



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:36 PM UTC

PDB ID : 2GH5 / pdb_00002gh5
Title : Crystal Structure of human Glutathione Reductase complexed with a Fluoro-Analogue of the Menadione Derivative M5
Authors : Fritz-Wolf, K.; Winzer, A.; Bauer, H.; Schirmer, H.; Davioud-Charvet, E.
Deposited on : 2006-03-25
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

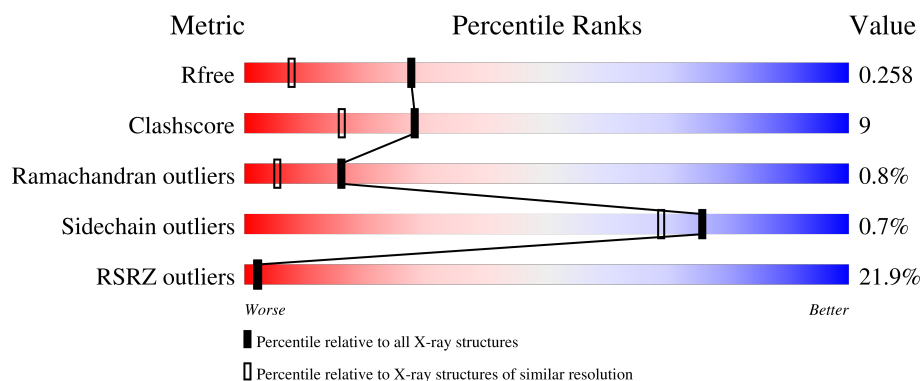
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	478	
1	B	478	

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
5	GOL	A	808	-	X	-	-
5	GOL	A	809	-	X	-	-
5	GOL	A	810	-	X	-	-
5	GOL	A	813	-	X	-	-
5	GOL	A	817	-	X	-	-
5	GOL	B	801	-	X	-	-
5	GOL	B	802	-	X	-	-
5	GOL	B	803	-	X	-	-
5	GOL	B	805	-	X	-	-
5	GOL	B	806	-	X	-	-
5	GOL	B	811	-	X	-	-
5	GOL	B	812	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7941 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 glutathione reductase, mitochondrial.

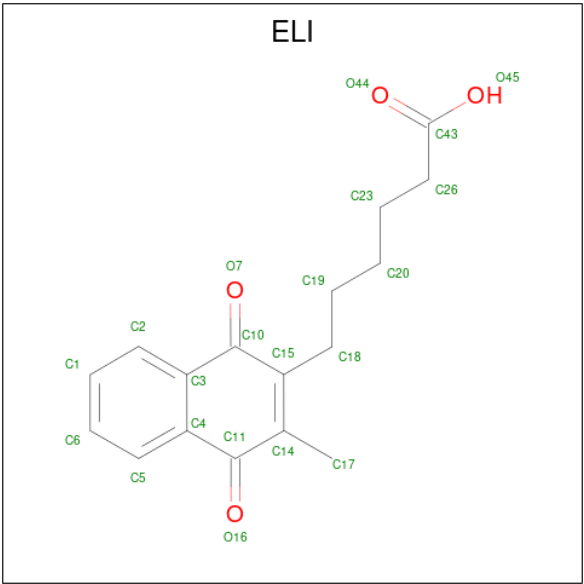
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	0	0
			3499	2212	603	660	24			
1	B	461	Total	C	N	O	S	0	0	0
			3499	2212	603	660	24			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



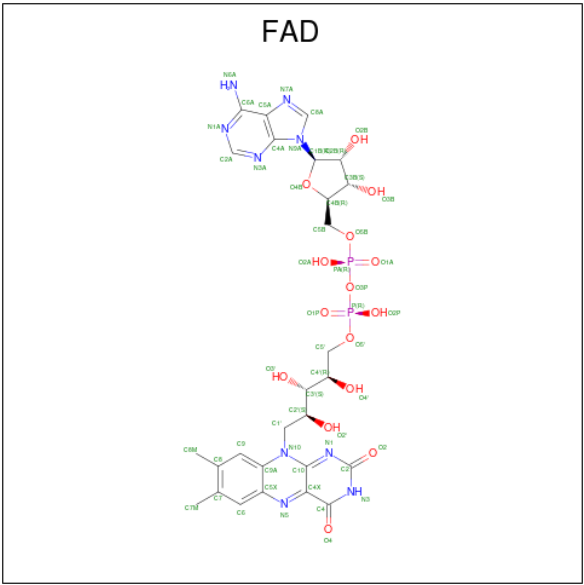
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 6-(3-METHYL-1,4-DIOXO-1,4-DIHYDRONAPHTHALEN-2-YL)HEXANOIC ACID (CCD ID: ELI) (formula: C₁₇H₁₈O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			21	17	4		
3	B	1	Total	C	O	0	0
			21	17	4		

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: C₂₇H₃₃N₉O₁₅P₂).



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

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

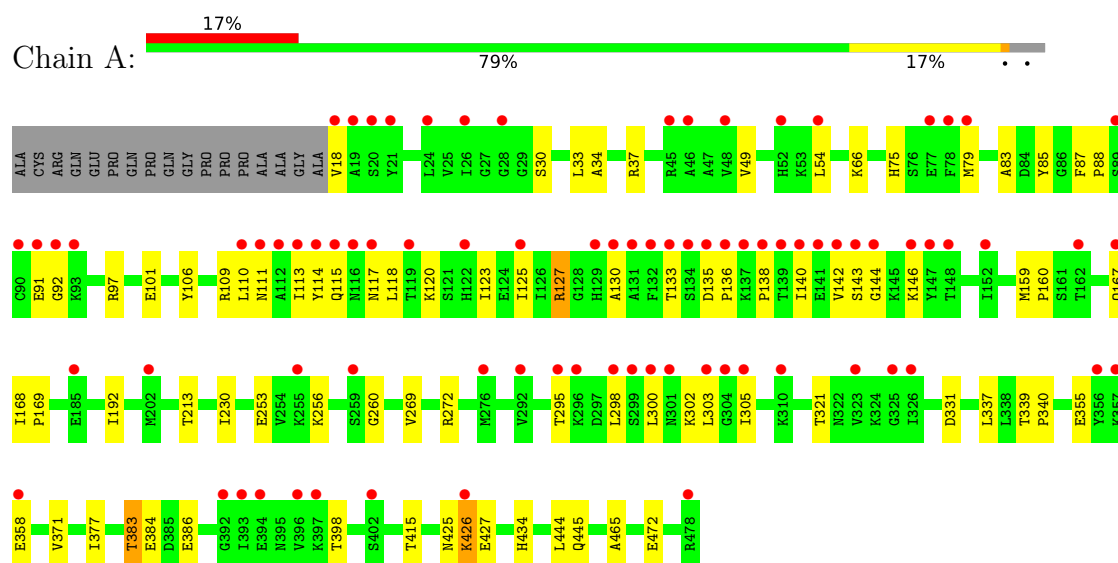
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	350	Total	O	0	0
			350	350		
6	B	353	Total	O	0	0
			353	353		

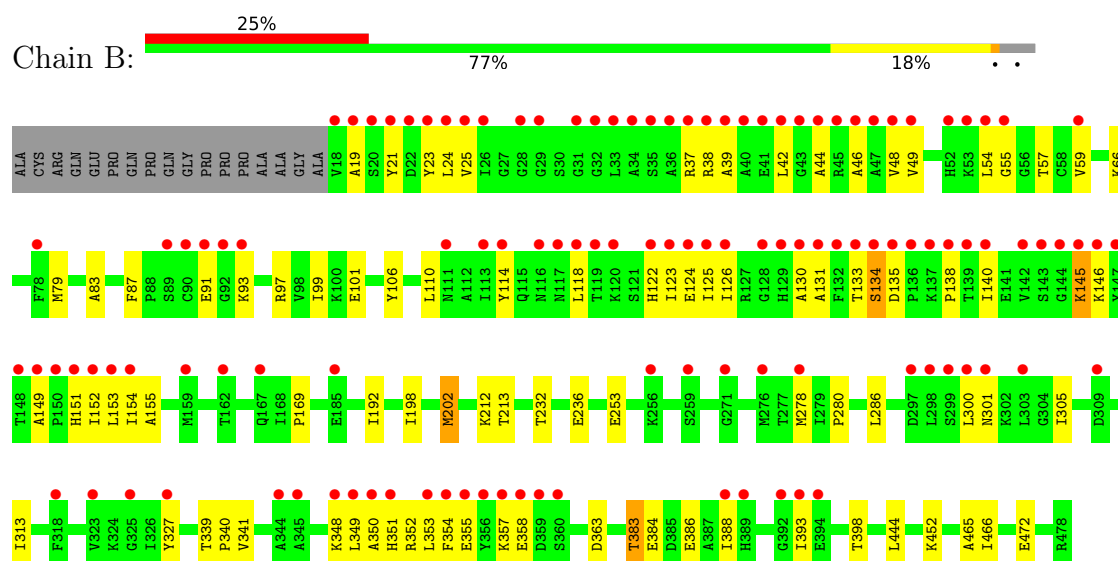
3 Residue-property plots [i](#)

