3	O	111/111 (100%)	107 (96%)	4 (4%)	35	64
4	D	97/97 (100%)	92 (95%)	5 (5%)	23	55
4	P	97/97 (100%)	96 (99%)	1 (1%)	76	87
All	All	1746/1746 (100%)	1659 (95%)	87 (5%)	24	56

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	38	VAL
1	A	42	ARG
1	A	49	GLU
1	A	52	SER
1	A	74	ASP
1	A	76	LEU
1	A	243	MET
1	A	284	LEU
1	A	299	ARG
1	A	346	GLU
1	A	413	ARG
1	A	419	ASN
1	A	465	ILE
1	A	485	ARG
1	A	490	ARG
1	A	570	ILE
1	A	572	THR
2	B	19	THR
2	B	27	GLU
2	B	109	PHE
2	B	113	LEU
2	B	116	ILE
2	B	132	ASN
2	B	154	CYS
2	B	178	ARG
2	B	237	ILE
2	B	243	ARG
3	C	12	THR
3	C	21	PHE
3	C	27	LEU
3	C	84	LYS
4	D	9	ASP
4	D	47	ASP
4	D	62	ILE
4	D	113	ILE
4	D	118	ILE
1	M	3	PHE
1	M	6	ASP
1	M	17	LEU
1	M	18	ARG
1	M	42	ARG
1	M	74	ASP

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Mol	Chain	Res	Type
1	M	76	LEU
1	M	89	CYS
1	M	93	MET
1	M	111	VAL
1	M	140	PHE
1	M	155	HIS
1	M	164	ASP
1	M	170	LEU
1	M	173	MET
1	M	180	LEU
1	M	197	ARG
1	M	202	ASN
1	M	221	VAL
1	M	243	MET
1	M	288	ASP
1	M	295	TRP
1	M	299	ARG
1	M	318	HIS
1	M	324	LEU
1	M	348	ILE
1	M	382	SER
1	M	413	ARG
1	M	439	LEU
1	M	463	CYS
1	M	485	ARG
1	M	502	LEU
1	M	537	GLU
1	M	543	ASP
1	M	544	ASP
1	M	552	LEU
2	N	5	ASN
2	N	82	ARG
2	N	121	ILE
2	N	125	ARG
2	N	184	ARG
2	N	189	LYS
2	N	206	PHE
2	N	214	CYS
2	N	243	ARG
3	O	19	LEU
3	O	39	SER
3	O	53	PRO

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

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

Mol	Chain	Res	Type
1	A	87	HIS
1	A	141	GLN
1	A	182	GLN
1	A	279	ASN
1	A	292	GLN
1	A	442	GLN
2	B	108	HIS
2	B	123	ASN
2	B	132	ASN
2	B	150	ASN
2	B	194	GLN
3	C	72	ASN
4	D	59	GLN
4	D	92	HIS
1	M	44	HIS
1	M	134	HIS
1	M	137	HIS
1	M	145	GLN
1	M	219	HIS
1	M	292	GLN
1	M	442	GLN
1	M	473	GLN
2	N	5	ASN
2	N	46	ASN
2	N	95	ASN
2	N	150	ASN
2	N	225	GLN
3	O	95	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	F3S	B	245	2	0,9,9	-	-	-		
5	FAD	M	601	-	54,58,58	2.12	7 (12%)	71,89,89	1.79	13 (18%)
9	SF4	N	244	2	0,12,12	-	-	-		
9	SF4	B	246	2	0,12,12	-	-	-		
5	FAD	A	601	-	54,58,58	1.03	4 (7%)	71,89,89	1.56	15 (21%)
7	FES	B	244	2	0,4,4	-	-	-		
6	OAA	A	702	-	8,8,8	2.25	3 (37%)	8,10,10	1.29	0
6	OAA	M	802	-	8,8,8	2.27	4 (50%)	8,10,10	1.42	1 (12%)
7	FES	N	245	2	0,4,4	-	-	-		
8	F3S	N	246	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
8	F3S	B	245	2	-	-	0/3/3/3
5	FAD	M	601	-	-	20/30/50/50	0/6/6/6
9	SF4	N	244	2	-	-	0/6/5/5
9	SF4	B	246	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FAD	A	601	-	-	4/30/50/50	0/6/6/6
7	FES	B	244	2	-	-	0/1/1/1
6	OAA	A	702	-	-	4/8/8/8	-
6	OAA	M	802	-	-	1/8/8/8	-
7	FES	N	245	2	-	-	0/1/1/1
8	F3S	N	246	2	-	-	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	M	601	FAD	O4B-C1B	8.80	1.52	1.40
5	M	601	FAD	C4A-N3A	6.74	1.44	1.35
5	M	601	FAD	C2A-N3A	-5.52	1.23	1.32
5	M	601	FAD	C2A-N1A	5.04	1.42	1.33
6	A	702	OAA	O3-C3	3.98	1.31	1.23
6	M	802	OAA	O3-C3	3.96	1.31	1.23
6	A	702	OAA	O4-C4	3.68	1.31	1.22
6	M	802	OAA	O4-C4	3.55	1.31	1.22
5	M	601	FAD	P-O3P	3.13	1.62	1.59
6	A	702	OAA	O1-C1	3.03	1.32	1.22
6	M	802	OAA	O1-C1	2.84	1.31	1.22
5	M	601	FAD	C4X-N5	2.81	1.36	1.30
5	A	601	FAD	C4X-N5	2.61	1.36	1.30
5	M	601	FAD	PA-O3P	2.61	1.62	1.59
5	A	601	FAD	C10-N10	2.49	1.42	1.37
5	A	601	FAD	O2B-C2B	-2.43	1.36	1.43
5	A	601	FAD	O3B-C3B	-2.30	1.37	1.43
6	M	802	OAA	C3-C4	-2.19	1.50	1.53

