



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:08 AM UTC

PDB ID : 8AUP / pdb_00008aup
Title : Structure of hARG1 with a novel inhibitor.
Authors : Napiorkowska-Gromadzka, A.; Nowak, E.; Nowotny, M.
Deposited on : 2022-08-25
Resolution : 2.17 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

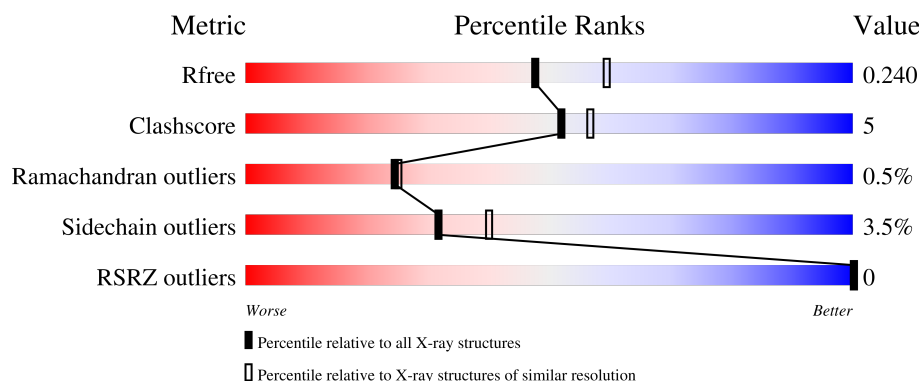
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.17 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	322	
1	B	322	
1	C	322	
1	D	322	
1	E	322	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	322	82% 16% ..

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15307 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.

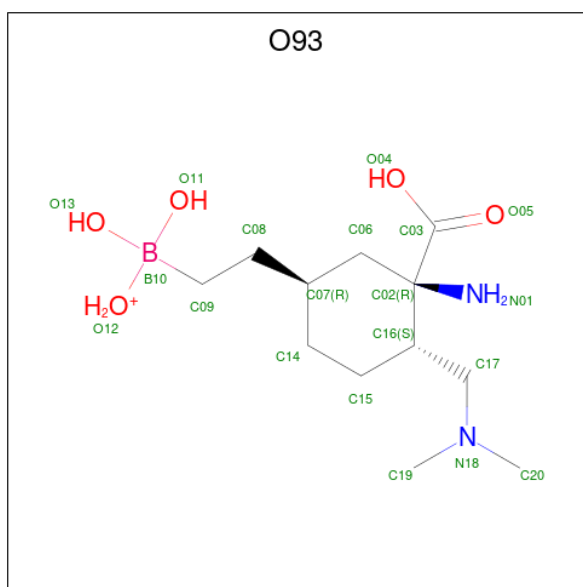
- Molecule 1 is a protein called Arginase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	1	0
			2390	1523	408	453	6			
1	B	318	Total	C	N	O	S	1	1	0
			2417	1541	412	458	6			
1	C	316	Total	C	N	O	S	0	0	0
			2374	1515	403	450	6			
1	D	318	Total	C	N	O	S	0	0	0
			2382	1517	403	456	6			
1	E	318	Total	C	N	O	S	0	0	0
			2390	1523	403	458	6			
1	F	317	Total	C	N	O	S	0	0	0
			2368	1507	399	456	6			

- Molecule 2 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

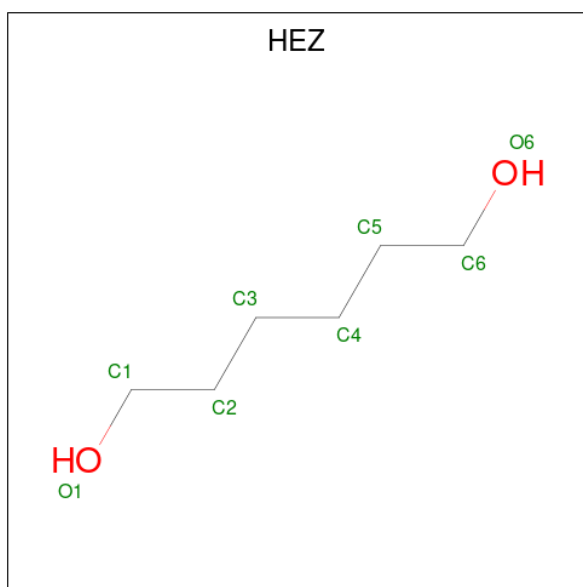
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	B	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		
2	D	2	Total	Mn	0	0
			2	2		
2	E	2	Total	Mn	0	0
			2	2		
2	F	2	Total	Mn	0	0
			2	2		

- Molecule 3 is 2-[(1 {R},3 {R},4 {S})-3-azanyl-3-carboxy-4-[(dimethylamino)methyl]cyclohexyl]ethyl- $\text{B}(\text{OH})_3$ -oxidanyl-bis(oxidanyl)boron (CCD ID: O93) (formula: $\text{C}_{12}\text{H}_{27}\text{BN}_2\text{O}_5$) (labeled as "Ligand of Interest" by depositor).



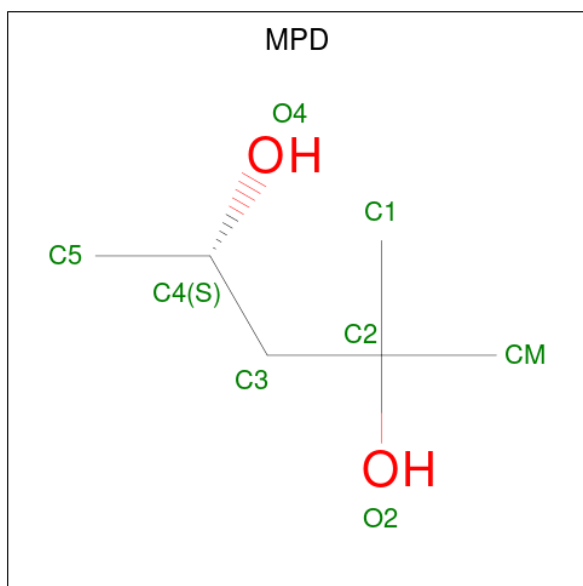
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	B	C	N	O	0	0
			20	1	12	2	5		
3	B	1	Total	B	C	N	O	0	0
			20	1	12	2	5		
3	C	1	Total	B	C	N	O	0	0
			20	1	12	2	5		
3	D	1	Total	B	C	N	O	0	0
			20	1	12	2	5		
3	E	1	Total	B	C	N	O	0	0
			20	1	12	2	5		
3	F	1	Total	B	C	N	O	0	0
			20	1	12	2	5		

- Molecule 4 is HEXANE-1,6-DIOL (CCD ID: HEZ) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			8	6	2		

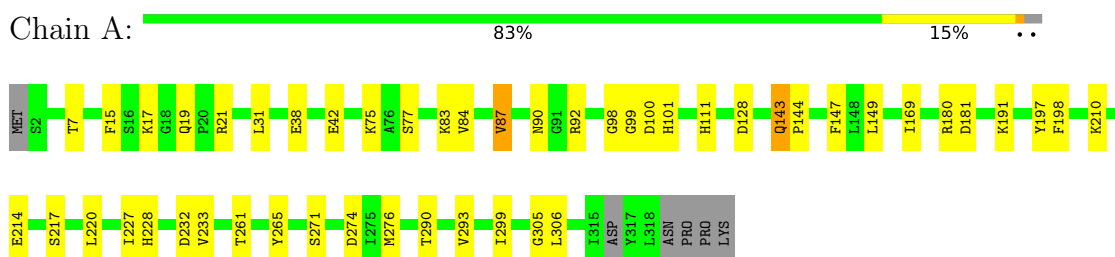
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	166	Total 166	O 166	0	0
6	B	165	Total 165	O 165	0	0
6	C	133	Total 133	O 133	0	0
6	D	141	Total 141	O 141	0	0
6	E	120	Total 120	O 120	0	0
6	F	113	Total 113	O 113	0	0

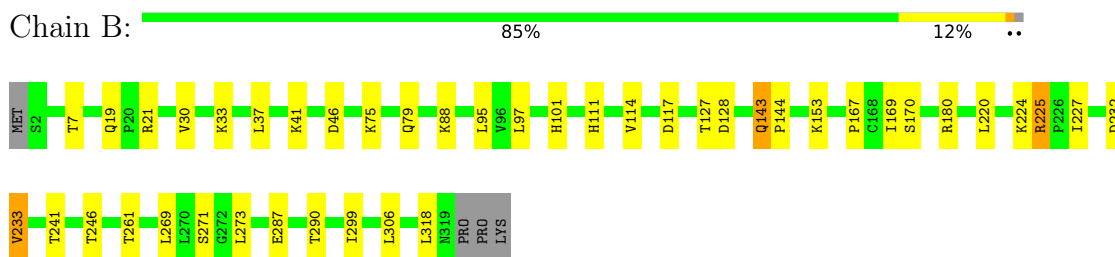
3 Residue-property plots

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.

