



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 4, 2021 – 02:08 PM JST

PDB ID : 6LPU
Title : Crystal structure of human D-2-hydroxyglutarate dehydrogenase in complex with L-2-hydroxyglutarate (L-2-HG)
Authors : Yang, J.; Zhu, H.; Ding, J.
Deposited on : 2020-01-12
Resolution : 2.92 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.16
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.16

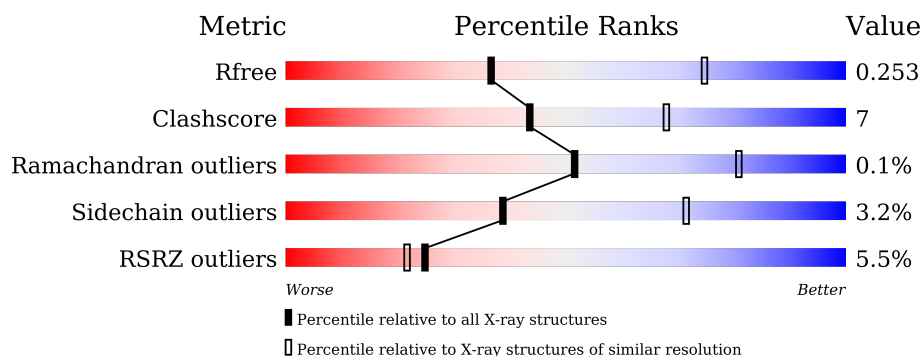
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.92 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2307 (2.94-2.90)
Clashscore	141614	2531 (2.94-2.90)
Ramachandran outliers	138981	2462 (2.94-2.90)
Sidechain outliers	138945	2464 (2.94-2.90)
RSRZ outliers	127900	2248 (2.94-2.90)

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	481	<div> <div>8%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	481	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>17%</div> <div>..</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7155 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 D-2-hydroxyglutarate dehydrogenase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	0	0	0
			3511	2228	618	646	19			
1	B	467	Total	C	N	O	S	0	0	0
			3516	2230	613	654	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	47	GLY	-	expression tag	UNP Q8N465
A	48	PRO	-	expression tag	UNP Q8N465
A	49	GLY	-	expression tag	UNP Q8N465
A	50	SER	-	expression tag	UNP Q8N465
A	522	HIS	-	expression tag	UNP Q8N465
A	523	HIS	-	expression tag	UNP Q8N465
A	524	HIS	-	expression tag	UNP Q8N465
A	525	HIS	-	expression tag	UNP Q8N465
A	526	HIS	-	expression tag	UNP Q8N465
A	527	HIS	-	expression tag	UNP Q8N465
B	47	GLY	-	expression tag	UNP Q8N465
B	48	PRO	-	expression tag	UNP Q8N465
B	49	GLY	-	expression tag	UNP Q8N465
B	50	SER	-	expression tag	UNP Q8N465
B	522	HIS	-	expression tag	UNP Q8N465
B	523	HIS	-	expression tag	UNP Q8N465
B	524	HIS	-	expression tag	UNP Q8N465
B	525	HIS	-	expression tag	UNP Q8N465
B	526	HIS	-	expression tag	UNP Q8N465
B	527	HIS	-	expression tag	UNP Q8N465

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$) (labeled as "Ligand of Interest" by depositor).

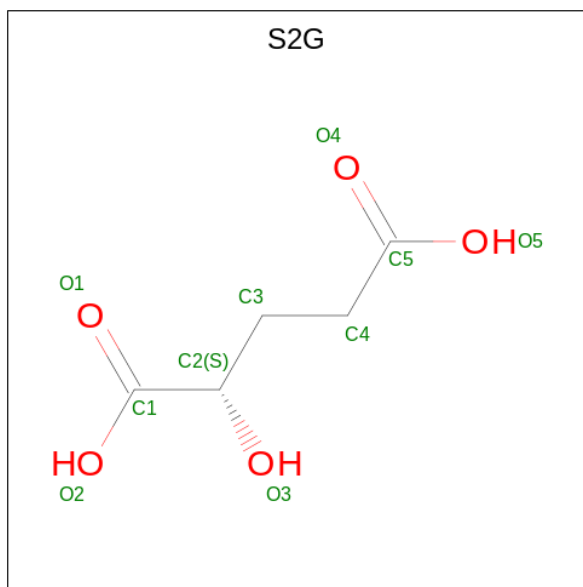


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is (2S)-2-HYDROXYPENTANEDIOIC ACID (three-letter code: S2G) (formula: C₅H₈O₅) (labeled as "Ligand of Interest" by depositor).

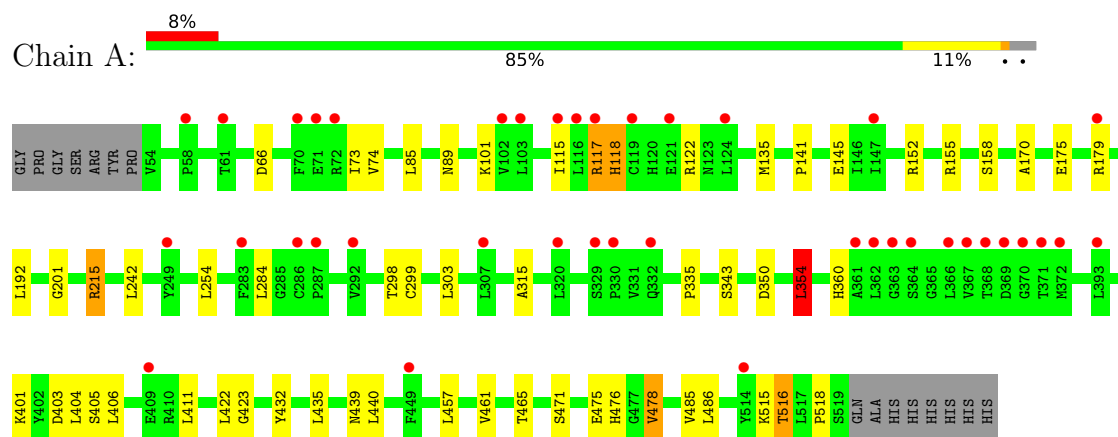


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	5	5		
4	B	1	Total	C	O	0	0
			10	5	5		