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	601	FAD	N3A-C2A-N1A	-6.58	119.74	128.67
5	A	601	FAD	N3A-C2A-N1A	-6.03	120.48	128.67
5	M	601	FAD	C4B-O4B-C1B	-5.88	104.54	109.92
5	M	601	FAD	C1B-N9A-C4A	-4.38	118.94	126.64
5	M	601	FAD	O4B-C1B-N9A	3.86	113.87	108.75
5	A	601	FAD	O4B-C1B-N9A	3.41	113.26	108.75
5	M	601	FAD	C4A-C5A-N7A	3.28	112.80	109.34
5	A	601	FAD	C1B-N9A-C4A	-3.19	121.04	126.64
5	A	601	FAD	C4-N3-C2	-3.05	120.23	125.64
5	M	601	FAD	C4X-C4-N3	2.90	120.63	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	601	FAD	C4-C4X-N5	2.83	122.11	118.21
5	M	601	FAD	C4-N3-C2	-2.83	120.62	125.64
5	A	601	FAD	C5X-N5-C4X	2.82	122.65	118.09
5	A	601	FAD	C4X-C4-N3	2.82	120.44	113.25
5	M	601	FAD	O4B-C4B-C5B	-2.71	100.67	109.33
6	M	802	OAA	O4-C4-C3	-2.65	118.52	121.81
5	A	601	FAD	O2B-C2B-C3B	-2.64	103.34	111.82
5	M	601	FAD	C9A-C5X-N5	-2.48	119.82	122.45
5	A	601	FAD	C4X-C10-N1	-2.44	118.60	124.59
5	A	601	FAD	C4A-C5A-N7A	-2.35	106.86	109.34
5	A	601	FAD	O4-C4-C4X	-2.33	120.38	126.53
5	A	601	FAD	C9A-C5X-N5	-2.30	120.01	122.45
5	M	601	FAD	O4-C4-C4X	-2.27	120.53	126.53
5	A	601	FAD	C10-C4X-N5	-2.26	120.19	124.81
5	A	601	FAD	C10-N1-C2	2.24	121.70	116.85
5	A	601	FAD	C4-C4X-N5	2.17	121.20	118.21
5	M	601	FAD	C10-C4X-N5	-2.15	120.42	124.81
5	M	601	FAD	C5X-N5-C4X	2.10	121.49	118.09
5	A	601	FAD	O3P-P-O1P	-2.10	104.39	110.70

There are no chirality outliers.

