WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Sep 19, 2023 – 11:23 AM EDT

PDB ID	:	5FDO
Title	:	Mcl-1 complexed with small molecule inhibitor
Authors	:	Zhao, B.
Deposited on	:	2015-12-16
Resolution	:	2.80 Å(reported)

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	:	2.35.1
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

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 2.80 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.
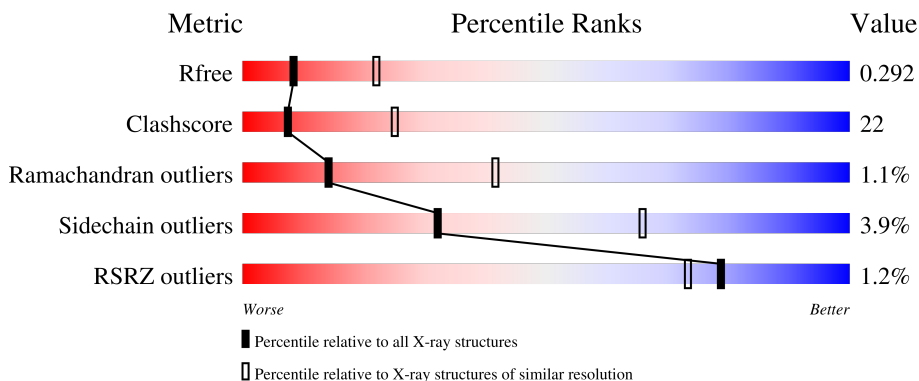
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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% 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	150	
1	B	150	
1	C	150	
1	D	150	

2   Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 4727 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 Induced myeloid leukemia cell differentiation protein Mcl-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	142	Total	C	N	O	S	0	0	0
			1145	721	211	210	3			
1	B	150	Total	C	N	O	S	0	0	0
			1187	744	218	221	4			
1	C	143	Total	C	N	O	S	0	0	0
			1146	721	211	211	3			
1	D	137	Total	C	N	O	S	0	0	0
			1113	702	205	203	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	171	GLY	-	expression tag	UNP Q07820
B	171	GLY	-	expression tag	UNP Q07820
C	171	GLY	-	expression tag	UNP Q07820
D	171	GLY	-	expression tag	UNP Q07820

- Molecule 2 is 3-[3-(4-chloranyl-3,5-dimethyl-phenoxy)propyl]- {N}-(phenylsulfonyl)-1 {H}-indole-2-carboxamide (three-letter code: 5X2) (formula: $C_{26}H_{25}ClN_2O_4S$).

5X2
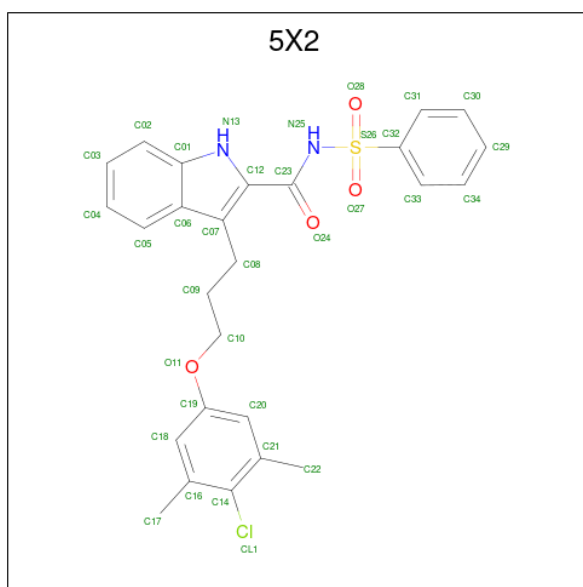
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	S	0	0
			34	26	1	2	4	1		
2	B	1	Total	C	Cl	N	O	S	0	0
			34	26	1	2	4	1		
2	C	1	Total	C	Cl	N	O	S	0	0
			34	26	1	2	4	1		
2	D	1	Total	C	Cl	N	O	S	0	0
			34	26	1	2	4	1		

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 secon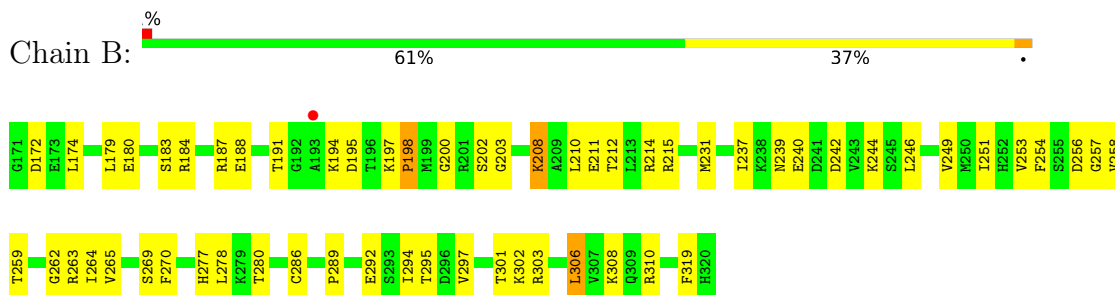d graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates 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: Induced myeloid leukemia cell differentiation protein Mcl-1
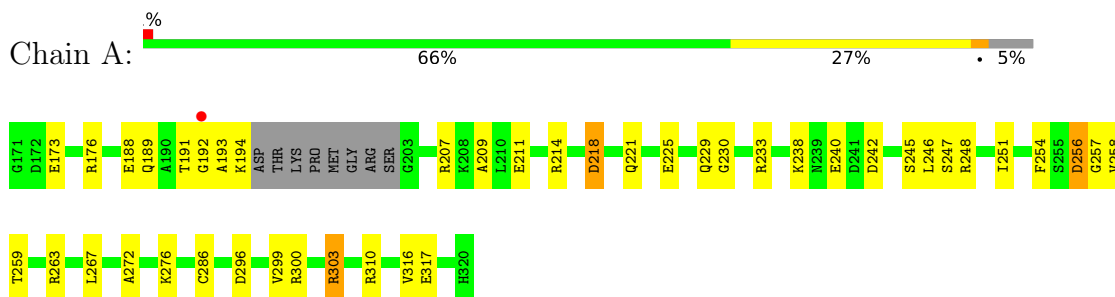
• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

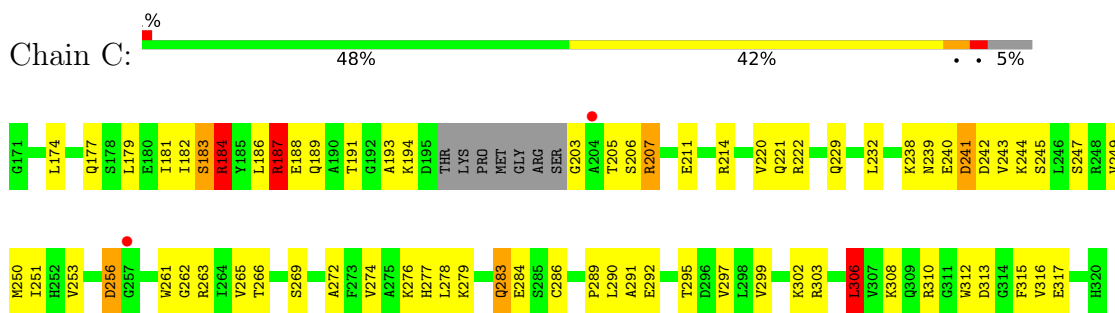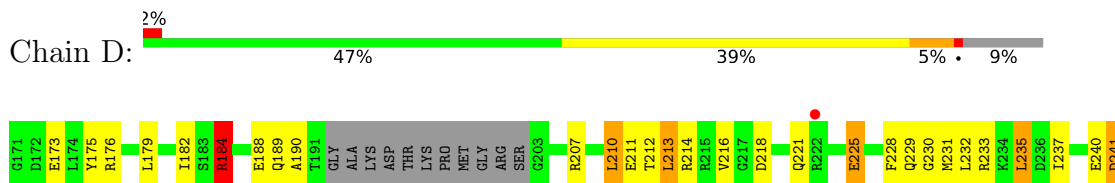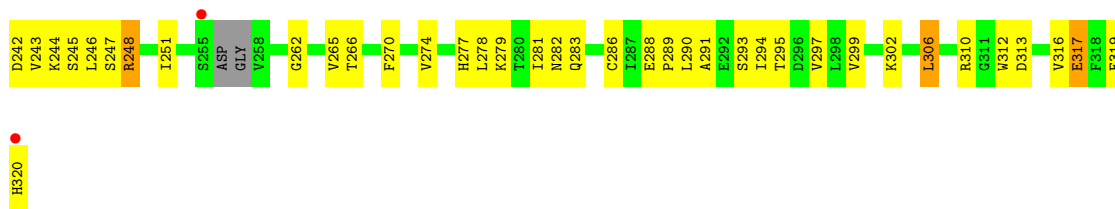

