



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:50 AM UTC

PDB ID : 5FDR / pdb_00005fdr
Title : Mcl-1 complexed with small molecule inhibitor
Authors : Zhao, B.
Deposited on : 2015-12-16
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

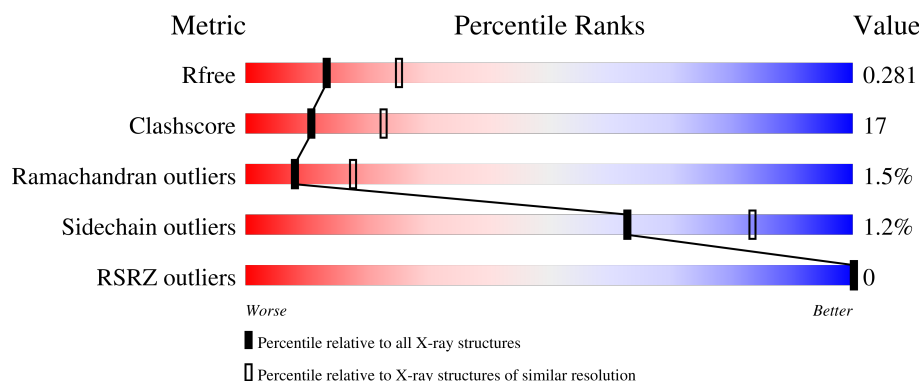
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	158	 62% 34% 2% 2% 2%
1	B	158	 60% 33% 3% 3% 3%
1	C	158	 66% 23% 5% 5% 5%
1	D	158	 58% 34% 3% 3% 3%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4937 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.

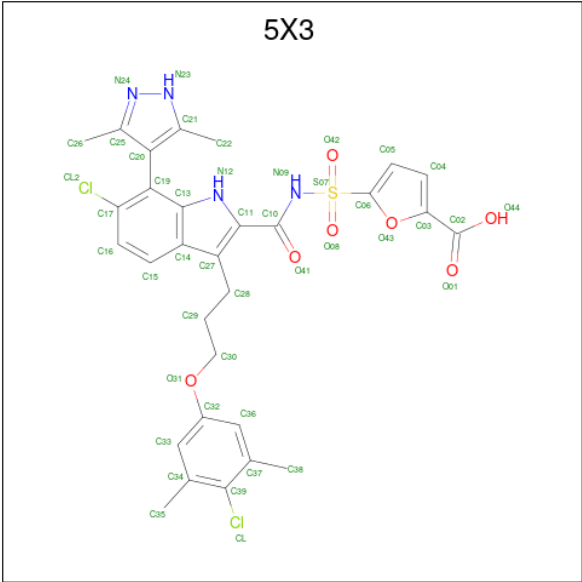
- Molecule 1 is a protein called Induced myeloid leukemia cell differentiation protein Mcl-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	155	Total	C	N	O	S	0	1	0
			1233	774	224	231	4			
1	B	149	Total	C	N	O	S	0	1	0
			1188	745	220	219	4			
1	C	143	Total	C	N	O	S	0	1	0
			1159	730	211	215	3			
1	D	148	Total	C	N	O	S	0	1	0
			1181	741	219	217	4			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	170	GLY	-	expression tag	UNP Q07820
A	171	ASP	-	expression tag	UNP Q07820
B	170	GLY	-	expression tag	UNP Q07820
B	171	ASP	-	expression tag	UNP Q07820
C	170	GLY	-	expression tag	UNP Q07820
C	171	ASP	-	expression tag	UNP Q07820
D	170	GLY	-	expression tag	UNP Q07820
D	171	ASP	-	expression tag	UNP Q07820

- Molecule 2 is 5-[[6-chloranyl-3-[3-(4-chloranyl-3,5-dimethyl-phenoxy)propyl]-7-(3,5-dimethyl-1 {H}-pyrazol-4-yl)-1 {H}-indol-2-yl]carbonylsulfamoyl]furan-2-carboxylic acid (CCD ID: 5X3) (formula: C₃₀H₂₈Cl₂N₄O₇S).

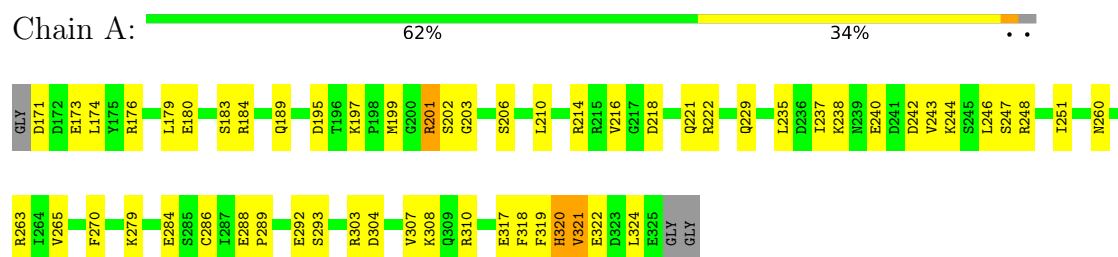


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 44	C 30	Cl 2	N 4	O 7	S 1	0	0
2	B	1	Total 44	C 30	Cl 2	N 4	O 7	S 1	0	0
2	C	1	Total 44	C 30	Cl 2	N 4	O 7	S 1	0	0
2	D	1	Total 44	C 30	Cl 2	N 4	O 7	S 1	0	0

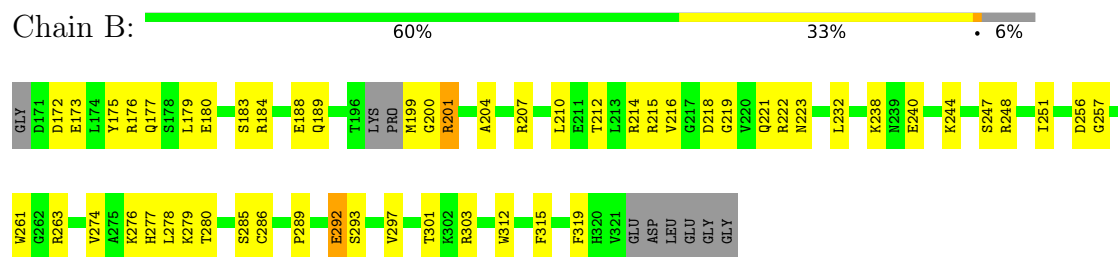
3 Residue-property plots

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 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.

