Full wwPDB X-ray Structure Validation Report (i)

Aug 21, 2020 – 03:47 PM BST

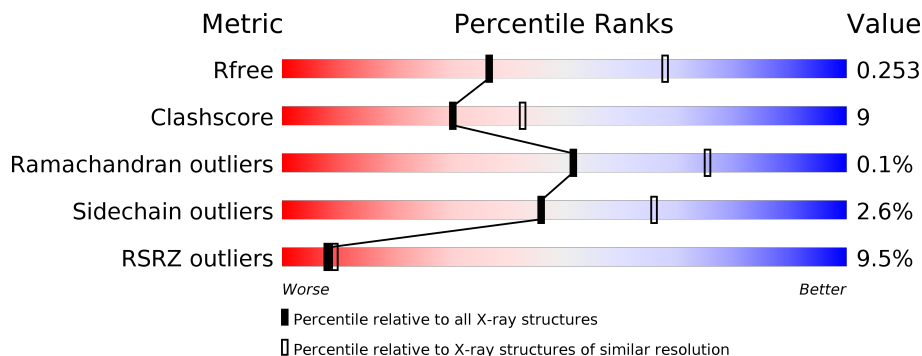|		
PDB ID	:	5K3L
Title	:	Crystal structure of Retinoic acid receptor-related orphan receptor (ROR) gamma ligand binding domain complex with 444
Authors	:	Huang, P.; Rastinejad, F.
Deposited on	:	2016-05-19
Resolution	:	2.75 Å(reported)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.253
Clashscore		9
Ramachandran outliers		0.1%
Sidechain outliers		2.6%
RSRZ outliers		9.5%

Worse　　　　　　　　　　　　　　　　　*Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 on 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	247	8% / 72% / 18% / 9%
1	B	247	10% / 68% / 23% / 9%
1	C	247	7% / 68% / 23% / 9%
1	D	247	10% / 69% / 21% / • / 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	444	A	900	-	X	-	-

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7516 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 Nuclear receptor ROR-gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	225	Total	C	N	O	S	0	0	0
			1840	1165	333	328	14			
1	B	226	Total	C	N	O	S	0	0	0
			1850	1171	336	329	14			
1	C	226	Total	C	N	O	S	0	0	0
			1850	1171	336	329	14			
1	D	226	Total	C	N	O	S	0	0	0
			1850	1171	336	329	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	261	GLY	-	expression tag	UNP P51449
A	262	SER	-	expression tag	UNP P51449
A	263	HIS	-	expression tag	UNP P51449
A	264	MET	-	expression tag	UNP P51449
B	261	GLY	-	expression tag	UNP P51449
B	262	SER	-	expression tag	UNP P51449
B	263	HIS	-	expression tag	UNP P51449
B	264	MET	-	expression tag	UNP P51449
C	261	GLY	-	expression tag	UNP P51449
C	262	SER	-	expression tag	UNP P51449
C	263	HIS	-	expression tag	UNP P51449
C	264	MET	-	expression tag	UNP P51449
D	261	GLY	-	expression tag	UNP P51449
D	262	SER	-	expression tag	UNP P51449
D	263	HIS	-	expression tag	UNP P51449
D	264	MET	-	expression tag	UNP P51449

- Molecule 2 is N-(2,2,2-TRIFLUOROETHYL)-N-{4-[2,2,2-TRIFLUORO-1-HYDROXY-1-(TRIFLUOROMETHYL)ETHYL]PHENYL}BENZENESULFONAMIDE (three-letter code: 444) (formula: $C_{17}H_{12}F_9NO_3S$).

444
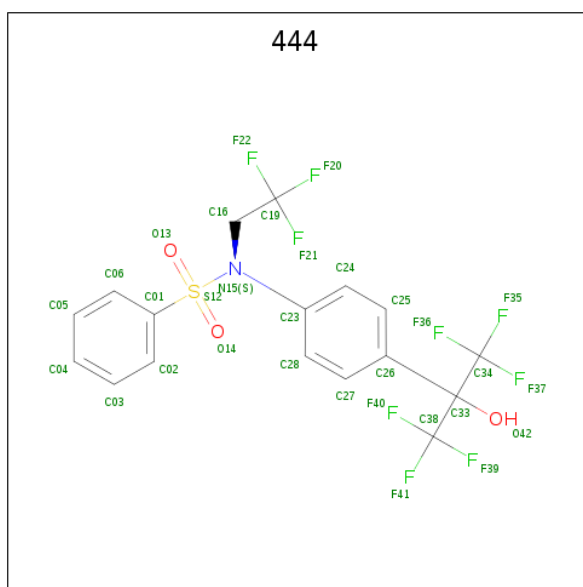
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			31	17	9	1	3	1		
2	B	1	Total	C	F	N	O	S	0	0
			31	17	9	1	3	1		
2	C	1	Total	C	F	N	O	S	0	0
			31	17	9	1	3	1		
2	D	1	Total	C	F	N	O	S	0	0
			31	17	9	1	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total	O	0	0
			2	2		

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, yel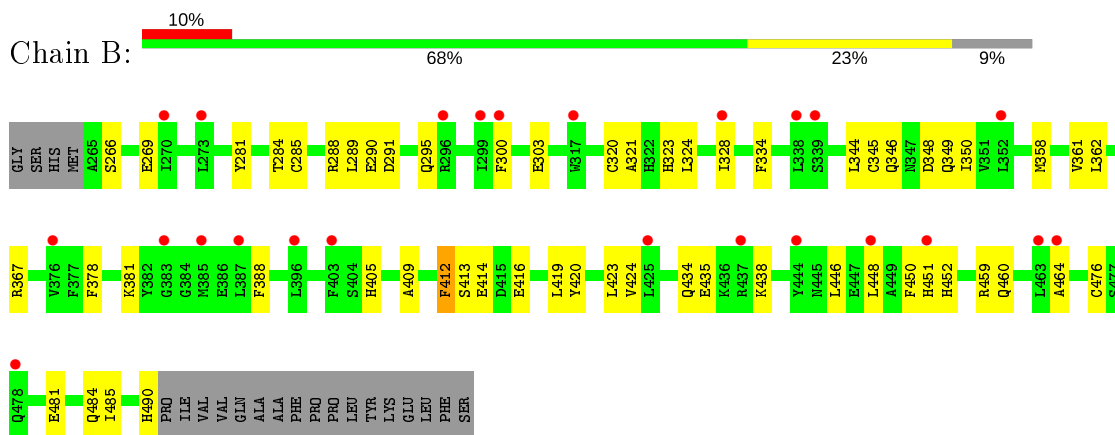low = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Nuclear receptor ROR-gamma
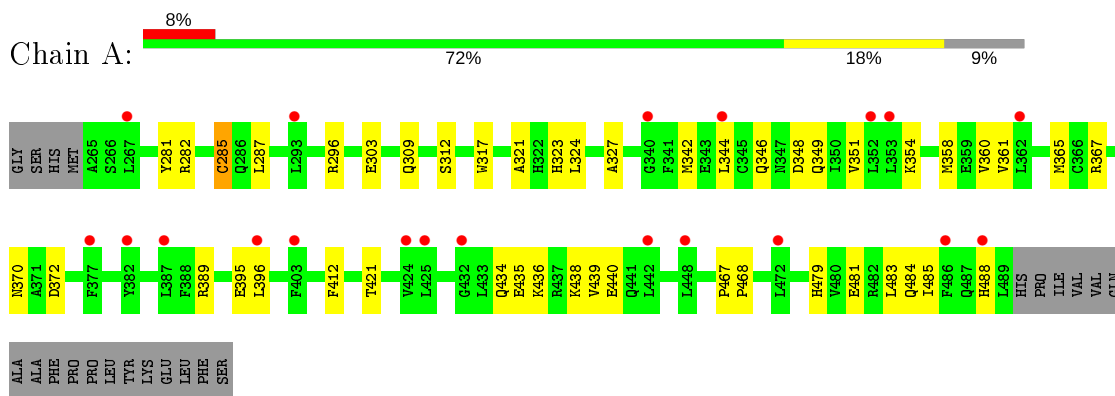
Chain A:

- Molecule 1: Nuclear receptor ROR-gamma

Chain B:

