



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 03:02 AM BST

PDB ID : 2ZNP
Title : Human PPAR delta ligand binding domain in complex with a synthetic agonist TIPP204
Authors : Oyama, T.; Hirakawa, Y.; Nagasawa, N.; Miyachi, H.; Morikawa, K.
Deposited on : 2008-04-30
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

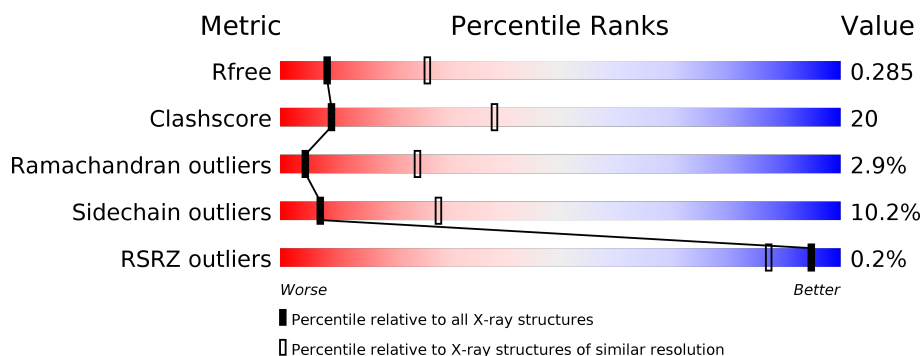
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 $\leq 5\%$. 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	276	
1	B	276	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4305 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.

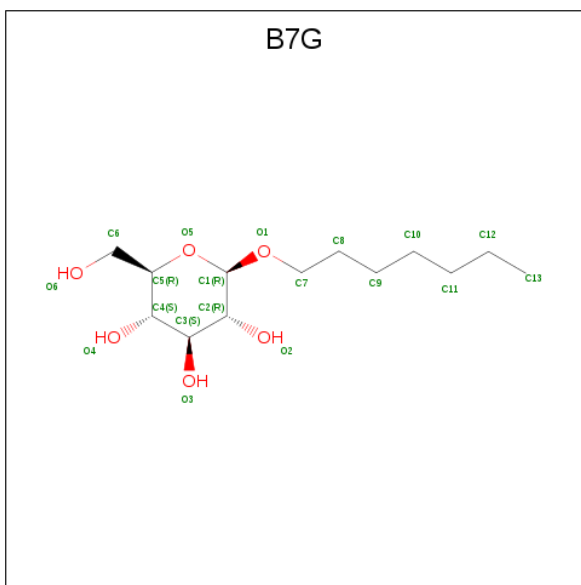
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	259	Total	C	N	O	S	0	0	0
			2083	1349	351	373	10			
1	B	262	Total	C	N	O	S	0	0	0
			2113	1370	355	378	10			

There are 8 discrepancies between the modelled and reference sequences:

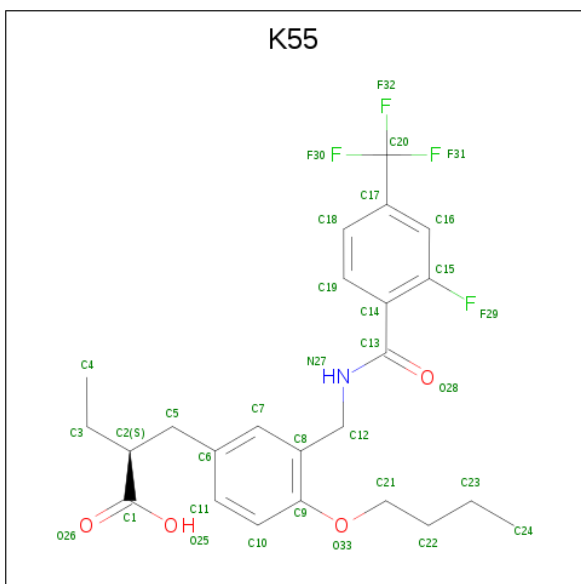
Chain	Residue	Modelled	Actual	Comment	Reference
A	202	GLY	-	expression tag	UNP Q03181
A	203	SER	-	expression tag	UNP Q03181
A	204	HIS	-	expression tag	UNP Q03181
A	205	MET	-	expression tag	UNP Q03181
B	202	GLY	-	expression tag	UNP Q03181
B	203	SER	-	expression tag	UNP Q03181
B	204	HIS	-	expression tag	UNP Q03181
B	205	MET	-	expression tag	UNP Q03181

