



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:04 AM UTC

PDB ID : 3CNT / pdb_00003cnt
Title : Crystal structure of fms1 in complex with R-Bz-MeSpermidine
Authors : Huang, Q.; Hao, Q.
Deposited on : 2008-03-26
Resolution : 2.70 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

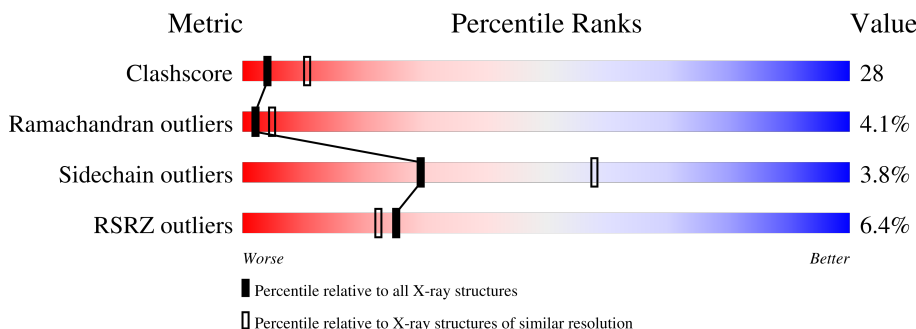
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	516	4% 54% 37% 5%
1	B	516	8% 49% 42% .

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
3	SP9	B	518	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7899 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 fms1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	495	Total	C	N	O	S	0	0	0
			3816	2407	664	723	22			
1	A	497	Total	C	N	O	S	0	0	0
			3907	2471	683	731	22			

There are 16 discrepancies between the modelled and reference sequences:

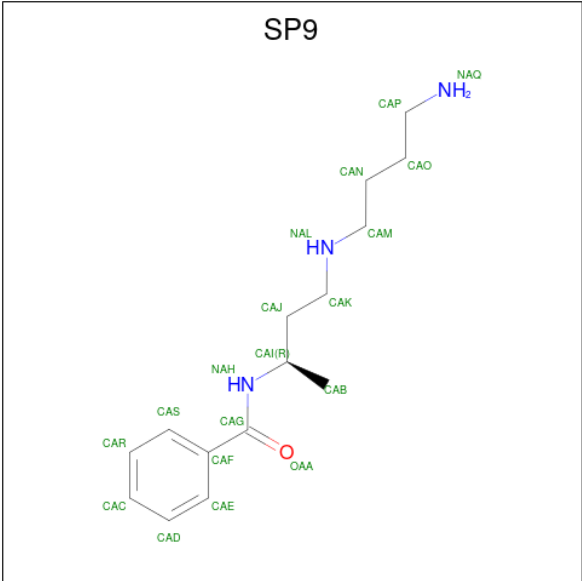
Chain	Residue	Modelled	Actual	Comment	Reference
B	509	LEU	-	expression tag	UNP P50264
B	510	GLU	-	expression tag	UNP P50264
B	511	HIS	-	expression tag	UNP P50264
B	512	HIS	-	expression tag	UNP P50264
B	513	HIS	-	expression tag	UNP P50264
B	514	HIS	-	expression tag	UNP P50264
B	515	HIS	-	expression tag	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 FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



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

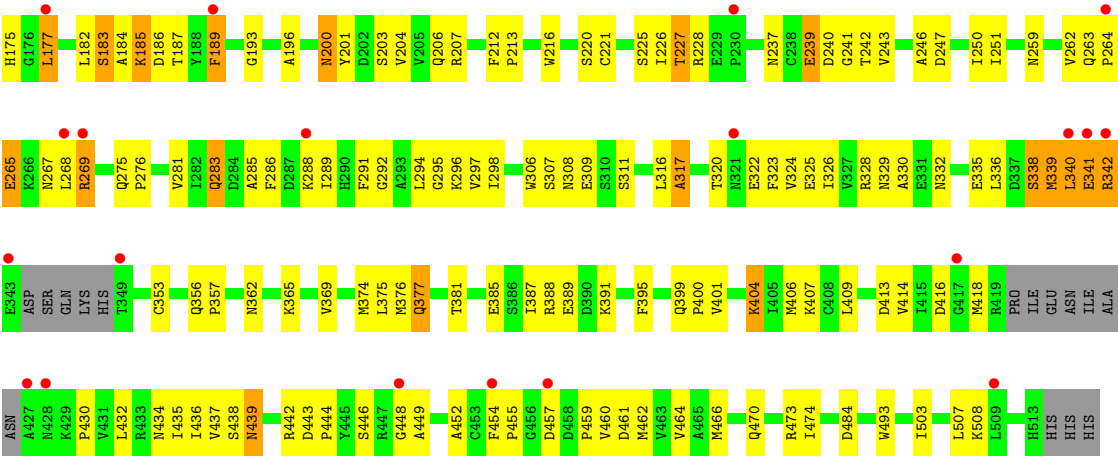
- Molecule 3 is N-{(1R)-3-[(4-aminobutyl)amino]-1-methylpropyl}benzamide (CCD ID: SP9) (formula: C₁₅H₂₅N₃O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			19	15	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	21	Total 21	O 21	0	0
4	A	30	Total 30	O 30	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	161.86Å 102.41Å 77.20Å 90.00° 94.94° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 50.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.6 (50.00-2.70) 91.6 (50.00-2.70)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.97 (at 2.51Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.223 , 0.290 0.227 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7899	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.23% 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, SP9

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	0.51	0/3989	0.96	7/5396 (0.1%)
1	B	0.47	0/3893	0.97	19/5267 (0.4%)
All	All	0.49	0/7882	0.97	26/10663 (0.2%)

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	419	ARG	CA-C-N	8.42	130.37	119.84
1	B	419	ARG	C-N-CA	8.42	130.37	119.84
1	B	174	TRP	N-CA-C	-8.07	103.95	113.88
1	A	66	HIS	N-CA-C	-7.17	97.05	108.73
1	A	201	TYR	N-CA-C	-6.92	103.51	112.23
1	B	188	TYR	N-CA-C	6.55	119.79	110.68
1	B	419	ARG	N-CA-C	-6.44	99.71	109.30
1	B	170	TYR	N-CA-C	-6.21	104.80	112.38
1	B	201	TYR	N-CA-C	-5.99	105.93	113.18
1	A	174	TRP	N-CA-C	-5.97	103.45	112.04
1	B	420	PRO	N-CA-C	5.88	124.58	112.47
1	B	163	TYR	N-CA-C	5.85	118.89	111.69
1	B	279	LYS	CA-C-N	5.81	127.11	119.84
1	B	279	LYS	C-N-CA	5.81	127.11	119.84
1	B	119	ASP	N-CA-C	-5.67	105.24	111.82
1	A	454	PHE	N-CA-C	-5.60	103.59	110.31
1	A	170	TYR	N-CA-C	-5.58	105.58	112.38
1	B	104	ARG	N-CA-C	5.42	118.11	111.82
1	B	414	VAL	N-CA-C	5.40	116.05	109.30
1	B	203	SER	N-CA-C	-5.38	105.52	111.71
1	B	85	ASP	N-CA-C	5.38	118.95	112.93
1	B	332	ASN	N-CA-C	5.28	116.23	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	TRP	N-CA-C	5.26	118.13	109.72
1	B	232	LYS	N-CA-C	5.13	121.73	110.80
1	A	225	SER	N-CA-C	5.06	116.93	108.99
1	A	104	ARG	N-CA-C	5.05	116.47	111.07

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	3907	0	3773	199	2
1	B	3816	0	3610	224	0
2	A	53	0	31	8	0
2	B	53	0	31	12	0
3	B	19	0	25	19	0
4	A	30	0	0	1	0
4	B	21	0	0	1	0
All	All	7899	0	7470	423	2

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 28.