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: glutathione reductase, mitochondrial



- Molecule 1: glutathione reductase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.70Å 63.60Å 103.99Å 90.00° 101.12° 90.00°	Depositor
Resolution (Å)	19.74 – 1.70 19.74 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (19.74-1.70) 98.9 (19.74-1.70)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.00 (at 1.70Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.224 , 0.256 0.225 , 0.258	Depositor DCC
R_{free} test set	5908 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	21.2	Xtriage
Anisotropy	0.370	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 50.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7941	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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 77.33 % 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 8.6982e-07. 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, ELI, GOL, 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	0.35	0/3566	0.83	5/4824 (0.1%)
1	B	0.36	0/3566	0.81	4/4824 (0.1%)
All	All	0.35	0/7132	0.82	9/9648 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	444	LEU	N-CA-C	8.19	120.29	111.36
1	B	444	LEU	N-CA-C	8.19	120.28	111.36
1	A	213	THR	N-CA-C	6.15	119.49	109.59
1	B	213	THR	N-CA-C	5.82	118.96	109.59
1	A	383	THR	N-CA-C	-5.65	103.24	110.53
1	A	355	GLU	N-CA-C	-5.60	105.22	113.61
1	B	212	LYS	N-CA-C	-5.58	100.03	108.67
1	B	383	THR	N-CA-C	-5.26	103.75	110.53
1	A	321	THR	N-CA-C	-5.05	101.92	109.79

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3499	0	3537	60	0
1	B	3499	0	3537	71	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
3	A	21	0	14	5	0
3	B	21	0	14	2	0
4	A	53	0	31	0	0
4	B	53	0	31	1	0
5	A	30	0	20	1	0
5	B	42	0	28	0	0
6	A	350	0	0	5	0
6	B	353	0	0	11	0
All	All	7941	0	7212	128	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 9.

All (128) 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:130:ALA:HB1	1:B:140:ILE:HD11	1.51	0.92
1:A:169:PRO:HG2	1:A:253:GLU:HG3	1.63	0.80
1:B:133:THR:HG22	1:B:134:SER:H	1.50	0.77
1:B:352:ARG:HA	6:B:6024:HOH:O	1.85	0.77
1:A:33:LEU:HD13	1:A:114:TYR:CE2	2.21	0.76
1:B:54:LEU:HD23	1:B:55:GLY:N	2.01	0.76
1:B:155:ALA:HB3	6:B:5818:HOH:O	1.85	0.75
1:B:169:PRO:HG2	1:B:253:GLU:HG3	1.71	0.72
1:B:130:ALA:HB1	1:B:140:ILE:CD1	2.19	0.71
1:B:23:TYR:HB3	1:B:46:ALA:HB2	1.72	0.71
1:B:466:ILE:HB	6:B:5707:HOH:O	1.90	0.71
1:A:79:MET:SD	1:A:92:GLY:HA2	2.30	0.70
1:B:145:LYS:HD3	1:B:146:LYS:N	2.07	0.70
1:A:30:SER:HA	3:A:958:ELI:H201	1.75	0.67
1:B:19:ALA:H	1:B:145:LYS:HE2	1.59	0.67
1:B:97:ARG:O	1:B:101:GLU:HG3	1.95	0.66
1:A:49:VAL:HG11	1:A:130:ALA:HB2	1.77	0.66
1:A:140:ILE:HB	6:A:5858:HOH:O	1.96	0.65
1:A:298:LEU:HD11	6:A:6049:HOH:O	1.95	0.65
1:A:33:LEU:HD22	1:A:118:LEU:HD21	1.78	0.65
1:B:351:HIS:O	1:B:355:GLU:HB2	1.96	0.65
1:A:97:ARG:O	1:A:101:GLU:HG3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:VAL:HG12	1:A:146:LYS:HB2	1.79	0.63
1:A:230:ILE:HD11	1:A:434:HIS:HB3	1.80	0.63
1:A:383:THR:OG1	1:A:386:GLU:HG3	1.99	0.62
1:B:341:VAL:HG23	6:B:5709:HOH:O	1.99	0.62
1:B:202:MET:SD	1:B:286:LEU:HD11	2.40	0.62
1:A:117:ASN:HA	1:A:120:LYS:HZ2	1.64	0.62
1:B:152:ILE:HD12	1:B:152:ILE:N	2.16	0.61
1:B:133:THR:HG22	1:B:134:SER:N	2.16	0.60
1:A:295:THR:HA	1:A:298:LEU:HD13	1.83	0.60
1:B:126:ILE:HD12	1:B:126:ILE:N	2.16	0.60
1:B:300:LEU:HB2	1:B:305:ILE:HB	1.84	0.60
1:B:388:ILE:HG23	1:B:393:ILE:HG12	1.84	0.59
1:B:24:LEU:HD22	1:B:152:ILE:HG23	1.85	0.57
1:A:331:ASP:HA	1:A:337:LEU:HD22	1.86	0.57
1:A:358:GLU:HG2	6:A:5978:HOH:O	2.04	0.57
1:B:348:LYS:O	1:B:351:HIS:HB3	2.05	0.56
1:A:85:TYR:HA	1:B:99:ILE:HD11	1.87	0.56
1:A:120:LYS:HZ2	1:A:120:LYS:HB2	1.69	0.56
1:A:465:ALA:HB1	1:A:472:GLU:HB2	1.87	0.56
1:B:57:THR:HG21	6:B:5879:HOH:O	2.05	0.55
1:A:88:PRO:HG2	1:B:91:GLU:OE2	2.06	0.55
1:A:120:LYS:HB2	1:A:120:LYS:NZ	2.21	0.55
1:A:37:ARG:HD3	3:A:958:ELI:O44	2.07	0.55
1:A:384:GLU:HG3	1:A:398:THR:HG21	1.89	0.55
1:B:37:ARG:HA	1:B:123:ILE:HD11	1.88	0.54
1:A:30:SER:HA	3:A:958:ELI:C20	2.37	0.54
1:A:302:LYS:C	1:A:303:LEU:HD22	2.32	0.54
1:B:49:VAL:HG22	1:B:126:ILE:HB	1.90	0.53
1:B:349:LEU:HG	6:B:5933:HOH:O	2.08	0.53
1:A:415:THR:HG21	5:A:817:GOL:H12	1.89	0.53
1:A:79:MET:HA	1:B:79:MET:HE1	1.91	0.53
1:B:383:THR:OG1	1:B:386:GLU:HG3	2.09	0.52
1:B:340:PRO:HB2	6:B:5709:HOH:O	2.09	0.52
1:B:149:ALA:O	1:B:152:ILE:HD11	2.08	0.52
1:B:388:ILE:CG2	1:B:393:ILE:HG12	2.40	0.52
1:A:106:TYR:O	1:A:110:LEU:HG	2.10	0.52
1:B:39:ALA:O	1:B:44:ALA:HB3	2.10	0.51
1:B:49:VAL:HG12	4:B:479:FAD:H2A	1.93	0.51
1:A:135:ASP:OD1	1:A:136:PRO:HD2	2.10	0.51
1:A:427:GLU:H	1:A:427:GLU:CD	2.18	0.51
1:B:49:VAL:HG11	1:B:130:ALA:HB2	1.90	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:ARG:O	1:A:113:ILE:HG22	2.11	0.51
1:A:117:ASN:HA	1:A:120:LYS:NZ	2.25	0.51
1:A:127:ARG:HG3	1:A:127:ARG:HH11	1.75	0.50
1:A:426:LYS:HB3	1:A:426:LYS:NZ	2.26	0.50
1:B:38:ARG:NH1	1:B:351:HIS:HB2	2.26	0.50
1:A:106:TYR:CE1	1:A:110:LEU:HD21	2.47	0.50
1:A:425:ASN:HB2	1:A:427:GLU:OE2	2.11	0.50
1:A:33:LEU:HB3	1:A:114:TYR:OH	2.11	0.50
1:A:192:ILE:HD12	1:A:192:ILE:N	2.28	0.49
1:A:66:LYS:HD2	1:A:66:LYS:C	2.37	0.49
1:B:151:HIS:C	1:B:152:ILE:HD12	2.37	0.49
1:A:54:LEU:HD11	1:A:125:ILE:HD13	1.94	0.49
1:A:167:GLN:HG2	1:A:168:ILE:HG13	1.95	0.48
1:B:465:ALA:HB1	1:B:472:GLU:HB2	1.95	0.48
1:A:133:THR:HG21	1:A:146:LYS:HD2	1.95	0.48
1:B:118:LEU:CD2	1:B:125:ILE:HD11	2.43	0.48
1:A:37:ARG:HA	1:A:123:ILE:HD11	1.96	0.48
1:A:83:ALA:HA	1:A:87:PHE:O	2.14	0.48
1:B:384:GLU:HG3	1:B:398:THR:HG21	1.95	0.47
1:B:25:VAL:HB	1:B:48:VAL:HG12	1.95	0.47
1:B:355:GLU:HB2	6:B:5808:HOH:O	2.13	0.47
1:A:114:TYR:O	1:A:117:ASN:N	2.44	0.47
1:A:256:LYS:HD2	1:A:260:GLY:O	2.14	0.47
1:A:300:LEU:HB3	1:A:305:ILE:HB	1.96	0.47
1:A:445:GLN:HB2	6:B:5707:HOH:O	2.14	0.47
1:B:21:TYR:HE2	1:B:124:GLU:OE2	1.98	0.46
1:B:66:LYS:C	1:B:66:LYS:HD2	2.40	0.46
1:A:295:THR:C	1:A:298:LEU:HD13	2.40	0.46
1:B:192:ILE:N	1:B:192:ILE:HD12	2.31	0.46
1:B:42:LEU:HD22	1:B:355:GLU:OE1	2.16	0.46
1:A:111:ASN:O	1:A:115:GLN:HG3	2.16	0.46
1:B:351:HIS:HE1	1:B:357:LYS:HG3	1.80	0.46
1:B:24:LEU:HD23	1:B:24:LEU:C	2.41	0.45
1:B:37:ARG:HD3	3:B:958:ELI:O45	2.17	0.45
1:A:295:THR:CA	1:A:298:LEU:HD13	2.47	0.45
1:B:23:TYR:OH	1:B:153:LEU:HD22	2.17	0.45
1:A:426:LYS:HG2	6:A:6005:HOH:O	2.17	0.44
1:B:232:THR:O	1:B:236:GLU:HG3	2.18	0.44
1:B:114:TYR:HB2	3:B:958:ELI:H2	1.99	0.44
1:B:198:ILE:O	1:B:202:MET:HG3	2.18	0.44
1:A:339:THR:HB	1:A:340:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:278:MET:O	1:B:280:PRO:HD3	2.18	0.43
1:B:83:ALA:HA	1:B:87:PHE:O	2.19	0.43
1:A:142:VAL:O	1:A:143:SER:HB2	2.18	0.43
1:A:159:MET:HB2	1:A:160:PRO:HD2	2.01	0.43
1:B:54:LEU:HD23	1:B:54:LEU:C	2.43	0.43
1:B:118:LEU:HD21	1:B:125:ILE:HD11	2.00	0.43
1:B:38:ARG:HH12	1:B:351:HIS:CD2	2.36	0.43
1:B:339:THR:HB	1:B:340:PRO:HD3	2.01	0.42
1:A:114:TYR:HB2	3:A:958:ELI:H2	2.02	0.42
1:A:426:LYS:HD3	6:A:5983:HOH:O	2.19	0.41
1:B:106:TYR:O	1:B:110:LEU:HG	2.20	0.41
1:B:327:TYR:N	1:B:327:TYR:CD1	2.87	0.41
1:B:300:LEU:HD12	1:B:301:ASN:N	2.36	0.41
1:A:371:VAL:HB	1:A:377:ILE:HB	2.02	0.41
1:A:269:VAL:HB	1:A:272:ARG:HD2	2.02	0.41
1:B:131:ALA:O	1:B:140:ILE:HG13	2.21	0.41
1:B:363:ASP:OD2	1:B:452:LYS:HE3	2.21	0.41
1:A:34:ALA:HA	3:A:958:ELI:O45	2.20	0.41
1:B:350:ALA:O	1:B:354:PHE:HD1	2.04	0.41
1:B:93:LYS:O	1:B:93:LYS:HG3	2.20	0.40
1:B:353:LEU:HB2	1:B:354:PHE:CE1	2.56	0.40
1:B:59:VAL:HG22	6:B:5762:HOH:O	2.21	0.40
1:B:154:ILE:HG21	1:B:313:ILE:CD1	2.52	0.40
1:B:138:PRO:HB2	6:B:6035:HOH:O	2.20	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	459/478 (96%)	439 (96%)	17 (4%)	3 (1%)	18 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	459/478 (96%)	432 (94%)	23 (5%)	4 (1%)	14	4
All	All	918/956 (96%)	871 (95%)	40 (4%)	7 (1%)	16	5

