



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:07 PM UTC

PDB ID : 3CNP / pdb_00003cnp
Title : Crystal structure of fms1 in complex with S-N1-AcMeSpermidine
Authors : Huang, Q.; Hao, Q.
Deposited on : 2008-03-26
Resolution : 2.50 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

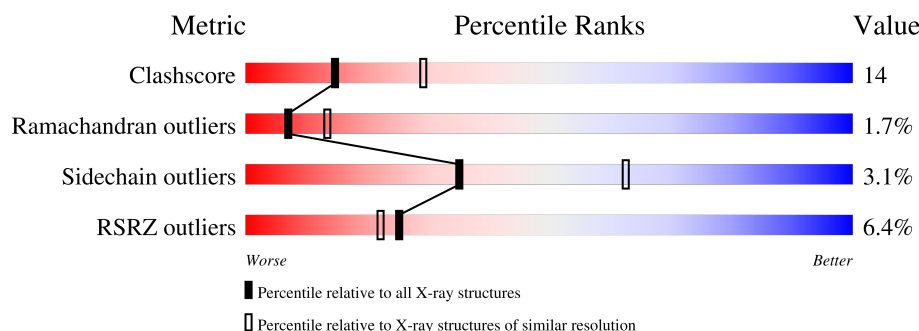
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	5% 70% 24% • •
1	B	516	7% 66% 28% • •

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	SP7	A	518	-	-	X	-
3	SP7	B	518	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	519	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8095 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.

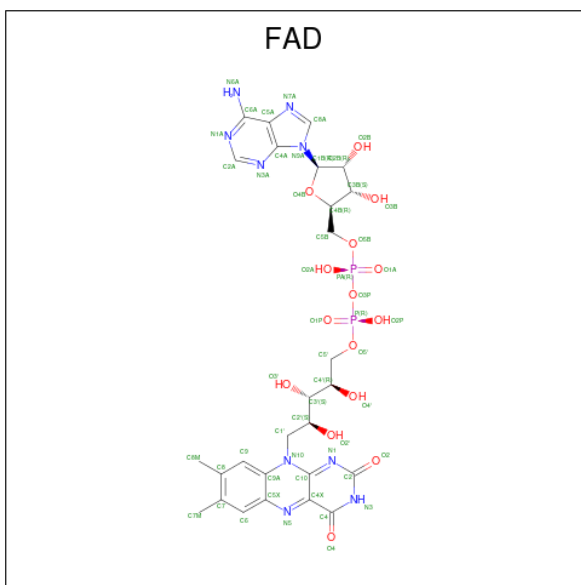
- Molecule 1 is a protein called fms1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	499	Total	C	N	O	S	0	0	0
			3914	2472	680	740	22			
1	A	493	Total	C	N	O	S	0	0	0
			3886	2458	675	731	22			

There are 16 discrepancies between the modelled and reference sequences:

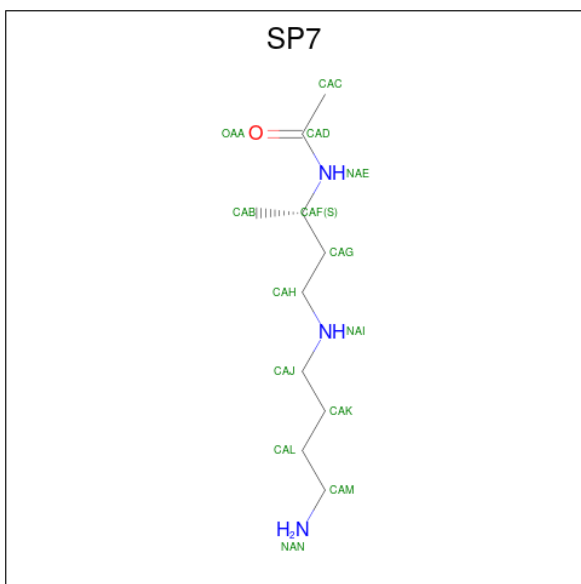
Chain	Residue	Modelled	Actual	Comment	Reference
B	509	LEU	-	insertion	UNP P50264
B	510	GLU	-	insertion	UNP P50264
B	511	HIS	-	insertion	UNP P50264
B	512	HIS	-	insertion	UNP P50264
B	513	HIS	-	insertion	UNP P50264
B	514	HIS	-	insertion	UNP P50264
B	515	HIS	-	insertion	UNP P50264
B	516	HIS	-	insertion	UNP P50264
A	509	LEU	-	insertion	UNP P50264
A	510	GLU	-	insertion	UNP P50264
A	511	HIS	-	insertion	UNP P50264
A	512	HIS	-	insertion	UNP P50264
A	513	HIS	-	insertion	UNP P50264
A	514	HIS	-	insertion	UNP P50264
A	515	HIS	-	insertion	UNP P50264
A	516	HIS	-	insertion	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-{(1S)-3-[(4-aminobutyl)amino]-1-methylpropyl}acetamide (CCD ID: SP7) (formula: $C_{10}H_{23}N_3O$).



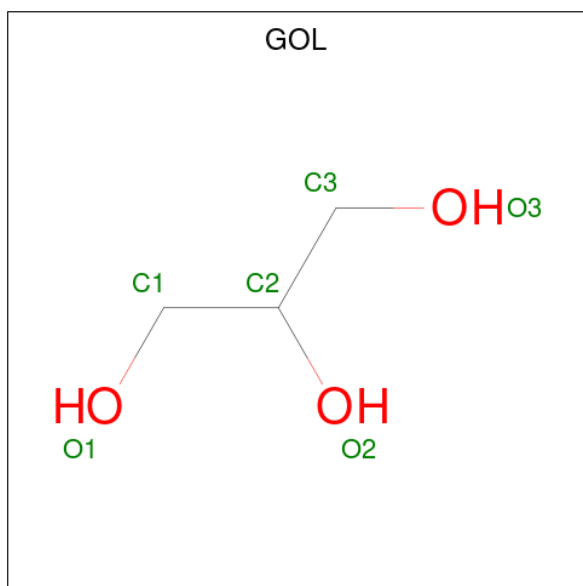
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	10	3	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	10	3	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	68	Total	O	0	0
			68	68		
5	A	87	Total	O	0	0
			87	87		