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

• Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1

D242 V243 K244 S245 L246 S247 R248 I251 S255 ASP GLY V258 G262 V265 T266 F270 V274 H277 L278 K279 T280 I281 N282 Q283 C286 I287 E288 P289 L290 A291 E292 S293 I294 T295 D296 V297 L298 V299 K302 L306 R310 G311 W312 D313 V316 E317 F318 F319

H320

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 63 2 2	Depositor
Cell constants a, b, c, α, β, γ	149.87Å　149.87Å　121.38Å 90.00°　　90.00°　　120.00°	Depositor
Resolution (Å)	29.78　–　2.80 44.33　–　2.60	Depositor EDS
% Data completeness (in resolution range)	95.6 (29.78-2.80) 85.1 (44.33-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.43 (at 2.61Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.213　,　0.291 0.217　,　0.292	Depositor DCC
R_{free} test set	1105 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å^2)	48.1	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 47.7	EDS
L-test for twinning[2]	$< |L| > = 0.43, < L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4727	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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 ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: 5X2

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	0.61	0/1163	0.84	0/1562
1	B	0.57	0/1206	0.81	3/1623 (0.2%)
1	C	0.69	3/1164 (0.3%)	0.87	4/1565 (0.3%)
1	D	0.51	0/1130	0.97	9/1517 (0.6%)
All	All	0.60	3/4663 (0.1%)	0.87	16/6267 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	279	LYS	CD-CE	-6.71	1.34	1.51
1	C	187	ARG	NE-CZ	-5.90	1.25	1.33
1	C	187	ARG	CZ-NH1	-5.76	1.25	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	210	LEU	CA-CB-CG	8.74	135.40	115.30
1	D	317	GLU	CA-CB-CG	7.05	128.92	113.40
1	B	198	PRO	N-CA-CB	6.53	111.14	103.30
1	B	306	LEU	CA-CB-CG	6.14	129.43	115.30
1	C	306	LEU	CA-CB-CG	5.78	128.60	115.30
1	D	235	LEU	CA-CB-CG	5.71	128.43	115.30
1	D	213	LEU	CA-CB-CG	5.63	128.25	115.30
1	D	306	LEU	CA-CB-CG	5.61	128.19	115.30
1	D	184	ARG	NE-CZ-NH1	-5.52	117.54	120.30
1	D	317	GLU	CB-CA-C	-5.50	99.41	110.40
1	C	187	ARG	CA-CB-CG	5.34	125.14	113.40
1	D	225	GLU	CB-CA-C	-5.32	99.76	110.40
1	C	184	ARG	CG-CD-NE	5.31	122.94	111.80
1	B	208	LYS	CA-CB-CG	5.26	124.98	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	306	LEU	CB-CG-CD1	-5.07	102.38	111.00
1	D	184	ARG	CG-CD-NE	5.06	122.42	111.80

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	1145	0	1152	33	1
1	B	1187	0	1170	41	1
1	C	1146	0	1143	71	1
1	D	1113	0	1116	62	0
2	A	34	0	0	3	0
2	B	34	0	0	3	0
2	C	34	0	0	0	0
2	D	34	0	0	1	0
All	All	4727	0	4581	207	2

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 22.