All (423) 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:278:LEU:HA	1:B:470:GLN:HE22	1.08	1.11
1:B:66:HIS:HB2	1:B:196:ALA:HB3	1.43	1.01
1:B:488:CYS:SG	3:B:518:SP9:HAN	2.03	0.98
1:B:359:PHE:CE2	3:B:518:SP9:HAR	1.99	0.96
1:B:177:LEU:HD11	1:B:292:GLY:HA2	1.48	0.96
1:B:353:CYS:SG	1:B:400:PRO:HG2	2.10	0.92
1:B:67:HIS:CD2	3:B:518:SP9:HABA	2.06	0.90
1:A:171:LEU:HD13	1:A:187:THR:HG22	1.54	0.90
1:A:377:GLN:H	1:A:377:GLN:NE2	1.70	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:GLN:HE21	1:A:377:GLN:N	1.69	0.89
1:B:81:LEU:HD11	1:B:207:ARG:NH1	1.88	0.88
1:B:50:THR:HG21	1:B:58:LYS:HE2	1.55	0.88
1:A:377:GLN:H	1:A:377:GLN:HE21	0.91	0.88
1:B:278:LEU:HA	1:B:470:GLN:NE2	1.89	0.86
1:B:72:ASN:C	1:B:72:ASN:HD22	1.84	0.85
1:A:54:TYR:HE2	1:A:55:GLN:HE21	1.24	0.85
1:B:237:ASN:ND2	1:B:243:VAL:HG22	1.93	0.83
1:B:237:ASN:OD1	1:B:243:VAL:HG13	1.79	0.83
1:A:335:GLU:HG2	1:A:339:MET:HE2	1.60	0.82
1:B:60:ASP:HB3	1:B:63:ALA:O	1.81	0.81
1:B:486:ALA:O	3:B:518:SP9:HANA	1.80	0.81
1:B:359:PHE:HE2	3:B:518:SP9:HAR	1.42	0.81
1:B:192:GLN:HE21	1:A:128:LEU:HD21	1.46	0.80
1:A:353:CYS:SG	1:A:400:PRO:HG2	2.21	0.80
1:A:85:ASP:CG	1:A:87:ARG:HG3	2.08	0.78
1:B:47:ARG:HH21	1:B:254:PRO:HB3	1.49	0.78
1:B:177:LEU:CD1	1:B:292:GLY:HA2	2.14	0.77
1:B:282:ILE:HD13	1:B:465:ALA:HB1	1.67	0.77
1:B:412:GLU:OE2	1:B:429:LYS:HG2	1.87	0.75
1:A:443:ASP:HB3	1:A:446:SER:HB3	1.67	0.75
1:B:302:GLU:HG2	1:B:433:ARG:HD3	1.67	0.75
1:B:271:ARG:O	1:B:271:ARG:HD3	1.86	0.75
1:B:377:GLN:H	1:B:377:GLN:NE2	1.85	0.74
1:A:263:GLN:HB3	1:A:264:PRO:HD2	1.70	0.74
1:B:466:MET:HB3	1:B:481:THR:HG22	1.68	0.73
1:A:213:PRO:HB2	1:A:216:TRP:CD1	2.23	0.73
1:A:22:LYS:HG3	1:A:493:TRP:CD1	2.24	0.72
1:B:172:GLU:HG2	1:B:177:LEU:O	1.90	0.71
1:B:358:LEU:HD22	1:B:374:MET:HE3	1.72	0.71
1:A:227:THR:HG23	1:A:275:GLN:HB2	1.72	0.71
1:B:67:HIS:NE2	3:B:518:SP9:HABA	2.05	0.70
1:B:72:ASN:ND2	1:B:75:PHE:H	1.88	0.70
1:B:332:ASN:C	1:B:332:ASN:HD22	2.00	0.70
1:B:139:CYS:SG	1:B:147:LYS:NZ	2.64	0.70
1:B:226:ILE:HA	1:B:236:VAL:HG12	1.73	0.69
1:A:239:GLU:HG3	1:A:240:ASP:N	2.05	0.69
1:B:415:ILE:HD13	1:B:426:ASN:OD1	1.91	0.69
1:B:271:ARG:NH2	1:B:273:GLU:HG3	2.07	0.69
1:B:192:GLN:NE2	1:A:128:LEU:HD21	2.08	0.69
1:A:177:LEU:HD21	1:A:452:ALA:HB1	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:LEU:O	1:B:340:LEU:HG	1.92	0.69
1:A:63:ALA:HA	2:A:517:FAD:N5	2.09	0.68
1:A:183:SER:HB2	1:A:455:PRO:HA	1.76	0.68
1:B:140:SER:N	1:B:143:GLN:OE1	2.26	0.68
1:B:278:LEU:CA	1:B:470:GLN:HE22	1.97	0.68
1:B:423:ASN:ND2	1:B:425:ALA:HB3	2.09	0.68
1:B:374:MET:HE1	1:B:398:PHE:CE2	2.29	0.67
1:A:283:GLN:O	1:A:286:PHE:HB2	1.94	0.67
1:B:479:GLU:HB2	1:B:487:GLY:HA2	1.77	0.67
1:B:77:GLU:HG2	1:B:207:ARG:HH22	1.60	0.66
1:B:332:ASN:ND2	1:B:335:GLU:H	1.94	0.66
1:A:240:ASP:OD1	1:A:242:THR:HG23	1.95	0.66
1:A:144:LEU:HD22	1:A:184:ALA:HB1	1.77	0.66
1:B:271:ARG:HH21	1:B:273:GLU:HG3	1.60	0.66
1:A:283:GLN:HA	1:A:286:PHE:HD1	1.61	0.66
1:A:39:GLU:OE2	2:A:517:FAD:H1B	1.96	0.66
1:A:470:GLN:HB3	1:A:474:ILE:HB	1.78	0.65
1:A:99:TYR:CE2	1:A:167:LEU:HG	2.31	0.65
1:A:391:LYS:O	1:A:418:MET:HE1	1.95	0.65
1:B:308:ASN:O	1:B:365:LYS:HD2	1.96	0.65
1:B:377:GLN:H	1:B:377:GLN:HE21	1.44	0.64
1:A:177:LEU:HD11	1:A:292:GLY:HA2	1.78	0.64
1:A:404:LYS:HA	1:A:404:LYS:HE3	1.80	0.64
1:B:47:ARG:NH2	1:B:254:PRO:HB3	2.12	0.63
1:B:391:LYS:O	1:B:418:MET:HE1	1.98	0.63
1:A:385:GLU:HG2	1:A:438:SER:O	1.99	0.63
1:B:141:PHE:CD1	1:B:187:THR:HG21	2.34	0.63
1:B:297:VAL:HG22	1:B:437:VAL:HG13	1.81	0.63
1:A:439:ASN:ND2	1:A:442:ARG:HB2	2.14	0.62
1:B:121:GLU:HG3	1:A:193:GLY:HA2	1.82	0.62
1:A:104:ARG:CZ	1:A:113:LEU:HD11	2.29	0.62
1:B:50:THR:CG2	1:B:58:LYS:HE2	2.29	0.62
1:B:9:LYS:O	1:B:246:ALA:HA	2.00	0.61
1:A:306:TRP:CE3	1:A:406:MET:HE1	2.35	0.61
1:A:267:ASN:HD21	1:A:269:ARG:HH22	1.47	0.61
1:A:325:GLU:HA	1:A:328:ARG:HB2	1.82	0.61
3:B:518:SP9:HAJA	3:B:518:SP9:OAA	2.01	0.61
1:A:95:ASP:OD2	1:A:365:LYS:NZ	2.32	0.61
1:A:377:GLN:NE2	1:A:377:GLN:N	2.40	0.61
1:B:401:VAL:O	1:B:405:ILE:HG13	2.01	0.61
1:A:416:ASP:OD1	1:A:416:ASP:C	2.44	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:ARG:HB3	1:A:444:PRO:HB2	1.83	0.60
1:B:479:GLU:HG2	2:B:517:FAD:O3'	2.02	0.60
1:B:12:ILE:HG13	1:B:246:ALA:HB2	1.83	0.60
1:A:55:GLN:NE2	1:A:57:ARG:HH21	1.98	0.60
1:B:57:ARG:HD3	1:B:369:VAL:CG1	2.32	0.60
1:B:506:LEU:O	1:B:510:GLU:HG3	2.02	0.60
1:B:237:ASN:CG	1:B:243:VAL:HG22	2.26	0.60
1:A:13:ILE:HD13	1:A:23:ALA:HB3	1.83	0.60
1:A:288:LYS:HD2	1:A:461:ASP:OD1	2.02	0.59
1:A:404:LYS:NZ	1:A:407:LYS:HD3	2.17	0.59
1:B:486:ALA:O	3:B:518:SP9:CAN	2.50	0.59
1:B:502:ARG:HG2	1:B:502:ARG:HH11	1.68	0.59
1:A:265:GLU:OE2	1:A:267:ASN:HB3	2.02	0.59
1:A:466:MET:HE2	1:A:466:MET:HA	1.84	0.59
1:A:78:GLU:CD	1:A:204:VAL:HG22	2.28	0.59
1:A:395:PHE:CD1	1:A:432:LEU:HD23	2.38	0.59
1:B:253:VAL:HG11	1:B:272:ILE:HD11	1.85	0.59
1:A:169:ARG:O	1:A:172:GLU:HG3	2.03	0.59
1:B:67:HIS:CD2	3:B:518:SP9:CAB	2.83	0.59
1:B:157:THR:OG1	1:B:160:GLN:HG3	2.03	0.59
1:B:267:ASN:O	1:B:268:LEU:C	2.46	0.59
1:B:479:GLU:HB2	1:B:487:GLY:CA	2.32	0.59
1:B:249:VAL:O	1:B:249:VAL:HG13	2.01	0.58
1:B:213:PRO:HG2	1:B:216:TRP:CD2	2.39	0.58
1:B:258:LEU:HD21	1:B:476:PHE:CE2	2.38	0.58
1:A:177:LEU:CD2	1:A:452:ALA:HB1	2.33	0.58
1:B:176:GLY:O	1:B:177:LEU:HD12	2.03	0.58
1:B:502:ARG:HG2	1:B:502:ARG:NH1	2.19	0.58
1:A:283:GLN:HA	1:A:286:PHE:CD1	2.39	0.58
1:A:442:ARG:HG2	1:A:442:ARG:HH11	1.68	0.57
1:B:359:PHE:HD2	1:B:375:LEU:HD22	1.68	0.57
1:A:200:ASN:O	1:A:203:SER:HB3	2.05	0.57
1:B:271:ARG:HD3	1:B:271:ARG:C	2.30	0.57
1:B:271:ARG:HH21	1:B:273:GLU:CG	2.18	0.57
1:A:167:LEU:HA	1:A:316:LEU:CD2	2.34	0.57
1:A:324:VAL:O	1:A:328:ARG:HG2	2.05	0.56
1:A:353:CYS:SG	1:A:401:VAL:HG13	2.44	0.56
1:B:12:ILE:HG12	1:B:36:LEU:HB2	1.87	0.56
1:A:237:ASN:OD1	1:A:243:VAL:HG22	2.05	0.56
1:A:388:ARG:HB2	1:A:437:VAL:HB	1.87	0.56
1:B:37:VAL:HB	1:B:217:LEU:HD12	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:295:GLY:HA3	1:B:381:THR:HG23	1.88	0.56
1:A:138:ASP:OD2	1:A:455:PRO:HA	2.06	0.56
1:A:228:ARG:HG2	1:A:228:ARG:HH11	1.70	0.56
1:B:226:ILE:HD12	1:B:274:PHE:CE2	2.41	0.56
1:A:434:ASN:ND2	1:A:435:ILE:H	2.03	0.56
1:B:362:ASN:ND2	1:B:364:SER:H	2.04	0.56