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	102.21Å 215.20Å 117.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.70 – 2.50 31.70 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (31.70-2.50) 99.6 (31.70-2.50)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 1.95Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.216 , 0.267 0.211 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.716	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8095	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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: GOL, FAD, SP7

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	0.44	0/3965	0.91	12/5361 (0.2%)
1	B	0.41	0/3995	0.91	14/5405 (0.3%)
All	All	0.43	0/7960	0.91	26/10766 (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	A	351	VAL	N-CA-C	8.01	119.46	108.89
1	A	138	ASP	N-CA-C	7.65	121.11	111.24
1	B	454	PHE	N-CA-C	-6.72	101.35	110.36
1	B	66	HIS	N-CA-C	-6.67	96.80	108.20
1	A	238	CYS	N-CA-C	-6.62	101.61	110.55
1	B	321	ASN	N-CA-C	-6.26	104.74	112.38
1	A	454	PHE	N-CA-C	-6.21	102.03	110.36
1	A	17	GLY	N-CA-C	-6.05	102.69	112.31
1	B	201	TYR	N-CA-C	-5.89	105.35	112.54
1	A	453	CYS	N-CA-C	5.79	118.34	108.90
1	B	458	ASP	CA-C-N	5.64	125.75	119.32
1	B	458	ASP	C-N-CA	5.64	125.75	119.32
1	A	201	TYR	N-CA-C	-5.62	105.68	112.54
1	B	182	LEU	N-CA-C	5.59	118.64	109.76
1	B	440	TRP	N-CA-C	5.58	117.36	111.28
1	B	83	LEU	N-CA-C	-5.50	105.44	111.82
1	A	66	HIS	N-CA-C	-5.49	98.82	108.20
1	A	199	LEU	N-CA-C	-5.48	103.75	110.65
1	B	424	ILE	N-CA-C	5.35	116.13	110.72
1	B	470	GLN	N-CA-C	-5.34	106.27	112.89
1	A	94	ASP	N-CA-C	-5.30	103.02	110.50
1	A	470	GLN	N-CA-C	-5.29	105.69	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	170	TYR	N-CA-C	-5.22	106.02	112.38
1	A	100	ILE	N-CA-C	5.19	115.59	108.12
1	B	453	CYS	N-CA-C	5.11	117.23	108.90
1	B	380	LEU	N-CA-C	5.10	116.84	111.28

