WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 11:43 PM EDT

PDB ID	:	3BPF
Title	:	Crystal Structure of Falcipain-2 with Its inhibitor, E64
Authors	:	kerr, I.D.; Lee, J.H.; Brinen, L.S.
Deposited on	:	2007-12-18
Resolution	:	2.90 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:

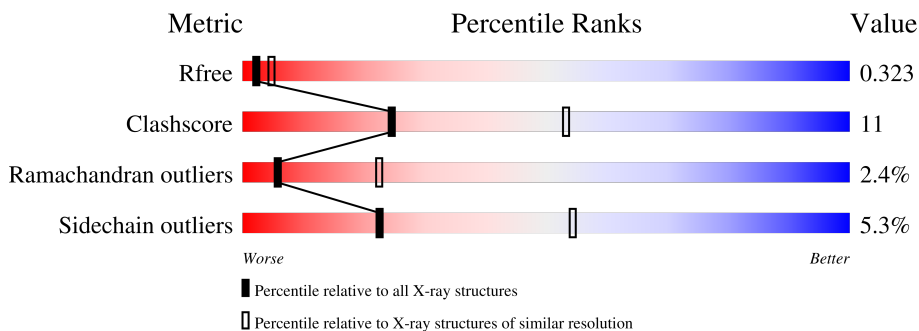|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.90 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	Percentile Ranks	Value
Rfree		0.323
Clashscore		11
Ramachandran outliers		2.4%
Sidechain outliers		5.3%

Worse *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 <=5%

Mol	Chain	Length	Quality of chain
1	A	241	67% 25% 6% •
1	B	241	77% 21% •
1	C	241	77% 20% • •
1	D	241	67% 21% • 11%

2　Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 7453 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.
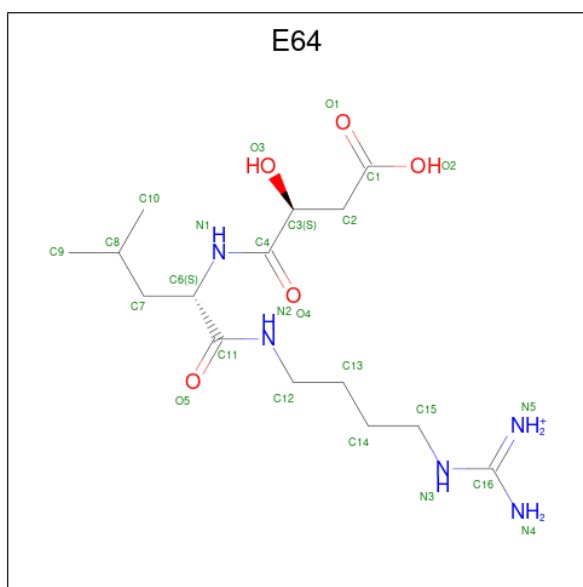
- Molecule 1 is a protein called Cysteine protease falcipain-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	0	0	0
			1868	1183	308	363	14			
1	B	240	Total	C	N	O	S	0	0	0
			1898	1205	314	365	14			
1	C	234	Total	C	N	O	S	0	0	0
			1847	1174	303	356	14			
1	D	215	Total	C	N	O	S	0	0	0
			1692	1076	275	328	13			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	GLN	GLU	SEE REMARK 999	UNP Q9NBD4
B	171	GLN	GLU	SEE REMARK 999	UNP Q9NBD4
C	171	GLN	GLU	SEE REMARK 999	UNP Q9NBD4
D	171	GLN	GLU	SEE REMARK 999	UNP Q9NBD4

- Molecule 2 is N-[N-[1-HYDROXYCARBOXYETHYL-CARBONYL]LEUCYLAMINO-BU TYL]-GUANIDINE (three-letter code: E64) (formula: $C_{15}H_{30}N_5O_5$).

E64

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 25	C 15	N 5	O 5	0	0
2	B	1	Total 25	C 15	N 5	O 5	0	0
2	C	1	Total 25	C 15	N 5	O 5	0	0
2	D	1	Total 25	C 15	N 5	O 5	0	0

• Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

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

- Molecule 4 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	10	Total 10	O 10	0	0
4	B	13	Total 13	O 13	0	0
4	C	15	Total 15	O 15	0	0
4	D	4	Total 4	O 4	0	0