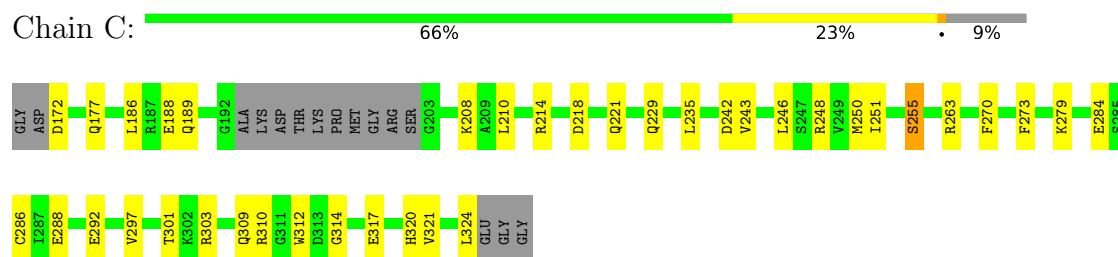
- Molecule 1: Induced myeloid leukemia cell differentiation protein Mcl-1



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D256	G257	V258	R263	I264	V265	I268	K279	E284	S285	C286	T295	D296	V297	R300	V307	K308	Q309	G314	V321	GLU	ASP	LEU	GLU	GLY	GLY
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	35.04Å 115.00Å 95.33Å 90.00° 91.17° 90.00°	Depositor
Resolution (Å)	28.75 – 2.60 28.75 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.9 (28.75-2.60) 89.5 (28.75-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.98 (at 2.58Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.224 , 0.283 0.237 , 0.281	Depositor DCC
R_{free} test set	1086 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	32.6	Xtriage
Anisotropy	0.610	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 15.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.239 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4937	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.67% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 5X3

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	0/1253	0.78	0/1688
1	B	0.46	0/1206	0.77	0/1621
1	C	0.47	0/1177	0.81	0/1583
1	D	0.50	0/1199	0.84	3/1611 (0.2%)
All	All	0.47	0/4835	0.80	3/6503 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	308	LYS	CA-CB-CG	-6.18	101.73	114.10
1	D	201	ARG	CD-NE-CZ	5.46	132.04	124.40
1	D	308	LYS	CB-CG-CD	-5.11	99.54	111.30

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	1233	0	1223	45	1
1	B	1188	0	1175	46	1
1	C	1159	0	1161	29	0
1	D	1181	0	1174	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	44	0	0	3	0
2	B	44	0	0	1	0
2	C	44	0	0	3	0
2	D	44	0	0	2	0
All	All	4937	0	4733	160	1

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 17.