All (207) 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:C:184:ARG:HA	1:C:187:ARG:NH1	1.57	1.20
1:C:205:THR:HG21	1:C:313:ASP:OD1	1.52	1.09
1:C:184:ARG:HG3	1:C:187:ARG:HH12	1.26	0.99
1:C:184:ARG:HA	1:C:187:ARG:HH12	1.33	0.92
1:A:193:ALA:HB1	1:A:194:LYS:HB2	1.52	0.92
1:B:301:THR:HG23	1:B:302:LYS:HG2	1.49	0.91
1:B:263:ARG:NH2	2:B:400:5X2:O28	2.12	0.82
1:D:190:ALA:O	1:D:279:LYS:NZ	2.13	0.81
1:C:184:ARG:HA	1:C:187:ARG:HH11	1.43	0.81
1:D:237:ILE:HD11	1:D:242:ASP:HB3	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:ARG:NH2	1:C:317:GLU:OE1	2.13	0.80
1:C:240:GLU:HG3	1:C:286:CYS:SG	2.21	0.79
1:C:203:GLY:O	1:C:207:ARG:NH2	2.14	0.78
1:A:310:ARG:NH2	1:A:317:GLU:OE2	2.17	0.78
1:C:184:ARG:HG3	1:C:187:ARG:NH1	2.01	0.76
1:C:184:ARG:CG	1:C:187:ARG:HH12	2.00	0.75
1:D:241:ASP:HA	1:D:244:LYS:HG2	1.68	0.74
1:D:175:TYR:HD2	1:D:299:VAL:HG21	1.52	0.74
1:D:231:MET:O	1:D:235:LEU:HD22	1.88	0.74
1:D:274:VAL:O	1:D:278:LEU:HD12	1.88	0.73
1:C:205:THR:HG21	1:C:313:ASP:CG	2.10	0.71
1:C:188:GLU:OE2	1:C:214:ARG:NH1	2.24	0.71
1:D:182:ILE:HD12	1:D:295:THR:HG22	1.72	0.71
1:A:296:ASP:O	1:A:300:ARG:HG2	1.91	0.70
1:D:225:GLU:HA	1:D:228:PHE:HB2	1.73	0.69
1:A:173:GLU:OE1	1:A:176:ARG:NH1	2.24	0.69
1:A:263:ARG:NH2	2:A:400:5X2:O28	2.26	0.69
1:C:262:GLY:O	1:C:266:THR:HG23	1.93	0.69
1:D:211:GLU:O	1:D:214:ARG:HB2	1.94	0.68
1:D:237:ILE:CD1	1:D:242:ASP:HB3	2.22	0.68
1:D:229:GLN:O	1:D:233:ARG:HG3	1.94	0.67
1:D:310:ARG:HH21	1:D:317:GLU:HG3	1.61	0.66
1:C:184:ARG:CA	1:C:187:ARG:HH12	2.08	0.66
1:A:188:GLU:CD	1:A:214:ARG:HH21	1.99	0.66
1:B:200:GLY:O	1:B:203:GLY:HA2	1.98	0.63
1:A:225:GLU:O	1:A:229:GLN:HG2	1.99	0.62
1:C:182:ILE:HD12	1:C:295:THR:HG22	1.81	0.62
1:C:205:THR:CG2	1:C:313:ASP:OD1	2.39	0.62
1:D:232:LEU:HD11	1:D:277:HIS:CD2	2.34	0.62
1:A:191:THR:O	1:A:193:ALA:N	2.29	0.61
1:A:256:ASP:HB2	1:A:263:ARG:HH12	1.65	0.61
1:D:179:LEU:HA	1:D:295:THR:HG21	1.82	0.61
1:A:221:GLN:HE22	1:A:276:LYS:HE2	1.66	0.60
1:C:232:LEU:HD21	1:C:277:HIS:CG	2.36	0.60
1:D:212:THR:O	1:D:216:VAL:HG12	2.02	0.60
1:D:290:LEU:O	1:D:294:ILE:HG13	2.01	0.60
1:D:242:ASP:O	1:D:245:SER:OG	2.12	0.60
1:B:277:HIS:O	1:B:280:THR:OG1	2.20	0.60
1:D:173:GLU:OE2	1:D:176:ARG:NH2	2.35	0.59
1:A:254:PHE:O	1:A:263:ARG:HD3	2.03	0.59
1:C:299:VAL:CG1	1:C:303:ARG:HH11	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:ASP:OD2	1:B:303:ARG:NH2	2.36	0.59
1:B:231:MET:HG3	2:B:400:5X2:C03	2.32	0.59
1:B:265:VAL:O	1:B:269:SER:OG	2.16	0.59
1:D:283:GLN:HB3	1:D:286:CYS:SG	2.42	0.58
1:C:188:GLU:HG3	1:C:193:ALA:HB3	1.85	0.58
1:B:251:ILE:HG12	1:B:297:VAL:HG23	1.85	0.58
1:C:306:LEU:HD12	1:C:306:LEU:H	1.69	0.57
1:B:208:LYS:HA	1:B:211:GLU:HB2	1.86	0.57
1:B:297:VAL:O	1:B:301:THR:HG22	2.05	0.57
1:B:237:ILE:HD11	1:B:246:LEU:HD21	1.86	0.57
1:B:257:GLY:HA3	1:B:258:VAL:C	2.25	0.57
1:C:179:LEU:HA	1:C:295:THR:HG21	1.86	0.57
1:C:177:GLN:O	1:C:181:ILE:HG13	2.05	0.56
1:B:215:ARG:NH2	1:B:319:PHE:O	2.34	0.56
1:C:289:PRO:HA	1:C:292:GLU:HG2	1.87	0.56
1:D:313:ASP:O	1:D:316:VAL:HG22	2.05	0.56
1:D:221:GLN:HA	1:D:228:PHE:HE2	1.71	0.56
1:A:230:GLY:HA2	1:A:233:ARG:NH2	2.21	0.56
1:C:256:ASP:HB2	1:C:263:ARG:HH12	1.71	0.56
1:C:241:ASP:N	1:C:241:ASP:OD1	2.39	0.55
1:C:256:ASP:HB2	1:C:263:ARG:HH22	1.71	0.55
1:B:278:LEU:HD13	1:B:286:CYS:HB2	1.89	0.55
1:B:254:PHE:HZ	1:B:264:ILE:HD13	1.71	0.55
1:B:240:GLU:O	1:B:244:LYS:HG3	2.07	0.55
1:D:312:TRP:O	1:D:316:VAL:HG13	2.07	0.55
1:B:180:GLU:O	1:B:184:ARG:HG3	2.07	0.55
1:B:208:LYS:O	1:B:212:THR:HG22	2.06	0.54
1:C:262:GLY:O	1:C:265:VAL:HG12	2.07	0.54
1:D:302:LYS:O	1:D:306:LEU:HD12	2.07	0.54
1:B:187:ARG:O	1:B:191:THR:HG22	2.08	0.54
1:C:291:ALA:O	1:C:295:THR:HG23	2.07	0.54
1:D:225:GLU:HG2	1:D:229:GLN:HG2	1.90	0.54
1:A:256:ASP:HB2	1:A:263:ARG:NH1	2.23	0.54
1:D:175:TYR:CD2	1:D:299:VAL:HG21	2.39	0.54
1:D:291:ALA:O	1:D:295:THR:HG23	2.08	0.54
1:C:299:VAL:O	1:C:303:ARG:HB2	2.08	0.53
1:D:248:ARG:O	1:D:251:ILE:HG12	2.08	0.53
1:C:247:SER:O	1:C:251:ILE:HG13	2.08	0.53
1:D:282:ASN:O	1:D:282:ASN:ND2	2.41	0.53
1:B:179:LEU:HD23	1:B:183:SER:OG	2.09	0.53
1:C:249:VAL:O	1:C:253:VAL:HG12	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:GLY:O	1:A:259:THR:N	2.43	0.52
1:C:232:LEU:HD21	1:C:277:HIS:CD2	2.45	0.52
1:B:191:THR:HG23	1:B:194:LYS:H	1.75	0.52
1:B:184:ARG:O	1:B:188:GLU:HB2	2.10	0.51
1:C:207:ARG:O	1:C:211:GLU:HG3	2.09	0.51
1:D:243:VAL:HA	1:D:246:LEU:HG	1.91	0.51
1:D:288:GLU:HB2	1:D:289:PRO:HD3	1.92	0.51
1:A:247:SER:O	1:A:251:ILE:HG13	2.11	0.51
1:D:310:ARG:NH2	1:D:317:GLU:HG3	2.23	0.51
1:D:212:THR:CG2	1:D:319:PHE:HB2	2.41	0.50
1:B:179:LEU:HB2	1:B:295:THR:HG21	1.92	0.50
1:D:317:GLU:HA	1:D:320:HIS:NE2	2.26	0.50
1:C:239:ASN:HA	1:C:283:GLN:OE1	2.12	0.50
1:D:189:GLN:OE1	1:D:221:GLN:NE2	2.39	0.50
1:D:241:ASP:OD1	1:D:241:ASP:N	2.44	0.50
1:A:207:ARG:HD3	1:A:211:GLU:OE2	2.11	0.49
1:A:230:GLY:HA2	1:A:233:ARG:HH21	1.75	0.49
1:B:286:CYS:C	1:B:289:PRO:HD2	2.33	0.49
1:C:242:ASP:O	1:C:245:SER:OG	2.24	0.49
1:A:221:GLN:HE22	1:A:276:LYS:CE	2.25	0.49
1:C:211:GLU:HG2	1:C:214:ARG:HH21	1.77	0.49
1:C:220:VAL:HG21	1:C:266:THR:HG22	1.94	0.49
1:B:256:ASP:HB2	1:B:263:ARG:NH1	2.27	0.48
1:A:188:GLU:OE1	1:A:214:ARG:NH2	2.42	0.48
1:B:240:GLU:HG3	1:B:286:CYS:SG	2.54	0.48
1:D:295:THR:O	1:D:299:VAL:HG22	2.14	0.48
1:A:300:ARG:HH11	1:A:303:ARG:HH22	1.60	0.48
1:B:262:GLY:O	1:B:265:VAL:HG12	2.14	0.48
1:C:299:VAL:HG12	1:C:303:ARG:HH11	1.77	0.48
1:B:174:LEU:HD23	1:B:303:ARG:NH1	2.28	0.48
1:C:184:ARG:CA	1:C:187:ARG:NH1	2.50	0.48
1:C:274:VAL:HG23	1:C:290:LEU:HD21	1.94	0.48
1:B:249:VAL:O	1:B:253:VAL:HG23	2.14	0.48
1:D:188:GLU:CD	1:D:214:ARG:HH21	2.17	0.48
1:D:188:GLU:OE1	1:D:214:ARG:NH2	2.46	0.47
1:D:274:VAL:HG12	1:D:278:LEU:HD11	1.95	0.47
1:D:317:GLU:HA	1:D:320:HIS:CE1	2.49	0.47
1:B:270:PHE:HD1	2:B:400:5X2:C16	2.28	0.47
1:D:247:SER:O	1:D:251:ILE:HG23	2.14	0.47
1:A:238:LYS:HE2	1:A:242:ASP:OD2	2.14	0.47
1:C:182:ILE:HB	1:C:295:THR:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:GLN:HG3	1:C:272:ALA:HB1	1.97	0.47
1:C:240:GLU:O	1:C:244:LYS:HG3	2.14	0.47
1:C:240:GLU:O	1:C:243:VAL:HG22	2.14	0.47
1:C:299:VAL:CG1	1:C:303:ARG:NH1	2.77	0.47
1:D:184:ARG:O	1:D:188:GLU:CB	2.63	0.47
1:A:221:GLN:NE2	1:A:276:LYS:HE2	2.27	0.47
1:D:221:GLN:HA	1:D:228:PHE:CE2	2.51	0.46
1:B:286:CYS:O	1:B:289:PRO:HD2	2.15	0.46
1:D:262:GLY:O	1:D:266:THR:HG23	2.15	0.46
1:C:278:LEU:HD13	1:C:286:CYS:HB2	1.98	0.46
1:D:179:LEU:O	1:D:179:LEU:HD23	2.16	0.46
1:B:256:ASP:HB2	1:B:263:ARG:HH12	1.81	0.45
1:C:306:LEU:HD12	1:C:306:LEU:N	2.31	0.45
1:C:256:ASP:HB2	1:C:263:ARG:NH1	2.31	0.45
1:A:209:ALA:HA	1:A:316:VAL:HG22	1.98	0.45
1:B:188:GLU:HG3	1:B:195:ASP:OD1	2.16	0.45
1:C:188:GLU:OE1	1:C:214:ARG:HD3	2.16	0.45
1:D:188:GLU:OE2	1:D:214:ARG:NH2	2.50	0.45
1:B:183:SER:O	1:B:187:ARG:HG3	2.16	0.45
1:D:278:LEU:HD22	1:D:286:CYS:HB2	1.98	0.45
1:C:188:GLU:O	1:C:191:THR:O	2.34	0.45
1:C:221:GLN:NE2	1:C:276:LYS:HE2	2.32	0.45
1:A:189:GLN:HG3	1:A:272:ALA:HB1	1.99	0.44
1:C:229:GLN:HA	1:C:229:GLN:OE1	2.17	0.44
1:D:207:ARG:O	1:D:210:LEU:HB3	2.16	0.44
1:C:256:ASP:HB2	1:C:263:ARG:NH2	2.31	0.44
1:D:237:ILE:HD12	1:D:237:ILE:HA	1.59	0.44
1:D:302:LYS:HB2	1:D:306:LEU:HD11	1.99	0.44
1:C:188:GLU:CD	1:C:214:ARG:HH11	2.20	0.43
1:A:254:PHE:CE1	1:A:263:ARG:HG2	2.53	0.43
1:B:239:ASN:N	1:B:242:ASP:OD1	2.37	0.43
1:C:265:VAL:O	1:C:269:SER:OG	2.24	0.43
1:C:250:MET:SD	1:C:297:VAL:HG11	2.58	0.43
1:D:262:GLY:O	1:D:265:VAL:HG12	2.18	0.43
1:C:229:GLN:OE1	1:C:232:LEU:HD23	2.19	0.43
1:D:240:GLU:CD	1:D:286:CYS:SG	2.97	0.43
1:C:186:LEU:HD22	1:C:291:ALA:HB2	2.01	0.43
1:C:179:LEU:O	1:C:183:SER:HB3	2.19	0.43
1:D:230:GLY:HA2	1:D:233:ARG:NH2	2.34	0.43
1:B:294:ILE:O	1:B:297:VAL:HG12	2.19	0.43
1:C:302:LYS:O	1:C:306:LEU:HD12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ASP:OD1	1:A:218:ASP:N	2.53	0.42
1:A:173:GLU:CD	1:A:176:ARG:HH11	2.23	0.42
1:A:299:VAL:HG12	1:A:303:ARG:CZ	2.50	0.42
1:B:254:PHE:CE1	1:B:263:ARG:HG2	2.54	0.42
1:C:308:LYS:HB3	1:C:308:LYS:HE3	1.87	0.42
1:B:308:LYS:O	1:B:308:LYS:HG3	2.20	0.42
1:C:312:TRP:O	1:C:316:VAL:HG23	2.20	0.42
1:A:299:VAL:O	1:A:303:ARG:HB2	2.19	0.42
1:A:246:LEU:HD13	2:A:400:5X2:CL1	2.57	0.42
1:C:261:TRP:CE3	1:C:315:PHE:HD1	2.37	0.42
1:D:184:ARG:O	1:D:188:GLU:HB2	2.20	0.41
1:C:189:GLN:NE2	1:C:189:GLN:HA	2.34	0.41
1:D:213:LEU:HA	1:D:216:VAL:CG1	2.50	0.41
1:C:284:GLU:H	1:C:284:GLU:HG3	1.68	0.41
1:D:173:GLU:O	1:D:173:GLU:HG3	2.20	0.41
1:D:281:ILE:HG13	1:D:283:GLN:HG3	2.01	0.41
1:C:256:ASP:CB	1:C:263:ARG:HH22	2.34	0.41
1:B:172:ASP:CG	1:B:303:ARG:HH22	2.22	0.41
1:B:180:GLU:OE2	1:B:184:ARG:HD2	2.21	0.41
1:A:267:LEU:HD12	2:A:400:5X2:C18	2.51	0.41
1:D:279:LYS:HB3	1:D:279:LYS:HE2	1.79	0.41
1:A:193:ALA:HB1	1:A:194:LYS:HE2	2.03	0.41
1:C:283:GLN:HB3	1:C:286:CYS:SG	2.61	0.41
1:D:270:PHE:HD2	2:D:400:5X2:C16	2.34	0.41
1:D:282:ASN:C	1:D:283:GLN:HG2	2.41	0.41
1:A:240:GLU:HB2	1:A:286:CYS:SG	2.61	0.40
1:C:206:SER:HB2	1:C:207:ARG:NH1	2.36	0.40
1:C:302:LYS:CB	1:C:306:LEU:HD11	2.51	0.40
1:B:210:LEU:HD21	1:B:214:ARG:NH2	2.36	0.40
1:C:174:LEU:HB3	1:C:303:ARG:NH2	2.37	0.40
1:C:177:GLN:HG3	1:C:312:TRP:CD1	2.57	0.40
1:D:240:GLU:O	1:D:244:LYS:HG2	2.21	0.40
1:D:293:SER:O	1:D:297:VAL:HG23	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:GLU:OE1	1:C:238:LYS:NZ[2_665]	2.18	0.02
1:A:245:SER:OG	1:A:248:ARG:NH1[7_555]	2.19	0.01