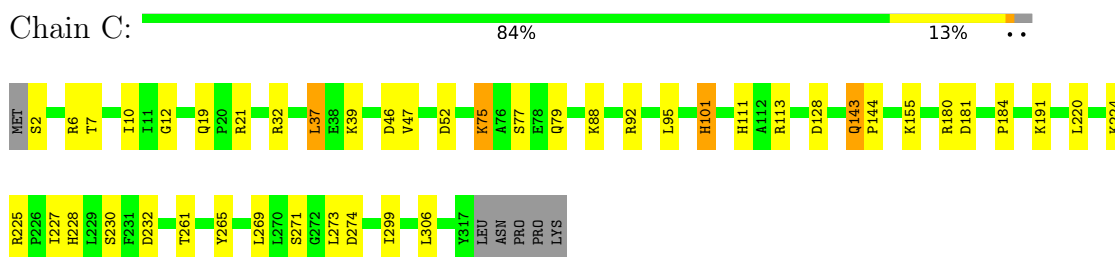
• Molecule 1: Arginase-1



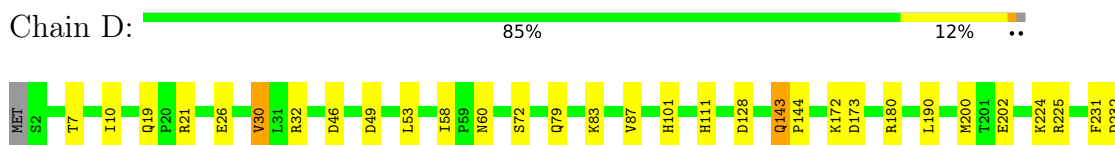
• Molecule 1: Arginase-1



• Molecule 1: Arginase-1



• Molecule 1: Arginase-1





- Molecule 1: Arginase-1

Chain E: 84% 14% ..



- Molecule 1: Arginase-1

Chain F: 82% 16% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.36Å 52.75Å 283.60Å 90.00° 90.65° 90.00°	Depositor
Resolution (Å)	49.11 – 2.17 49.11 – 2.17	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.11-2.17) 87.0 (49.11-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.18Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158, PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.207 , 0.240 0.207 , 0.240	Depositor DCC
R_{free} test set	2101 reflections (1.98%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.928	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.229 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15307	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN, HEZ, O93, MPD

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	0.12	0/2442	0.31	0/3313
1	B	0.12	0/2470	0.34	2/3351 (0.1%)
1	C	0.11	0/2424	0.31	0/3293
1	D	0.12	0/2432	0.30	0/3309
1	E	0.13	0/2440	0.31	0/3317
1	F	0.13	0/2418	0.32	0/3293
All	All	0.12	0/14626	0.32	2/19876 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	97	LEU	CA-C-N	-5.24	117.03	122.69
1	B	97	LEU	C-N-CA	-5.24	117.03	122.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2390	0	2420	23	0
1	B	2417	0	2462	20	0
1	C	2374	0	2398	31	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2382	0	2381	22	0
1	E	2390	0	2403	28	0
1	F	2368	0	2353	26	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
3	A	20	0	0	0	0
3	B	20	0	0	0	0
3	C	20	0	0	0	0
3	D	20	0	0	0	0
3	E	20	0	0	1	0
3	F	20	0	0	0	0
4	A	8	0	14	0	0
5	B	8	0	14	1	0
6	A	166	0	0	3	0
6	B	165	0	0	0	0
6	C	133	0	0	6	0
6	D	141	0	0	2	0
6	E	120	0	0	5	0
6	F	113	0	0	2	0
All	All	15307	0	14445	148	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 5.