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	134	SER
1	A	91	GLU
1	B	135	ASP
1	A	144	GLY
1	B	358	GLU
1	B	122	HIS
1	A	138	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	382/393 (97%)	379 (99%)	3 (1%)	73	65
1	B	382/393 (97%)	380 (100%)	2 (0%)	81	76
All	All	764/786 (97%)	759 (99%)	5 (1%)	76	69

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	A	127	ARG
1	A	426	LYS
1	B	145	LYS
1	B	202	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	116	ASN
1	A	164	HIS
1	A	182	GLN
1	A	365	ASN
1	A	395	ASN
1	A	425	ASN
1	B	52	HIS
1	B	111	ASN
1	B	115	GLN
1	B	167	GLN
1	B	250	GLN
1	B	351	HIS
1	B	365	ASN
1	B	366	ASN
1	B	425	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

20 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	FAD	A	479	-	58,58,58	1.65	10 (17%)	85,89,89	1.12	5 (5%)
5	GOL	B	805	-	5,5,5	4.78	5 (100%)	5,5,5	6.08	3 (60%)
5	GOL	B	803	-	5,5,5	4.78	5 (100%)	5,5,5	6.13	3 (60%)
2	PO4	A	5706	-	4,4,4	1.80	0	6,6,6	0.46	0
5	GOL	A	817	-	5,5,5	4.78	5 (100%)	5,5,5	6.12	3 (60%)
5	GOL	A	813	-	5,5,5	4.79	5 (100%)	5,5,5	6.11	3 (60%)
2	PO4	B	5705	-	4,4,4	1.79	1 (25%)	6,6,6	0.47	0
3	ELI	B	958	1	22,22,22	5.16	13 (59%)	27,30,30	3.80	6 (22%)
5	GOL	B	811	-	5,5,5	4.77	5 (100%)	5,5,5	6.14	3 (60%)
5	GOL	B	806	-	5,5,5	4.77	5 (100%)	5,5,5	6.11	3 (60%)
2	PO4	B	5704	-	4,4,4	1.74	1 (25%)	6,6,6	0.45	0
5	GOL	A	809	-	5,5,5	4.77	5 (100%)	5,5,5	6.12	3 (60%)
5	GOL	A	810	-	5,5,5	4.75	5 (100%)	5,5,5	6.12	3 (60%)
5	GOL	B	801	-	5,5,5	4.77	5 (100%)	5,5,5	6.09	3 (60%)
4	FAD	B	479	-	58,58,58	1.68	8 (13%)	85,89,89	1.22	9 (10%)
2	PO4	A	5703	-	4,4,4	1.74	0	6,6,6	0.46	0
3	ELI	A	958	1	22,22,22	5.50	17 (77%)	27,30,30	3.18	6 (22%)
5	GOL	B	802	-	5,5,5	4.80	5 (100%)	5,5,5	6.12	3 (60%)
5	GOL	A	808	-	5,5,5	4.77	5 (100%)	5,5,5	6.11	3 (60%)
5	GOL	B	812	-	5,5,5	4.78	5 (100%)	5,5,5	6.11	3 (60%)

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
5	GOL	B	801	-	-	2/4/4/4	-
4	FAD	B	479	-	-	3/34/50/50	0/6/6/6
3	ELI	B	958	1	-	5/8/28/28	0/2/2/2
5	GOL	A	817	-	-	4/4/4/4	-
5	GOL	B	811	-	-	4/4/4/4	-
5	GOL	B	806	-	-	2/4/4/4	-
5	GOL	A	813	-	-	3/4/4/4	-
4	FAD	A	479	-	-	3/34/50/50	0/6/6/6
3	ELI	A	958	1	-	1/8/28/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	B	805	-	-	3/4/4/4	-
5	GOL	B	802	-	-	2/4/4/4	-
5	GOL	B	803	-	-	2/4/4/4	-
5	GOL	A	809	-	-	2/4/4/4	-
5	GOL	A	808	-	-	2/4/4/4	-
5	GOL	A	810	-	-	4/4/4/4	-
5	GOL	B	812	-	-	2/4/4/4	-