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	3886	0	3772	94	0
1	B	3914	0	3759	120	0
2	A	53	0	31	3	0
2	B	53	0	31	2	0
3	A	14	0	23	14	0
3	B	14	0	23	8	0
4	A	6	0	8	4	0
5	A	87	0	0	0	0
5	B	68	0	0	0	0
All	All	8095	0	7647	217	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 (217) 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:487:GLY:O	3:A:518:SP7:HAB	1.50	1.12
1:B:451:SER:O	3:B:518:SP7:HABB	1.55	1.04
1:A:487:GLY:C	3:A:518:SP7:HAB	1.82	1.03
1:A:103:GLU:HG3	1:A:104:ARG:H	1.33	0.93
1:B:451:SER:O	3:B:518:SP7:CAB	2.18	0.91
1:B:278:LEU:HA	1:B:470:GLN:HE22	1.37	0.88
1:B:224:LYS:HE2	1:B:224:LYS:HA	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:CYS:SG	1:A:400:PRO:HG2	2.17	0.85
1:B:237:ASN:HB3	1:B:243:VAL:HG22	1.58	0.84
1:A:487:GLY:O	3:A:518:SP7:CAB	2.28	0.81
1:B:353:CYS:SG	1:B:400:PRO:HG2	2.25	0.76
1:B:423:ASN:HD22	1:B:426:ASN:ND2	1.84	0.76
3:A:518:SP7:HACA	4:A:519:GOL:O2	1.86	0.76
1:A:122:MET:HE1	1:A:145:VAL:HG22	1.68	0.75
1:B:252:THR:HG22	1:B:477:ALA:HB3	1.68	0.75
1:A:150:LEU:O	1:A:153:ARG:HD2	1.87	0.74
3:A:518:SP7:HAC	3:A:518:SP7:HABB	1.69	0.74
1:B:8:LYS:N	1:B:245:ASN:HD21	1.86	0.73
1:B:315:THR:HG21	1:B:401:VAL:CG2	2.18	0.72
1:A:418:MET:O	1:A:419:ARG:HG3	1.91	0.70
1:B:278:LEU:HA	1:B:470:GLN:NE2	2.07	0.70
1:A:487:GLY:C	3:A:518:SP7:CAB	2.65	0.69
1:A:377:GLN:NE2	1:A:377:GLN:H	1.90	0.69
1:B:67:HIS:NE2	3:B:518:SP7:HAL	2.07	0.69
1:B:315:THR:HG21	1:B:401:VAL:HG22	1.74	0.69
1:A:332:ASN:ND2	1:A:335:GLU:H	1.92	0.68
1:A:213:PRO:O	1:A:216:TRP:HB2	1.95	0.66
1:A:406:MET:HE2	1:A:406:MET:HA	1.78	0.66
1:A:264:PRO:O	1:A:265:GLU:HB3	1.95	0.66
1:B:247:ASP:O	1:B:473:ARG:HD2	1.95	0.65
1:B:9:LYS:O	1:B:246:ALA:HA	1.96	0.65
1:A:442:ARG:HG2	1:A:442:ARG:HH11	1.62	0.65
1:B:48:LEU:CD2	1:B:63:ALA:HB3	2.28	0.64
1:B:332:ASN:HD21	1:B:334:ASP:HB2	1.62	0.64
1:A:133:HIS:O	1:A:136:VAL:HG23	1.98	0.64
1:B:412:GLU:HB2	1:B:429:LYS:HD3	1.79	0.64
1:A:157:THR:OG1	1:A:160:GLN:HG3	1.98	0.63
1:B:311:SER:HA	1:B:362:ASN:HB3	1.81	0.62
1:A:103:GLU:HG3	1:A:104:ARG:N	2.10	0.62
1:B:377:GLN:H	1:B:377:GLN:NE2	1.97	0.62
1:B:271:ARG:HG3	1:B:271:ARG:HH11	1.63	0.62
1:B:227:THR:HB	1:B:235:THR:HB	1.83	0.61
1:B:264:PRO:HG2	1:B:265:GLU:OE2	2.00	0.61
1:B:133:HIS:HB3	1:B:136:VAL:HG21	1.83	0.60
1:A:451:SER:OG	4:A:519:GOL:H12	2.00	0.60
1:A:167:LEU:O	1:A:170:TYR:HD2	1.84	0.60
1:B:14:ILE:CD1	1:B:226:ILE:HD11	2.32	0.60
1:A:412:GLU:OE1	1:A:429:LYS:HG2	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:VAL:HA	1:A:430:PRO:HG2	1.84	0.60
1:A:415:ILE:HD11	1:A:429:LYS:HD3	1.83	0.60
1:B:153:ARG:NH1	1:B:327:VAL:O	2.34	0.60
1:B:68:ASP:HB3	1:B:192:GLN:HB2	1.83	0.59
1:A:451:SER:OG	4:A:519:GOL:C1	2.50	0.59
1:B:336:LEU:HD22	1:B:340:LEU:HD11	1.85	0.58
1:B:250:ILE:HD11	1:B:503:ILE:HD12	1.85	0.58
1:B:190:GLY:O	1:B:191:HIS:C	2.45	0.58
1:B:14:ILE:HD12	1:B:251:ILE:HG12	1.84	0.58
1:B:23:ALA:O	1:B:27:LEU:HG	2.04	0.58
3:A:518:SP7:HABB	3:A:518:SP7:CAC	2.34	0.58
1:B:67:HIS:NE2	3:B:518:SP7:CAL	2.67	0.57
1:A:479:GLU:OE1	1:A:487:GLY:HA2	2.04	0.57
1:B:72:ASN:C	1:B:72:ASN:HD22	2.12	0.57
1:B:254:PRO:HD3	2:B:517:FAD:H51A	1.86	0.57
1:A:259:ASN:O	1:A:262:VAL:HG22	2.04	0.57
1:B:54:TYR:O	1:B:57:ARG:HG3	2.04	0.57
1:B:213:PRO:O	1:B:216:TRP:HB2	2.04	0.57
1:B:362:ASN:C	1:B:362:ASN:HD22	2.13	0.56
1:A:487:GLY:HA3	3:A:518:SP7:HABB	1.86	0.56
1:B:63:ALA:HA	2:B:517:FAD:N5	2.20	0.56
1:A:64:SER:OG	1:A:296:LYS:NZ	2.38	0.56
1:A:332:ASN:C	1:A:332:ASN:HD22	2.13	0.56
1:A:504:SER:O	1:A:508:LYS:HG2	2.06	0.56
1:B:128:LEU:HD21	1:A:192:GLN:NE2	2.21	0.56
1:A:252:THR:HG22	1:A:477:ALA:HB3	1.88	0.55
1:B:392:GLU:HG2	1:B:419:ARG:NH1	2.21	0.55
1:B:48:LEU:HD23	1:B:63:ALA:HB3	1.89	0.55
1:A:48:LEU:CD2	1:A:63:ALA:HB3	2.37	0.55
1:A:165:PRO:O	1:A:169:ARG:HG3	2.06	0.55
1:B:311:SER:O	1:B:312:LYS:HE3	2.06	0.55
1:B:381:THR:O	1:B:385:GLU:HG3	2.07	0.55
1:B:392:GLU:HG2	1:B:419:ARG:HH12	1.71	0.55
1:B:479:GLU:OE1	1:B:487:GLY:HA2	2.07	0.54
1:A:189:PHE:CZ	1:A:191:HIS:NE2	2.76	0.54
1:A:164:LEU:N	1:A:165:PRO:HD2	2.22	0.53
1:B:240:ASP:OD1	1:B:242:THR:HG23	2.09	0.53
1:B:285:ALA:O	1:B:289:ILE:HG22	2.09	0.53
1:B:8:LYS:N	1:B:245:ASN:ND2	2.56	0.53
1:A:150:LEU:HD13	1:A:336:LEU:HD22	1.91	0.53
1:B:57:ARG:HD3	1:B:369:VAL:CG1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:GLN:HE22	1:B:289:ILE:HG13	1.74	0.53
1:B:362:ASN:C	1:B:362:ASN:ND2	2.64	0.52
1:B:452:ALA:HA	3:B:518:SP7:HABB	1.90	0.52
1:B:271:ARG:HG3	1:B:271:ARG:NH1	2.24	0.52
1:B:47:ARG:NH2	1:B:254:PRO:HB3	2.24	0.52
1:A:239:GLU:C	1:A:241:GLY:H	2.17	0.52
1:A:122:MET:HG2	1:A:148:TYR:CG	2.45	0.52
1:A:213:PRO:HB2	1:A:216:TRP:CD1	2.45	0.52
1:A:293:ALA:HB3	1:A:378:ALA:HB2	1.89	0.52
1:A:487:GLY:HA3	3:A:518:SP7:CAB	2.40	0.52
1:A:278:LEU:HA	1:A:470:GLN:NE2	2.25	0.51
1:B:423:ASN:HB3	1:B:426:ASN:HD22	1.76	0.51
1:A:442:ARG:HG2	1:A:442:ARG:NH1	2.25	0.51
1:B:165:PRO:O	1:B:169:ARG:HG3	2.10	0.51
1:B:263:GLN:HG3	1:B:264:PRO:HD2	1.92	0.51
1:B:265:GLU:C	1:B:267:ASN:H	2.19	0.51
3:A:518:SP7:CAC	4:A:519:GOL:O2	2.57	0.51
1:B:136:VAL:O	1:B:136:VAL:HG23	2.11	0.51
