



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 12:50 AM UTC

PDB ID : 3T58 / pdb_00003t58
Title : C76A/C455S mutant of mouse QSOX1 containing an interdomain disulfide
Authors : Fass, D.; Alon, A.; Gat, Y.
Deposited on : 2011-07-27
Resolution : 2.40 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

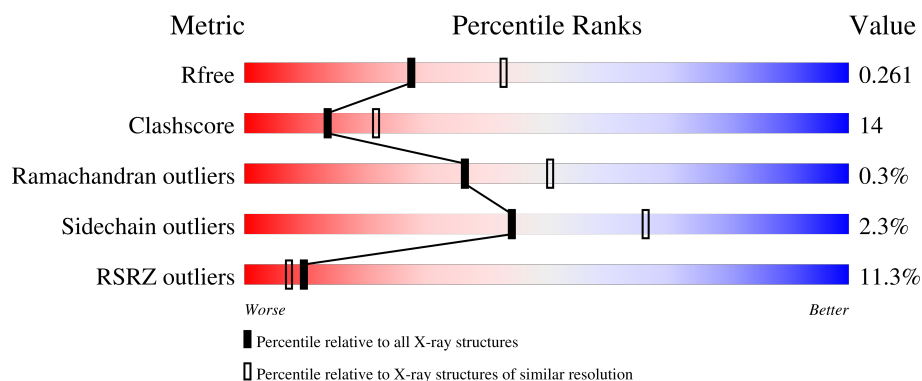
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (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 $\leq 5\%$. 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	519	
1	B	519	
1	C	519	
1	D	519	

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	FAD	D	601	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17335 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 Sulfhydryl oxidase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	502	Total	C	N	O	S	0	5	0
			4031	2585	702	727	17			
1	B	504	Total	C	N	O	S	0	5	0
			4050	2595	708	730	17			
1	C	501	Total	C	N	O	S	0	1	0
			3989	2556	697	721	15			
1	D	500	Total	C	N	O	S	0	1	0
			3982	2554	693	720	15			

There are 24 discrepancies between the modelled and reference sequences:

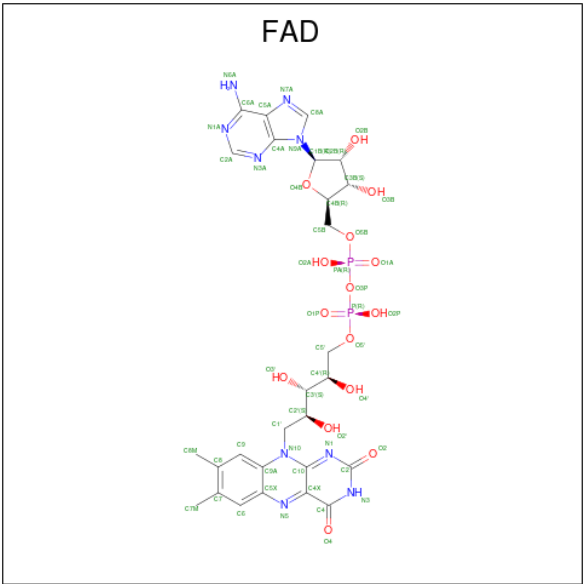
Chain	Residue	Modelled	Actual	Comment	Reference
A	32	GLY	-	expression tag	UNP Q8BND5
A	33	SER	-	expression tag	UNP Q8BND5
A	34	HIS	-	expression tag	UNP Q8BND5
A	35	MET	-	expression tag	UNP Q8BND5
A	76	ALA	CYS	engineered mutation	UNP Q8BND5
A	455	SER	CYS	engineered mutation	UNP Q8BND5
B	32	GLY	-	expression tag	UNP Q8BND5
B	33	SER	-	expression tag	UNP Q8BND5
B	34	HIS	-	expression tag	UNP Q8BND5
B	35	MET	-	expression tag	UNP Q8BND5
B	76	ALA	CYS	engineered mutation	UNP Q8BND5
B	455	SER	CYS	engineered mutation	UNP Q8BND5
C	32	GLY	-	expression tag	UNP Q8BND5
C	33	SER	-	expression tag	UNP Q8BND5
C	34	HIS	-	expression tag	UNP Q8BND5
C	35	MET	-	expression tag	UNP Q8BND5
C	76	ALA	CYS	engineered mutation	UNP Q8BND5
C	455	SER	CYS	engineered mutation	UNP Q8BND5
D	32	GLY	-	expression tag	UNP Q8BND5
D	33	SER	-	expression tag	UNP Q8BND5
D	34	HIS	-	expression tag	UNP Q8BND5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	35	MET	-	expression tag	UNP Q8BND5
D	76	ALA	CYS	engineered mutation	UNP Q8BND5
D	455	SER	CYS	engineered mutation	UNP Q8BND5

- 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	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	C	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	D	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

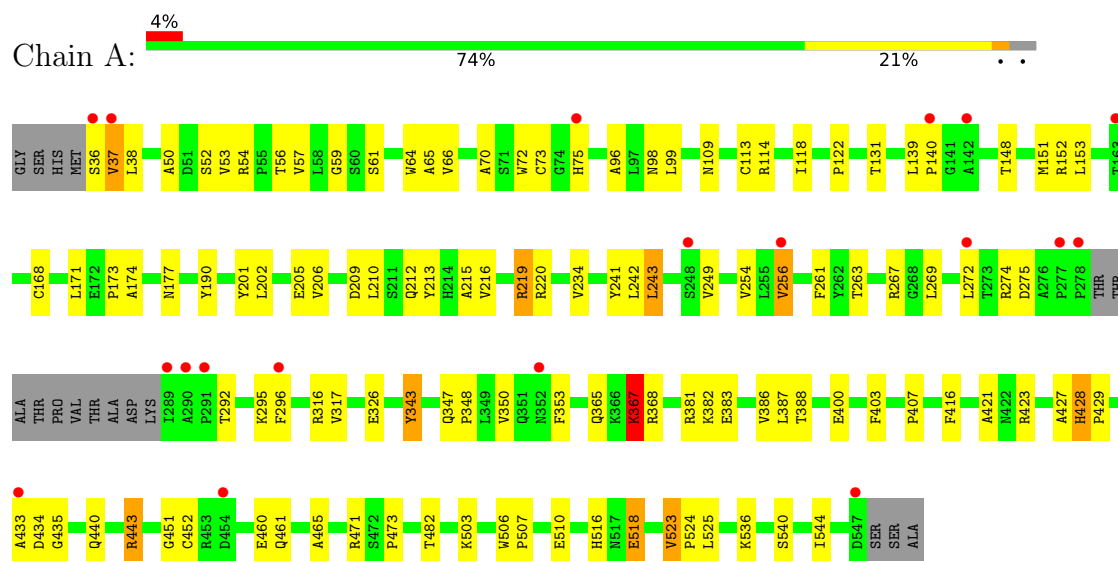
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	341	Total	O	0	0
			341	341		
3	B	339	Total	O	0	0
			339	339		
3	C	211	Total	O	0	0
			211	211		
3	D	180	Total	O	0	0
			180	180		

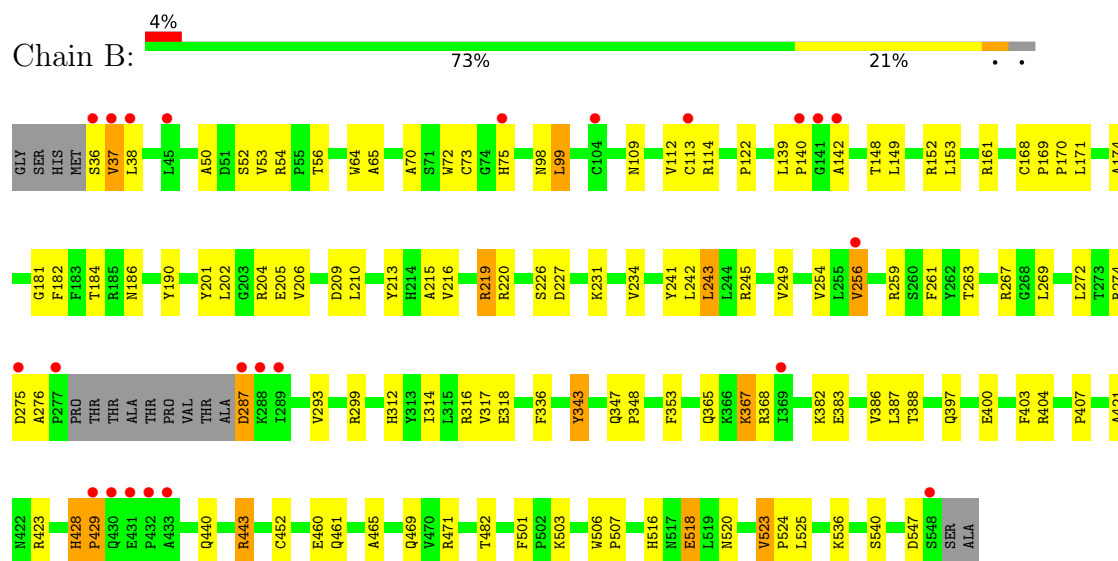
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

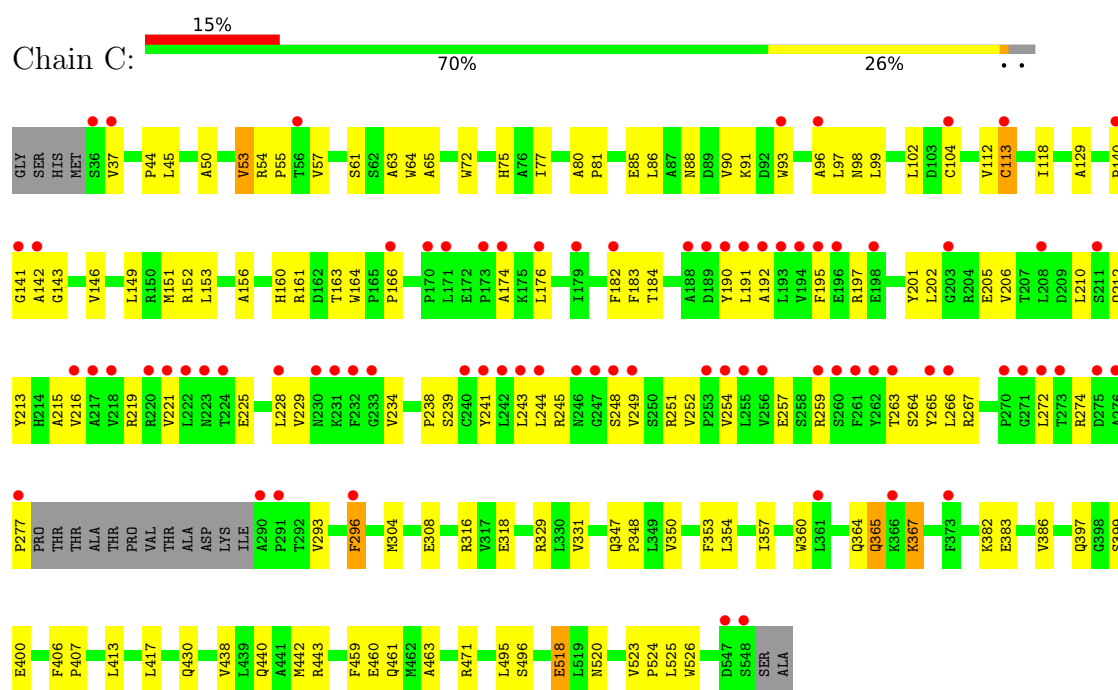
• Molecule 1: Sulfhydryl oxidase 1



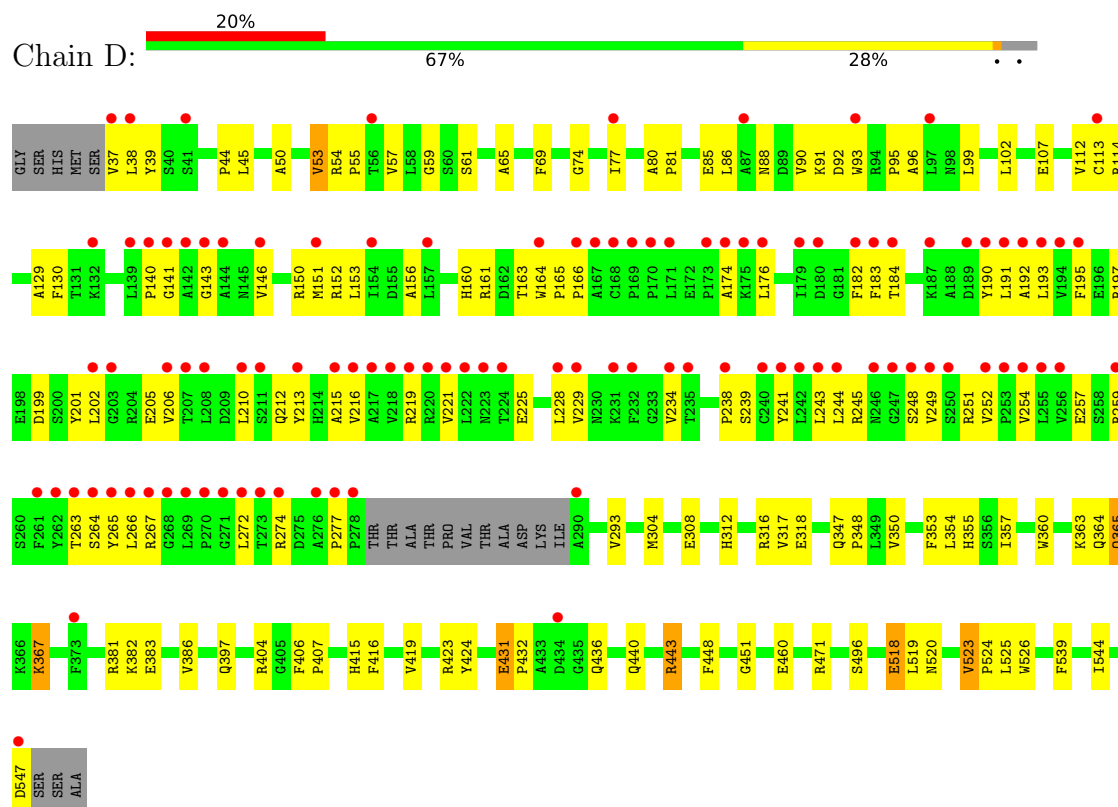
• Molecule 1: Sulfhydryl oxidase 1



• Molecule 1: Sulfhydryl oxidase 1



• Molecule 1: Sulfhydryl oxidase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.87Å 148.64Å 215.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (50.00-2.40) 99.2 (50.00-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.86 (at 2.39Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.259 0.221 , 0.261	Depositor DCC
R_{free} test set	7280 reflections (7.01%)	wwPDB-VP
Wilson B-factor (Å ²)	38.9	Xtriage
Anisotropy	0.758	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 42.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17335	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.07 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.6094e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.42	0/4148	0.87	12/5651 (0.2%)
1	B	0.42	0/4166	0.87	10/5672 (0.2%)
1	C	0.37	0/4102	0.83	4/5584 (0.1%)
1	D	0.38	0/4096	0.85	11/5578 (0.2%)
All	All	0.40	0/16512	0.85	37/22485 (0.2%)