All (110) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	958	ELI	C4-C3	12.13	1.60	1.40
3	B	958	ELI	C4-C3	10.19	1.57	1.40
3	A	958	ELI	C15-C14	8.51	1.50	1.35
3	B	958	ELI	C5-C4	8.17	1.52	1.39
5	B	812	GOL	C3-C2	-8.11	1.20	1.51
5	A	813	GOL	C3-C2	-8.06	1.21	1.51
5	B	802	GOL	C3-C2	-8.05	1.21	1.51
5	B	803	GOL	C3-C2	-8.04	1.21	1.51
5	A	817	GOL	C3-C2	-8.03	1.21	1.51
5	A	808	GOL	C3-C2	-8.00	1.21	1.51
5	A	809	GOL	C3-C2	-8.00	1.21	1.51
5	B	805	GOL	C3-C2	-7.98	1.21	1.51
5	B	811	GOL	C3-C2	-7.97	1.21	1.51
5	A	810	GOL	C3-C2	-7.97	1.21	1.51
5	B	806	GOL	C3-C2	-7.97	1.21	1.51
5	B	801	GOL	C3-C2	-7.94	1.21	1.51
3	B	958	ELI	C15-C10	7.78	1.66	1.47
3	A	958	ELI	C5-C4	7.57	1.51	1.39
3	A	958	ELI	C1-C2	7.25	1.51	1.38
3	B	958	ELI	C2-C3	7.14	1.50	1.39
3	A	958	ELI	C15-C10	6.86	1.64	1.47
3	A	958	ELI	C14-C11	6.73	1.63	1.47
3	B	958	ELI	C14-C11	6.73	1.63	1.47
3	A	958	ELI	C2-C3	6.65	1.50	1.39
3	B	958	ELI	C1-C2	6.56	1.50	1.38
3	A	958	ELI	C6-C5	6.55	1.50	1.38
3	A	958	ELI	C6-C1	6.49	1.52	1.38
3	B	958	ELI	C6-C5	6.46	1.49	1.38
3	B	958	ELI	C6-C1	6.34	1.52	1.38
3	B	958	ELI	C4-C11	6.30	1.60	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	958	ELI	C4-C11	6.24	1.60	1.48
3	B	958	ELI	C15-C14	6.20	1.46	1.35
3	A	958	ELI	C3-C10	5.67	1.59	1.48
4	B	479	FAD	C4X-N5	5.63	1.42	1.30
4	A	479	FAD	C4X-N5	5.22	1.42	1.30
3	B	958	ELI	C3-C10	5.17	1.58	1.48
5	B	805	GOL	O1-C1	4.65	1.61	1.42
5	B	806	GOL	O1-C1	4.57	1.61	1.42
5	B	811	GOL	O1-C1	4.56	1.61	1.42
5	A	813	GOL	O1-C1	4.55	1.61	1.42
5	B	802	GOL	O1-C1	4.55	1.61	1.42
5	A	809	GOL	O1-C1	4.53	1.61	1.42
5	A	817	GOL	O1-C1	4.52	1.61	1.42
5	B	801	GOL	O1-C1	4.50	1.61	1.42
5	A	808	GOL	O1-C1	4.49	1.61	1.42
5	A	810	GOL	O1-C1	4.47	1.61	1.42
5	B	812	GOL	O1-C1	4.44	1.61	1.42
4	A	479	FAD	C9A-C5X	4.43	1.48	1.41
5	B	803	GOL	O1-C1	4.42	1.61	1.42
4	B	479	FAD	C9A-C5X	4.37	1.48	1.41
4	B	479	FAD	C9-C8	4.11	1.45	1.39
4	A	479	FAD	C4A-N3A	3.76	1.41	1.34
3	B	958	ELI	C17-C14	3.74	1.58	1.50
3	A	958	ELI	O44-C43	-3.73	1.09	1.22
4	B	479	FAD	C4A-N3A	3.71	1.41	1.34
4	B	479	FAD	C2A-N1A	3.51	1.40	1.33
4	A	479	FAD	C2A-N1A	3.48	1.40	1.33
5	B	801	GOL	O3-C3	3.48	1.57	1.42
4	A	479	FAD	C6-C5X	3.47	1.45	1.40
5	B	805	GOL	O3-C3	3.46	1.56	1.42
5	B	811	GOL	O3-C3	3.43	1.56	1.42
5	A	810	GOL	O3-C3	3.43	1.56	1.42
5	B	802	GOL	O3-C3	3.43	1.56	1.42
5	B	806	GOL	O3-C3	3.39	1.56	1.42
5	A	817	GOL	O3-C3	3.39	1.56	1.42
5	A	809	GOL	O3-C3	3.39	1.56	1.42
5	A	808	GOL	O3-C3	3.38	1.56	1.42
5	B	803	GOL	O3-C3	3.36	1.56	1.42
5	A	813	GOL	O3-C3	3.32	1.56	1.42
5	B	812	GOL	O3-C3	3.32	1.56	1.42
4	A	479	FAD	C10-N10	3.31	1.44	1.37
5	B	801	GOL	C1-C2	-3.17	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	803	GOL	C1-C2	-3.15	1.39	1.51
5	A	808	GOL	C1-C2	-3.15	1.39	1.51
4	B	479	FAD	C10-N10	3.14	1.44	1.37
5	A	817	GOL	C1-C2	-3.11	1.39	1.51
5	B	812	GOL	C1-C2	-3.09	1.40	1.51
5	A	810	GOL	C1-C2	-3.09	1.40	1.51
5	A	809	GOL	C1-C2	-3.09	1.40	1.51
5	B	802	GOL	C1-C2	-3.08	1.40	1.51
5	B	806	GOL	C1-C2	-3.08	1.40	1.51
5	A	813	GOL	C1-C2	-3.06	1.40	1.51
4	B	479	FAD	C6-C5X	3.05	1.44	1.40
4	A	479	FAD	C9-C8	3.03	1.43	1.39
5	B	811	GOL	C1-C2	-3.03	1.40	1.51
5	B	805	GOL	C1-C2	-3.02	1.40	1.51
5	B	803	GOL	O2-C2	-2.96	1.34	1.43
5	A	813	GOL	O2-C2	-2.92	1.34	1.43
5	B	812	GOL	O2-C2	-2.91	1.34	1.43
5	B	802	GOL	O2-C2	-2.91	1.34	1.43
5	B	806	GOL	O2-C2	-2.88	1.35	1.43
5	B	801	GOL	O2-C2	-2.87	1.35	1.43
5	B	811	GOL	O2-C2	-2.87	1.35	1.43
5	A	809	GOL	O2-C2	-2.86	1.35	1.43
5	A	808	GOL	O2-C2	-2.85	1.35	1.43
5	B	805	GOL	O2-C2	-2.83	1.35	1.43
3	B	958	ELI	O7-C10	2.82	1.29	1.23
5	A	817	GOL	O2-C2	-2.82	1.35	1.43
5	A	810	GOL	O2-C2	-2.81	1.35	1.43
4	B	479	FAD	PA-O3P	2.74	1.62	1.59
4	A	479	FAD	PA-O3P	2.63	1.62	1.59
3	A	958	ELI	C19-C18	2.49	1.61	1.52
4	A	479	FAD	C6-C7	2.24	1.42	1.39
4	A	479	FAD	C9A-N10	2.21	1.45	1.41
3	A	958	ELI	C17-C14	2.21	1.55	1.50
3	A	958	ELI	C23-C20	-2.21	1.40	1.51
3	A	958	ELI	O7-C10	2.20	1.27	1.23
2	B	5705	PO4	P-O2	-2.13	1.48	1.54
2	B	5704	PO4	P-O3	-2.12	1.48	1.54
3	A	958	ELI	C26-C43	-2.05	1.45	1.50