- Molecule 1: Nuclear receptor ROR-gamma
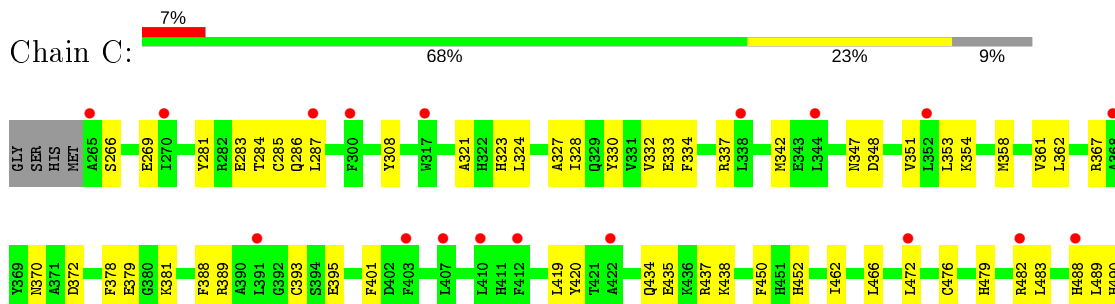
Chain C:

PRO ILE VAL VAL GLN ALA ALA PHE PRO PRO LEU TYR LYS GLU LEU PHE SER

• Molecule 1: Nuclear receptor ROR-gamma

Chain D:

GLY SER HIS MET A265 S266 E269 I270 E271 H272 K279 S280 Y281 R282 E283 T284 C285 R288 L289 E290 L293 R296 F300 S301 R302 E303 E304 V305 T306 G307 Y308 Q309 R310 K311 C320 A321 L324 I328 V332 E333 F334 A335 K336 R337 F341 D348 L352

L353 M358 E359 L362 M365 C366 R367 A368 N373 V376 F377 F378 K381 E386 L396 S404 F412 L419 L425 I426 E435 K436 R437 K438 Y444 F450 H451 H452 H453 K456 R459 Q460 A464 L472 L475 C476 S477 Q478 H479 V480

E481 R482 L483 Q484 I485 H490 PRO ILE VAL VAL GLN ALA ALA PHE PRO PRO LEU TYR LYS GLU LEU PHE SER

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	89.56Å 89.56Å 153.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.78 – 2.75 44.78 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.2 (44.78-2.75) 98.1 (44.78-2.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.10_2155	Depositor
R, R_{free}	0.239 , 0.264 0.227 , 0.253	Depositor DCC
R_{free} test set	1765 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	84.4	Xtriage
Anisotropy	0.460	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 67.5	EDS
L-test for twinning[2]	$< |L| > = 0.52, < L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.479 for -h,-k,l 0.480 for h,-h-k,-l 0.479 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for -h,-k,l	Depositor
Outliers	0 of 35103 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7516	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 444

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	0.26	0/1876	0.41	0/2522
1	B	0.25	0/1887	0.39	0/2537
1	C	0.25	0/1887	0.41	0/2537
1	D	0.25	0/1887	0.40	0/2537
All	All	0.25	0/7537	0.40	0/10133

There are no bond length outliers.

There are no bond angle outliers.