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	138/150 (92%)	125 (91%)	11 (8%)	2 (1%)	11	34
1	B	148/150 (99%)	125 (84%)	20 (14%)	3 (2%)	7	24
1	C	139/150 (93%)	128 (92%)	10 (7%)	1 (1%)	22	53
1	D	131/150 (87%)	120 (92%)	11 (8%)	0	100	100
All	All	556/600 (93%)	498 (90%)	52 (9%)	6 (1%)	14	41

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	197	LYS
1	B	198	PRO
1	A	192	GLY
1	A	258	VAL
1	C	194	LYS
1	B	202	SER

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	123/130 (95%)	120 (98%)	3 (2%)	49	81
1	B	125/130 (96%)	122 (98%)	3 (2%)	49	81
1	C	122/130 (94%)	113 (93%)	9 (7%)	13	37
1	D	120/130 (92%)	116 (97%)	4 (3%)	38	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	490/520 (94%)	471 (96%)	19 (4%)	32	66

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	218	ASP
1	A	256	ASP
1	A	303	ARG
1	B	259	THR
1	B	306	LEU
1	B	310	ARG
1	C	183	SER
1	C	184	ARG
1	C	187	ARG
1	C	207	ARG
1	C	222	ARG
1	C	241	ASP
1	C	256	ASP
1	C	283	GLN
1	C	306	LEU
1	D	184	ARG
1	D	218	ASP
1	D	241	ASP
1	D	248	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	221	GLN
1	C	189	GLN
1	C	221	GLN
1	D	224	HIS

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 ⓘ

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	5X2	C	400	-	35,37,37	5.36	24 (68%)	47,53,53	2.98	11 (23%)
2	5X2	B	400	-	35,37,37	5.17	24 (68%)	47,53,53	2.35	5 (10%)
2	5X2	D	400	-	35,37,37	5.30	24 (68%)	47,53,53	2.46	6 (12%)
2	5X2	A	400	-	35,37,37	4.86	24 (68%)	47,53,53	2.25	7 (14%)

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	5X2	C	400	-	-	9/18/22/22	0/4/4/4
2	5X2	B	400	-	-	6/18/22/22	0/4/4/4
2	5X2	D	400	-	-	6/18/22/22	0/4/4/4
2	5X2	A	400	-	-	0/18/22/22	0/4/4/4