- Molecule 2 is heptyl beta-D-glucopyranoside (three-letter code: B7G) (formula: C₁₃H₂₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			19	13	6		
2	B	1	Total	C	O	0	0
			19	13	6		

- Molecule 3 is (2S)-2-{4-butoxy-3-[(2-fluoro-4-(trifluoromethyl)phenyl)carbonyl]amino)methyl}benzyl}butanoic acid (three-letter code: K55) (formula: C₂₄H₂₇F₄NO₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			33	24	4	1	4		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	F	N	O	0	0
			33	24	4	1	4		

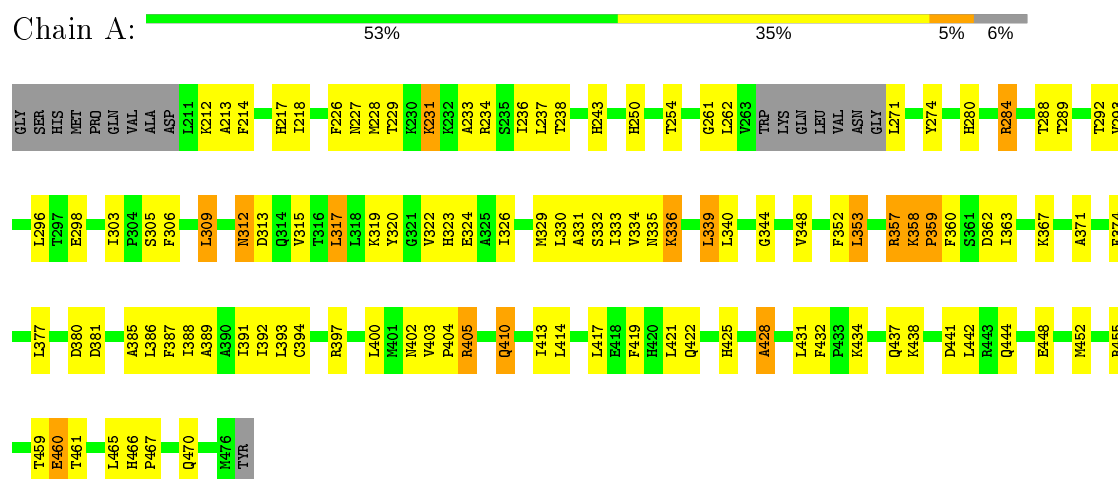
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	O	0	0
			2	2		
4	B	3	Total	O	0	0
			3	3		

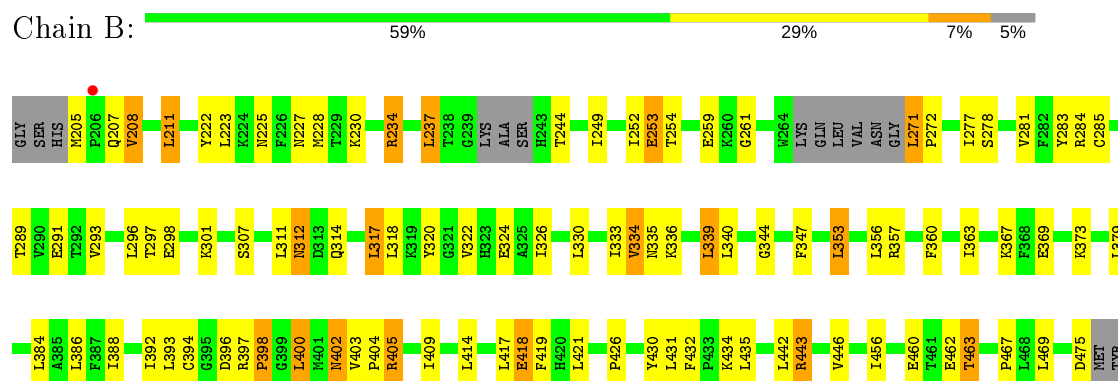
3 Residue-property plots

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: Peroxisome proliferator-activated receptor delta



- Molecule 1: Peroxisome proliferator-activated receptor delta



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	39.49Å 93.15Å 96.37Å 90.00° 97.48° 90.00°	Depositor
Resolution (Å)	38.01 – 3.00 47.77 – 2.99	Depositor EDS
% Data completeness (in resolution range)	93.4 (38.01-3.00) 92.8 (47.77-2.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.288 0.227 , 0.285	Depositor DCC
R_{free} test set	686 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	49.8	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4305	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.78% 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: K55, B7G

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	0.47	0/2127	0.64	0/2873
1	B	0.48	0/2159	0.63	0/2919
All	All	0.48	0/4286	0.64	0/5792

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

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	222	TYR	Sidechain

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	2083	0	2131	89	0
1	B	2113	0	2150	86	0
2	A	19	0	26	1	0
2	B	19	0	26	4	0
3	A	33	0	26	2	0
3	B	33	0	27	5	0
4	A	2	0	0	1	0
4	B	3	0	0	0	0
All	All	4305	0	4386	174	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 20.