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	39	TYR	N-CA-C	8.09	123.18	110.32
1	A	435	GLY	N-CA-C	-7.39	105.03	115.30
1	A	428	HIS	CA-C-N	6.78	127.34	119.47
1	A	428	HIS	C-N-CA	6.78	127.34	119.47
1	A	343	TYR	N-CA-C	6.46	122.23	113.97
1	D	53	VAL	N-CA-C	6.18	116.30	110.30
1	B	465	ALA	N-CA-C	6.10	118.72	111.71
1	C	53	VAL	N-CA-C	5.83	115.96	110.30
1	A	61	SER	N-CA-C	-5.78	106.19	113.18
1	C	438	VAL	N-CA-C	5.69	115.88	110.53
1	B	343	TYR	N-CA-C	5.68	121.25	113.97
1	A	451	GLY	N-CA-C	5.52	118.91	112.50
1	D	520	ASN	N-CA-C	5.48	118.52	110.30
1	D	451	GLY	N-CA-C	5.47	119.30	112.73
1	B	317	VAL	N-CA-C	5.46	116.62	111.48
1	C	526	TRP	N-CA-C	5.45	118.35	110.28
1	D	526	TRP	N-CA-C	5.45	118.14	109.96
1	D	523	VAL	N-CA-C	-5.41	103.65	108.95
1	D	39	TYR	N-CA-CB	-5.38	101.64	110.41
1	B	226	SER	N-CA-C	5.34	117.51	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	516	HIS	N-CA-C	5.32	117.30	108.20
1	A	66	VAL	N-CA-C	5.32	115.61	108.17
1	A	317	VAL	N-CA-C	5.31	116.47	111.48
1	B	428	HIS	CA-C-N	5.26	126.42	119.84
1	B	428	HIS	C-N-CA	5.26	126.42	119.84
1	B	523	VAL	N-CA-C	-5.26	103.23	108.96
1	D	415	HIS	N-CA-C	-5.24	105.46	111.07
1	C	520	ASN	N-CA-C	5.19	118.09	110.30
1	D	431	GLU	CA-C-N	5.17	126.30	119.84
1	D	431	GLU	C-N-CA	5.17	126.30	119.84
1	B	516	HIS	N-CA-C	5.17	117.04	108.20
1	A	367	LYS	N-CA-C	-5.12	107.20	113.50
1	A	465	ALA	N-CA-C	5.10	117.73	111.82
1	D	448	PHE	N-CA-C	5.07	119.61	113.38
1	B	520	ASN	N-CA-C	5.06	118.13	110.64
1	A	523	VAL	N-CA-C	-5.02	104.03	108.95
1	B	404	ARG	CB-CA-C	-5.00	110.78	116.54