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	1840	0	1842	31	0
1	B	1850	0	1849	42	0
1	C	1850	0	1849	30	0
1	D	1850	0	1849	39	0
2	A	31	0	12	3	0
2	B	31	0	12	3	0
2	C	31	0	12	3	0
2	D	31	0	12	4	0
3	D	2	0	0	0	0
All	All	7516	0	7437	139	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (139) 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:362:LEU:HD11	1:C:476:CYS:HB3	1.66	0.78
1:C:283:GLU:OE2	1:C:337:ARG:NH2	2.21	0.73
1:A:281:TYR:O	1:A:285:CYS:N	2.23	0.71
1:A:321:ALA:HB2	1:A:483:LEU:HD11	1.74	0.70
1:B:451:HIS:HB3	1:D:451:HIS:HB3	1.76	0.68
1:D:281:TYR:O	1:D:285:CYS:N	2.27	0.68
1:B:344:LEU:O	1:B:349:GLN:NE2	2.29	0.65
2:A:900:444:F39	2:A:900:444:F35	1.89	0.65
1:C:347:ASN:ND2	1:C:434:GLN:OE1	2.29	0.65
1:C:370:ASN:ND2	1:C:372:ASP:OD2	2.30	0.64
1:C:287:LEU:O	1:C:367:ARG:NH2	2.31	0.64
1:D:265:ALA:N	1:D:269:GLU:OE2	2.31	0.63
2:C:900:444:F39	2:C:900:444:H27	1.89	0.63
1:A:287:LEU:O	1:A:367:ARG:NH2	2.29	0.62
1:B:460:GLN:HB3	1:D:451:HIS:NE2	2.15	0.62
1:C:342:MET:N	1:C:342:MET:SD	2.73	0.61
1:B:362:LEU:HD11	1:B:476:CYS:HB3	1.83	0.61
1:B:346:GLN:HE21	1:B:350:ILE:HD11	1.66	0.60
2:D:900:444:F41	2:D:900:444:F36	1.97	0.60
1:C:351:VAL:HA	1:C:354:LYS:HD3	1.84	0.60
1:B:452:HIS:CD2	1:D:452:HIS:HD2	2.20	0.59
1:B:451:HIS:NE2	1:D:460:GLN:HB2	2.18	0.59
2:A:900:444:H27	2:A:900:444:F40	1.93	0.59
1:C:388:PHE:CZ	2:C:900:444:H05	2.37	0.59
1:A:370:ASN:ND2	1:A:372:ASP:OD2	2.37	0.58
1:C:321:ALA:HB2	1:C:483:LEU:HD11	1.86	0.58
1:C:348:ASP:OD2	1:C:435:GLU:N	2.33	0.57
1:B:288:ARG:NH2	1:B:290:GLU:OE2	2.37	0.57
1:B:328:ILE:HG12	1:B:361:VAL:HG21	1.86	0.57
1:D:303:GLU:OE1	1:D:303:GLU:N	2.38	0.56
1:B:423:LEU:HD11	1:B:446:LEU:HB3	1.88	0.56
1:D:348:ASP:OD2	1:D:435:GLU:N	2.33	0.56
1:B:345:CYS:N	1:B:435:GLU:OE1	2.32	0.55
1:D:435:GLU:HG2	1:D:438:LYS:HB2	1.86	0.55
1:A:342:MET:SD	1:A:342:MET:N	2.79	0.55
1:A:348:ASP:OD2	1:A:435:GLU:N	2.39	0.55
1:C:284:THR:HG1	1:C:334:PHE:HD1	1.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:479:HIS:CE1	2:D:900:444:H42	2.25	0.55
1:B:324:LEU:O	1:B:328:ILE:HG13	2.08	0.54
1:A:344:LEU:HB2	1:A:349:GLN:HG3	1.89	0.54
1:D:453:HIS:HA	1:D:456:LYS:HD3	1.89	0.54
1:A:324:LEU:HD12	2:A:900:444:C25	2.37	0.54
1:D:396:LEU:HD21	1:D:479:HIS:HB2	1.90	0.53
1:A:309:GLN:OE1	1:A:389:ARG:NH1	2.41	0.53
1:D:358:MET:HB3	1:D:476:CYS:HB2	1.90	0.53
2:C:900:444:F41	2:C:900:444:F36	2.03	0.53
1:A:479:HIS:CE1	1:A:483:LEU:HB2	2.43	0.52
1:B:285:CYS:HB2	1:B:367:ARG:HH12	1.74	0.52
1:B:464:ALA:HA	1:D:464:ALA:HA	1.92	0.52
1:B:289:LEU:HB2	1:B:367:ARG:HH21	1.75	0.52
1:B:320:CYS:O	1:B:324:LEU:N	2.37	0.51
1:B:281:TYR:OH	1:B:367:ARG:NH1	2.44	0.51
1:A:395:GLU:N	1:A:395:GLU:OE2	2.38	0.51
1:A:296:ARG:HH21	1:A:370:ASN:ND2	2.09	0.51
1:A:484:GLN:HG2	1:A:488:HIS:HA	1.92	0.51
1:B:423:LEU:CD1	1:B:446:LEU:HB3	2.40	0.51
1:D:302:ARG:O	1:D:306:THR:OG1	2.27	0.51
1:D:309:GLN:NE2	1:D:386:GLU:O	2.38	0.51
1:A:351:VAL:HA	1:A:354:LYS:HD3	1.91	0.51
1:B:419:LEU:HD13	1:B:450:PHE:HA	1.93	0.51
1:C:332:VAL:HG23	1:C:333:GLU:H	1.75	0.50
1:D:300:PHE:CZ	1:D:381:LYS:HB2	2.46	0.50
1:C:393:CYS:SG	1:C:482:ARG:NH1	2.84	0.50
1:B:405:HIS:O	1:B:409:ALA:N	2.44	0.50
1:C:266:SER:HB3	1:C:269:GLU:HG2	1.94	0.50
1:A:296:ARG:HH21	1:A:370:ASN:HD22	1.60	0.50
1:D:373:ASN:OD1	1:D:373:ASN:N	2.44	0.50
1:B:324:LEU:HG	1:B:328:ILE:HD11	1.93	0.49
1:D:481:GLU:O	1:D:485:ILE:HG13	2.13	0.49
1:C:324:LEU:HD11	1:C:358:MET:SD	2.52	0.49
1:C:323:HIS:O	1:C:327:ALA:N	2.38	0.49
1:A:317:TRP:HZ3	1:A:479:HIS:HE1	1.60	0.49
1:A:346:GLN:HA	1:A:349:GLN:HE21	1.78	0.49
1:A:312:SER:HB3	1:B:414:GLU:HB2	1.95	0.49
1:B:460:GLN:CD	1:B:460:GLN:H	2.15	0.49
1:C:395:GLU:N	1:C:395:GLU:OE2	2.39	0.49
1:A:396:LEU:HD21	1:A:479:HIS:HB2	1.95	0.48
1:C:378:PHE:N	1:C:381:LYS:O	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:481:GLU:O	1:A:485:ILE:HG12	2.14	0.48
1:D:362:LEU:HD11	1:D:476:CYS:HB3	1.96	0.48
1:A:360:VAL:HG13	1:A:421:THR:HB	1.95	0.48
1:C:281:TYR:O	1:C:285:CYS:N	2.47	0.47
1:A:361:VAL:O	1:A:365:MET:HG3	2.14	0.47
1:B:435:GLU:HG2	1:B:438:LYS:HD3	1.96	0.47
1:D:324:LEU:HG	1:D:328:ILE:HD11	1.97	0.47
1:B:448:LEU:O	1:B:452:HIS:HB2	2.14	0.47
1:B:413:SER:N	1:B:416:GLU:OE1	2.39	0.47
1:B:388:PHE:CE1	2:B:900:444:H05	2.50	0.47
1:D:324:LEU:O	1:D:328:ILE:HG13	2.16	0.46
1:D:283:GLU:OE1	1:D:337:ARG:NH1	2.49	0.46
1:B:484:GLN:HG3	1:B:490:HIS:CE1	2.50	0.46
1:A:323:HIS:O	1:A:327:ALA:N	2.38	0.46
1:B:321:ALA:HA	1:B:324:LEU:HB3	1.98	0.46
1:C:308:TYR:OH	1:C:379:GLU:OE1	2.27	0.46
1:C:286:GLN:HB2	1:C:330:TYR:CG	2.51	0.46
1:A:435:GLU:O	1:A:439:VAL:HG23	2.17	0.45
1:A:484:GLN:HA	1:A:488:HIS:HA	1.99	0.45
1:C:328:ILE:HG12	1:C:361:VAL:HG21	1.98	0.45
1:B:412:PHE:HD1	1:B:412:PHE:HA	1.71	0.45
1:A:348:ASP:CG	1:A:434:GLN:H	2.21	0.44
1:B:291:ASP:O	1:B:295:GLN:HG2	2.18	0.44
1:C:321:ALA:HB1	1:C:489:LEU:HD23	1.99	0.44
1:D:308:TYR:HA	1:D:311:LYS:HE2	1.98	0.44
1:D:359:GLU:HB3	1:D:472:LEU:HG	2.00	0.44
1:B:420:TYR:O	1:B:424:VAL:HG23	2.17	0.44
1:C:353:LEU:HD23	1:C:353:LEU:HA	1.84	0.43
1:A:303:GLU:N	1:A:303:GLU:OE2	2.38	0.43
1:A:436:LYS:NZ	1:A:440:GLU:OE2	2.40	0.43
1:D:479:HIS:HE2	2:D:900:444:C38	2.31	0.43
1:B:481:GLU:O	1:B:485:ILE:HG12	2.18	0.43
1:D:321:ALA:HA	1:D:324:LEU:HB3	2.00	0.43
1:D:358:MET:O	1:D:362:LEU:HG	2.19	0.43
1:C:420:TYR:OH	1:C:472:LEU:HD11	2.18	0.43
1:D:284:THR:OG1	1:D:334:PHE:HB2	2.18	0.43
1:D:300:PHE:CD2	1:D:381:LYS:HD2	2.54	0.43
1:B:348:ASP:OD2	1:B:434:GLN:N	2.52	0.43
1:D:336:LYS:HA	1:D:341:PHE:CD2	2.54	0.43
1:A:349:GLN:HE21	1:A:349:GLN:HB2	1.66	0.42
1:D:479:HIS:NE2	2:D:900:444:F40	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:300:PHE:CZ	1:B:381:LYS:HB2	2.55	0.42
1:B:358:MET:HB3	1:B:476:CYS:HB2	2.00	0.42
1:D:288:ARG:HB3	1:D:290:GLU:HG2	2.02	0.42
1:D:482:ARG:HA	1:D:482:ARG:HD3	1.89	0.41
1:D:332:VAL:HG22	1:D:353:LEU:HD22	2.03	0.41
1:D:475:LEU:O	1:D:479:HIS:HB3	2.20	0.41
1:D:366:CYS:HA	1:D:404:SER:OG	2.20	0.41
1:B:388:PHE:CZ	2:B:900:444:H05	2.55	0.41
1:B:284:THR:OG1	1:B:334:PHE:HB2	2.20	0.41
1:B:320:CYS:HB3	2:B:900:444:F40	2.11	0.41
1:D:266:SER:HB3	1:D:269:GLU:HG3	2.01	0.41
1:A:467:PRO:HA	1:A:468:PRO:HD3	1.92	0.41
1:B:323:HIS:CD2	1:B:378:PHE:HE2	2.39	0.41
1:C:324:LEU:O	1:C:328:ILE:HG13	2.21	0.41
1:C:389:ARG:NH1	1:D:459:ARG:HD3	2.35	0.41
1:A:389:ARG:NH2	1:B:459:ARG:HD3	2.36	0.40
1:C:419:LEU:HB3	1:C:450:PHE:CD1	2.56	0.40
1:C:462:ILE:O	1:C:466:LEU:HG	2.21	0.40
1:B:266:SER:HB3	1:B:269:GLU:HG3	2.03	0.40
1:C:324:LEU:HD23	1:C:489:LEU:HD21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	223/247 (90%)	211 (95%)	11 (5%)	1 (0%)	34	53
1	B	224/247 (91%)	209 (93%)	15 (7%)	0	100	100
1	C	224/247 (91%)	217 (97%)	7 (3%)	0	100	100
1	D	224/247 (91%)	217 (97%)	7 (3%)	0	100	100
All	All	895/988 (91%)	854 (95%)	40 (4%)	1 (0%)	51	75

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	285	CYS

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	201/220 (91%)	197 (98%)	4 (2%)	55	72
1	B	202/220 (92%)	200 (99%)	2 (1%)	76	85
1	C	202/220 (92%)	195 (96%)	7 (4%)	36	56
1	D	202/220 (92%)	194 (96%)	8 (4%)	31	51
All	All	807/880 (92%)	786 (97%)	21 (3%)	46	66

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	282	ARG
1	A	358	MET
1	A	412	PHE
1	A	438	LYS
1	B	303	GLU
1	B	412	PHE
1	C	401	PHE
1	C	437	ARG
1	C	438	LYS
1	C	452	HIS
1	C	479	HIS
1	C	488	HIS
1	C	490	HIS
1	D	279	LYS
1	D	285	CYS
1	D	302	ARG
1	D	365	MET
1	D	378	PHE
1	D	412	PHE