3 Residue-property plots ⓘ

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. 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. 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.
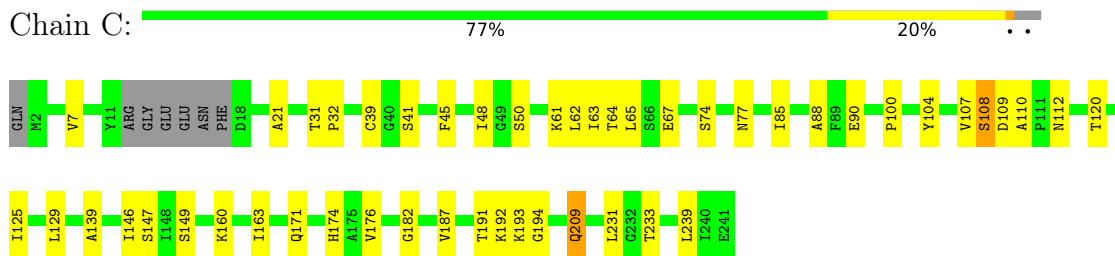
• Molecule 1: Cysteine protease falcipain-2
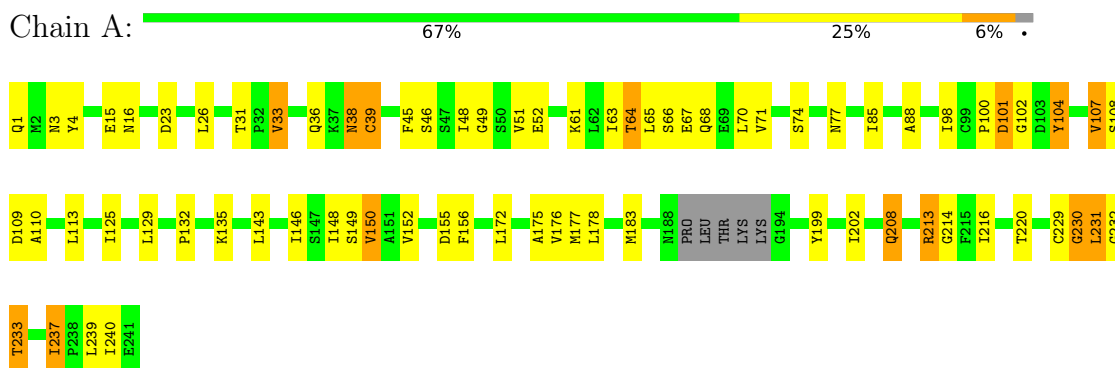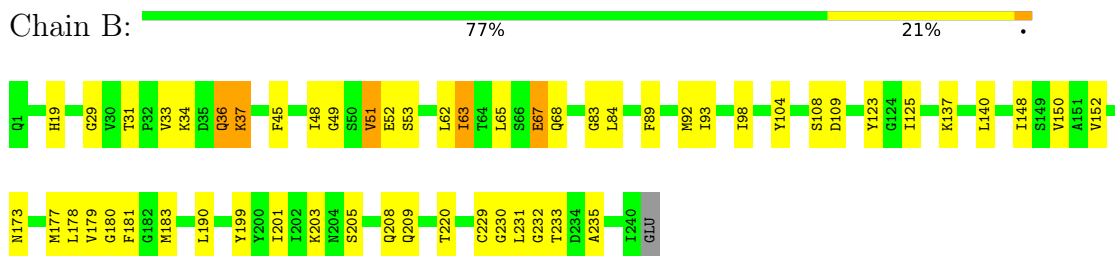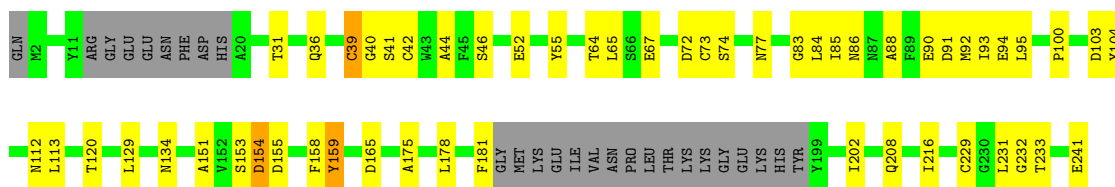
Chain A:

• Molecule 1: Cysteine protease falcipain-2

Chain B:

• Molecule 1: Cysteine protease falcipain-2

Chain C:

• Molecule 1: Cysteine protease falcipain-2

Chain D:

GLN M2 Y11 ARG GLY GLU GLU ASN PHE ASP HIS A20 T31 Q36 C39 G40 S41 C42 W43 A44 F45 S46 E52 Y55 T64 L65 S66 E67 D72 C73 S74 N77 G83 L84 I85 N86 N87 A88 F89 E90 D91 M92 I93 E94 L95 P100 D103 Y104

N112 L113 T120 L129 N134 A151 V152 S153 D154 D155 F158 Y159 D165 A175 L178 F181 GLY MET LYS GLU ILE VAL ASN PRO LEU THR LYS LYS GLY GLU LYS HIS TYR Y199 I202 Q208 I216 C229 G230 L231 G232 T233 E241

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	143.78Å 167.81Å 177.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.67 – 2.90 66.65 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.9 (66.67-2.90) 99.9 (66.65-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$< I/\sigma(I) >$ [1]	1.32 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.275 , 0.325 0.275 , 0.323	Depositor DCC
R_{free} test set	2677 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	69.8	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 108.3	EDS
L-test for twinning[2]	$< |L| > = 0.44, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	7453	wwPDB-VP
Average B, all atoms (Å^2)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, E64

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	0.46	0/1909	0.58	0/2572
1	B	0.37	0/1941	0.51	0/2618
1	C	0.39	0/1888	0.50	0/2545
1	D	0.40	0/1728	0.51	0/2330
All	All	0.41	0/7466	0.53	0/10065

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	36	GLN	Peptide

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.

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1868	0	1774	56	0
1	B	1898	0	1820	32	0
1	C	1847	0	1773	29	0
1	D	1692	0	1613	22	0
2	A	25	0	28	1	0
2	B	25	0	28	0	0
2	C	25	0	28	1	0
2	D	25	0	28	1	0
3	C	6	0	8	0	0
4	A	10	0	0	0	0
4	B	13	0	0	0	0
4	C	15	0	0	0	0
4	D	4	0	0	0	0
All	All	7453	0	7100	137	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 11.