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	4031	0	3913	109	0
1	B	4050	0	3935	105	0
1	C	3989	0	3885	119	0
1	D	3982	0	3875	134	0
2	A	53	0	30	1	0
2	B	53	0	29	1	0
2	C	53	0	30	0	0
2	D	53	0	30	0	0
3	A	341	0	0	8	0
3	B	339	0	0	10	0
3	C	211	0	0	5	0
3	D	180	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	17335	0	15727	463	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 (463) 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:73[A]:CYS:HB3	1:A:75[A]:HIS:CE1	1.61	1.33
1:A:73[A]:CYS:CB	1:A:75[A]:HIS:CE1	2.22	1.22
1:A:73[A]:CYS:SG	1:A:75[A]:HIS:HE1	1.64	1.20
1:A:73[B]:CYS:HB3	1:A:75[B]:HIS:CE1	1.92	1.04
1:A:73[A]:CYS:SG	1:A:75[A]:HIS:CE1	2.50	1.03
1:B:140:PRO:HG3	1:B:152:ARG:HG3	1.42	0.98
1:B:73[B]:CYS:HB3	1:B:75[B]:HIS:CE1	2.01	0.95
1:A:73[A]:CYS:HB3	1:A:75[A]:HIS:ND1	1.81	0.94
1:B:65:ALA:HB3	1:B:99:LEU:HD22	1.52	0.92
1:A:518:GLU:HG3	1:A:525:LEU:N	1.89	0.88
1:A:73[B]:CYS:CB	1:A:75[B]:HIS:CE1	2.58	0.85
1:A:65:ALA:HB3	1:A:99:LEU:HD22	1.59	0.84
1:C:129:ALA:O	1:C:163:THR:HG21	1.79	0.83
1:A:263:THR:O	1:A:267:ARG:HG2	1.77	0.83
1:A:518:GLU:HG3	1:A:525:LEU:H	1.45	0.82
1:B:367:LYS:HD3	1:B:367:LYS:H	1.44	0.81
1:D:129:ALA:O	1:D:163:THR:HG21	1.82	0.80
1:B:518:GLU:HG3	1:B:525:LEU:N	1.96	0.80
1:D:518:GLU:HG3	1:D:525:LEU:H	1.46	0.80
1:B:263:THR:O	1:B:267:ARG:HG2	1.83	0.78
1:B:518:GLU:HG2	1:B:524:PRO:HA	1.66	0.78
1:C:316:ARG:HH21	1:C:383:GLU:HG3	1.46	0.77
1:B:73[B]:CYS:CB	1:B:75[B]:HIS:CE1	2.68	0.77
1:B:36:SER:C	1:B:38:LEU:H	1.93	0.76
1:C:518:GLU:HG3	1:C:525:LEU:H	1.48	0.76
1:B:518:GLU:HG3	1:B:525:LEU:H	1.49	0.75
1:D:65:ALA:HB3	1:D:99:LEU:HD22	1.70	0.74
1:C:443:ARG:HD2	1:C:460:GLU:OE1	1.87	0.73
1:A:243:LEU:HD22	1:A:249:VAL:HG22	1.68	0.73
1:A:210:LEU:HD12	1:A:216:VAL:HG11	1.71	0.72
1:C:65:ALA:HB3	1:C:99:LEU:HD22	1.72	0.72
1:A:213:TYR:OH	1:A:274:ARG:HD2	1.90	0.72
1:D:518:GLU:HG3	1:D:525:LEU:N	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:GLU:CG	1:B:524:PRO:HA	2.20	0.72
1:B:213:TYR:OH	1:B:274:ARG:HD2	1.89	0.71
1:D:367:LYS:HD3	1:D:367:LYS:H	1.54	0.71
1:A:72:TRP:CE3	1:A:407:PRO:HG3	2.26	0.71
1:A:367:LYS:H	1:A:367:LYS:HD3	1.55	0.71
1:B:276:ALA:HB2	3:B:1017:HOH:O	1.90	0.71
1:B:72:TRP:CE3	1:B:407:PRO:HG3	2.26	0.70
1:D:431:GLU:HG3	1:D:432:PRO:HD2	1.73	0.70
1:A:140:PRO:HG2	1:A:152:ARG:HG3	1.71	0.70
1:B:423[B]:ARG:HH21	1:B:540:SER:HB3	1.57	0.70
1:C:367:LYS:H	1:C:367:LYS:HD3	1.55	0.69
1:C:518:GLU:HG2	1:C:524:PRO:HA	1.73	0.69
1:A:36:SER:C	1:A:38:LEU:H	2.00	0.69
1:C:293:VAL:HG12	1:C:397:GLN:OE1	1.92	0.68
1:D:212:GLN:NE2	1:D:277:PRO:HD3	2.09	0.68
1:B:367:LYS:HD3	1:B:367:LYS:N	2.08	0.68
1:C:212:GLN:NE2	1:C:277:PRO:HD3	2.09	0.66
1:D:293:VAL:HG12	1:D:397:GLN:OE1	1.95	0.66
1:D:50:ALA:HA	1:D:112:VAL:HG21	1.78	0.66
1:A:367:LYS:HD3	1:A:367:LYS:N	2.11	0.65
1:A:174:ALA:HB2	1:A:219:ARG:HG3	1.79	0.65
1:D:206:VAL:HG13	1:D:263:THR:HG22	1.77	0.64
1:A:73[B]:CYS:HB3	1:A:75[B]:HIS:HE1	1.61	0.64
1:C:77:ILE:HD13	1:C:496:SER:HA	1.79	0.64
1:A:518:GLU:CG	1:A:524:PRO:HA	2.27	0.63
1:C:367:LYS:HD3	1:C:367:LYS:N	2.13	0.63
1:B:210:LEU:HD12	1:B:216:VAL:HG11	1.80	0.63
1:A:387:LEU:O	1:A:388:THR:HG23	1.99	0.63
1:B:243:LEU:HD22	1:B:249:VAL:HG22	1.78	0.62
1:A:518:GLU:CG	1:A:525:LEU:H	2.10	0.62
1:C:518:GLU:CG	1:C:525:LEU:H	2.11	0.62
1:A:254:VAL:HA	3:A:884:HOH:O	1.99	0.62
1:C:518:GLU:HG3	1:C:525:LEU:N	2.15	0.62
1:B:423[B]:ARG:NH2	1:B:536:LYS:O	2.33	0.62
1:B:347:GLN:HB3	1:B:348:PRO:HD2	1.82	0.62
1:B:387:LEU:O	1:B:388:THR:HG23	2.00	0.62
1:B:423[B]:ARG:HG2	1:B:423[B]:ARG:HH11	1.65	0.62
1:D:213:TYR:CE1	1:D:274:ARG:HB2	2.35	0.62
1:A:213:TYR:CZ	1:A:274:ARG:HD2	2.35	0.61
1:A:70:ALA:HB3	1:A:73[B]:CYS:SG	2.40	0.61
1:D:367:LYS:HD3	1:D:367:LYS:N	2.14	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:471[A]:ARG:HA	1:C:471[A]:ARG:NE	2.15	0.61
1:A:518:GLU:HG2	1:A:524:PRO:HA	1.81	0.61
1:C:316:ARG:HH21	1:C:383:GLU:CG	2.14	0.61
1:C:518:GLU:CG	1:C:524:PRO:HA	2.29	0.61
1:B:75[B]:HIS:CD2	1:B:122:PRO:HD3	2.36	0.61
1:A:428:HIS:N	1:A:429:PRO:HD3	2.16	0.60
1:C:440:GLN:HG3	3:C:726:HOH:O	2.01	0.60
1:C:80:ALA:HB3	1:C:81:PRO:HD3	1.82	0.60
1:C:263:THR:O	1:C:267:ARG:HG2	2.00	0.60
1:D:151:MET:HE3	1:D:201:TYR:CE2	2.37	0.60
1:D:243:LEU:HD22	1:D:249:VAL:HG22	1.83	0.60
1:B:400:GLU:HB2	1:B:403:PHE:CD2	2.37	0.60
1:A:201:TYR:O	1:A:205:GLU:HG3	2.01	0.59
1:D:213:TYR:OH	1:D:274:ARG:HD2	2.01	0.59
1:B:518:GLU:CG	1:B:525:LEU:H	2.14	0.59
1:C:252:VAL:HG12	1:C:254:VAL:HG13	1.85	0.59
1:D:174:ALA:HB2	1:D:219:ARG:HG3	1.84	0.59
1:A:212:GLN:HB2	3:A:805:HOH:O	2.02	0.59
1:B:213:TYR:CZ	1:B:274:ARG:HD2	2.37	0.59
1:D:263:THR:O	1:D:267:ARG:HG2	2.02	0.59
1:B:201:TYR:O	1:B:205:GLU:HG3	2.02	0.59
1:B:443:ARG:HD2	1:B:460:GLU:OE1	2.02	0.59
1:C:151:MET:HE3	1:C:201:TYR:CE2	2.36	0.59
1:A:518:GLU:CG	1:A:525:LEU:N	2.65	0.58
1:B:190:TYR:CD1	1:B:269:LEU:HD13	2.39	0.58
1:B:259:ARG:O	1:B:263:THR:HG23	2.03	0.58
1:C:213:TYR:CE1	1:C:274:ARG:HB2	2.39	0.58
1:B:299:ARG:HD3	1:B:501:PHE:HE1	1.69	0.58
1:C:293:VAL:HG12	1:C:397:GLN:CD	2.28	0.58
1:A:400:GLU:HB2	1:A:403:PHE:CD2	2.39	0.58
1:C:365:GLN:CD	1:C:365:GLN:H	2.11	0.58
1:A:72:TRP:CZ3	1:A:452[A]:CYS:SG	2.97	0.57
1:B:36:SER:C	1:B:38:LEU:N	2.61	0.57
1:D:65:ALA:HB3	1:D:99:LEU:CD2	2.34	0.57
1:D:471:ARG:HA	1:D:471:ARG:NE	2.20	0.57
1:C:86:LEU:O	1:C:90:VAL:HG22	2.05	0.57
1:C:206:VAL:HG13	1:C:263:THR:HG22	1.86	0.56
1:C:244:LEU:HD12	1:C:248:SER:HB2	1.87	0.56
1:C:140:PRO:HB2	1:C:152:ARG:NH1	2.20	0.56
1:D:80:ALA:HB3	1:D:81:PRO:HD3	1.87	0.56
1:D:191:LEU:HD23	1:D:243:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:LEU:HD22	1:C:249:VAL:HG22	1.88	0.56
1:D:85:GLU:OE2	1:D:146:VAL:HG21	2.05	0.56
1:D:151:MET:HG2	1:D:201:TYR:CD2	2.41	0.56
1:D:215:ALA:HB3	1:D:272:LEU:HD23	1.86	0.56
1:C:174:ALA:HB2	1:C:219:ARG:HG3	1.87	0.56
1:C:213:TYR:OH	1:C:274:ARG:HD2	2.06	0.56
1:D:518:GLU:CG	1:D:524:PRO:HA	2.35	0.56
1:D:293:VAL:HG12	1:D:397:GLN:CD	2.31	0.56
1:D:365:GLN:CD	1:D:365:GLN:H	2.12	0.56
1:B:50:ALA:HB2	1:B:109:ASN:HA	1.88	0.55
1:C:215:ALA:HB3	1:C:272:LEU:HD23	1.86	0.55
1:A:36:SER:C	1:A:38:LEU:N	2.63	0.55
1:D:423:ARG:HD2	3:D:767:HOH:O	2.07	0.55
1:B:174:ALA:HB2	1:B:219:ARG:HG3	1.88	0.55
1:D:53:VAL:HG13	1:D:54:ARG:N	2.22	0.55
1:D:77:ILE:HD13	1:D:496:SER:HA	1.87	0.55
1:D:518:GLU:HG2	1:D:524:PRO:HA	1.88	0.55
1:D:86:LEU:O	1:D:90:VAL:HG22	2.06	0.55
1:D:252:VAL:HG12	1:D:254:VAL:HG13	1.89	0.55
1:A:365:GLN:H	1:A:365:GLN:CD	2.15	0.55
1:C:244:LEU:HB2	1:C:248:SER:HB2	1.89	0.55
1:C:347:GLN:HB3	1:C:348:PRO:HD2	1.88	0.55
1:A:52:SER:O	1:A:56:THR:HG23	2.06	0.54
1:A:296:PHE:HD1	1:B:443:ARG:CZ	2.20	0.54
1:D:201:TYR:O	1:D:205:GLU:HG3	2.07	0.54
1:D:304:MET:O	1:D:308:GLU:HG3	2.07	0.54
1:A:148:THR:O	1:A:152:ARG:HG2	2.07	0.54
1:A:347:GLN:HB3	1:A:348:PRO:HD2	1.89	0.54
1:B:518:GLU:CG	1:B:525:LEU:N	2.68	0.54
1:A:37:VAL:HG12	1:A:37:VAL:O	2.08	0.54
1:C:202:LEU:HA	1:C:205:GLU:OE1	2.08	0.54
1:B:367:LYS:H	1:B:367:LYS:CD	2.17	0.54
1:D:347:GLN:HB3	1:D:348:PRO:HD2	1.89	0.54
1:B:213:TYR:CE2	1:B:274:ARG:HB2	2.43	0.54
1:D:244:LEU:HD12	1:D:248:SER:HB2	1.89	0.54
1:B:267:ARG:HD2	3:B:832:HOH:O	2.07	0.54
1:A:518:GLU:CD	1:A:524:PRO:HA	2.31	0.54
1:D:266:LEU:O	1:D:272:LEU:HD11	2.08	0.54
1:B:206:VAL:HG13	1:B:263:THR:HG22	1.90	0.53
1:B:70:ALA:HB3	1:B:73[B]:CYS:SG	2.48	0.53
1:C:225:GLU:O	1:C:229:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:LEU:O	1:C:272:LEU:HD11	2.09	0.53
1:D:518:GLU:CG	1:D:525:LEU:H	2.17	0.53
1:A:50:ALA:HB2	1:A:109:ASN:HA	1.90	0.53
1:D:140:PRO:HB2	1:D:152:ARG:NH1	2.24	0.53
1:A:53:VAL:O	1:A:57:VAL:HG22	2.09	0.53
1:A:213:TYR:CE2	1:A:274:ARG:HB2	2.44	0.53
1:B:209:ASP:OD2	1:B:263:THR:HG21	2.09	0.53
1:D:202:LEU:HA	1:D:205:GLU:OE1	2.08	0.53
1:D:244:LEU:HB2	1:D:248:SER:HB2	1.91	0.53
1:D:53:VAL:HG13	1:D:54:ARG:H	1.73	0.53
1:B:37:VAL:HG12	1:B:37:VAL:O	2.08	0.53
1:C:151:MET:HG2	1:C:201:TYR:CD2	2.44	0.53
1:B:428:HIS:N	1:B:429:PRO:HD3	2.24	0.52
1:C:238:PRO:HG2	1:C:257:GLU:HB3	1.91	0.52
1:B:72:TRP:HE3	1:B:407:PRO:HG3	1.74	0.52
1:B:72:TRP:CZ3	1:B:452[A]:CYS:SG	3.02	0.52
1:B:518:GLU:CD	1:B:524:PRO:HA	2.34	0.52
1:A:443:ARG:HD2	1:A:460:GLU:OE1	2.09	0.52
1:A:113:CYS:HB3	1:A:118:ILE:HB	1.92	0.52
1:B:52:SER:O	1:B:56:THR:HG23	2.10	0.52
1:C:53:VAL:HG13	1:C:54:ARG:N	2.25	0.52
1:C:195:PHE:HA	1:C:221:VAL:O	2.10	0.52
1:C:304:MET:O	1:C:308:GLU:HG3	2.08	0.52
1:C:65:ALA:HB3	1:C:99:LEU:CD2	2.40	0.52
1:C:331:VAL:HG21	1:D:547:ASP:HB3	1.91	0.52
1:D:152:ARG:HG3	1:D:152:ARG:HH11	1.75	0.52
1:A:220:ARG:HG2	3:A:711:HOH:O	2.09	0.51
1:B:365:GLN:H	1:B:365:GLN:CD	2.19	0.51
1:C:113:CYS:HB3	1:C:118:ILE:HB	1.92	0.51
1:D:112:VAL:C	1:D:114:ARG:H	2.18	0.51
1:A:190:TYR:CD1	1:A:269:LEU:HD13	2.45	0.51
1:A:256:VAL:HG13	1:A:261:PHE:CD2	2.45	0.51
1:B:353:PHE:CE1	1:B:383:GLU:HB3	2.46	0.51
1:D:37:VAL:HG12	1:D:37:VAL:O	2.10	0.51
1:D:195:PHE:HE2	1:D:241:TYR:HD2	1.58	0.51
1:A:423:ARG:HD2	3:A:737:HOH:O	2.10	0.51
1:D:151:MET:HE3	1:D:201:TYR:HE2	1.75	0.51
1:D:195:PHE:HA	1:D:221:VAL:O	2.11	0.51
1:D:202:LEU:HD21	1:D:259:ARG:HA	1.93	0.51
1:A:427:ALA:C	1:A:429:PRO:HD3	2.35	0.51
1:C:316:ARG:NH2	1:C:383:GLU:HG3	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:518:GLU:HG2	1:B:524:PRO:CA	2.38	0.51
1:D:431:GLU:HB3	3:D:727:HOH:O	2.10	0.51
1:A:433:ALA:HB1	1:A:473:PRO:CG	2.41	0.51
1:D:176:LEU:HA	1:D:228:LEU:HD21	1.91	0.51
1:A:75[A]:HIS:CD2	1:A:122:PRO:HD3	2.46	0.50
1:D:183:PHE:HB3	1:D:245:ARG:NH1	2.26	0.50
1:B:139:LEU:HD21	1:B:153:LEU:HD23	1.92	0.50
1:C:201:TYR:O	1:C:205:GLU:HG3	2.11	0.50
1:D:238:PRO:HG2	1:D:257:GLU:HB3	1.91	0.50
1:D:225:GLU:O	1:D:229:VAL:HG23	2.11	0.50
1:A:292:THR:HB	1:A:295:LYS:HD2	1.94	0.50
1:D:416:PHE:CZ	1:D:544:ILE:HD11	2.47	0.50
1:B:139:LEU:HG	1:B:140:PRO:HD2	1.93	0.50
1:C:202:LEU:HD21	1:C:259:ARG:HA	1.94	0.50
1:A:243:LEU:CD2	1:A:249:VAL:HG13	2.42	0.50
1:C:85:GLU:OE2	1:C:146:VAL:HG21	2.11	0.50
1:C:239:SER:HA	1:C:257:GLU:OE2	2.12	0.50
1:D:363:LYS:HD3	3:D:784:HOH:O	2.11	0.50
1:D:107:GLU:HG3	1:D:317:VAL:HG22	1.93	0.50
1:D:234:VAL:HG22	1:D:241:TYR:HE2	1.77	0.50
1:D:443:ARG:HD2	1:D:460[A]:GLU:OE1	2.12	0.49
1:C:191:LEU:HD23	1:C:243:LEU:HD12	1.94	0.49
1:C:296:PHE:N	1:C:296:PHE:CD1	2.78	0.49
1:D:316:ARG:HH21	1:D:383:GLU:HG3	1.77	0.49
1:A:503:LYS:NZ	2:A:601:FAD:O5'	2.46	0.49
1:A:206:VAL:HG13	1:A:263:THR:HG22	1.95	0.49
1:A:381:ARG:HH11	1:A:381:ARG:HG3	1.78	0.49
1:C:495:LEU:HD12	3:C:751:HOH:O	2.13	0.49
1:C:54:ARG:N	1:C:55:PRO:HD2	2.27	0.49
1:A:518:GLU:CD	1:A:518:GLU:H	2.20	0.49
1:A:114:ARG:NH2	3:A:915:HOH:O	2.45	0.49
1:A:54:ARG:HG3	3:A:720:HOH:O	2.13	0.48
1:B:220:ARG:NH2	3:B:973:HOH:O	2.47	0.48
1:D:107:GLU:HG3	1:D:317:VAL:CG2	2.42	0.48
1:D:252:VAL:HG13	1:D:265:TYR:CD2	2.48	0.48
1:B:50:ALA:HA	1:B:112:VAL:CG2	2.43	0.48
1:A:518:GLU:HG2	1:A:523:VAL:O	2.13	0.48
1:B:518:GLU:CD	1:B:518:GLU:H	2.21	0.48
1:C:252:VAL:HG13	1:C:265:TYR:CD2	2.48	0.48
1:C:234:VAL:HG22	1:C:241:TYR:HE2	1.79	0.48
1:C:461:GLN:NE2	3:C:854:HOH:O	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:VAL:HG22	1:D:241:TYR:CE2	2.47	0.48
1:B:256:VAL:HG13	1:B:261:PHE:CD2	2.48	0.48
1:D:213:TYR:HE1	1:D:274:ARG:HB2	1.78	0.48
1:A:219:ARG:HG3	1:A:219:ARG:HH11	1.78	0.48
1:C:152:ARG:HG3	1:C:152:ARG:HH11	1.79	0.48
1:A:367:LYS:H	1:A:367:LYS:CD	2.23	0.48
1:C:61:SER:O	1:C:166:PRO:HD2	2.13	0.48
1:C:88:ASN:O	1:C:91:LYS:HG2	2.14	0.48
1:D:245:ARG:HG3	1:D:245:ARG:HH11	1.79	0.48
1:D:44:PRO:HG3	1:D:88:ASN:OD1	2.14	0.48
1:B:148:THR:O	1:B:152:ARG:HG2	2.14	0.48
1:D:518:GLU:HG2	1:D:523:VAL:O	2.14	0.47
1:B:423[B]:ARG:NH2	1:B:540:SER:HB3	2.28	0.47
1:C:350:VAL:O	1:C:353:PHE:HB3	2.15	0.47
1:C:518:GLU:HG2	1:C:523:VAL:O	2.14	0.47
1:D:114:ARG:NH1	3:D:864:HOH:O	2.47	0.47
1:B:440:GLN:HG3	3:B:1030:HOH:O	2.14	0.47
1:A:242:LEU:C	1:A:243:LEU:HD23	2.40	0.47
1:B:243:LEU:CD2	1:B:249:VAL:HG13	2.45	0.47
1:C:210:LEU:HD22	1:C:210:LEU:N	2.29	0.47
1:C:399:SER:O	1:C:400:GLU:HG3	2.15	0.47
1:B:243:LEU:HD22	1:B:249:VAL:HG13	1.95	0.47
1:B:275:ASP:CG	1:B:275:ASP:O	2.57	0.47
1:C:518:GLU:CD	1:C:524:PRO:HA	2.40	0.47
1:D:202:LEU:O	1:D:202:LEU:HD23	2.15	0.47
1:D:37:VAL:HG12	3:D:827:HOH:O	2.13	0.47
1:C:195:PHE:HE2	1:C:241:TYR:HD2	1.63	0.46
1:C:329:ARG:HD2	3:C:843:HOH:O	2.14	0.46
1:C:382:LYS:O	1:C:386:VAL:HG23	2.14	0.46
1:A:275:ASP:CG	1:A:275:ASP:O	2.57	0.46
1:C:176:LEU:HA	1:C:228:LEU:HD21	1.96	0.46
1:D:264:SER:HA	1:D:267:ARG:HD2	1.96	0.46
1:C:241:TYR:CE1	1:C:251:ARG:HD3	2.51	0.46
1:D:141:GLY:O	1:D:143:GLY:N	2.48	0.46
1:A:73[A]:CYS:HA	1:A:452[A]:CYS:SG	2.55	0.46
1:B:518:GLU:HG2	1:B:523:VAL:O	2.15	0.46
1:A:75[B]:HIS:CD2	1:A:122:PRO:HD3	2.49	0.46
1:A:243:LEU:HD22	1:A:249:VAL:HG13	1.97	0.46
1:B:234:VAL:HG22	1:B:241:TYR:CE1	2.50	0.46
1:B:299:ARG:HD2	3:B:767:HOH:O	2.16	0.46
1:D:355:HIS:HD2	3:D:728:HOH:O	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:TRP:CG	1:A:507:PRO:HA	2.51	0.46
1:C:53:VAL:HG13	1:C:54:ARG:H	1.81	0.46
1:D:192:ALA:HB2	1:D:266:LEU:HD21	1.97	0.46
1:A:434[B]:ASP:OD1	1:A:434[B]:ASP:N	2.45	0.46
1:B:36:SER:O	1:B:38:LEU:N	2.48	0.46
1:B:382:LYS:O	1:B:386:VAL:HG23	2.16	0.46
1:C:413:LEU:O	1:C:417:LEU:HG	2.16	0.46
1:D:88:ASN:O	1:D:91:LYS:HG2	2.16	0.46
1:D:163:THR:HG22	1:D:164:TRP:N	2.30	0.46
1:A:174:ALA:HB2	1:A:219:ARG:CG	2.45	0.46
1:A:343:TYR:CE1	1:A:421:ALA:HA	2.51	0.46
1:B:174:ALA:HB2	1:B:219:ARG:CG	2.46	0.46
1:C:75:HIS:CE1	1:C:142:ALA:HA	2.51	0.45
1:D:191:LEU:HB3	1:D:243:LEU:HB2	1.98	0.45
1:B:140:PRO:HG2	1:B:149:LEU:HD23	1.97	0.45
1:D:195:PHE:CE2	1:D:241:TYR:HD2	2.33	0.45
1:D:202:LEU:O	1:D:206:VAL:HG23	2.15	0.45
1:C:202:LEU:HD23	1:C:202:LEU:O	2.17	0.45
1:D:424:TYR:HE1	1:D:431:GLU:HG2	1.81	0.45
1:A:518:GLU:HG2	1:A:524:PRO:CA	2.45	0.45
1:B:267:ARG:NH2	3:B:969:HOH:O	2.39	0.45
1:B:471:ARG:HA	1:B:471:ARG:NE	2.31	0.45
1:C:160:HIS:HB3	1:C:163:THR:O	2.16	0.45
1:D:350:VAL:O	1:D:353:PHE:HB3	2.17	0.45
1:D:61:SER:O	1:D:166:PRO:HD2	2.17	0.45
1:D:190:TYR:HB2	1:D:216:VAL:HG23	1.97	0.45
1:D:436:GLN:O	1:D:440:GLN:HB2	2.17	0.45
1:D:239:SER:HA	1:D:257:GLU:OE2	2.17	0.45
1:D:443:ARG:NH1	1:D:460[A]:GLU:OE2	2.50	0.45
1:A:215:ALA:HB3	1:A:272:LEU:CD2	2.46	0.45
1:A:64:TRP:CZ3	1:A:98:ASN:HB3	2.51	0.45
1:A:173:PRO:HA	1:A:220:ARG:HG3	1.98	0.45
1:B:171:LEU:O	1:B:220:ARG:HD3	2.17	0.45
1:D:360:TRP:O	1:D:364:GLN:HG2	2.17	0.45
1:D:54:ARG:N	1:D:55:PRO:HD2	2.31	0.45
1:D:95:PRO:HD3	1:D:277:PRO:HB3	1.99	0.45
1:D:197:ARG:HG3	1:D:197:ARG:HH11	1.81	0.45
1:C:219:ARG:HG3	1:C:219:ARG:HH11	1.80	0.45
1:D:59:GLY:HA2	1:D:130:PHE:HA	1.98	0.45
1:A:440:GLN:HG3	3:A:992:HOH:O	2.16	0.44
1:D:241:TYR:HE1	1:D:251:ARG:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:102:LEU:C	1:C:102:LEU:HD23	2.42	0.44
1:D:219:ARG:HG3	1:D:219:ARG:HH11	1.81	0.44
1:C:443:ARG:HD3	1:C:463:ALA:CB	2.47	0.44
1:D:50:ALA:HA	1:D:112:VAL:CG2	2.45	0.44
1:D:210:LEU:N	1:D:210:LEU:HD22	2.33	0.44
1:B:181:GLY:O	1:B:184:THR:HB	2.17	0.44
1:C:183:PHE:HB3	1:C:245:ARG:NH1	2.32	0.44
1:C:234:VAL:HG22	1:C:241:TYR:CE2	2.51	0.44
1:D:182:PHE:C	1:D:184:THR:H	2.26	0.44
1:B:254:VAL:HA	3:B:987:HOH:O	2.18	0.44
1:C:151:MET:HE3	1:C:201:TYR:HE2	1.80	0.44
1:C:153:LEU:O	1:C:156:ALA:HB3	2.18	0.44
1:C:182:PHE:C	1:C:184:THR:H	2.26	0.44
1:A:96:ALA:HB1	1:A:168:CYS:HB2	2.00	0.44
1:B:170:PRO:HD2	3:B:937:HOH:O	2.16	0.44
1:D:153:LEU:O	1:D:156:ALA:HB3	2.18	0.44
1:D:241:TYR:CE1	1:D:251:ARG:HB2	2.53	0.44
1:B:287:ASP:OD1	1:B:287:ASP:N	2.50	0.44
1:A:73[B]:CYS:HB3	1:A:75[B]:HIS:ND1	2.26	0.43
1:A:368:ARG:HB3	1:A:368:ARG:NH1	2.33	0.43
1:B:227:ASP:O	1:B:231:LYS:HB2	2.18	0.43
1:C:93:TRP:O	1:C:96:ALA:HB3	2.18	0.43
1:C:202:LEU:O	1:C:206:VAL:HG23	2.18	0.43
1:D:102:LEU:HD23	1:D:102:LEU:C	2.42	0.43
1:C:241:TYR:HE1	1:C:251:ARG:HB2	1.83	0.43
1:D:382:LYS:O	1:D:386:VAL:HG23	2.19	0.43
1:A:36:SER:O	1:A:38:LEU:N	2.51	0.43
1:A:381:ARG:HG3	1:A:381:ARG:NH1	2.32	0.43
1:C:72:TRP:CE3	1:C:407:PRO:HG3	2.52	0.43
1:D:241:TYR:CE1	1:D:251:ARG:HD3	2.54	0.43
1:A:59:GLY:N	1:A:131:THR:O	2.47	0.43
1:A:382:LYS:O	1:A:386:VAL:HG23	2.18	0.43
1:D:312:HIS:CE1	1:D:316:ARG:HG3	2.54	0.43
1:C:44:PRO:HG3	1:C:88:ASN:OD1	2.18	0.43
1:A:234:VAL:HG22	1:A:241:TYR:CE1	2.53	0.43
1:C:241:TYR:CE1	1:C:251:ARG:HB2	2.54	0.43
1:C:195:PHE:CE2	1:C:241:TYR:HD2	2.36	0.43
1:A:296:PHE:CD1	1:B:443:ARG:CZ	3.01	0.43
1:B:423[B]:ARG:HG2	1:B:423[B]:ARG:NH1	2.31	0.43
1:C:63:ALA:O	1:C:97:LEU:HD12	2.18	0.43
1:D:102:LEU:HD11	1:D:112:VAL:HG11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:406:PHE:HB3	1:D:407:PRO:HD3	2.01	0.43
1:A:53:VAL:HG13	1:A:54:ARG:N	2.34	0.43
1:A:316:ARG:NH2	1:A:383:GLU:HG3	2.34	0.43
1:A:209:ASP:OD2	1:A:263:THR:HG21	2.18	0.43
1:B:368:ARG:NH1	1:B:368:ARG:HB3	2.34	0.42
1:C:244:LEU:HD12	1:C:248:SER:CB	2.48	0.42
1:A:510:GLU:OE1	1:A:510:GLU:N	2.45	0.42
1:C:64:TRP:CZ3	1:C:98:ASN:HB3	2.55	0.42
1:A:256:VAL:CG1	1:A:261:PHE:CE2	3.02	0.42
1:A:387:LEU:O	1:A:388:THR:CG2	2.68	0.42
1:B:64:TRP:CZ3	1:B:98:ASN:HB3	2.54	0.42
1:B:245:ARG:NH2	3:B:942:HOH:O	2.51	0.42
1:B:343:TYR:CE1	1:B:421:ALA:HA	2.54	0.42
1:C:182:PHE:CZ	1:C:191:LEU:HD13	2.54	0.42
1:C:191:LEU:HB3	1:C:243:LEU:HB2	2.01	0.42
1:C:406:PHE:HB3	1:C:407:PRO:HD3	2.01	0.42
1:D:164:TRP:HA	1:D:165:PRO:HD3	1.89	0.42
1:D:354:LEU:HA	1:D:357:ILE:HG22	2.01	0.42
1:B:152:ARG:HA	1:B:152:ARG:HD3	1.86	0.42
1:B:312:HIS:CE1	1:B:316:ARG:HG3	2.53	0.42
1:C:163:THR:HG22	1:C:164:TRP:N	2.33	0.42
1:D:419:VAL:HG21	1:D:539:PHE:HB2	2.01	0.42
1:D:182:PHE:CZ	1:D:191:LEU:HD13	2.54	0.42
1:B:469:GLN:HB2	1:D:519:LEU:HD13	2.02	0.42
1:C:190:TYR:HB2	1:C:216:VAL:HG23	2.01	0.42
1:D:74:GLY:O	1:D:77:ILE:CG2	2.68	0.42
1:D:350:VAL:HG22	1:D:386:VAL:HG12	2.01	0.42
1:A:139:LEU:HD21	1:A:153:LEU:HD23	2.01	0.42
1:A:428:HIS:N	1:A:429:PRO:CD	2.83	0.42
1:B:220:ARG:HG2	3:B:905:HOH:O	2.20	0.42
1:C:161:ARG:HA	1:C:161:ARG:HD3	1.86	0.42
1:C:367:LYS:H	1:C:367:LYS:CD	2.27	0.42
1:D:92:ASP:OD1	1:D:274:ARG:NH2	2.53	0.42
1:A:151:MET:HE3	1:A:201:TYR:CD1	2.55	0.41
1:B:293:VAL:CG1	1:B:397:GLN:CD	2.93	0.41
1:B:353:PHE:CZ	1:B:383:GLU:HB3	2.55	0.41
1:A:416:PHE:CZ	1:A:544:ILE:HD11	2.55	0.41
1:B:53:VAL:HG13	1:B:54:ARG:N	2.35	0.41
1:B:387:LEU:O	1:B:388:THR:CG2	2.68	0.41
1:C:245:ARG:HG3	1:C:245:ARG:HH11	1.84	0.41
1:C:442:MET:HE2	1:C:459:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381:ARG:HG3	1:D:381:ARG:HH11	1.85	0.41
1:C:50:ALA:HA	1:C:112:VAL:HG21	2.02	0.41
1:C:241:TYR:CD1	1:C:251:ARG:HA	2.55	0.41
1:C:354:LEU:HA	1:C:357:ILE:HG22	2.01	0.41
1:D:252:VAL:HG13	1:D:265:TYR:CE2	2.55	0.41
1:C:360:TRP:O	1:C:364:GLN:HG2	2.20	0.41
1:D:245:ARG:NH1	1:D:245:ARG:HG3	2.34	0.41
1:D:367:LYS:H	1:D:367:LYS:CD	2.26	0.41
1:B:140:PRO:CG	1:B:152:ARG:HG3	2.32	0.41
1:B:204:ARG:HG3	1:B:220:ARG:HD2	2.03	0.41
1:B:503:LYS:NZ	2:B:601:FAD:O5'	2.53	0.41
1:D:193:LEU:HA	1:D:219:ARG:O	2.20	0.41
1:D:304:MET:HE2	1:D:544:ILE:HG21	2.02	0.41
1:A:171:LEU:O	1:A:220:ARG:HD3	2.21	0.41
1:A:367:LYS:N	1:A:367:LYS:CD	2.77	0.41
1:D:241:TYR:CD1	1:D:251:ARG:HA	2.55	0.41
1:D:518:GLU:CD	1:D:524:PRO:HA	2.45	0.41
1:A:215:ALA:HB3	1:A:272:LEU:HD23	2.02	0.41
1:B:213:TYR:CZ	1:B:267:ARG:NH1	2.87	0.41
1:B:314:ILE:HG21	1:B:336:PHE:HE2	1.85	0.41
1:B:367:LYS:N	1:B:367:LYS:CD	2.76	0.41
1:C:430:GLN:HB2	3:C:722:HOH:O	2.20	0.41
1:D:160:HIS:O	1:D:161:ARG:HD3	2.21	0.41
1:B:242:LEU:C	1:B:243:LEU:HD23	2.46	0.41
1:C:212:GLN:HE22	1:C:277:PRO:HD3	1.85	0.41
1:A:177:ASN:ND2	3:A:1019:HOH:O	2.52	0.41
1:A:326:GLU:CD	1:A:326:GLU:C	2.88	0.41
1:B:215:ALA:HB3	1:B:272:LEU:CD2	2.51	0.41
1:C:53:VAL:O	1:C:57:VAL:HG22	2.21	0.41
1:C:195:PHE:CD1	1:C:221:VAL:HB	2.56	0.41
1:C:316:ARG:HE	1:C:383:GLU:CD	2.29	0.41
1:C:367:LYS:N	1:C:367:LYS:CD	2.81	0.41
1:D:53:VAL:O	1:D:57:VAL:HG22	2.21	0.41
1:D:160:HIS:HB3	1:D:163:THR:O	2.21	0.41
1:D:316:ARG:HE	1:D:383:GLU:CD	2.29	0.41
1:D:518:GLU:CG	1:D:525:LEU:N	2.78	0.41
1:A:316:ARG:HH21	1:A:383:GLU:HG3	1.86	0.41
1:B:168:CYS:HA	1:B:169:PRO:HD3	1.88	0.41
1:C:141:GLY:O	1:C:143:GLY:N	2.54	0.41
1:C:252:VAL:HG13	1:C:265:TYR:CE2	2.56	0.41
1:D:112:VAL:C	1:D:114:ARG:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:ALA:HB2	1:C:266:LEU:HD21	2.03	0.40
1:D:93:TRP:O	1:D:96:ALA:HB3	2.21	0.40
1:D:150:ARG:NE	1:D:259:ARG:HH12	2.19	0.40
1:D:244:LEU:HD12	1:D:248:SER:CB	2.50	0.40
1:D:404:ARG:O	1:D:407:PRO:HD2	2.21	0.40
1:A:471:ARG:NE	1:A:471:ARG:HA	2.37	0.40
1:B:73[B]:CYS:HB3	1:B:75[B]:HIS:HE1	1.75	0.40
1:B:182:PHE:O	1:B:186:ASN:HB2	2.21	0.40
1:C:197:ARG:HG3	1:C:197:ARG:HH11	1.86	0.40
1:D:197:ARG:C	1:D:199:ASP:H	2.30	0.40
1:B:506:TRP:CG	1:B:507:PRO:HA	2.57	0.40
1:C:149:LEU:O	1:C:152:ARG:HB2	2.22	0.40
1:D:38:LEU:HD23	1:D:69:PHE:CE2	2.57	0.40
1:A:73[B]:CYS:CB	1:A:75[B]:HIS:HE1	2.21	0.40
1:A:210:LEU:HD12	1:A:216:VAL:CG1	2.48	0.40
1:B:293:VAL:HG12	1:B:397:GLN:OE1	2.21	0.40
1:A:350:VAL:O	1:A:353:PHE:HB3	2.22	0.40
1:A:536:LYS:O	1:A:540:SER:HB3	2.22	0.40
1:C:195:PHE:O	1:C:238:PRO:HA	2.22	0.40
1:C:264:SER:HA	1:C:267:ARG:HD2	2.03	0.40