All (148) 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:19:GLN:NE2	1:A:21:ARG:O	2.13	0.80
1:A:181:ASP:OD2	6:A:501:HOH:O	2.02	0.77
1:F:32:ARG:NH1	1:F:52:ASP:OD1	2.18	0.76
1:B:227:ILE:HD12	1:B:269:LEU:HB2	1.67	0.76
1:F:128:ASP:HB3	1:F:144:PRO:HD2	1.67	0.75
1:D:173:ASP:OD1	1:D:225:ARG:NH1	2.15	0.74
1:D:261:THR:HG21	1:D:299:ILE:HG23	1.70	0.73
1:B:318:LEU:HD13	1:C:155:LYS:HG2	1.69	0.72
5:B:404:MPD:H31	1:C:184:PRO:HG3	1.71	0.72
1:C:181:ASP:OD2	6:C:501:HOH:O	2.08	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:261:THR:HG21	1:F:299:ILE:HG23	1.74	0.70
1:F:236:LEU:HD11	1:F:299:ILE:HD11	1.75	0.69
1:B:128:ASP:HB3	1:B:144:PRO:HD2	1.75	0.69
1:C:10:ILE:HD13	1:C:37:LEU:HD22	1.73	0.69
1:E:128:ASP:HB3	1:E:144:PRO:HD2	1.74	0.69
1:C:79:GLN:NE2	6:C:502:HOH:O	2.21	0.68
1:A:128:ASP:HB3	1:A:144:PRO:HD2	1.75	0.67
1:B:220:LEU:HD11	1:B:227:ILE:HD11	1.80	0.64
1:A:220:LEU:HD11	1:A:227:ILE:HD11	1.80	0.64
1:C:111:HIS:ND1	1:C:228:HIS:HD2	1.98	0.61
1:C:224:LYS:NZ	6:C:508:HOH:O	2.33	0.61
1:E:32:ARG:O	6:E:501:HOH:O	2.16	0.61
1:C:261:THR:HG21	1:C:299:ILE:HG23	1.82	0.60
1:D:19:GLN:NE2	1:D:21:ARG:O	2.28	0.60
1:F:15:PHE:HB3	1:F:103:LEU:HD11	1.84	0.59
1:B:111:HIS:CE1	1:B:271:SER:HB3	2.38	0.58
1:D:128:ASP:HB3	1:D:144:PRO:HD2	1.84	0.58
1:C:128:ASP:HB3	1:C:144:PRO:HD2	1.86	0.58
1:A:90:ASN:ND2	6:A:511:HOH:O	2.37	0.58
1:D:32:ARG:NH1	1:D:49:ASP:OD2	2.24	0.58
1:D:60:ASN:OD1	1:E:196:LYS:NZ	2.36	0.58
1:E:88:LYS:O	6:E:502:HOH:O	2.17	0.58
1:F:220:LEU:HD11	1:F:227:ILE:HD11	1.86	0.57
1:F:180:ARG:NH1	1:F:248:VAL:O	2.38	0.56
1:C:7:THR:HG22	1:C:92:ARG:HG2	1.86	0.56
1:C:180:ARG:NH2	6:C:513:HOH:O	2.39	0.55
1:B:88:LYS:HB2	1:B:114:VAL:HG21	1.88	0.55
1:C:19:GLN:NE2	1:C:21:ARG:O	2.32	0.55
1:B:7:THR:HG22	1:B:46:ASP:HB3	1.87	0.55
1:E:261:THR:HG21	1:E:299:ILE:HG23	1.89	0.54
1:D:224:LYS:HE2	1:D:269:LEU:HD11	1.90	0.54
1:A:19:GLN:HG2	1:A:100:ASP:HB3	1.90	0.53
1:C:75:LYS:O	1:C:79:GLN:HG3	2.08	0.53
1:C:32:ARG:NH1	1:C:52:ASP:OD1	2.35	0.53
1:C:39:LYS:NZ	6:C:514:HOH:O	2.41	0.53
1:E:4:LYS:NZ	6:E:509:HOH:O	2.33	0.53
1:D:231:PHE:CZ	1:D:299:ILE:HD13	2.45	0.52
1:B:19:GLN:NE2	1:B:21:ARG:O	2.35	0.52
1:B:261:THR:HG21	1:B:299:ILE:HG23	1.90	0.51
1:A:31:LEU:HD23	1:A:293:VAL:HG13	1.92	0.51
1:A:101:HIS:CE1	1:A:232:ASP:HB2	2.46	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:LYS:O	1:A:87:VAL:HG12	2.10	0.51
1:F:146:SER:HA	1:F:152:LEU:HD12	1.93	0.50
1:A:111:HIS:NE2	1:A:271:SER:OG	2.42	0.50
1:A:191:LYS:NZ	1:A:197:TYR:OH	2.42	0.50
1:D:53:LEU:HD21	1:D:83:LYS:HG2	1.94	0.50
1:D:7:THR:HG22	1:D:46:ASP:HB3	1.94	0.49
1:F:180:ARG:NH2	1:F:235:GLY:O	2.45	0.49
1:A:38:GLU:O	1:A:42:GLU:HG3	2.12	0.49
1:B:153:LYS:HG3	1:B:167:PRO:HG2	1.95	0.49
1:C:220:LEU:HD11	1:C:227:ILE:HD11	1.94	0.49
1:D:233:VAL:HG13	1:D:241:THR:HB	1.94	0.48
1:B:117:ASP:O	1:B:225:ARG:HD3	2.13	0.48
1:F:21:ARG:HH11	1:F:21:ARG:HG3	1.77	0.48
1:B:101:HIS:CE1	1:B:232:ASP:HB2	2.49	0.48
1:D:111:HIS:CE1	1:D:271:SER:HB3	2.49	0.48
1:E:139:ASN:ND2	6:E:518:HOH:O	2.47	0.48
1:B:233:VAL:HG13	1:B:241:THR:HB	1.95	0.48
1:B:287:GLU:HA	1:B:290:THR:HG22	1.96	0.47
1:B:224:LYS:HD2	1:B:269:LEU:HD11	1.96	0.47
1:E:124:ASP:OD1	1:E:125:ALA:N	2.46	0.47
1:C:101:HIS:CE1	1:C:232:ASP:HB2	2.50	0.47
1:C:227:ILE:HD12	1:C:269:LEU:HB2	1.96	0.47
1:B:37:LEU:O	1:B:41:LYS:HG3	2.14	0.47
1:F:101:HIS:CD2	1:F:276:MET:HG3	2.50	0.47
1:A:228:HIS:HE1	1:A:274:ASP:OD2	1.97	0.47
1:C:113:ARG:NH1	6:C:516:HOH:O	2.46	0.46
1:E:84:VAL:O	1:E:88:LYS:HG2	2.16	0.46
1:C:111:HIS:NE2	1:C:271:SER:OG	2.48	0.46
1:E:84:VAL:HG21	1:E:107:SER:HA	1.97	0.45
1:E:220:LEU:HD13	1:E:269:LEU:HD12	1.98	0.45
1:F:28:PRO:HG3	1:F:97:LEU:O	2.16	0.45
1:A:149:LEU:HD23	1:A:169:ILE:HG13	1.98	0.45
1:C:6:ARG:NH1	1:C:265:TYR:OH	2.48	0.45
1:C:75:LYS:HA	1:C:75:LYS:HD2	1.78	0.45
1:E:233:VAL:HG22	1:E:241:THR:HG21	1.97	0.45
1:D:202:GLU:OE2	6:D:501:HOH:O	2.21	0.45
1:E:19:GLN:NE2	1:E:21:ARG:O	2.34	0.45
1:C:230:SER:HA	1:C:274:ASP:HB2	1.97	0.45
1:E:37:LEU:H	1:E:37:LEU:HD12	1.82	0.45
1:F:88:LYS:HA	1:F:88:LYS:HD2	1.61	0.45
1:A:15:PHE:CZ	1:A:17:LYS:HB2	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:75:LYS:O	1:E:79:GLN:HG3	2.16	0.45
1:F:10:ILE:HD12	1:F:47:VAL:HG13	1.98	0.45
1:C:12:GLY:HA3	1:C:52:ASP:OD1	2.16	0.45
1:F:15:PHE:HE2	1:F:73:VAL:HG22	1.80	0.45
1:F:53:LEU:HD21	1:F:83:LYS:HG2	1.98	0.45
1:C:10:ILE:HD12	1:C:47:VAL:HG13	1.97	0.45
1:A:261:THR:HG21	1:A:299:ILE:HG23	1.99	0.44
1:D:274:ASP:HB3	1:D:276:MET:SD	2.57	0.44
1:F:319:ASN:ND2	6:F:519:HOH:O	2.50	0.44
1:E:7:THR:HG22	1:E:92:ARG:HA	2.00	0.44
1:E:126:HIS:ND1	3:E:403:O93:O12	2.49	0.44
1:D:200:MET:HE1	1:D:252:LEU:HD23	1.99	0.44
1:C:228:HIS:HE1	1:C:274:ASP:OD2	2.01	0.44
1:C:191:LYS:HA	1:C:191:LYS:HD2	1.76	0.44
1:F:21:ARG:NH1	1:F:245:GLY:O	2.50	0.44
1:A:98:GLY:HA3	1:A:276:MET:SD	2.58	0.43
1:E:230:SER:HA	1:E:274:ASP:HB2	2.00	0.43
1:F:3:ALA:N	6:F:520:HOH:O	2.50	0.43
1:F:297:VAL:O	1:F:301:LEU:HG	2.17	0.43
1:B:143:GLN:N	1:B:144:PRO:CD	2.82	0.43
1:D:101:HIS:CE1	1:D:232:ASP:HB2	2.54	0.43
1:D:236:LEU:HD11	1:D:299:ILE:CD1	2.48	0.43
1:A:147:PHE:O	6:A:502:HOH:O	2.21	0.43
1:E:40:LEU:O	1:E:45:CYS:HB2	2.18	0.43
1:A:198:PHE:HZ	1:A:214:GLU:HG2	1.84	0.43
1:B:30:VAL:HA	1:B:33:LYS:HG2	2.01	0.43
1:E:258:LEU:HD23	1:E:299:ILE:HD13	2.01	0.43
1:E:109:SER:O	1:E:113:ARG:HG3	2.19	0.42
1:A:143:GLN:N	1:A:144:PRO:CD	2.82	0.42
1:A:265:TYR:CE2	1:A:305:GLY:HA2	2.54	0.42
1:D:143:GLN:N	1:D:144:PRO:CD	2.82	0.42
1:F:265:TYR:CE2	1:F:305:GLY:HA2	2.54	0.42
1:D:58:ILE:HD12	1:D:72:SER:HA	2.01	0.42
1:C:95:LEU:HD13	1:C:273:LEU:HD23	2.02	0.42
1:C:143:GLN:N	1:C:144:PRO:CD	2.83	0.42
1:D:265:TYR:CE2	1:D:305:GLY:HA2	2.54	0.42
1:A:15:PHE:O	1:A:99:GLY:HA3	2.20	0.42
1:F:143:GLN:N	1:F:144:PRO:CD	2.83	0.42
1:E:58:ILE:HD12	1:E:72:SER:HA	2.01	0.41
1:E:143:GLN:N	1:E:144:PRO:CD	2.83	0.41
1:F:208:ILE:HB	1:F:256:GLU:HG2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:GLU:O	1:D:30:VAL:HG22	2.20	0.41
1:B:75[A]:LYS:HE3	1:B:79:GLN:HG3	2.02	0.41
1:F:240:PHE:CE1	1:F:254:TYR:HB2	2.55	0.41
1:C:88:LYS:HD2	1:C:88:LYS:HA	1.83	0.41
1:B:95:LEU:HD13	1:B:273:LEU:HD23	2.01	0.41
1:D:79:GLN:NE2	6:D:502:HOH:O	2.30	0.41
1:E:15:PHE:HB3	1:E:103:LEU:HD11	2.03	0.41
1:E:233:VAL:HG13	1:E:241:THR:HB	2.02	0.41
1:C:2:SER:HB2	1:C:46:ASP:HB2	2.03	0.40
1:E:66:ILE:HG12	1:E:138:GLY:HA3	2.02	0.40
1:E:200:MET:HE3	1:E:200:MET:HA	2.03	0.40
1:F:66:ILE:HD12	1:F:66:ILE:HA	1.89	0.40
1:E:37:LEU:HD12	6:E:501:HOH:O	2.21	0.40
1:F:240:PHE:CD1	1:F:254:TYR:HB2	2.56	0.40
1:A:7:THR:HG22	1:A:92:ARG:HG2	2.02	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	313/322 (97%)	307 (98%)	4 (1%)	2 (1%)	21	20
1	B	317/322 (98%)	307 (97%)	8 (2%)	2 (1%)	21	20
1	C	314/322 (98%)	307 (98%)	6 (2%)	1 (0%)	36	39
1	D	316/322 (98%)	306 (97%)	8 (2%)	2 (1%)	21	20
1	E	316/322 (98%)	310 (98%)	5 (2%)	1 (0%)	36	39
1	F	315/322 (98%)	305 (97%)	9 (3%)	1 (0%)	36	39
All	All	1891/1932 (98%)	1842 (97%)	40 (2%)	9 (0%)	24	25