All (160) 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:251:ILE:O	1:C:255:SER:HB2	1.73	0.86
1:A:310:ARG:NH2	1:A:317:GLU:OE2	2.10	0.85
1:A:248:ARG:HB3	1:D:249:VAL:HG21	1.56	0.85
1:C:214:ARG:O	1:C:218:ASP:HB2	1.77	0.84
1:A:176:ARG:NH2	1:A:201:ARG:O	2.14	0.81
1:D:201:ARG:HG3	1:D:202:SER:H	1.44	0.80
1:A:235:LEU:O	1:D:248:ARG:NH1	2.13	0.80
1:D:201:ARG:HE	1:D:202:SER:N	1.80	0.80
1:A:199:MET:HE3	1:A:206:SER:HB3	1.64	0.80
1:B:176:ARG:NH1	1:B:180:GLU:OE1	2.14	0.79
1:B:215:ARG:NH2	1:B:319:PHE:O	2.18	0.76
1:A:189:GLN:NE2	1:A:221:GLN:HE22	1.84	0.75
1:D:201:ARG:HE	1:D:201:ARG:C	1.95	0.75
1:B:289:PRO:O	1:B:292:GLU:HB3	1.87	0.74
1:A:263:ARG:HD3	2:A:400:5X3:O42	1.89	0.73
1:B:286:CYS:HA	1:B:289:PRO:HG2	1.69	0.72
1:C:310:ARG:NH2	1:C:317:GLU:OE2	2.25	0.70
1:C:172:ASP:N	1:C:303:ARG:HH22	1.91	0.69
1:D:201:ARG:CG	1:D:202:SER:H	2.06	0.67
1:A:179:LEU:O	1:A:183:SER:OG	2.06	0.67
1:C:248:ARG:HA	1:C:251:ILE:HG22	1.75	0.67
1:D:251:ILE:HD11	1:D:297:VAL:HG22	1.78	0.65
1:D:203:GLY:O	1:D:207:ARG:HG3	1.96	0.65
1:D:250:MET:HE3	1:D:297:VAL:HG21	1.79	0.64
1:A:189:GLN:HE22	1:A:221:GLN:HE22	1.44	0.64
1:A:304:ASP:O	1:A:308:LYS:HG2	1.99	0.63
1:D:256:ASP:O	1:D:263:ARG:NH2	2.29	0.63
1:A:216:VAL:HG12	1:A:265:VAL:HG11	1.79	0.63
1:A:318:PHE:O	1:B:223:ASN:ND2	2.24	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:GLU:O	1:B:244:LYS:HG3	1.99	0.61
1:C:229:GLN:HG3	1:C:273:PHE:HZ	1.66	0.61
1:D:279:LYS:O	1:D:279:LYS:HD3	2.00	0.60
1:A:319:PHE:HA	1:B:223:ASN:ND2	2.15	0.60
1:D:263:ARG:HD3	2:D:400:5X3:O08	2.01	0.60
1:B:247:SER:O	1:B:251:ILE:HG13	2.02	0.59
1:D:211:GLU:HA	1:D:214:ARG:HG3	1.84	0.59
1:B:261:TRP:CH2	1:B:315:PHE:HB2	2.38	0.59
1:A:218:ASP:O	1:A:222:ARG:HG2	2.03	0.58
1:B:289:PRO:HA	1:B:292:GLU:HB3	1.84	0.58
1:A:199:MET:HB2	1:A:203:GLY:HA2	1.84	0.58
1:C:263:ARG:NE	2:C:400:5X3:O42	2.36	0.58
1:D:237:ILE:HD13	1:D:246:LEU:HD11	1.85	0.58
1:C:208:LYS:HB3	1:C:208:LYS:NZ	2.19	0.58
1:A:248:ARG:HA	1:A:251:ILE:HG22	1.86	0.57
1:B:248:ARG:HH22	1:C:242:ASP:HB3	1.70	0.57
1:D:223:ASN:HB2	1:D:224:HIS:HD2	1.71	0.56
1:A:279:LYS:NZ	1:A:284:GLU:OE1	2.35	0.56
1:B:173:GLU:OE2	1:B:176:ARG:NE	2.35	0.56
1:B:210:LEU:O	1:B:214:ARG:HG3	2.04	0.56
1:B:232:LEU:HD13	1:B:274:VAL:HG22	1.88	0.56
1:D:187:ARG:HH11	1:D:187:ARG:HB3	1.70	0.56
1:A:210:LEU:O	1:A:214:ARG:HG3	2.06	0.56
1:D:183:SER:O	1:D:187:ARG:HG3	2.06	0.56
1:D:217:GLY:O	1:D:221:GLN:HG3	2.06	0.56
1:D:279:LYS:NZ	1:D:284:GLU:OE1	2.34	0.55
1:B:172:ASP:OD2	1:B:303:ARG:NH2	2.40	0.55
1:B:297:VAL:O	1:B:301:THR:OG1	2.23	0.55
1:D:250:MET:HE3	1:D:297:VAL:CG2	2.36	0.55
1:A:180:GLU:O	1:A:184:ARG:HG3	2.07	0.55
1:D:187:ARG:O	1:D:191:THR:HG22	2.07	0.55
1:B:179:LEU:HD23	1:B:183:SER:OG	2.05	0.54
1:A:310:ARG:NH2	1:A:317:GLU:CD	2.66	0.54
1:D:201:ARG:CG	1:D:202:SER:N	2.70	0.54
1:A:247:SER:HB3	1:A:293:SER:OG	2.07	0.54
1:D:189:GLN:NE2	1:D:221:GLN:HE22	2.06	0.54
1:C:279:LYS:NZ	1:C:284:GLU:OE1	2.37	0.54
1:C:288:GLU:O	1:C:292:GLU:HG3	2.07	0.53
1:A:173:GLU:OE2	1:A:176:ARG:NH2	2.41	0.53
1:D:307:VAL:HG12	1:D:308:LYS:HG2	1.89	0.53
1:C:310:ARG:NH2	1:C:317:GLU:CD	2.67	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:180:GLU:HG2	1:B:184:ARG:NH1	2.24	0.52
1:A:184:ARG:CZ	1:A:199:MET:SD	2.97	0.52
1:A:303:ARG:HG3	1:A:304:ASP:N	2.24	0.52
1:A:321:VAL:HG11	1:A:324:LEU:HD12	1.92	0.52
1:D:256:ASP:C	1:D:263:ARG:HH22	2.16	0.52
1:D:201:ARG:HG3	1:D:202:SER:N	2.20	0.52
1:D:309:GLN:O	1:D:314:GLY:HA3	2.10	0.52
1:B:240:GLU:HG2	1:B:244:LYS:HE3	1.91	0.52
1:C:177:GLN:HE21	1:C:312:TRP:HD1	1.58	0.51
1:A:248:ARG:CB	1:D:249:VAL:HG21	2.33	0.51
1:A:237:ILE:HD13	1:A:246:LEU:HD11	1.93	0.51
1:D:216:VAL:HG22	1:D:265:VAL:HG11	1.93	0.51
1:D:247:SER:O	1:D:251:ILE:HG12	2.11	0.51
1:D:223:ASN:CB	1:D:224:HIS:HD2	2.24	0.50
1:B:256:ASP:O	1:B:263:ARG:NH1	2.41	0.50
1:D:212:THR:O	1:D:216:VAL:HG12	2.11	0.49
1:B:200:GLY:O	1:B:201:ARG:HB2	2.12	0.49
1:A:319:PHE:O	1:A:320:HIS:C	2.56	0.49
1:B:172:ASP:CG	1:B:303:ARG:HH21	2.21	0.48
1:B:221:GLN:HE22	1:B:276[A]:LYS:HE2	1.78	0.48
1:A:248:ARG:O	1:A:251:ILE:HG22	2.13	0.48
1:D:218:ASP:O	1:D:222:ARG:HG2	2.13	0.48
1:A:171:ASP:OD2	1:A:303:ARG:HD2	2.14	0.48
1:B:177:GLN:NE2	1:B:312:TRP:HD1	2.12	0.48
1:D:184:ARG:HH12	1:D:199:MET:HE2	1.78	0.48
1:A:260:ASN:ND2	2:A:400:5X3:O44	2.45	0.47
1:B:292:GLU:HG3	1:B:293:SER:N	2.29	0.47
1:D:188:GLU:CD	1:D:214:ARG:HH21	2.22	0.47
1:A:322:GLU:OE2	1:B:219:GLY:HA3	2.15	0.47
1:C:210:LEU:O	1:C:214:ARG:HG3	2.13	0.47
1:D:213:LEU:HD11	1:D:268:ILE:HG21	1.96	0.47
1:B:279:LYS:C	1:B:279:LYS:HD2	2.39	0.47
1:C:297:VAL:O	1:C:301:THR:OG1	2.23	0.47
1:C:309:GLN:O	1:C:314:GLY:HA3	2.14	0.46
1:A:242:ASP:HB3	1:D:248:ARG:NH2	2.31	0.46
1:D:172:ASP:OD2	1:D:172:ASP:N	2.48	0.46
1:A:307:VAL:HG12	1:A:308:LYS:HD3	1.97	0.46
1:C:310:ARG:HD3	1:D:258:VAL:HG21	1.98	0.46
1:D:296:ASP:OD1	1:D:300:ARG:NH2	2.49	0.46
1:A:288:GLU:OE2	1:A:288:GLU:N	2.46	0.46
1:C:321:VAL:CG1	1:C:324:LEU:HA	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:321:VAL:O	1:C:321:VAL:HG12	2.16	0.46
1:B:248:ARG:NH2	1:C:235:LEU:O	2.49	0.46
1:C:310:ARG:NH2	1:C:317:GLU:OE1	2.45	0.45
1:D:200:GLY:O	1:D:203:GLY:N	2.47	0.45
1:D:179:LEU:O	1:D:183:SER:OG	2.17	0.45
1:B:278:LEU:HD13	1:B:286:CYS:HB2	1.97	0.45
1:B:179:LEU:HD23	1:B:183:SER:HG	1.81	0.45
1:A:243:VAL:HG21	1:A:286:CYS:HB3	1.97	0.45
1:B:172:ASP:CG	1:B:303:ARG:NH2	2.75	0.45
1:B:175:TYR:CE2	1:B:179:LEU:HD12	2.52	0.45
1:B:238:LYS:HB2	1:B:238:LYS:HE2	1.80	0.45
1:D:178:SER:HB2	1:D:295:THR:HG23	1.98	0.45
1:D:243:VAL:HG21	1:D:286:CYS:HB3	1.99	0.45
1:B:199:MET:HB3	1:B:207:ARG:HH21	1.82	0.44
1:B:257:GLY:HA3	2:B:400:5X3:O01	2.18	0.44
1:C:243:VAL:HA	1:C:246:LEU:HD12	1.99	0.44
1:A:270:PHE:HD2	2:A:400:5X3:C37	2.31	0.44
1:C:189:GLN:NE2	1:C:221:GLN:HE22	2.16	0.44
1:D:208:LYS:HE2	1:D:211:GLU:OE2	2.18	0.44
1:D:240:GLU:O	1:D:244:LYS:HG3	2.17	0.44
1:C:250:MET:HE2	2:C:400:5X3:C38	2.48	0.43
1:C:270:PHE:HD2	2:C:400:5X3:C37	2.31	0.43
1:D:184:ARG:NH1	1:D:195:ASP:O	2.51	0.43
1:C:208:LYS:HB3	1:C:208:LYS:HZ3	1.81	0.43
1:D:251:ILE:CD1	1:D:297:VAL:HG22	2.48	0.43
1:A:171:ASP:HA	1:A:174:LEU:HB3	2.01	0.43
1:B:289:PRO:C	1:B:292:GLU:HB3	2.43	0.42
1:B:274:VAL:O	1:B:277:HIS:HB3	2.18	0.42
1:C:210:LEU:HD12	1:C:210:LEU:HA	1.79	0.42
1:A:171:ASP:HA	1:A:174:LEU:H	1.85	0.42
1:B:189:GLN:NE2	1:B:218:ASP:OD2	2.53	0.42
1:B:212:THR:O	1:B:216:VAL:HG22	2.20	0.42
1:A:240:GLU:O	1:A:244:LYS:HG3	2.20	0.42
1:A:238:LYS:HE2	1:A:238:LYS:HB2	1.61	0.41
1:A:310:ARG:HH22	1:A:317:GLU:CD	2.27	0.41
1:B:285:SER:O	1:B:289:PRO:HD2	2.20	0.41
1:A:289:PRO:HA	1:A:292:GLU:OE2	2.20	0.41
1:C:188:GLU:OE2	1:C:214:ARG:NE	2.48	0.41
1:D:213:LEU:HD23	1:D:213:LEU:HA	1.89	0.41
1:B:221:GLN:HE22	1:B:276[A]:LYS:CE	2.34	0.41
1:B:188:GLU:OE2	1:B:214:ARG:NE	2.47	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:VAL:HG21	1:C:286:CYS:HB3	2.03	0.41
1:D:254:PHE:HB2	2:D:400:5X3:C29	2.50	0.41
1:B:218:ASP:O	1:B:222:ARG:HG3	2.21	0.41
1:B:261:TRP:CE3	1:B:315:PHE:HD1	2.40	0.40
1:A:243:VAL:HA	1:A:246:LEU:HD12	2.03	0.40
1:A:319:PHE:HA	1:B:223:ASN:HD21	1.84	0.40
1:B:214:ARG:HH11	1:B:214:ARG:HD2	1.73	0.40
1:D:188:GLU:HG2	1:D:194:LYS:HA	2.02	0.40