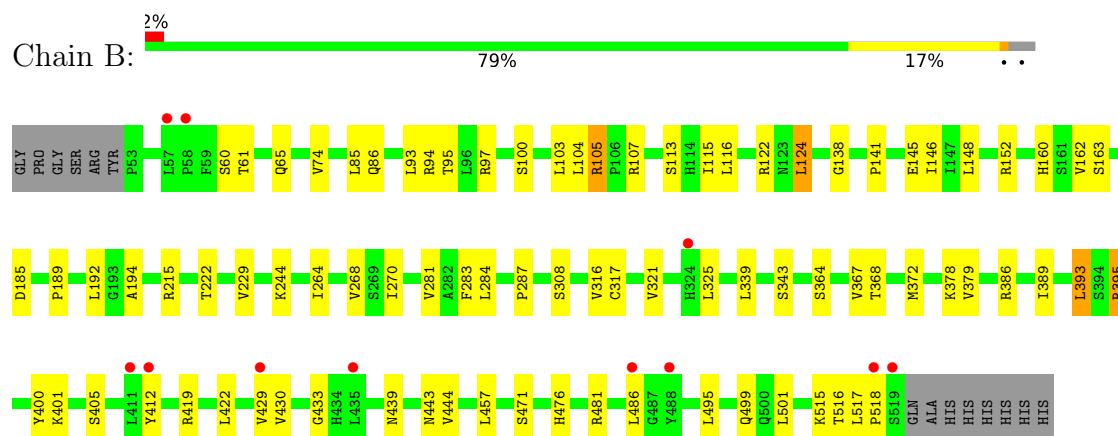
3 Residue-property plots [i](#)

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: D-2-hydroxyglutarate dehydrogenase, mitochondrial



- Molecule 1: D-2-hydroxyglutarate dehydrogenase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.71Å 94.53Å 72.79Å 90.00° 112.25° 90.00°	Depositor
Resolution (Å)	47.27 – 2.92 47.27 – 2.92	Depositor EDS
% Data completeness (in resolution range)	97.0 (47.27-2.92) 97.4 (47.27-2.92)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.15rc1 _3420	Depositor
R, R_{free}	0.224 , 0.255 0.222 , 0.253	Depositor DCC
R_{free} test set	946 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.746	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 26.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.038 for l,-k,h	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7155	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.10% 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: ZN, S2G, 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	0.28	0/3584	0.61	4/4869 (0.1%)
1	B	0.28	0/3589	0.55	1/4877 (0.0%)
All	All	0.28	0/7173	0.58	5/9746 (0.1%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	354	LEU	CA-CB-CG	10.23	138.84	115.30
1	A	516	THR	C-N-CA	7.36	140.10	121.70
1	A	117	ARG	CB-CG-CD	5.98	127.14	111.60
1	A	435	LEU	CA-CB-CG	5.46	127.87	115.30
1	B	372	MET	CB-CA-C	5.16	120.72	110.40

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	3511	0	3509	36	0
1	B	3516	0	3504	59	0
2	A	53	0	31	2	0
2	B	53	0	31	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	10	0	6	3	0
4	B	10	0	6	2	0
All	All	7155	0	7087	96	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 7.