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Mol	Chain	Res	Type
1	D	437	ARG
1	D	479	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	349	GLN
1	B	346	GLN
1	C	347	ASN
1	C	434	GLN
1	C	441	GLN
1	C	445	ASN
1	D	452	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 monosaccharides 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	444	A	900	-	31,32,32	4.04	4 (12%)	52,52,52	3.09	20 (38%)
2	444	B	900	-	31,32,32	3.96	2 (6%)	52,52,52	2.67	12 (23%)
2	444	C	900	-	31,32,32	4.07	2 (6%)	52,52,52	2.73	17 (32%)
2	444	D	900	-	31,32,32	4.04	2 (6%)	52,52,52	2.66	14 (26%)

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	444	A	900	-	-	36/45/45/45	0/2/2/2
2	444	B	900	-	-	26/45/45/45	0/2/2/2
2	444	C	900	-	-	33/45/45/45	0/2/2/2
2	444	D	900	-	-	32/45/45/45	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	900	444	S12-N15	16.22	1.88	1.65
2	D	900	444	S12-N15	16.01	1.87	1.65
2	C	900	444	C23-N15	15.94	1.67	1.44
2	C	900	444	S12-N15	15.89	1.87	1.65
2	B	900	444	S12-N15	15.64	1.87	1.65
2	D	900	444	C23-N15	15.49	1.66	1.44
2	B	900	444	C23-N15	15.21	1.66	1.44
2	A	900	444	C23-N15	14.77	1.65	1.44
2	A	900	444	C01-S12	2.48	1.79	1.76
2	A	900	444	C27-C28	-2.27	1.34	1.38

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	900	444	O14-S12-O13	-11.25	101.28	119.52
2	D	900	444	O14-S12-O13	-11.01	101.67	119.52
2	C	900	444	O14-S12-O13	-10.80	102.01	119.52
2	B	900	444	O14-S12-O13	-10.58	102.38	119.52
2	B	900	444	C19-C16-N15	-8.41	103.97	112.14
2	A	900	444	C19-C16-N15	-8.31	104.07	112.14
2	C	900	444	C19-C16-N15	-7.61	104.74	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	900	444	C19-C16-N15	-7.54	104.81	112.14
2	A	900	444	C23-N15-S12	-7.31	103.07	117.73
2	D	900	444	C23-N15-S12	-6.68	104.34	117.73
2	B	900	444	C23-N15-S12	-6.43	104.84	117.73
2	C	900	444	C23-N15-S12	-5.98	105.73	117.73
2	D	900	444	C16-N15-S12	-5.59	109.21	117.00
2	A	900	444	F40-C38-C33	4.99	121.38	111.85
2	A	900	444	C01-S12-N15	4.92	113.63	106.92
2	A	900	444	C38-C33-C26	4.89	118.65	110.34
2	B	900	444	C16-N15-S12	-4.82	110.28	117.00
2	A	900	444	C28-C23-N15	-4.71	113.15	120.16
2	C	900	444	C16-N15-S12	-4.68	110.48	117.00
2	A	900	444	C16-N15-C23	-4.55	111.51	117.59
2	C	900	444	C38-C33-C34	-4.53	104.60	110.28
2	C	900	444	C38-C33-C26	4.46	117.92	110.34
2	B	900	444	C16-N15-C23	-4.40	111.71	117.59
2	C	900	444	O13-S12-N15	4.26	111.75	106.71
2	B	900	444	O13-S12-N15	3.81	111.22	106.71
2	D	900	444	O13-S12-N15	3.78	111.18	106.71
2	A	900	444	C16-N15-S12	-3.72	111.81	117.00
2	C	900	444	C16-N15-C23	-3.56	112.83	117.59
2	A	900	444	O13-S12-N15	3.51	110.86	106.71
2	A	900	444	F41-C38-C33	-3.47	105.24	111.85
2	A	900	444	O14-S12-N15	3.34	110.66	106.71
2	D	900	444	C16-N15-C23	-3.30	113.18	117.59
2	C	900	444	O14-S12-N15	3.27	110.58	106.71
2	A	900	444	C24-C23-N15	3.27	125.03	120.16
2	D	900	444	O14-S12-N15	3.15	110.43	106.71
2	D	900	444	O13-S12-C01	3.06	111.91	108.05
2	B	900	444	O13-S12-C01	3.04	111.89	108.05
2	B	900	444	O14-S12-N15	3.00	110.26	106.71
2	C	900	444	O13-S12-C01	2.91	111.73	108.05
2	A	900	444	F36-C34-C33	-2.87	106.37	111.85
2	C	900	444	F40-C38-C33	-2.87	106.37	111.85
2	A	900	444	F22-C19-C16	-2.87	107.43	112.13
2	C	900	444	F39-C38-C33	2.84	117.28	111.85
2	D	900	444	C34-C33-C26	2.83	115.16	110.34
2	B	900	444	F39-C38-C33	-2.82	106.48	111.85
2	B	900	444	O14-S12-C01	2.78	111.56	108.05
2	A	900	444	C03-C02-C01	2.76	121.82	118.95
2	C	900	444	C28-C23-N15	-2.68	116.17	120.16
2	A	900	444	C06-C01-C02	-2.61	116.80	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	900	444	C01-S12-N15	2.58	110.44	106.92
2	D	900	444	F40-C38-C33	-2.57	106.94	111.85
2	B	900	444	F22-C19-C16	-2.56	107.92	112.13
2	C	900	444	F22-C19-C16	-2.51	108.01	112.13
2	D	900	444	F22-C19-C16	-2.51	108.01	112.13
2	A	900	444	C05-C06-C01	2.48	121.53	118.95
2	C	900	444	C24-C23-N15	2.41	123.75	120.16
2	A	900	444	C25-C24-C23	-2.40	117.16	120.32
2	B	900	444	O42-C33-C38	2.31	111.44	106.09
2	D	900	444	O14-S12-C01	2.27	110.92	108.05
2	A	900	444	C06-C01-S12	2.23	122.10	119.76
2	C	900	444	O14-S12-C01	2.18	110.80	108.05
2	D	900	444	C28-C23-N15	-2.11	117.02	120.16
2	C	900	444	C01-S12-N15	2.10	109.78	106.92

There are no chirality outliers.

All (127) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	900	444	C23-N15-S12-C01
2	A	900	444	C19-C16-N15-C23
2	A	900	444	N15-C16-C19-F22
2	A	900	444	N15-C16-C19-F21
2	A	900	444	N15-C16-C19-F20
2	A	900	444	C25-C26-C33-O42
2	A	900	444	C25-C26-C33-C38
2	A	900	444	C27-C26-C33-O42
2	A	900	444	C38-C33-C34-F36
2	A	900	444	C38-C33-C34-F37
2	A	900	444	C38-C33-C34-F35
2	A	900	444	C34-C33-C38-F41
2	B	900	444	C23-N15-S12-C01
2	B	900	444	C19-C16-N15-C23
2	B	900	444	N15-C16-C19-F22
2	B	900	444	N15-C16-C19-F21
2	B	900	444	N15-C16-C19-F20
2	C	900	444	C23-N15-S12-C01
2	C	900	444	C19-C16-N15-C23
2	C	900	444	N15-C16-C19-F22
2	C	900	444	N15-C16-C19-F21
2	C	900	444	N15-C16-C19-F20
2	C	900	444	C27-C26-C33-O42