All (1) 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:A:292:GLU:OE1	1:B:207:ARG:NH2[2_755]	2.11	0.09

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	153/158 (97%)	143 (94%)	5 (3%)	5 (3%)	3	5
1	B	145/158 (92%)	139 (96%)	3 (2%)	3 (2%)	5	11
1	C	139/158 (88%)	133 (96%)	5 (4%)	1 (1%)	18	38
1	D	144/158 (91%)	137 (95%)	7 (5%)	0	100	100
All	All	581/632 (92%)	552 (95%)	20 (3%)	9 (2%)	8	18

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	204	ALA
1	C	320	HIS

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Mol	Chain	Res	Type
1	A	320	HIS
1	B	201	ARG
1	A	201	ARG
1	B	292	GLU
1	A	195	ASP
1	A	321	VAL
1	A	197	LYS

5.3.2 Protein sidechains [i](#)

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	132/136 (97%)	130 (98%)	2 (2%)	57	80
1	B	125/136 (92%)	124 (99%)	1 (1%)	73	88
1	C	126/136 (93%)	124 (98%)	2 (2%)	55	79
1	D	125/136 (92%)	124 (99%)	1 (1%)	73	88
All	All	508/544 (93%)	502 (99%)	6 (1%)	63	83

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	202	SER
1	A	229	GLN
1	B	280	THR
1	C	186	LEU
1	C	255	SER
1	D	172	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	A	283	GLN
1	B	177	GLN

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Mol	Chain	Res	Type
1	B	221	GLN
1	C	177	GLN
1	C	189	GLN
1	C	252	HIS
1	D	189	GLN
1	D	224	HIS
1	D	229	GLN
1	D	252	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	5X3	D	400	-	45,48,48	3.73	15 (33%)	63,72,72	2.12	13 (20%)
2	5X3	A	400	-	45,48,48	3.69	15 (33%)	63,72,72	2.14	17 (26%)
2	5X3	C	400	-	45,48,48	3.66	17 (37%)	63,72,72	2.19	20 (31%)
2	5X3	B	400	-	45,48,48	3.78	19 (42%)	63,72,72	2.00	14 (22%)

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	5X3	D	400	-	-	3/29/30/30	0/5/5/5
2	5X3	A	400	-	-	6/29/30/30	0/5/5/5
2	5X3	C	400	-	-	7/29/30/30	0/5/5/5
2	5X3	B	400	-	-	12/29/30/30	0/5/5/5

All (66) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	5X3	O42-S07	15.45	1.66	1.43
2	D	400	5X3	O42-S07	15.26	1.65	1.43
2	C	400	5X3	O08-S07	14.94	1.65	1.43
2	A	400	5X3	O08-S07	14.84	1.65	1.43
2	D	400	5X3	O08-S07	14.64	1.64	1.43
2	C	400	5X3	O42-S07	14.47	1.64	1.43
2	A	400	5X3	O42-S07	14.35	1.64	1.43
2	B	400	5X3	O08-S07	14.19	1.64	1.43
2	A	400	5X3	C10-N09	5.90	1.45	1.38
2	D	400	5X3	S07-N09	5.51	1.69	1.64
2	D	400	5X3	C10-N09	5.44	1.45	1.38
2	C	400	5X3	C10-N09	5.15	1.44	1.38
2	B	400	5X3	S07-N09	5.07	1.69	1.64
2	B	400	5X3	C10-N09	4.97	1.44	1.38
2	B	400	5X3	C11-N12	-4.88	1.31	1.38
2	A	400	5X3	S07-N09	4.83	1.68	1.64
2	A	400	5X3	O43-C03	-4.79	1.30	1.38
2	C	400	5X3	S07-N09	4.71	1.68	1.64
2	A	400	5X3	C11-N12	-4.46	1.32	1.38
2	D	400	5X3	C11-N12	-4.26	1.32	1.38
2	D	400	5X3	O43-C03	-4.23	1.31	1.38
2	C	400	5X3	C11-N12	-4.23	1.32	1.38
2	C	400	5X3	O43-C03	-4.17	1.31	1.38
2	B	400	5X3	O43-C03	-4.14	1.31	1.38
2	B	400	5X3	C21-N23	-3.99	1.27	1.34
2	C	400	5X3	C14-C13	-3.06	1.37	1.41
2	B	400	5X3	C39-CL	3.00	1.79	1.72
2	D	400	5X3	C39-CL	2.76	1.78	1.72
2	C	400	5X3	C03-C02	2.47	1.54	1.48
2	D	400	5X3	C03-C02	2.46	1.54	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	5X3	O41-C10	-2.44	1.18	1.23
2	B	400	5X3	C11-C10	2.44	1.52	1.47
2	A	400	5X3	C04-C03	2.44	1.41	1.35
2	A	400	5X3	C14-C13	-2.40	1.38	1.41
2	A	400	5X3	C28-C27	2.38	1.54	1.51
2	C	400	5X3	C39-CL	2.35	1.77	1.72
2	B	400	5X3	C38-C37	2.33	1.55	1.51
2	D	400	5X3	C21-N23	-2.33	1.30	1.34
2	C	400	5X3	C04-C03	2.33	1.40	1.35
2	A	400	5X3	C39-CL	2.32	1.77	1.72
2	B	400	5X3	C13-N12	-2.31	1.33	1.38
2	B	400	5X3	O31-C32	2.31	1.42	1.37
2	C	400	5X3	C11-C10	2.30	1.52	1.47
2	D	400	5X3	C19-C20	2.30	1.54	1.50
2	A	400	5X3	C11-C10	2.22	1.51	1.47
2	C	400	5X3	C21-N23	-2.21	1.30	1.34
2	C	400	5X3	C17-CL2	2.17	1.78	1.73
2	A	400	5X3	C13-N12	-2.17	1.34	1.38
2	D	400	5X3	C26-C25	2.15	1.54	1.49
2	D	400	5X3	C04-C03	2.13	1.40	1.35
2	B	400	5X3	C25-N24	-2.13	1.29	1.34
2	D	400	5X3	C13-N12	-2.11	1.34	1.38
2	A	400	5X3	C03-C02	2.11	1.53	1.48
2	C	400	5X3	C22-C21	2.11	1.53	1.49
2	B	400	5X3	C03-C02	2.09	1.53	1.48
2	D	400	5X3	O41-C10	-2.07	1.19	1.23
2	A	400	5X3	C22-C21	2.07	1.53	1.49
2	C	400	5X3	C13-N12	-2.06	1.34	1.38
2	C	400	5X3	O41-C10	-2.05	1.19	1.23
2	A	400	5X3	O31-C32	2.05	1.42	1.37
2	B	400	5X3	C26-C25	2.05	1.53	1.49
2	C	400	5X3	O01-C02	2.04	1.27	1.22
2	D	400	5X3	C11-C10	2.04	1.51	1.47
2	B	400	5X3	N23-N24	-2.02	1.32	1.36
2	B	400	5X3	C33-C34	-2.02	1.36	1.39
2	B	400	5X3	C19-C20	2.01	1.53	1.50