All (96) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:PRO:HB3	1:B:145:GLU:HG2	1.56	0.84
1:B:95:THR:OG1	1:B:481:ARG:NH2	2.12	0.81
1:B:189:PRO:HG3	1:B:222:THR:HG21	1.66	0.76
1:B:105:ARG:HH11	1:B:152:ARG:NH1	1.89	0.69
1:A:350:ASP:O	1:A:354:LEU:HD23	1.94	0.68
1:B:215:ARG:HB2	1:B:308:SER:HA	1.78	0.66
1:B:316:VAL:HG13	1:B:430:VAL:HG12	1.79	0.65
1:B:105:ARG:HH11	1:B:152:ARG:HH12	1.44	0.64
1:A:73:ILE:HD11	1:A:118:HIS:HD2	1.64	0.63
1:B:386:ARG:NH2	1:B:433:GLY:HA2	2.14	0.63
1:B:93:LEU:HD12	1:B:481:ARG:HH12	1.64	0.63
1:B:104:LEU:HB2	1:B:148:LEU:HD12	1.82	0.62
1:A:215:ARG:NH1	1:A:343:SER:O	2.33	0.62
1:A:432:TYR:OH	4:A:603:S2G:O5	2.12	0.61
1:A:476:HIS:CE1	4:A:603:S2G:H4A	2.36	0.60
1:B:283:PHE:HD1	1:B:339:LEU:HD12	1.67	0.60
1:B:476:HIS:CE1	4:B:603:S2G:H4A	2.36	0.60
1:B:515:LYS:HB3	1:B:516:THR:HG22	1.84	0.59
1:B:321:VAL:HG13	1:B:325:LEU:HD12	1.83	0.59
1:A:478:VAL:CG1	1:A:486:LEU:HD21	2.33	0.58
1:B:386:ARG:HH21	1:B:433:GLY:HA2	1.68	0.58
1:B:189:PRO:CG	1:B:222:THR:HG21	2.33	0.57
1:B:116:LEU:HD11	1:B:264:ILE:HD12	1.85	0.57
1:B:395:ARG:HD3	1:B:395:ARG:N	2.19	0.57
1:B:412:TYR:OH	1:B:419:ARG:NH2	2.38	0.57
1:A:101:LYS:HG2	1:A:101:LYS:O	2.05	0.57
1:B:60:SER:HB3	1:B:124:LEU:HD12	1.86	0.56
1:A:74:VAL:HG21	1:A:115:ILE:HD11	1.86	0.56
1:A:170:ALA:HB1	1:A:201:GLY:HA3	1.89	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:LEU:HD22	2:A:601:FAD:C4	2.37	0.55
1:B:105:ARG:HD3	1:B:152:ARG:NH1	2.21	0.55
1:B:268:VAL:HG12	1:B:270:ILE:HG13	1.89	0.55
1:B:74:VAL:HG21	1:B:115:ILE:HD11	1.88	0.55
1:A:315:ALA:HB2	1:A:335:PRO:HA	1.88	0.54
1:A:406:LEU:HB2	1:A:411:LEU:HD12	1.89	0.54
1:B:495:LEU:O	1:B:499:GLN:HG3	2.07	0.54
1:A:515:LYS:HB3	1:A:516:THR:CG2	2.38	0.53
1:A:478:VAL:HG23	1:A:516:THR:HB	1.90	0.53
1:B:400:TYR:HB2	1:B:444:VAL:HB	1.90	0.53
1:A:66:ASP:OD2	1:A:122:ARG:NH1	2.42	0.53
1:A:404:LEU:HD22	1:A:465:THR:HG21	1.91	0.53
1:B:405:SER:HB2	1:B:471:SER:HB3	1.89	0.52
1:B:284:LEU:HD13	1:B:367:VAL:HG21	1.92	0.52
1:B:422:LEU:HD11	1:B:457:LEU:HD21	1.91	0.52
1:B:103:LEU:HD22	1:B:105:ARG:HH21	1.74	0.52
1:B:94:ARG:HH11	1:B:395:ARG:HH22	1.57	0.51
1:B:124:LEU:HD23	1:B:146:ILE:HD11	1.93	0.51
1:B:107:ARG:HG2	1:B:152:ARG:HB3	1.92	0.51
1:A:405:SER:HB2	1:A:471:SER:HB3	1.93	0.51
1:A:242:LEU:HD22	1:B:405:SER:HB3	1.93	0.50
1:A:461:VAL:O	1:A:465:THR:HG23	2.12	0.49
1:B:215:ARG:NH2	1:B:343:SER:OG	2.45	0.49
1:A:515:LYS:HB3	1:A:516:THR:HG22	1.95	0.48
1:A:475:GLU:OE1	1:B:244:LYS:NZ	2.43	0.48
1:B:317:CYS:SG	1:B:430:VAL:HB	2.54	0.48
1:A:403:ASP:OD1	1:A:475:GLU:N	2.47	0.48
1:B:115:ILE:HD13	1:B:148:LEU:HD11	1.96	0.48
1:B:162:VAL:HG13	1:B:163:SER:H	1.79	0.48
2:B:601:FAD:H2'	2:B:601:FAD:N1	2.29	0.48
1:A:485:VAL:HG12	1:A:485:VAL:O	2.13	0.47
1:A:85:LEU:O	1:A:89:ASN:ND2	2.48	0.47
1:B:386:ARG:HH12	4:B:603:S2G:C1	2.29	0.46
1:B:281:VAL:HG12	1:B:379:VAL:HG22	1.98	0.46
1:B:113:SER:HA	1:B:229:VAL:HG11	1.98	0.45
1:B:194:ALA:HB2	2:B:601:FAD:C8	2.46	0.45
1:A:478:VAL:HG12	1:A:486:LEU:HD21	1.98	0.45
1:A:411:LEU:HG	1:A:440:LEU:HB2	1.99	0.45
1:B:401:LYS:HG2	1:B:443:ASN:OD1	2.17	0.44
1:B:100:SER:HB2	1:B:141:PRO:HG2	1.99	0.44
1:B:93:LEU:CD1	1:B:481:ARG:HH12	2.30	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:PRO:HB3	1:A:145:GLU:HB2	1.99	0.43
1:A:478:VAL:HG11	1:A:486:LEU:HD21	1.99	0.43
1:A:486:LEU:HD12	1:A:518:PRO:HD3	2.00	0.43
2:B:601:FAD:H1'2	2:B:601:FAD:H9	1.80	0.43
1:B:283:PHE:HD1	1:B:339:LEU:CD1	2.30	0.43
1:B:287:PRO:HD3	1:B:368:THR:HG23	2.00	0.43
1:A:175:GLU:HG2	1:A:179:ARG:NH2	2.33	0.43
1:B:501:LEU:HA	1:B:501:LEU:HD23	1.83	0.43
1:B:138:GLY:HA2	1:B:515:LYS:HE2	2.01	0.42
1:B:516:THR:H	1:B:517:LEU:HD12	1.84	0.42
1:B:486:LEU:HD12	1:B:518:PRO:HD3	2.00	0.42
1:A:476:HIS:NE2	4:A:603:S2G:H4A	2.35	0.42
1:B:364:SER:OG	1:B:364:SER:O	2.38	0.42
1:B:389:ILE:O	1:B:393:LEU:HD13	2.19	0.42
1:B:122:ARG:HB3	1:B:124:LEU:HD13	2.02	0.42
1:A:422:LEU:HD11	1:A:457:LEU:HD21	2.02	0.42
2:A:601:FAD:N1	2:A:601:FAD:H2'	2.35	0.41
1:B:515:LYS:HB3	1:B:516:THR:CG2	2.49	0.41
1:B:97:ARG:HB2	1:B:97:ARG:NH1	2.35	0.41
1:A:401:LYS:HB2	1:A:401:LYS:HE2	1.88	0.41
1:B:419:ARG:NH1	1:B:429:VAL:O	2.53	0.41
1:B:86:GLN:OE1	1:B:97:ARG:HD2	2.21	0.41
1:A:486:LEU:HA	1:A:486:LEU:HD23	1.76	0.40
1:B:85:LEU:HD23	1:B:85:LEU:HA	1.75	0.40
1:A:299:CYS:SG	1:A:303:LEU:HD12	2.62	0.40
1:A:117:ARG:NH2	1:A:118:HIS:CD2	2.90	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	464/481 (96%)	456 (98%)	7 (2%)	1 (0%)	47	77
1	B	465/481 (97%)	455 (98%)	10 (2%)	0	100	100
All	All	929/962 (97%)	911 (98%)	17 (2%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	423	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	375/397 (94%)	362 (96%)	13 (4%)	36	68
1	B	377/397 (95%)	366 (97%)	11 (3%)	42	74
All	All	752/794 (95%)	728 (97%)	24 (3%)	39	71

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	HIS
1	A	135	MET
1	A	152	ARG
1	A	155	ARG
1	A	158	SER
1	A	215	ARG
1	A	254	LEU
1	A	284	LEU
1	A	298	THR
1	A	354	LEU
1	A	360	HIS
1	A	439	ASN
1	A	478	VAL
1	B	61	THR
1	B	65	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	105	ARG
1	B	124	LEU
1	B	160	HIS
1	B	185	ASP
1	B	192	LEU
1	B	378	LYS
1	B	393	LEU
1	B	395	ARG
1	B	439	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

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	S2G	B	603	3	3,9,9	0.83	0	5,11,11	2.12	3 (60%)
4	S2G	A	603	1,3	3,9,9	0.80	0	5,11,11	1.95	2 (40%)
2	FAD	B	601	-	51,58,58	1.22	5 (9%)	60,89,89	2.22	8 (13%)
2	FAD	A	601	-	51,58,58	1.22	6 (11%)	60,89,89	2.22	8 (13%)

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	S2G	B	603	3	-	2/3/9/9	-
4	S2G	A	603	1,3	-	2/3/9/9	-
2	FAD	B	601	-	-	9/30/50/50	0/6/6/6
2	FAD	A	601	-	-	10/30/50/50	0/6/6/6