All (62) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	958	ELI	C20-C19-C18	16.18	172.57	113.13
3	A	958	ELI	C20-C19-C18	13.03	160.99	113.13
5	B	803	GOL	O3-C3-C2	11.13	160.47	110.38
5	B	811	GOL	O3-C3-C2	11.12	160.44	110.38
5	B	802	GOL	O3-C3-C2	11.11	160.38	110.38
5	A	810	GOL	O3-C3-C2	11.09	160.32	110.38
5	A	809	GOL	O3-C3-C2	11.09	160.29	110.38
5	A	808	GOL	O3-C3-C2	11.08	160.28	110.38
5	B	806	GOL	O3-C3-C2	11.08	160.24	110.38
5	A	817	GOL	O3-C3-C2	11.07	160.23	110.38
5	A	813	GOL	O3-C3-C2	11.07	160.22	110.38
5	B	801	GOL	O3-C3-C2	11.05	160.10	110.38
5	B	812	GOL	O3-C3-C2	11.04	160.07	110.38
5	B	805	GOL	O3-C3-C2	11.04	160.06	110.38
5	A	817	GOL	O2-C2-C3	7.23	139.11	109.18
5	B	803	GOL	O2-C2-C3	7.23	139.10	109.18
5	A	810	GOL	O2-C2-C3	7.22	139.09	109.18
5	B	811	GOL	O2-C2-C3	7.21	139.05	109.18
5	B	812	GOL	O2-C2-C3	7.21	139.05	109.18
5	A	808	GOL	O2-C2-C3	7.21	139.04	109.18
5	B	801	GOL	O2-C2-C3	7.20	138.99	109.18
5	A	809	GOL	O2-C2-C3	7.20	138.98	109.18
5	B	802	GOL	O2-C2-C3	7.19	138.96	109.18
5	A	813	GOL	O2-C2-C3	7.17	138.87	109.18
5	B	806	GOL	O2-C2-C3	7.17	138.85	109.18
5	B	805	GOL	O2-C2-C3	7.14	138.73	109.18
3	B	958	ELI	C23-C26-C43	6.49	131.45	114.51
3	B	958	ELI	C20-C23-C26	-6.43	89.50	113.13
3	A	958	ELI	C19-C18-C15	-4.44	100.36	113.10
3	A	958	ELI	C20-C23-C26	-4.43	96.84	113.13
3	A	958	ELI	C23-C20-C19	-4.08	93.74	114.37
3	A	958	ELI	C23-C26-C43	3.80	124.42	114.51
5	B	806	GOL	O1-C1-C2	3.49	126.11	110.38
5	A	813	GOL	O1-C1-C2	3.45	125.90	110.38
5	B	812	GOL	O1-C1-C2	3.44	125.88	110.38
5	B	802	GOL	O1-C1-C2	3.44	125.84	110.38
5	B	811	GOL	O1-C1-C2	3.42	125.79	110.38
4	B	479	FAD	N3A-C2A-N1A	-3.41	123.42	128.58
5	A	809	GOL	O1-C1-C2	3.40	125.66	110.38
5	B	805	GOL	O1-C1-C2	3.39	125.66	110.38
5	A	817	GOL	O1-C1-C2	3.39	125.65	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	958	ELI	O44-C43-C26	3.39	133.83	123.09
5	A	810	GOL	O1-C1-C2	3.38	125.58	110.38
3	B	958	ELI	O45-C43-O44	-3.37	114.68	123.33
5	A	808	GOL	O1-C1-C2	3.33	125.37	110.38
5	B	801	GOL	O1-C1-C2	3.33	125.36	110.38
4	A	479	FAD	N3A-C2A-N1A	-3.33	123.55	128.58
5	B	803	GOL	O1-C1-C2	3.31	125.27	110.38
3	B	958	ELI	C23-C20-C19	-3.26	97.91	114.37
3	B	958	ELI	O44-C43-C26	2.92	132.34	123.09
4	A	479	FAD	C8M-C8-C7	2.86	126.60	120.76
4	B	479	FAD	O2A-PA-O1A	2.79	125.44	112.44
4	A	479	FAD	C8M-C8-C9	-2.62	114.95	119.57
4	B	479	FAD	C8M-C8-C7	2.58	126.03	120.76
4	B	479	FAD	C4-C4X-N5	2.24	121.30	118.21
4	A	479	FAD	O2A-PA-O1A	2.22	122.79	112.44
4	B	479	FAD	O5B-PA-O1A	-2.21	100.19	108.94
4	B	479	FAD	C2B-C1B-N9A	2.17	118.70	113.30
4	B	479	FAD	C9-C9A-N10	2.13	124.72	121.85
4	B	479	FAD	C8M-C8-C9	-2.11	115.85	119.57
4	A	479	FAD	C2B-C1B-N9A	2.05	118.41	113.30
4	B	479	FAD	O2B-C2B-C3B	2.01	118.27	111.82

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	479	FAD	PA-O3P-P-O5'
4	B	479	FAD	PA-O3P-P-O5'
5	A	808	GOL	C1-C2-C3-O3
5	A	809	GOL	O1-C1-C2-C3
5	A	813	GOL	C1-C2-C3-O3
5	B	801	GOL	O1-C1-C2-C3
5	B	802	GOL	O1-C1-C2-C3
5	B	803	GOL	C1-C2-C3-O3
5	B	805	GOL	C1-C2-C3-O3
5	B	811	GOL	O1-C1-C2-C3
5	B	812	GOL	C1-C2-C3-O3
3	A	958	ELI	C15-C18-C19-C20
5	B	806	GOL	O2-C2-C3-O3
5	A	810	GOL	O1-C1-C2-C3
5	A	810	GOL	C1-C2-C3-O3
5	A	817	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
5	A	817	GOL	C1-C2-C3-O3
5	B	803	GOL	O1-C1-C2-C3
5	B	805	GOL	O1-C1-C2-C3
5	B	806	GOL	O1-C1-C2-C3
5	B	811	GOL	C1-C2-C3-O3
5	A	809	GOL	O2-C2-C3-O3
5	A	810	GOL	O2-C2-C3-O3
5	A	813	GOL	O1-C1-C2-O2
5	A	817	GOL	O2-C2-C3-O3
5	B	801	GOL	O2-C2-C3-O3
3	B	958	ELI	C18-C19-C20-C23
5	A	808	GOL	O1-C1-C2-O2
5	B	802	GOL	O2-C2-C3-O3
5	B	812	GOL	O1-C1-C2-O2
3	B	958	ELI	C20-C23-C26-C43
5	B	805	GOL	O1-C1-C2-O2
4	B	479	FAD	P-O3P-PA-O1A
5	B	811	GOL	O1-C1-C2-O2
5	A	813	GOL	O1-C1-C2-C3
4	A	479	FAD	P-O3P-PA-O1A
3	B	958	ELI	C15-C18-C19-C20
5	A	817	GOL	O1-C1-C2-O2
5	B	811	GOL	O2-C2-C3-O3
4	A	479	FAD	P-O3P-PA-O2A
3	B	958	ELI	C23-C26-C43-O44
5	A	810	GOL	O1-C1-C2-O2
3	B	958	ELI	C23-C26-C43-O45
4	B	479	FAD	P-O3P-PA-O2A

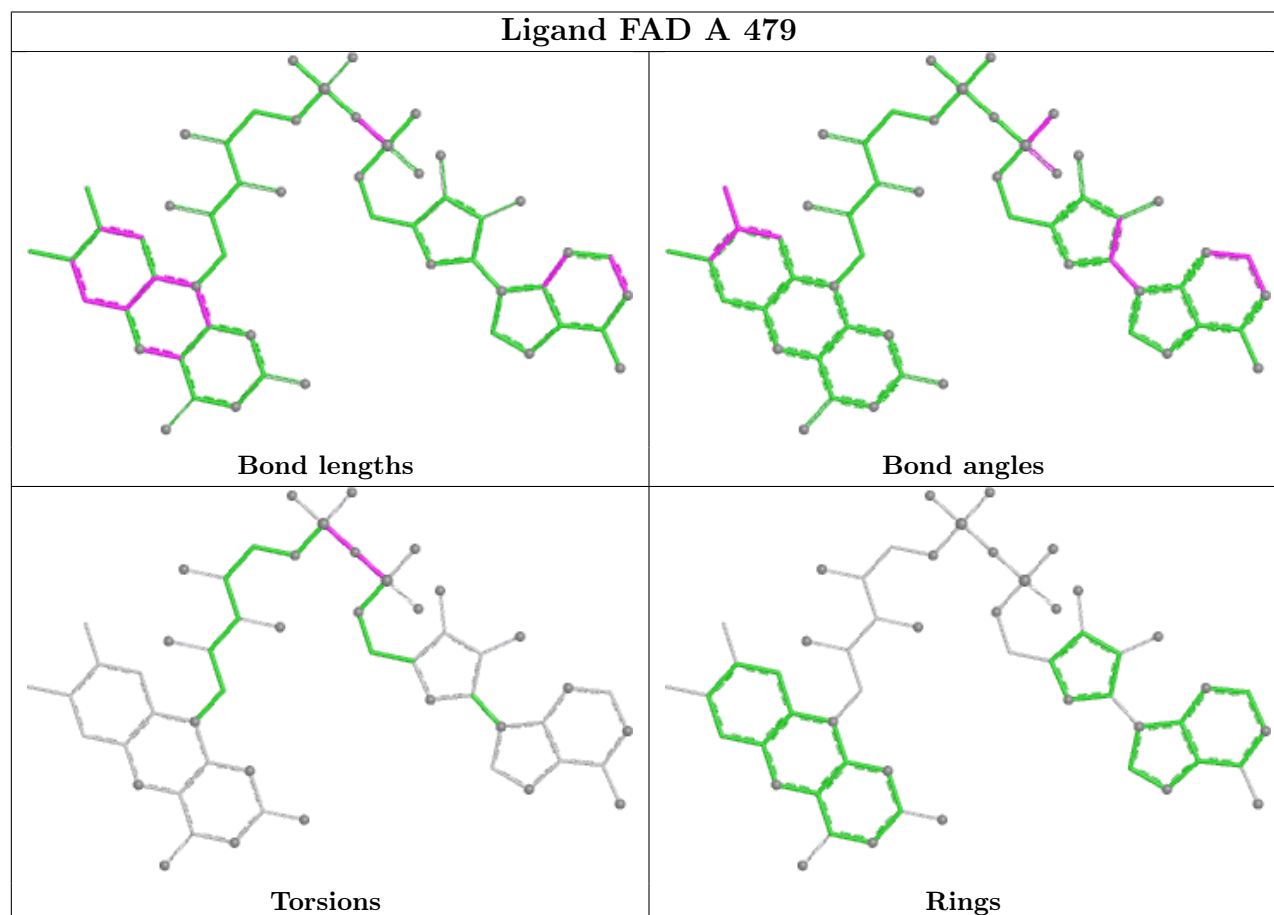
There are no ring outliers.

