Full wwPDB X-ray Structure Validation Report (i)

Aug 23, 2023 – 10:33 AM EDT

PDB ID	:	3CN8
Title	:	Crystal structure of fms1 in complex with spermidine
Authors	:	Huang, Q.; Hao, Q.
Deposited on	:	2008-03-25
Resolution	:	2.40 Å(reported)

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

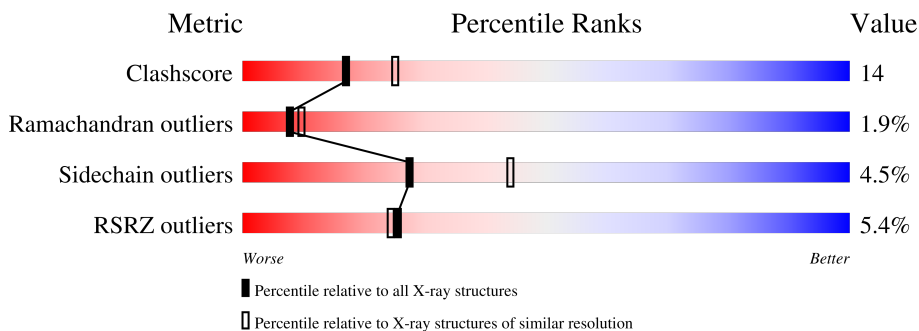|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 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 2.40 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	Percentile Ranks	Value
Clashscore		14
Ramachandran outliers		1.9%
Sidechain outliers		4.5%
RSRZ outliers		5.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	516	3% 73% 21% · ·
1	B	516	8% 64% 29% · ·

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
2	SPD	A	517	-	-	X	-

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 7956 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 Polyamine oxidase FMS1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	499	Total	C	N	O	S	0	0	0
			3845	2425	668	730	22			
1	A	494	Total	C	N	O	S	0	0	0
			3866	2446	674	724	22			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	509	LEU	-	expression tag	UNP P50264
B	510	GLU	-	expression tag	UNP P50264
B	511	HIS	-	expression tag	UNP P50264
B	512	HIS	-	expression tag	UNP P50264
B	513	HIS	-	expression tag	UNP P50264
B	514	HIS	-	expression tag	UNP P50264
B	515	HIS	-	expression tag	UNP P50264
B	516	HIS	-	expression tag	UNP P50264
A	509	LEU	-	expression tag	UNP P50264
A	510	GLU	-	expression tag	UNP P50264
A	511	HIS	-	expression tag	UNP P50264
A	512	HIS	-	expression tag	UNP P50264
A	513	HIS	-	expression tag	UNP P50264
A	514	HIS	-	expression tag	UNP P50264
A	515	HIS	-	expression tag	UNP P50264
A	516	HIS	-	expression tag	UNP P50264

- Molecule 2 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).

SPD
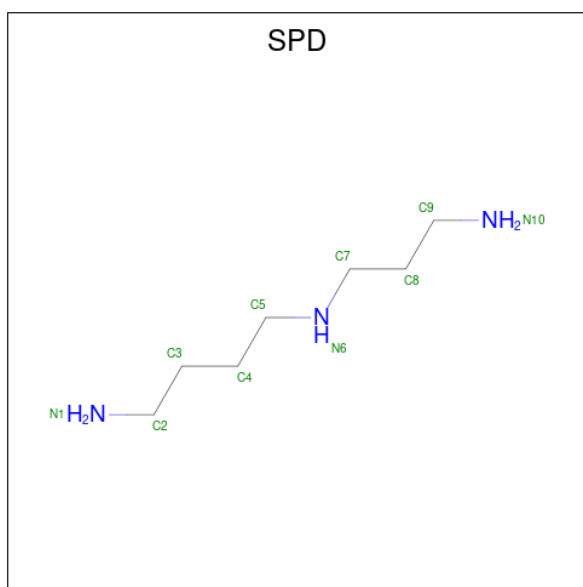
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total 10	C 7	N 3	0	0
2	A	1	Total 10	C 7	N 3	0	0

- Molecule 3 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).

FAD
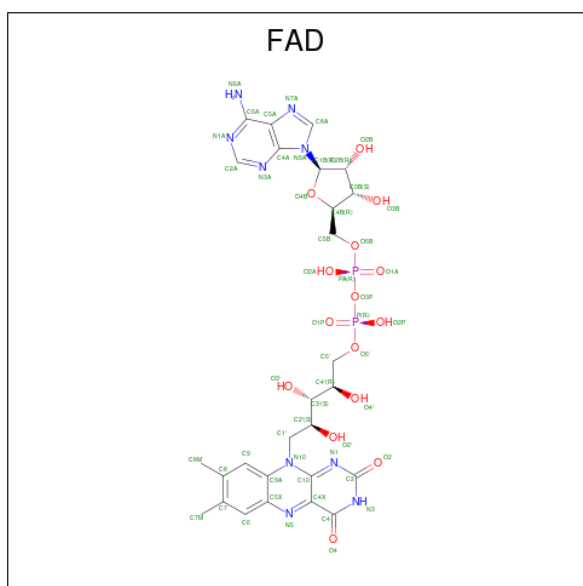
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total 53	C 27	N 9	O 15	P 2	0	0

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	56	Total 56	O 56	0	0
4	A	63	Total 63	O 63	0	0