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	FAD	C4X-C10	5.67	1.44	1.38
2	B	601	FAD	C4X-C10	5.64	1.44	1.38
2	A	601	FAD	C4-N3	3.07	1.38	1.33
2	B	601	FAD	C4-N3	3.03	1.38	1.33
2	B	601	FAD	C4-C4X	2.39	1.45	1.41
2	A	601	FAD	C4-C4X	2.35	1.45	1.41
2	A	601	FAD	C9A-N10	2.27	1.41	1.38
2	B	601	FAD	C9A-N10	2.26	1.41	1.38
2	B	601	FAD	C5X-N5	2.12	1.38	1.35
2	A	601	FAD	C5X-N5	2.08	1.38	1.35
2	A	601	FAD	C4X-N5	-2.06	1.30	1.33

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	FAD	C4-N3-C2	13.00	126.12	115.14
2	A	601	FAD	C4-N3-C2	12.94	126.07	115.14
2	B	601	FAD	C4X-C4-N3	-6.98	113.89	123.43
2	A	601	FAD	C4X-C4-N3	-6.97	113.89	123.43
2	B	601	FAD	C10-C4X-N5	4.86	124.62	121.26
2	A	601	FAD	C10-C4X-N5	4.76	124.55	121.26

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	FAD	C4-C4X-C10	-3.67	117.52	119.95
2	B	601	FAD	C4-C4X-C10	-3.65	117.54	119.95
2	B	601	FAD	C4X-C10-N10	-3.56	116.65	120.30
2	A	601	FAD	C4X-C10-N10	-3.51	116.69	120.30
4	B	603	S2G	C4-C3-C2	3.42	119.47	114.44
4	A	603	S2G	C4-C3-C2	3.10	119.00	114.44
2	A	601	FAD	C1'-N10-C9A	2.69	120.41	118.29
2	B	601	FAD	C1'-N10-C9A	2.66	120.38	118.29
4	B	603	S2G	C3-C2-C1	2.46	119.45	112.34
4	A	603	S2G	C3-C2-C1	2.42	119.36	112.34
2	B	601	FAD	P-O3P-PA	-2.37	124.70	132.83
2	B	601	FAD	C5A-C6A-N6A	2.32	123.88	120.35
2	A	601	FAD	P-O3P-PA	-2.32	124.86	132.83
2	A	601	FAD	C5A-C6A-N6A	2.31	123.86	120.35
4	B	603	S2G	O3-C2-C1	-2.08	105.40	111.66

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	603	S2G	C1-C2-C3-C4
4	A	603	S2G	O3-C2-C3-C4
4	B	603	S2G	C1-C2-C3-C4
4	B	603	S2G	O3-C2-C3-C4
2	B	601	FAD	C2'-C1'-N10-C9A
2	B	601	FAD	N10-C1'-C2'-O2'
2	B	601	FAD	C2'-C3'-C4'-O4'
2	B	601	FAD	C2'-C3'-C4'-C5'
2	B	601	FAD	O3'-C3'-C4'-O4'
2	B	601	FAD	O3'-C3'-C4'-C5'
2	B	601	FAD	C3'-C4'-C5'-O5'
2	B	601	FAD	O4'-C4'-C5'-O5'
2	A	601	FAD	C2'-C1'-N10-C9A
2	A	601	FAD	C2'-C1'-N10-C10
2	A	601	FAD	N10-C1'-C2'-O2'
2	A	601	FAD	N10-C1'-C2'-C3'
2	A	601	FAD	C2'-C3'-C4'-O4'
2	A	601	FAD	O3'-C3'-C4'-O4'
2	A	601	FAD	C3'-C4'-C5'-O5'
2	A	601	FAD	O4'-C4'-C5'-O5'
2	A	601	FAD	O3'-C3'-C4'-C5'
2	A	601	FAD	C2'-C3'-C4'-C5'

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	601	FAD	N10-C1'-C2'-C3'

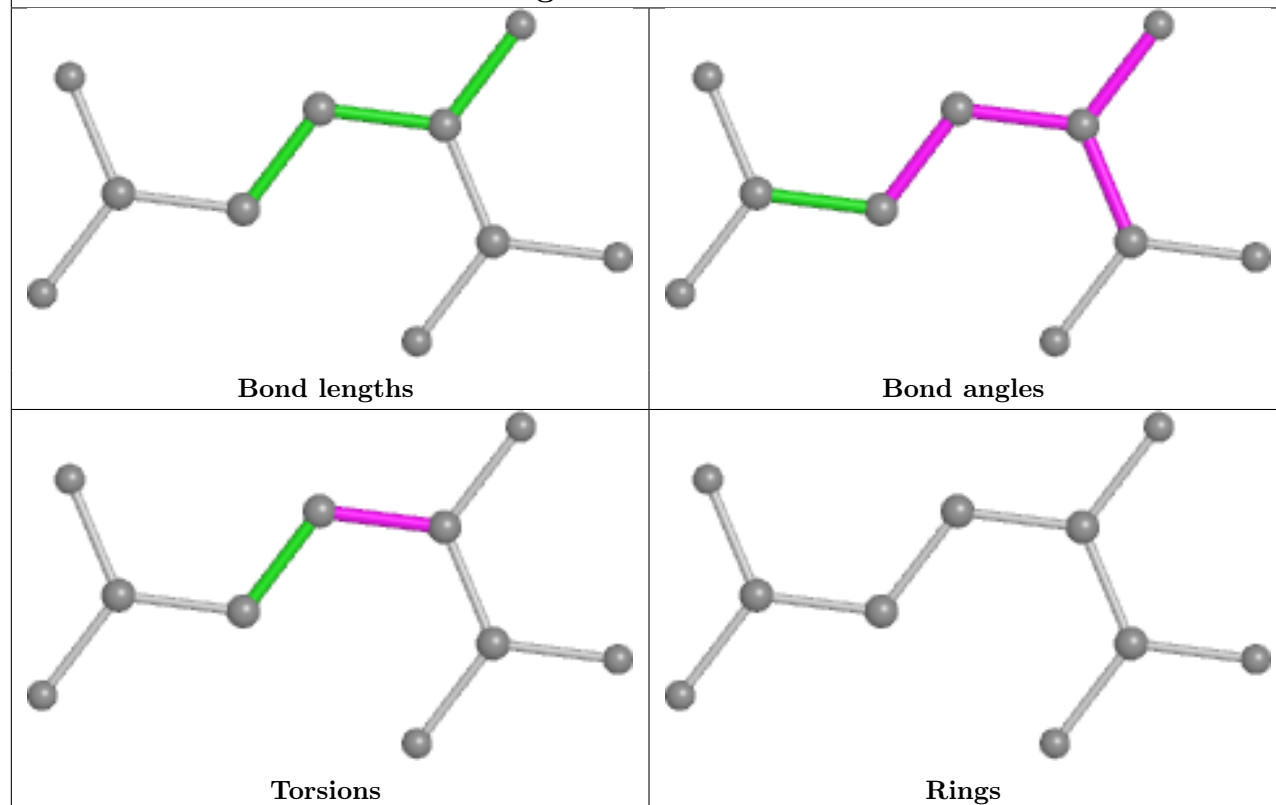
There are no ring outliers.