4 monomers are involved in 9 short contacts:

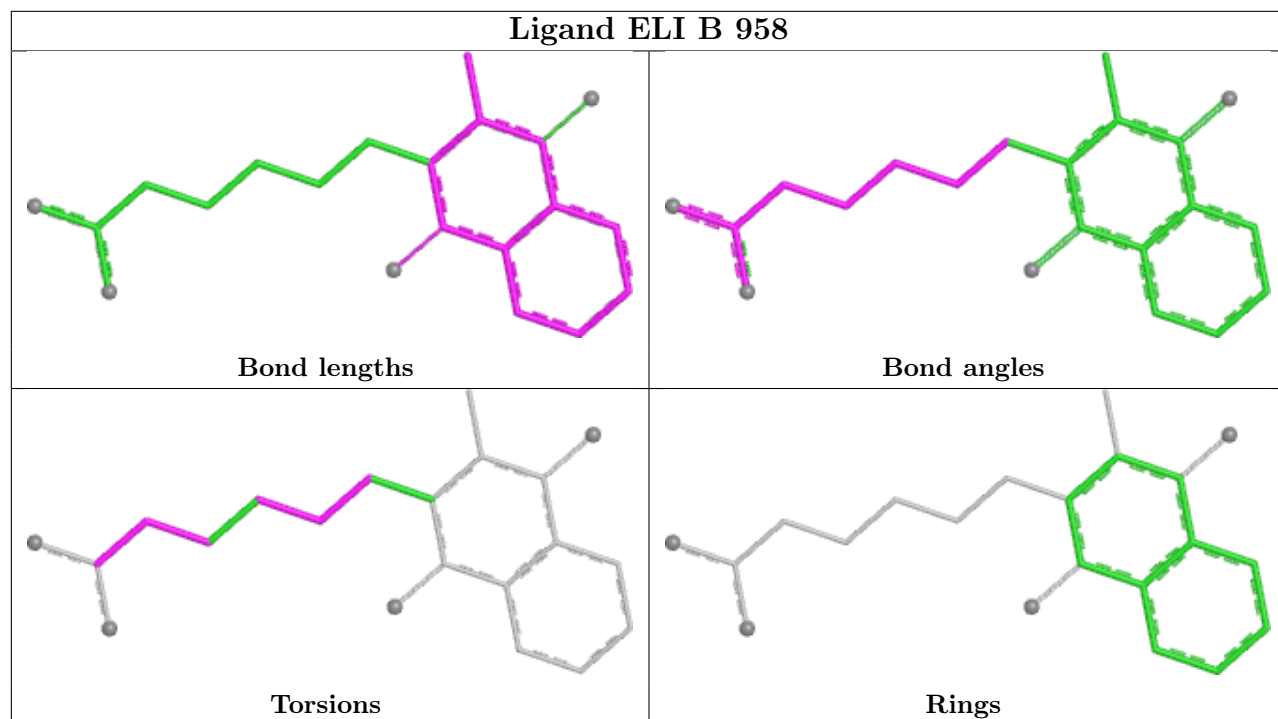
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	817	GOL	1	0
3	B	958	ELI	2	0
4	B	479	FAD	1	0
3	A	958	ELI	5	0

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

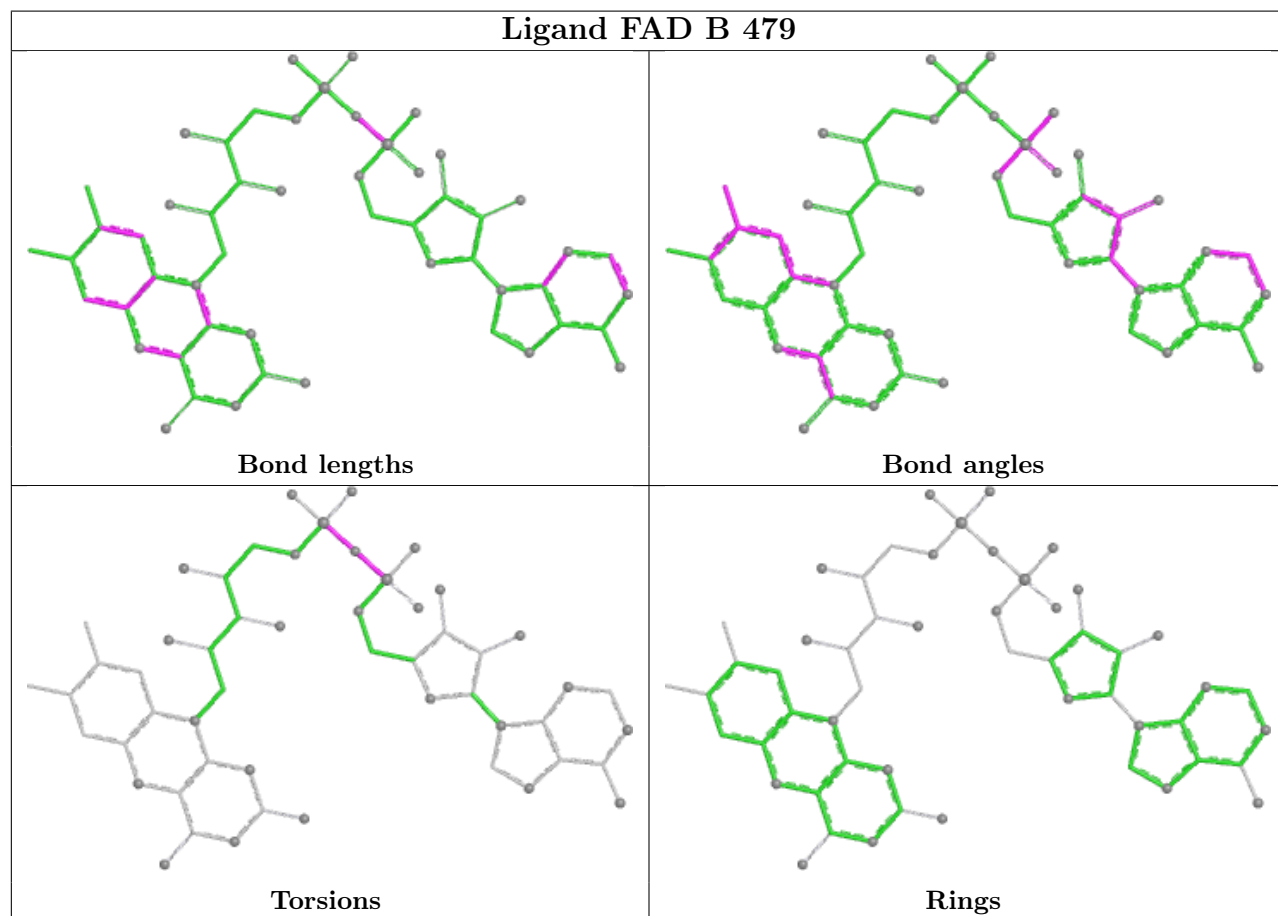
within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