All (137) 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:67:GLU:O	1:A:71:VAL:HG23	1.63	0.97
1:C:129:LEU:HD23	1:C:239:LEU:HD11	1.41	0.97
1:A:129:LEU:HD22	1:A:239:LEU:HD11	1.61	0.82
1:C:174:HIS:CD2	1:C:176:VAL:HG13	2.21	0.76
1:D:83:GLY:O	1:D:84:LEU:HD23	1.87	0.75
1:A:129:LEU:CD2	1:A:237:ILE:HG23	2.21	0.70
1:C:7:VAL:HG21	1:C:129:LEU:HD22	1.75	0.68
1:A:129:LEU:HD21	1:A:237:ILE:HG23	1.75	0.68
1:C:108:SER:OG	1:C:109:ASP:N	2.21	0.68
1:B:63:ILE:HG21	1:B:123:TYR:CE1	2.29	0.68
1:C:21:ALA:HB2	1:C:182:GLY:HA2	1.77	0.67
1:B:48:ILE:HD12	1:B:49:GLY:N	2.11	0.66
1:A:23:ASP:HB3	1:A:26:LEU:HD12	1.77	0.65
1:B:199:TYR:HA	1:B:220:THR:HG22	1.78	0.65
1:A:178:LEU:HD23	1:A:202:ILE:HD13	1.79	0.64
1:A:113:LEU:HD21	1:C:31:THR:HA	1.79	0.64
1:D:72:ASP:OD2	1:D:112:ASN:ND2	2.31	0.63
1:B:33:VAL:HG13	1:B:208:GLN:HG2	1.80	0.63
1:A:178:LEU:HD23	1:A:202:ILE:CD1	2.28	0.62
1:A:143:LEU:HB3	1:A:237:ILE:HD13	1.80	0.62
1:C:107:VAL:HG12	1:C:110:ALA:HB3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:LYS:NZ	1:C:63:ILE:HD11	2.14	0.62
1:A:107:VAL:O	1:A:107:VAL:HG23	2.01	0.61
1:A:48:ILE:HD11	1:A:98:ILE:HD13	1.83	0.61
1:C:21:ALA:CB	1:C:182:GLY:HA2	2.31	0.59
1:C:174:HIS:HD2	1:C:176:VAL:HG13	1.68	0.58
1:B:33:VAL:CG1	1:B:208:GLN:HG2	2.34	0.58
1:D:151:ALA:HB3	1:D:229:CYS:HB3	1.86	0.58
1:A:199:TYR:HA	1:A:220:THR:HG22	1.85	0.58
1:A:33:VAL:HG11	1:A:214:GLY:HA3	1.86	0.57
1:B:177:MET:HE3	1:B:203:LYS:HD3	1.85	0.57
1:B:148:ILE:HD11	1:B:178:LEU:HD13	1.85	0.57
1:A:31:THR:HG22	1:D:113:LEU:HD21	1.86	0.56
1:B:29:GLY:O	1:B:53:SER:OG	2.16	0.56
1:A:150:VAL:HG23	1:A:229:CYS:O	2.06	0.55
1:A:202:ILE:HB	1:A:216:ILE:HG23	1.88	0.54
1:D:39:CYS:O	1:D:41:SER:N	2.40	0.54
1:B:150:VAL:HG23	1:B:229:CYS:HB2	1.91	0.53
1:B:33:VAL:HG22	1:B:34:LYS:O	2.08	0.53
1:D:85:ILE:O	1:D:88:ALA:HB3	2.09	0.53
1:A:107:VAL:HG23	1:A:110:ALA:HB3	1.91	0.53
1:B:108:SER:OG	1:B:109:ASP:N	2.35	0.52
1:D:86:ASN:N	1:D:86:ASN:OD1	2.40	0.52
1:A:108:SER:OG	1:A:109:ASP:N	2.41	0.52
1:D:52:GLU:OE2	1:D:64:THR:HA	2.09	0.52
1:A:70:LEU:HD12	1:A:74:SER:HB2	1.92	0.52
1:A:149:SER:HB2	1:A:172:LEU:HD22	1.92	0.52
1:A:208:GLN:HB3	1:A:213:ARG:HG2	1.90	0.52
1:A:4:TYR:HA	1:A:129:LEU:HD12	1.92	0.51
1:A:101:ASP:OD1	1:A:102:GLY:N	2.44	0.51
1:B:36:GLN:HG2	1:B:205:SER:O	2.10	0.51
1:A:74:SER:OG	1:A:77:ASN:ND2	2.41	0.51
1:C:39:CYS:SG	1:C:41:SER:OG	2.69	0.51
1:D:44:ALA:HB1	1:D:67:GLU:HB2	1.93	0.51
1:A:199:TYR:CA	1:A:220:THR:HG22	2.40	0.51
1:B:19:HIS:O	1:B:137:LYS:NZ	2.38	0.50
1:A:46:SER:CB	1:A:175:ALA:HB1	2.42	0.50
1:A:33:VAL:HG22	1:A:208:GLN:HG2	1.94	0.50
1:B:140:LEU:HD11	1:B:179:VAL:C	2.32	0.50
1:D:88:ALA:O	1:D:92:MET:HG3	2.12	0.50
1:C:74:SER:OG	1:C:77:ASN:ND2	2.39	0.49
1:A:176:VAL:CG2	1:A:202:ILE:HD12	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:ALA:CB	1:C:146:ILE:HD11	2.42	0.49
1:C:107:VAL:CG1	1:C:110:ALA:HB3	2.42	0.49
1:A:156:PHE:CZ	1:A:216:ILE:HD13	2.47	0.49
1:D:93:ILE:HG22	1:D:94:GLU:N	2.26	0.49
1:C:50:SER:HB2	1:C:147:SER:OG	2.12	0.49
1:B:181:PHE:HA	1:B:201:ILE:HD12	1.94	0.49
1:A:150:VAL:HG23	1:A:229:CYS:HB2	1.94	0.48
1:B:48:ILE:HA	1:B:92:MET:HE1	1.95	0.48
1:C:45:PHE:CE2	1:C:67:GLU:HG3	2.49	0.48
1:C:191:THR:O	1:C:193:LYS:N	2.47	0.48
1:A:85:ILE:O	1:A:88:ALA:HB3	2.13	0.47
1:A:176:VAL:HG21	1:A:202:ILE:HD12	1.96	0.47
1:B:148:ILE:HG22	1:B:235:ALA:HA	1.95	0.47
1:A:129:LEU:HD23	1:A:237:ILE:HG23	1.96	0.47
1:A:172:LEU:HD11	1:A:233:THR:OG1	2.14	0.47
1:D:91:ASP:O	1:D:95:LEU:HD12	2.15	0.46
1:C:31:THR:HB	1:C:32:PRO:HD2	1.97	0.46
1:D:36:GLN:NE2	2:D:242:E64:O2	2.48	0.46
1:D:158:PHE:O	1:D:159:TYR:C	2.53	0.46
1:D:178:LEU:HA	1:D:202:ILE:HG22	1.98	0.46
1:A:23:ASP:CB	1:A:26:LEU:HD12	2.46	0.45
1:A:49:GLY:HA3	1:A:177:MET:SD	2.56	0.45
1:A:132:PRO:HG2	1:A:135:LYS:HB2	1.98	0.45
1:B:177:MET:HE3	1:B:203:LYS:CD	2.46	0.45
1:C:48:ILE:HD12	1:C:67:GLU:HA	1.98	0.45
1:A:152:VAL:HG22	1:A:156:PHE:CD2	2.51	0.45
1:D:46:SER:CB	1:D:175:ALA:HB1	2.47	0.45
1:B:83:GLY:O	1:B:84:LEU:HD23	2.17	0.45
1:D:65:LEU:HA	1:D:100:PRO:HA	1.99	0.45
1:A:68:GLN:O	1:A:71:VAL:N	2.50	0.44
1:B:148:ILE:HG22	1:B:235:ALA:CB	2.47	0.44
1:A:15:GLU:HB3	1:A:16:ASN:C	2.37	0.44
1:B:51:VAL:CG2	1:B:65:LEU:HD12	2.47	0.44
1:B:152:VAL:HG22	1:B:173:ASN:OD1	2.17	0.44
1:A:229:CYS:O	1:A:231:LEU:N	2.51	0.44
1:A:230:GLY:O	1:A:231:LEU:C	2.55	0.44
1:A:66:SER:HB2	1:A:104:TYR:HB3	1.99	0.44
1:A:125:ILE:HA	1:A:240:ILE:HG22	2.00	0.43
1:A:38:ASN:O	1:A:39:CYS:HB2	2.18	0.43
1:A:36:GLN:NE2	2:A:242:E64:O2	2.51	0.43
1:D:153:SER:O	1:D:155:ASP:N	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:LEU:HD21	1:B:180:GLY:N	2.34	0.43
1:A:52:GLU:OE2	1:A:64:THR:HG22	2.20	0.42
1:C:187:VAL:HA	1:C:194:GLY:HA2	2.02	0.42
1:B:45:PHE:CE1	1:B:67:GLU:HG3	2.54	0.42
1:D:42:CYS:HB2	1:D:175:ALA:HB3	2.01	0.42
1:B:209:GLN:OE1	1:B:209:GLN:N	2.52	0.42
1:B:65:LEU:HD22	1:B:98:ILE:O	2.19	0.42
1:B:181:PHE:CA	1:B:201:ILE:HD12	2.50	0.42
1:C:209:GLN:CD	1:C:209:GLN:H	2.21	0.42
1:D:232:GLY:O	1:D:233:THR:C	2.59	0.41
1:B:89:PHE:O	1:B:93:ILE:HD12	2.20	0.41
1:C:61:LYS:HZ2	1:C:63:ILE:HD11	1.84	0.41
1:C:62:LEU:O	1:C:63:ILE:HD13	2.21	0.41
1:D:74:SER:OG	1:D:77:ASN:ND2	2.53	0.41
1:A:52:GLU:HG2	1:A:63:ILE:O	2.20	0.41
1:D:73:CYS:HB3	1:D:95:LEU:HD21	2.01	0.41
1:C:65:LEU:HA	1:C:100:PRO:HA	2.02	0.41
1:A:45:PHE:CZ	1:A:67:GLU:HG3	2.55	0.41
1:C:85:ILE:O	1:C:88:ALA:HB3	2.21	0.41
1:C:139:ALA:HB3	1:C:146:ILE:HD11	2.02	0.41
1:C:139:ALA:HB1	1:C:146:ILE:HD11	2.03	0.41
1:C:149:SER:OG	2:C:242:E64:H103	2.21	0.41
1:B:230:GLY:O	1:B:232:GLY:N	2.53	0.40
1:C:62:LEU:C	1:C:62:LEU:HD23	2.41	0.40
1:A:146:ILE:O	1:A:148:ILE:HG23	2.21	0.40
1:A:38:ASN:OD1	1:A:38:ASN:C	2.59	0.40
1:A:52:GLU:OE2	1:A:64:THR:HA	2.20	0.40
1:A:100:PRO:O	1:A:102:GLY:N	2.55	0.40
1:A:230:GLY:O	1:A:232:GLY:N	2.53	0.40
1:B:31:THR:HG21	1:B:52:GLU:HB3	2.02	0.40
1:B:36:GLN:HG3	1:B:37:LYS:N	2.36	0.40
1:B:93:ILE:HD12	1:B:125:ILE:HD11	2.04	0.40
1:A:65:LEU:HA	1:A:100:PRO:HA	2.03	0.40
1:A:178:LEU:HD23	1:A:202:ILE:HD11	2.00	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	232/241 (96%)	205 (88%)	20 (9%)	7 (3%)	4	17
1	B	238/241 (99%)	217 (91%)	18 (8%)	3 (1%)	12	37
1	C	230/241 (95%)	198 (86%)	28 (12%)	4 (2%)	9	31
1	D	209/241 (87%)	172 (82%)	29 (14%)	8 (4%)	3	13
All	All	909/964 (94%)	792 (87%)	95 (10%)	22 (2%)	6	22