1:B:475:ARG:HB3	1:B:499:GLU:OE1	2.06	0.56
1:A:395:PHE:CE2	1:A:416:ASP:HB2	2.41	0.56
1:B:39:GLU:OE2	2:B:517:FAD:H1B	2.05	0.55
1:A:336:LEU:HA	1:A:339:MET:HE3	1.89	0.55
1:A:108:ASP:O	1:A:109:HIS:C	2.50	0.55
1:A:171:LEU:HD13	1:A:187:THR:CG2	2.34	0.55
1:B:77:GLU:O	1:B:80:GLN:HB2	2.07	0.55
1:B:353:CYS:SG	1:B:401:VAL:HG13	2.47	0.55
1:B:377:GLN:NE2	1:B:377:GLN:N	2.55	0.55
1:A:184:ALA:O	1:A:186:ASP:N	2.41	0.55
1:B:70:LEU:HD23	1:A:152:ARG:CZ	2.37	0.54
1:B:259:ASN:O	1:B:262:VAL:HG22	2.07	0.54
1:B:421:ILE:O	1:B:421:ILE:HG22	2.05	0.54
1:A:138:ASP:OD1	1:A:185:LYS:HB2	2.07	0.54
1:A:306:TRP:HE1	1:A:362:ASN:HD21	1.56	0.54
1:B:102:GLU:HG3	1:B:354:TRP:CZ2	2.42	0.54
1:B:375:LEU:CD2	3:B:518:SP9:HAS	2.38	0.54
1:A:138:ASP:O	1:A:139:CYS:CB	2.56	0.54
1:A:341:GLU:O	1:A:342:ARG:C	2.50	0.54
1:B:226:ILE:O	1:B:274:PHE:HA	2.08	0.54
1:A:125:PHE:CD2	1:A:148:TYR:HB2	2.42	0.54
1:B:67:HIS:CE1	3:B:518:SP9:HAE	2.43	0.54
1:B:485:GLY:O	1:B:488:CYS:HB2	2.08	0.54
1:B:242:THR:HB	1:B:244:TYR:CE1	2.42	0.54
1:B:302:GLU:HG3	1:B:431:VAL:HB	1.89	0.53
1:A:432:LEU:HD21	1:A:435:ILE:HD11	1.91	0.53
1:B:14:ILE:CD1	1:B:226:ILE:HD11	2.38	0.53
1:B:119:ASP:O	1:B:122:MET:HB3	2.09	0.53
1:A:48:LEU:CD2	1:A:63:ALA:HB3	2.39	0.53
1:B:14:ILE:HD12	1:B:226:ILE:HD11	1.91	0.53
1:B:193:GLY:HA2	1:A:121:GLU:HG3	1.90	0.53
1:A:265:GLU:CG	1:A:268:LEU:HG	2.38	0.53
1:A:414:VAL:HA	1:A:430:PRO:HG2	1.91	0.53
1:B:63:ALA:HA	2:B:517:FAD:N5	2.23	0.53
1:B:72:ASN:C	1:B:72:ASN:ND2	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:226:ILE:HG12	1:B:236:VAL:CG1	2.39	0.53
1:A:98:ILE:HG12	1:A:106:ARG:NH2	2.24	0.53
1:A:320:THR:O	1:A:323:PHE:HB3	2.09	0.53
1:A:322:GLU:O	1:A:326:ILE:HG13	2.09	0.53
1:A:449:ALA:O	2:A:517:FAD:HM81	2.08	0.53
1:B:279:LYS:HE2	1:B:470:GLN:HA	1.91	0.53
1:A:289:ILE:HG21	1:A:462:MET:HB2	1.92	0.52
1:B:99:TYR:H	1:B:108:ASP:HB3	1.74	0.52
1:A:267:ASN:ND2	1:A:269:ARG:HH22	2.08	0.52
1:A:395:PHE:HD1	1:A:432:LEU:HD23	1.75	0.52
1:A:503:ILE:O	1:A:507:LEU:HG	2.10	0.52
1:B:362:ASN:HD21	1:B:364:SER:CB	2.22	0.52
1:A:99:TYR:H	1:A:108:ASP:HB3	1.75	0.52
1:A:177:LEU:HD21	1:A:452:ALA:CB	2.39	0.52
1:A:434:ASN:ND2	1:A:435:ILE:N	2.58	0.52
1:B:67:HIS:ND1	1:B:195:ASN:OD1	2.43	0.52
1:B:36:LEU:HB3	1:B:38:LEU:HD21	1.92	0.52
1:B:48:LEU:CD2	1:B:63:ALA:HB3	2.40	0.51
1:A:55:GLN:NE2	1:A:57:ARG:NH2	2.59	0.51
1:B:104:ARG:CZ	1:B:113:LEU:HD11	2.40	0.51
1:A:89:ARG:HG3	1:A:89:ARG:HH11	1.75	0.51
1:A:265:GLU:HG2	1:A:268:LEU:HG	1.91	0.51
1:B:81:LEU:HD11	1:B:207:ARG:HH11	1.73	0.51
1:A:5:SER:HB2	1:A:6:PRO:CD	2.41	0.51
1:B:279:LYS:HG2	1:B:470:GLN:OE1	2.11	0.51
1:A:259:ASN:O	1:A:262:VAL:HG22	2.11	0.51
1:B:72:ASN:HD21	1:B:74:LEU:HB3	1.75	0.51
1:B:359:PHE:CD2	1:B:375:LEU:HD22	2.46	0.51
1:B:485:GLY:HA3	1:B:490:TYR:CE1	2.46	0.51
1:A:130:PHE:O	1:A:131:HIS:C	2.54	0.51
1:B:178:ASP:OD1	1:B:179:TRP:HD1	1.94	0.50
1:B:362:ASN:ND2	1:B:362:ASN:C	2.68	0.50
1:A:356:GLN:HB2	1:A:357:PRO:HD2	1.93	0.50
1:B:171:LEU:HD13	1:B:187:THR:HG22	1.93	0.50
1:B:440:TRP:HB3	1:B:448:GLY:O	2.11	0.50
1:A:295:GLY:HA3	1:A:381:THR:HG23	1.94	0.50
1:B:226:ILE:HG12	1:B:236:VAL:HG12	1.94	0.50
1:B:288:LYS:O	1:B:289:ILE:O	2.30	0.50
1:B:405:ILE:HG22	1:B:409:LEU:HD12	1.93	0.50
1:A:449:ALA:HA	2:A:517:FAD:C8M	2.42	0.50
1:A:77:GLU:HG2	1:A:207:ARG:NH2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:VAL:HG23	1:A:376:MET:HE2	1.93	0.50
1:B:52:THR:HA	1:B:57:ARG:O	2.11	0.50
1:B:212:PHE:HB2	1:B:213:PRO:HD2	1.94	0.50
1:A:73:PRO:HB2	1:A:493:TRP:CZ3	2.47	0.49
1:B:57:ARG:HD3	1:B:369:VAL:HG11	1.94	0.49
1:A:63:ALA:HA	2:A:517:FAD:C4X	2.42	0.49
1:A:91:VAL:HG13	1:A:91:VAL:O	2.10	0.49
1:A:164:LEU:N	1:A:165:PRO:HD2	2.27	0.49
1:B:488:CYS:SG	3:B:518:SP9:CAN	2.91	0.49
1:A:449:ALA:HA	2:A:517:FAD:HM81	1.94	0.49
1:B:36:LEU:CD1	1:B:244:TYR:CD2	2.96	0.49
1:A:399:GLN:N	1:A:400:PRO:HD2	2.28	0.49
1:B:37:VAL:C	1:B:38:LEU:HD23	2.38	0.49
1:B:453:CYS:HA	1:B:457:ASP:OD2	2.12	0.49
1:A:184:ALA:C	1:A:186:ASP:N	2.69	0.49
1:B:113:LEU:CD2	1:B:159:ASP:HB3	2.43	0.49
1:A:60:ASP:HB3	1:A:63:ALA:O	2.13	0.49
1:A:457:ASP:O	1:A:459:PRO:HD3	2.13	0.49
1:A:133:HIS:HB3	1:A:136:VAL:HG21	1.94	0.49
1:A:113:LEU:HB3	1:A:115:LEU:HG	1.95	0.48
1:A:157:THR:OG1	1:A:160:GLN:HG3	2.13	0.48
1:B:265:GLU:O	1:B:267:ASN:N	2.45	0.48
1:A:311:SER:HA	1:A:362:ASN:HB3	1.95	0.48
1:B:176:GLY:C	1:B:177:LEU:HD12	2.38	0.48
1:B:254:PRO:HD3	2:B:517:FAD:H51A	1.95	0.48
1:B:294:LEU:HD22	1:B:450:TYR:OH	2.13	0.48
1:A:5:SER:HB2	1:A:6:PRO:HD3	1.95	0.48
1:A:12:ILE:HG13	1:A:246:ALA:HB2	1.94	0.48
1:A:133:HIS:HB3	1:A:136:VAL:CG2	2.43	0.48
1:B:22:LYS:HG3	1:B:493:TRP:CD1	2.48	0.48
1:B:16:ALA:HB2	1:B:39:GLU:HB2	1.96	0.48
1:B:67:HIS:NE2	3:B:518:SP9:CAB	2.76	0.48
1:B:177:LEU:HD21	1:B:454:PHE:CE2	2.49	0.48
1:B:305:CYS:O	1:B:305:CYS:SG	2.72	0.48
1:A:434:ASN:HD22	1:A:435:ILE:H	1.62	0.48
1:B:412:GLU:CD	1:B:429:LYS:HG2	2.39	0.48
1:B:296:LYS:HE2	1:B:373:MET:SD	2.54	0.47
1:A:442:ARG:HG2	1:A:442:ARG:NH1	2.29	0.47
1:B:74:LEU:HD13	1:B:493:TRP:NE1	2.29	0.47
1:A:122:MET:O	1:A:125:PHE:HB3	2.15	0.47
1:A:87:ARG:HB2	1:A:89:ARG:HH12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ALA:C	1:A:186:ASP:H	2.22	0.47
1:B:338:SER:C	1:B:340:LEU:N	2.72	0.47
1:A:66:HIS:HB2	1:A:196:ALA:HB3	1.96	0.47
1:B:38:LEU:HD23	1:B:38:LEU:N	2.30	0.47
1:A:28:HIS:CD2	1:A:213:PRO:HD3	2.50	0.47
1:A:158:ASN:ND2	1:A:328:ARG:HH21	2.13	0.47
1:A:177:LEU:CD1	1:A:292:GLY:HA2	2.45	0.47
1:B:358:LEU:HD22	1:B:374:MET:CE	2.43	0.47
1:A:107:VAL:O	1:A:115:LEU:HD12	2.15	0.47
1:A:374:MET:HG2	1:A:375:LEU:N	2.30	0.47
1:B:499:GLU:O	1:B:503:ILE:HG13	2.14	0.46
1:A:135:GLY:O	1:A:136:VAL:C	2.58	0.46
1:A:212:PHE:O	1:A:213:PRO:C	2.57	0.46
1:B:331:GLU:O	1:B:332:ASN:HB3	2.15	0.46
1:A:228:ARG:HG2	1:A:228:ARG:NH1	2.30	0.46
1:B:22:LYS:HE3	1:B:493:TRP:CZ2	2.50	0.46
1:A:262:VAL:CG1	1:A:283:GLN:HB3	2.46	0.46
1:A:298:ILE:HB	1:A:436:ILE:HB	1.96	0.46
1:A:439:ASN:HD21	1:A:442:ARG:HD3	1.80	0.46
1:B:48:LEU:HD22	1:B:63:ALA:HB3	1.97	0.46
1:A:387:ILE:O	1:A:387:ILE:HG13	2.16	0.46
1:B:260:LEU:HD11	1:B:447:ARG:NH1	2.31	0.46
1:B:382:ASN:HB3	4:B:522:HOH:O	2.15	0.46
1:A:46:GLY:C	1:A:48:LEU:H	2.23	0.46
1:A:138:ASP:O	1:A:139:CYS:HB3	2.14	0.46
1:A:165:PRO:O	1:A:169:ARG:HG3	2.15	0.46