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Mol	Chain	Res	Type	Atoms
2	C	900	444	C27-C26-C33-C38
2	D	900	444	C23-N15-S12-C01
2	D	900	444	C19-C16-N15-C23
2	D	900	444	N15-C16-C19-F22
2	D	900	444	N15-C16-C19-F21
2	D	900	444	N15-C16-C19-F20
2	D	900	444	C38-C33-C34-F36
2	D	900	444	C38-C33-C34-F37
2	D	900	444	C38-C33-C34-F35
2	C	900	444	C26-C33-C38-F39
2	C	900	444	C26-C33-C38-F40
2	C	900	444	C26-C33-C38-F41
2	D	900	444	C26-C33-C38-F39
2	D	900	444	C26-C33-C38-F40
2	D	900	444	C26-C33-C38-F41
2	B	900	444	C23-N15-S12-O14
2	C	900	444	C23-N15-S12-O14
2	A	900	444	C26-C33-C34-F36
2	A	900	444	C26-C33-C34-F37
2	A	900	444	C26-C33-C34-F35
2	A	900	444	O42-C33-C34-F36
2	A	900	444	O42-C33-C34-F37
2	A	900	444	O42-C33-C34-F35
2	A	900	444	C26-C33-C38-F39
2	A	900	444	C26-C33-C38-F40
2	A	900	444	O42-C33-C38-F40
2	A	900	444	O42-C33-C38-F41
2	B	900	444	C26-C33-C34-F36
2	B	900	444	C26-C33-C34-F37
2	B	900	444	C26-C33-C34-F35
2	B	900	444	O42-C33-C34-F36
2	B	900	444	O42-C33-C34-F37
2	B	900	444	O42-C33-C34-F35
2	C	900	444	O42-C33-C38-F39
2	C	900	444	O42-C33-C38-F40
2	C	900	444	O42-C33-C38-F41
2	D	900	444	C26-C33-C34-F36
2	D	900	444	C26-C33-C34-F37
2	D	900	444	C26-C33-C34-F35
2	D	900	444	O42-C33-C34-F36
2	D	900	444	O42-C33-C34-F37
2	D	900	444	O42-C33-C34-F35

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Mol	Chain	Res	Type	Atoms
2	D	900	444	O42-C33-C38-F39
2	D	900	444	O42-C33-C38-F40
2	D	900	444	O42-C33-C38-F41
2	A	900	444	C34-C33-C38-F39
2	A	900	444	C34-C33-C38-F40
2	B	900	444	C38-C33-C34-F36
2	B	900	444	C38-C33-C34-F37
2	B	900	444	C38-C33-C34-F35
2	C	900	444	C38-C33-C34-F36
2	C	900	444	C38-C33-C34-F35
2	C	900	444	C34-C33-C38-F39
2	C	900	444	C34-C33-C38-F40
2	D	900	444	C34-C33-C38-F39
2	D	900	444	C34-C33-C38-F40
2	D	900	444	C34-C33-C38-F41
2	D	900	444	C23-N15-S12-O14
2	A	900	444	C26-C33-C38-F41
2	A	900	444	O42-C33-C38-F39
2	C	900	444	C38-C33-C34-F37
2	C	900	444	C34-C33-C38-F41
2	B	900	444	C16-N15-S12-O13
2	B	900	444	C16-N15-S12-O14
2	C	900	444	C16-N15-S12-O14
2	D	900	444	C16-N15-S12-O14
2	B	900	444	C23-N15-S12-O13
2	A	900	444	C24-C23-N15-C16
2	A	900	444	C28-C23-N15-C16
2	B	900	444	C28-C23-N15-C16
2	C	900	444	C24-C23-N15-C16
2	C	900	444	C28-C23-N15-C16
2	D	900	444	C24-C23-N15-C16
2	D	900	444	C28-C23-N15-C16
2	B	900	444	C26-C33-C38-F40
2	A	900	444	C16-N15-S12-O14
2	A	900	444	C16-N15-S12-C01
2	B	900	444	C16-N15-S12-C01
2	C	900	444	C16-N15-S12-C01
2	D	900	444	C16-N15-S12-C01
2	A	900	444	C27-C26-C33-C38
2	C	900	444	C25-C26-C33-C38
2	B	900	444	C24-C23-N15-C16
2	A	900	444	C23-N15-S12-O14

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Mol	Chain	Res	Type	Atoms
2	C	900	444	C26-C33-C34-F37
2	A	900	444	C16-N15-S12-O13
2	C	900	444	C16-N15-S12-O13
2	D	900	444	C16-N15-S12-O13
2	A	900	444	C23-N15-S12-O13
2	C	900	444	C23-N15-S12-O13
2	C	900	444	C25-C26-C33-O42
2	D	900	444	C23-N15-S12-O13
2	A	900	444	C06-C01-S12-O13
2	C	900	444	C26-C33-C34-F35
2	A	900	444	C02-C01-S12-O13
2	B	900	444	C26-C33-C38-F39
2	B	900	444	C26-C33-C38-F41
2	C	900	444	C26-C33-C34-F36
2	B	900	444	C34-C33-C38-F40
2	C	900	444	O42-C33-C34-F36
2	C	900	444	O42-C33-C34-F37
2	B	900	444	C34-C33-C38-F39
2	D	900	444	C02-C01-S12-O13
2	D	900	444	C06-C01-S12-O13

There are no ring outliers.

4 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	444	3	0
2	B	900	444	3	0
2	C	900	444	3	0
2	D	900	444	4	0