There are no symmetry-related clashes.

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	503/519 (97%)	486 (97%)	16 (3%)	1 (0%)	43	58
1	B	505/519 (97%)	480 (95%)	22 (4%)	3 (1%)	21	32
1	C	498/519 (96%)	463 (93%)	34 (7%)	1 (0%)	43	58
1	D	497/519 (96%)	465 (94%)	32 (6%)	0	100	100
All	All	2003/2076 (96%)	1894 (95%)	104 (5%)	5 (0%)	36	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	37	VAL
1	B	142	ALA
1	A	37	VAL
1	B	429	PRO
1	C	37	VAL

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	433/441 (98%)	424 (98%)	9 (2%)	47	69
1	B	435/441 (99%)	419 (96%)	16 (4%)	30	51
1	C	428/441 (97%)	420 (98%)	8 (2%)	50	71
1	D	427/441 (97%)	420 (98%)	7 (2%)	55	76
All	All	1723/1764 (98%)	1683 (98%)	40 (2%)	44	66

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	LEU
1	A	219	ARG
1	A	243	LEU
1	A	256	VAL
1	A	367	LYS
1	A	443	ARG
1	A	461	GLN
1	A	482	THR
1	A	518	GLU
1	B	99	LEU
1	B	113	CYS
1	B	114	ARG
1	B	161	ARG
1	B	202	LEU
1	B	219	ARG

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Mol	Chain	Res	Type
1	B	243	LEU
1	B	256	VAL
1	B	287	ASP
1	B	318	GLU
1	B	367	LYS
1	B	443	ARG
1	B	461	GLN
1	B	482	THR
1	B	518	GLU
1	B	547	ASP
1	C	45	LEU
1	C	104	CYS
1	C	113	CYS
1	C	296	PHE
1	C	318	GLU
1	C	365	GLN
1	C	367	LYS
1	C	518	GLU
1	D	45	LEU
1	D	113	CYS
1	D	318	GLU
1	D	365	GLN
1	D	367	LYS
1	D	443	ARG
1	D	518	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	355	HIS
1	A	358	ASN
1	A	364	GLN
1	A	402	HIS
1	A	436	GLN
1	A	440	GLN
1	A	447	GLN
1	A	520	ASN
1	B	98	ASN
1	B	347	GLN
1	B	364	GLN
1	B	397	GLN