1:A:166:GLN:OE1	1:A:317:ALA:HB3	2.16	0.46
1:A:239:GLU:C	1:A:241:GLY:H	2.24	0.46
1:A:268:LEU:O	1:A:269:ARG:C	2.59	0.46
1:B:13:ILE:HD12	1:B:24:ALA:HB2	1.98	0.46
1:B:36:LEU:HD13	1:B:244:TYR:CD2	2.51	0.46
1:B:102:GLU:HG3	1:B:354:TRP:CE2	2.50	0.46
1:B:332:ASN:C	1:B:332:ASN:ND2	2.69	0.46
1:B:36:LEU:HD11	1:B:244:TYR:HD2	1.80	0.45
1:B:113:LEU:HD21	1:B:159:ASP:HB3	1.97	0.45
1:B:142:PHE:HB2	1:B:179:TRP:O	2.16	0.45
2:B:517:FAD:C2	3:B:518:SP9:CAB	2.95	0.45
1:A:240:ASP:OD1	1:A:240:ASP:C	2.60	0.45
1:B:67:HIS:NE2	3:B:518:SP9:CAI	2.80	0.45
1:A:32:ILE:HD12	1:A:507:LEU:HD12	1.99	0.45
1:B:125:PHE:CD2	1:B:148:TYR:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:HIS:HE1	3:B:518:SP9:CAE	2.29	0.45
1:B:169:ARG:HD2	1:B:179:TRP:CE2	2.52	0.45
2:B:517:FAD:N3	3:B:518:SP9:HABA	2.31	0.45
1:B:95:ASP:OD2	1:B:365:LYS:NZ	2.40	0.45
1:B:268:LEU:O	1:B:269:ARG:C	2.58	0.45
1:A:306:TRP:CZ3	1:A:406:MET:HE1	2.51	0.45
1:B:110:ASP:HB3	1:B:113:LEU:HB2	1.98	0.45
1:B:275:GLN:HA	1:B:276:PRO:C	2.40	0.45
1:B:353:CYS:HB3	1:B:397:PHE:O	2.16	0.45
1:B:485:GLY:O	1:B:486:ALA:C	2.60	0.45
1:A:72:ASN:HB3	1:A:75:PHE:HB3	1.98	0.45
1:A:162:ARG:HB2	1:A:324:VAL:HG22	1.99	0.45
1:A:460:VAL:O	1:A:464:VAL:HG23	2.17	0.45
1:A:40:ALA:O	1:A:220:SER:HA	2.16	0.45
1:A:158:ASN:HD22	1:A:328:ARG:HH21	1.62	0.45
1:A:185:LYS:HB2	1:A:185:LYS:HE3	1.81	0.45
1:A:338:SER:O	1:A:339:MET:C	2.59	0.45
1:B:479:GLU:OE1	1:B:487:GLY:HA2	2.17	0.45
1:A:291:PHE:CD2	1:A:448:GLY:HA3	2.51	0.44
1:A:326:ILE:HG21	1:A:340:LEU:CD2	2.46	0.44
1:B:41:ARG:NH1	2:B:517:FAD:O2B	2.51	0.44
1:A:87:ARG:HB2	1:A:89:ARG:NH1	2.31	0.44
1:A:175:HIS:CD2	1:A:182:LEU:HD21	2.51	0.44
1:B:13:ILE:HD13	1:B:23:ALA:HB3	1.99	0.44
1:B:16:ALA:HB1	1:B:44:VAL:HG12	1.99	0.44
1:B:54:TYR:CE2	1:B:55:GLN:HG3	2.53	0.44
1:B:169:ARG:NE	1:B:172:GLU:OE2	2.43	0.44
1:A:395:PHE:CZ	1:A:416:ASP:HB2	2.52	0.44
1:A:462:MET:SD	1:A:466:MET:HG2	2.56	0.44
1:B:167:LEU:HD23	1:B:167:LEU:C	2.43	0.44
1:A:118:VAL:CG2	1:A:164:LEU:HD22	2.47	0.44
1:B:115:LEU:HB3	1:B:167:LEU:HD13	1.98	0.44
1:A:158:ASN:ND2	1:A:328:ARG:HE	2.16	0.44
1:B:262:VAL:O	1:B:262:VAL:HG23	2.18	0.44
1:B:313:ILE:HG22	1:B:314:VAL:N	2.33	0.43
1:B:36:LEU:HD11	1:B:244:TYR:CD2	2.53	0.43
1:A:262:VAL:O	1:A:262:VAL:HG23	2.18	0.43
1:A:329:ASN:O	1:A:330:ALA:C	2.61	0.43
1:A:206:GLN:O	1:A:207:ARG:C	2.61	0.43
1:B:214:GLN:C	1:B:216:TRP:H	2.27	0.43
2:B:517:FAD:C10	3:B:518:SP9:HABB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:267:ASN:ND2	1:A:267:ASN:O	2.52	0.43
1:B:124:LYS:HD3	1:B:124:LYS:HA	1.88	0.42
1:B:141:PHE:CZ	1:B:171:LEU:HD12	2.54	0.42
1:B:251:ILE:HD13	1:B:274:PHE:HE2	1.82	0.42
1:A:11:VAL:HB	1:A:35:CYS:SG	2.58	0.42
1:A:11:VAL:HG11	1:A:27:LEU:HD11	2.01	0.42
1:A:414:VAL:HG22	1:A:430:PRO:HG2	2.01	0.42
1:B:314:VAL:HA	1:B:358:LEU:O	2.19	0.42
1:A:335:GLU:CG	1:A:339:MET:HE2	2.41	0.42
1:A:340:LEU:O	1:A:342:ARG:N	2.52	0.42
1:B:249:VAL:CG1	1:B:474:ILE:HG23	2.50	0.42
1:B:404:LYS:HD2	1:B:404:LYS:HA	1.85	0.42
1:A:189:PHE:CD1	1:A:189:PHE:C	2.97	0.42
1:B:41:ARG:HH21	1:B:443:ASP:CG	2.28	0.42
1:B:169:ARG:HD2	1:B:179:TRP:CD2	2.54	0.42
1:A:150:LEU:C	1:A:150:LEU:HD13	2.44	0.42
1:B:17:GLY:O	1:B:21:LEU:HG	2.19	0.42
1:B:59:TYR:HE1	1:B:300:GLU:OE2	2.01	0.42
1:B:219:LEU:O	1:B:220:SER:HB2	2.20	0.42
1:B:362:ASN:HD21	1:B:364:SER:HB2	1.85	0.42
1:A:158:ASN:HD21	1:A:328:ARG:HE	1.68	0.42
1:B:63:ALA:HB2	2:B:517:FAD:O2'	2.20	0.42
1:A:296:LYS:HA	1:A:374:MET:O	2.20	0.42
1:B:39:GLU:CD	2:B:517:FAD:HO3A	2.28	0.42
1:B:268:LEU:O	1:B:271:ARG:HB3	2.19	0.42
1:A:14:ILE:HD12	1:A:14:ILE:N	2.35	0.42
1:A:275:GLN:HA	1:A:276:PRO:C	2.44	0.42
1:A:308:ASN:HB3	1:A:365:LYS:HB2	2.01	0.42
1:B:35:CYS:HB2	1:B:216:TRP:CE2	2.54	0.42
1:B:46:GLY:C	1:B:48:LEU:H	2.28	0.42
1:B:240:ASP:OD1	1:B:241:GLY:N	2.53	0.42
2:B:517:FAD:C2	3:B:518:SP9:HABA	2.50	0.42
1:A:294:LEU:H	1:A:449:ALA:CB	2.33	0.42
1:A:294:LEU:HD12	1:A:376:MET:O	2.19	0.42
1:B:63:ALA:HA	2:B:517:FAD:C4X	2.50	0.42
1:B:68:ASP:C	1:B:70:LEU:H	2.28	0.42
1:A:437:VAL:HG12	1:A:438:SER:N	2.34	0.42
1:A:106:ARG:HH12	1:A:309:GLU:CD	2.28	0.41
2:A:517:FAD:HM71	2:A:517:FAD:HM83	1.89	0.41
1:A:164:LEU:C	1:A:164:LEU:HD12	2.45	0.41
1:B:199:LEU:HD23	1:B:199:LEU:HA	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:SER:H	1:B:143:GLN:CD	2.26	0.41
1:B:154:GLN:NE2	1:A:83:LEU:HB2	2.35	0.41
1:B:429:LYS:H	1:B:429:LYS:HG3	1.51	0.41
1:A:57:ARG:HD3	1:A:369:VAL:HG13	2.02	0.41
1:B:59:TYR:OH	1:B:300:GLU:HG2	2.21	0.41
1:B:356:GLN:CD	1:B:356:GLN:N	2.78	0.41
1:B:447:ARG:HG2	1:B:447:ARG:HH11	1.86	0.41
1:A:247:ASP:O	1:A:473:ARG:HD3	2.21	0.41
1:B:169:ARG:C	1:B:171:LEU:N	2.74	0.41
1:B:274:PHE:CD1	1:B:274:PHE:N	2.88	0.41
1:B:349:THR:O	1:B:350:SER:CB	2.69	0.41
1:A:239:GLU:C	1:A:241:GLY:N	2.78	0.41
1:A:340:LEU:O	1:A:341:GLU:C	2.64	0.41
1:B:226:ILE:HB	1:B:274:PHE:CD2	2.56	0.41
1:A:169:ARG:C	1:A:171:LEU:N	2.75	0.41
1:A:170:TYR:CD1	1:A:170:TYR:C	2.98	0.41
1:A:226:ILE:HD13	1:A:251:ILE:HD11	2.03	0.41
1:A:285:ALA:O	1:A:289:ILE:HG22	2.20	0.41
1:A:35:CYS:HB2	1:A:216:TRP:CH2	2.56	0.41
1:A:138:ASP:O	1:A:139:CYS:SG	2.79	0.41
1:B:9:LYS:HG3	1:B:36:LEU:CD1	2.50	0.41
1:B:88:THR:HG22	1:B:199:LEU:HD12	2.02	0.41
1:B:91:VAL:HG13	1:B:91:VAL:O	2.21	0.41
1:B:93:ASP:OD2	1:B:197:PHE:HB2	2.20	0.41
1:B:152:ARG:O	1:B:153:ARG:C	2.62	0.41
1:B:311:SER:OG	1:B:312:LYS:NZ	2.54	0.41
1:B:502:ARG:HH11	1:B:502:ARG:CG	2.33	0.41
1:A:339:MET:O	1:A:340:LEU:C	2.64	0.41
1:B:213:PRO:HG2	1:B:216:TRP:CG	2.55	0.41
1:A:171:LEU:CD1	1:A:187:THR:HG22	2.38	0.41
1:A:307:SER:O	1:A:409:LEU:HD22	2.21	0.41
1:B:148:TYR:CE1	1:B:152:ARG:HG3	2.55	0.40
1:B:217:LEU:HD21	1:B:219:LEU:HD21	2.02	0.40
1:A:129:GLU:OE1	1:A:129:GLU:HA	2.21	0.40
1:A:263:GLN:HB3	1:A:264:PRO:CD	2.45	0.40
1:B:466:MET:CB	1:B:481:THR:HG22	2.43	0.40
1:A:115:LEU:O	1:A:118:VAL:HG22	2.20	0.40
1:A:200:ASN:N	4:A:518:HOH:O	2.54	0.40
1:A:250:ILE:HD11	1:A:503:ILE:HD12	2.03	0.40
1:B:12:ILE:O	1:B:249:VAL:HG23	2.21	0.40
1:B:234:VAL:CG2	1:B:473:ARG:HB3	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ARG:HG3	1:B:445:TYR:CE2	2.57	0.40
1:A:326:ILE:HD13	1:A:340:LEU:HD23	2.04	0.40
1:B:387:ILE:O	1:B:387:ILE:HG13	2.22	0.40
1:A:449:ALA:CA	2:A:517:FAD:HM81	2.51	0.40