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	5X3	C20-C25-N24	-8.23	105.66	110.88
2	C	400	5X3	C20-C25-N24	-7.74	105.97	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	400	5X3	C20-C25-N24	-7.11	106.37	110.88
2	A	400	5X3	C20-C25-N24	-6.95	106.47	110.88
2	D	400	5X3	O42-S07-O08	-6.44	108.02	119.82
2	A	400	5X3	C03-O43-C06	5.50	111.46	105.17
2	A	400	5X3	O42-S07-O08	-5.45	109.82	119.82
2	B	400	5X3	O42-S07-O08	-5.44	109.85	119.82
2	D	400	5X3	C03-O43-C06	5.37	111.31	105.17
2	A	400	5X3	O42-S07-C06	5.17	114.86	107.07
2	C	400	5X3	C03-O43-C06	5.02	110.91	105.17
2	C	400	5X3	O42-S07-O08	-4.45	111.66	119.82
2	C	400	5X3	C26-C25-N24	4.41	127.65	120.99
2	B	400	5X3	C03-O43-C06	4.27	110.05	105.17
2	A	400	5X3	C26-C25-N24	4.21	127.34	120.99
2	A	400	5X3	C22-C21-C20	-4.14	125.83	131.62
2	C	400	5X3	C21-C20-C25	3.98	106.91	104.91
2	D	400	5X3	C22-C21-C20	-3.91	126.14	131.62
2	B	400	5X3	C10-N09-S07	-3.81	118.41	123.84
2	D	400	5X3	O08-S07-C06	3.80	112.79	107.07
2	B	400	5X3	C04-C03-C02	-3.77	122.55	132.59
2	D	400	5X3	C26-C25-N24	3.69	126.55	120.99
2	C	400	5X3	C22-C21-N23	3.49	127.32	121.81
2	D	400	5X3	C22-C21-N23	3.48	127.29	121.81
2	C	400	5X3	C22-C21-C20	-3.37	126.91	131.62
2	C	400	5X3	O41-C10-C11	3.35	125.34	120.87
2	C	400	5X3	O44-C02-C03	3.34	121.63	114.06
2	C	400	5X3	O42-S07-C06	3.32	112.08	107.07
2	A	400	5X3	C05-C04-C03	-3.10	104.17	106.94
2	D	400	5X3	O44-C02-C03	3.05	120.98	114.06
2	B	400	5X3	C13-C19-C20	-3.03	116.82	120.48
2	C	400	5X3	O08-S07-C06	2.96	111.53	107.07
2	B	400	5X3	O41-C10-C11	2.91	124.76	120.87
2	A	400	5X3	C30-O31-C32	-2.79	110.69	117.93
2	C	400	5X3	C16-C17-C19	-2.78	118.13	121.86
2	C	400	5X3	C14-C13-C19	-2.75	119.95	122.41
2	C	400	5X3	C05-C04-C03	-2.61	104.61	106.94
2	B	400	5X3	C04-C05-C06	-2.58	103.71	110.58
2	C	400	5X3	C11-C10-N09	-2.54	110.52	116.05
2	A	400	5X3	C22-C21-N23	2.54	125.81	121.81
2	B	400	5X3	O42-S07-C06	2.54	110.89	107.07
2	D	400	5X3	C04-C03-C02	-2.50	125.92	132.59
2	A	400	5X3	C25-N24-N23	2.47	111.94	106.51
2	A	400	5X3	O41-C10-N09	2.44	125.47	121.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	5X3	C04-C05-C06	-2.42	104.13	110.58
2	D	400	5X3	O08-S07-N09	2.42	112.55	106.66
2	A	400	5X3	C14-C27-C11	-2.38	104.04	106.79
2	A	400	5X3	C28-C29-C30	-2.37	107.56	112.33
2	A	400	5X3	C11-C10-N09	-2.36	110.91	116.05
2	C	400	5X3	C04-C03-C02	-2.36	126.30	132.59
2	C	400	5X3	O42-S07-N09	2.36	112.41	106.66
2	A	400	5X3	O42-S07-N09	2.35	112.39	106.66
2	B	400	5X3	C28-C27-C14	2.32	130.74	124.71
2	C	400	5X3	C38-C37-C39	-2.31	117.08	122.28
2	C	400	5X3	C17-C19-C20	-2.25	118.32	121.67
2	D	400	5X3	C25-N24-N23	2.24	111.45	106.51
2	B	400	5X3	C14-C13-N12	2.23	110.99	108.13
2	B	400	5X3	C25-N24-N23	2.21	111.37	106.51
2	A	400	5X3	C04-C05-C06	-2.16	104.84	110.58
2	A	400	5X3	C28-C27-C14	2.15	130.29	124.71
2	D	400	5X3	C21-C20-C25	2.13	105.98	104.91
2	C	400	5X3	C32-C36-C37	-2.10	118.40	120.61
2	B	400	5X3	C38-C37-C39	-2.07	117.62	122.28
2	B	400	5X3	C13-C14-C27	-2.06	104.57	106.93

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	5X3	C05-C06-S07-N09
2	B	400	5X3	N09-C10-C11-N12
2	B	400	5X3	N09-C10-C11-C27
2	B	400	5X3	C14-C27-C28-C29
2	B	400	5X3	C27-C28-C29-C30
2	B	400	5X3	C05-C06-S07-N09
2	B	400	5X3	C05-C06-S07-O42
2	B	400	5X3	O43-C06-S07-O42
2	C	400	5X3	C27-C28-C29-C30
2	C	400	5X3	C05-C06-S07-N09
2	D	400	5X3	C05-C06-S07-N09
2	D	400	5X3	C05-C06-S07-O42
2	D	400	5X3	O43-C06-S07-O42
2	C	400	5X3	C28-C29-C30-O31
2	B	400	5X3	C11-C27-C28-C29
2	C	400	5X3	C36-C32-O31-C30
2	C	400	5X3	C33-C32-O31-C30