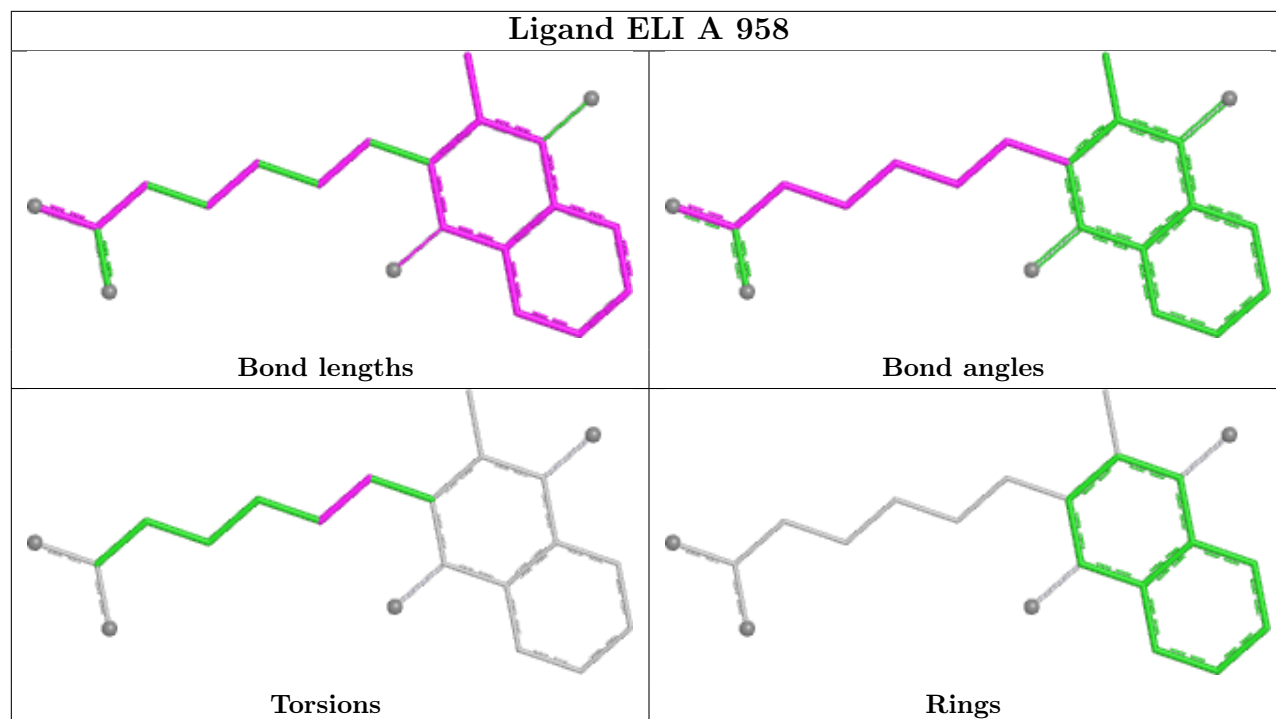


Ligand ELI B 958



Ligand FAD B 479





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	461/478 (96%)	0.91	83 (18%) 3 3	12, 25, 45, 62	0
1	B	461/478 (96%)	1.22	119 (25%) 1 1	13, 26, 62, 75	0
All	All	922/956 (96%)	1.07	202 (21%) 2 2	12, 25, 56, 75	0

All (202) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	92	GLY	7.7
1	B	354	PHE	7.3
1	A	78	PHE	7.0
1	B	21	TYR	6.8
1	B	350	ALA	6.7
1	B	24	LEU	6.5
1	B	125	ILE	6.5
1	B	300	LEU	6.4
1	B	351	HIS	6.3
1	B	42	LEU	6.1
1	B	138	PRO	6.0
1	B	136	PRO	5.8
1	B	48	VAL	5.8
1	B	45	ARG	5.7
1	B	44	ALA	5.7
1	B	78	PHE	5.5
1	A	142	VAL	5.4
1	B	90	CYS	5.4
1	B	28	GLY	5.4
1	B	356	TYR	5.4
1	B	134	SER	5.3
1	B	40	ALA	5.1
1	B	23	TYR	5.1
1	B	18	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
1	B	22	ASP	4.9
1	B	130	ALA	4.8
1	B	123	ILE	4.8
1	B	91	GLU	4.8
1	A	90	CYS	4.7
1	B	131	ALA	4.7
1	B	139	THR	4.6
1	A	138	PRO	4.6
1	A	140	ILE	4.6
1	A	144	GLY	4.6
1	B	140	ILE	4.6
1	B	133	THR	4.5
1	A	92	GLY	4.5
1	B	132	PHE	4.5
1	B	119	THR	4.4
1	B	126	ILE	4.4
1	A	18	VAL	4.3
1	B	142	VAL	4.3
1	B	150	PRO	4.3
1	B	355	GLU	4.3
1	B	358	GLU	4.3
1	A	114	TYR	4.2
1	B	118	LEU	4.2
1	B	39	ALA	4.2
1	A	299	SER	4.1
1	A	255	LYS	4.1
1	B	32	GLY	4.0
1	B	41	GLU	4.0
1	A	91	GLU	3.9
1	B	93	LYS	3.9
1	B	152	ILE	3.9
1	B	353	LEU	3.9
1	B	144	GLY	3.9
1	B	147	TYR	3.8
1	A	298	LEU	3.8
1	B	349	LEU	3.7
1	B	114	TYR	3.7
1	B	323	VAL	3.7
1	B	148	THR	3.7
1	B	151	HIS	3.7
1	B	55	GLY	3.7
1	A	131	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	136	PRO	3.6
1	A	77	GLU	3.6
1	B	43	GLY	3.6
1	A	139	THR	3.6
1	B	393	ILE	3.5
1	A	143	SER	3.5
1	A	132	PHE	3.5
1	A	303	LEU	3.5
1	B	303	LEU	3.5
1	A	130	ALA	3.4
1	B	128	GLY	3.4
1	A	113	ILE	3.4
1	B	46	ALA	3.4
1	A	167	GLN	3.4
1	A	79	MET	3.3
1	B	360	SER	3.3
1	B	19	ALA	3.3
1	B	325	GLY	3.2
1	B	53	LYS	3.2
1	B	359	ASP	3.2
1	B	38	ARG	3.2
1	B	394	GLU	3.2
1	B	20	SER	3.2
1	A	52	HIS	3.2
1	A	358	GLU	3.2
1	A	117	ASN	3.2
1	B	54	LEU	3.2
1	B	137	LYS	3.1
1	B	146	LYS	3.1
1	A	357	LYS	3.1
1	B	149	ALA	3.1
1	A	296	LYS	3.0
1	A	116	ASN	3.0
1	A	89	SER	3.0
1	A	135	ASP	3.0
1	B	143	SER	3.0
1	A	162	THR	3.0
1	B	344	ALA	3.0
1	B	299	SER	3.0
1	A	397	LYS	2.9
1	B	33	LEU	2.9
1	B	318	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	35	SER	2.9
1	A	146	LYS	2.9
1	B	25	VAL	2.9
1	A	326	ILE	2.9
1	A	141	GLU	2.9
1	A	394	GLU	2.9
1	B	124	GLU	2.9
1	A	137	LYS	2.9
1	B	256	LYS	2.9
1	B	301	ASN	2.9
1	B	47	ALA	2.8
1	B	297	ASP	2.8
1	A	28	GLY	2.8
1	A	110	LEU	2.8
1	B	357	LYS	2.8
1	A	148	THR	2.8
1	A	112	ALA	2.7
1	A	478	ARG	2.7
1	B	36	ALA	2.7
1	A	48	VAL	2.7
1	B	49	VAL	2.7
1	A	259	SER	2.7
1	A	185	GLU	2.7
1	A	292	VAL	2.7
1	A	300	LEU	2.7
1	B	162	THR	2.7
1	B	116	ASN	2.7
1	B	348	LYS	2.7
1	B	129	HIS	2.7
1	A	393	ILE	2.7
1	A	45	ARG	2.6
1	B	113	ILE	2.6
1	B	388	ILE	2.6
1	B	120	LYS	2.6
1	A	392	GLY	2.6
1	B	271	GLY	2.6
1	A	54	LEU	2.6
1	B	52	HIS	2.6
1	B	135	ASP	2.6
1	B	298	LEU	2.6
1	A	147	TYR	2.6
1	A	276	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	276	MET	2.6
1	A	19	ALA	2.6
1	B	117	ASN	2.6
1	B	37	ARG	2.6
1	B	185	GLU	2.6
1	A	129	HIS	2.5
1	A	134	SER	2.5
1	B	153	LEU	2.5
1	A	111	ASN	2.5
1	B	122	HIS	2.5
1	A	295	THR	2.5
1	A	125	ILE	2.5
1	B	154	ILE	2.4
1	B	259	SER	2.4
1	A	21	TYR	2.4
1	B	59	VAL	2.4
1	A	93	LYS	2.4
1	A	304	GLY	2.4
1	B	327	TYR	2.4
1	B	392	GLY	2.3
1	A	26	ILE	2.3
1	B	145	LYS	2.3
1	A	24	LEU	2.3
1	A	115	GLN	2.3
1	A	356	TYR	2.3
1	B	309	ASP	2.3
1	B	278	MET	2.3
1	A	305	ILE	2.2
1	A	122	HIS	2.2
1	A	133	THR	2.2
1	B	34	ALA	2.2
1	B	26	ILE	2.2
1	A	301	ASN	2.2
1	A	323	VAL	2.2
1	A	396	VAL	2.2
1	A	325	GLY	2.2
1	B	31	GLY	2.2
1	A	46	ALA	2.1
1	B	89	SER	2.1
1	B	167	GLN	2.1
1	A	310	LYS	2.1
1	B	29	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	159	MET	2.1
1	A	152	ILE	2.1
1	A	119	THR	2.0
1	A	202	MET	2.0
1	B	111	ASN	2.0
1	B	345	ALA	2.0
1	A	20	SER	2.0
1	A	402	SER	2.0
1	A	426	LYS	2.0
1	B	389	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
5	GOL	B	801	6/6	0.53	0.25	50,51,52,52	0
5	GOL	B	805	6/6	0.57	0.20	38,42,43,45	0
5	GOL	A	810	6/6	0.67	0.20	37,46,48,49	0
5	GOL	A	809	6/6	0.70	0.18	67,68,68,68	0
5	GOL	A	813	6/6	0.70	0.19	55,57,58,58	0
5	GOL	B	802	6/6	0.73	0.20	67,67,67,68	0
5	GOL	A	817	6/6	0.73	0.19	57,60,60,60	0
3	ELI	A	958	21/21	0.77	0.17	31,38,46,49	0
5	GOL	B	812	6/6	0.77	0.23	55,58,58,58	0
3	ELI	B	958	21/21	0.78	0.17	33,40,43,45	0
5	GOL	A	808	6/6	0.78	0.14	40,42,44,48	0
5	GOL	B	811	6/6	0.81	0.15	62,63,63,63	0
5	GOL	B	806	6/6	0.87	0.12	27,39,41,43	0