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	CYS
1	C	163	ILE
1	C	192	LYS
1	D	154	ASP
1	A	101	ASP
1	A	213	ARG
1	A	230	GLY
1	B	231	LEU
1	C	231	LEU
1	D	40	GLY
1	D	208	GLN
1	D	231	LEU
1	A	61	LYS
1	A	231	LEU
1	B	37	LYS
1	B	190	LEU
1	C	160	LYS
1	D	39	CYS
1	D	159	TYR
1	D	165	ASP
1	D	134	ASN
1	A	150	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	201/206 (98%)	188 (94%)	13 (6%)	17	45
1	B	205/206 (100%)	197 (96%)	8 (4%)	32	66
1	C	200/206 (97%)	190 (95%)	10 (5%)	24	57
1	D	183/206 (89%)	172 (94%)	11 (6%)	19	49
All	All	789/824 (96%)	747 (95%)	42 (5%)	22	54

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	3	ASN
1	A	33	VAL
1	A	38	ASN
1	A	51	VAL
1	A	64	THR
1	A	104	TYR
1	A	107	VAL
1	A	155	ASP
1	A	183	MET
1	A	208	GLN
1	A	233	THR
1	A	237	ILE
1	B	51	VAL
1	B	62	LEU
1	B	63	ILE
1	B	67	GLU
1	B	68	GLN
1	B	104	TYR
1	B	183	MET
1	B	233	THR
1	C	64	THR
1	C	90	GLU
1	C	104	TYR

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Mol	Chain	Res	Type
1	C	108	SER
1	C	112	ASN
1	C	120	THR
1	C	125	ILE
1	C	171	GLN
1	C	209	GLN
1	C	233	THR
1	D	31	THR
1	D	55	TYR
1	D	90	GLU
1	D	103	ASP
1	D	104	TYR
1	D	120	THR
1	D	129	LEU
1	D	154	ASP
1	D	181	PHE
1	D	216	ILE
1	D	241	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	68	GLN
1	C	38	ASN
1	D	112	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	E64	C	242	1	24,24,24	0.70	0	27,30,30	0.82	1 (3%)
2	E64	D	242	1	24,24,24	0.70	0	27,30,30	0.75	0
2	E64	B	242	1	24,24,24	0.64	0	27,30,30	0.78	0
3	GOL	C	243	-	5,5,5	0.37	0	5,5,5	0.22	0
2	E64	A	242	1	24,24,24	0.61	0	27,30,30	0.82	0