All (96) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	400	5X2	C31-C32	9.72	1.54	1.38
2	C	400	5X2	C18-C16	9.59	1.53	1.39
2	D	400	5X2	C02-C01	9.24	1.57	1.41
2	D	400	5X2	C18-C16	9.24	1.53	1.39
2	D	400	5X2	C33-C32	9.15	1.53	1.38
2	D	400	5X2	C31-C32	9.07	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	5X2	C20-C21	9.06	1.52	1.39
2	C	400	5X2	C02-C01	8.95	1.57	1.41
2	B	400	5X2	C33-C32	8.92	1.52	1.38
2	B	400	5X2	C18-C16	8.89	1.52	1.39
2	C	400	5X2	C33-C32	8.84	1.52	1.38
2	B	400	5X2	C31-C32	8.60	1.52	1.38
2	A	400	5X2	C20-C21	8.59	1.52	1.39
2	D	400	5X2	C20-C21	8.52	1.52	1.39
2	C	400	5X2	C20-C21	8.50	1.52	1.39
2	C	400	5X2	C20-C19	8.37	1.53	1.38
2	D	400	5X2	C18-C19	8.37	1.53	1.38
2	B	400	5X2	C02-C01	8.37	1.56	1.41
2	A	400	5X2	C02-C01	8.21	1.56	1.41
2	A	400	5X2	C33-C32	8.17	1.51	1.38
2	C	400	5X2	C18-C19	8.11	1.53	1.38
2	B	400	5X2	C20-C19	7.98	1.52	1.38
2	A	400	5X2	C31-C32	7.95	1.51	1.38
2	A	400	5X2	C18-C16	7.93	1.51	1.39
2	B	400	5X2	C18-C19	7.86	1.52	1.38
2	D	400	5X2	C20-C19	7.70	1.52	1.38
2	B	400	5X2	C05-C06	7.62	1.57	1.42
2	D	400	5X2	C05-C06	7.59	1.57	1.42
2	C	400	5X2	C05-C06	7.56	1.57	1.42
2	A	400	5X2	C05-C06	7.47	1.57	1.42
2	A	400	5X2	C18-C19	7.40	1.51	1.38
2	C	400	5X2	C30-C31	7.27	1.54	1.38
2	C	400	5X2	C34-C33	7.20	1.54	1.38
2	A	400	5X2	C20-C19	6.98	1.51	1.38
2	D	400	5X2	C30-C31	6.90	1.53	1.38
2	D	400	5X2	C34-C33	6.74	1.53	1.38
2	B	400	5X2	C34-C33	6.61	1.52	1.38
2	B	400	5X2	C30-C31	6.56	1.52	1.38
2	A	400	5X2	C34-C33	6.55	1.52	1.38
2	C	400	5X2	C03-C02	6.38	1.51	1.36
2	D	400	5X2	C04-C05	6.37	1.51	1.36
2	C	400	5X2	C04-C05	6.32	1.51	1.36
2	A	400	5X2	C30-C31	6.27	1.52	1.38
2	C	400	5X2	C34-C29	6.23	1.54	1.38
2	B	400	5X2	C04-C05	6.10	1.50	1.36
2	B	400	5X2	C30-C29	6.04	1.54	1.38
2	D	400	5X2	C03-C02	6.04	1.50	1.36
2	D	400	5X2	C30-C29	5.89	1.53	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	5X2	C34-C29	5.84	1.53	1.38
2	D	400	5X2	C34-C29	5.79	1.53	1.38
2	B	400	5X2	C03-C02	5.78	1.49	1.36
2	C	400	5X2	C30-C29	5.75	1.53	1.38
2	A	400	5X2	C03-C02	5.72	1.49	1.36
2	A	400	5X2	C04-C05	5.71	1.49	1.36
2	A	400	5X2	C34-C29	5.67	1.53	1.38
2	A	400	5X2	C30-C29	5.39	1.52	1.38
2	D	400	5X2	C23-N25	5.21	1.45	1.39
2	B	400	5X2	C14-C16	4.96	1.53	1.40
2	C	400	5X2	C14-C16	4.92	1.53	1.40
2	D	400	5X2	C14-C16	4.85	1.53	1.40
2	B	400	5X2	C14-C21	4.60	1.52	1.40
2	D	400	5X2	C14-C21	4.52	1.52	1.40
2	A	400	5X2	C14-C16	4.46	1.52	1.40
2	C	400	5X2	C23-N25	4.37	1.44	1.39
2	C	400	5X2	C14-C21	4.30	1.51	1.40
2	A	400	5X2	C23-N25	4.29	1.44	1.39
2	B	400	5X2	C23-N25	4.22	1.44	1.39
2	C	400	5X2	C04-C03	4.14	1.49	1.38
2	A	400	5X2	C14-C21	4.11	1.51	1.40
2	B	400	5X2	C04-C03	4.03	1.48	1.38
2	C	400	5X2	C32-S26	3.99	1.82	1.76
2	A	400	5X2	C04-C03	3.89	1.48	1.38
2	D	400	5X2	C32-S26	3.85	1.82	1.76
2	D	400	5X2	C04-C03	3.84	1.48	1.38
2	B	400	5X2	C32-S26	3.56	1.82	1.76
2	D	400	5X2	O28-S26	3.48	1.47	1.43
2	A	400	5X2	O27-S26	3.45	1.47	1.43
2	B	400	5X2	O27-S26	3.33	1.47	1.43
2	B	400	5X2	O28-S26	3.29	1.47	1.43
2	A	400	5X2	O28-S26	3.18	1.47	1.43
2	C	400	5X2	O27-S26	3.03	1.47	1.43
2	C	400	5X2	O28-S26	2.95	1.46	1.43
2	D	400	5X2	S26-N25	2.90	1.70	1.64
2	D	400	5X2	C14-CL1	2.80	1.78	1.72
2	C	400	5X2	C14-CL1	2.59	1.78	1.72
2	D	400	5X2	O27-S26	2.58	1.46	1.43
2	B	400	5X2	C14-CL1	2.57	1.78	1.72
2	A	400	5X2	C14-CL1	2.56	1.78	1.72
2	A	400	5X2	C32-S26	2.41	1.80	1.76
2	A	400	5X2	O24-C23	-2.22	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	400	5X2	S26-N25	2.18	1.69	1.64
2	B	400	5X2	S26-N25	2.13	1.68	1.64
2	C	400	5X2	O24-C23	-2.12	1.19	1.23
2	A	400	5X2	S26-N25	2.08	1.68	1.64
2	B	400	5X2	O24-C23	-2.08	1.19	1.23
2	D	400	5X2	O24-C23	-2.00	1.19	1.23

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	5X2	O28-S26-O27	-13.92	102.44	119.55
2	B	400	5X2	O28-S26-O27	-13.06	103.49	119.55
2	C	400	5X2	O28-S26-O27	-12.93	103.66	119.55
2	A	400	5X2	O28-S26-O27	-11.55	105.35	119.55
2	C	400	5X2	C32-S26-N25	-6.79	95.69	105.97
2	C	400	5X2	O28-S26-C32	6.69	116.21	107.97
2	C	400	5X2	C23-N25-S26	-6.53	114.94	123.36
2	C	400	5X2	O27-S26-C32	6.26	115.68	107.97
2	D	400	5X2	O28-S26-C32	5.57	114.83	107.97
2	B	400	5X2	C32-S26-N25	4.37	112.59	105.97
2	A	400	5X2	O28-S26-C32	4.21	113.16	107.97
2	B	400	5X2	O28-S26-C32	4.14	113.06	107.97
2	A	400	5X2	O24-C23-N25	4.00	125.99	121.08
2	C	400	5X2	C30-C31-C32	3.30	122.38	118.95
2	C	400	5X2	C33-C32-S26	3.11	123.15	119.77
2	B	400	5X2	O24-C23-C12	2.83	124.83	120.59
2	A	400	5X2	O24-C23-C12	2.63	124.52	120.59
2	A	400	5X2	C31-C32-S26	-2.51	117.03	119.77
2	A	400	5X2	O27-S26-C32	2.50	111.04	107.97
2	C	400	5X2	O28-S26-N25	2.38	113.44	106.74
2	D	400	5X2	C12-N13-C01	2.30	108.63	103.90
2	D	400	5X2	C16-C14-CL1	2.20	122.54	118.19
2	B	400	5X2	C08-C09-C10	-2.14	106.13	113.34
2	C	400	5X2	O27-S26-N25	2.08	112.59	106.74
2	D	400	5X2	O24-C23-C12	2.05	123.65	120.59
2	D	400	5X2	O28-S26-N25	2.02	112.41	106.74
2	C	400	5X2	C05-C06-C01	2.01	120.84	118.17
2	C	400	5X2	C05-C06-C07	-2.01	130.70	134.17
2	A	400	5X2	C16-C14-CL1	2.00	122.15	118.19