All (2) 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:269:ARG:NH2	1:A:269:ARG:NH2[2_555]	1.98	0.22
1:A:269:ARG:NE	1:A:269:ARG:NE[2_555]	2.19	0.01

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	491/516 (95%)	428 (87%)	47 (10%)	16 (3%)	3	7
1	B	489/516 (95%)	405 (83%)	60 (12%)	24 (5%)	1	3
All	All	980/1032 (95%)	833 (85%)	107 (11%)	40 (4%)	2	5

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	266	LYS
1	B	289	ILE
1	B	290	HIS
1	B	341	GLU
1	A	131	HIS
1	A	136	VAL
1	A	139	CYS
1	A	317	ALA

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Mol	Chain	Res	Type
1	A	338	SER
1	B	55	GLN
1	B	342	ARG
1	B	427	ALA
1	B	460	VAL
1	B	469	GLY
1	A	185	LYS
1	A	200	ASN
1	A	339	MET
1	B	69	THR
1	B	232	LYS
1	B	242	THR
1	A	132	GLN
1	A	340	LEU
1	A	341	GLU
1	A	342	ARG
1	B	44	VAL
1	B	86	GLY
1	B	231	SER
1	B	239	GLU
1	B	268	LEU
1	B	455	PRO
1	A	47	ARG
1	A	265	GLU
1	A	413	ASP
1	B	200	ASN
1	B	350	SER
1	B	370	ALA
1	B	420	PRO
1	B	421	ILE
1	A	138	ASP
1	B	241	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	420/457 (92%)	403 (96%)	17 (4%)	28	56
1	B	400/457 (88%)	386 (96%)	14 (4%)	32	61
All	All	820/914 (90%)	789 (96%)	31 (4%)	29	58