1:B:191:HIS:HE1	1:B:195:ASN:HD21	1.57	0.50
1:A:67:HIS:NE2	3:A:518:SP7:NAI	2.44	0.50
1:A:108:ASP:O	1:A:109:HIS:C	2.53	0.50
1:A:54:TYR:O	1:A:57:ARG:HG3	2.11	0.50
1:B:110:ASP:HB3	1:B:113:LEU:HB2	1.93	0.50
1:A:5:SER:N	1:A:6:PRO:HD2	2.27	0.49
1:A:14:ILE:HD12	1:A:14:ILE:N	2.28	0.49
1:B:254:PRO:HG2	1:B:257:VAL:HG23	1.93	0.49
1:B:439:ASN:HD21	1:B:442:ARG:HD3	1.78	0.49
1:B:398:PHE:O	1:B:401:VAL:HG12	2.12	0.49
1:B:439:ASN:HD21	1:B:442:ARG:HH11	1.59	0.49
1:B:190:GLY:O	1:B:192:GLN:N	2.45	0.49
1:B:224:LYS:HA	1:B:224:LYS:CE	2.38	0.49
1:B:116:GLU:OE1	1:B:116:GLU:N	2.36	0.48
1:B:141:PHE:O	1:B:145:VAL:HG23	2.13	0.48
1:A:72:ASN:HB3	1:A:75:PHE:HB3	1.94	0.48
2:A:517:FAD:C4X	3:A:518:SP7:HAJA	2.43	0.48
1:B:451:SER:HB3	3:B:518:SP7:HACA	1.96	0.48
1:A:362:ASN:HD21	1:A:364:SER:HB3	1.78	0.48
1:A:116:GLU:OE2	1:A:116:GLU:N	2.36	0.47
1:B:130:PHE:CD2	1:B:185:LYS:HG3	2.49	0.47
1:B:450:TYR:CE2	3:B:518:SP7:HAH	2.48	0.47
1:B:412:GLU:CB	1:B:429:LYS:HD3	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:ASP:OD2	1:A:455:PRO:HA	2.15	0.47
1:A:432:LEU:HD21	1:A:435:ILE:HD11	1.96	0.47
1:A:282:ILE:HG12	1:A:465:ALA:HB1	1.96	0.47
1:A:388:ARG:HB2	1:A:437:VAL:HB	1.97	0.47
1:A:250:ILE:HD11	1:A:503:ILE:HD12	1.96	0.47
1:B:135:GLY:O	1:B:136:VAL:C	2.58	0.47
1:B:282:ILE:HD13	1:B:465:ALA:HB1	1.96	0.47
1:A:278:LEU:HA	1:A:470:GLN:HE22	1.80	0.47
1:A:63:ALA:HA	2:A:517:FAD:N5	2.30	0.47
1:B:279:LYS:HE2	1:B:470:GLN:HA	1.97	0.46
1:B:395:PHE:O	1:B:399:GLN:HB2	2.15	0.46
1:A:44:VAL:CG1	1:A:217:LEU:HD21	2.45	0.46
1:B:141:PHE:CD1	1:B:187:THR:HG21	2.50	0.46
1:B:439:ASN:ND2	1:B:442:ARG:HD3	2.30	0.46
1:B:504:SER:O	1:B:508:LYS:HG3	2.15	0.46
1:B:460:VAL:O	1:B:464:VAL:HG23	2.16	0.46
1:A:336:LEU:O	1:A:340:LEU:HG	2.16	0.46
1:B:502:ARG:HG2	1:B:502:ARG:HH11	1.80	0.46
1:A:9:LYS:O	1:A:246:ALA:HA	2.15	0.46
1:B:502:ARG:HG2	1:B:502:ARG:NH1	2.32	0.45
1:B:262:VAL:HG12	1:B:283:GLN:HG2	1.97	0.45
1:B:362:ASN:ND2	1:B:364:SER:H	2.14	0.45
1:A:189:PHE:CE1	1:A:191:HIS:CD2	3.04	0.45
1:B:359:PHE:HD2	1:B:375:LEU:HD22	1.81	0.45
1:B:412:GLU:HB3	1:B:429:LYS:HZ2	1.82	0.45
1:A:118:VAL:HG23	1:A:164:LEU:HD13	1.97	0.45
1:B:113:LEU:O	1:B:114:LEU:C	2.60	0.45
1:B:199:LEU:HD23	1:B:199:LEU:HA	1.84	0.45
1:B:432:LEU:HD21	1:B:435:ILE:HD11	1.99	0.45
1:B:110:ASP:O	1:B:114:LEU:HD23	2.17	0.45
2:A:517:FAD:N5	3:A:518:SP7:HAJA	2.31	0.45
1:B:8:LYS:HB2	1:B:245:ASN:OD1	2.16	0.44
1:B:11:VAL:HG11	1:B:27:LEU:HD11	1.99	0.44
1:B:68:ASP:CB	1:B:192:GLN:HB2	2.46	0.44
1:B:271:ARG:HD3	1:B:271:ARG:C	2.42	0.44
1:A:122:MET:HG2	1:A:148:TYR:CD2	2.51	0.44
1:A:167:LEU:O	1:A:170:TYR:CD2	2.68	0.44
1:A:167:LEU:HA	1:A:316:LEU:CD2	2.47	0.44
1:B:167:LEU:HD23	1:B:167:LEU:C	2.43	0.44
1:B:115:LEU:HB3	1:B:167:LEU:HD13	1.99	0.44
1:B:191:HIS:HE1	1:B:195:ASN:ND2	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:PRO:O	1:B:284:ASP:OD2	2.36	0.44
1:A:297:VAL:HG23	1:A:376:MET:HE2	2.00	0.44
1:B:225:SER:HA	1:B:272:ILE:HG23	2.00	0.43
1:A:470:GLN:HB3	1:A:474:ILE:HB	2.00	0.43
1:A:466:MET:HE2	1:A:466:MET:HA	2.00	0.43
1:A:150:LEU:CD1	1:A:336:LEU:HD22	2.48	0.43
1:A:189:PHE:CD2	1:A:189:PHE:N	2.87	0.43
1:A:418:MET:HA	1:A:433:ARG:O	2.18	0.43
1:A:41:ARG:NH1	1:A:443:ASP:OD2	2.50	0.43
1:A:122:MET:O	1:A:125:PHE:HB3	2.19	0.43
1:A:311:SER:HA	1:A:362:ASN:HB3	2.00	0.43
1:B:414:VAL:HA	1:B:430:PRO:HG2	2.02	0.42
1:B:475:ARG:HB3	1:B:499:GLU:OE1	2.19	0.42
1:B:507:LEU:O	1:B:510:GLU:HB2	2.20	0.42
1:A:213:PRO:HB2	1:A:216:TRP:CG	2.54	0.42
1:B:316:LEU:N	1:B:316:LEU:CD1	2.82	0.42
1:B:362:ASN:HD21	1:B:364:SER:HB3	1.84	0.42
1:A:46:GLY:C	1:A:48:LEU:H	2.27	0.42
1:A:110:ASP:HB3	1:A:113:LEU:HB2	2.02	0.42
1:A:332:ASN:HD21	1:A:335:GLU:H	1.64	0.42
1:A:470:GLN:OE1	1:A:470:GLN:HA	2.20	0.42
1:A:487:GLY:CA	3:A:518:SP7:CAB	2.97	0.42
1:B:316:LEU:N	1:B:316:LEU:HD12	2.34	0.42
1:B:365:LYS:NZ	1:A:111:LYS:HB2	2.35	0.42
1:B:451:SER:O	3:B:518:SP7:CAF	2.67	0.41
1:A:78:GLU:CD	1:A:204:VAL:HG22	2.44	0.41
1:A:434:ASN:ND2	1:A:435:ILE:H	2.17	0.41
1:B:150:LEU:O	1:B:153:ARG:HG2	2.21	0.41
1:B:164:LEU:N	1:B:165:PRO:HD2	2.35	0.41
1:B:278:LEU:CA	1:B:470:GLN:HE22	2.20	0.41
1:B:312:LYS:HD3	1:B:359:PHE:CZ	2.55	0.41
1:B:70:LEU:HB2	1:B:192:GLN:O	2.20	0.41
1:B:141:PHE:CE1	1:B:187:THR:HG21	2.56	0.41
1:A:218:LYS:HE2	1:A:218:LYS:HB3	1.88	0.41
1:B:41:ARG:HH21	1:B:443:ASP:CG	2.28	0.41
1:B:193:GLY:HA2	1:A:121:GLU:HG3	2.02	0.41
1:A:113:LEU:HB3	1:A:115:LEU:HG	2.03	0.41
1:A:183:SER:HB2	1:A:455:PRO:HA	2.01	0.41
1:B:72:ASN:HD21	1:B:490:TYR:HB3	1.86	0.40
1:A:148:TYR:CE1	1:A:152:ARG:HG3	2.56	0.40
1:A:237:ASN:OD1	1:A:243:VAL:HG22	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:405:ILE:O	1:A:409:LEU:HG	2.22	0.40
1:B:214:GLN:HA	1:B:214:GLN:OE1	2.22	0.40
1:B:157:THR:O	1:B:161:ILE:HG13	2.22	0.40
1:A:99:TYR:O	1:A:106:ARG:HA	2.22	0.40
1:A:167:LEU:HA	1:A:316:LEU:HD22	2.02	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	487/516 (94%)	450 (92%)	30 (6%)	7 (1%)	9	17
1	B	495/516 (96%)	447 (90%)	38 (8%)	10 (2%)	6	10
All	All	982/1032 (95%)	897 (91%)	68 (7%)	17 (2%)	7	13