There are no chirality outliers.
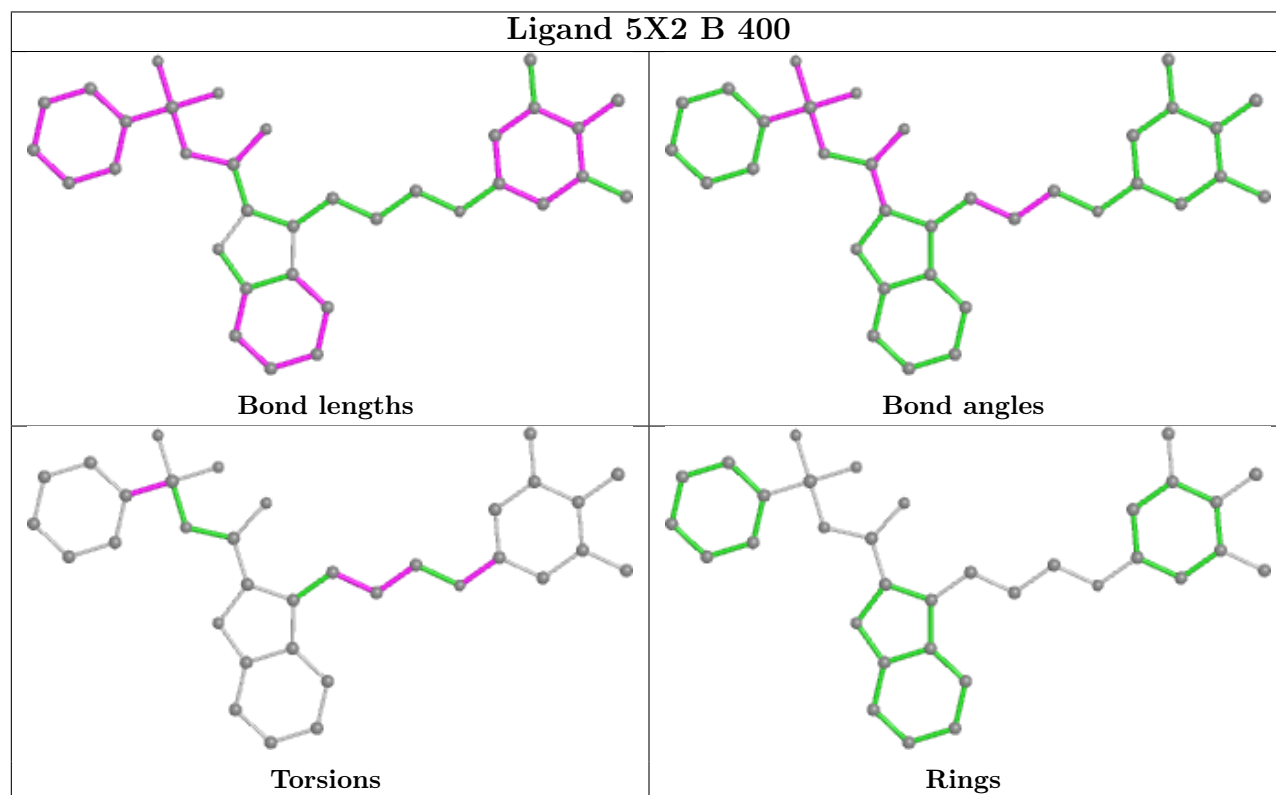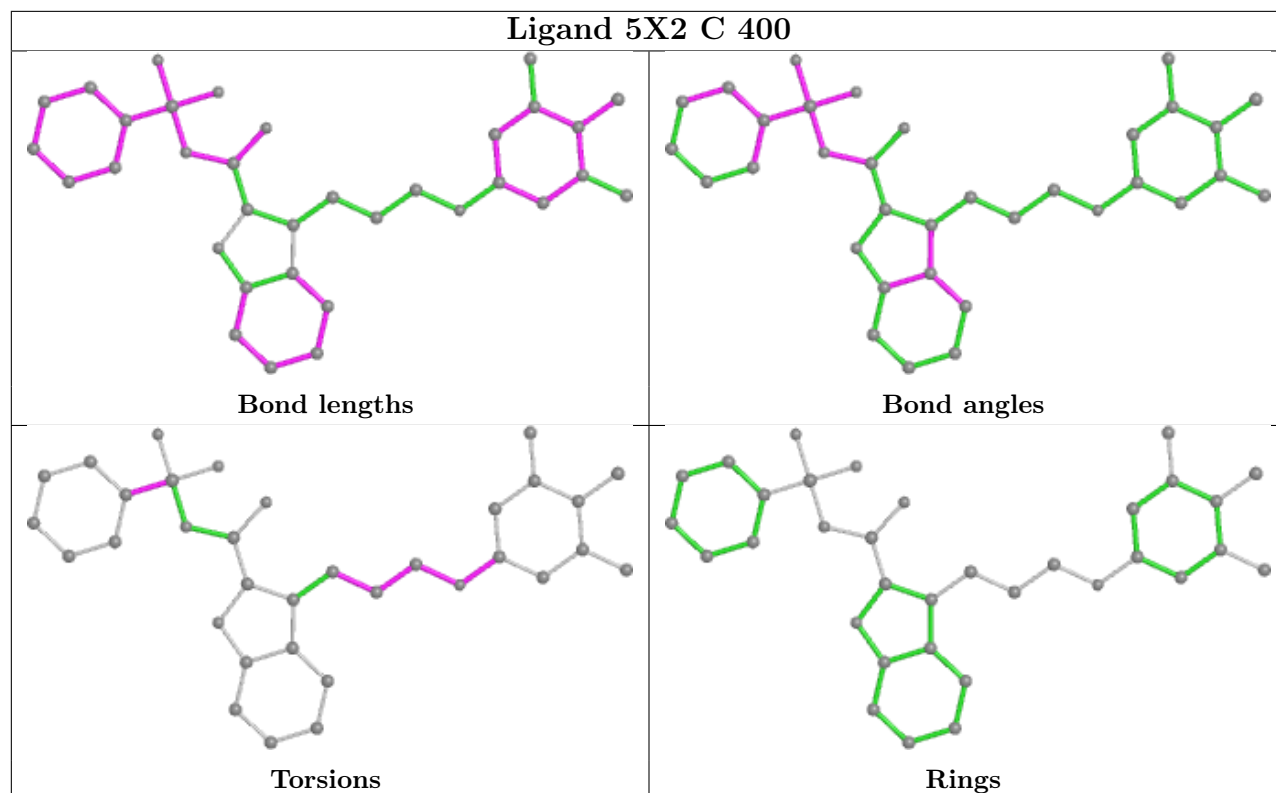
All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	400	5X2	C07-C08-C09-C10
2	D	400	5X2	C07-C08-C09-C10
2	C	400	5X2	C20-C19-O11-C10
2	C	400	5X2	C18-C19-O11-C10
2	B	400	5X2	C18-C19-O11-C10
2	B	400	5X2	C20-C19-O11-C10
2	B	400	5X2	C08-C09-C10-O11
2	C	400	5X2	C33-C32-S26-O27
2	C	400	5X2	C07-C08-C09-C10
2	C	400	5X2	C31-C32-S26-O27
2	D	400	5X2	C31-C32-S26-O27
2	D	400	5X2	C08-C09-C10-O11
2	D	400	5X2	C33-C32-S26-O27
2	C	400	5X2	C31-C32-S26-N25
2	B	400	5X2	C31-C32-S26-O27
2	B	400	5X2	C33-C32-S26-O27
2	C	400	5X2	C33-C32-S26-N25
2	C	400	5X2	C09-C10-O11-C19
2	C	400	5X2	C08-C09-C10-O11
2	D	400	5X2	C31-C32-S26-N25
2	D	400	5X2	C33-C32-S26-N25