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	180	ARG
1	B	180	ARG
1	D	143	GLN
1	A	180	ARG
1	B	143	GLN
1	F	143	GLN
1	A	143	GLN
1	C	143	GLN
1	E	143	GLN

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	260/270 (96%)	250 (96%)	10 (4%)	29	37
1	B	265/270 (98%)	258 (97%)	7 (3%)	40	51
1	C	257/270 (95%)	251 (98%)	6 (2%)	44	56
1	D	257/270 (95%)	249 (97%)	8 (3%)	35	45
1	E	260/270 (96%)	251 (96%)	9 (4%)	32	40
1	F	255/270 (94%)	240 (94%)	15 (6%)	18	19
All	All	1554/1620 (96%)	1499 (96%)	55 (4%)	32	40

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75[A]	LYS
1	A	75[B]	LYS
1	A	77	SER
1	A	84	VAL
1	A	87	VAL
1	A	210	LYS
1	A	217	SER
1	A	233	VAL
1	A	290	THR
1	A	306	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	127	THR
1	B	169	ILE
1	B	170	SER
1	B	225	ARG
1	B	233	VAL
1	B	246	THR
1	B	306	LEU
1	C	37	LEU
1	C	75	LYS
1	C	77	SER
1	C	101	HIS
1	C	225	ARG
1	C	306	LEU
1	D	10	ILE
1	D	30	VAL
1	D	87	VAL
1	D	172	LYS
1	D	190	LEU
1	D	233	VAL
1	D	246	THR
1	D	299	ILE
1	E	39	LYS
1	E	87	VAL
1	E	225	ARG
1	E	230	SER
1	E	233	VAL
1	E	284	LYS
1	E	290	THR
1	E	306	LEU
1	E	315	ILE
1	F	36	LEU
1	F	37	LEU
1	F	62	SER
1	F	67	VAL
1	F	77	SER
1	F	95	LEU
1	F	136	THR
1	F	180	ARG
1	F	190	LEU
1	F	191	LYS
1	F	225	ARG
1	F	230	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	233	VAL
1	F	299	ILE
1	F	306	LEU

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

Mol	Chain	Res	Type
1	A	65	GLN
1	A	139	ASN
1	A	228	HIS
1	B	143	GLN
1	C	65	GLN
1	C	228	HIS
1	D	43	GLN
1	D	65	GLN
1	D	79	GLN
1	D	115	HIS
1	E	79	GLN
1	E	90	ASN
1	E	130	ASN
1	F	90	ASN
1	F	139	ASN
1	F	319	ASN

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](#)

Of 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	O93	E	403	2	16,20,20	4.53	4 (25%)	16,30,30	1.79	4 (25%)
5	MPD	B	404	-	7,7,7	0.31	0	9,10,10	0.28	0
3	O93	B	403	2	16,20,20	4.51	4 (25%)	16,30,30	1.80	3 (18%)
3	O93	C	403	2	16,20,20	4.56	4 (25%)	16,30,30	1.59	3 (18%)
3	O93	D	403	2	16,20,20	4.53	4 (25%)	16,30,30	1.53	4 (25%)
3	O93	F	403	2	16,20,20	4.57	4 (25%)	16,30,30	1.35	3 (18%)
3	O93	A	403	2	16,20,20	4.55	4 (25%)	16,30,30	1.71	3 (18%)
4	HEZ	A	404	-	7,7,7	0.12	0	6,6,6	0.08	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
3	O93	E	403	2	-	3/11/32/32	0/1/1/1
5	MPD	B	404	-	-	2/5/5/5	-
3	O93	B	403	2	-	5/11/32/32	0/1/1/1
3	O93	C	403	2	-	4/11/32/32	0/1/1/1
3	O93	D	403	2	-	6/11/32/32	0/1/1/1
3	O93	F	403	2	-	5/11/32/32	0/1/1/1
3	O93	A	403	2	-	4/11/32/32	0/1/1/1
4	HEZ	A	404	-	-	1/5/5/5	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	403	O93	B10-O13	10.44	1.69	1.47
3	B	403	O93	B10-O13	10.41	1.69	1.47
3	A	403	O93	B10-O13	10.41	1.69	1.47
3	F	403	O93	B10-O13	10.38	1.69	1.47
3	E	403	O93	B10-O13	10.33	1.69	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	403	O93	B10-O13	10.28	1.69	1.47
3	E	403	O93	B10-O11	10.23	1.69	1.47
3	F	403	O93	B10-O11	10.22	1.69	1.47
3	A	403	O93	B10-O11	10.20	1.69	1.47
3	C	403	O93	B10-O11	10.18	1.69	1.47
3	D	403	O93	B10-O11	10.13	1.69	1.47
3	B	403	O93	B10-O11	10.12	1.69	1.47
3	F	403	O93	B10-O12	9.96	1.68	1.47
3	D	403	O93	B10-O12	9.91	1.68	1.47
3	A	403	O93	B10-O12	9.86	1.68	1.47
3	C	403	O93	B10-O12	9.86	1.68	1.47
3	E	403	O93	B10-O12	9.85	1.68	1.47
3	B	403	O93	B10-O12	9.67	1.68	1.47
3	C	403	O93	B10-C09	3.94	1.68	1.58
3	F	403	O93	B10-C09	3.94	1.68	1.58
3	A	403	O93	B10-C09	3.84	1.68	1.58
3	D	403	O93	B10-C09	3.81	1.67	1.58
3	B	403	O93	B10-C09	3.77	1.67	1.58
3	E	403	O93	B10-C09	3.67	1.67	1.58

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	403	O93	C09-C08-C07	-5.19	110.67	114.64
3	E	403	O93	C06-C07-C14	3.99	113.20	109.48
3	D	403	O93	C09-C08-C07	-3.82	111.72	114.64
3	A	403	O93	C09-C08-C07	-3.76	111.77	114.64
3	A	403	O93	C06-C07-C14	3.74	112.97	109.48
3	C	403	O93	C09-C08-C07	-3.49	111.97	114.64
3	E	403	O93	C09-C08-C07	-3.43	112.02	114.64
3	C	403	O93	C06-C07-C14	3.38	112.63	109.48
3	E	403	O93	B10-C09-C08	-2.72	106.16	115.56
3	D	403	O93	C06-C07-C14	2.72	112.01	109.48
3	A	403	O93	O04-C03-C02	2.71	120.58	113.53
3	B	403	O93	C06-C07-C14	2.70	112.00	109.48
3	C	403	O93	O04-C03-C02	2.62	120.34	113.53
3	B	403	O93	O04-C03-C02	2.60	120.30	113.53
3	F	403	O93	O04-C03-C02	2.51	120.08	113.53
3	E	403	O93	O04-C03-C02	2.50	120.04	113.53
3	F	403	O93	C06-C07-C14	2.45	111.77	109.48
3	D	403	O93	O04-C03-C02	2.29	119.50	113.53
3	F	403	O93	C09-C08-C07	-2.20	112.95	114.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	403	O93	B10-C09-C08	-2.03	108.54	115.56

There are no chirality outliers.