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: Polyamine oxidase FMS1
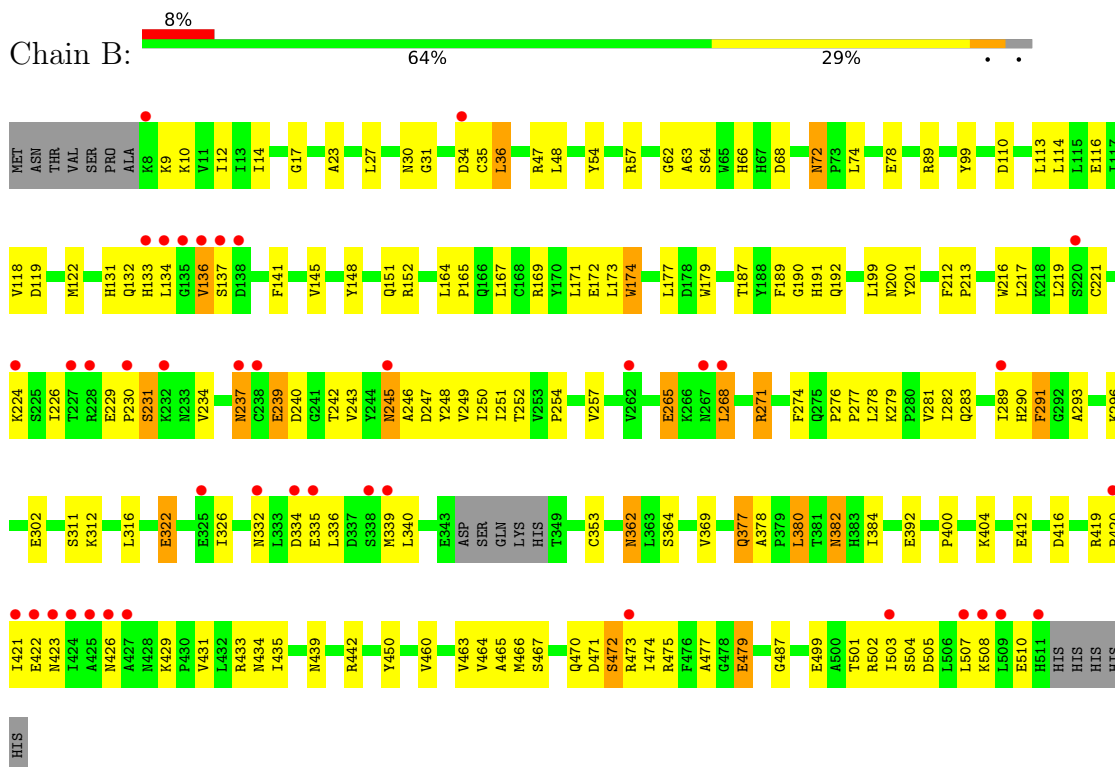
• Molecule 1: Polyamine oxidase FMS1
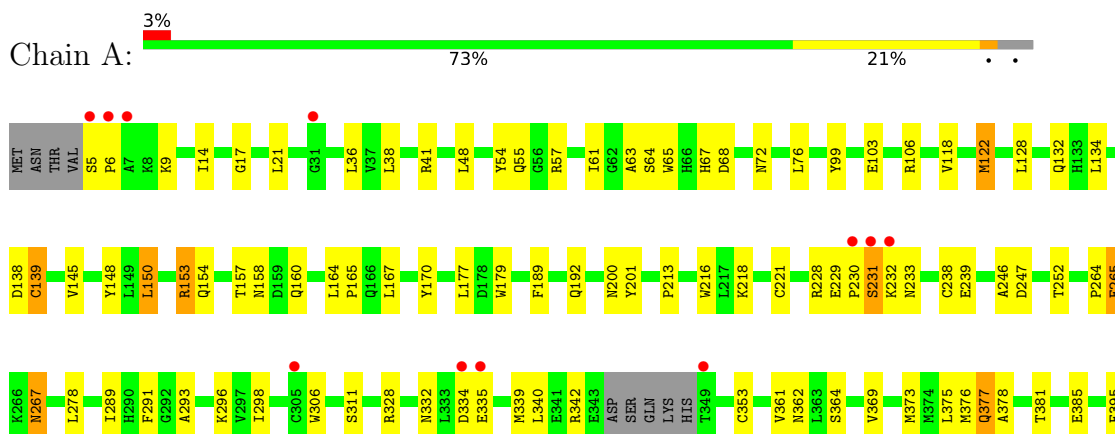
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	102.52Å 215.46Å 119.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 47.09 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.9 (50.00-2.40) 89.8 (47.09-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	3.10 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.226 , 0.272 0.225 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	42.4	Xtriage
Anisotropy	0.730	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 49.3	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7956	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: SPD, FAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.38	0/3945	0.61	1/5336 (0.0%)
1	B	0.36	0/3923	0.59	1/5310 (0.0%)
All	All	0.37	0/7868	0.60	2/10646 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	238	CYS	CA-CB-SG	5.33	123.60	114.00
1	B	66	HIS	N-CA-C	-5.28	96.75	111.00

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	3866	0	3730	80	1
1	B	3845	0	3642	132	0
2	A	10	0	19	8	0
2	B	10	0	19	2	0
3	A	53	0	31	3	0
3	B	53	0	31	3	0
4	A	63	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	56	0	0	0	0
All	All	7956	0	7472	214	1