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	400	5X2	3	0
2	D	400	5X2	1	0
2	A	400	5X2	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

Full wwPDB X-ray Structure Validation Report

Ligand 5X2 C 400

Bond lengths

Bond angles

Torsions

Rings

Ligand 5X2 B 400

Bond lengths

Bond angles

Torsions

Rings

Ligand 5X2 D 400

Bond lengths

Bond angles

Torsions

Rings

Ligand 5X2 A 400

Bond lengths

Bond angles

Torsions

Rings
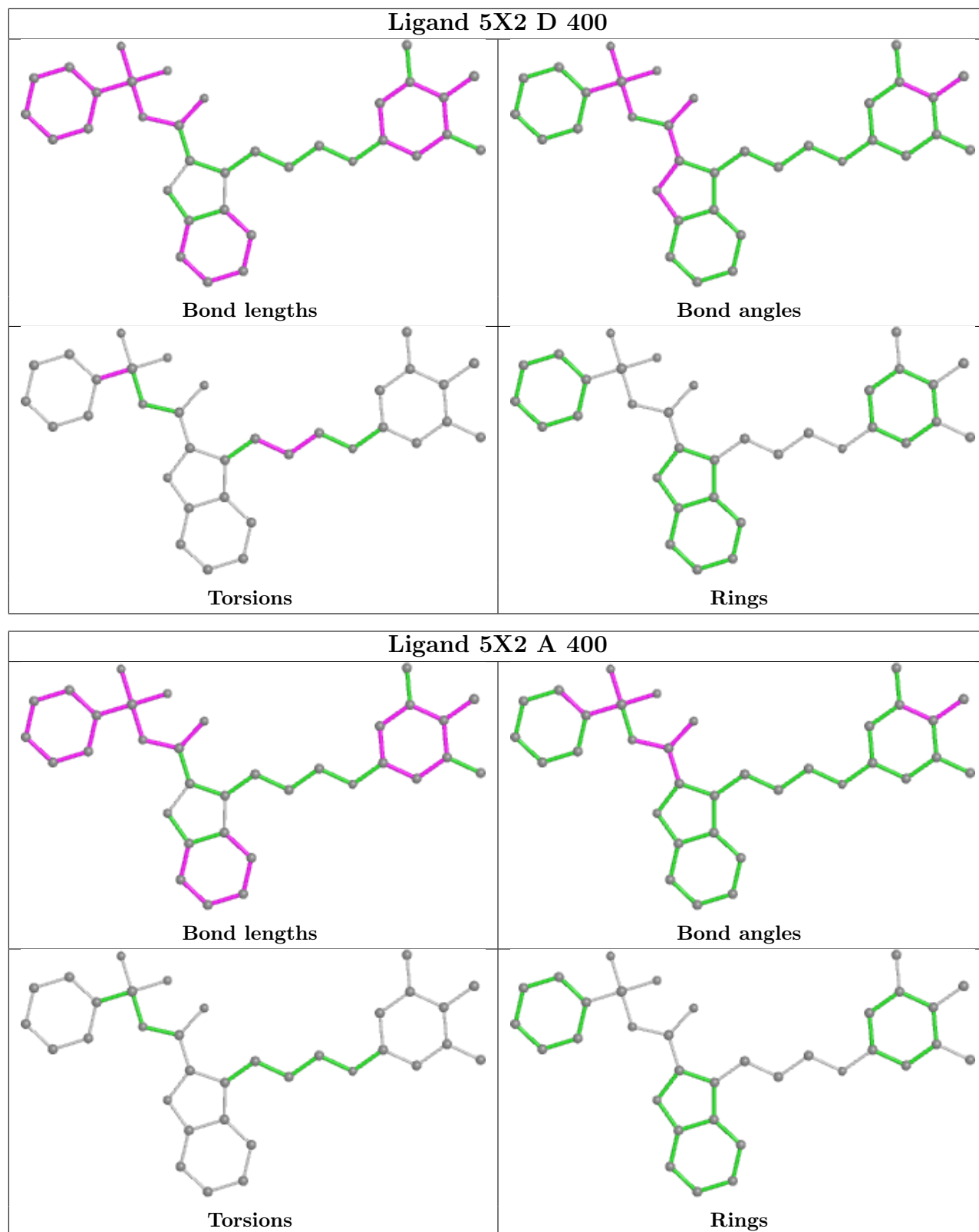
5.7 Other polymers ⓘ

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(Å²)	Q<0.9
1	A	142/150 (94%)	-0.63	1 (0%)	87	84	20, 42, 69, 87	0
1	B	150/150 (100%)	-0.53	1 (0%)	87	84	38, 58, 87, 94	0
1	C	143/150 (95%)	-0.21	2 (1%)	75	70	56, 82, 115, 127	0
1	D	137/150 (91%)	-0.08	3 (2%)	62	52	54, 95, 129, 141	0
All	All	572/600 (95%)	-0.37	7 (1%)	79	73	20, 67, 118, 141	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	320	HIS	4.5
1	B	193	ALA	3.0
1	D	222	ARG	2.9
1	C	204	ALA	2.9
1	C	257	GLY	2.6
1	A	192	GLY	2.5
1	D	255	SER	2.3