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	E64	C	242	1	-	16/29/29/29	-
2	E64	D	242	1	-	8/29/29/29	-
2	E64	B	242	1	-	8/29/29/29	-
3	GOL	C	243	-	-	1/4/4/4	-
2	E64	A	242	1	-	9/29/29/29	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	242	E64	O1-C1-C2	-2.00	116.38	122.80

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	242	E64	O3-C3-C4-N1

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Mol	Chain	Res	Type	Atoms
2	B	242	E64	O3-C3-C4-N1
2	C	242	E64	O3-C3-C4-N1
2	D	242	E64	C2-C3-C4-O4
2	D	242	E64	C2-C3-C4-N1
2	A	242	E64	N1-C6-C7-C8
2	A	242	E64	C11-C6-C7-C8
2	B	242	E64	C13-C14-C15-N3
2	A	242	E64	N2-C12-C13-C14
2	D	242	E64	N1-C6-C7-C8
2	C	242	E64	N2-C12-C13-C14
2	D	242	E64	C11-C6-C7-C8
2	C	242	E64	C6-C7-C8-C9
2	C	242	E64	C6-C7-C8-C10
2	D	242	E64	C13-C14-C15-N3
2	A	242	E64	O3-C3-C4-O4
2	C	242	E64	O3-C3-C4-O4
2	B	242	E64	C12-C13-C14-C15
2	C	242	E64	C12-C13-C14-C15
2	A	242	E64	C12-C13-C14-C15
2	C	242	E64	C1-C2-C3-O3
2	B	242	E64	C11-C6-C7-C8
2	B	242	E64	O3-C3-C4-O4
3	C	243	GOL	O1-C1-C2-O2
2	D	242	E64	O3-C3-C4-N1
2	C	242	E64	O5-C11-C6-C7
2	B	242	E64	N1-C6-C7-C8
2	C	242	E64	C1-C2-C3-C4
2	D	242	E64	N2-C12-C13-C14
2	A	242	E64	C2-C3-C4-N1
2	C	242	E64	C13-C14-C15-N3
2	C	242	E64	N2-C11-C6-C7
2	D	242	E64	O3-C3-C4-O4
2	C	242	E64	O5-C11-C6-N1
2	A	242	E64	O2-C1-C2-C3
2	C	242	E64	N2-C11-C6-N1
2	C	242	E64	C14-C15-N3-C16
2	A	242	E64	C2-C3-C4-O4
2	B	242	E64	C2-C3-C4-O4
2	C	242	E64	C2-C3-C4-O4
2	B	242	E64	C2-C3-C4-N1
2	C	242	E64	C2-C3-C4-N1

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	242	E64	1	0
2	D	242	E64	1	0
2	A	242	E64	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 then 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 E64 C 242