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 (214) 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:B:332:ASN:HD21	1:B:334:ASP:HB2	1.28	0.98
1:A:353:CYS:SG	1:A:400:PRO:HG2	2.13	0.89
1:B:353:CYS:SG	1:B:400:PRO:HG2	2.17	0.85
1:B:237:ASN:HB3	1:B:243:VAL:HG22	1.58	0.84
1:A:158:ASN:ND2	1:A:328:ARG:HH21	1.73	0.84
1:A:377:GLN:NE2	1:A:377:GLN:H	1.76	0.84
1:B:282:ILE:HD13	1:B:465:ALA:HB1	1.59	0.83
1:B:382:ASN:H	1:B:382:ASN:ND2	1.75	0.81
1:A:252:THR:HG22	1:A:477:ALA:HB3	1.64	0.80
2:A:517:SPD:H71	2:A:517:SPD:H32	1.64	0.79
1:B:192:GLN:HE21	1:A:128:LEU:HD21	1.47	0.78
1:B:133:HIS:HB3	1:B:136:VAL:HG13	1.64	0.78
1:B:377:GLN:H	1:B:377:GLN:NE2	1.84	0.75
1:B:423:ASN:HB3	1:B:426:ASN:ND2	2.04	0.73
1:B:382:ASN:H	1:B:382:ASN:HD22	1.37	0.72
1:B:423:ASN:HB3	1:B:426:ASN:HD22	1.56	0.71
1:A:229:GLU:O	1:A:231:SER:N	2.23	0.70
1:A:264:PRO:O	1:A:265:GLU:HB3	1.91	0.70
1:A:158:ASN:HD21	1:A:328:ARG:HE	1.40	0.69
1:B:278:LEU:HA	1:B:470:GLN:HE22	1.58	0.69
1:A:335:GLU:HG2	1:A:339:MET:HE2	1.75	0.68
1:B:99:TYR:HB3	1:B:316:LEU:HD21	1.76	0.68
1:A:157:THR:OG1	1:A:160:GLN:HG3	1.94	0.67
1:B:48:LEU:CD2	1:B:63:ALA:HB3	2.25	0.67
1:B:271:ARG:HG3	1:B:271:ARG:HH11	1.59	0.67
1:B:133:HIS:O	1:B:134:LEU:HB2	1.94	0.67
1:A:158:ASN:HD22	1:A:328:ARG:HH21	1.41	0.66
1:B:189:PHE:CE1	1:B:191:HIS:HB2	2.32	0.65
1:A:332:ASN:HD21	1:A:334:ASP:HB2	1.59	0.65
1:B:9:LYS:HB2	1:B:246:ALA:HB2	1.81	0.63
1:A:122:MET:HE1	1:A:145:VAL:HG22	1.79	0.63
1:A:377:GLN:H	1:A:377:GLN:HE21	1.43	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:THR:HG22	1:B:477:ALA:HB3	1.81	0.63
1:A:278:LEU:HA	1:A:470:GLN:NE2	2.14	0.62
1:B:72:ASN:C	1:B:72:ASN:HD22	2.03	0.62
1:A:213:PRO:O	1:A:216:TRP:HB2	2.01	0.61
1:B:254:PRO:HG2	1:B:257:VAL:HG23	1.83	0.60
1:B:439:ASN:HD21	1:B:442:ARG:HH11	1.49	0.60
1:B:30:ASN:HB3	1:B:508:LYS:HD2	1.81	0.60
1:A:278:LEU:HA	1:A:470:GLN:HE22	1.67	0.60
1:A:381:THR:O	1:A:385:GLU:HG3	2.01	0.59
1:A:67:HIS:NE2	2:A:517:SPD:H72	2.17	0.59
1:A:63:ALA:HA	3:A:801:FAD:N5	2.17	0.59
1:B:463:VAL:O	1:B:467:SER:HB2	2.02	0.59
1:B:479:GLU:OE1	1:B:487:GLY:HA2	2.02	0.59
1:B:470:GLN:HB3	1:B:474:ILE:HB	1.84	0.59
1:B:116:GLU:OE1	1:B:116:GLU:N	2.30	0.58
1:B:265:GLU:O	1:B:268:LEU:HD12	2.04	0.58
1:A:479:GLU:OE1	1:A:487:GLY:HA2	2.03	0.58
1:B:237:ASN:HD22	1:B:243:VAL:CG2	2.17	0.58
1:B:189:PHE:HE1	1:B:191:HIS:HB2	1.68	0.57
2:A:517:SPD:H71	2:A:517:SPD:C3	2.33	0.57
1:B:271:ARG:HG3	1:B:271:ARG:NH1	2.19	0.57
1:B:279:LYS:HE2	1:B:470:GLN:HA	1.87	0.57
1:B:141:PHE:CD1	1:B:187:THR:HG21	2.40	0.56
1:A:293:ALA:HB3	1:A:378:ALA:HB2	1.88	0.56
1:B:14:ILE:HD12	1:B:251:ILE:HG12	1.86	0.56
1:B:10:LYS:O	1:B:247:ASP:HB2	2.06	0.56
1:B:171:LEU:HD13	1:B:187:THR:HG22	1.88	0.56
1:B:380:LEU:HD22	1:B:384:ILE:HG12	1.88	0.56
1:A:48:LEU:CD2	1:A:63:ALA:HB3	2.36	0.56
1:B:47:ARG:NH2	1:B:254:PRO:HB3	2.21	0.56
1:B:434:ASN:ND2	1:B:435:ILE:H	2.04	0.56
1:B:332:ASN:ND2	1:B:334:ASP:HB2	2.11	0.55
1:A:361:VAL:HB	1:A:373:MET:HB3	1.88	0.55
1:B:420:PRO:O	1:B:421:ILE:HD13	2.06	0.55
1:A:122:MET:CE	1:A:145:VAL:HG22	2.36	0.55
1:B:63:ALA:HA	3:B:802:FAD:N5	2.22	0.55
1:B:250:ILE:HD11	1:B:503:ILE:HD12	1.87	0.55
1:B:473:ARG:HG3	1:B:473:ARG:HH11	1.72	0.55
1:B:110:ASP:O	1:B:114:LEU:HD23	2.08	0.54
1:B:501:THR:O	1:B:504:SER:HB3	2.08	0.54
1:A:64:SER:OG	1:A:296:LYS:NZ	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:LEU:CD2	2:A:517:SPD:H42	2.38	0.54
1:A:311:SER:HA	1:A:362:ASN:HB3	1.90	0.53
1:B:332:ASN:ND2	1:B:334:ASP:H	2.06	0.53
1:A:68:ASP:HB3	1:A:192:GLN:HB2	1.90	0.53
1:B:335:GLU:O	1:B:339:MET:HB2	2.09	0.53
1:B:190:GLY:O	1:B:191:HIS:HB3	2.09	0.52
1:A:54:TYR:CZ	1:A:433:ARG:HG3	2.44	0.52
1:B:119:ASP:O	1:B:122:MET:HB3	2.10	0.52
1:B:237:ASN:HD22	1:B:243:VAL:HG22	1.73	0.52
1:A:5:SER:N	1:A:6:PRO:HD2	2.25	0.52
1:A:150:LEU:O	1:A:153:ARG:HD2	2.09	0.52
1:B:282:ILE:HD12	1:B:466:MET:CE	2.40	0.52
1:A:54:TYR:CD2	1:A:55:GLN:HG3	2.44	0.52
1:A:401:VAL:O	1:A:405:ILE:HG13	2.09	0.52
1:B:229:GLU:C	1:B:231:SER:H	2.13	0.51
1:A:41:ARG:HD2	4:A:805:HOH:O	2.10	0.51
1:A:48:LEU:HD23	1:A:63:ALA:HB3	1.93	0.51
1:A:14:ILE:HD12	1:A:14:ILE:N	2.24	0.51
1:A:158:ASN:ND2	1:A:328:ARG:HE	2.08	0.51
1:B:213:PRO:HB2	1:B:216:TRP:CD1	2.46	0.51
1:A:122:MET:HG2	1:A:148:TYR:CD2	2.45	0.51
1:B:164:LEU:N	1:B:165:PRO:HD2	2.25	0.50
1:A:332:ASN:ND2	1:A:334:ASP:HB2	2.26	0.50
1:B:229:GLU:O	1:B:231:SER:N	2.43	0.50
1:B:460:VAL:O	1:B:464:VAL:HG23	2.11	0.50
1:B:336:LEU:HD23	1:B:340:LEU:HG	1.93	0.50
1:A:353:CYS:SG	1:A:401:VAL:HG13	2.51	0.50
1:B:281:VAL:HG13	1:B:282:ILE:N	2.27	0.50
1:A:395:PHE:O	1:A:399:GLN:HB2	2.12	0.49
1:B:278:LEU:HA	1:B:470:GLN:NE2	2.27	0.49
2:A:517:SPD:H32	2:A:517:SPD:C7	2.40	0.49
1:A:264:PRO:O	1:A:265:GLU:CB	2.60	0.49
2:A:517:SPD:HN6	3:A:801:FAD:C4	2.25	0.49
1:B:377:GLN:H	1:B:377:GLN:HE21	1.61	0.49
1:A:164:LEU:N	1:A:165:PRO:HD2	2.27	0.49
1:B:271:ARG:HD3	1:B:271:ARG:C	2.34	0.49