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	136	VAL
1	B	191	HIS
1	B	200	ASN
1	A	200	ASN
1	B	137	SER
1	B	510	GLU
1	B	479	GLU
1	A	104	ARG
1	A	132	GLN
1	A	139	CYS
1	B	420	PRO
1	A	262	VAL
1	B	135	GLY

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Mol	Chain	Res	Type
1	A	232	LYS
1	A	341	GLU
1	B	262	VAL
1	B	264	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	420/457 (92%)	410 (98%)	10 (2%)	43	70
1	B	420/457 (92%)	404 (96%)	16 (4%)	29	56
All	All	840/914 (92%)	814 (97%)	26 (3%)	35	62

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	22	LYS
1	B	118	VAL
1	B	134	LEU
1	B	173	LEU
1	B	177	LEU
1	B	201	TYR
1	B	221	CYS
1	B	237	ASN
1	B	239	GLU
1	B	249	VAL
1	B	265	GLU
1	B	312	LYS
1	B	336	LEU
1	B	362	ASN
1	B	377	GLN
1	B	380	LEU
1	A	36	LEU
1	A	122	MET
1	A	150	LEU

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Mol	Chain	Res	Type
1	A	177	LEU
1	A	201	TYR
1	A	221	CYS
1	A	239	GLU
1	A	267	ASN
1	A	332	ASN
1	A	377	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	29	GLN
1	B	30	ASN
1	B	72	ASN
1	B	131	HIS
1	B	133	HIS
1	B	191	HIS
1	B	215	ASN
1	B	255	GLN
1	B	259	ASN
1	B	283	GLN
1	B	290	HIS
1	B	321	ASN
1	B	329	ASN
1	B	332	ASN
1	B	362	ASN
1	B	377	GLN
1	B	426	ASN
1	B	434	ASN
1	B	439	ASN
1	B	468	ASN
1	A	28	HIS
1	A	29	GLN
1	A	33	GLN
1	A	192	GLN
1	A	259	ASN
1	A	267	ASN
1	A	321	ASN
1	A	332	ASN
1	A	362	ASN
1	A	377	GLN
1	A	434	ASN

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Mol	Chain	Res	Type
1	A	439	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

5 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	$\# Z > 2$
4	GOL	A	519	-	5,5,5	0.45	0	5,5,5	0.08	0
3	SP7	B	518	-	13,13,13	0.61	0	13,14,14	0.99	0
2	FAD	B	517	-	58,58,58	1.35	8 (13%)	85,89,89	1.63	20 (23%)
3	SP7	A	518	-	13,13,13	0.61	0	13,14,14	0.99	0
2	FAD	A	517	-	58,58,58	1.35	7 (12%)	85,89,89	1.63	20 (23%)

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
4	GOL	A	519	-	-	4/4/4/4	-
3	SP7	B	518	-	-	8/12/12/12	-
2	FAD	B	517	-	-	1/34/50/50	0/6/6/6
3	SP7	A	518	-	-	11/12/12/12	-
2	FAD	A	517	-	-	1/34/50/50	0/6/6/6

All (15) 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	4.51	1.40	1.30
2	B	517	FAD	C10-N1	3.58	1.40	1.33
2	A	517	FAD	C10-N1	3.55	1.40	1.33
2	A	517	FAD	C5A-N7A	-3.14	1.33	1.39
2	B	517	FAD	C5A-N7A	-3.09	1.33	1.39
2	A	517	FAD	P-O1P	3.07	1.61	1.50
2	A	517	FAD	PA-O1A	3.04	1.61	1.50
2	B	517	FAD	P-O1P	3.04	1.61	1.50
2	B	517	FAD	PA-O1A	3.01	1.61	1.50
2	B	517	FAD	C8A-N9A	-2.31	1.33	1.37
2	A	517	FAD	C8A-N9A	-2.29	1.33	1.37
2	A	517	FAD	C4A-N9A	-2.08	1.33	1.37
2	B	517	FAD	C4A-N9A	-2.05	1.33	1.37
2	B	517	FAD	PA-O3P	2.01	1.61	1.59