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

Ligand 444 A 900

Bond lengths

Bond angles

Torsions

Rings

Ligand 444 B 900

Bond lengths

Bond angles

Torsions

Rings

Ligand 444 C 900

Bond lengths

Bond angles

Torsions

Rings

Ligand 444 D 900

Bond lengths

Bond angles

Torsions

Rings
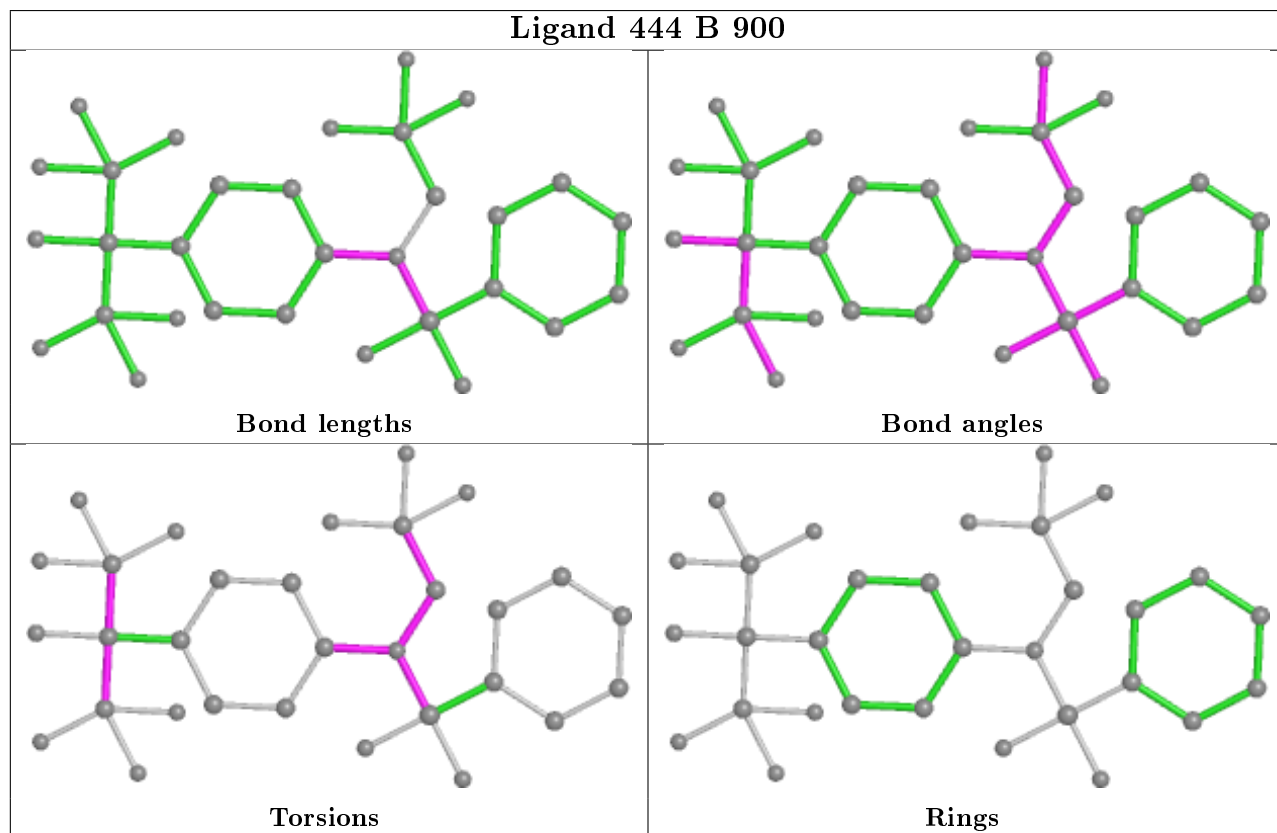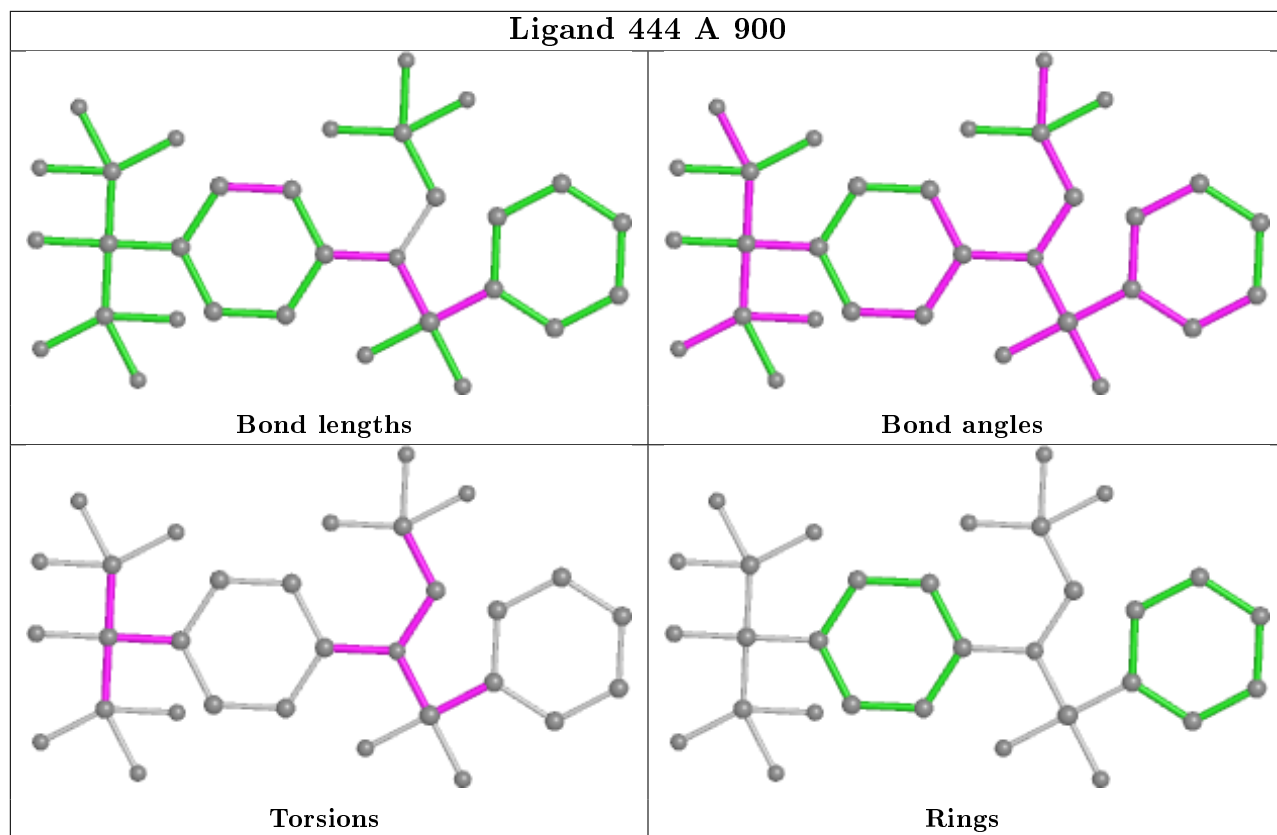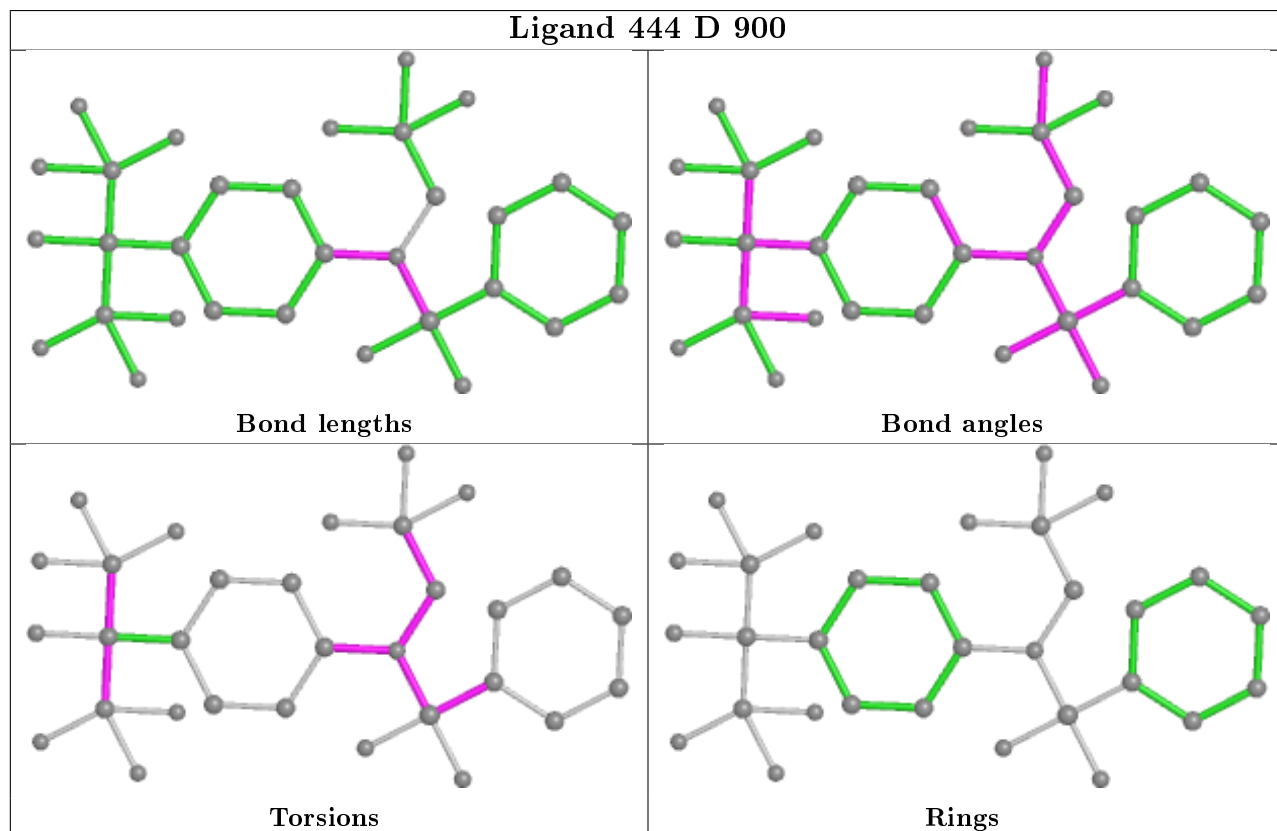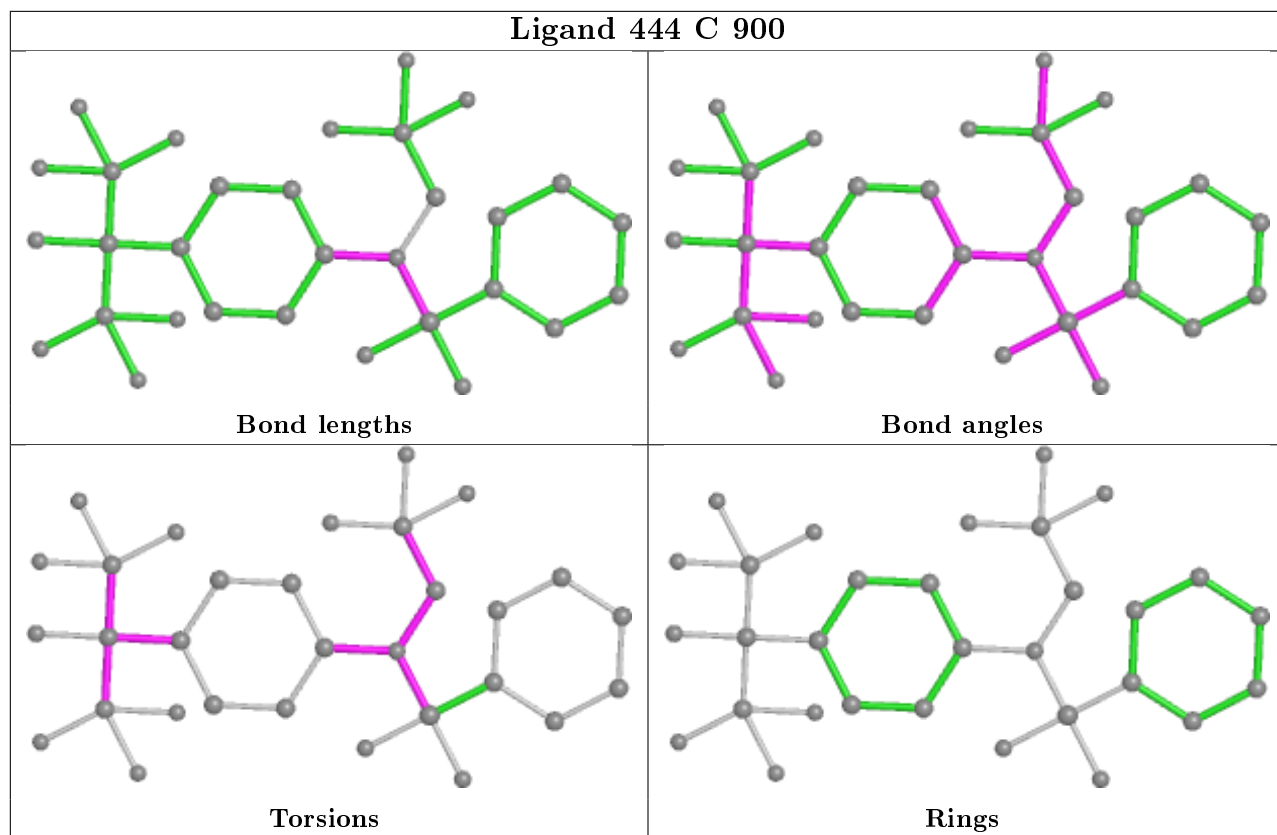
5.7 Other polymers (i)