1:B:63:ALA:HA	3:B:802:FAD:C4X	2.43	0.48
1:B:291:PHE:HA	1:B:450:TYR:O	2.13	0.48
1:B:57:ARG:HD3	1:B:369:VAL:CG1	2.44	0.48
1:B:335:GLU:OE2	1:B:339:MET:HE1	2.13	0.48
1:A:375:LEU:HD21	2:A:517:SPD:H42	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:TYR:CE2	1:B:433:ARG:HG3	2.49	0.48
1:B:226:ILE:HD12	1:B:274:PHE:CE2	2.49	0.48
1:B:311:SER:O	1:B:312:LYS:HD3	2.14	0.48
1:A:376:MET:HG3	1:A:381:THR:OG1	2.14	0.48
1:B:151:GLN:HG2	1:B:151:GLN:O	2.13	0.47
1:B:247:ASP:O	1:B:473:ARG:HD2	2.14	0.47
1:A:158:ASN:ND2	1:A:328:ARG:NH2	2.51	0.47
1:A:247:ASP:O	1:A:473:ARG:HD2	2.14	0.47
1:B:118:VAL:HG23	1:B:164:LEU:HD13	1.96	0.47
1:B:254:PRO:HG2	1:B:257:VAL:CG2	2.44	0.47
1:B:473:ARG:HG3	1:B:473:ARG:NH1	2.30	0.47
1:B:9:LYS:HE3	1:B:36:LEU:HD23	1.97	0.47
1:B:302:GLU:HB2	1:B:433:ARG:HD3	1.97	0.46
1:B:110:ASP:HB3	1:B:113:LEU:HB2	1.98	0.46
1:A:63:ALA:HA	3:A:801:FAD:C4X	2.45	0.46
1:A:362:ASN:HD21	1:A:364:SER:HB3	1.80	0.46
1:A:167:LEU:O	1:A:170:TYR:HD2	1.97	0.46
1:B:248:TYR:CE2	1:B:473:ARG:HD3	2.51	0.46
1:B:54:TYR:O	1:B:57:ARG:HG3	2.15	0.46
1:B:217:LEU:HD21	1:B:219:LEU:HD21	1.97	0.46
1:B:276:PRO:HB2	1:B:277:PRO:HD2	1.97	0.45
1:B:416:ASP:C	1:B:416:ASP:OD1	2.53	0.45
1:B:475:ARG:HB3	1:B:499:GLU:OE1	2.16	0.45
1:B:439:ASN:HD21	1:B:442:ARG:NH1	2.12	0.45
1:B:293:ALA:HB3	1:B:378:ALA:HB2	1.97	0.45
1:A:65:TRP:CZ3	2:A:517:SPD:H41	2.51	0.45
1:B:224:LYS:HE2	1:B:239:GLU:HA	1.98	0.45
1:B:141:PHE:CE1	1:B:187:THR:HG21	2.51	0.45
1:B:12:ILE:HB	1:B:249:VAL:HG22	1.99	0.45
1:B:141:PHE:O	1:B:145:VAL:HG23	2.17	0.45
1:A:228:ARG:HD2	1:A:233:ASN:O	2.17	0.45
1:A:398:PHE:O	1:A:402:LEU:HG	2.17	0.45
1:B:382:ASN:ND2	1:B:382:ASN:N	2.54	0.44
1:B:377:GLN:NE2	1:B:377:GLN:N	2.60	0.44
1:A:9:LYS:O	1:A:246:ALA:HA	2.17	0.44
1:B:36:LEU:O	1:B:36:LEU:HD12	2.18	0.44
1:B:234:VAL:O	1:B:245:ASN:HA	2.17	0.44
1:B:431:VAL:HG11	1:B:433:ARG:HH11	1.82	0.44
1:B:322:GLU:O	1:B:326:ILE:HG13	2.17	0.44
1:B:362:ASN:ND2	1:B:364:SER:H	2.16	0.44
1:B:316:LEU:HD22	1:B:316:LEU:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:505:ASP:C	1:B:507:LEU:N	2.70	0.43
1:B:240:ASP:OD2	1:B:242:THR:HG23	2.18	0.43
1:B:362:ASN:HD21	1:B:364:SER:HB3	1.83	0.43
1:A:17:GLY:O	1:A:21:LEU:HG	2.18	0.43
1:A:103:GLU:HA	1:A:103:GLU:OE1	2.19	0.43
1:A:41:ARG:HG2	1:A:41:ARG:HH11	1.84	0.43
1:A:72:ASN:O	1:A:76:LEU:HG	2.19	0.43
1:B:199:LEU:HD23	1:B:199:LEU:HA	1.82	0.43
1:B:167:LEU:HA	1:B:316:LEU:CD1	2.48	0.43
1:B:282:ILE:HD12	1:B:466:MET:HE1	2.00	0.43
1:A:57:ARG:HD3	1:A:369:VAL:CG1	2.49	0.43
1:A:61:ILE:HD12	1:A:61:ILE:HA	1.92	0.43
1:B:17:GLY:HA3	3:B:802:FAD:H52A	2.01	0.43
1:A:298:ILE:HB	1:A:436:ILE:HB	2.01	0.42
1:B:212:PHE:HB2	1:B:213:PRO:HD2	2.01	0.42
1:B:283:GLN:HE21	1:B:283:GLN:HB3	1.64	0.42
1:B:72:ASN:HD21	1:B:74:LEU:HB3	1.84	0.42
1:B:148:TYR:CE1	1:B:152:ARG:HG3	2.55	0.42
1:B:35:CYS:O	1:B:216:TRP:CG	2.73	0.42
1:B:174:TRP:CE2	2:B:517:SPD:H21	2.55	0.42
1:A:38:LEU:HD22	1:A:218:LYS:HD3	2.02	0.42
1:A:470:GLN:HB3	1:A:474:ILE:HB	2.00	0.42
1:B:404:LYS:HD2	1:B:404:LYS:HA	1.83	0.42
1:A:505:ASP:O	1:A:508:LYS:HB3	2.20	0.42
1:A:306:TRP:HE1	1:A:362:ASN:HD21	1.68	0.42
1:B:131:HIS:O	1:B:132:GLN:C	2.58	0.42
1:B:212:PHE:HB2	1:B:213:PRO:CD	2.50	0.42
1:B:472:SER:CA	1:B:502:ARG:HH22	2.32	0.42
1:B:237:ASN:CB	1:B:243:VAL:HG22	2.40	0.42
1:A:377:GLN:NE2	1:A:377:GLN:N	2.58	0.41
1:B:35:CYS:O	1:B:216:TRP:CD1	2.74	0.41
1:A:399:GLN:HB3	1:A:400:PRO:CD	2.51	0.41
1:A:505:ASP:HA	1:A:508:LYS:HE2	2.02	0.41
1:B:412:GLU:HG3	1:B:429:LYS:HD3	2.02	0.41
1:B:78:GLU:OE1	1:B:89:ARG:HD3	2.20	0.41
1:B:239:GLU:OE1	1:B:239:GLU:O	2.38	0.41
1:A:154:GLN:O	1:A:154:GLN:HG2	2.20	0.41
1:A:265:GLU:OE2	1:A:267:ASN:N	2.43	0.41
1:A:414:VAL:HA	1:A:430:PRO:HG2	2.01	0.41
1:B:173:LEU:O	2:B:517:SPD:H32	2.21	0.41
1:A:340:LEU:O	1:A:342:ARG:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:GLY:O	1:B:296:LYS:NZ	2.52	0.41
1:A:189:PHE:CD2	1:A:189:PHE:N	2.88	0.41
1:A:232:LYS:C	1:A:473:ARG:HH12	2.25	0.41
1:B:68:ASP:HB3	1:B:192:GLN:HB2	2.03	0.41
1:B:72:ASN:C	1:B:72:ASN:ND2	2.73	0.41
1:B:326:ILE:HG23	1:B:339:MET:SD	2.61	0.41
1:B:505:ASP:C	1:B:507:LEU:H	2.23	0.41
1:A:289:ILE:HA	1:A:457:ASP:OD2	2.20	0.41
1:B:169:ARG:C	1:B:171:LEU:N	2.74	0.40
1:B:23:ALA:O	1:B:27:LEU:HG	2.21	0.40
1:B:412:GLU:HG3	1:B:429:LYS:CD	2.51	0.40
1:A:138:ASP:O	1:A:139:CYS:SG	2.79	0.40
1:A:54:TYR:O	1:A:57:ARG:HG3	2.22	0.40
1:B:172:GLU:HG2	1:B:177:LEU:O	2.21	0.40
1:B:192:GLN:HE21	1:A:128:LEU:CD2	2.25	0.40
1:B:229:GLU:C	1:B:231:SER:N	2.74	0.40
1:B:422:GLU:HG2	1:B:423:ASN:N	2.36	0.40
1:A:99:TYR:O	1:A:106:ARG:HA	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASN:ND2	1:A:267:ASN:ND2[4_556]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	488/516 (95%)	453 (93%)	30 (6%)	5 (1%)	15	23
1	B	495/516 (96%)	442 (89%)	39 (8%)	14 (3%)	5	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	983/1032 (95%)	895 (91%)	69 (7%)	19 (2%)	8 10