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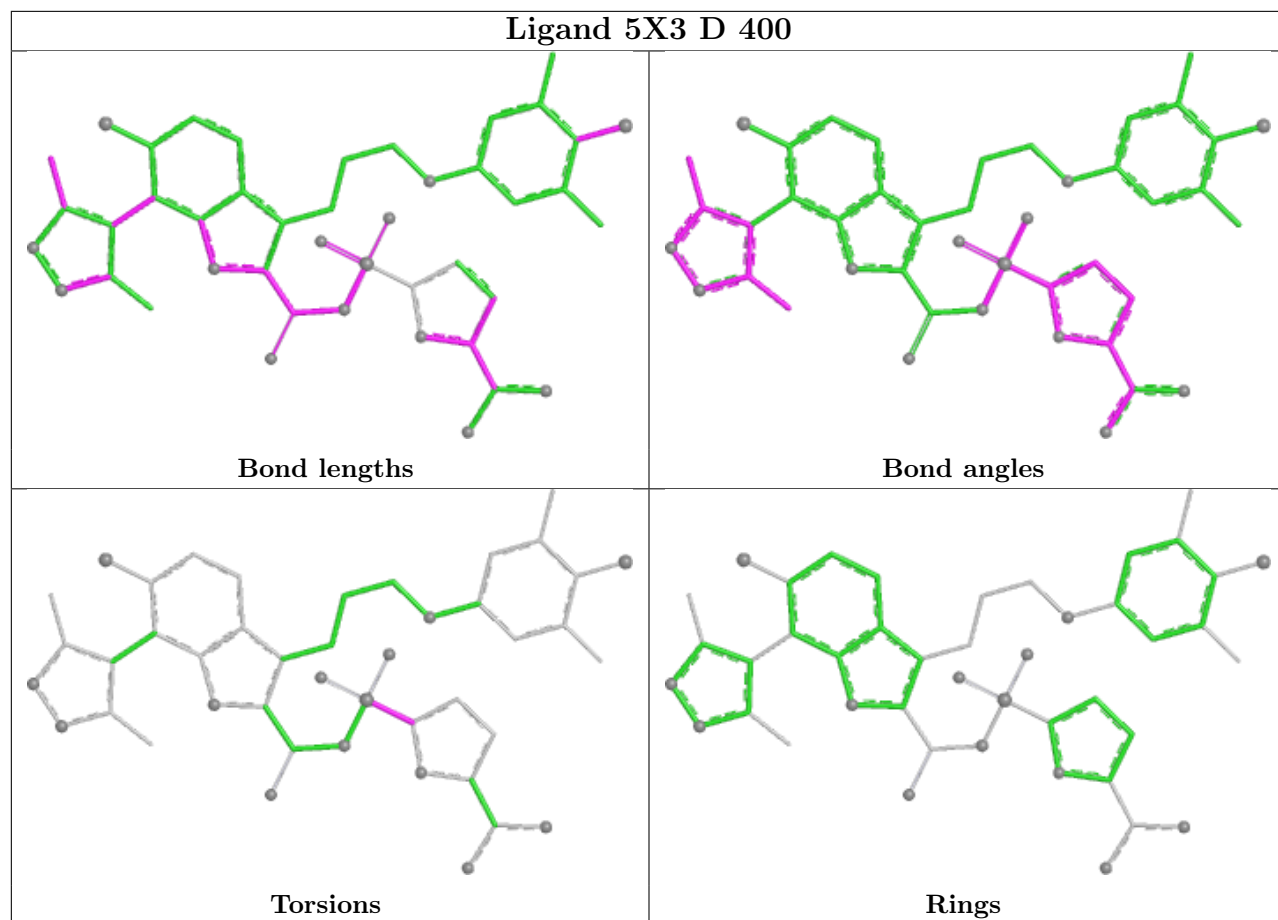
Mol	Chain	Res	Type	Atoms
2	A	400	5X3	C05-C06-S07-O08
2	C	400	5X3	C05-C06-S07-O08
2	B	400	5X3	C28-C29-C30-O31
2	B	400	5X3	C29-C30-O31-C32
2	A	400	5X3	O01-C02-C03-C04
2	A	400	5X3	O01-C02-C03-O43
2	A	400	5X3	O44-C02-C03-C04
2	A	400	5X3	O44-C02-C03-O43
2	B	400	5X3	C36-C32-O31-C30
2	B	400	5X3	C33-C32-O31-C30
2	C	400	5X3	O43-C06-S07-O08

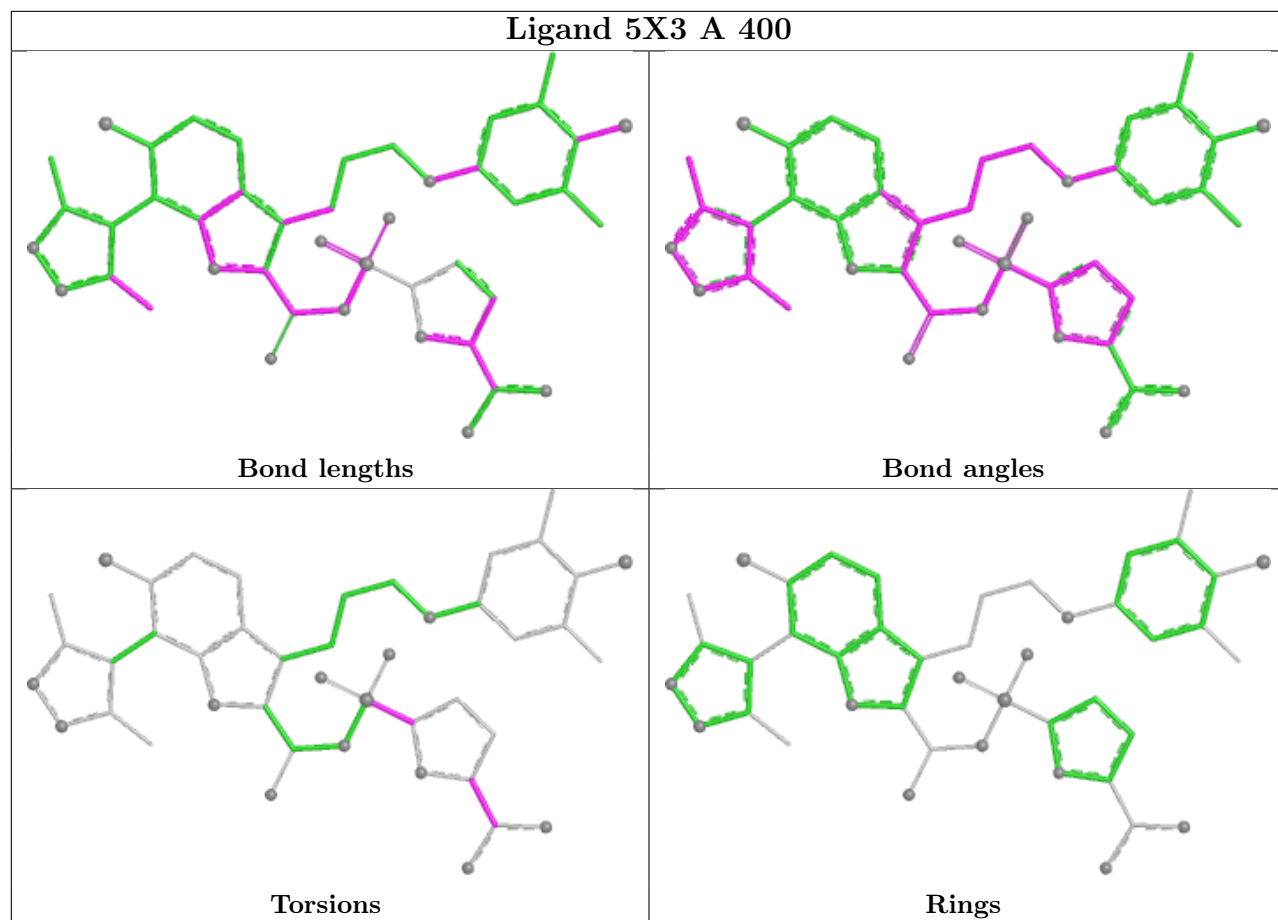
There are no ring outliers.