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	517	FAD	C5A-C4A-N3A	-5.29	119.43	126.72
2	A	517	FAD	C5A-C4A-N3A	-5.25	119.48	126.72
2	B	517	FAD	N3A-C2A-N1A	-4.44	121.87	128.58
2	A	517	FAD	N3A-C2A-N1A	-4.41	121.91	128.58
2	B	517	FAD	N3A-C4A-N9A	3.82	133.66	127.17
2	A	517	FAD	N3A-C4A-N9A	3.76	133.56	127.17
2	B	517	FAD	C2A-N3A-C4A	3.50	120.39	111.83
2	A	517	FAD	C2A-N3A-C4A	3.47	120.30	111.83
2	B	517	FAD	C4-N3-C2	-3.18	119.99	125.64
2	A	517	FAD	N9A-C8A-N7A	-3.05	109.60	113.94
2	B	517	FAD	N9A-C8A-N7A	-3.03	109.63	113.94
2	A	517	FAD	C4-N3-C2	-3.00	120.32	125.64
2	A	517	FAD	O2P-P-O3P	2.89	115.08	107.27
2	B	517	FAD	C4B-O4B-C1B	-2.80	103.29	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	517	FAD	O4B-C1B-C2B	-2.74	100.74	106.62
2	A	517	FAD	C5A-N7A-C8A	2.74	107.76	103.45
2	A	517	FAD	C9A-C5X-N5	-2.74	119.55	122.45
2	B	517	FAD	C5A-N7A-C8A	2.72	107.73	103.45
2	B	517	FAD	C4X-C4-N3	2.72	120.17	113.25
2	A	517	FAD	C4X-C4-N3	2.71	120.16	113.25
2	B	517	FAD	O4B-C1B-C2B	-2.70	100.83	106.62
2	B	517	FAD	C9A-C5X-N5	-2.70	119.59	122.45
2	A	517	FAD	O4-C4-C4X	-2.64	119.55	126.53
2	A	517	FAD	C4A-C5A-N7A	-2.64	107.56	110.58
2	B	517	FAD	C4A-C5A-N7A	-2.63	107.58	110.58
2	B	517	FAD	O2A-PA-O3P	2.59	114.26	107.27
2	B	517	FAD	O2P-P-O3P	2.54	114.14	107.27
2	B	517	FAD	C10-C4X-N5	-2.50	119.70	124.81
2	A	517	FAD	C4B-O4B-C1B	-2.49	103.97	109.47
2	B	517	FAD	O4-C4-C4X	-2.47	120.01	126.53
2	A	517	FAD	C10-C4X-N5	-2.43	119.85	124.81
2	A	517	FAD	C4X-C10-N10	2.40	119.92	116.48
2	B	517	FAD	C4X-C10-N10	2.39	119.90	116.48
2	A	517	FAD	C5'-C4'-C3'	-2.38	107.73	112.22
2	B	517	FAD	C4A-N9A-C8A	2.30	108.15	105.74
2	A	517	FAD	O2A-PA-O3P	2.29	113.46	107.27
2	A	517	FAD	C4A-N9A-C8A	2.27	108.12	105.74
2	A	517	FAD	C5X-C9A-N10	2.14	119.90	117.97
2	B	517	FAD	C5X-C9A-N10	2.08	119.84	117.97
2	B	517	FAD	C5'-C4'-C3'	-2.04	108.37	112.22

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	518	SP7	CAC-CAD-NAE-CAF
3	B	518	SP7	OAA-CAD-NAE-CAF
3	B	518	SP7	CAB-CAF-NAE-CAD
3	B	518	SP7	NAE-CAF-CAG-CAH
4	A	519	GOL	C1-C2-C3-O3
4	A	519	GOL	O2-C2-C3-O3
3	B	518	SP7	NAI-CAJ-CAK-CAL
3	A	518	SP7	CAC-CAD-NAE-CAF
3	A	518	SP7	OAA-CAD-NAE-CAF
3	A	518	SP7	NAI-CAJ-CAK-CAL
3	A	518	SP7	CAK-CAJ-NAI-CAH