All (30) torsion outliers are listed below:

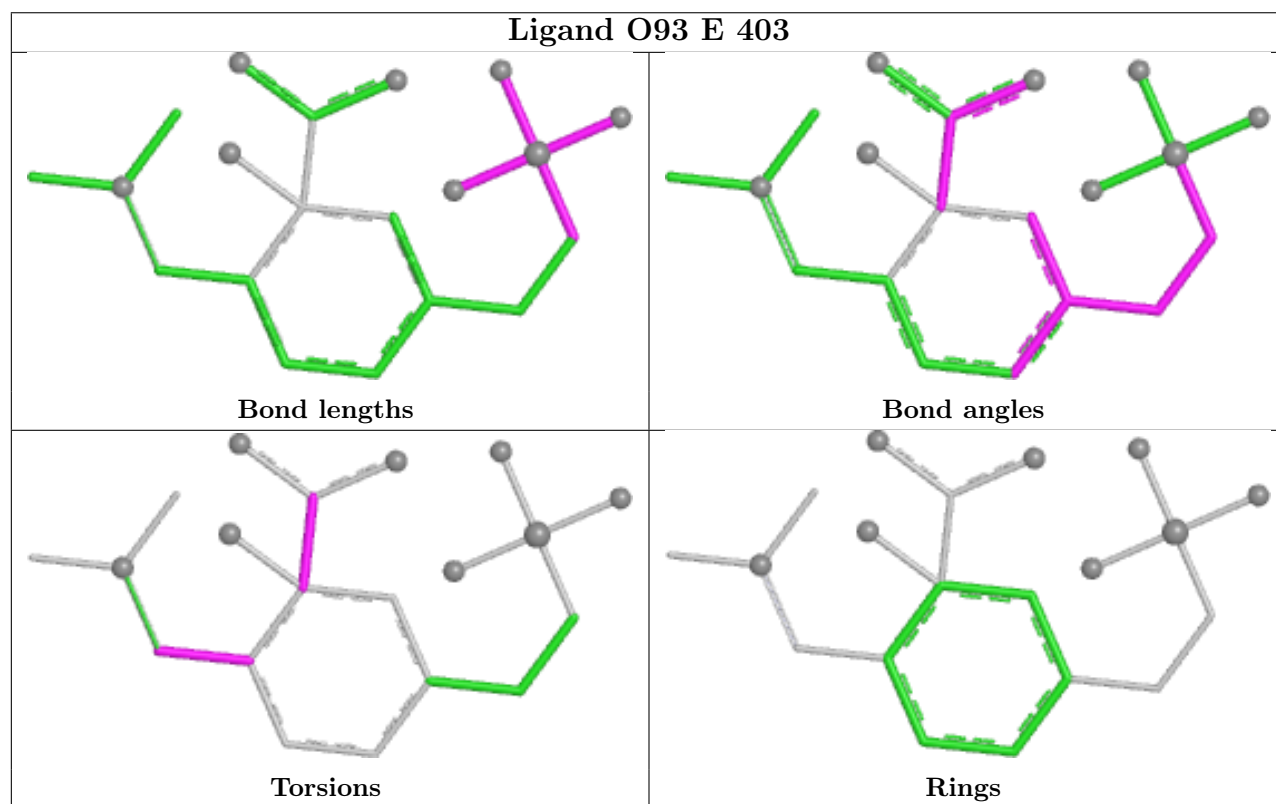
Mol	Chain	Res	Type	Atoms
3	A	403	O93	C15-C16-C17-N18
3	B	403	O93	C15-C16-C17-N18
3	C	403	O93	C15-C16-C17-N18
3	D	403	O93	C15-C16-C17-N18
3	D	403	O93	C16-C17-N18-C19
3	E	403	O93	C15-C16-C17-N18
3	F	403	O93	C15-C16-C17-N18
3	D	403	O93	C16-C02-C03-O04
4	A	404	HEZ	C1-C2-C3-C4
3	B	403	O93	C02-C16-C17-N18
3	D	403	O93	C02-C16-C17-N18
3	E	403	O93	C02-C16-C17-N18
3	F	403	O93	C02-C16-C17-N18
5	B	404	MPD	O2-C2-C3-C4
3	D	403	O93	C16-C02-C03-O05
3	A	403	O93	C06-C07-C08-C09
3	A	403	O93	C14-C07-C08-C09
3	B	403	O93	C06-C07-C08-C09
3	B	403	O93	C14-C07-C08-C09
3	C	403	O93	C06-C07-C08-C09
3	C	403	O93	C14-C07-C08-C09
3	D	403	O93	C06-C07-C08-C09
3	F	403	O93	C06-C07-C08-C09
3	F	403	O93	C14-C07-C08-C09
3	A	403	O93	C02-C16-C17-N18
3	C	403	O93	C02-C16-C17-N18
3	B	403	O93	C16-C02-C03-O04
3	E	403	O93	C16-C02-C03-O04
3	F	403	O93	C16-C02-C03-O05
5	B	404	MPD	C2-C3-C4-O4

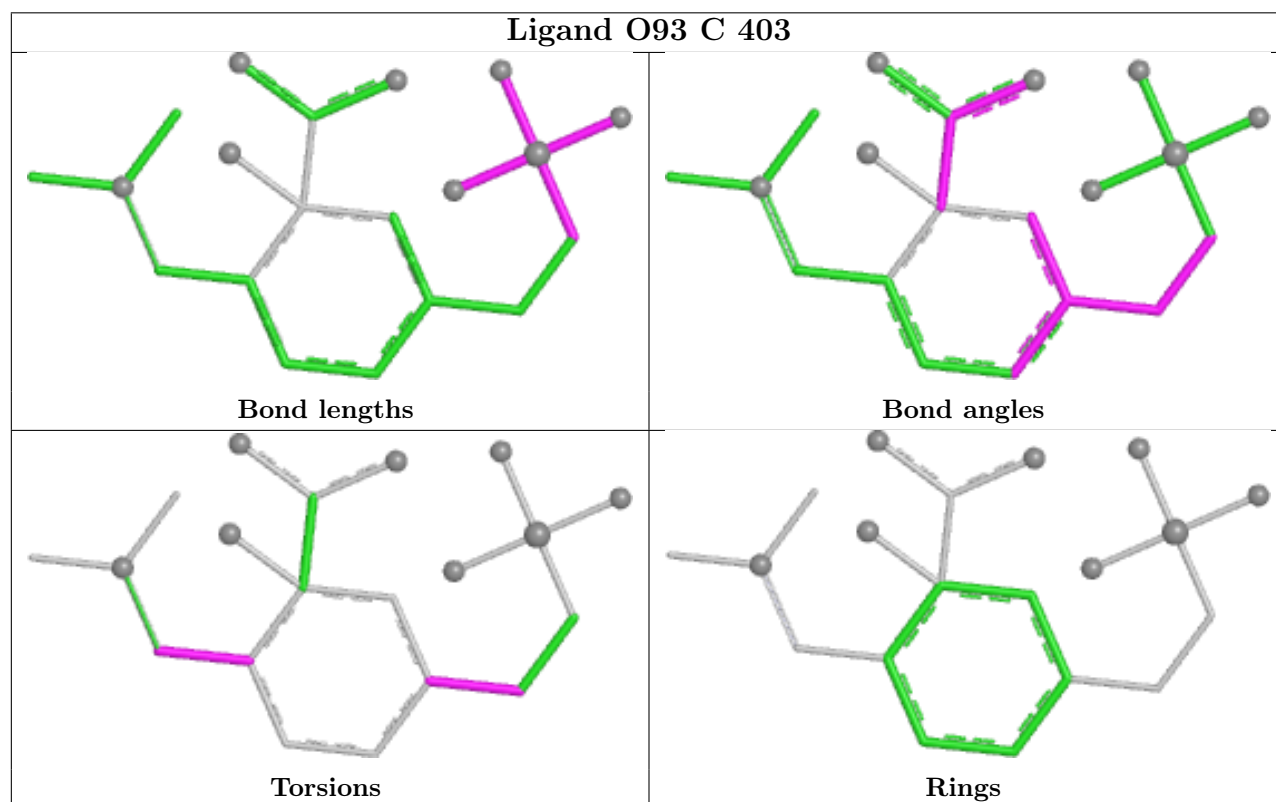
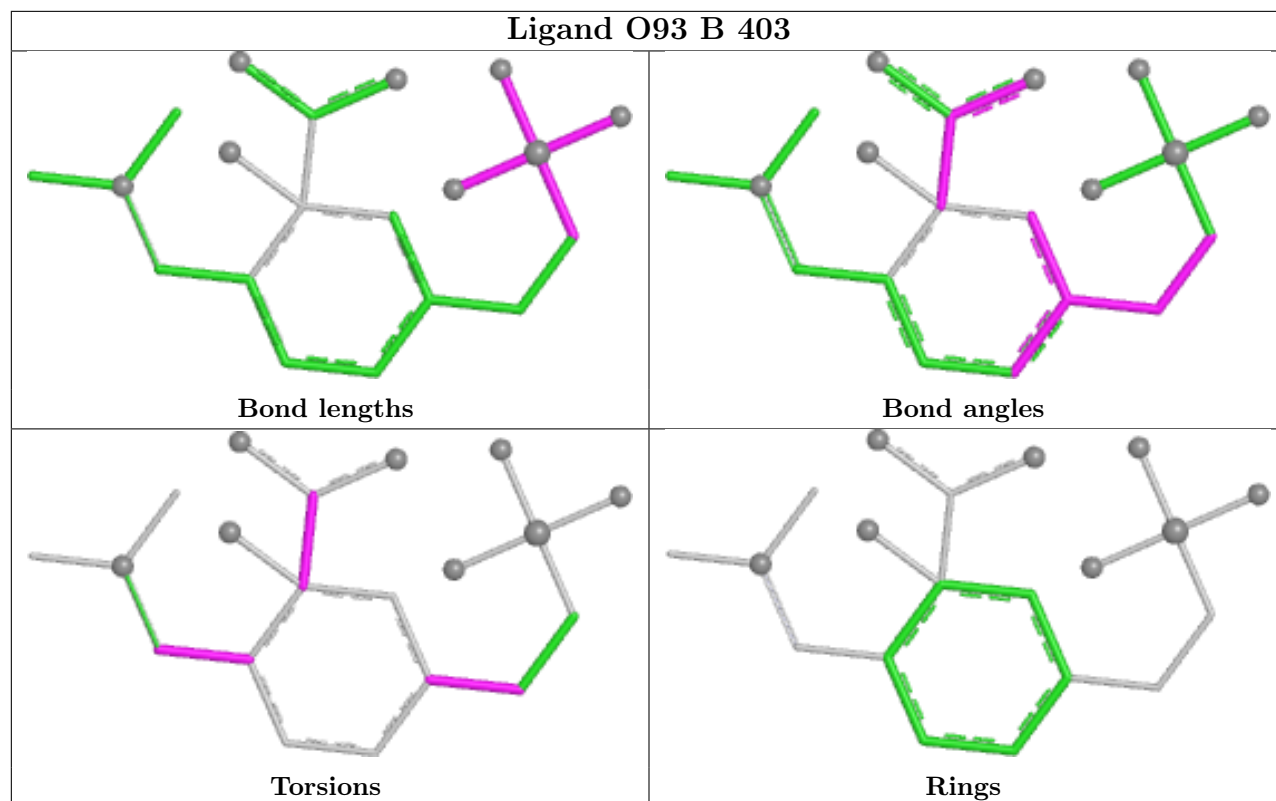
There are no ring outliers.