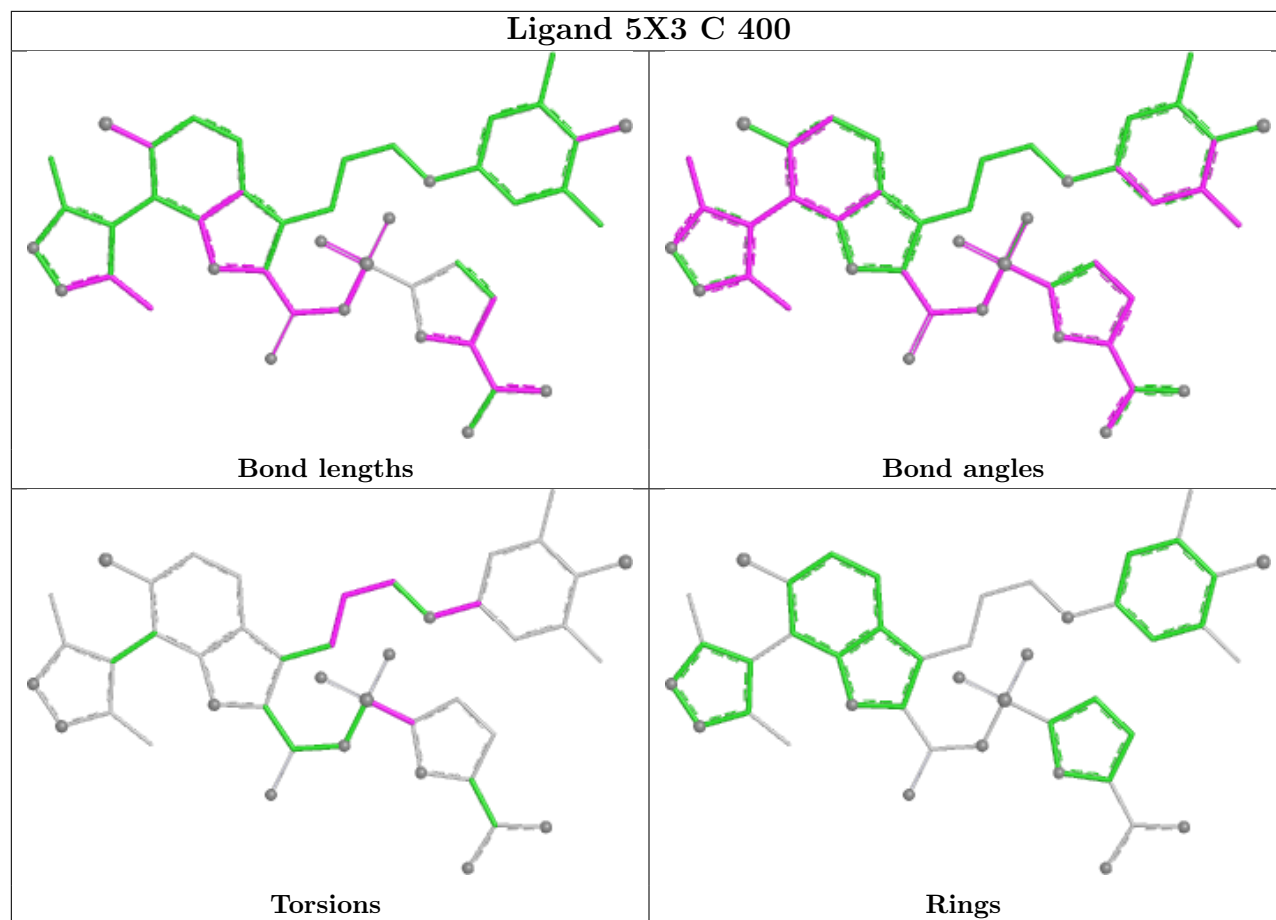
4 monomers are involved in 9 short contacts:

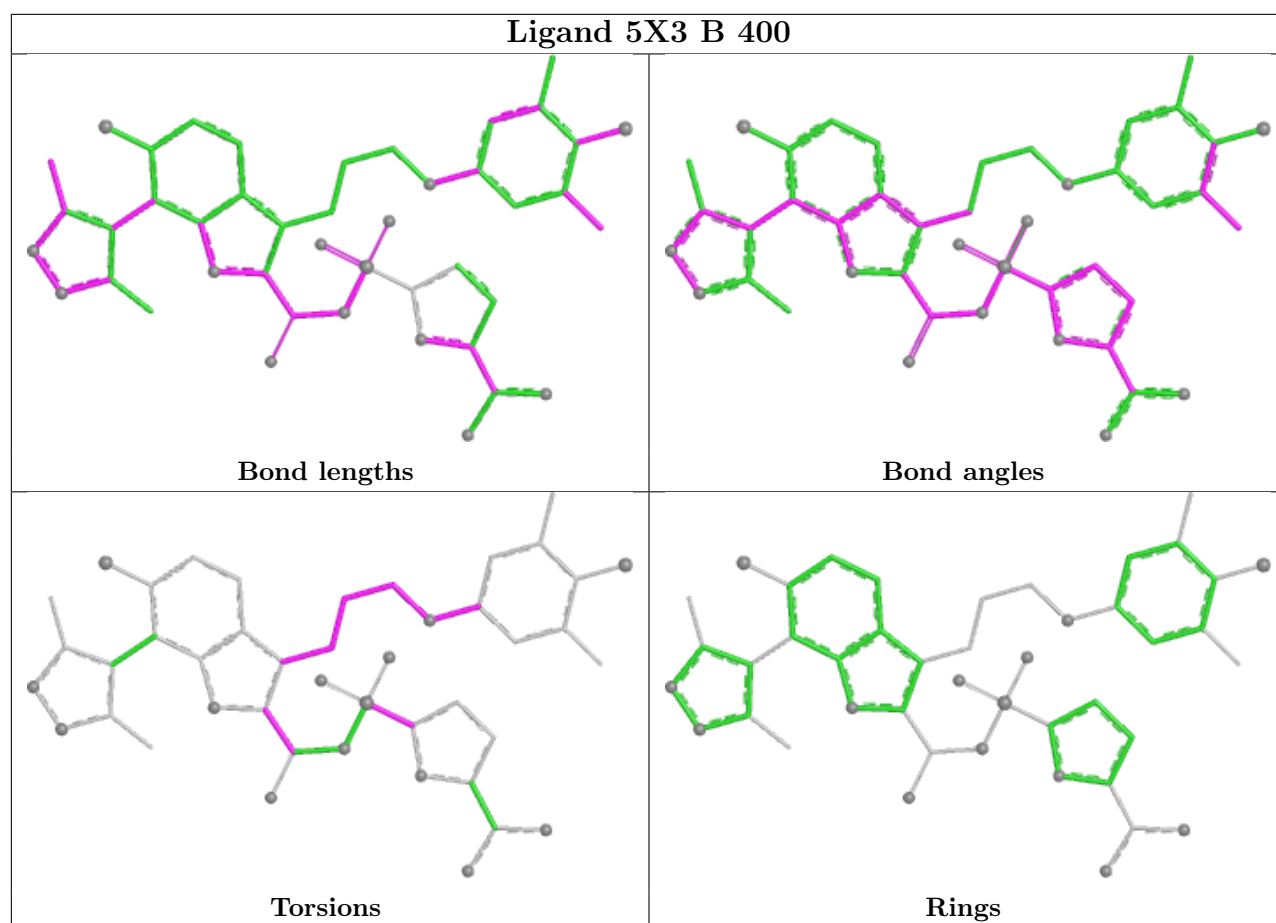
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	400	5X3	2	0
2	A	400	5X3	3	0
2	C	400	5X3	3	0
2	B	400	5X3	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	155/158 (98%)	-1.09	0 100 100	21, 35, 55, 82	0
1	B	149/158 (94%)	-0.96	0 100 100	27, 41, 64, 79	0
1	C	143/158 (90%)	-1.04	0 100 100	23, 37, 55, 69	0
1	D	148/158 (93%)	-0.87	0 100 100	22, 44, 74, 93	0
All	All	595/632 (94%)	-0.99	0 100 100	21, 40, 64, 93	0

There are no RSRZ outliers to report.