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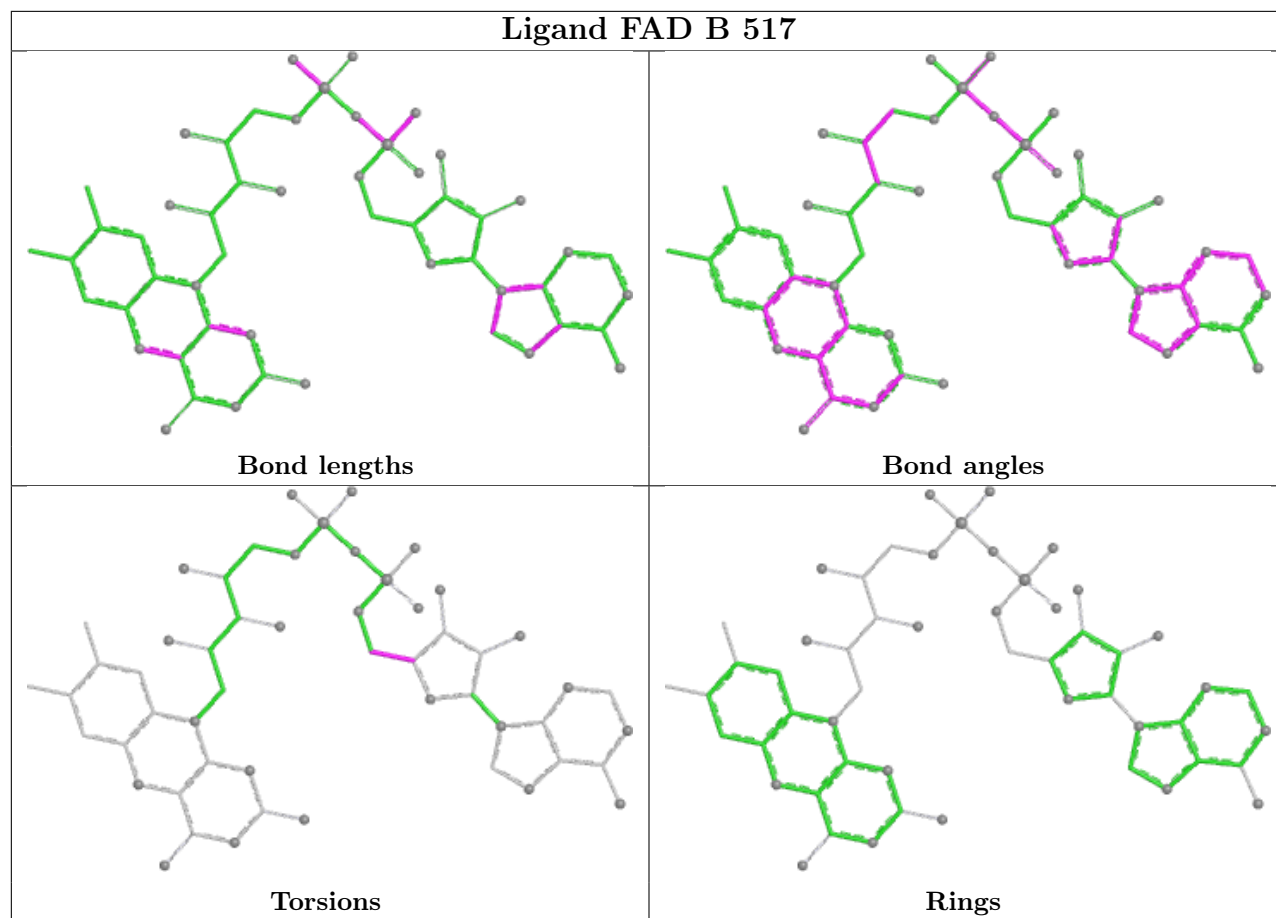
Mol	Chain	Res	Type	Atoms
4	A	519	GOL	O1-C1-C2-C3
4	A	519	GOL	O1-C1-C2-O2
3	B	518	SP7	CAB-CAF-CAG-CAH
3	A	518	SP7	CAB-CAF-CAG-CAH
3	A	518	SP7	NAE-CAF-CAG-CAH
3	A	518	SP7	CAG-CAF-NAE-CAD
3	A	518	SP7	CAJ-CAK-CAL-CAM
3	B	518	SP7	CAK-CAL-CAM-NAN
3	A	518	SP7	CAK-CAL-CAM-NAN
3	B	518	SP7	CAK-CAJ-NAI-CAH
3	A	518	SP7	CAB-CAF-NAE-CAD
2	A	517	FAD	O4B-C4B-C5B-O5B
2	B	517	FAD	O4B-C4B-C5B-O5B
3	A	518	SP7	CAG-CAH-NAI-CAJ

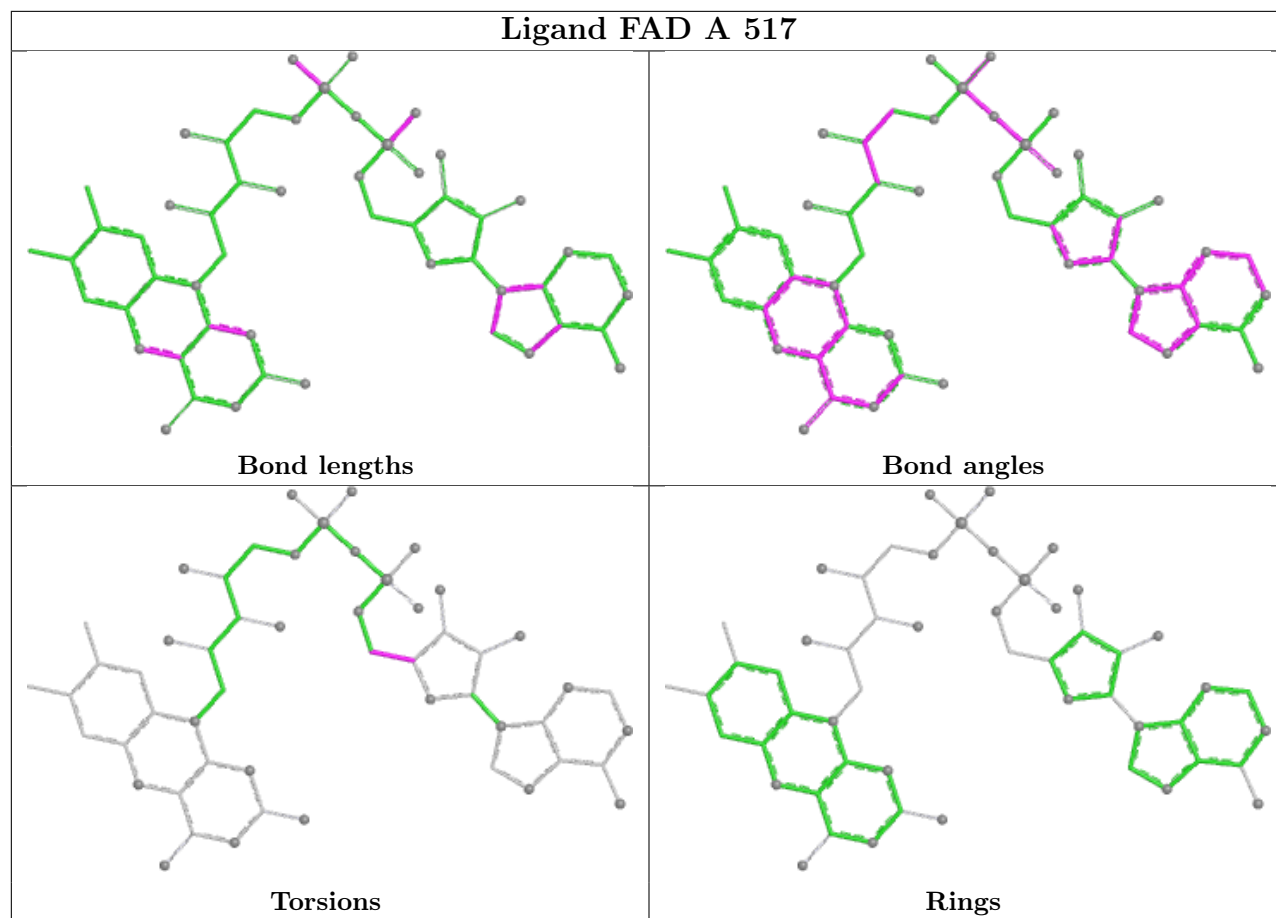
There are no ring outliers.