4 monomers are involved in 10 short contacts:

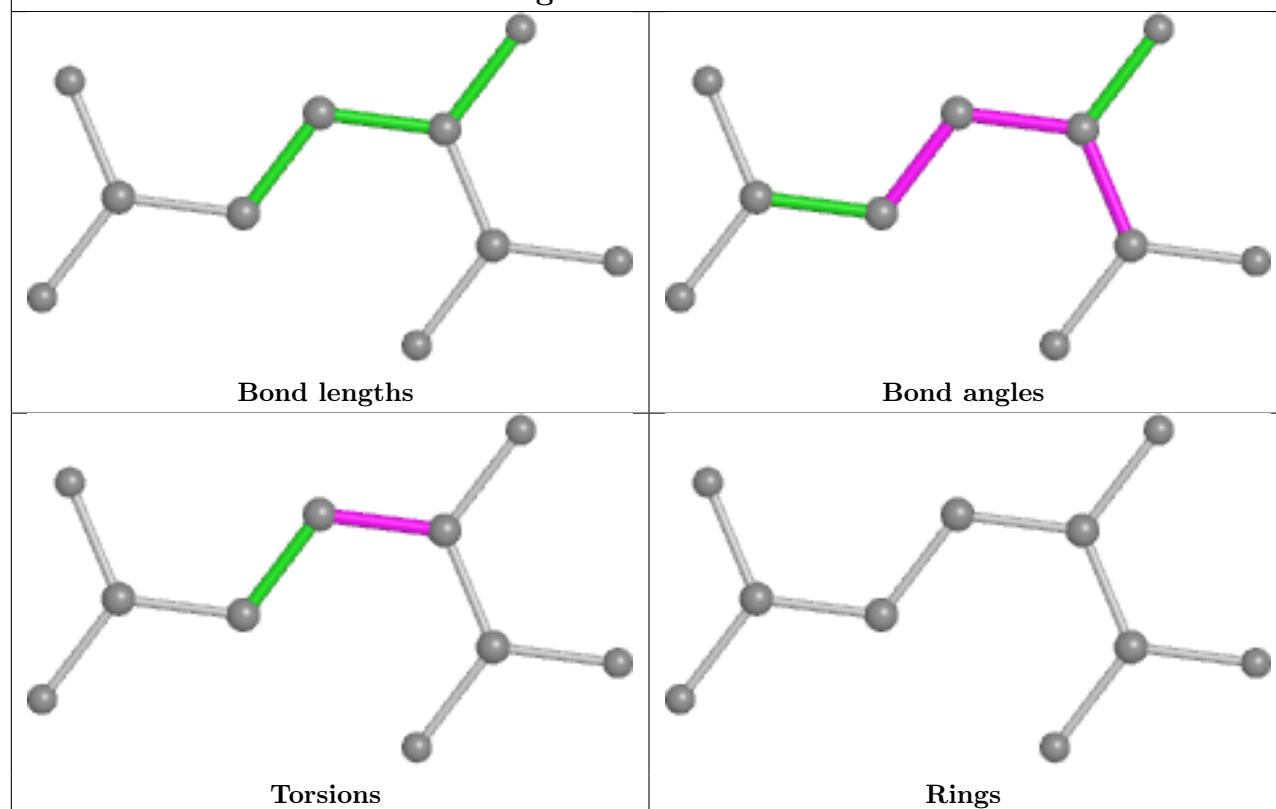
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	603	S2G	2	0
4	A	603	S2G	3	0
2	B	601	FAD	3	0
2	A	601	FAD	2	0

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.