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](#)

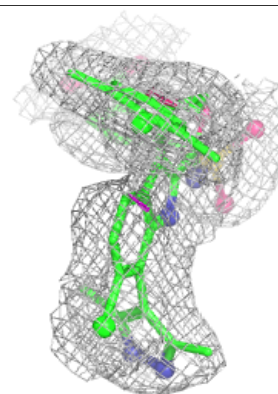
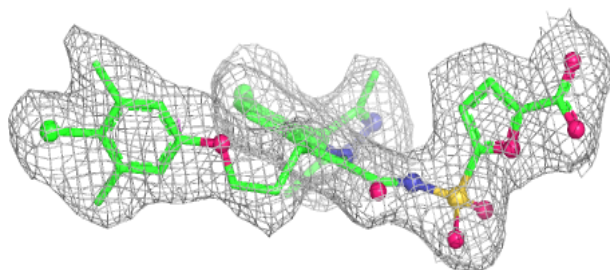
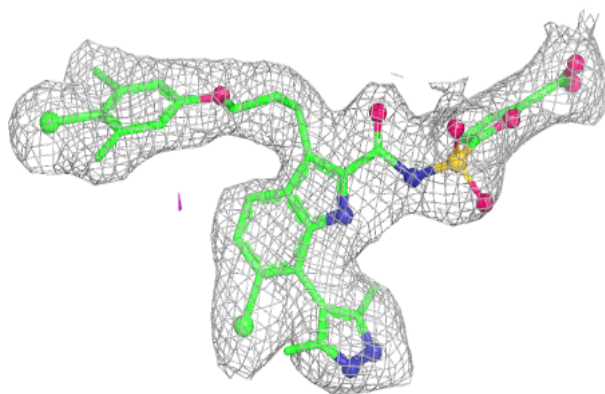
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	5X3	A	400	44/44	0.99	0.04	11,29,44,46	0
2	5X3	B	400	44/44	0.99	0.04	14,28,42,51	0
2	5X3	C	400	44/44	0.99	0.04	9,30,54,60	0
2	5X3	D	400	44/44	0.99	0.05	0,30,45,63	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.

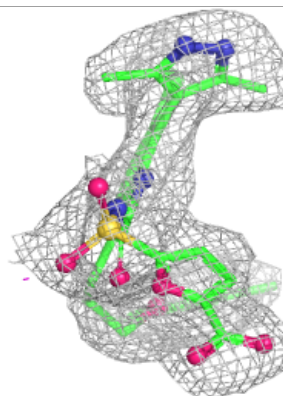
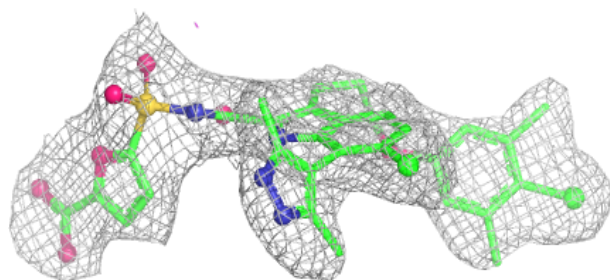
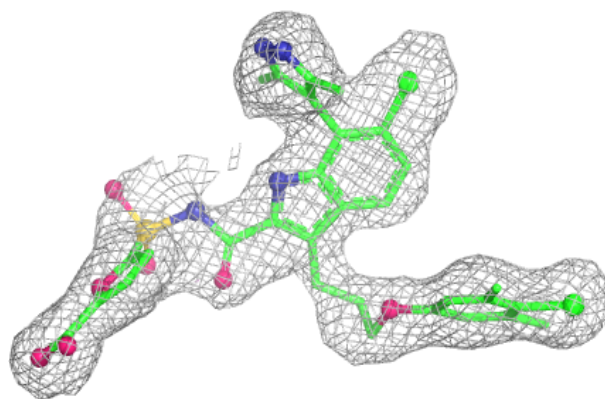
Electron density around 5X3 A 400:

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

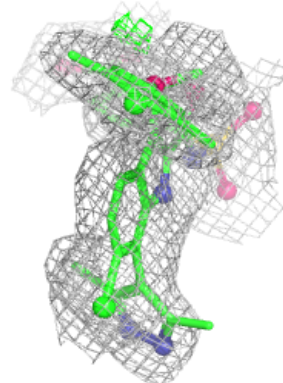
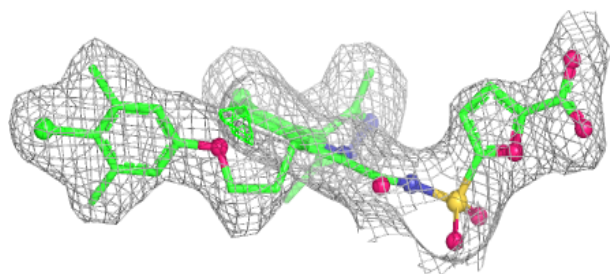
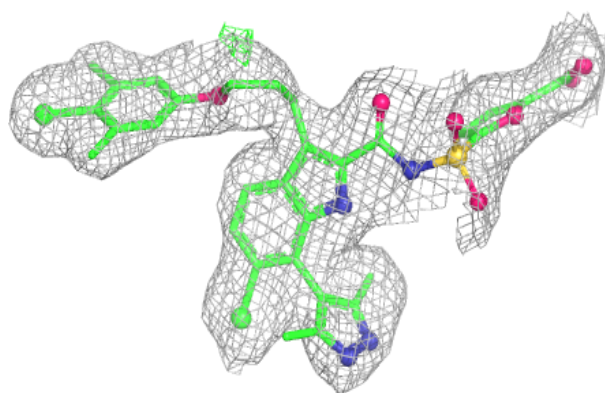


Electron density around 5X3 B 400:

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

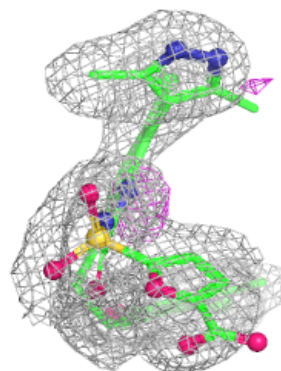
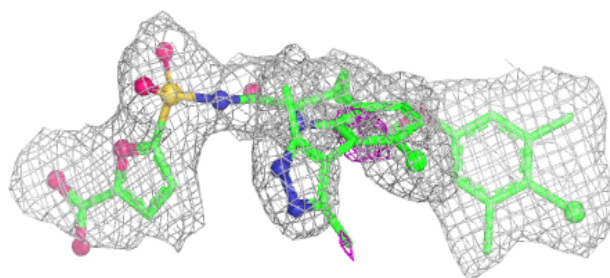
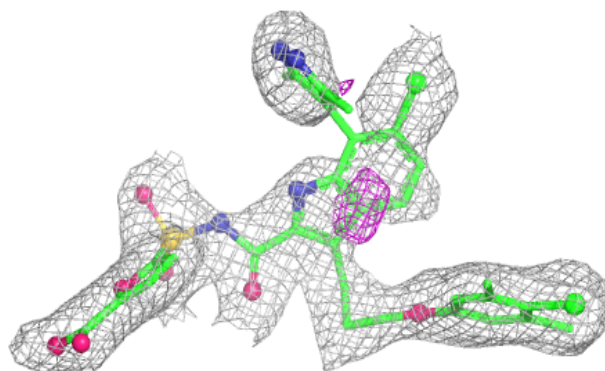
**Electron density around 5X3 C 400:**

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



Electron density around 5X3 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.