Bond lengths

Bond angles

Torsions

Rings

Ligand E64 D 242

Bond lengths

Bond angles

Torsions

Rings

Ligand E64 B 242

Bond lengths

Bond angles

Torsions

Rings

Ligand E64 A 242

Bond lengths

Bond angles

Torsions

Rings
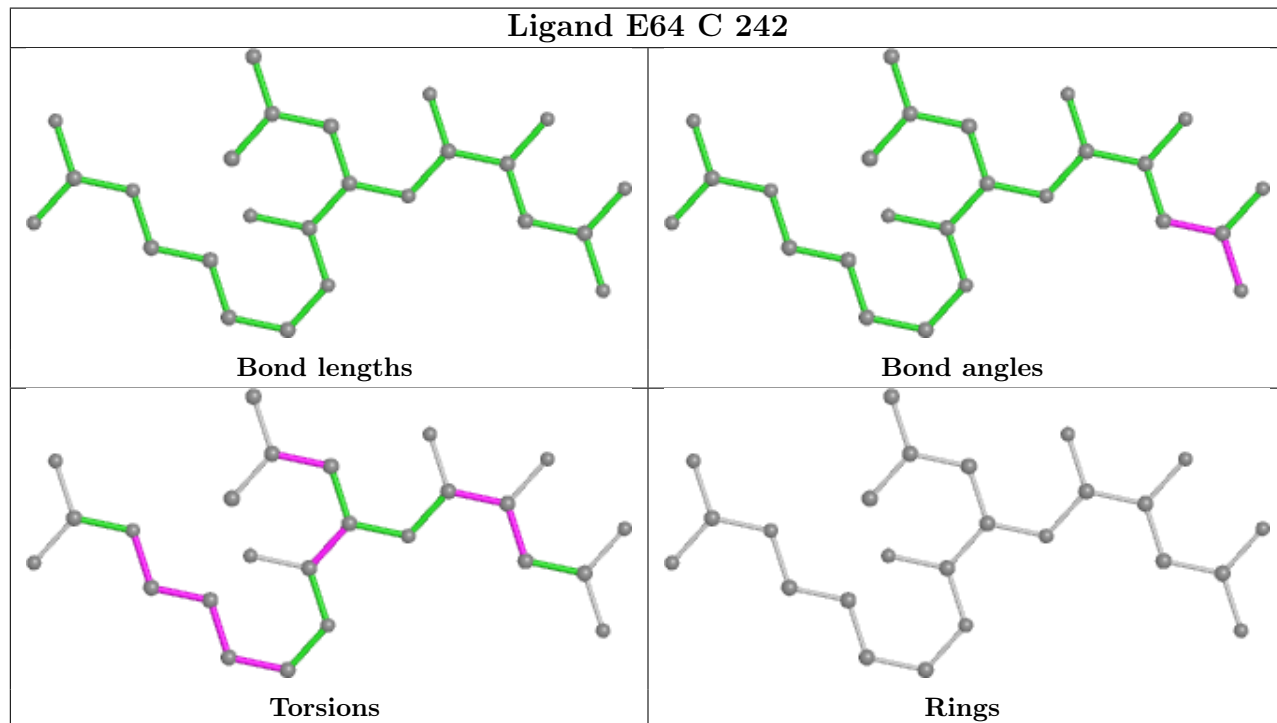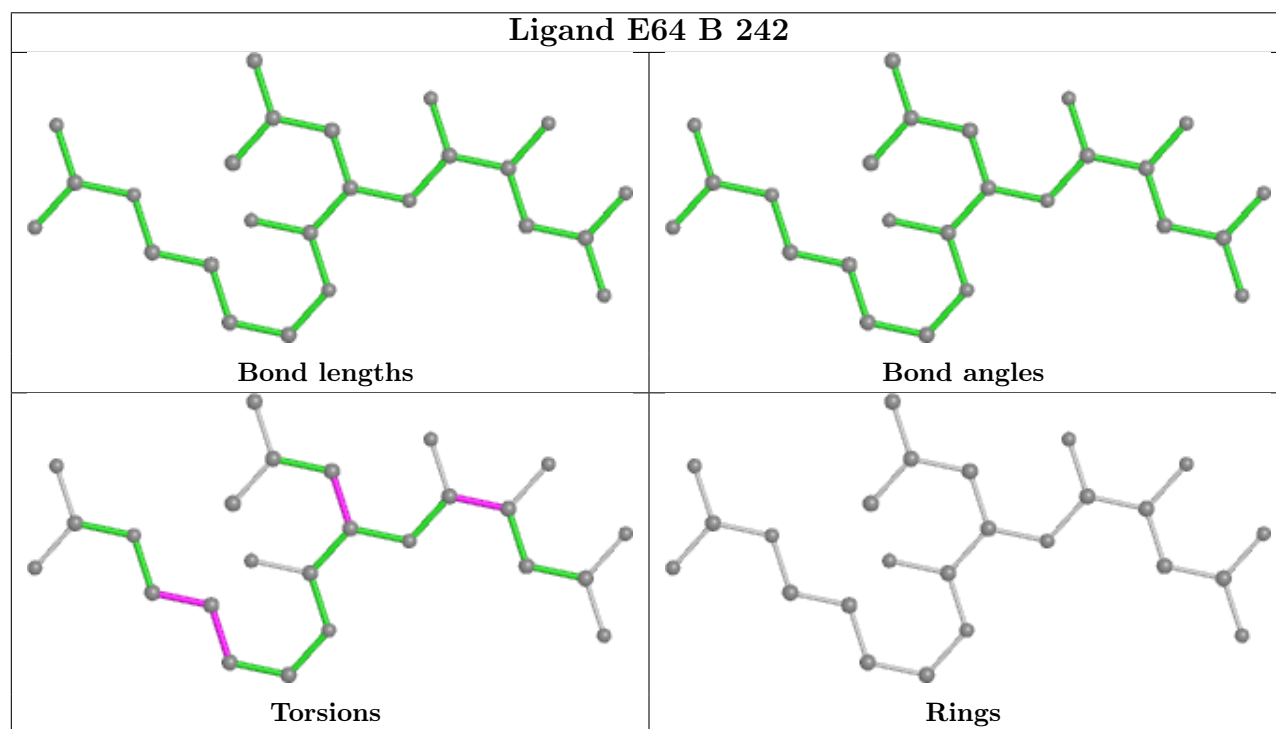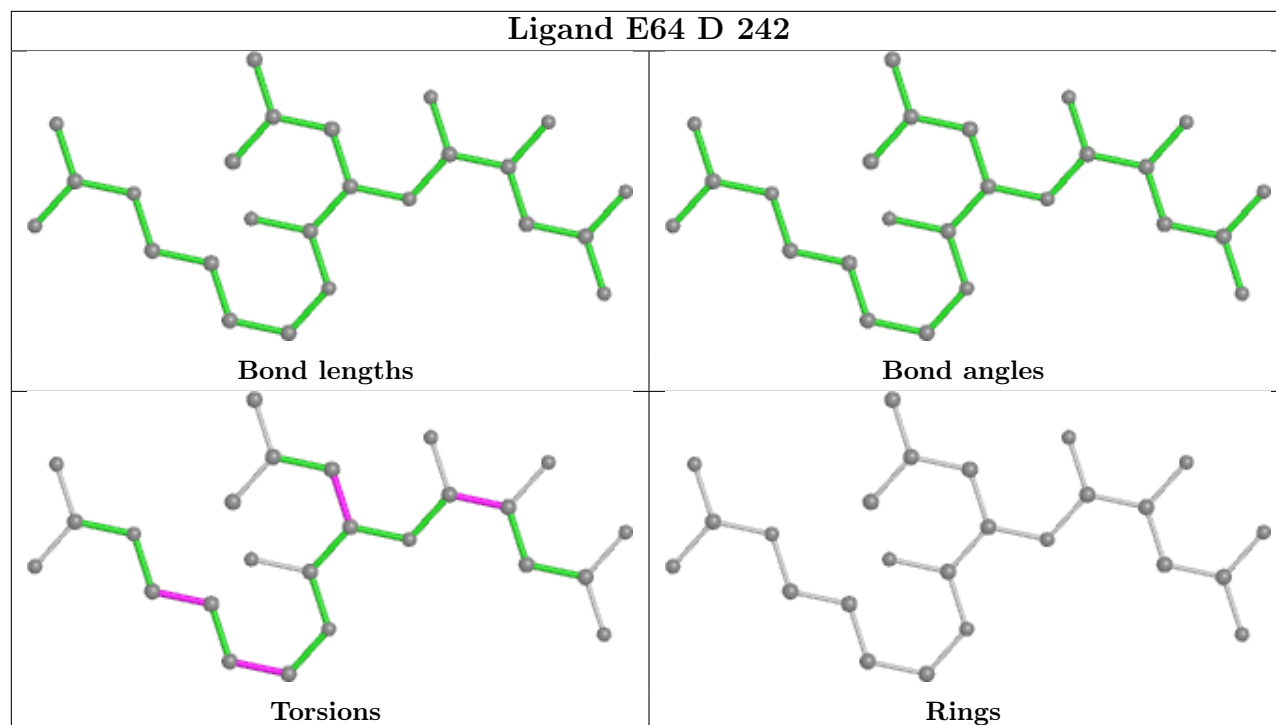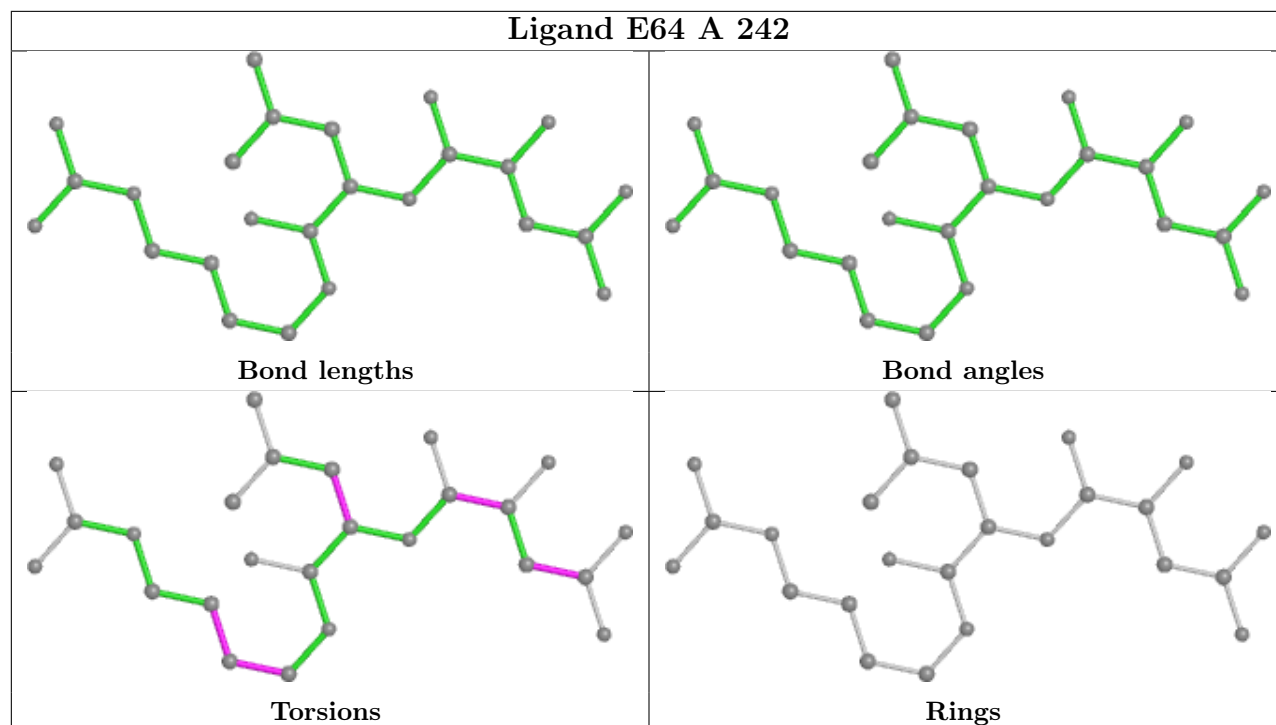