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	136	VAL
1	B	200	ASN
1	B	289	ILE
1	B	290	HIS
1	B	510	GLU
1	A	200	ASN
1	B	137	SER
1	B	231	SER
1	B	265	GLU
1	B	291	PHE
1	B	31	GLY
1	B	472	SER
1	A	132	GLN
1	A	265	GLU
1	B	230	PRO
1	B	479	GLU
1	A	231	SER
1	B	471	ASP
1	A	230	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	413/457 (90%)	396 (96%)	17 (4%)	30	48
1	B	404/457 (88%)	384 (95%)	20 (5%)	24	40
All	All	817/914 (89%)	780 (96%)	37 (4%)	27	44

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	34	ASP
1	B	36	LEU
1	B	64	SER
1	B	72	ASN
1	B	174	TRP
1	B	179	TRP
1	B	201	TYR
1	B	221	CYS
1	B	237	ASN
1	B	239	GLU
1	B	245	ASN
1	B	268	LEU
1	B	271	ARG
1	B	322	GLU
1	B	362	ASN
1	B	377	GLN
1	B	380	LEU
1	B	382	ASN
1	B	392	GLU
1	B	419	ARG
1	A	36	LEU
1	A	118	VAL
1	A	122	MET
1	A	134	LEU
1	A	139	CYS
1	A	150	LEU
1	A	153	ARG
1	A	177	LEU
1	A	179	TRP
1	A	201	TYR
1	A	221	CYS
1	A	239	GLU
1	A	267	ASN
1	A	291	PHE
1	A	377	GLN
1	A	442	ARG
1	A	484	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	29	GLN
1	B	72	ASN

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Mol	Chain	Res	Type
1	B	109	HIS
1	B	133	HIS
1	B	192	GLN
1	B	283	GLN
1	B	329	ASN
1	B	362	ASN
1	B	377	GLN
1	B	382	ASN
1	B	426	ASN
1	B	434	ASN
1	B	439	ASN
1	A	33	GLN
1	A	158	ASN
1	A	267	ASN
1	A	332	ASN
1	A	362	ASN
1	A	377	GLN
1	A	434	ASN
1	A	439	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 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	$\#|Z| > 2$
3	FAD	B	802	-	53,58,58	1.27	7 (13%)	68,89,89	1.40	11 (16%)
2	SPD	B	517	-	9,9,9	0.34	0	8,8,8	0.68	0
3	FAD	A	801	-	53,58,58	1.33	5 (9%)	68,89,89	1.34	9 (13%)
2	SPD	A	517	-	9,9,9	0.35	0	8,8,8	0.64	0

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
3	FAD	B	802	-	-	5/30/50/50	0/6/6/6
2	SPD	B	517	-	-	1/7/7/7	-
3	FAD	A	801	-	-	5/30/50/50	0/6/6/6
2	SPD	A	517	-	-	2/7/7/7	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	FAD	C4X-N5	4.86	1.40	1.30
3	B	802	FAD	C4X-N5	4.75	1.40	1.30
3	A	801	FAD	C2A-N3A	3.02	1.37	1.32
3	A	801	FAD	C2A-N1A	2.70	1.38	1.33
3	B	802	FAD	C2A-N3A	2.57	1.36	1.32
3	B	802	FAD	C2A-N1A	2.48	1.38	1.33
3	B	802	FAD	C10-N1	2.34	1.38	1.33
3	A	801	FAD	PA-O2A	-2.31	1.44	1.55
3	A	801	FAD	C10-N1	2.26	1.37	1.33
3	B	802	FAD	C10-N10	2.14	1.42	1.37
3	B	802	FAD	PA-O2A	-2.10	1.45	1.55
3	B	802	FAD	C9A-C5X	2.06	1.44	1.41