All (174) 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:B:205:MET:HG3	1:B:208:VAL:H	1.22	1.00
1:A:296:LEU:HD23	1:A:322:VAL:HG12	1.55	0.88
1:A:312:ASN:HB3	2:B:920:B7G:H91	1.56	0.86
2:A:921:B7G:H91	1:B:312:ASN:HB3	1.57	0.86
1:A:334:VAL:HG22	1:A:335:ASN:H	1.50	0.76
1:B:405:ARG:O	1:B:409:ILE:HG12	1.87	0.75
1:B:205:MET:HG3	1:B:208:VAL:N	2.01	0.75
1:B:272:PRO:HB2	1:B:283:TYR:CE2	2.25	0.72
1:A:334:VAL:HG11	1:A:371:ALA:HB1	1.70	0.72
1:A:228:MET:SD	1:A:233:ALA:HB2	2.32	0.70
1:A:320:TYR:HB2	1:A:397:ARG:HD2	1.74	0.70
1:A:444:GLN:O	1:A:448:GLU:HG3	1.91	0.70
1:B:403:VAL:HB	1:B:404:PRO:HD3	1.74	0.70
1:B:330:LEU:HG	3:B:923:K55:H24B	1.73	0.69
1:A:229:THR:OG1	1:A:231:LYS:HB3	1.92	0.69
1:B:252:ILE:HD12	1:B:277:ILE:HG21	1.75	0.68
1:B:289:THR:O	1:B:293:VAL:HG23	1.93	0.68
1:B:386:LEU:HD13	1:B:417:LEU:HA	1.76	0.67
1:A:312:ASN:N	1:A:312:ASN:HD22	1.91	0.67
1:A:292:THR:HG21	1:A:326:ILE:HG12	1.75	0.67
1:A:377:LEU:HD11	1:A:438:LYS:NZ	2.11	0.66
1:B:297:THR:HG22	1:B:301:LYS:HE2	1.78	0.66
1:A:388:ILE:O	1:A:392:ILE:HG12	1.96	0.65
1:A:309:LEU:HD22	1:A:313:ASP:HB2	1.79	0.65
1:A:357:ARG:HG2	1:A:357:ARG:HH11	1.60	0.64
1:A:284:ARG:HG3	1:A:284:ARG:HH11	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:456:ILE:O	1:B:460:GLU:HB2	1.98	0.62
1:B:367:LYS:HG2	3:B:923:K55:H10	1.81	0.62
1:A:226:PHE:HZ	1:A:296:LEU:HD12	1.63	0.62
1:B:205:MET:SD	1:B:207:GLN:HB3	2.40	0.62
1:B:230:LYS:O	1:B:234:ARG:HB2	2.00	0.62
1:B:394:CYS:O	1:B:397:ARG:HG2	1.99	0.62
1:B:234:ARG:HA	1:B:234:ARG:HE	1.64	0.62
1:B:230:LYS:HD2	1:B:234:ARG:HD2	1.82	0.61
1:B:234:ARG:HH21	1:B:237:LEU:HD23	1.65	0.60
1:A:234:ARG:HH21	1:A:237:LEU:HD12	1.66	0.60
1:A:403:VAL:HB	1:A:404:PRO:HD3	1.82	0.60
1:A:213:ALA:O	1:A:217:HIS:HB2	2.02	0.59
1:A:465:LEU:HD23	1:A:470:GLN:HG2	1.84	0.59
1:B:340:LEU:HB3	1:B:344:GLY:HA2	1.84	0.59
1:B:318:LEU:HD13	2:B:920:B7G:H133	1.85	0.59
1:B:320:TYR:HB2	1:B:397:ARG:HD2	1.83	0.59
1:B:318:LEU:CD1	2:B:920:B7G:H133	2.33	0.58
1:B:334:VAL:HG23	1:B:339:LEU:HB3	1.84	0.58
1:A:357:ARG:HB3	1:A:359:PRO:HD2	1.86	0.58
1:A:377:LEU:HD11	1:A:438:LYS:HZ3	1.69	0.58
1:B:237:LEU:HG	1:B:335:ASN:HD22	1.69	0.57
1:B:460:GLU:HB3	1:B:463:THR:HG23	1.87	0.57
1:B:363:ILE:O	1:B:367:LYS:HD3	2.05	0.56
1:B:225:ASN:OD1	1:B:298:GLU:HB3	2.06	0.56
1:A:312:ASN:H	1:A:312:ASN:HD22	1.52	0.56
1:A:437:GLN:NE2	1:A:437:GLN:HA	2.21	0.55
1:B:277:ILE:HG13	1:B:278:SER:N	2.21	0.55
1:A:292:THR:O	1:A:296:LEU:HB2	2.06	0.55
1:B:430:TYR:HB2	1:B:434:LYS:HZ2	1.70	0.55
1:A:466:HIS:O	1:A:470:GLN:HG3	2.07	0.55
1:B:402:ASN:OD1	1:B:405:ARG:HB2	2.06	0.55
1:B:205:MET:SD	1:B:207:GLN:CB	2.95	0.55
1:A:284:ARG:HG3	1:A:284:ARG:NH1	2.22	0.55