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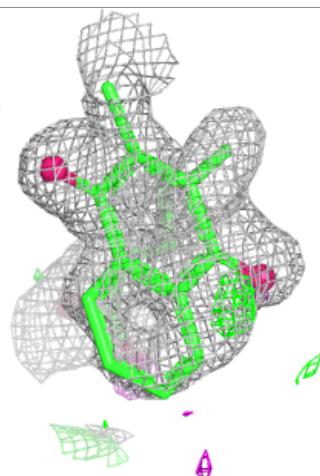
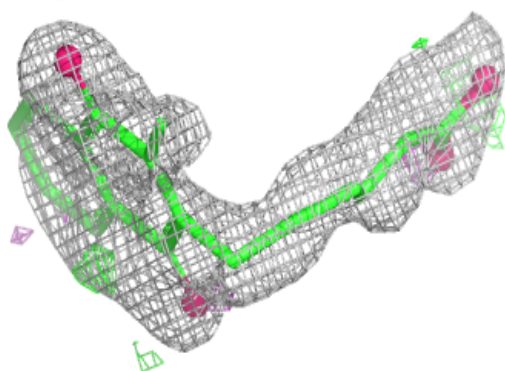
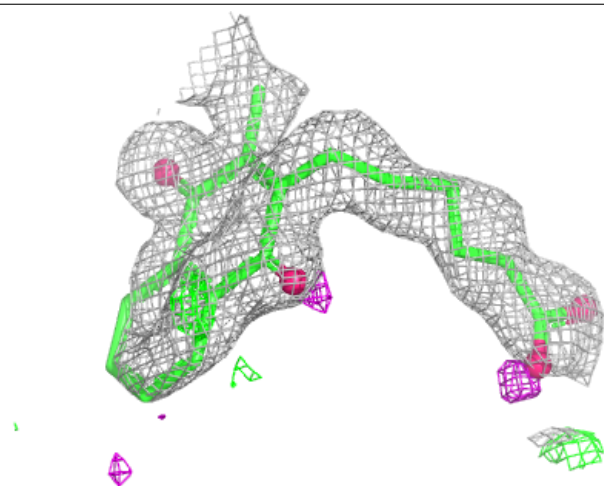
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GOL	B	803	6/6	0.88	0.12	28,38,40,44	0
2	PO4	B	5705	5/5	0.91	0.12	33,33,36,37	0
4	FAD	A	479	53/53	0.94	0.09	13,18,32,34	0
4	FAD	B	479	53/53	0.94	0.09	15,20,38,39	0
2	PO4	A	5703	5/5	0.95	0.08	34,36,36,37	0
2	PO4	B	5704	5/5	0.96	0.07	27,27,28,28	0
2	PO4	A	5706	5/5	0.96	0.09	29,33,34,34	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.

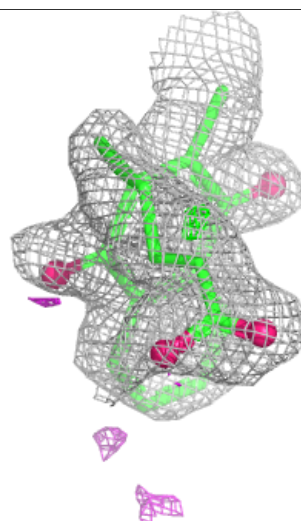
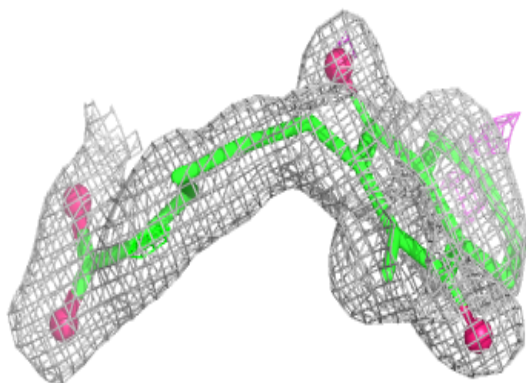
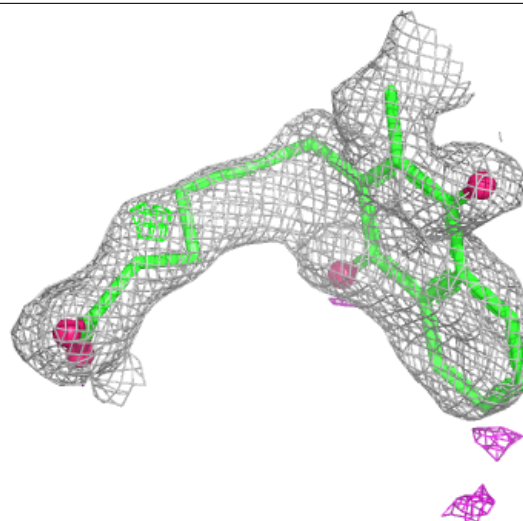
Electron density around ELI A 958:

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



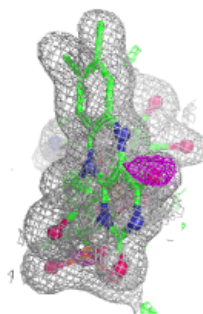
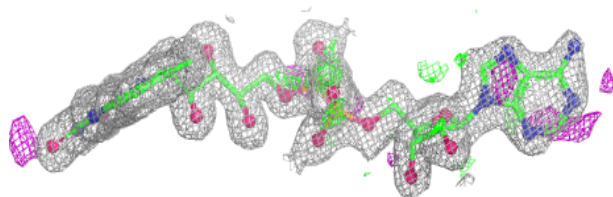
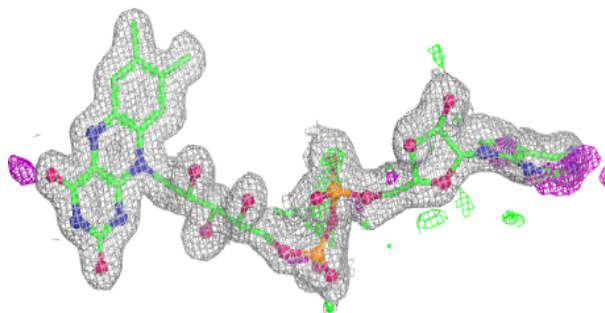
Electron density around ELI B 958:

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

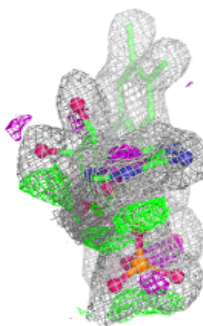
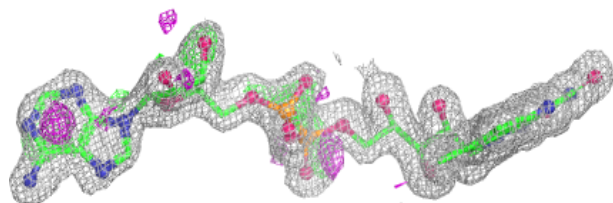
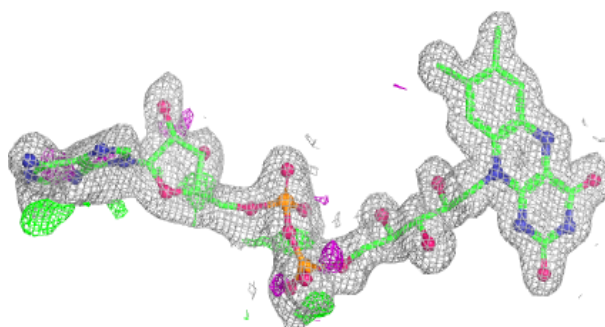


Electron density around FAD A 479:

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

**Electron density around FAD B 479:**

$2mF_o-DF_c$ (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.