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	FAD	O2A-PA-O1A	4.62	135.08	112.24
3	B	802	FAD	O2A-PA-O1A	4.52	134.57	112.24
3	B	802	FAD	O4B-C1B-C2B	-4.05	101.01	106.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	801	FAD	O4B-C1B-C2B	-3.65	101.59	106.93
3	B	802	FAD	O3'-C3'-C4'	-2.79	102.07	108.81
3	A	801	FAD	C9A-C5X-N5	-2.68	119.52	122.43
3	A	801	FAD	O3'-C3'-C4'	-2.57	102.60	108.81
3	B	802	FAD	C9A-C5X-N5	-2.43	119.79	122.43
3	B	802	FAD	C5'-C4'-C3'	-2.41	107.55	112.20
3	B	802	FAD	P-O3P-PA	2.36	140.92	132.83
3	A	801	FAD	N3A-C2A-N1A	-2.35	125.00	128.68
3	B	802	FAD	C5A-C6A-N6A	2.34	123.91	120.35
3	B	802	FAD	C4-C4X-N5	2.17	121.33	118.23
3	B	802	FAD	N3A-C2A-N1A	-2.10	125.40	128.68
3	A	801	FAD	C4-C4X-N5	2.10	121.22	118.23
3	B	802	FAD	C4'-C3'-C2'	2.07	117.67	113.36
3	B	802	FAD	C10-C4X-N5	-2.07	120.47	124.86
3	A	801	FAD	P-O3P-PA	2.05	139.88	132.83
3	A	801	FAD	C4X-C10-N10	2.05	119.48	116.48
3	A	801	FAD	C5A-C6A-N6A	2.02	123.42	120.35

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	802	FAD	C5B-O5B-PA-O2A
3	A	801	FAD	C5B-O5B-PA-O2A
3	B	802	FAD	C5B-O5B-PA-O3P
3	A	801	FAD	C5B-O5B-PA-O3P
3	B	802	FAD	P-O3P-PA-O2A
3	A	801	FAD	P-O3P-PA-O2A
3	B	802	FAD	C4B-C5B-O5B-PA
3	A	801	FAD	C4B-C5B-O5B-PA
3	B	802	FAD	C2'-C3'-C4'-O4'
2	A	517	SPD	C4-C5-N6-C7
3	A	801	FAD	P-O3P-PA-O1A
2	B	517	SPD	C2-C3-C4-C5
2	A	517	SPD	C8-C7-N6-C5

There are no ring outliers.

4 monomers are involved in 15 short contacts:

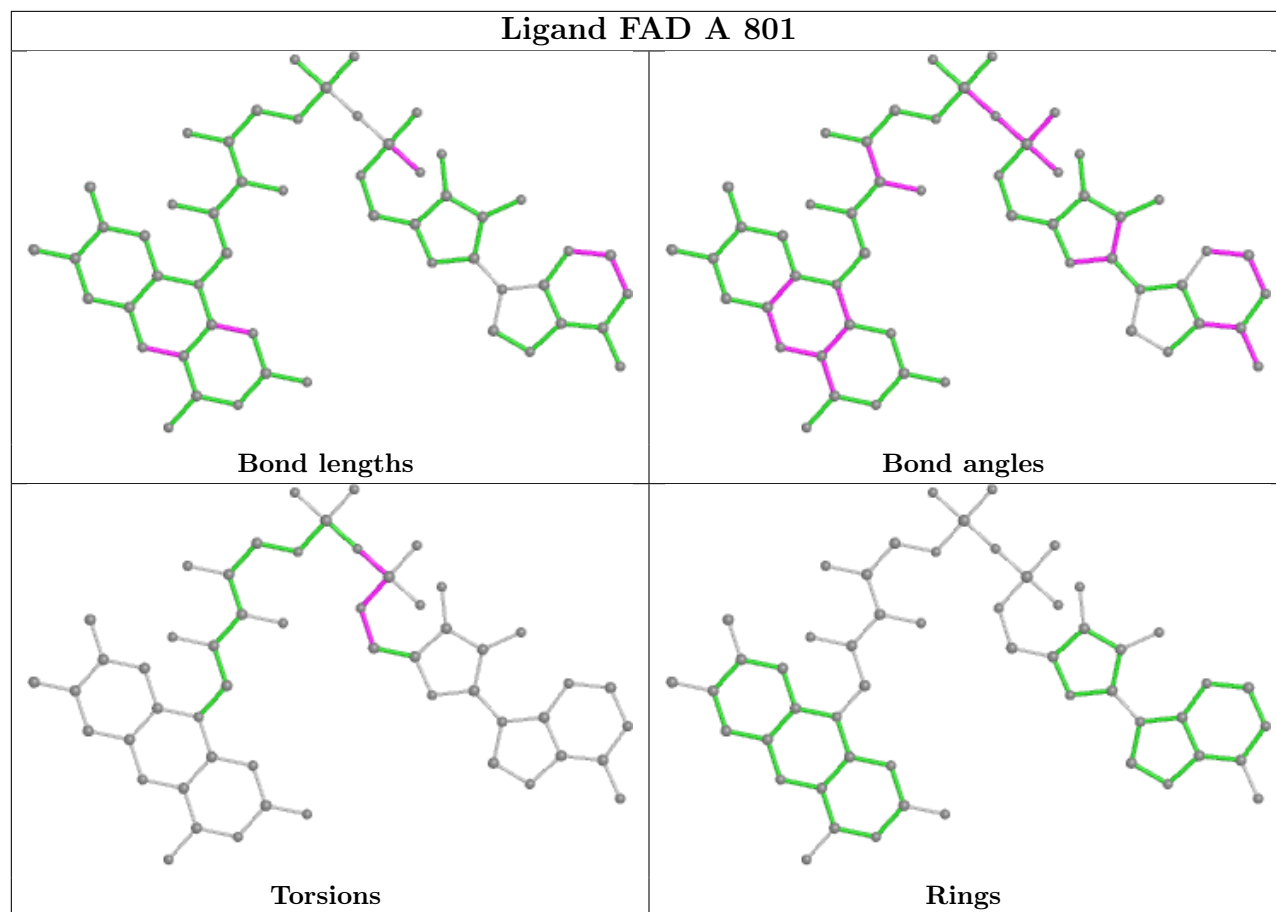| Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	802	FAD	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	517	SPD	2	0
3	A	801	FAD	3	0
2	A	517	SPD	8	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 B 802