1:A:237:LEU:HD13	1:A:335:ASN:HD22	1.71	0.55
1:B:281:VAL:HG11	1:B:356:LEU:HD11	1.89	0.54
1:A:226:PHE:CZ	1:A:296:LEU:HD12	2.43	0.54
1:B:317:LEU:HG	1:B:392:ILE:O	2.09	0.53
1:A:419:PHE:HA	1:A:422:GLN:HE21	1.73	0.53
1:B:205:MET:SD	1:B:207:GLN:N	2.72	0.53
1:A:363:ILE:HG22	1:A:452:MET:SD	2.48	0.52
1:B:312:ASN:H	1:B:312:ASN:HD22	1.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:430:TYR:HB2	1:B:434:LYS:NZ	2.24	0.52
1:A:394:CYS:O	1:A:397:ARG:HG2	2.09	0.52
1:A:320:TYR:CB	1:A:397:ARG:HD2	2.40	0.52
1:A:322:VAL:O	1:A:326:ILE:HG13	2.09	0.52
1:B:320:TYR:CE2	1:B:398:PRO:HB2	2.45	0.52
1:A:358:LYS:C	1:A:360:PHE:H	2.13	0.52
1:A:362:ASP:O	1:A:452:MET:SD	2.67	0.51
1:B:367:LYS:N	1:B:367:LYS:CD	2.73	0.51
1:B:277:ILE:O	1:B:281:VAL:HG23	2.10	0.51
1:B:205:MET:CG	1:B:208:VAL:H	2.10	0.51
1:A:363:ILE:O	1:A:367:LYS:HD3	2.11	0.51
1:A:431:LEU:O	1:A:434:LYS:HB2	2.11	0.51
1:A:323:HIS:HB2	4:A:1001:HOH:O	2.10	0.50
1:B:367:LYS:N	1:B:367:LYS:HD2	2.25	0.50
1:A:250:HIS:CE1	1:A:254:THR:HG21	2.47	0.50
1:A:334:VAL:HG11	1:A:371:ALA:CB	2.39	0.50
1:A:421:LEU:HD12	1:A:432:PHE:HB2	1.93	0.49
1:A:339:LEU:HD13	3:A:922:K55:H22A	1.93	0.49
1:A:358:LYS:O	1:A:360:PHE:N	2.46	0.49
1:A:334:VAL:CG1	1:A:371:ALA:HB1	2.40	0.49
1:A:274:TYR:CE1	1:A:280:HIS:HB2	2.48	0.49
1:A:317:LEU:HD13	1:A:400:LEU:HD21	1.94	0.49
1:A:358:LYS:N	1:A:359:PRO:HD2	2.28	0.49
1:A:214:PHE:HE1	1:A:413:ILE:HG12	1.77	0.49
1:A:250:HIS:HA	1:A:352:PHE:HB2	1.94	0.49
1:A:289:THR:O	1:A:293:VAL:HG23	2.13	0.49
1:B:271:LEU:HD13	1:B:272:PRO:HD2	1.95	0.49
1:A:319:LYS:HD3	1:A:320:TYR:CE2	2.48	0.48
1:A:425:HIS:HB3	1:A:428:ALA:HB2	1.95	0.48
1:B:234:ARG:HA	1:B:234:ARG:NE	2.29	0.48
1:B:384:LEU:O	1:B:388:ILE:HG12	2.13	0.48
1:B:211:LEU:HD23	1:B:419:PHE:CD1	2.48	0.48
1:B:421:LEU:HD13	1:B:431:LEU:HG	1.94	0.48
1:B:367:LYS:CD	1:B:367:LYS:H	2.27	0.48
1:B:249:ILE:HA	1:B:254:THR:HB	1.96	0.47
1:B:211:LEU:HD23	1:B:419:PHE:HD1	1.79	0.47
1:A:330:LEU:O	1:A:333:ILE:HG13	2.14	0.47
1:A:234:ARG:HE	1:A:234:ARG:HA	1.79	0.47
1:A:329:MET:O	1:A:332:SER:HB3	2.14	0.47
1:B:442:LEU:O	1:B:446:VAL:HG23	2.15	0.47
1:A:386:LEU:HD13	1:A:417:LEU:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:ASP:O	1:A:444:GLN:HB3	2.15	0.46
1:B:388:ILE:O	1:B:392:ILE:HG12	2.14	0.46
1:A:236:ILE:O	1:A:236:ILE:HG22	2.16	0.46
1:B:253:GLU:H	1:B:253:GLU:CD	2.19	0.46
1:A:360:PHE:O	1:A:363:ILE:HG12	2.16	0.46
1:A:459:THR:O	1:A:461:THR:N	2.48	0.46
1:B:318:LEU:O	1:B:322:VAL:HG22	2.15	0.46
1:B:307:SER:HA	1:B:314:GLN:HE22	1.80	0.46
1:A:455:ARG:O	1:A:459:THR:HG23	2.17	0.45
1:A:324:GLU:CD	1:A:397:ARG:HH22	2.20	0.45
1:B:397:ARG:HA	1:B:398:PRO:HD3	1.80	0.45
1:B:324:GLU:CD	1:B:397:ARG:HH22	2.19	0.45