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	34	ASP
1	B	72	ASN
1	B	123	SER
1	B	201	TYR
1	B	221	CYS
1	B	242	THR
1	B	273	GLU
1	B	316	LEU
1	B	332	ASN
1	B	377	GLN
1	B	380	LEU
1	B	447	ARG
1	B	474	ILE
1	B	479	GLU
1	A	22	LYS
1	A	177	LEU
1	A	183	SER
1	A	189	PHE
1	A	221	CYS
1	A	227	THR
1	A	239	GLU
1	A	269	ARG
1	A	281	VAL
1	A	283	GLN
1	A	332	ASN
1	A	377	GLN
1	A	389	GLU
1	A	404	LYS
1	A	439	ASN
1	A	484	ASP
1	A	508	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	28	HIS
1	B	30	ASN
1	B	72	ASN
1	B	80	GLN
1	B	151	GLN
1	B	192	GLN
1	B	255	GLN
1	B	259	ASN
1	B	275	GLN
1	B	318	ASN
1	B	329	ASN
1	B	332	ASN
1	B	362	ASN
1	B	377	GLN
1	B	382	ASN
1	B	423	ASN
1	B	434	ASN
1	B	439	ASN
1	B	470	GLN
1	A	28	HIS
1	A	33	GLN
1	A	49	GLN
1	A	55	GLN
1	A	158	ASN
1	A	245	ASN
1	A	267	ASN
1	A	362	ASN
1	A	377	GLN
1	A	434	ASN
1	A	439	ASN
1	A	468	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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$
2	FAD	B	517	-	58,58,58	1.34	7 (12%)	85,89,89	1.58	17 (20%)
3	SP9	B	518	-	19,19,19	0.48	0	21,22,22	0.58	0
2	FAD	A	517	-	58,58,58	1.34	7 (12%)	85,89,89	1.59	19 (22%)

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
2	FAD	B	517	-	-	2/34/50/50	0/6/6/6
3	SP9	B	518	-	-	13/16/16/16	0/1/1/1
2	FAD	A	517	-	-	1/34/50/50	0/6/6/6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	517	FAD	C4X-N5	4.51	1.40	1.30
2	A	517	FAD	C4X-N5	4.49	1.40	1.30
2	B	517	FAD	C10-N1	3.57	1.40	1.33
2	A	517	FAD	C10-N1	3.56	1.40	1.33
2	A	517	FAD	C5A-N7A	-3.19	1.33	1.39
2	B	517	FAD	C5A-N7A	-3.11	1.33	1.39
2	B	517	FAD	PA-O1A	3.07	1.61	1.50
2	A	517	FAD	PA-O1A	3.03	1.61	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	517	FAD	P-O1P	3.02	1.61	1.50
2	A	517	FAD	P-O1P	3.02	1.61	1.50
2	A	517	FAD	C8A-N9A	-2.32	1.33	1.37
2	B	517	FAD	C8A-N9A	-2.27	1.33	1.37
2	A	517	FAD	C4A-N9A	-2.11	1.33	1.37
2	B	517	FAD	C4A-N9A	-2.06	1.33	1.37

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	517	FAD	C5A-C4A-N3A	-5.02	119.80	126.72
2	A	517	FAD	C5A-C4A-N3A	-4.99	119.84	126.72
2	B	517	FAD	N3A-C2A-N1A	-4.60	121.62	128.58
2	A	517	FAD	N3A-C2A-N1A	-4.41	121.90	128.58
2	A	517	FAD	N3A-C4A-N9A	3.60	133.28	127.17
2	B	517	FAD	N3A-C4A-N9A	3.53	133.17	127.17
2	B	517	FAD	C2A-N3A-C4A	3.47	120.30	111.83
2	A	517	FAD	C2A-N3A-C4A	3.35	120.02	111.83
2	B	517	FAD	C4-N3-C2	-3.15	120.05	125.64
2	A	517	FAD	N9A-C8A-N7A	-3.07	109.58	113.94
2	B	517	FAD	N9A-C8A-N7A	-3.04	109.62	113.94
2	A	517	FAD	C4-N3-C2	-3.03	120.26	125.64
2	A	517	FAD	O4B-C1B-C2B	-3.01	100.18	106.62
2	B	517	FAD	C5A-N7A-C8A	2.75	107.77	103.45
2	A	517	FAD	C5A-N7A-C8A	2.73	107.73	103.45
2	B	517	FAD	C4X-C4-N3	2.70	120.11	113.25
2	B	517	FAD	C4A-C5A-N7A	-2.67	107.53	110.58
2	A	517	FAD	C4X-C4-N3	2.66	120.02	113.25
2	B	517	FAD	C9A-C5X-N5	-2.61	119.68	122.45
2	A	517	FAD	O2P-P-O3P	2.60	114.30	107.27
2	A	517	FAD	C4A-C5A-N7A	-2.59	107.62	110.58
2	A	517	FAD	O4-C4-C4X	-2.59	119.70	126.53
2	B	517	FAD	O2P-P-O3P	2.56	114.19	107.27
2	B	517	FAD	O4-C4-C4X	-2.56	119.78	126.53
2	A	517	FAD	C4B-O4B-C1B	-2.53	103.88	109.47
2	A	517	FAD	C9A-C5X-N5	-2.45	119.85	122.45
2	B	517	FAD	O4B-C1B-C2B	-2.44	101.38	106.62
2	B	517	FAD	C10-C4X-N5	-2.34	120.03	124.81
2	A	517	FAD	C4A-N9A-C8A	2.33	108.18	105.74
2	A	517	FAD	C10-C4X-N5	-2.28	120.16	124.81
2	A	517	FAD	C4X-C10-N10	2.28	119.74	116.48
2	A	517	FAD	C5X-C9A-N10	2.21	119.97	117.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	517	FAD	C4X-C10-N10	2.21	119.65	116.48
2	B	517	FAD	C4A-N9A-C8A	2.21	108.06	105.74
2	B	517	FAD	C5X-C9A-N10	2.21	119.96	117.97
2	A	517	FAD	O2A-PA-O3P	2.19	113.19	107.27

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	518	SP9	CAF-CAG-NAH-CAI
3	B	518	SP9	CAJ-CAI-NAH-CAG
3	B	518	SP9	NAH-CAI-CAJ-CAK
3	B	518	SP9	CAB-CAI-CAJ-CAK
3	B	518	SP9	OAA-CAG-NAH-CAI
3	B	518	SP9	NAL-CAM-CAN-CAO
3	B	518	SP9	CAS-CAF-CAG-OAA
3	B	518	SP9	CAS-CAF-CAG-NAH
3	B	518	SP9	CAM-CAN-CAO-CAP
3	B	518	SP9	CAE-CAF-CAG-OAA
3	B	518	SP9	CAE-CAF-CAG-NAH
3	B	518	SP9	CAN-CAM-NAL-CAK
3	B	518	SP9	CAN-CAO-CAP-NAQ
2	A	517	FAD	O4B-C4B-C5B-O5B
2	B	517	FAD	O4B-C4B-C5B-O5B
2	B	517	FAD	C2B-C1B-N9A-C8A

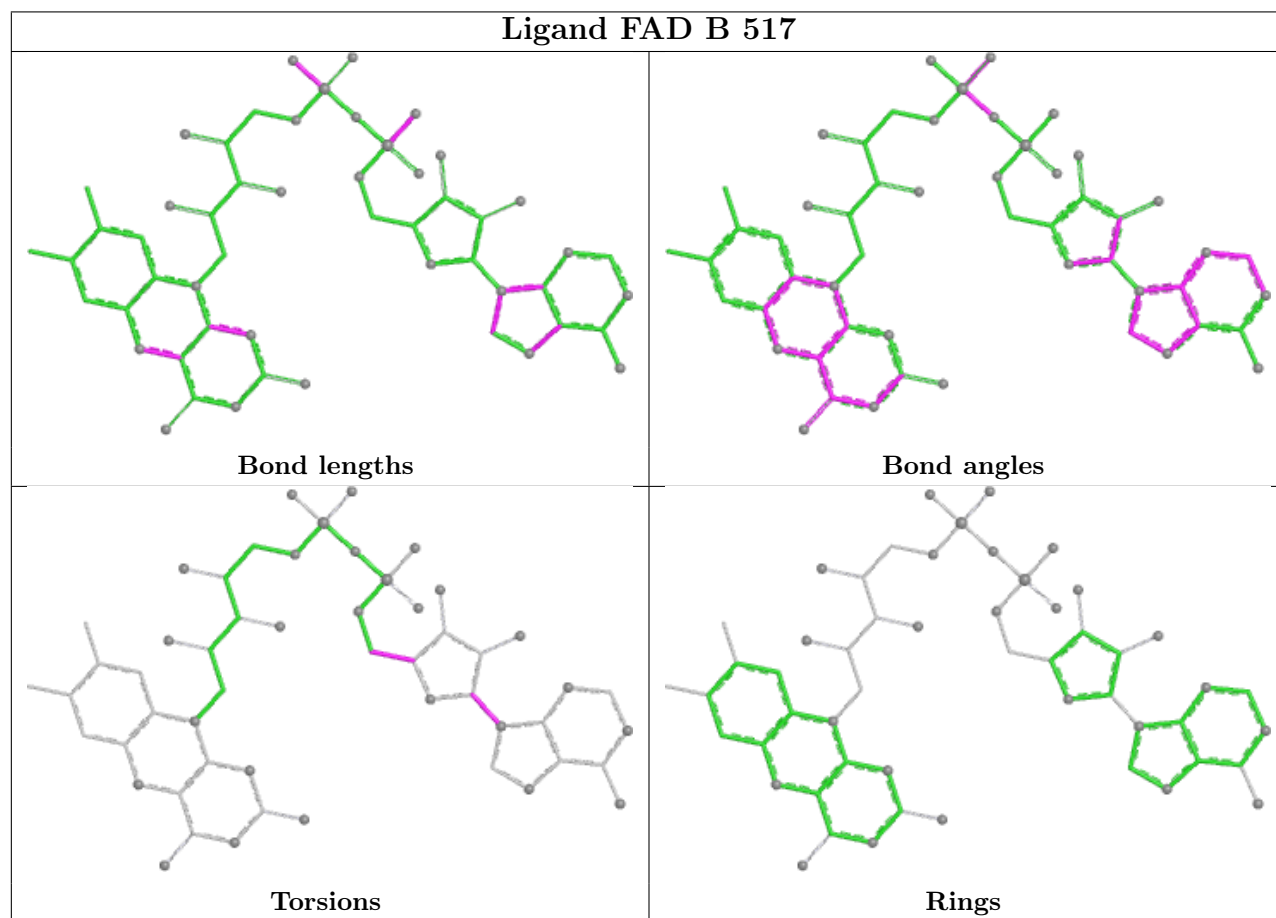
There are no ring outliers.