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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 E64 A 242:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
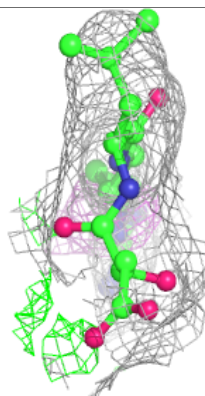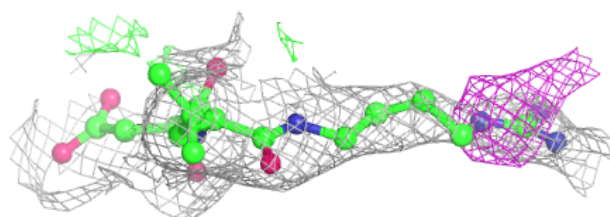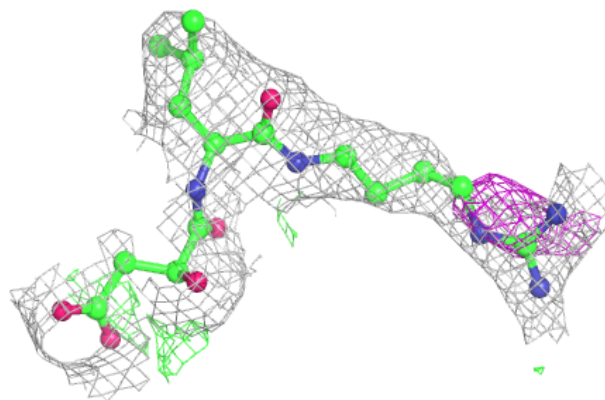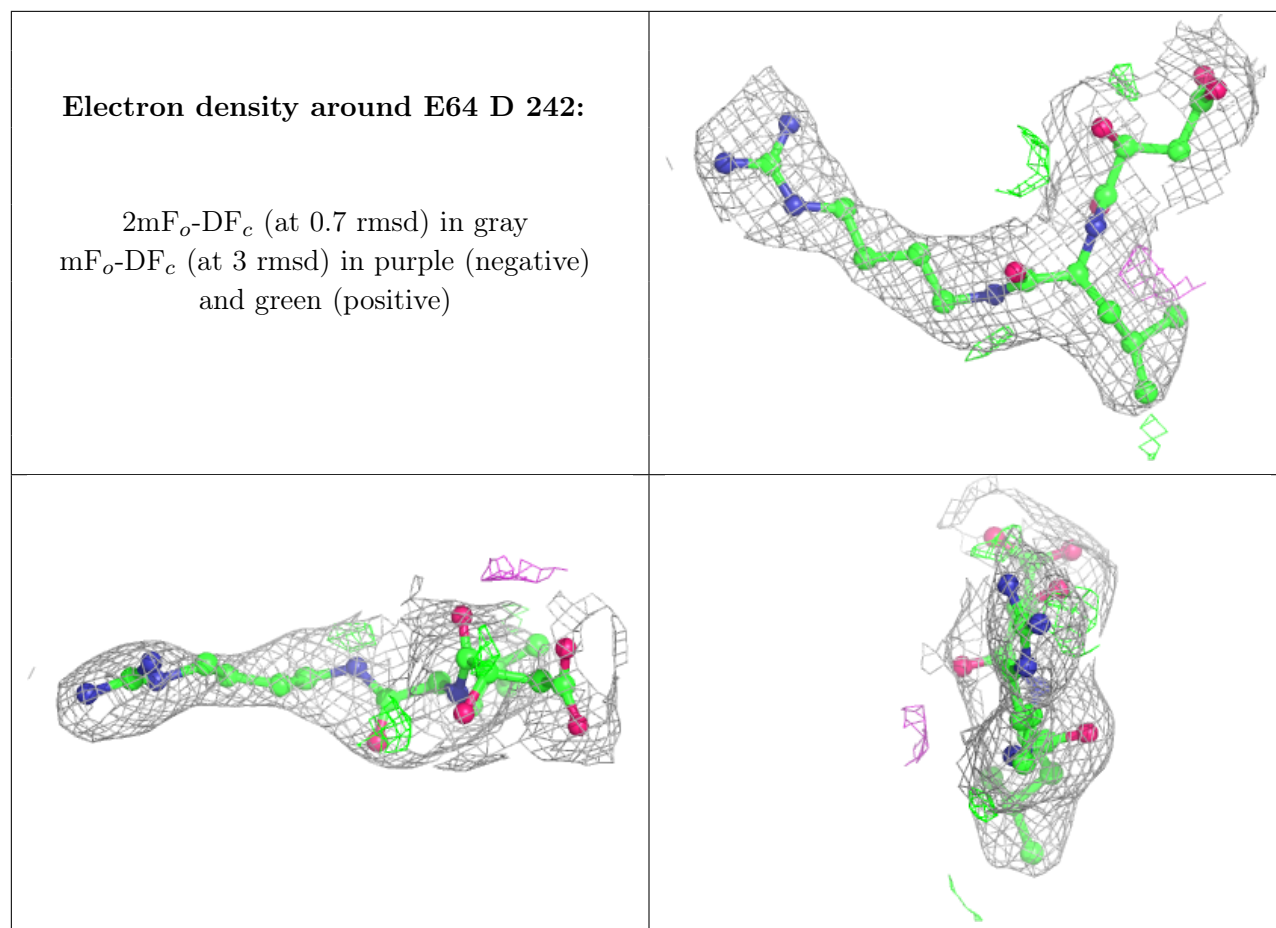and green (positive)
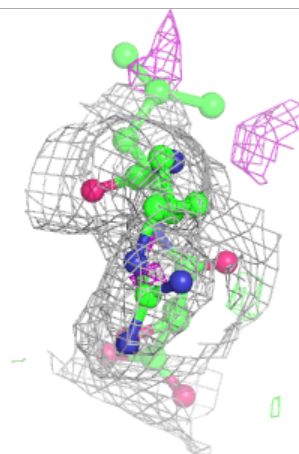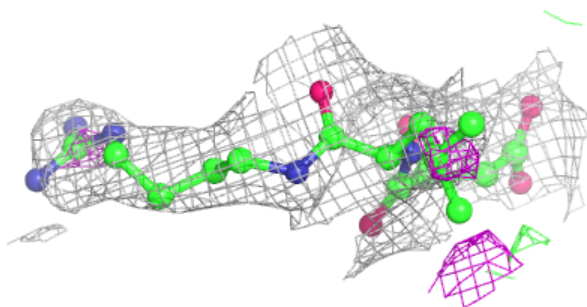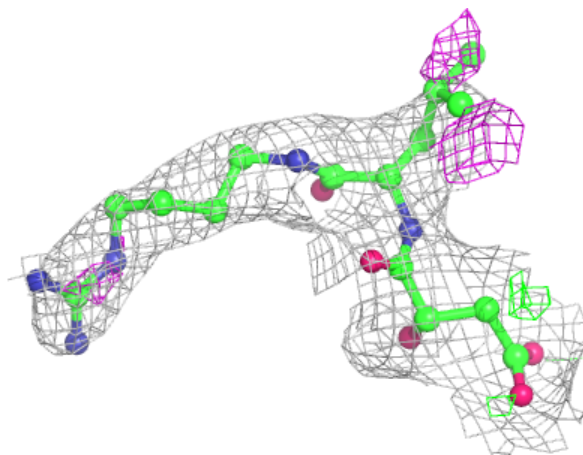