All (29) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
5	M	601	FAD	C3B-C4B-C5B-O5B
5	A	601	FAD	PA-O3P-P-O5'
6	A	702	OAA	C1-C2-C3-O3
6	A	702	OAA	O3-C3-C4-O4
6	A	702	OAA	C2-C3-C4-O4
5	M	601	FAD	C5'-O5'-P-O1P
5	M	601	FAD	C5'-O5'-P-O3P
5	M	601	FAD	PA-O3P-P-O1P
6	M	802	OAA	O1-C1-C2-C3
5	M	601	FAD	PA-O3P-P-O2P
5	A	601	FAD	PA-O3P-P-O2P

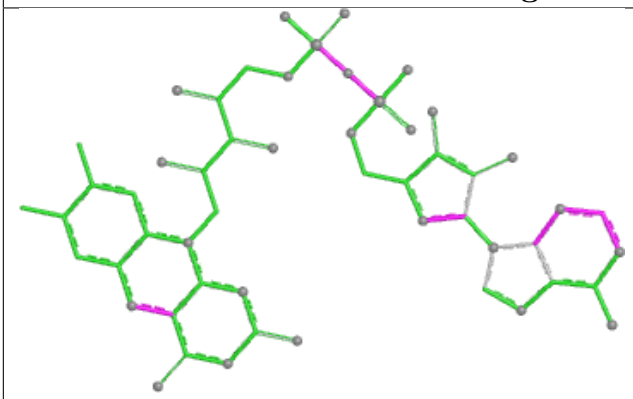
There are no ring outliers.

8 monomers are involved in 47 short contacts:

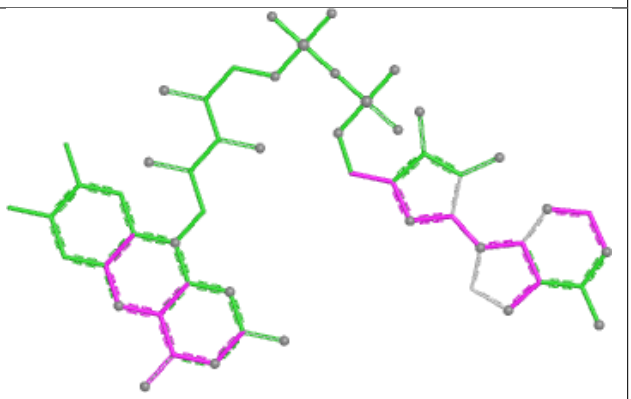
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	245	F3S	2	0
5	M	601	FAD	20	0
9	N	244	SF4	2	0
9	B	246	SF4	7	0
5	A	601	FAD	10	0
6	M	802	OAA	2	0
7	N	245	FES	1	0
8	N	246	F3S	3	0

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.