Bond lengths   Bond angles

Torsions   Rings

Ligand FAD A 801

Bond lengths

Bond angles

Torsions

Rings
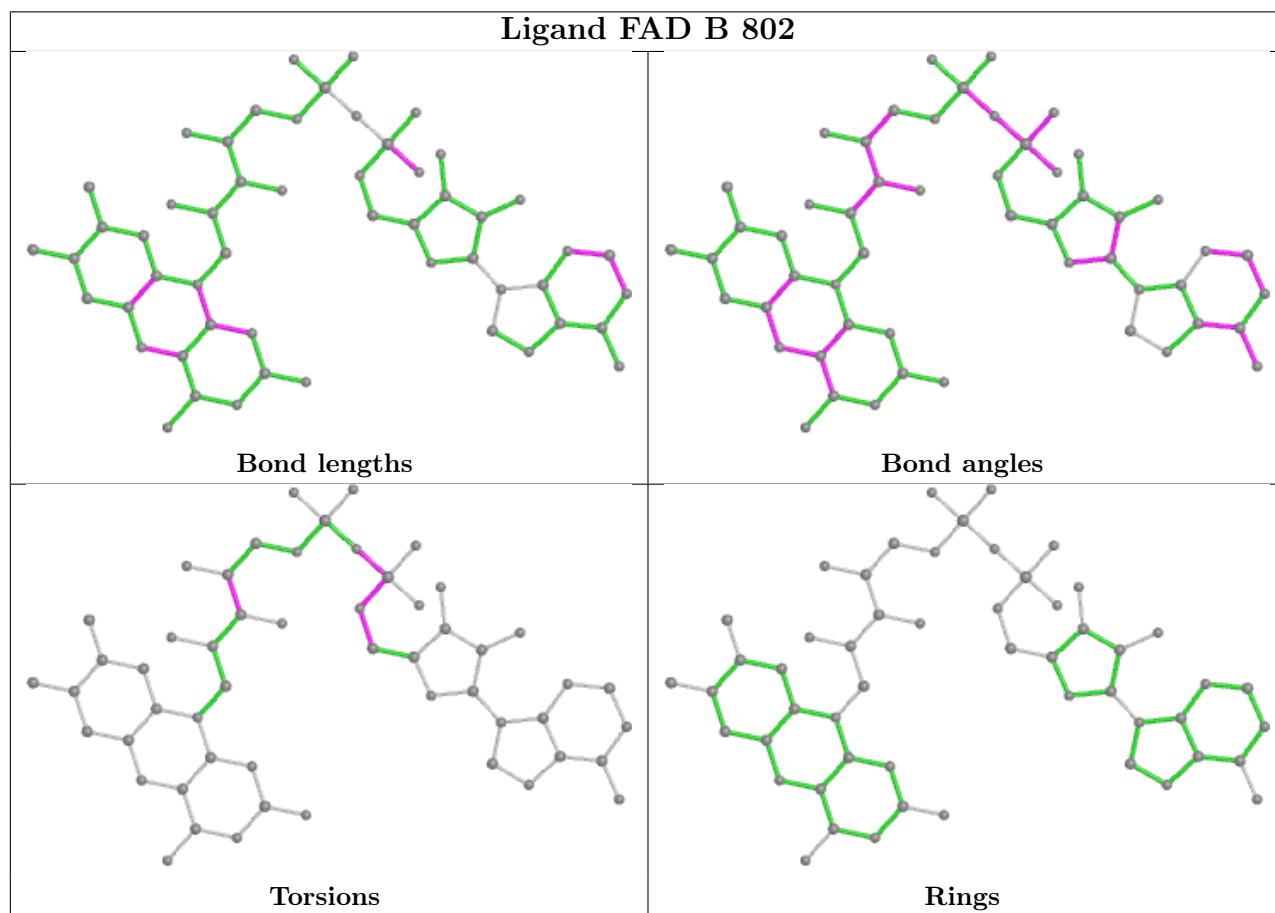
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	494/516 (95%)	0.02	13 (2%)	56	54	29, 45, 68, 86	0
1	B	499/516 (96%)	0.21	41 (8%)	11	10	29, 47, 82, 98	0
All	All	993/1032 (96%)	0.12	54 (5%)	25	24	29, 45, 78, 98	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	423	ASN	7.2
1	B	425	ALA	6.8
1	B	135	GLY	6.2
1	B	136	VAL	6.0
1	B	509	LEU	5.8
1	A	5	SER	5.5
1	B	134	LEU	5.3
1	A	231	SER	4.8
1	B	424	ILE	4.4
1	B	426	ASN	4.2
1	A	6	PRO	4.2
1	B	422	GLU	4.0
1	B	230	PRO	3.8
1	B	133	HIS	3.8
1	B	427	ALA	3.4
1	B	334	ASP	3.3
1	B	245	ASN	3.3
1	A	7	ALA	3.2
1	B	227	THR	3.2
1	B	289	ILE	3.2
1	B	332	ASN	3.2
1	A	508	LYS	2.9
1	B	325	GLU	2.9
1	B	335	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	305	CYS	2.8
1	B	503	ILE	2.8
1	B	137	SER	2.8
1	A	232	LYS	2.7
1	B	338	SER	2.7
1	A	230	PRO	2.6
1	B	421	ILE	2.6
1	B	138	ASP	2.5
1	A	349	THR	2.4
1	B	262	VAL	2.4
1	A	427	ALA	2.4
1	A	334	ASP	2.4
1	B	420	PRO	2.3
1	B	508	LYS	2.3
1	B	232	LYS	2.3
1	B	507	LEU	2.3
1	B	238	CYS	2.3
1	B	511	HIS	2.3
1	B	228	ARG	2.3
1	B	267	ASN	2.2
1	B	8	LYS	2.2
1	B	34	ASP	2.2
1	A	335	GLU	2.2
1	B	237	ASN	2.1
1	B	339	MET	2.1
1	B	268	LEU	2.1
1	A	31	GLY	2.1
1	B	220	SER	2.1
1	B	224	LYS	2.1
1	B	473	ARG	2.0