Electron density around E64 B 242:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
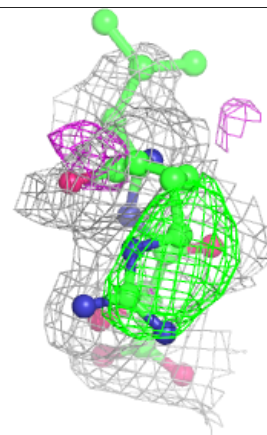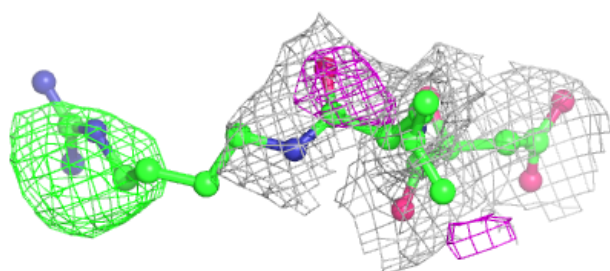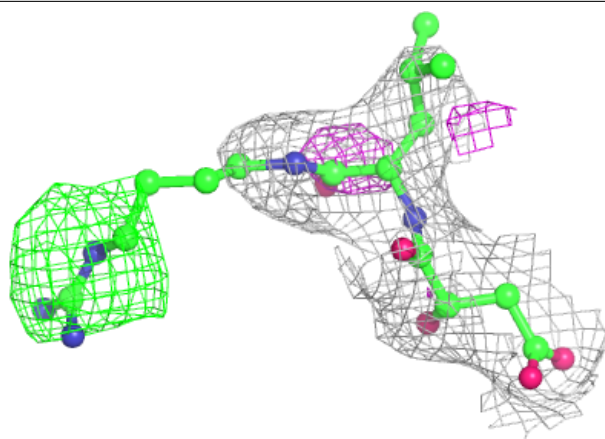
Electron density around E64 C 242:

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

Electron density around E64 D 242:

$2mF_o$-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)

Unable to reproduce the depositors R factor - this section is therefore empty.