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

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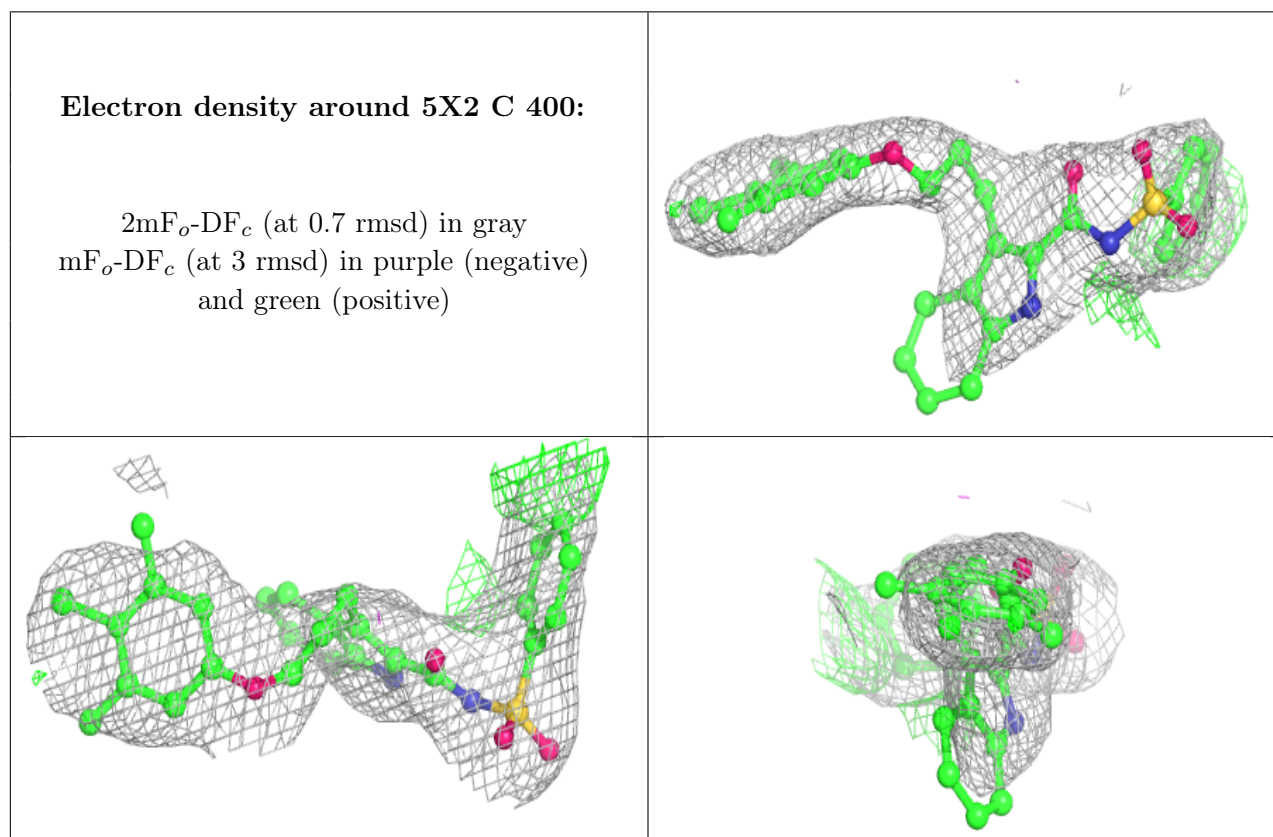
6.3   Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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($Å^2$)	Q<0.9
2	5X2	C	400	34/34	0.90	0.20	68,84,98,102	0
2	5X2	D	400	34/34	0.91	0.22	61,88,110,118	0
2	5X2	B	400	34/34	0.96	0.13	30,55,74,83	0
2	5X2	A	400	34/34	0.97	0.14	19,42,78,86	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.
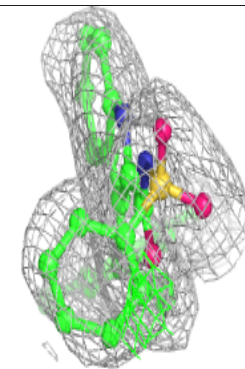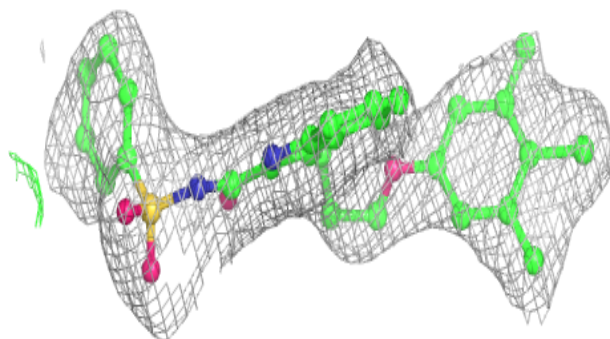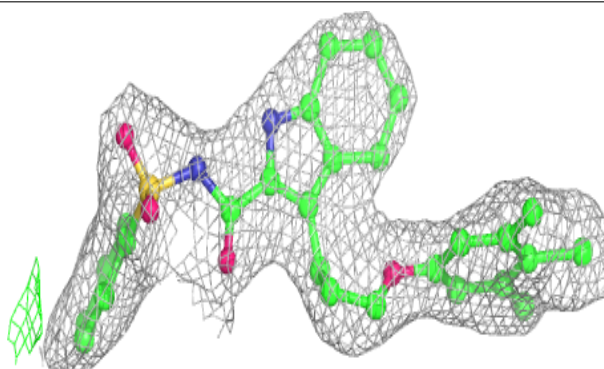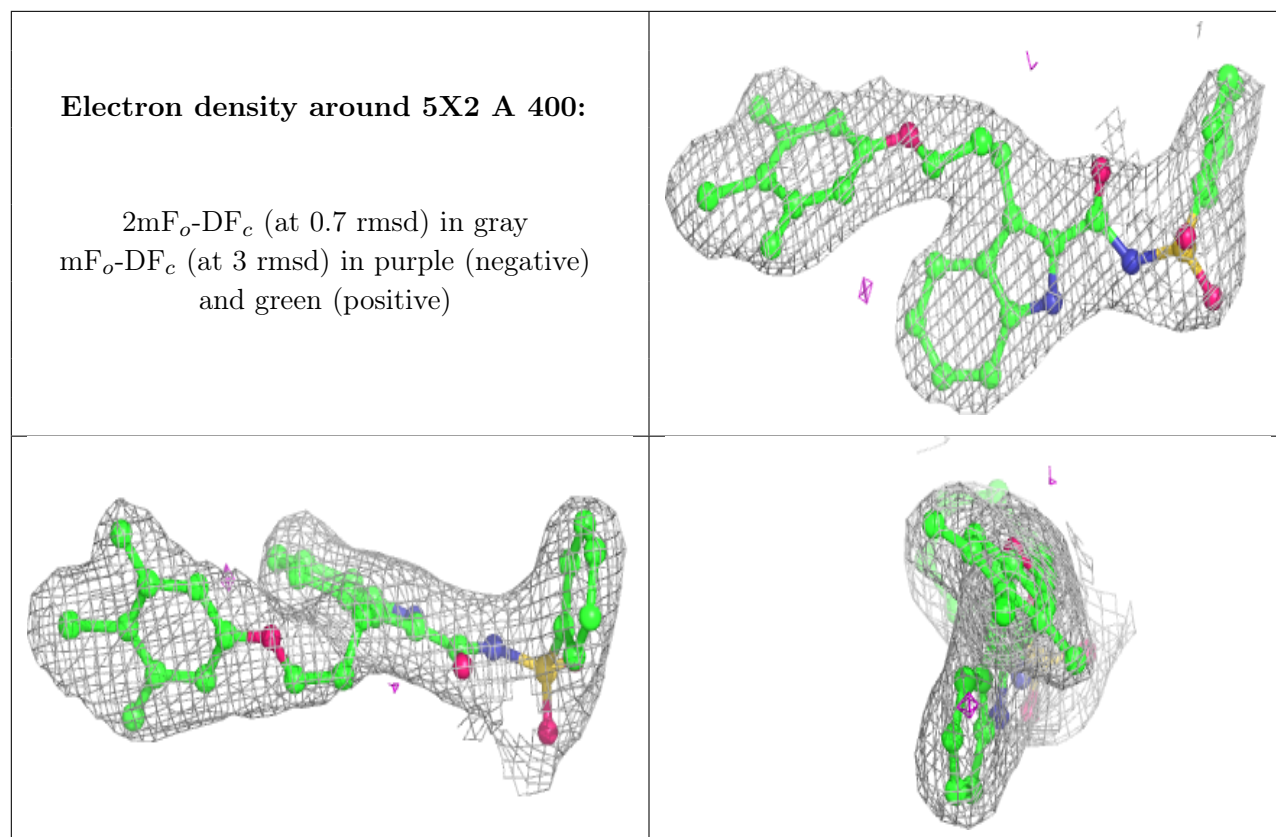
Electron density around 5X2 C 400:

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

Electron density around 5X2 D 400:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
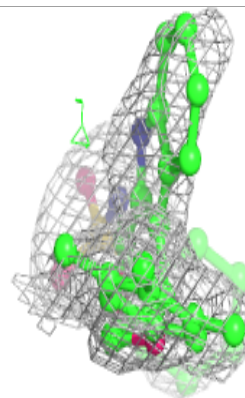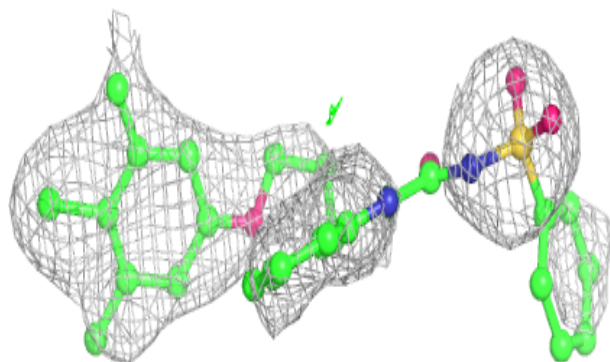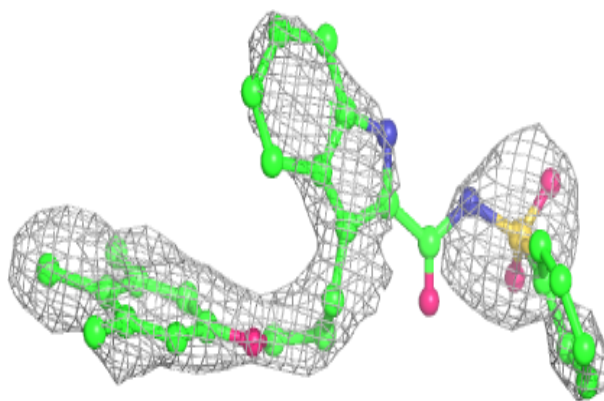
Electron density around 5X2 B 400:

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 5X2 A 400:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.