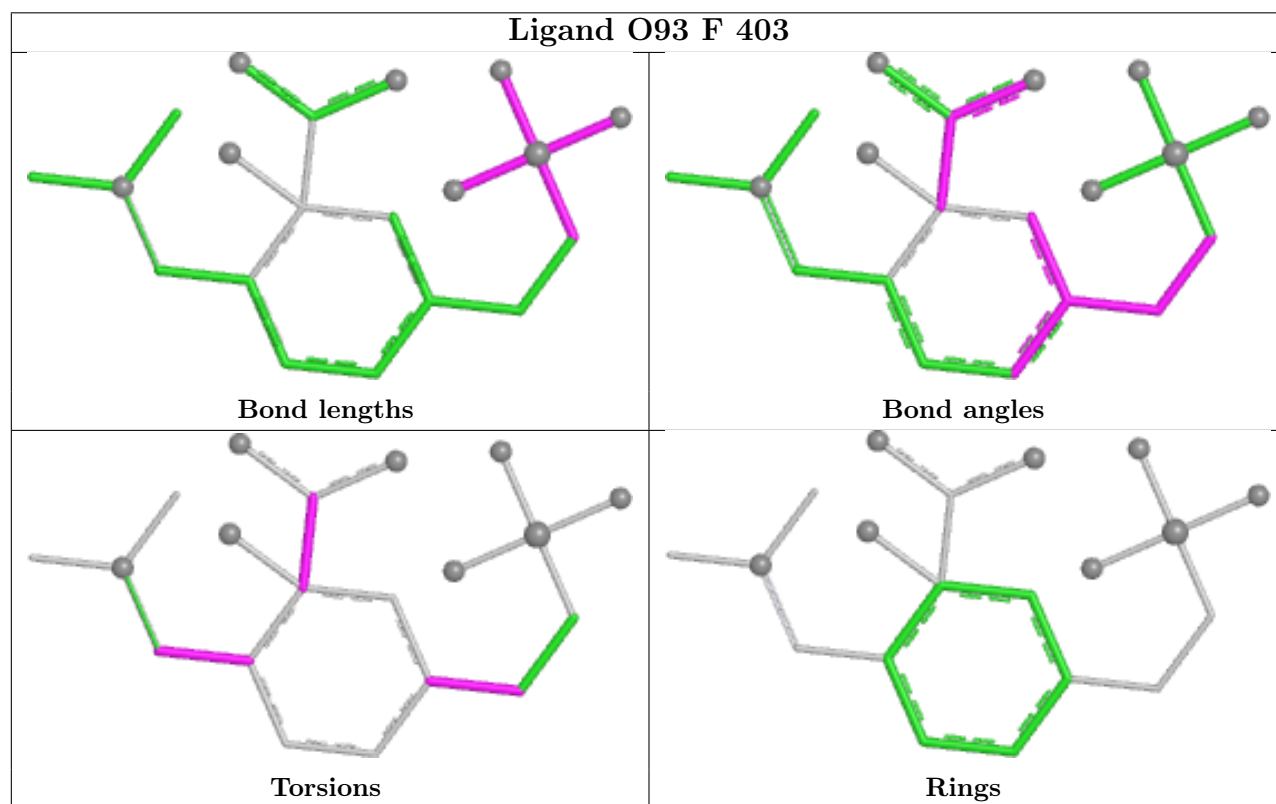
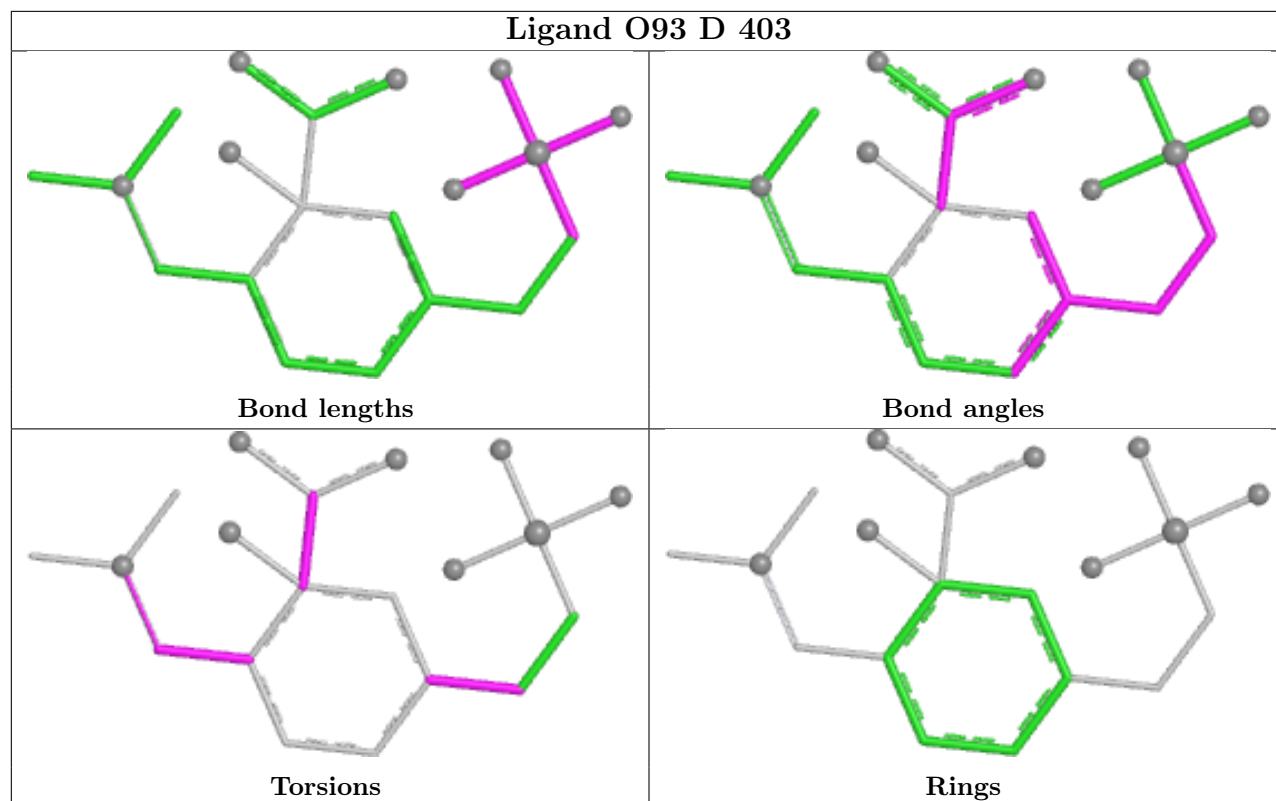
2 monomers are involved in 2 short contacts:

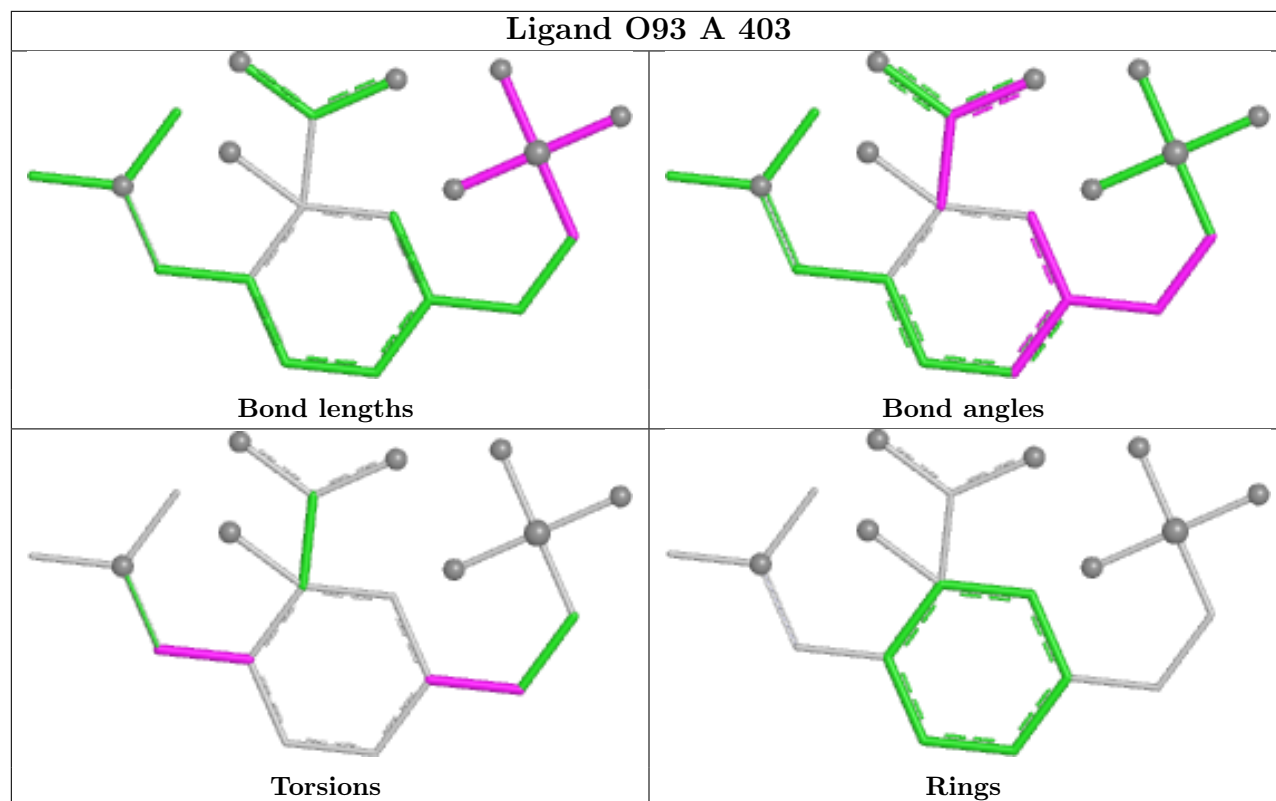
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	403	O93	1	0
5	B	404	MPD	1	0

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	316/322 (98%)	-1.61	0 100 100	24, 35, 56, 84	3 (0%)
1	B	318/322 (98%)	-1.66	0 100 100	21, 33, 48, 67	2 (0%)
1	C	316/322 (98%)	-1.63	0 100 100	25, 34, 51, 88	3 (0%)
1	D	318/322 (98%)	-1.63	0 100 100	25, 34, 48, 71	1 (0%)
1	E	318/322 (98%)	-1.59	0 100 100	25, 45, 64, 96	0
1	F	317/322 (98%)	-1.59	0 100 100	26, 46, 73, 98	0
All	All	1903/1932 (98%)	-1.62	0 100 100	21, 37, 61, 98	9 (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
4	HEZ	A	404	8/8	0.98	0.04	48,49,53,53	0

Continued on next page...

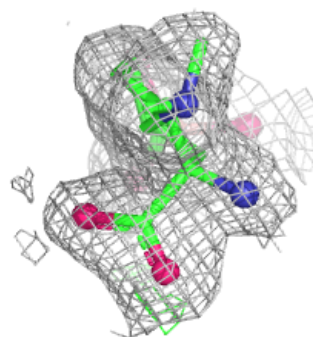
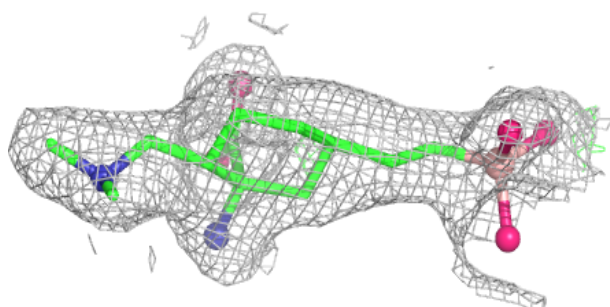
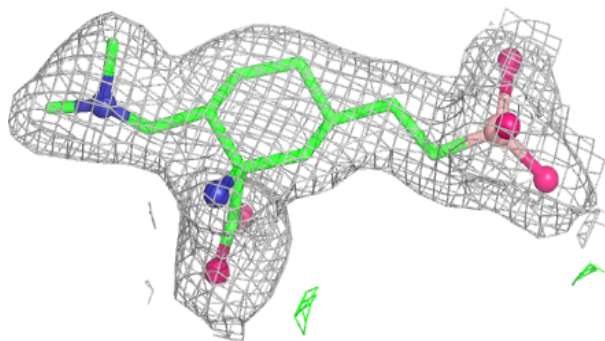
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	O93	D	403	20/20	0.99	0.03	25,32,38,39	0
3	O93	B	403	20/20	0.99	0.03	22,29,36,36	0
5	MPD	B	404	8/8	0.99	0.03	46,49,55,57	0
2	MN	C	401	1/1	1.00	0.01	29,29,29,29	0
2	MN	C	402	1/1	1.00	0.01	31,31,31,31	0
2	MN	D	401	1/1	1.00	0.01	26,26,26,26	0
2	MN	D	402	1/1	1.00	0.00	25,25,25,25	0
2	MN	E	401	1/1	1.00	0.01	35,35,35,35	0
2	MN	E	402	1/1	1.00	0.01	41,41,41,41	0
2	MN	F	401	1/1	1.00	0.01	42,42,42,42	0
2	MN	F	402	1/1	1.00	0.00	35,35,35,35	0
3	O93	A	403	20/20	1.00	0.02	23,36,39,42	0
2	MN	A	401	1/1	1.00	0.00	27,27,27,27	0
3	O93	C	403	20/20	1.00	0.02	26,36,42,46	0
2	MN	A	402	1/1	1.00	0.00	27,27,27,27	0
3	O93	E	403	20/20	1.00	0.02	38,43,51,53	0
3	O93	F	403	20/20	1.00	0.02	39,46,52,53	0
2	MN	B	401	1/1	1.00	0.01	25,25,25,25	0
2	MN	B	402	1/1	1.00	0.01	22,22,22,22	0