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	225/247 (91%)	0.62	20 (8%)	9	11	66, 101, 130, 175	0
1	B	226/247 (91%)	0.72	24 (10%)	6	6	72, 103, 131, 173	0
1	C	226/247 (91%)	0.64	18 (7%)	12	15	71, 105, 130, 175	0
1	D	226/247 (91%)	0.71	24 (10%)	6	6	76, 105, 134, 175	0
All	All	903/988 (91%)	0.67	86 (9%)	8	9	66, 103, 132, 175	0

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	296	ARG	5.7
1	C	287	LEU	4.8
1	C	352	LEU	4.7
1	D	490	HIS	4.5
1	B	270	ILE	4.5
1	C	391	LEU	4.1
1	D	444	TYR	4.1
1	C	472	LEU	3.6
1	C	338	LEU	3.6
1	B	437	ARG	3.4
1	A	293	LEU	3.3
1	C	265	ALA	3.3
1	C	488	HIS	3.2
1	B	352	LEU	3.1
1	B	317	TRP	3.1
1	A	362	LEU	3.0
1	B	338	LEU	3.0
1	C	270	ILE	2.9
1	A	344	LEU	2.9
1	D	352	LEU	2.9
1	D	353	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	383	GLY	2.8
1	A	267	LEU	2.8
1	D	358	MET	2.7
1	A	486	PHE	2.7
1	A	382	TYR	2.7
1	C	482	ARG	2.7
1	B	300	PHE	2.6
1	B	463	LEU	2.6
1	C	412	PHE	2.6
1	D	425	LEU	2.6
1	B	339	SER	2.6
1	A	353	LEU	2.5
1	D	270	ILE	2.5
1	A	396	LEU	2.5
1	D	296	ARG	2.5
1	B	273	LEU	2.5
1	B	448	LEU	2.5
1	B	451	HIS	2.5
1	A	377	PHE	2.4
1	D	272	HIS	2.4
1	D	483	LEU	2.4
1	C	300	PHE	2.4
1	A	352	LEU	2.4
1	B	396	LEU	2.4
1	C	344	LEU	2.4
1	C	403	PHE	2.4
1	D	368	ALA	2.4
1	A	424	VAL	2.3
1	D	396	LEU	2.3
1	A	403	PHE	2.3
1	D	478	GLN	2.3
1	B	403	PHE	2.3
1	B	387	LEU	2.3
1	B	444	TYR	2.3
1	C	368	ALA	2.3
1	D	281	TYR	2.3
1	B	478	GLN	2.3
1	B	464	ALA	2.3
1	D	336	LYS	2.2
1	A	442	LEU	2.2