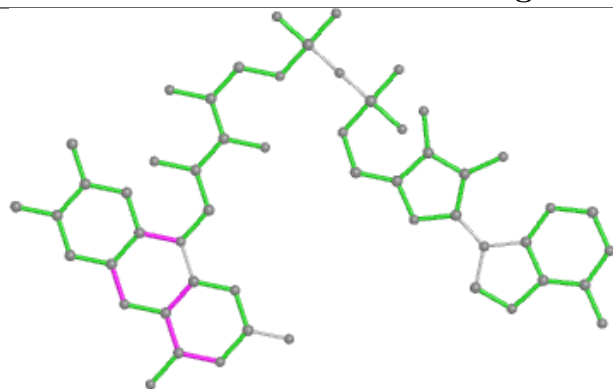
Ligand S2G B 603



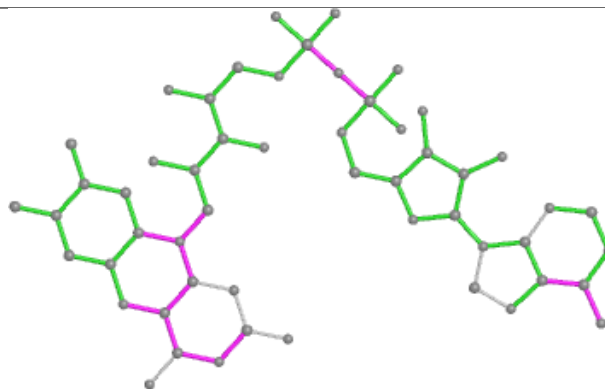
Ligand S2G A 603



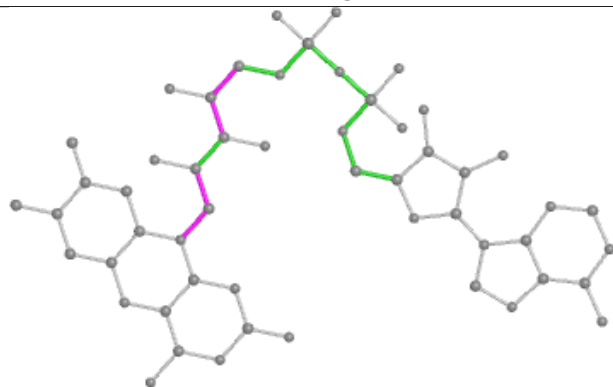
Ligand FAD B 601



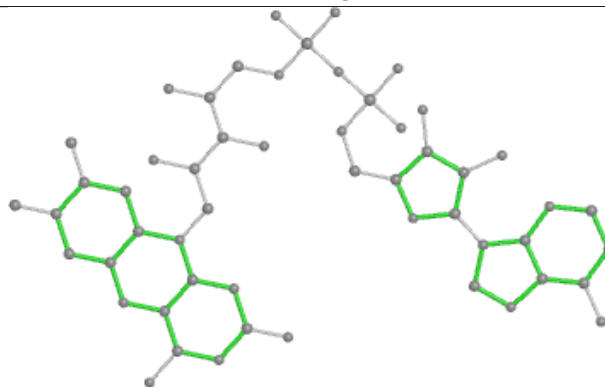
Bond lengths



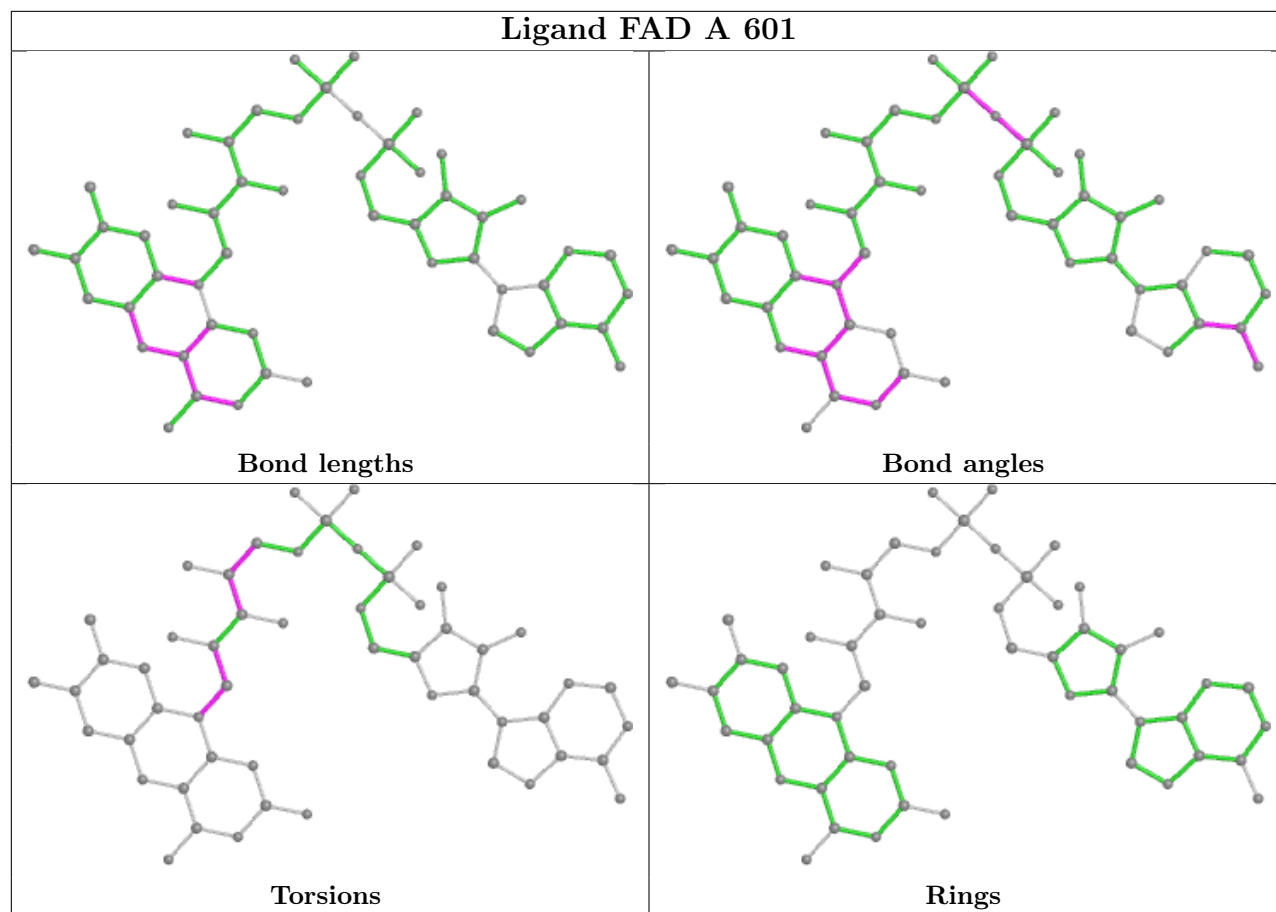
Bond angles



Torsions



Rings



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	466/481 (96%)	0.52	40 (8%) 10 8	28, 43, 61, 73	0
1	B	467/481 (97%)	0.24	11 (2%) 59 57	25, 37, 54, 80	0
All	All	933/962 (96%)	0.38	51 (5%) 25 22	25, 40, 60, 80	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	368	THR	4.6
1	A	362	LEU	4.3
1	A	124	LEU	4.3
1	A	286	CYS	4.1
1	A	367	VAL	3.5
1	A	102	VAL	3.5
1	A	115	ILE	3.2
1	A	393	LEU	3.1
1	A	119	CYS	3.1
1	A	61	THR	3.1
1	A	103	LEU	3.0
1	A	121	GLU	2.9
1	B	57	LEU	2.9
1	A	116	LEU	2.9
1	A	371	THR	2.8
1	A	364	SER	2.8
1	A	330	PRO	2.8
1	A	370	GLY	2.8
1	B	324	HIS	2.8
1	A	71	GLU	2.7
1	A	292	VAL	2.7
1	A	307	LEU	2.7
1	B	429	VAL	2.6
1	A	329	SER	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	411	LEU	2.5
1	B	412	TYR	2.5
1	A	58	PRO	2.4
1	A	283	PHE	2.4
1	A	361	ALA	2.4
1	B	519	SER	2.4
1	A	70	PHE	2.3
1	A	147	ILE	2.3
1	A	320	LEU	2.3
1	A	332	GLN	2.3
1	A	369	ASP	2.3
1	A	287	PRO	2.3
1	B	435	LEU	2.3
1	A	117	ARG	2.2
1	A	514	TYR	2.2
1	A	363	GLY	2.2
1	A	366	LEU	2.2
1	A	179	ARG	2.1
1	B	518	PRO	2.1
1	A	72	ARG	2.1
1	B	486	LEU	2.1
1	A	449	PHE	2.1
1	B	58	PRO	2.0
1	A	249	TYR	2.0
1	A	409	GLU	2.0
1	B	488	TYR	2.0
1	A	372	MET	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