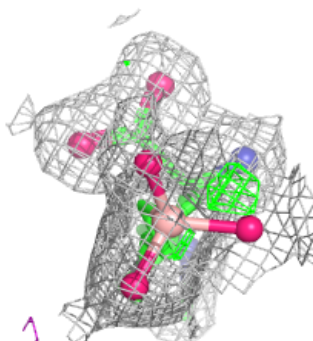
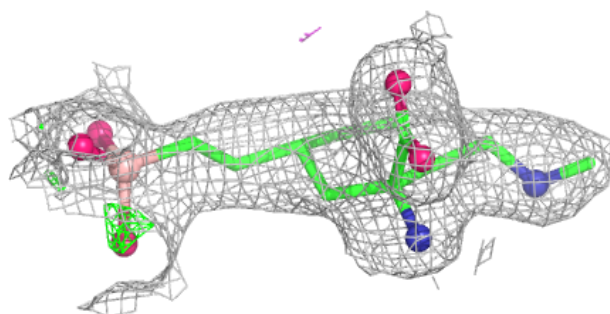
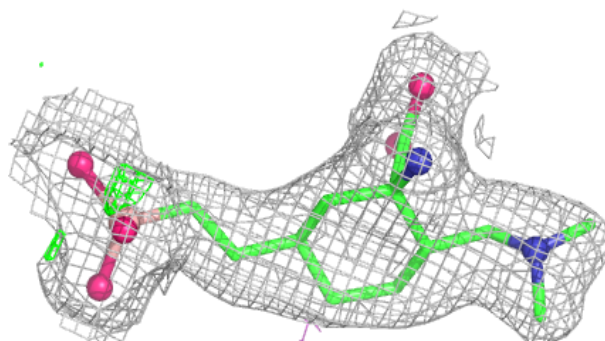
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around O93 D 403:

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

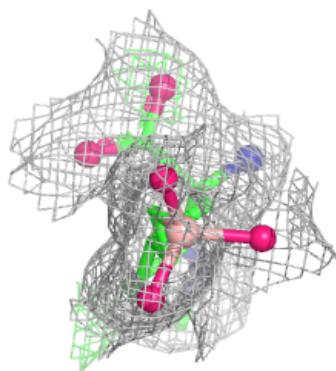
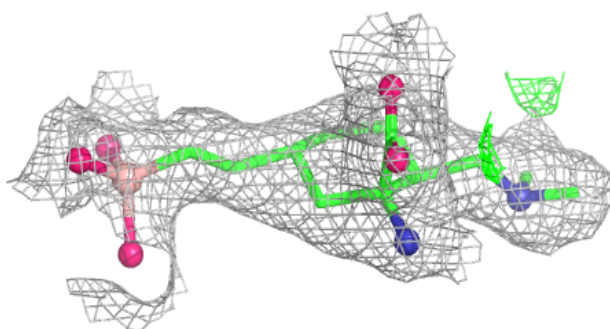
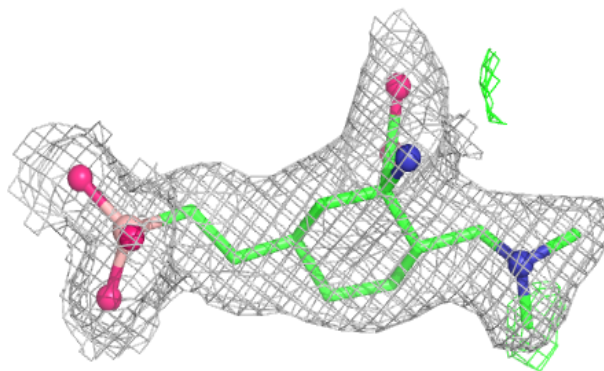
**Electron density around O93 B 403:**

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

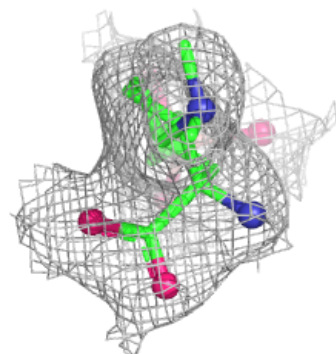
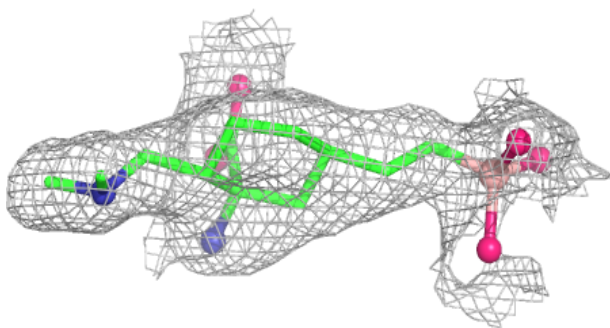
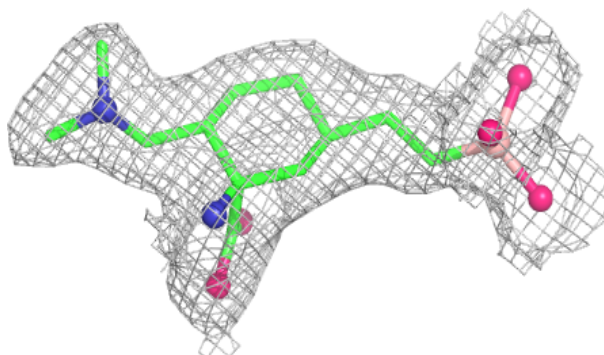


Electron density around O93 A 403:

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

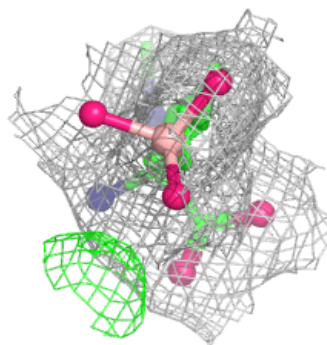
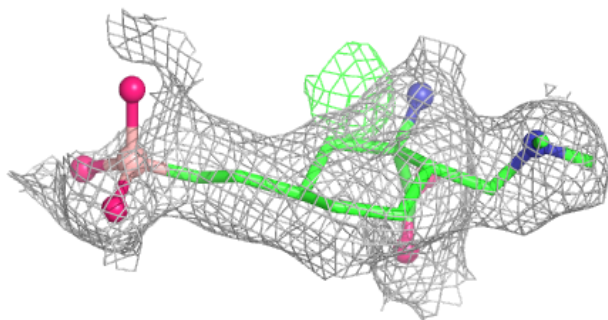
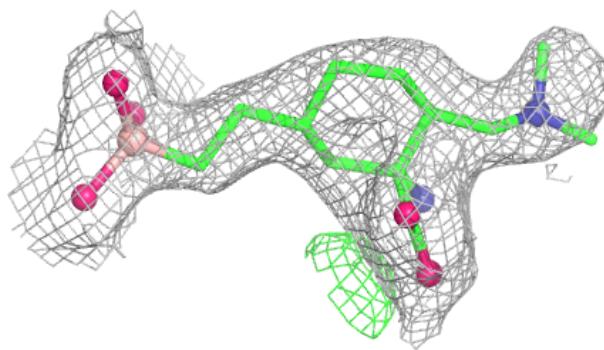
**Electron density around O93 C 403:**

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

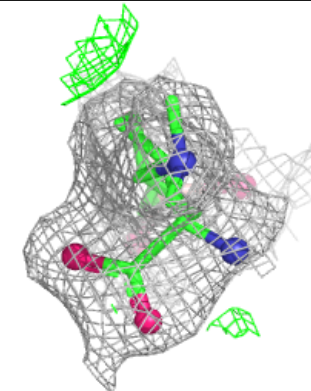
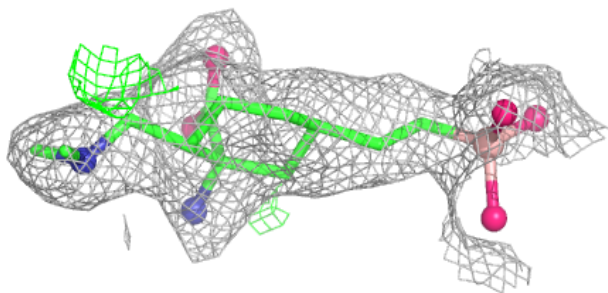
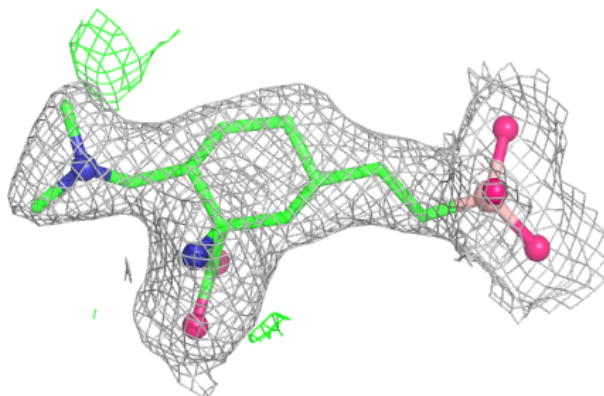


Electron density around O93 E 403:

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

**Electron density around O93 F 403:**

$2mF_o-DF_c$ (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.