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Mol	Chain	Res	Type
1	B	402	HIS
1	B	520	ASN
1	C	212	GLN
1	C	362	GLN
1	C	447	GLN
1	C	475	ASN
1	C	500	HIS
1	D	212	GLN
1	D	214	HIS
1	D	347	GLN
1	D	447	GLN
1	D	461	GLN

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](#)

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	$\# Z > 2$
2	FAD	B	601	-	58,58,58	2.00	13 (22%)	85,89,89	3.66	50 (58%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	FAD	D	601	-	58,58,58	2.00	12 (20%)	85,89,89	3.53	54 (63%)
2	FAD	C	601	-	58,58,58	2.04	15 (25%)	85,89,89	3.51	46 (54%)
2	FAD	A	601	-	58,58,58	2.05	14 (24%)	85,89,89	3.65	49 (57%)

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	601	-	-	14/34/50/50	0/6/6/6
2	FAD	D	601	-	-	17/34/50/50	0/6/6/6
2	FAD	C	601	-	-	13/34/50/50	0/6/6/6
2	FAD	A	601	-	-	13/34/50/50	0/6/6/6

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	FAD	C4X-N5	6.49	1.44	1.30
2	A	601	FAD	C4X-N5	6.31	1.44	1.30
2	D	601	FAD	C4X-N5	6.30	1.44	1.30
2	B	601	FAD	C4X-N5	5.93	1.43	1.30
2	B	601	FAD	C9A-C5X	5.19	1.49	1.41
2	A	601	FAD	C9A-C5X	5.06	1.49	1.41
2	D	601	FAD	C9A-C5X	5.05	1.49	1.41
2	C	601	FAD	C9A-N10	5.05	1.49	1.41
2	A	601	FAD	C9A-N10	5.04	1.49	1.41
2	B	601	FAD	C9A-N10	5.00	1.49	1.41
2	C	601	FAD	C9A-C5X	4.95	1.49	1.41
2	C	601	FAD	C4A-N3A	4.86	1.43	1.34
2	D	601	FAD	C9A-N10	4.68	1.49	1.41
2	B	601	FAD	C4A-N3A	4.41	1.42	1.34
2	D	601	FAD	C4A-N3A	4.24	1.42	1.34
2	B	601	FAD	C5A-C4A	-4.15	1.31	1.39
2	A	601	FAD	C4A-N3A	4.01	1.41	1.34
2	A	601	FAD	C5A-C4A	-4.00	1.31	1.39
2	D	601	FAD	C5A-C4A	-3.96	1.32	1.39
2	C	601	FAD	C2A-N3A	3.93	1.40	1.33
2	A	601	FAD	C2A-N3A	3.70	1.40	1.33
2	D	601	FAD	C2A-N3A	3.65	1.40	1.33
2	A	601	FAD	P-O3P	3.47	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	FAD	C5A-C4A	-3.45	1.32	1.39
2	B	601	FAD	C2A-N3A	3.27	1.39	1.33
2	B	601	FAD	C5'-C4'	-3.25	1.47	1.51
2	A	601	FAD	C5'-C4'	-3.06	1.47	1.51
2	D	601	FAD	C8A-N9A	3.05	1.42	1.37
2	C	601	FAD	C8A-N9A	2.96	1.42	1.37
2	A	601	FAD	C10-N1	2.82	1.38	1.33
2	C	601	FAD	C2B-C3B	-2.73	1.46	1.53
2	D	601	FAD	C2B-C3B	-2.70	1.46	1.53
2	B	601	FAD	C10-N1	2.70	1.38	1.33
2	D	601	FAD	C5'-C4'	-2.66	1.48	1.51
2	D	601	FAD	C10-N1	2.63	1.38	1.33
2	C	601	FAD	C10-N1	2.63	1.38	1.33
2	A	601	FAD	C6-C7	2.63	1.43	1.39
2	A	601	FAD	C8A-N9A	2.60	1.42	1.37
2	A	601	FAD	C2B-C3B	-2.58	1.46	1.53
2	C	601	FAD	C5'-C4'	-2.57	1.48	1.51
2	C	601	FAD	C6-C7	2.55	1.43	1.39
2	D	601	FAD	C6-C7	2.53	1.43	1.39
2	B	601	FAD	C8A-N9A	2.44	1.41	1.37
2	B	601	FAD	C2B-C3B	-2.40	1.46	1.53
2	D	601	FAD	O4-C4	2.35	1.28	1.23
2	B	601	FAD	C6-C7	2.17	1.42	1.39
2	B	601	FAD	P-O3P	2.16	1.61	1.59
2	A	601	FAD	C4-N3	2.14	1.42	1.38
2	C	601	FAD	C5X-N5	2.13	1.43	1.39
2	C	601	FAD	O4-C4	2.11	1.27	1.23
2	B	601	FAD	O4-C4	2.11	1.27	1.23
2	C	601	FAD	P-O3P	2.08	1.61	1.59
2	A	601	FAD	C5X-N5	2.01	1.43	1.39
2	C	601	FAD	C1'-N10	-2.00	1.43	1.47

All (199) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	FAD	C5X-C9A-N10	-10.07	108.86	117.97
2	C	601	FAD	C9-C9A-N10	9.78	135.01	121.85
2	B	601	FAD	C9-C9A-N10	9.71	134.92	121.85
2	B	601	FAD	C4'-C3'-C2'	9.66	129.64	113.57
2	A	601	FAD	C4A-N9A-C8A	-9.58	95.68	105.74
2	B	601	FAD	O4-C4-N3	-9.49	102.27	120.11
2	D	601	FAD	C5X-C9A-N10	-9.39	109.48	117.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C5X-C9A-N10	-9.04	109.79	117.97
2	C	601	FAD	C9A-N10-C10	8.88	134.29	120.75
2	A	601	FAD	C9-C9A-N10	8.73	133.60	121.85
2	D	601	FAD	C9-C9A-N10	8.61	133.43	121.85
2	A	601	FAD	N3A-C2A-N1A	-8.16	116.23	128.58
2	D	601	FAD	C9A-N10-C10	8.09	133.08	120.75
2	D	601	FAD	C4A-N9A-C8A	-8.09	97.24	105.74
2	B	601	FAD	N3A-C2A-N1A	-8.06	116.38	128.58
2	A	601	FAD	C9A-N10-C10	7.99	132.93	120.75
2	B	601	FAD	C9A-N10-C10	7.96	132.88	120.75
2	A	601	FAD	C5X-C9A-N10	-7.49	111.20	117.97
2	D	601	FAD	N3A-C2A-N1A	-7.49	117.25	128.58
2	B	601	FAD	C4A-N9A-C8A	-7.37	98.00	105.74
2	A	601	FAD	C4'-C3'-C2'	7.35	125.79	113.57
2	D	601	FAD	C8M-C8-C9	-7.02	107.21	119.57
2	A	601	FAD	C9A-C5X-N5	-6.79	115.25	122.45
2	C	601	FAD	C4A-N9A-C8A	-6.73	98.68	105.74
2	A	601	FAD	C5'-C4'-C3'	6.39	124.28	112.22
2	C	601	FAD	C4'-C3'-C2'	6.34	124.12	113.57
2	C	601	FAD	C2B-C1B-N9A	6.32	129.01	113.30
2	C	601	FAD	C4A-C5A-N7A	6.30	117.79	110.58
2	A	601	FAD	C5X-N5-C4X	6.28	128.25	118.09
2	D	601	FAD	C8M-C8-C7	6.27	133.56	120.76
2	A	601	FAD	C5A-C4A-N9A	6.07	112.42	105.81
2	C	601	FAD	O4-C4-N3	-6.05	108.75	120.11
2	B	601	FAD	C5X-N5-C4X	5.91	127.65	118.09
2	D	601	FAD	C10-N1-C2	5.68	129.14	116.85
2	A	601	FAD	C8M-C8-C9	-5.67	109.57	119.57
2	C	601	FAD	N9A-C8A-N7A	5.66	121.97	113.94
2	B	601	FAD	O3P-P-O1P	-5.57	93.95	110.70
2	A	601	FAD	C8M-C8-C7	5.50	131.99	120.76
2	D	601	FAD	C4-C4X-N5	5.45	125.74	118.21
2	D	601	FAD	N9A-C8A-N7A	5.40	121.60	113.94
2	B	601	FAD	C4-C4X-N5	5.39	125.66	118.21
2	A	601	FAD	C5B-C4B-C3B	5.37	134.53	115.21
2	B	601	FAD	C9A-C5X-N5	-5.31	116.82	122.45
2	D	601	FAD	O3'-C3'-C4'	5.29	120.96	108.93
2	B	601	FAD	C2B-C1B-N9A	5.27	126.39	113.30
2	C	601	FAD	C5A-N7A-C8A	-5.26	95.18	103.45
2	A	601	FAD	C4B-O4B-C1B	-5.24	97.90	109.47
2	C	601	FAD	C4-C4X-N5	5.23	125.43	118.21
2	D	601	FAD	C5X-N5-C4X	5.22	126.53	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	N9A-C8A-N7A	5.20	121.32	113.94
2	A	601	FAD	C4-C4X-N5	5.17	125.34	118.21
2	B	601	FAD	O2'-C2'-C3'	5.12	121.23	109.25
2	C	601	FAD	C5X-N5-C4X	5.07	126.29	118.09
2	C	601	FAD	N3A-C2A-N1A	-5.05	120.94	128.58
2	D	601	FAD	N3-C2-N1	-4.99	108.90	119.50
2	D	601	FAD	O4-C4-N3	-4.88	110.93	120.11
2	A	601	FAD	C10-N1-C2	4.86	127.37	116.85
2	C	601	FAD	O4B-C4B-C5B	-4.83	93.87	109.33
2	D	601	FAD	C5B-C4B-C3B	4.80	132.48	115.21
2	D	601	FAD	C2B-C1B-N9A	4.76	125.14	113.30
2	A	601	FAD	O2-C2-N3	4.74	127.68	118.58
2	C	601	FAD	O3'-C3'-C4'	4.72	119.65	108.93
2	C	601	FAD	O2B-C2B-C3B	4.71	126.91	111.82
2	A	601	FAD	O4-C4-N3	-4.67	111.34	120.11
2	D	601	FAD	C4'-C3'-C2'	4.66	121.32	113.57
2	B	601	FAD	C5B-C4B-C3B	4.63	131.88	115.21
2	D	601	FAD	C4A-C5A-N7A	4.60	115.84	110.58
2	B	601	FAD	C4B-O4B-C1B	-4.48	99.57	109.47
2	D	601	FAD	C5A-N7A-C8A	-4.47	96.42	103.45
2	D	601	FAD	C9A-C5X-N5	-4.43	117.75	122.45
2	C	601	FAD	C5B-C4B-C3B	4.38	130.99	115.21
2	C	601	FAD	C3B-C2B-C1B	-4.36	93.21	101.46
2	B	601	FAD	C8M-C8-C7	4.34	129.62	120.76
2	A	601	FAD	C2B-C1B-N9A	4.32	124.03	113.30
2	D	601	FAD	C5A-C6A-N6A	-4.31	112.61	123.29
2	C	601	FAD	C10-N1-C2	4.29	126.14	116.85
2	D	601	FAD	O4B-C4B-C5B	-4.26	95.68	109.33
2	C	601	FAD	O2'-C2'-C3'	4.24	119.18	109.25
2	A	601	FAD	O2A-PA-O5B	4.16	126.40	107.57
2	C	601	FAD	C5A-C6A-N6A	-4.03	113.31	123.29
2	C	601	FAD	C6A-C5A-C4A	-4.02	111.69	117.18
2	B	601	FAD	O4B-C4B-C3B	4.01	113.12	105.15
2	C	601	FAD	C9A-C5X-N5	-4.00	118.21	122.45
2	D	601	FAD	PA-O5B-C5B	3.99	144.19	121.35
2	B	601	FAD	C5A-C4A-N9A	3.98	110.15	105.81
2	A	601	FAD	N3-C2-N1	-3.96	111.09	119.50
2	A	601	FAD	O4B-C1B-C2B	3.87	114.90	106.62
2	C	601	FAD	C2B-C3B-C4B	3.82	109.99	102.61
2	B	601	FAD	C8M-C8-C9	-3.78	112.90	119.57
2	A	601	FAD	O3B-C3B-C2B	3.76	123.87	111.82
2	C	601	FAD	O3P-P-O1P	-3.72	99.51	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	O2'-C2'-C3'	3.69	117.89	109.25
2	B	601	FAD	N9A-C8A-N7A	3.68	119.15	113.94
2	B	601	FAD	O4-C4-C4X	3.68	136.24	126.53
2	B	601	FAD	C10-N1-C2	3.60	124.65	116.85
2	B	601	FAD	C7M-C7-C6	-3.59	113.24	119.57
2	A	601	FAD	C6-C5X-N5	3.46	124.19	118.44
2	B	601	FAD	O5'-C5'-C4'	3.44	118.54	109.36
2	C	601	FAD	C8M-C8-C9	-3.41	113.56	119.57
2	D	601	FAD	C6A-C5A-C4A	-3.41	112.52	117.18
2	B	601	FAD	C10-C4X-N5	-3.37	117.93	124.81
2	D	601	FAD	O4'-C4'-C5'	3.35	117.38	109.99
2	D	601	FAD	C10-C4X-N5	-3.32	118.03	124.81
2	C	601	FAD	C4X-C4-N3	3.32	121.70	113.25
2	B	601	FAD	O2P-P-O1P	3.29	127.77	112.44
2	B	601	FAD	PA-O5B-C5B	3.29	140.21	121.35
2	A	601	FAD	O5B-C5B-C4B	-3.28	97.82	108.99
2	B	601	FAD	C1'-N10-C9A	-3.28	114.27	120.63
2	D	601	FAD	O2-C2-N3	3.24	124.80	118.58
2	A	601	FAD	C10-C4X-N5	-3.22	118.24	124.81
2	C	601	FAD	C1'-N10-C9A	-3.20	114.41	120.63
2	B	601	FAD	P-O5'-C5'	3.19	139.65	121.35
2	B	601	FAD	C4X-C4-N3	3.19	121.38	113.25
2	A	601	FAD	P-O5'-C5'	3.16	139.47	121.35
2	D	601	FAD	P-O5'-C5'	3.14	139.32	121.35
2	A	601	FAD	N10-C10-N1	3.12	127.69	118.51
2	B	601	FAD	O2A-PA-O5B	3.09	121.55	107.57
2	A	601	FAD	C4X-C4-N3	3.08	121.09	113.25
2	A	601	FAD	C2A-N3A-C4A	3.07	119.33	111.83
2	A	601	FAD	O3P-P-O1P	-3.05	101.52	110.70
2	C	601	FAD	N3-C2-N1	-3.04	113.04	119.50
2	C	601	FAD	O4'-C4'-C5'	3.03	116.66	109.99
2	C	601	FAD	C10-C4X-N5	-3.02	118.65	124.81
2	D	601	FAD	O3B-C3B-C4B	2.99	119.67	111.08
2	D	601	FAD	N10-C10-N1	2.97	127.27	118.51
2	B	601	FAD	O3B-C3B-C2B	2.96	121.30	111.82
2	C	601	FAD	N10-C10-N1	2.96	127.22	118.51
2	A	601	FAD	C9A-C9-C8	2.92	125.09	119.22
2	D	601	FAD	O2P-P-O1P	2.92	126.02	112.44
2	C	601	FAD	C5A-C6A-N1A	2.91	124.89	117.51
2	D	601	FAD	C2'-C1'-N10	2.91	123.93	110.20
2	D	601	FAD	C1'-N10-C9A	-2.90	114.99	120.63
2	C	601	FAD	C8M-C8-C7	2.89	126.67	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C5A-N7A-C8A	-2.89	98.90	103.45
2	B	601	FAD	C2A-N3A-C4A	2.89	118.89	111.83
2	A	601	FAD	O4B-C4B-C3B	2.89	110.89	105.15
2	A	601	FAD	C4X-C10-N10	-2.89	112.35	116.48
2	A	601	FAD	C3B-C2B-C1B	-2.88	96.02	101.46
2	A	601	FAD	C9-C9A-C5X	-2.87	114.96	120.03
2	C	601	FAD	O3B-C3B-C2B	2.87	121.01	111.82
2	B	601	FAD	C9A-C9-C8	2.85	124.95	119.22
2	C	601	FAD	C4X-C10-N10	-2.84	112.42	116.48
2	B	601	FAD	O3'-C3'-C4'	2.82	115.33	108.93
2	A	601	FAD	O3B-C3B-C4B	2.77	119.03	111.08
2	B	601	FAD	C5'-C4'-C3'	2.76	117.43	112.22
2	B	601	FAD	C9-C9A-C5X	-2.75	115.17	120.03
2	B	601	FAD	O3B-C3B-C4B	2.74	118.96	111.08
2	D	601	FAD	N6A-C6A-N1A	2.73	124.45	118.38
2	D	601	FAD	C5A-C4A-N9A	2.64	108.69	105.81
2	A	601	FAD	C2'-C1'-N10	2.64	122.66	110.20
2	D	601	FAD	O2-C2-N1	2.63	126.17	121.80
2	D	601	FAD	C2B-C3B-C4B	2.62	107.67	102.61
2	B	601	FAD	C4A-N9A-C1B	2.61	132.73	126.63
2	D	601	FAD	C4X-C4-N3	2.60	119.87	113.25
2	A	601	FAD	C4A-N9A-C1B	2.59	132.70	126.63
2	B	601	FAD	C2A-N1A-C6A	2.59	122.98	118.73
2	C	601	FAD	P-O5'-C5'	2.58	136.12	121.35
2	B	601	FAD	N10-C10-N1	2.57	126.09	118.51
2	A	601	FAD	C2A-N1A-C6A	2.57	122.95	118.73
2	C	601	FAD	O5'-C5'-C4'	2.57	116.22	109.36
2	A	601	FAD	N3A-C4A-N9A	-2.57	122.80	127.17
2	B	601	FAD	N3-C2-N1	-2.55	114.09	119.50
2	C	601	FAD	O2-C2-N3	2.55	123.47	118.58
2	A	601	FAD	O2P-P-O5'	-2.54	96.06	107.57
2	D	601	FAD	O2A-PA-O1A	2.52	124.16	112.44
2	D	601	FAD	N3A-C4A-N9A	-2.51	122.90	127.17
2	D	601	FAD	O5'-C5'-C4'	2.49	116.00	109.36
2	D	601	FAD	C4A-N9A-C1B	2.48	132.43	126.63
2	C	601	FAD	O2P-P-O1P	2.46	123.89	112.44
2	A	601	FAD	PA-O5B-C5B	2.43	135.28	121.35
2	B	601	FAD	C4X-C10-N10	-2.41	113.03	116.48
2	D	601	FAD	O3B-C3B-C2B	2.41	119.53	111.82
2	C	601	FAD	C4A-N9A-C1B	2.40	132.24	126.63
2	B	601	FAD	O4B-C1B-C2B	2.36	111.68	106.62
2	C	601	FAD	C2'-C1'-N10	2.36	121.37	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	O5B-C5B-C4B	-2.35	100.98	108.99
2	D	601	FAD	C6-C5X-N5	2.35	122.34	118.44
2	B	601	FAD	O2-C2-N3	2.27	122.94	118.58
2	B	601	FAD	O2P-P-O3P	2.27	113.40	107.27
2	C	601	FAD	C1'-C2'-C3'	2.26	115.79	109.66
2	D	601	FAD	O2A-PA-O5B	2.24	117.72	107.57
2	D	601	FAD	C4X-C10-N1	-2.24	119.11	124.59
2	C	601	FAD	C9-C9A-C5X	-2.21	116.12	120.03
2	B	601	FAD	O2P-P-O5'	-2.19	97.63	107.57
2	D	601	FAD	O4B-C1B-N9A	2.17	112.27	108.09
2	B	601	FAD	C5A-N7A-C8A	-2.16	100.05	103.45
2	A	601	FAD	C1'-N10-C9A	-2.15	116.46	120.63
2	D	601	FAD	C2A-N3A-C4A	2.14	117.07	111.83
2	B	601	FAD	C6-C5X-N5	2.12	121.97	118.44
2	D	601	FAD	C2A-N1A-C6A	2.11	122.19	118.73
2	D	601	FAD	O4'-C4'-C3'	2.11	114.18	109.25
2	C	601	FAD	C9A-C9-C8	2.10	123.45	119.22
2	D	601	FAD	O2P-P-O5'	-2.10	98.06	107.57
2	C	601	FAD	O2P-P-O5'	-2.09	98.11	107.57
2	D	601	FAD	C5A-C6A-N1A	2.07	122.77	117.51
2	A	601	FAD	C2B-C3B-C4B	2.06	106.60	102.61
2	D	601	FAD	C4X-C10-N10	-2.04	113.57	116.48
2	A	601	FAD	C1'-C2'-C3'	2.01	115.12	109.66
2	D	601	FAD	C1'-C2'-C3'	2.01	115.11	109.66