5 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	519	GOL	4	0
3	B	518	SP7	8	0
2	B	517	FAD	2	0
3	A	518	SP7	14	0
2	A	517	FAD	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	493/516 (95%)	0.21	25 (5%)	33 29	22, 38, 61, 83	0
1	B	499/516 (96%)	0.43	38 (7%)	20 17	26, 41, 75, 99	0
All	All	992/1032 (96%)	0.32	63 (6%)	25 22	22, 39, 69, 99	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	509	LEU	5.9
1	B	135	GLY	5.5
1	B	238	CYS	5.2
1	B	427	ALA	4.9
1	B	230	PRO	4.6
1	B	136	VAL	4.2
1	A	349	THR	3.9
1	B	231	SER	3.8
1	A	510	GLU	3.6
1	B	134	LEU	3.5
1	A	230	PRO	3.5
1	A	221	CYS	3.4
1	B	189	PHE	3.4
1	B	191	HIS	3.4
1	B	421	ILE	3.4
1	B	349	THR	3.3
1	A	133	HIS	3.3
1	A	264	PRO	3.2
1	B	245	ASN	3.1
1	A	238	CYS	3.1
1	B	422	GLU	3.0
1	B	350	SER	3.0
1	A	189	PHE	2.9
1	A	340	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	264	PRO	2.8
1	B	420	PRO	2.8
1	A	427	ALA	2.8
1	B	511	HIS	2.8
1	A	428	ASN	2.8
1	B	132	GLN	2.7
1	B	428	ASN	2.7
1	B	508	LYS	2.6
1	B	338	SER	2.6
1	B	228	ARG	2.6
1	A	334	ASP	2.6
1	B	234	VAL	2.6
1	B	423	ASN	2.6
1	A	170	TYR	2.6
1	B	174	TRP	2.5
1	A	240	ASP	2.5
1	B	336	LEU	2.5
1	B	426	ASN	2.5
1	A	233	ASN	2.4
1	A	132	GLN	2.3
1	A	5	SER	2.3
1	B	229	GLU	2.3
1	A	7	ALA	2.2
1	A	339	MET	2.2
1	B	341	GLU	2.2
1	A	338	SER	2.2
1	A	191	HIS	2.1
1	B	233	ASN	2.1
1	B	246	ALA	2.1
1	B	343	GLU	2.1
1	B	11	VAL	2.1
1	A	245	ASN	2.1
1	A	342	ARG	2.1
1	A	419	ARG	2.1
1	B	472	SER	2.1
1	B	339	MET	2.1
1	A	509	LEU	2.0
1	B	8	LYS	2.0
1	B	133	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

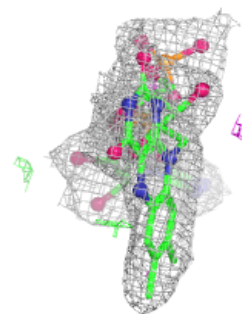
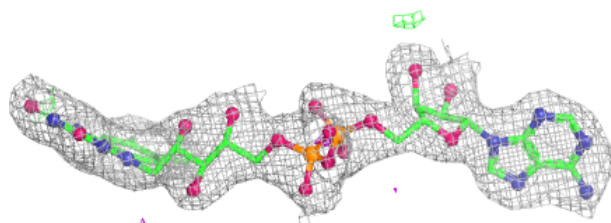
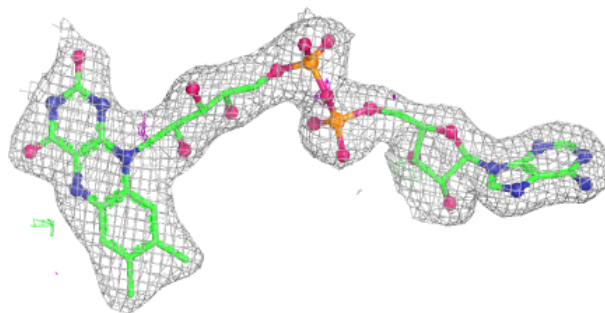
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	SP7	A	518	14/14	0.65	0.30	20,20,20,20	0
3	SP7	B	518	14/14	0.69	0.25	20,20,20,20	0
4	GOL	A	519	6/6	0.79	0.22	20,20,20,20	0
2	FAD	B	517	53/53	0.96	0.08	27,32,38,39	0
2	FAD	A	517	53/53	0.97	0.07	15,25,30,32	0

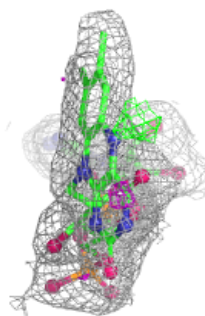
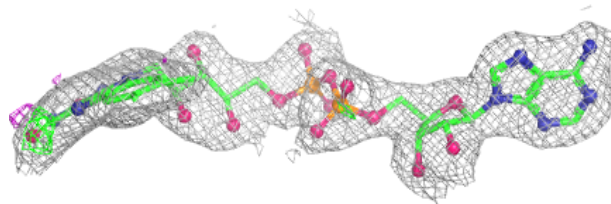
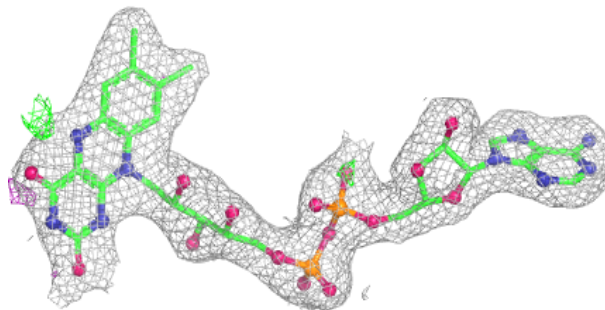
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around FAD B 517:

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

**Electron density around FAD A 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.