1:B:418:GLU:HG2	1:B:432:PHE:CD1	2.52	0.45
1:B:312:ASN:N	1:B:312:ASN:HD22	2.14	0.45
1:A:331:ALA:HB2	1:A:371:ALA:HA	1.99	0.45
1:A:218:ILE:HG22	1:A:385:ALA:HB1	1.97	0.45
1:A:289:THR:HG21	3:A:922:K55:O26	2.17	0.45
1:A:315:VAL:CG2	1:B:311:LEU:HD23	2.47	0.45
1:A:389:ALA:HB1	1:A:413:ILE:HD13	1.99	0.44
1:A:214:PHE:O	1:A:218:ILE:HD13	2.18	0.44
1:B:228:MET:HG2	1:B:333:ILE:HG21	1.97	0.44
1:A:367:LYS:HD2	1:A:367:LYS:N	2.33	0.44
1:B:211:LEU:HD12	1:B:211:LEU:HA	1.85	0.44
1:B:379:LEU:HD11	1:B:435:LEU:HD21	1.99	0.44
1:A:357:ARG:NH2	1:A:460:GLU:OE1	2.51	0.43
1:B:289:THR:HG21	1:B:469:LEU:HD21	2.00	0.43
1:A:331:ALA:HA	1:A:334:VAL:HG12	1.99	0.43
1:B:205:MET:O	1:B:208:VAL:HG12	2.18	0.43
1:A:339:LEU:CD2	1:A:348:VAL:HB	2.48	0.43
1:B:307:SER:HA	1:B:314:GLN:NE2	2.33	0.43
1:B:353:LEU:HD12	1:B:353:LEU:HA	1.88	0.43
1:A:357:ARG:CG	1:A:357:ARG:HH11	2.27	0.43
1:A:339:LEU:HD23	1:A:348:VAL:HB	2.00	0.43
1:B:284:ARG:HA	1:B:284:ARG:HD3	1.84	0.43
1:B:320:TYR:CB	1:B:397:ARG:HD2	2.47	0.43
1:B:414:LEU:HD23	1:B:417:LEU:HD23	2.01	0.42
1:A:334:VAL:HG13	1:A:335:ASN:N	2.35	0.42
1:A:237:LEU:HD21	1:A:340:LEU:HG	2.01	0.42
3:B:923:K55:H4B	3:B:923:K55:H5A	1.95	0.42
1:A:414:LEU:HA	1:A:414:LEU:HD23	1.86	0.42
1:B:367:LYS:HG2	3:B:923:K55:C10	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:402:ASN:CG	1:A:405:ARG:HB2	2.40	0.42
1:B:335:ASN:HD21	1:B:347:PHE:HE1	1.68	0.42
1:A:467:PRO:O	1:A:470:GLN:HB2	2.20	0.42
1:B:296:LEU:HA	1:B:296:LEU:HD12	1.89	0.41
1:B:334:VAL:HG23	1:B:339:LEU:CB	2.48	0.41
1:B:324:GLU:OE2	1:B:443:ARG:HD3	2.20	0.41
1:B:330:LEU:HA	1:B:330:LEU:HD12	1.82	0.41
1:A:334:VAL:HG22	1:A:335:ASN:N	2.27	0.41
1:A:387:PHE:O	1:A:391:ILE:HG13	2.21	0.41
1:A:442:LEU:HD23	1:A:442:LEU:HA	1.86	0.41
1:A:340:LEU:HB3	1:A:344:GLY:HA2	2.03	0.41
1:B:322:VAL:O	1:B:326:ILE:HG13	2.21	0.41
1:A:315:VAL:HG23	1:B:311:LEU:HD23	2.03	0.40
1:A:393:LEU:O	1:A:410:GLN:HB2	2.21	0.40
1:B:317:LEU:HD12	1:B:317:LEU:HA	1.89	0.40
1:A:303:ILE:O	1:A:306:PHE:HB3	2.21	0.40
1:B:369:GLU:O	1:B:373:LYS:HG3	2.20	0.40
1:B:317:LEU:HD11	1:B:400:LEU:HD11	2.02	0.40
1:B:318:LEU:O	1:B:322:VAL:HG13	2.22	0.40
1:B:435:LEU:HA	1:B:435:LEU:HD23	1.94	0.40
1:A:312:ASN:ND2	1:A:312:ASN:N	2.63	0.40
1:A:353:LEU:HD12	1:A:353:LEU:HA	1.83	0.40
1:B:285:CYS:SG	3:B:923:K55:N27	2.89	0.40
1:B:430:TYR:O	1:B:434:LYS:HG3	2.21	0.40
1:B:297:THR:OG1	2:B:920:B7G:H131	2.22	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	255/276 (92%)	217 (85%)	28 (11%)	10 (4%)	3 17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	256/276 (93%)	220 (86%)	31 (12%)	5 (2%)	7	34
All	All	511/552 (93%)	437 (86%)	59 (12%)	15 (3%)	4	24