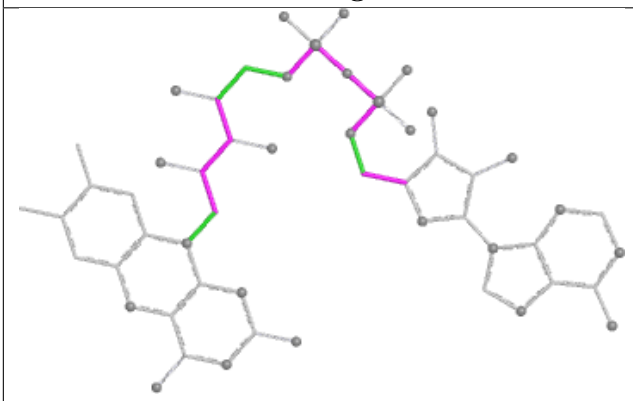
Ligand FAD M 601



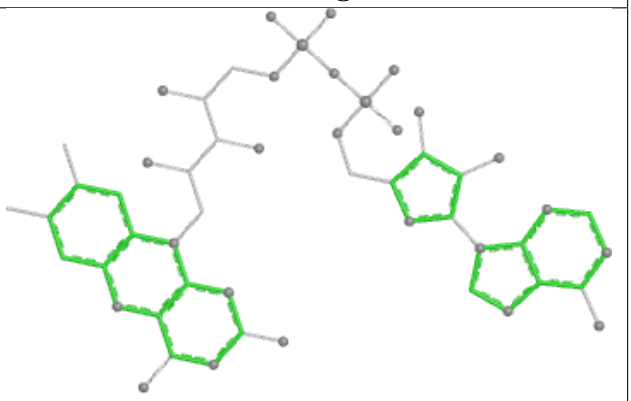
Bond lengths



Bond angles

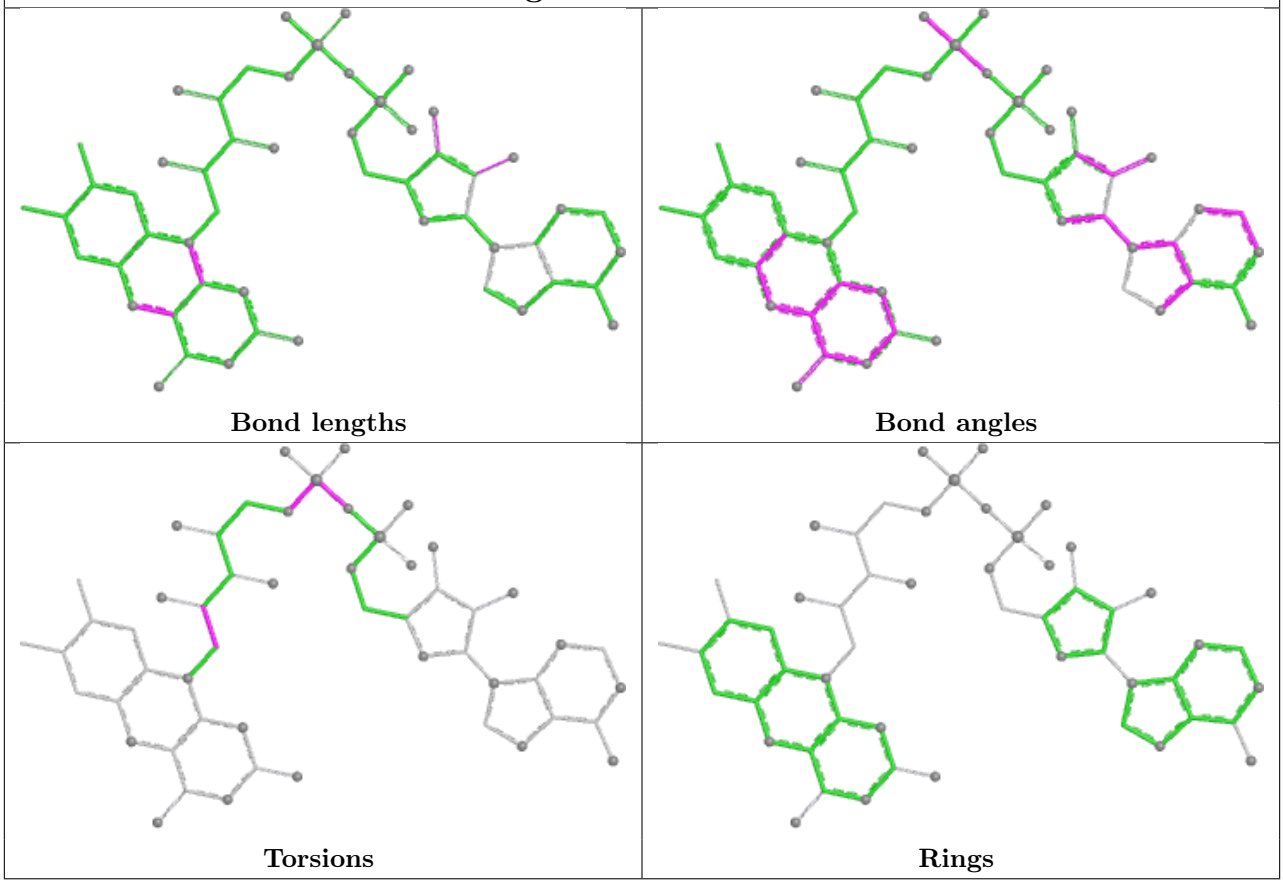


Torsions



Rings

Ligand FAD A 601



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	577/577 (100%)	-0.45	1 (0%) 95 97	29, 46, 91, 117	0
1	M	577/577 (100%)	0.89	88 (15%) 2 2	88, 155, 184, 215	0
2	B	243/243 (100%)	-0.41	1 (0%) 92 94	29, 51, 75, 133	0
2	N	243/243 (100%)	0.40	19 (7%) 13 15	76, 129, 206, 230	0
3	C	130/130 (100%)	-0.33	0 100 100	53, 69, 98, 108	0
3	O	130/130 (100%)	-0.09	3 (2%) 60 63	60, 93, 153, 194	0
4	D	119/119 (100%)	-0.40	1 (0%) 86 89	49, 65, 91, 108	0
4	P	119/119 (100%)	-0.30	0 100 100	57, 81, 139, 168	0
All	All	2138/2138 (100%)	0.05	113 (5%) 26 28	29, 80, 179, 230	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	172	ALA	7.3
1	M	188	VAL	6.8
1	M	411	THR	6.6
1	M	571	THR	6.1
1	M	206	GLY	5.5
1	M	573	LEU	5.3
1	M	7	LEU	5.3
1	M	572	THR	5.2
1	M	409	GLN	5.2
1	M	193	GLY	4.9
1	M	489	VAL	4.7
3	O	1	THR	4.6
1	M	205	GLY	4.4
1	M	192	THR	4.3
1	M	499	ASN	4.3
1	M	77	CYS	4.2

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Mol	Chain	Res	Type	RSRZ
1	M	189	VAL	4.2
1	M	373	GLY	4.1
2	N	1	ALA	4.1
1	M	545	VAL	4.0
1	M	179	THR	3.9
2	N	25	PHE	3.9
1	M	194	GLY	3.8
1	M	574	PRO	3.7
1	M	375	PHE	3.6
1	M	395	SER	3.5
2	N	26	TYR	3.5
3	O	96	ILE	3.5
1	M	380	CYS	3.4
1	M	204	ASN	3.4
1	M	357	THR	3.3
1	M	210	GLY	3.3