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	FAD	C5B-O5B-PA-O1A
2	A	601	FAD	C5B-O5B-PA-O3P
2	A	601	FAD	N10-C1'-C2'-O2'
2	A	601	FAD	C5'-O5'-P-O1P
2	A	601	FAD	C5'-O5'-P-O2P
2	A	601	FAD	C5'-O5'-P-O3P
2	B	601	FAD	C5B-O5B-PA-O1A
2	B	601	FAD	C5B-O5B-PA-O3P
2	B	601	FAD	N10-C1'-C2'-O2'
2	B	601	FAD	C5'-O5'-P-O2P
2	B	601	FAD	C5'-O5'-P-O3P
2	C	601	FAD	C5B-O5B-PA-O1A
2	C	601	FAD	C5B-O5B-PA-O2A

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Mol	Chain	Res	Type	Atoms
2	C	601	FAD	C5B-O5B-PA-O3P
2	C	601	FAD	N10-C1'-C2'-O2'
2	C	601	FAD	C1'-C2'-C3'-C4'
2	C	601	FAD	O2'-C2'-C3'-C4'
2	C	601	FAD	C3'-C4'-C5'-O5'
2	C	601	FAD	C5'-O5'-P-O2P
2	D	601	FAD	C5B-O5B-PA-O1A
2	D	601	FAD	C5B-O5B-PA-O2A
2	D	601	FAD	C5B-O5B-PA-O3P
2	D	601	FAD	N10-C1'-C2'-O2'
2	D	601	FAD	C1'-C2'-C3'-C4'
2	D	601	FAD	C5'-O5'-P-O2P
2	D	601	FAD	C5'-O5'-P-O3P
2	D	601	FAD	C3B-C4B-C5B-O5B
2	A	601	FAD	O4B-C4B-C5B-O5B
2	B	601	FAD	O4B-C4B-C5B-O5B
2	C	601	FAD	O4B-C4B-C5B-O5B
2	C	601	FAD	C3B-C4B-C5B-O5B
2	D	601	FAD	O4B-C4B-C5B-O5B
2	D	601	FAD	C2'-C3'-C4'-O4'
2	D	601	FAD	O2'-C2'-C3'-C4'
2	B	601	FAD	O2'-C2'-C3'-C4'
2	D	601	FAD	PA-O3P-P-O1P
2	A	601	FAD	PA-O3P-P-O5'
2	B	601	FAD	PA-O3P-P-O5'
2	C	601	FAD	PA-O3P-P-O5'
2	C	601	FAD	C2'-C3'-C4'-O4'
2	D	601	FAD	C2B-C1B-N9A-C8A
2	A	601	FAD	C5B-O5B-PA-O2A
2	B	601	FAD	C5B-O5B-PA-O2A
2	B	601	FAD	C5'-O5'-P-O1P
2	D	601	FAD	C5'-O5'-P-O1P
2	A	601	FAD	O2'-C2'-C3'-C4'
2	B	601	FAD	PA-O3P-P-O1P
2	A	601	FAD	C2B-C1B-N9A-C8A
2	D	601	FAD	PA-O3P-P-O5'
2	D	601	FAD	O3'-C3'-C4'-C5'
2	B	601	FAD	C2B-C1B-N9A-C8A
2	B	601	FAD	O4B-C1B-N9A-C8A
2	B	601	FAD	C2'-C3'-C4'-O4'
2	A	601	FAD	PA-O3P-P-O1P
2	C	601	FAD	O4B-C1B-N9A-C8A

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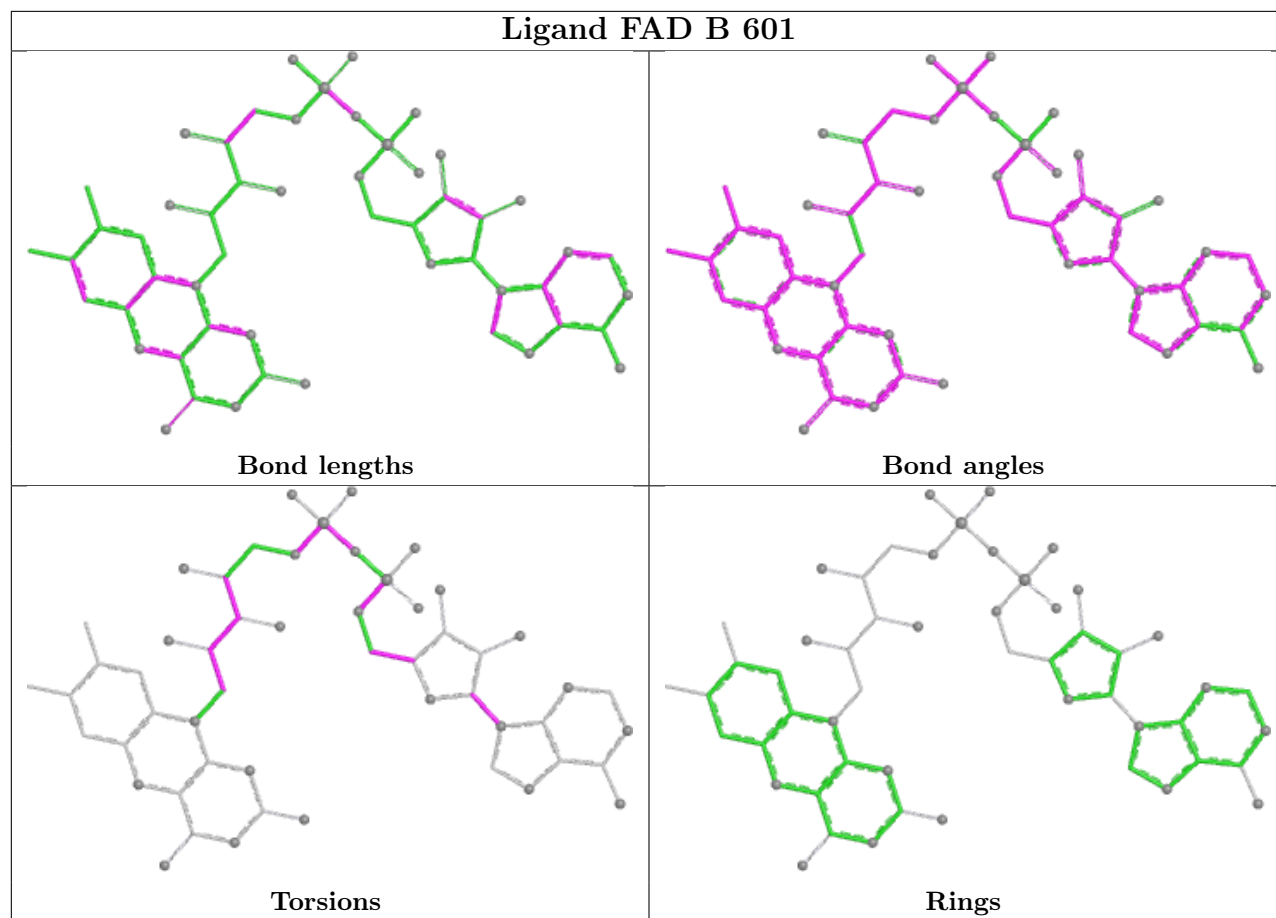
Mol	Chain	Res	Type	Atoms
2	D	601	FAD	O4B-C1B-N9A-C8A
2	A	601	FAD	O4B-C1B-N9A-C8A

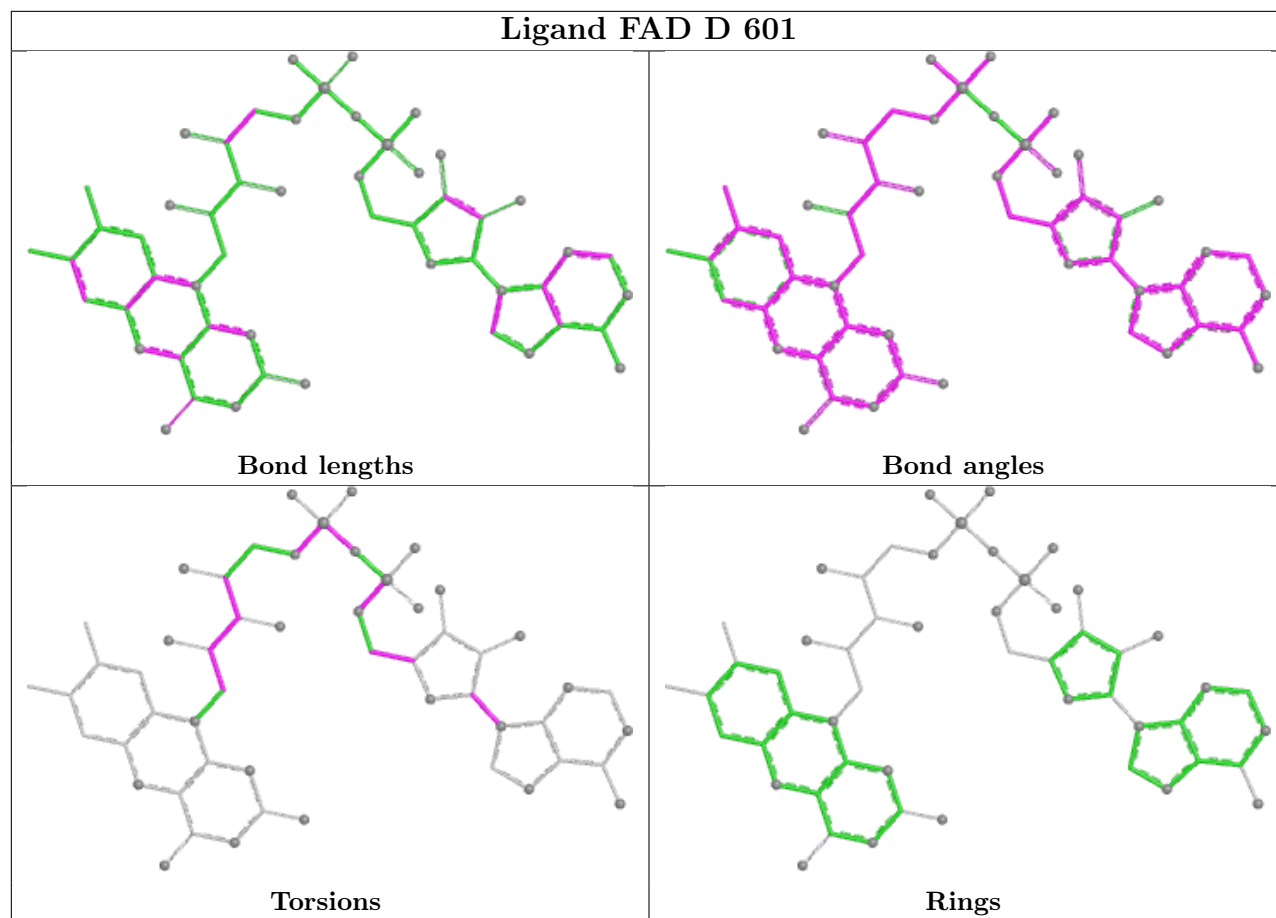
There are no ring outliers.