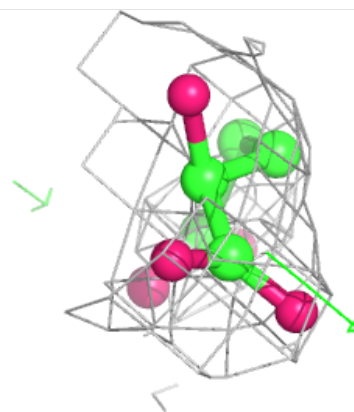
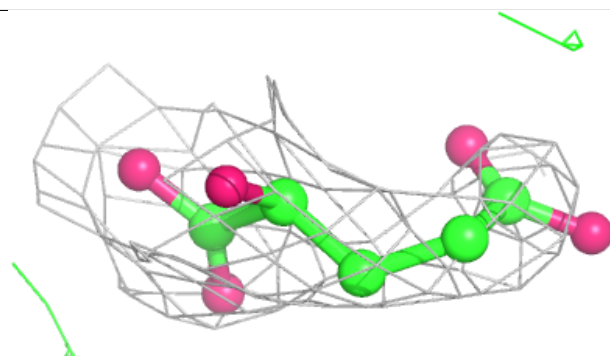
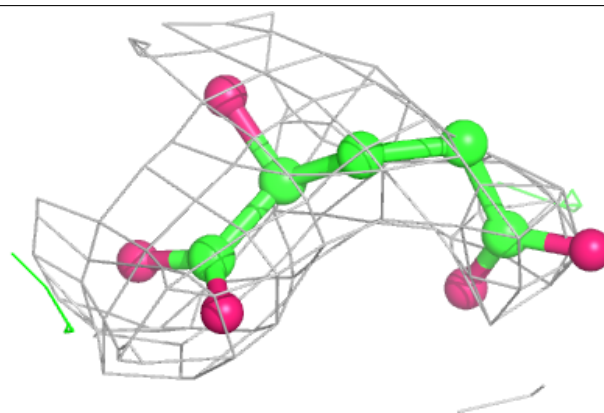
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	S2G	B	603	10/10	0.92	0.26	33,36,42,46	3
4	S2G	A	603	10/10	0.94	0.24	36,42,51,54	3
2	FAD	A	601	53/53	0.95	0.17	26,38,45,49	0
2	FAD	B	601	53/53	0.96	0.16	24,34,39,41	0
3	ZN	A	602	1/1	0.98	0.16	35,35,35,35	0
3	ZN	B	602	1/1	0.99	0.09	39,39,39,39	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.

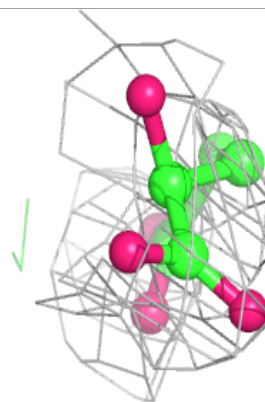
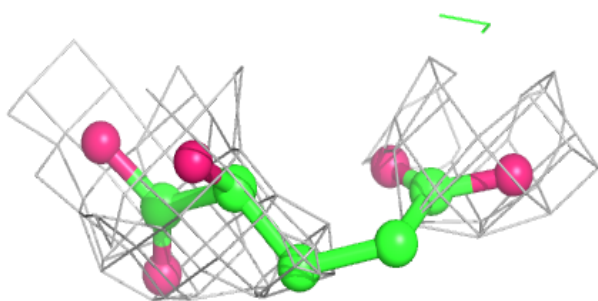
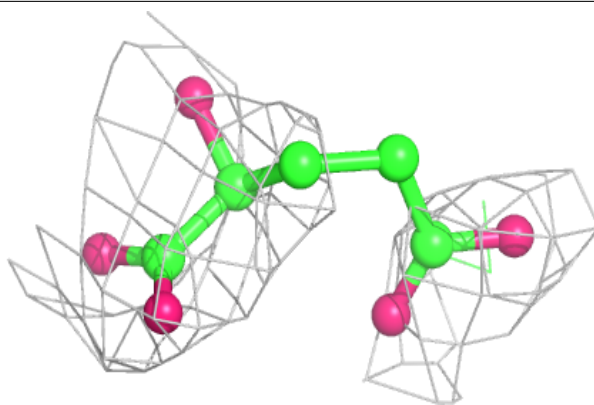
Electron density around S2G B 603:

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

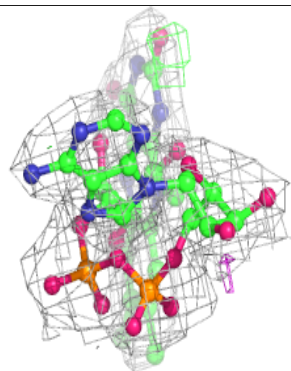
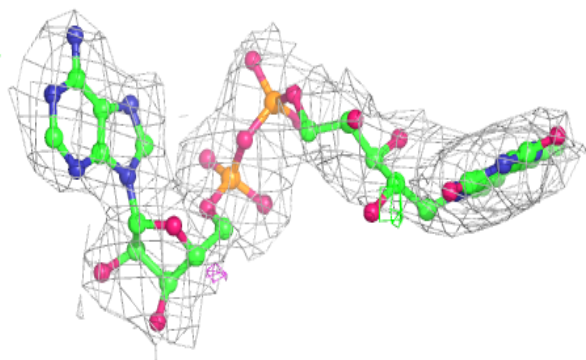
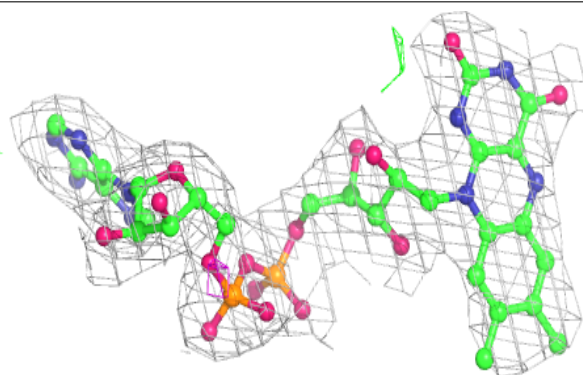