1	M	44	HIS	3.3
1	M	491	ILE	3.3
1	M	8	ALA	3.2
1	M	423	ALA	3.2
1	M	27	ASN	3.2
1	M	28	PRO	3.2
2	N	56	SER	3.2
2	N	2	GLU	3.2
1	M	387	GLY	3.2
2	N	52	SER	3.2
1	M	480	ALA	3.2
1	M	6	ASP	3.1
1	M	203	THR	3.1
1	M	322	LYS	3.1
2	N	57	CYS	3.1
1	M	393	SER	3.1
1	M	484	GLU	3.0
1	M	405	LEU	2.9
1	M	45	THR	2.9
2	N	241	LYS	2.9
1	M	475	THR	2.9
1	M	165	GLY	2.9
2	N	11	VAL	2.9
1	M	378	GLY	2.8
2	B	1	ALA	2.8
4	D	118	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	M	202	ASN	2.8
1	M	170	LEU	2.7
2	N	237	ILE	2.7
1	M	107	PRO	2.7
2	N	27	GLU	2.7
1	M	26	ALA	2.7
1	M	169	GLY	2.7
2	N	88	MET	2.7
2	N	20	ALA	2.7
1	M	167	VAL	2.6
1	M	79	GLN	2.6
1	M	181	VAL	2.6
1	M	498	PHE	2.6
1	M	219	HIS	2.5
1	M	477	ASP	2.5
2	N	29	PRO	2.5
1	M	548	LEU	2.5
1	M	422	GLU	2.5
2	N	24	ALA	2.5
1	M	222	PRO	2.4
1	M	218	SER	2.4
1	M	304	ILE	2.4
3	O	2	THR	2.4
1	M	197	ARG	2.4
1	M	482	LEU	2.4
2	N	62	CYS	2.3
1	M	32	ILE	2.3
1	M	318	HIS	2.3
1	M	554	PHE	2.3
1	M	168	ARG	2.3
1	M	252	GLY	2.2
1	M	250	GLU	2.2
1	M	160	ILE	2.2
2	N	99	GLU	2.2
1	M	376	ALA	2.2
1	M	419	ASN	2.2
1	M	180	LEU	2.2
2	N	122	GLY	2.2
1	M	173	MET	2.2
1	M	410	ALA	2.2
1	M	415	ALA	2.2
1	M	552	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	M	517	CYS	2.1
1	A	322	LYS	2.1
1	M	377	VAL	2.1
1	M	490	ARG	2.1
1	M	251	GLY	2.1
1	M	125	TRP	2.1
1	M	473	GLN	2.1
1	M	326	GLU	2.1
2	N	137	ALA	2.1
1	M	51	GLY	2.1
1	M	209	THR	2.1
1	M	295	TRP	2.0
1	M	59	HIS	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)