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

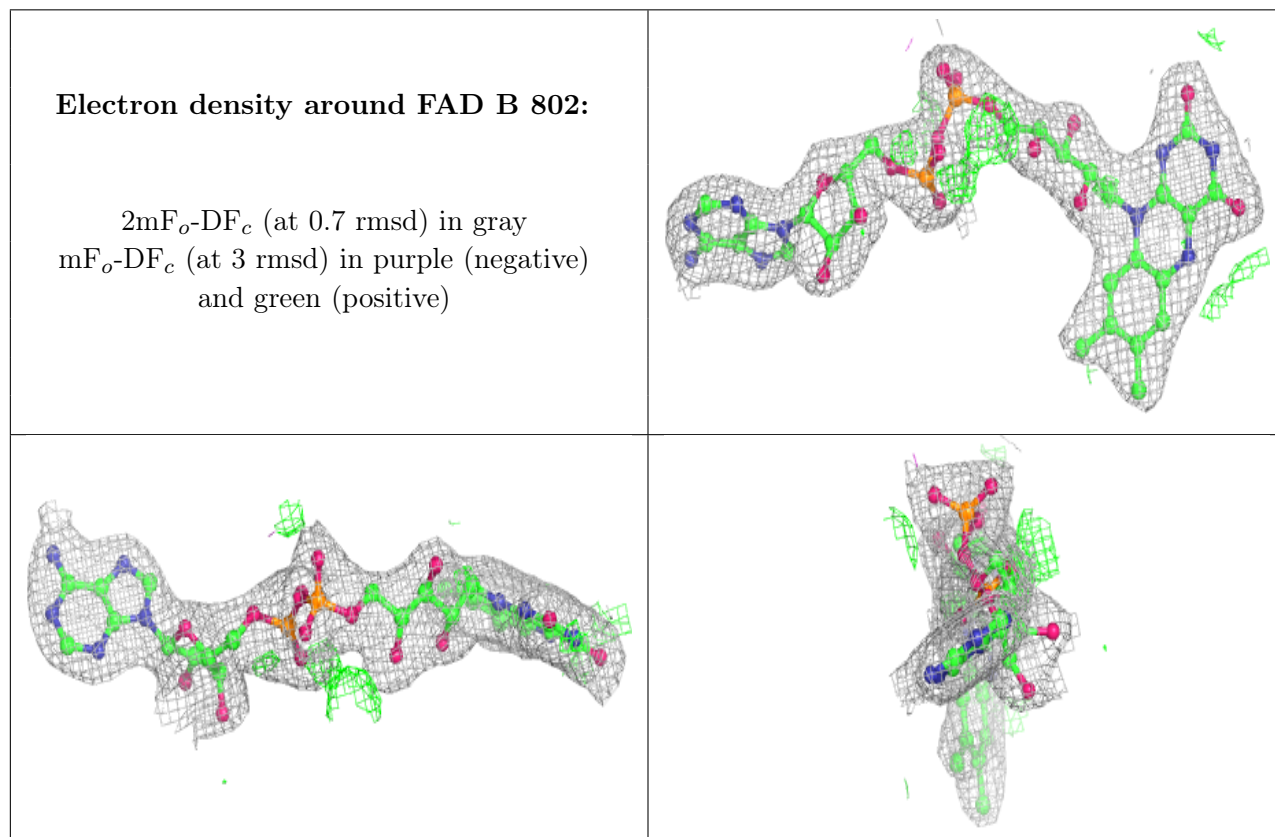There are no non-standard protein/DNA/RNA residues in this entry.

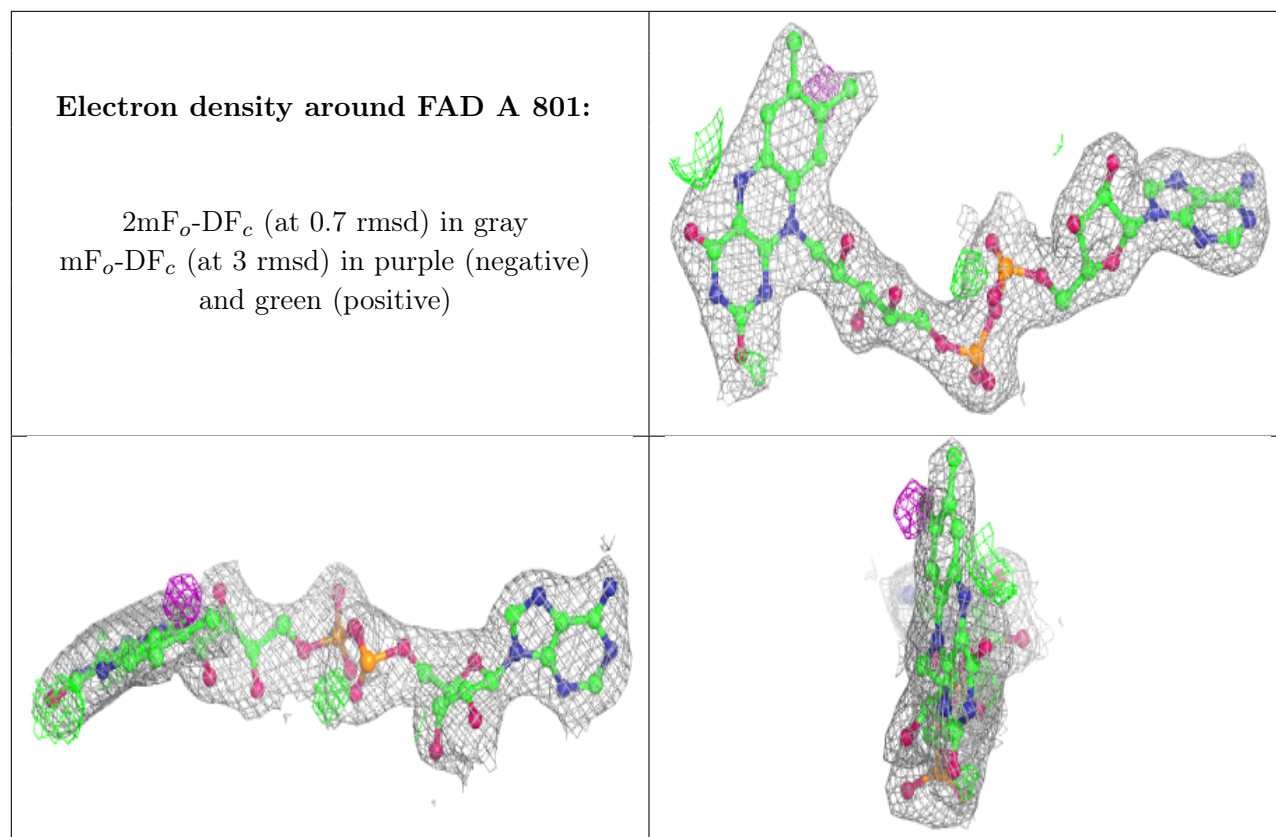## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SPD	A	517	10/10	0.77	0.32	63,64,65,66	0
2	SPD	B	517	10/10	0.78	0.37	66,67,68,69	0
3	FAD	B	802	53/53	0.96	0.15	24,36,43,44	0
3	FAD	A	801	53/53	0.96	0.17	28,34,41,42	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 B 802:

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

Electron density around FAD A 801:

$2mF_o$-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 ⓘ

There are no such residues in this entry.