Electron density around S2G A 603:

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

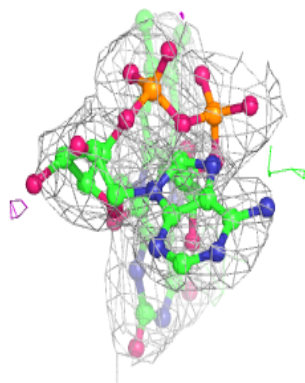
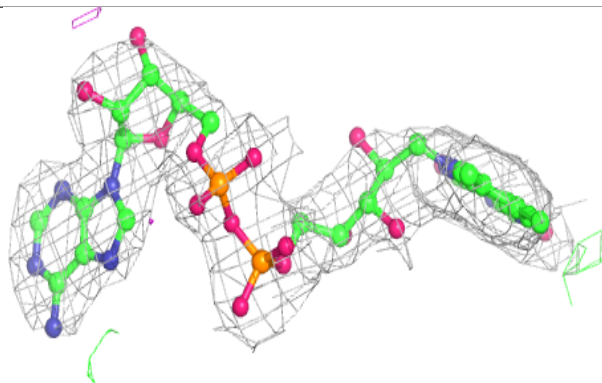
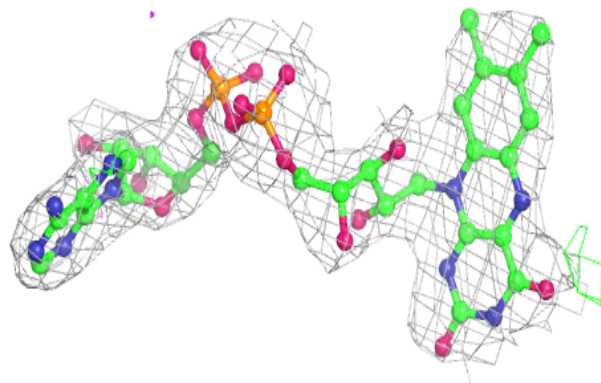
**Electron density around FAD A 601:**

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



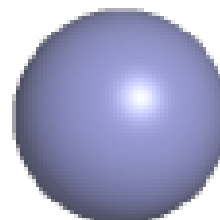
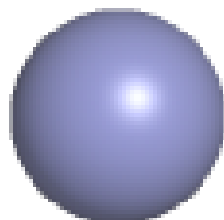
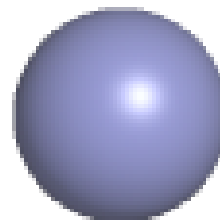
Electron density around FAD B 601:

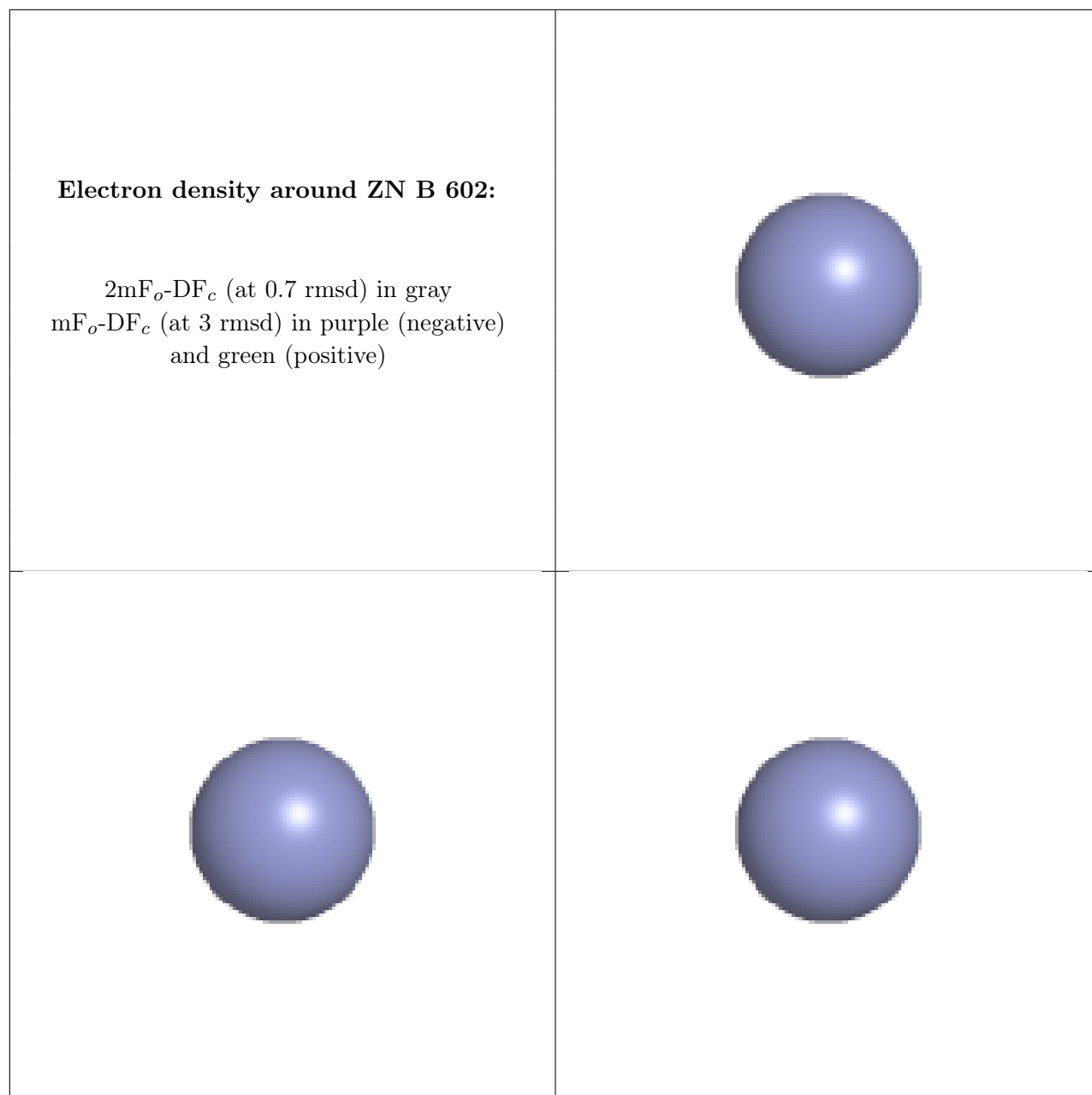
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN A 602:

$2mF_o-DF_c$ (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.