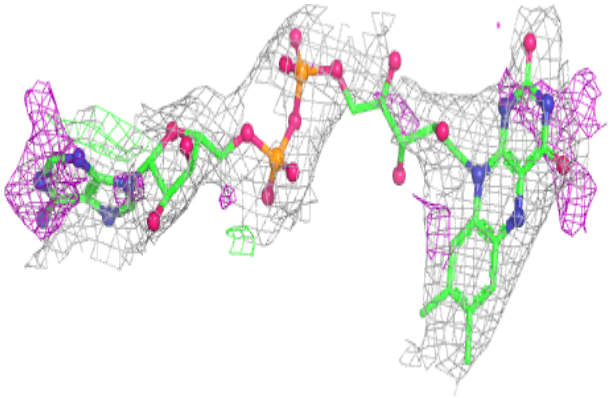
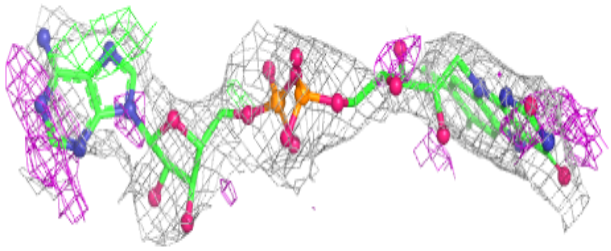
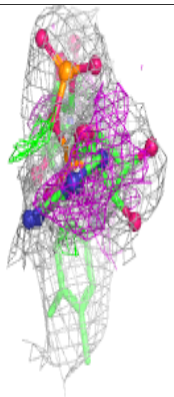
There are no monosaccharides in this entry.

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

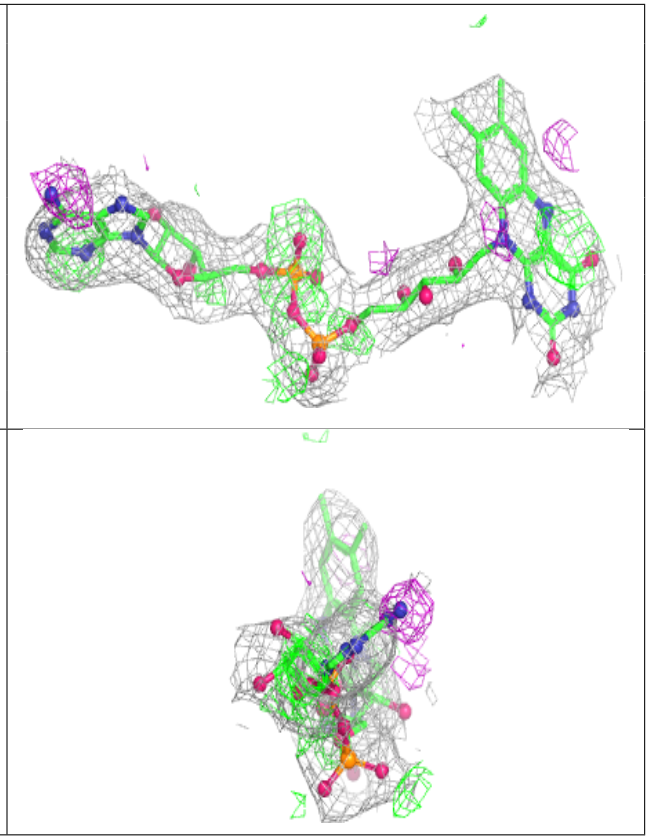
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	OAA	M	802	9/9	0.66	0.45	114,114,115,115	0
5	FAD	M	601	53/53	0.82	0.36	95,109,125,126	0
6	OAA	A	702	9/9	0.89	0.31	45,48,49,50	0
5	FAD	A	601	53/53	0.96	0.28	43,47,57,61	0
7	FES	N	245	4/4	0.98	0.18	88,88,89,90	0
8	F3S	N	246	7/7	0.98	0.14	75,75,76,76	0
9	SF4	B	246	8/8	0.98	0.20	63,65,66,66	0
9	SF4	N	244	8/8	0.98	0.16	82,82,83,83	0
8	F3S	B	245	7/7	1.00	0.14	45,47,47,47	0
7	FES	B	244	4/4	1.00	0.18	32,34,34,35	0

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

Electron density around FAD M 601: $2mF_o$-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 A 601:

$2mF_o$-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.