1	A	488	HIS	2.2
1	A	425	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	410	LEU	2.2
1	D	305	VAL	2.1
1	C	422	ALA	2.1
1	B	425	LEU	2.1
1	B	385	MET	2.1
1	D	365	MET	2.1
1	A	448	LEU	2.1
1	D	293	LEU	2.1
1	B	376	VAL	2.1
1	D	450	PHE	2.1
1	A	432	GLY	2.1
1	B	299	ILE	2.1
1	B	328	ILE	2.1
1	D	376	VAL	2.1
1	D	419	LEU	2.1
1	C	317	TRP	2.1
1	A	387	LEU	2.1
1	A	340	GLY	2.0
1	C	407	LEU	2.0
1	D	426	ILE	2.0
1	D	320	CYS	2.0
1	D	476	CYS	2.0
1	A	472	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	444	B	900	31/31	0.81	0.78	125,167,266,280	0
2	444	A	900	31/31	0.85	0.57	140,159,240,265	0
2	444	D	900	31/31	0.85	0.69	121,159,239,260	0
2	444	C	900	31/31	0.91	0.50	102,158,220,231	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.
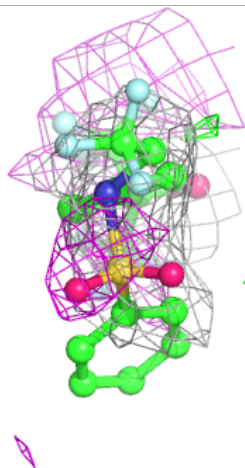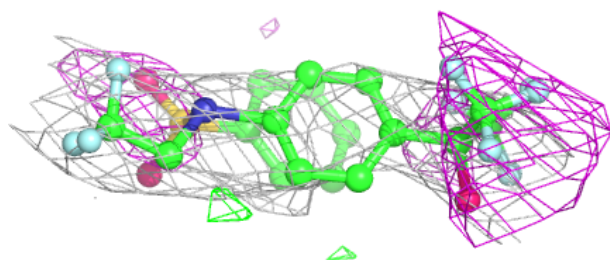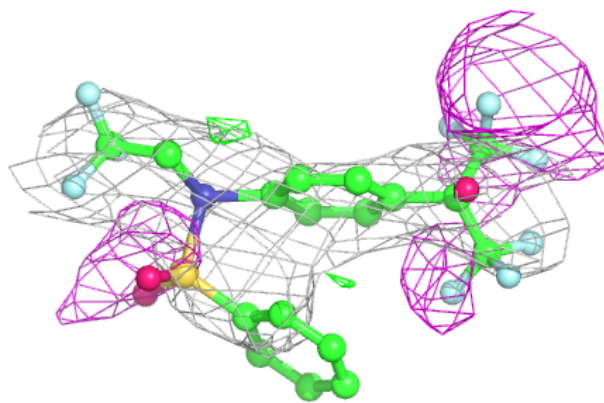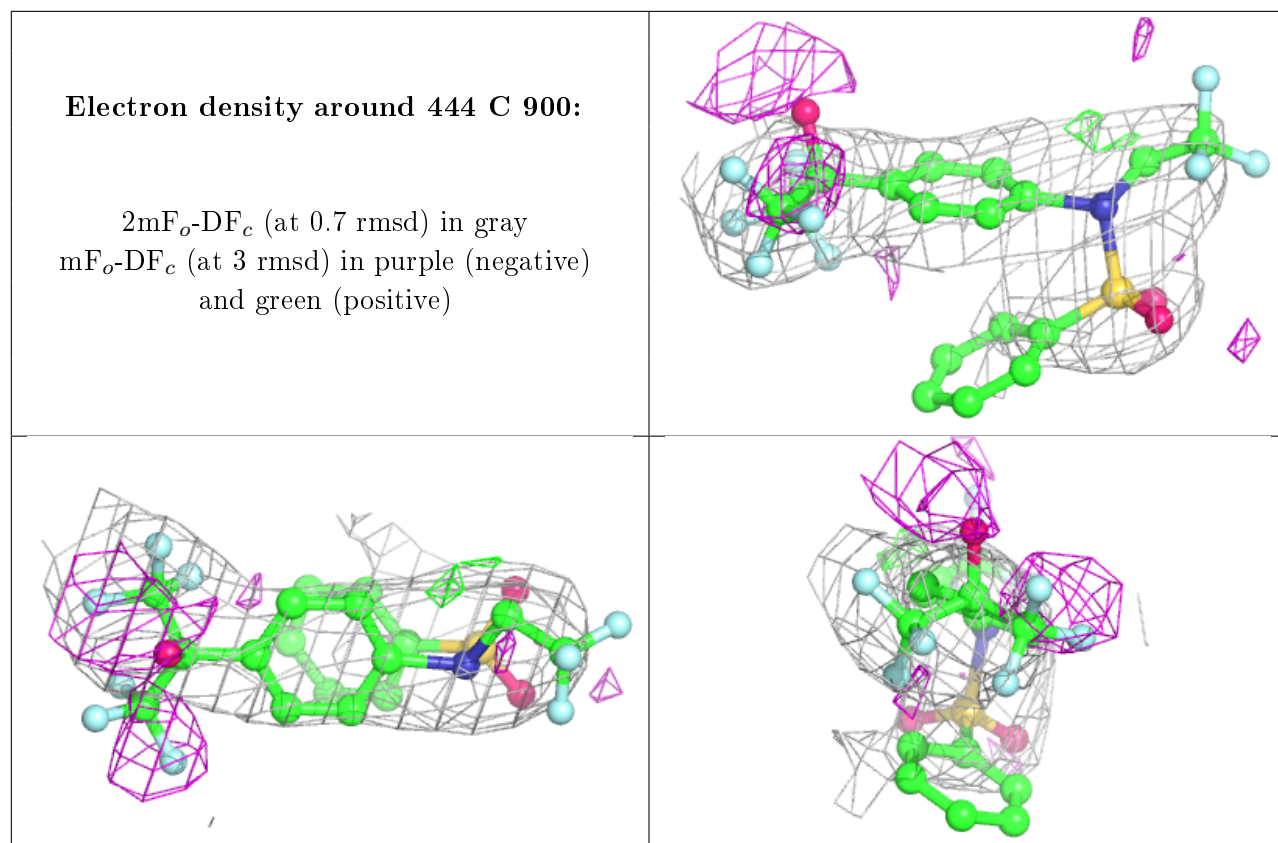
Electron density around 444 B 900:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
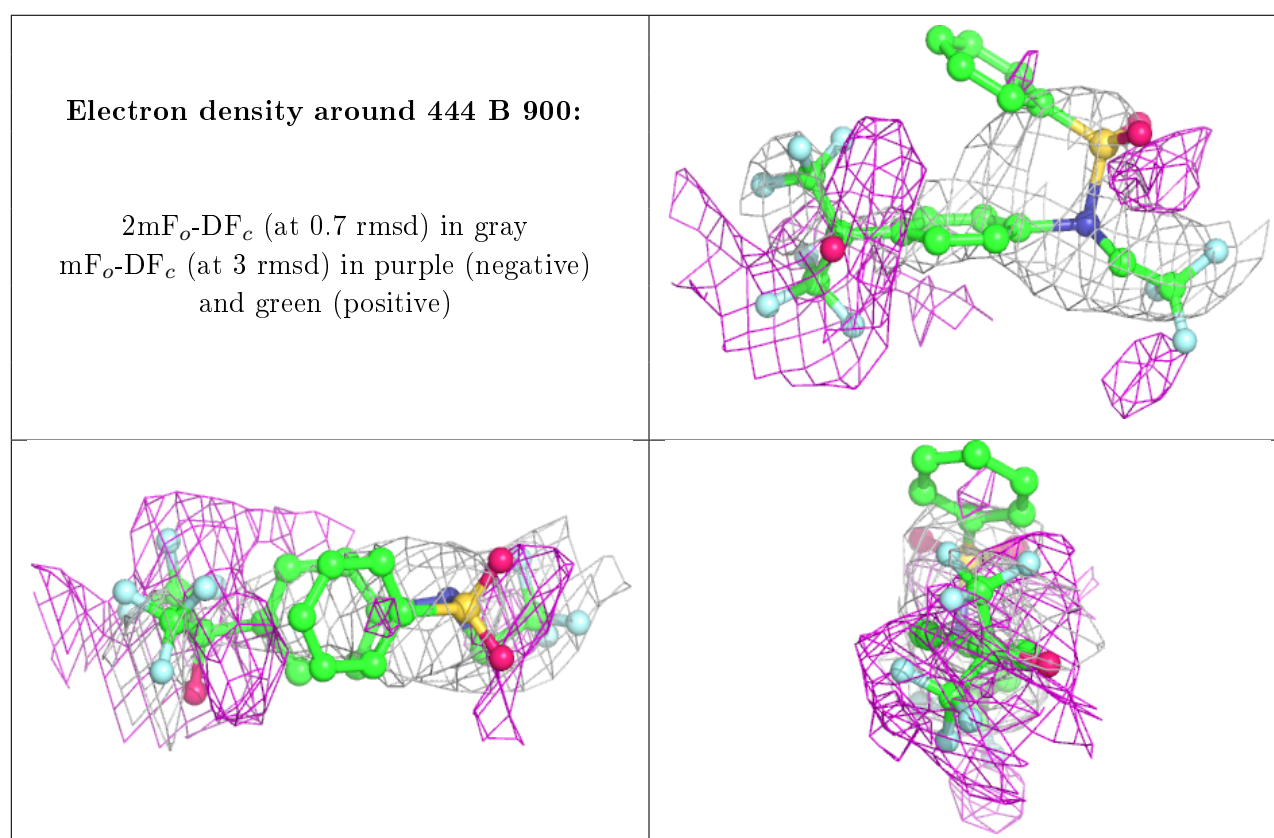
Electron density around 444 A 900:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
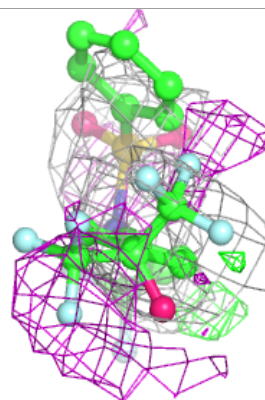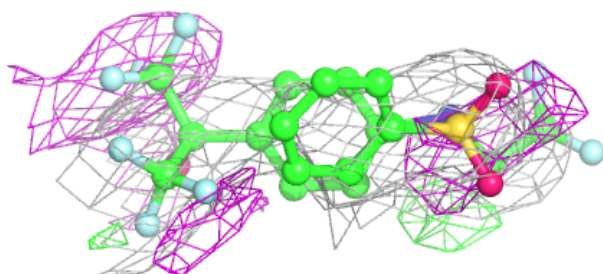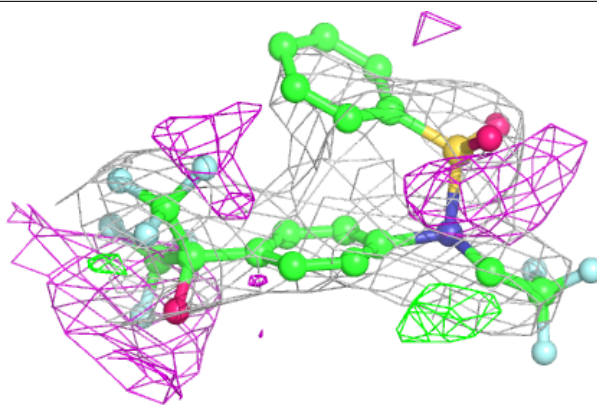
Electron density around 444 D 900:

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 444 C 900:

$2mF_o\text{-}DF_c$ (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.