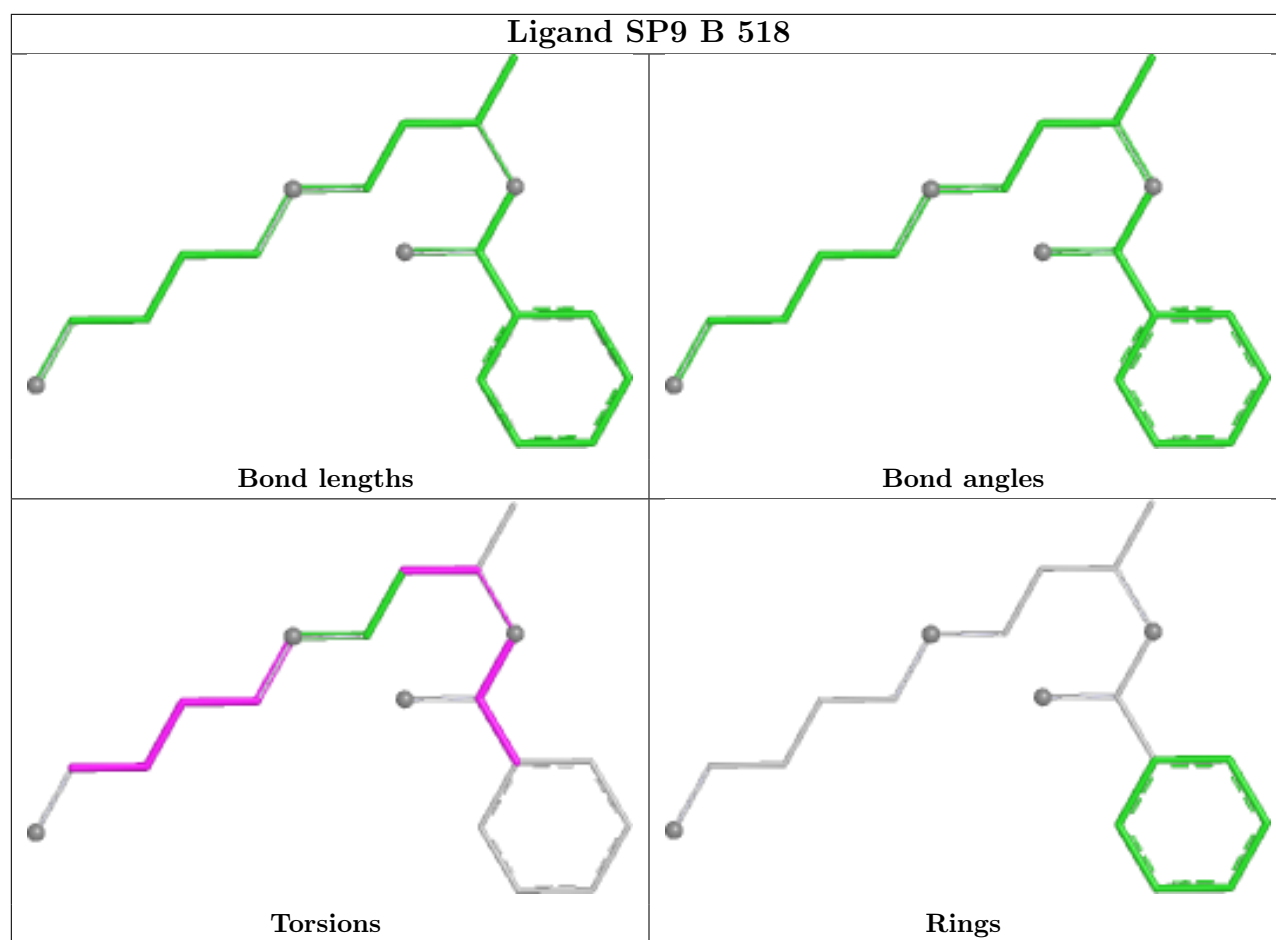
3 monomers are involved in 35 short contacts:

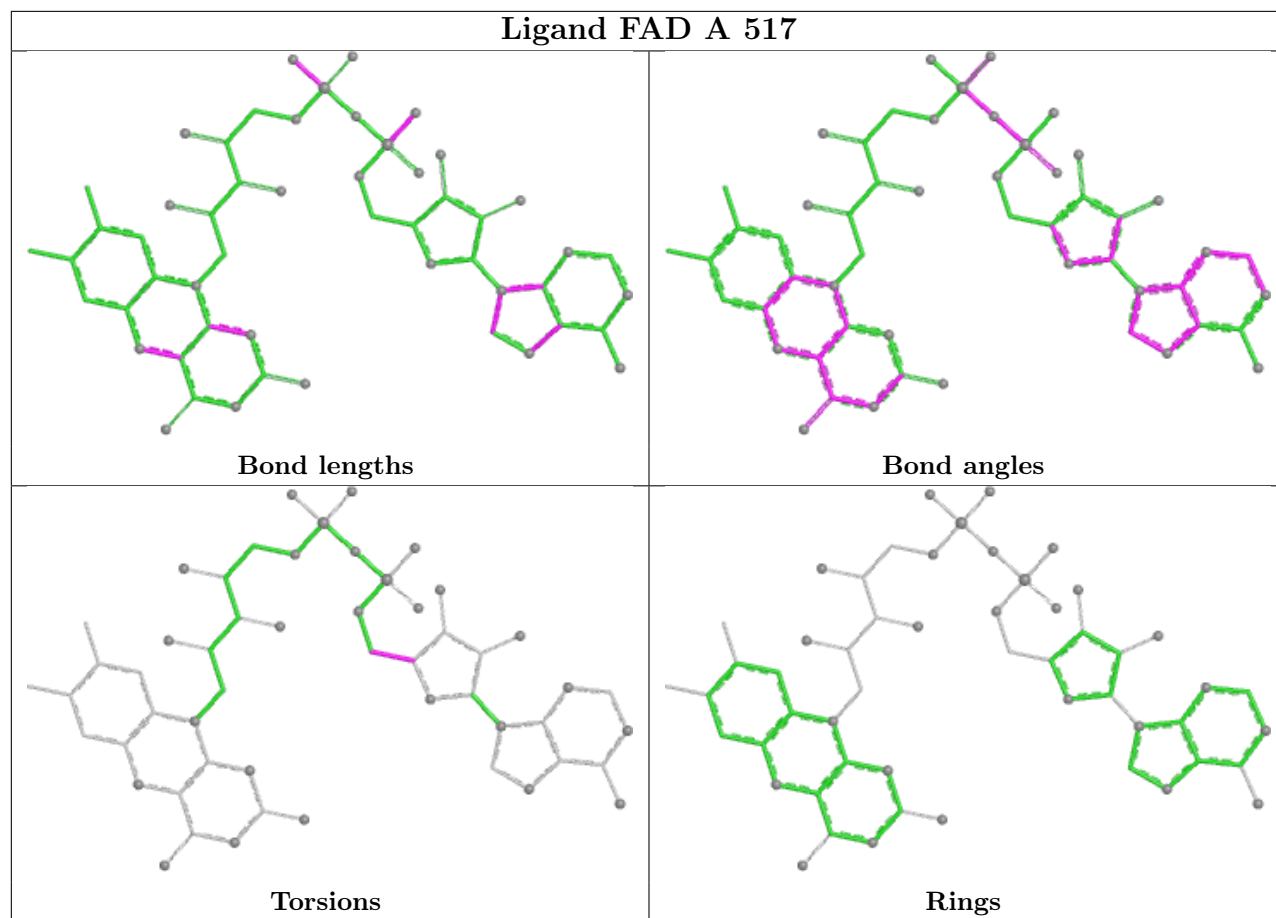
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	517	FAD	12	0
3	B	518	SP9	19	0
2	A	517	FAD	8	0