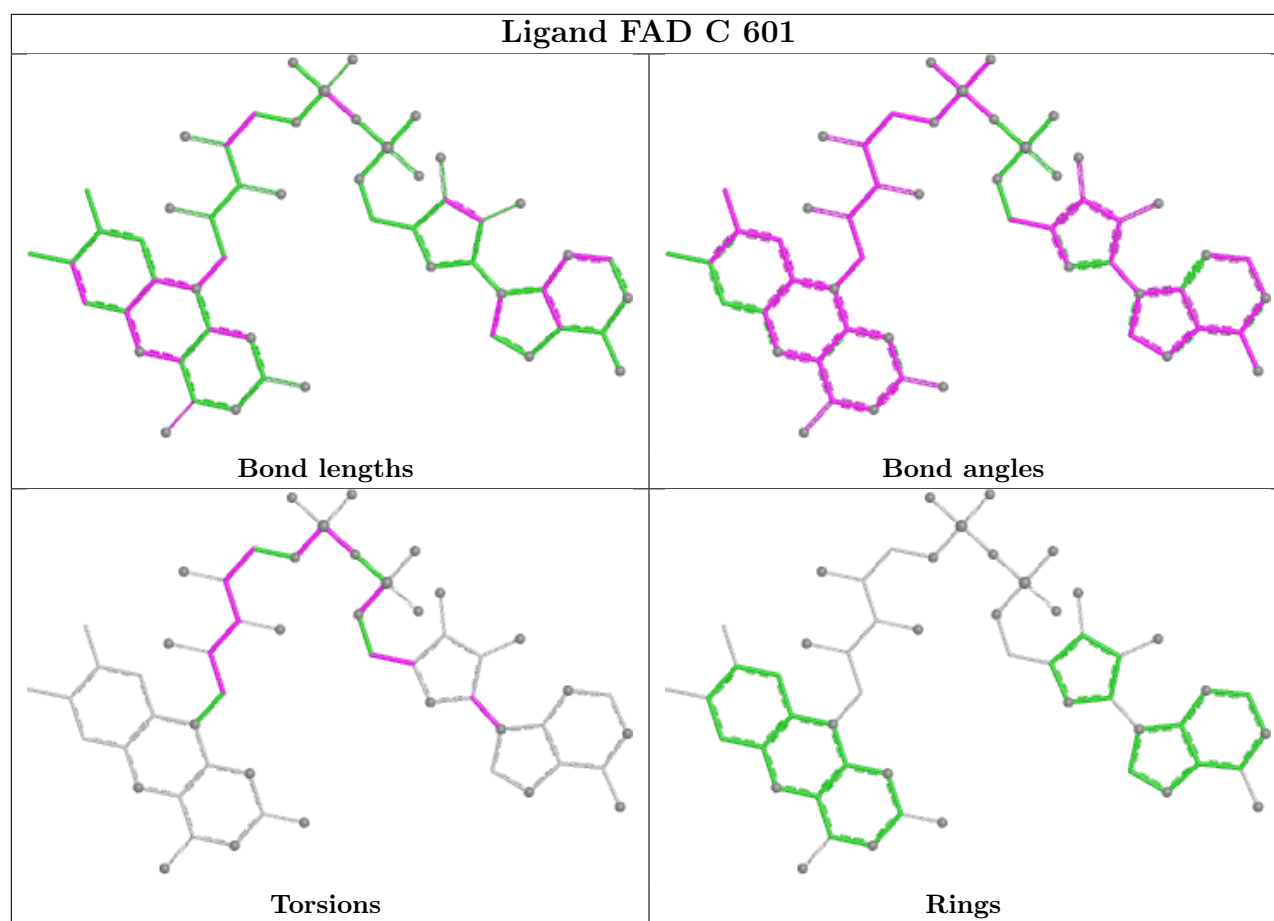
2 monomers are involved in 2 short contacts:

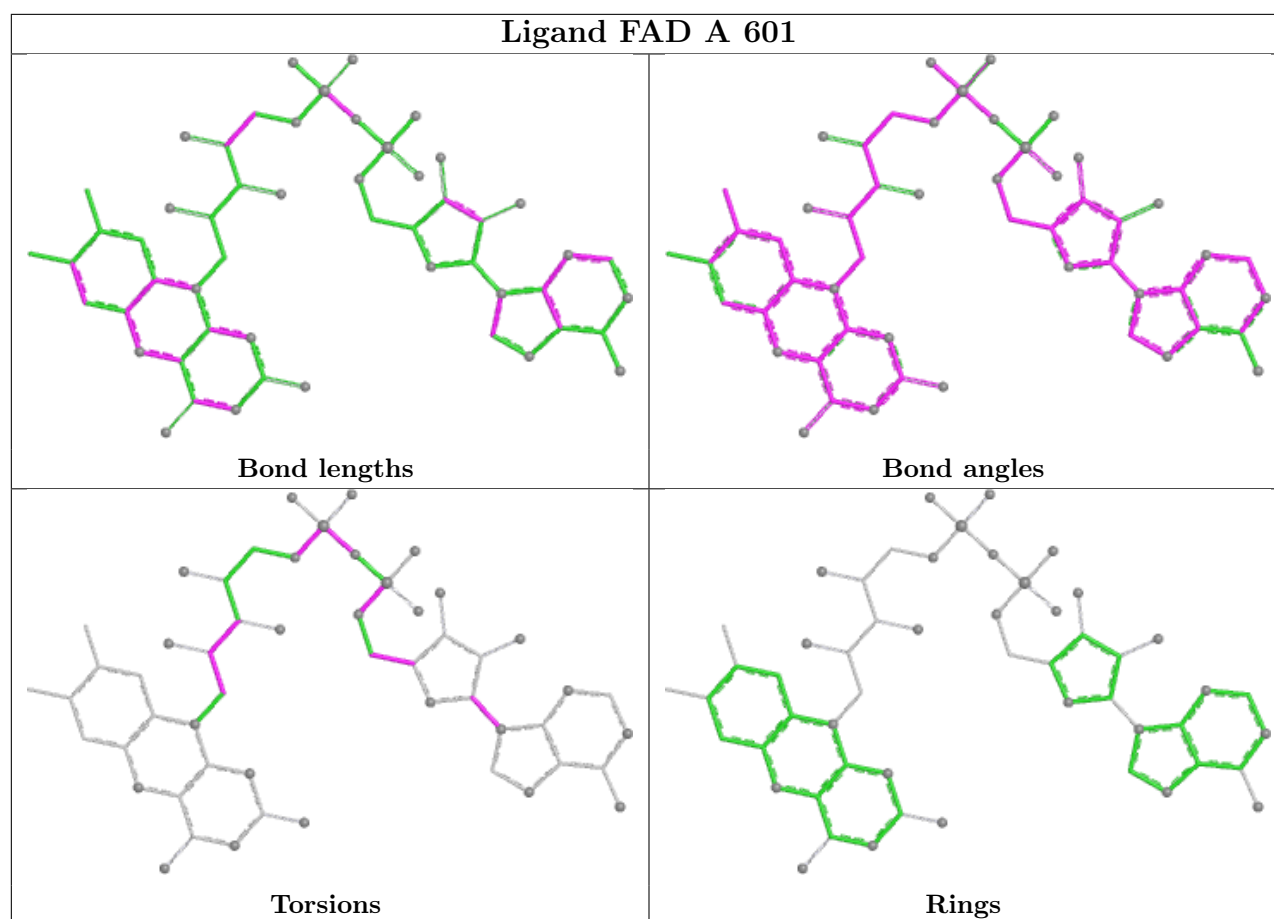
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	FAD	1	0
2	A	601	FAD	1	0

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	502/519 (96%)	0.01	19 (3%)	44	40	18, 40, 68, 96	6 (1%)
1	B	504/519 (97%)	0.01	23 (4%)	37	33	19, 38, 68, 96	6 (1%)
1	C	501/519 (96%)	0.75	79 (15%)	5	4	20, 53, 132, 141	2 (0%)
1	D	500/519 (96%)	0.93	106 (21%)	2	2	17, 55, 136, 146	2 (0%)
All	All	2007/2076 (96%)	0.42	227 (11%)	10	7	17, 44, 128, 146	16 (0%)

All (227) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	433	ALA	7.1
1	D	113	CYS	6.8
1	B	432	PRO	6.3
1	D	242	LEU	6.0
1	D	142	ALA	6.0
1	C	242	LEU	5.8
1	D	256	VAL	5.1
1	D	278	PRO	5.1
1	C	277	PRO	4.9
1	B	142	ALA	4.9
1	D	221	VAL	4.8
1	C	37	VAL	4.8
1	D	243	LEU	4.8
1	D	232	PHE	4.6
1	D	249	VAL	4.6
1	B	37	VAL	4.5
1	D	266	LEU	4.5
1	D	265	TYR	4.5
1	C	232	PHE	4.4
1	D	174	ALA	4.4
1	C	276	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	278	PRO	4.3
1	D	195	PHE	4.3
1	B	431	GLU	4.3
1	C	113	CYS	4.3
1	C	142	ALA	4.3
1	D	262	TYR	4.3
1	D	255	LEU	4.2
1	A	37	VAL	4.2
1	D	269	LEU	4.2
1	C	171	LEU	4.2
1	C	256	VAL	4.1
1	C	192	ALA	4.1
1	B	113	CYS	4.1
1	D	191	LEU	4.1
1	D	248	SER	4.1
1	C	255	LEU	4.0
1	C	249	VAL	4.0
1	D	175	LYS	3.9
1	D	216	VAL	3.9
1	D	222	LEU	3.9
1	D	244	LEU	3.9
1	C	548	SER	3.9
1	C	266	LEU	3.8
1	D	171	LEU	3.8
1	D	224	THR	3.8
1	C	243	LEU	3.8
1	C	296	PHE	3.7
1	C	228	LEU	3.6
1	D	206	VAL	3.6
1	C	104	CYS	3.5
1	B	277	PRO	3.5
1	D	140	PRO	3.5
1	A	256	VAL	3.5
1	D	218	VAL	3.5
1	A	142	ALA	3.5
1	D	183	PHE	3.5
1	D	547	ASP	3.5
1	D	37	VAL	3.5
1	B	104	CYS	3.5
1	A	140	PRO	3.4
1	B	141	GLY	3.4
1	A	75[A]	HIS	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	261	PHE	3.4
1	D	210	LEU	3.4
1	D	211	SER	3.4
1	B	289	ILE	3.3
1	D	167	ALA	3.3
1	D	215	ALA	3.3
1	D	246	ASN	3.3
1	B	75[A]	HIS	3.3
1	C	182	PHE	3.3
1	C	191	LEU	3.2
1	D	176	LEU	3.2
1	D	184	THR	3.2
1	D	93	TRP	3.2
1	D	193	LEU	3.2
1	C	271	GLY	3.2
1	D	192	ALA	3.2
1	D	276	ALA	3.2
1	D	170	PRO	3.2
1	D	228	LEU	3.2
1	D	194	VAL	3.2
1	D	235	THR	3.2
1	D	164	TRP	3.1
1	C	194	VAL	3.1
1	D	263	THR	3.1
1	C	244	LEU	3.1
1	C	221	VAL	3.1
1	D	217	ALA	3.1
1	C	176	LEU	3.1
1	D	271	GLY	3.1
1	C	254	VAL	3.1
1	D	247	GLY	3.0
1	D	151	MET	3.0
1	D	182	PHE	3.0
1	D	220	ARG	3.0
1	A	289	ILE	3.0
1	C	265	TYR	3.0
1	D	139	LEU	3.0
1	B	288	LYS	3.0
1	D	141	GLY	3.0
1	D	56	THR	3.0
1	D	144	ALA	2.9
1	C	193	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	250	SER	2.9
1	D	252	VAL	2.9
1	D	273	THR	2.9
1	D	179	ILE	2.9
1	B	140	PRO	2.9
1	B	287	ASP	2.9
1	D	267	ARG	2.8
1	C	366	LYS	2.8
1	D	234	VAL	2.8
1	C	222	LEU	2.8
1	C	218	VAL	2.8
1	D	277	PRO	2.8
1	C	273	THR	2.8
1	D	132	LYS	2.8
1	C	140	PRO	2.8
1	C	240	CYS	2.8
1	C	233	GLY	2.8
1	D	190	TYR	2.8
1	A	352	ASN	2.8
1	C	216	VAL	2.8
1	C	211	SER	2.7
1	D	272	LEU	2.7
1	B	429	PRO	2.7
1	B	256	VAL	2.7
1	A	547	ASP	2.7
1	D	166	PRO	2.7
1	D	270	PRO	2.6
1	C	223	ASN	2.6
1	D	97	LEU	2.6
1	D	87	ALA	2.6
1	D	261	PHE	2.6
1	D	373	PHE	2.6
1	D	223	ASN	2.6
1	D	146	VAL	2.6
1	D	229	VAL	2.6
1	C	248	SER	2.6
1	A	36	SER	2.6
1	C	36	SER	2.6
1	D	208	LEU	2.6
1	C	290	ALA	2.6
1	C	275	ASP	2.5
1	C	195	PHE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	36	SER	2.5
1	B	548	SER	2.5
1	D	169	PRO	2.5
1	A	290	ALA	2.5
1	D	238	PRO	2.5
1	C	141	GLY	2.5
1	D	290	ALA	2.5
1	D	241	TYR	2.5
1	D	187	LYS	2.5
1	D	259	ARG	2.5
1	D	240	CYS	2.4
1	D	143	GLY	2.4
1	B	430	GLN	2.4
1	C	373	PHE	2.4
1	C	174	ALA	2.4
1	C	56	THR	2.4
1	D	264	SER	2.4
1	C	217	ALA	2.4
1	C	224	THR	2.4
1	C	231	LYS	2.4
1	C	220	ARG	2.4
1	C	179	ILE	2.4
1	B	275	ASP	2.4
1	D	254	VAL	2.4
1	D	219	ARG	2.3
1	B	45	LEU	2.3
1	C	188	ALA	2.3
1	C	170	PRO	2.3
1	C	173	PRO	2.3
1	C	208	LEU	2.3
1	D	189	ASP	2.3
1	A	433	ALA	2.3
1	D	253	PRO	2.3
1	C	247	GLY	2.3
1	C	260	SER	2.3
1	C	272	LEU	2.3
1	D	38	LEU	2.3
1	C	547	ASP	2.3
1	C	241	TYR	2.3
1	D	213	TYR	2.3
1	C	166	PRO	2.3
1	C	270	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	268	GLY	2.3
1	D	202	LEU	2.3
1	A	277	PRO	2.3
1	A	291	PRO	2.2
1	D	173	PRO	2.2
1	C	246	ASN	2.2
1	C	263	THR	2.2
1	B	369	ILE	2.2
1	D	180	ASP	2.2
1	C	262	TYR	2.2
1	C	203	GLY	2.2
1	C	361	LEU	2.2
1	D	154	ILE	2.2
1	C	189	ASP	2.2
1	A	296	PHE	2.2
1	C	291	PRO	2.2
1	C	96	ALA	2.2
1	C	230	ASN	2.2
1	A	272	LEU	2.2
1	D	157	LEU	2.2
1	C	196	GLU	2.2
1	C	259	ARG	2.2
1	D	207	THR	2.1
1	C	190	TYR	2.1
1	D	168	CYS	2.1
1	D	41	SER	2.1
1	D	231	LYS	2.1
1	C	93	TRP	2.1
1	B	38	LEU	2.1
1	D	203	GLY	2.1
1	C	198	GLU	2.1
1	D	434	ASP	2.1
1	D	274	ARG	2.1
1	D	77	ILE	2.0
1	A	248	SER	2.0
1	C	253	PRO	2.0
1	A	163	THR	2.0
1	A	454	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

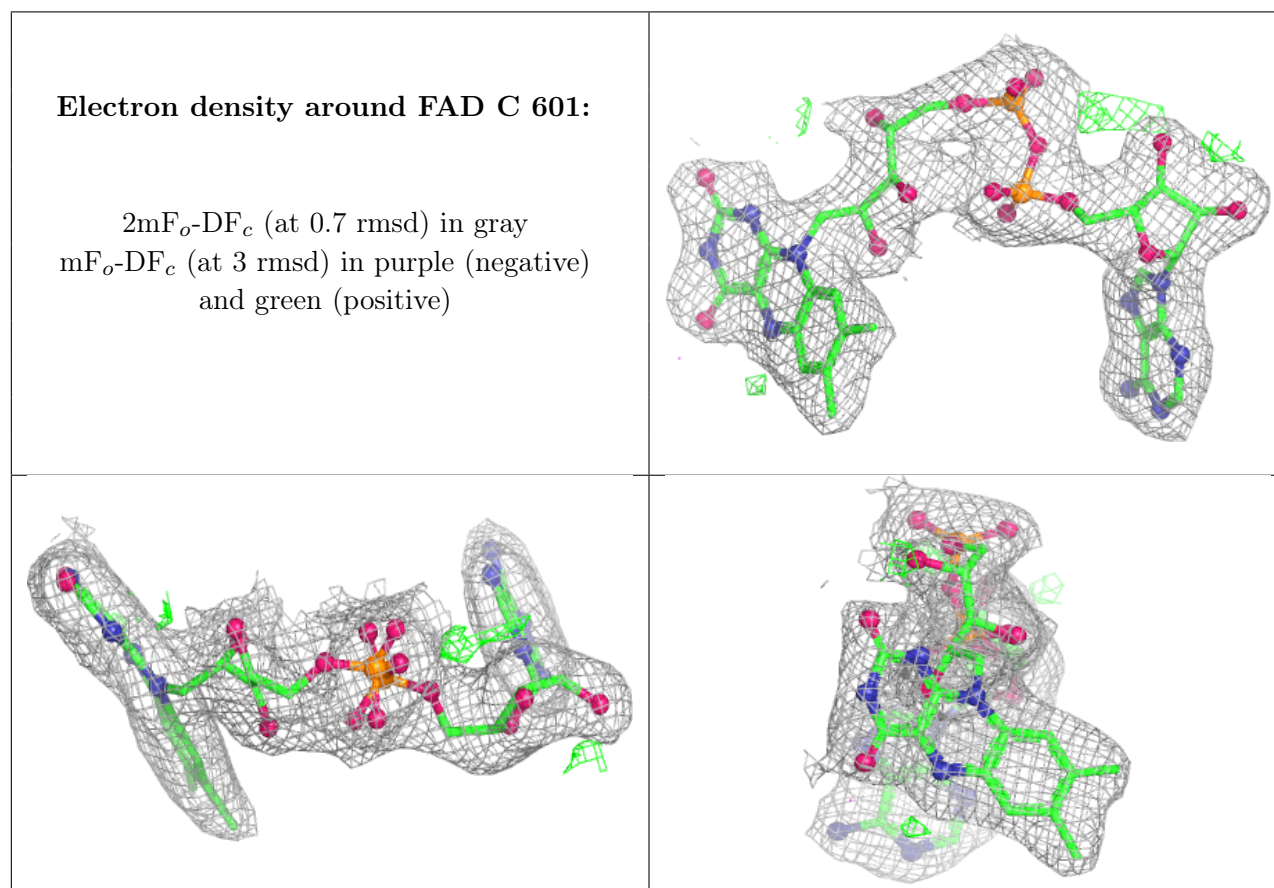
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

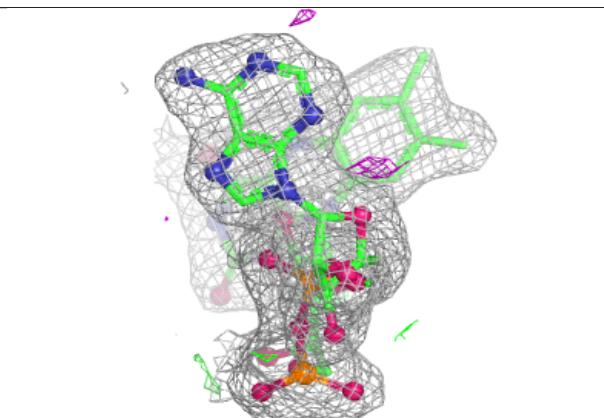
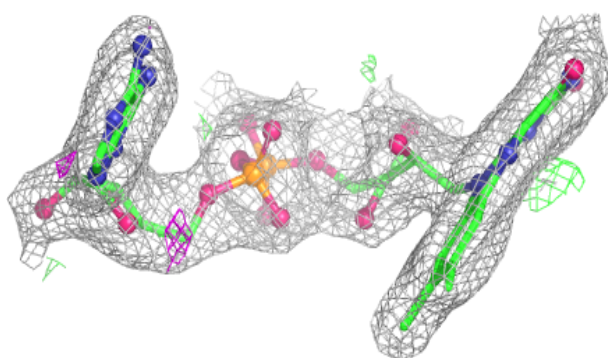
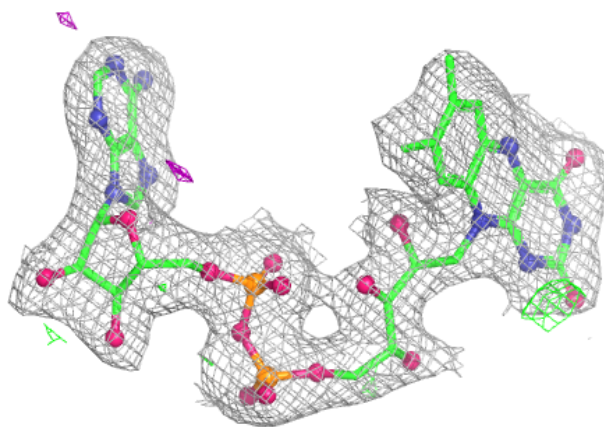
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FAD	C	601	53/53	0.96	0.07	28,39,47,51	0
2	FAD	B	601	53/53	0.97	0.07	19,33,39,42	0
2	FAD	A	601	53/53	0.97	0.07	21,33,41,43	0
2	FAD	D	601	53/53	0.97	0.06	24,36,42,44	0

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.

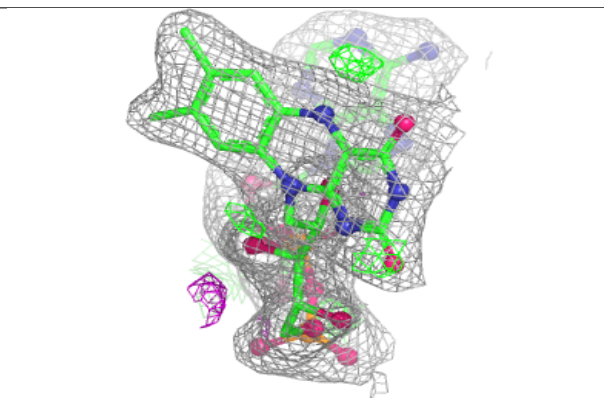
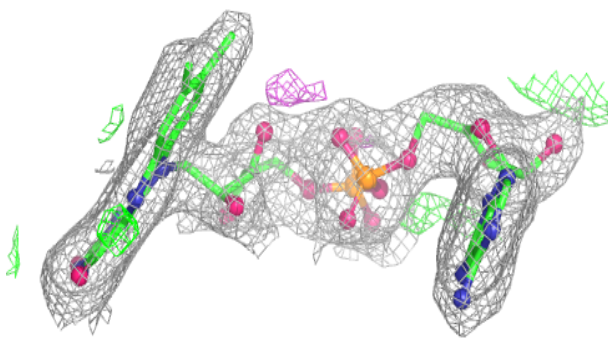
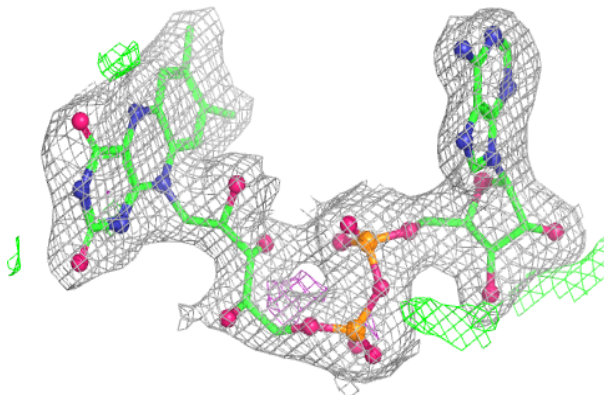


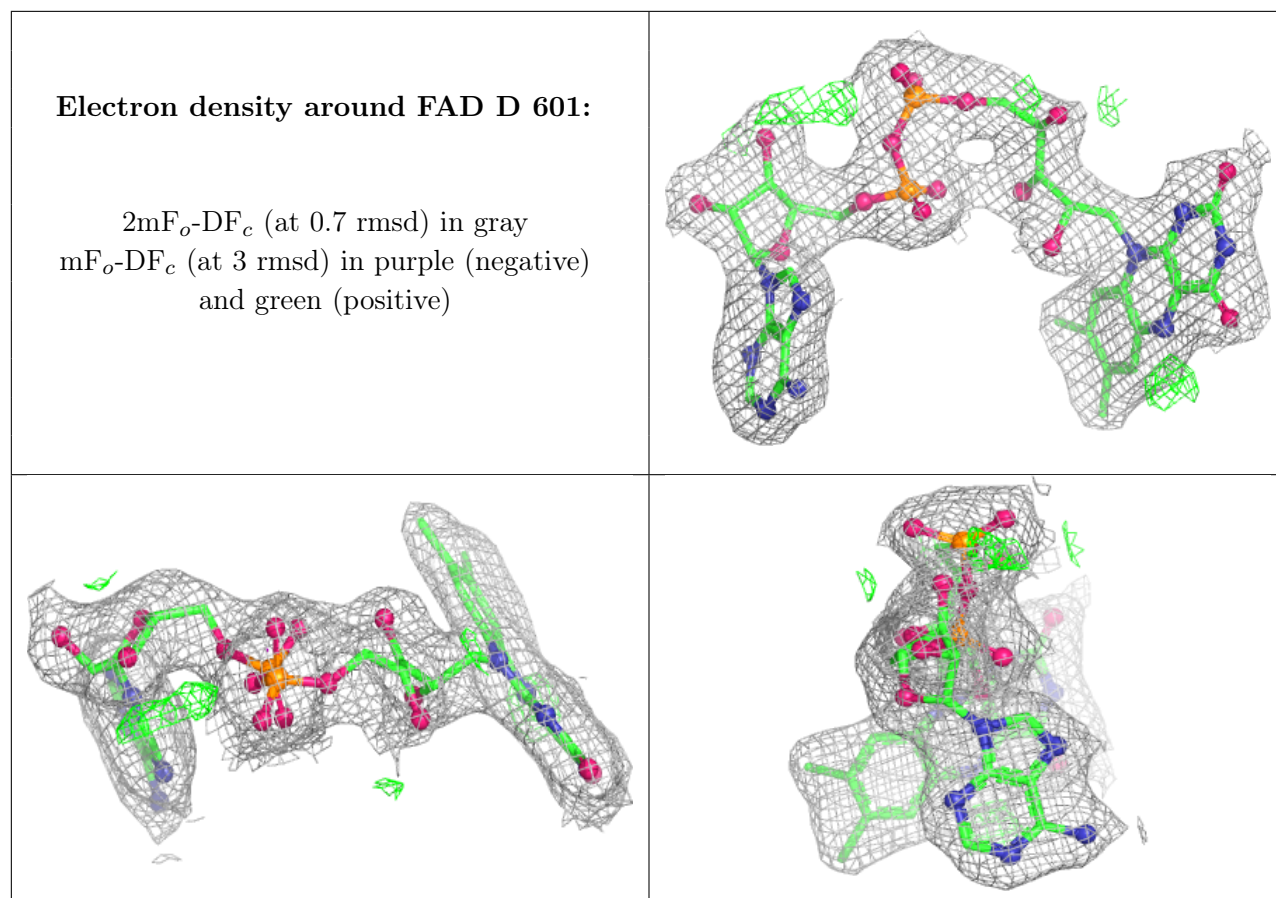
Electron density around FAD B 601:

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

**Electron density around FAD A 601:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.