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 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	497/516 (96%)	0.37	22 (4%)	39 35	29, 54, 83, 107	0
1	B	495/516 (95%)	0.64	41 (8%)	17 14	40, 62, 91, 98	0
All	All	992/1032 (96%)	0.51	63 (6%)	25 22	29, 57, 90, 107	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	449	ALA	5.3
1	B	467	SER	5.0
1	B	511	HIS	5.0
1	B	448	GLY	4.3
1	B	32	ILE	4.0
1	B	425	ALA	3.9
1	B	289	ILE	3.8
1	A	343	GLU	3.4
1	B	291	PHE	3.4
1	B	341	GLU	3.4
1	A	509	LEU	3.2
1	B	233	ASN	3.2
1	A	342	ARG	3.2
1	A	264	PRO	3.2
1	A	454	PHE	3.0
1	B	428	ASN	3.0
1	B	454	PHE	2.9
1	B	236	VAL	2.8
1	B	476	PHE	2.7
1	A	321	ASN	2.7
1	A	268	LEU	2.7
1	B	230	PRO	2.7
1	A	457	ASP	2.6
1	A	131	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	349	THR	2.6
1	B	288	LYS	2.6
1	B	342	ARG	2.5
1	A	448	GLY	2.4
1	B	133	HIS	2.4
1	A	136	VAL	2.4
1	B	227	THR	2.3
1	B	235	THR	2.3
1	B	38	LEU	2.3
1	B	17	GLY	2.3
1	B	262	VAL	2.3
1	B	452	ALA	2.2
1	B	349	THR	2.2
1	B	463	VAL	2.2
1	A	427	ALA	2.2
1	A	189	PHE	2.2
1	B	237	ASN	2.2
1	A	428	ASN	2.2
1	A	288	LYS	2.2
1	A	417	GLY	2.2
1	B	290	HIS	2.2
1	A	341	GLU	2.1
1	B	134	LEU	2.1
1	B	340	LEU	2.1
1	B	507	LEU	2.1
1	B	220	SER	2.1
1	A	269	ARG	2.1
1	B	509	LEU	2.1
1	B	15	GLY	2.1
1	B	343	GLU	2.1
1	B	280	PRO	2.1
1	B	466	MET	2.1
1	A	340	LEU	2.1
1	B	506	LEU	2.1
1	B	286	PHE	2.1
1	B	450	TYR	2.0
1	B	460	VAL	2.0
1	A	230	PRO	2.0
1	A	177	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

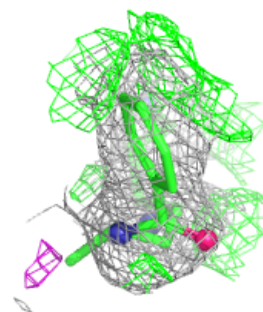
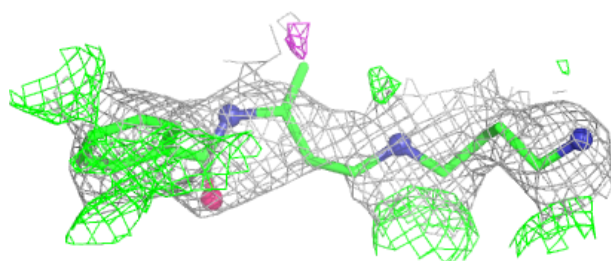
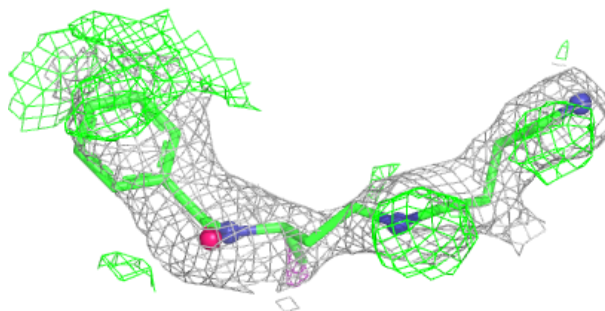
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SP9	B	518	19/19	0.71	0.22	53,70,75,75	0
2	FAD	B	517	53/53	0.92	0.10	47,52,55,57	0
2	FAD	A	517	53/53	0.96	0.08	27,35,41,44	0

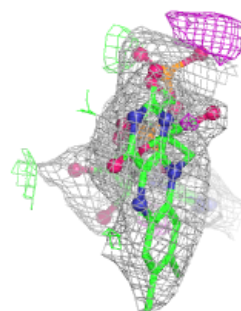
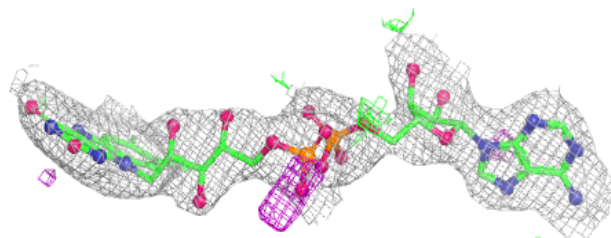
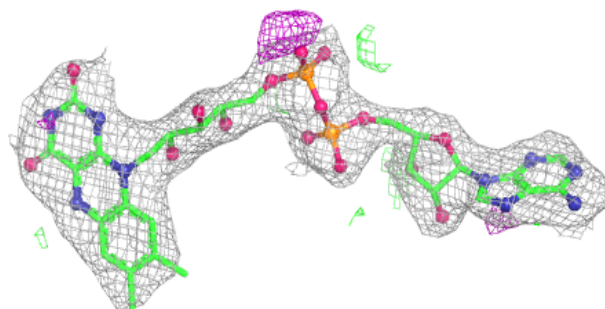
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

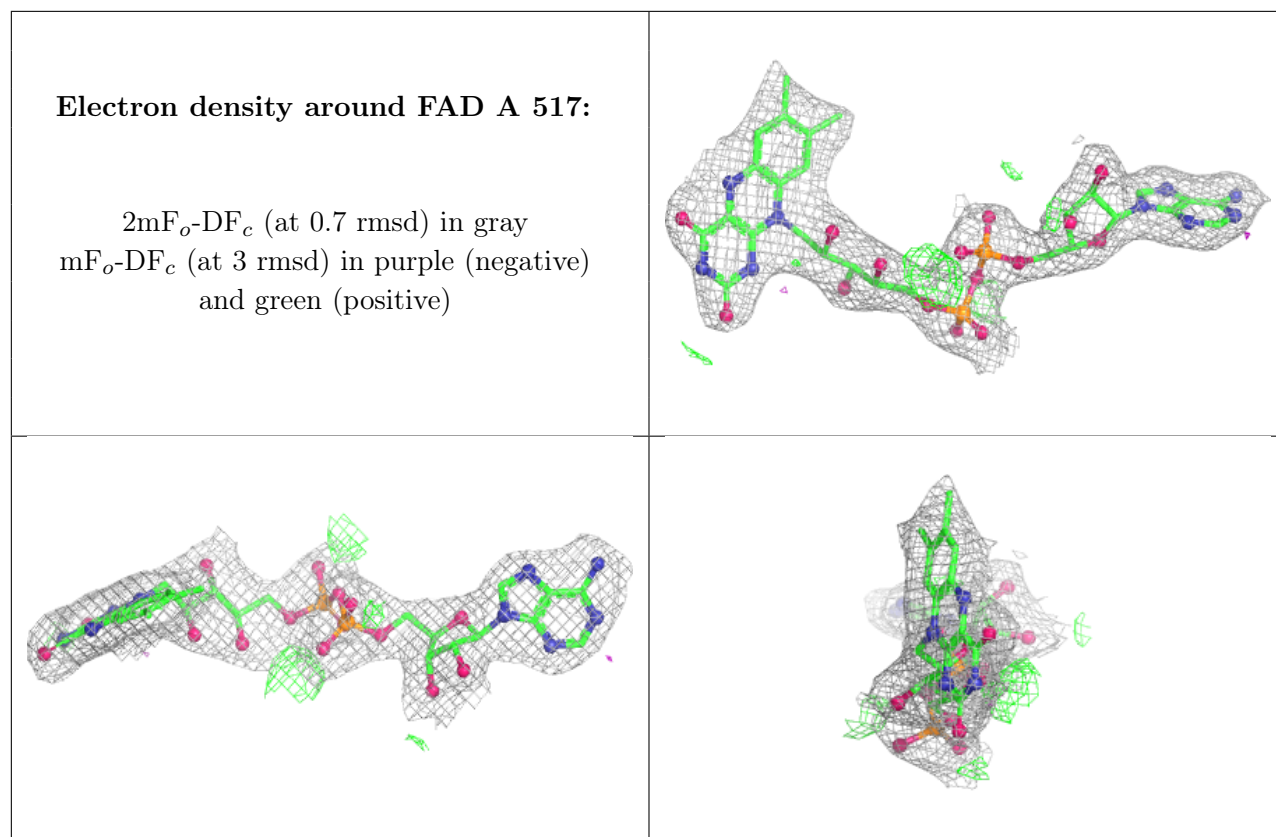
Electron density around SP9 B 518:

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

**Electron density around FAD B 517:**

$2mF_o-DF_c$ (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.