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	231	LYS
1	A	262	LEU
1	A	374	PHE
1	B	259	GLU
1	B	426	PRO
1	A	336	LYS
1	B	261	GLY
1	B	336	LYS
1	A	261	GLY
1	A	381	ASP
1	A	428	ALA
1	A	212	LYS
1	A	460	GLU
1	B	398	PRO
1	A	359	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	229/243 (94%)	210 (92%)	19 (8%)	11	39
1	B	232/243 (96%)	204 (88%)	28 (12%)	5	21
All	All	461/486 (95%)	414 (90%)	47 (10%)	7	28

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	227	ASN

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Mol	Chain	Res	Type
1	A	238	THR
1	A	243	HIS
1	A	271	LEU
1	A	284	ARG
1	A	288	THR
1	A	298	GLU
1	A	305	SER
1	A	309	LEU
1	A	312	ASN
1	A	317	LEU
1	A	336	LYS
1	A	339	LEU
1	A	353	LEU
1	A	357	ARG
1	A	358	LYS
1	A	380	ASP
1	A	405	ARG
1	A	410	GLN
1	B	208	VAL
1	B	211	LEU
1	B	223	LEU
1	B	227	ASN
1	B	234	ARG
1	B	237	LEU
1	B	244	THR
1	B	253	GLU
1	B	271	LEU
1	B	291	GLU
1	B	312	ASN
1	B	317	LEU
1	B	334	VAL
1	B	339	LEU
1	B	353	LEU
1	B	357	ARG
1	B	360	PHE
1	B	393	LEU
1	B	396	ASP
1	B	400	LEU
1	B	402	ASN
1	B	405	ARG
1	B	418	GLU
1	B	443	ARG

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Mol	Chain	Res	Type
1	B	462	GLU
1	B	463	THR
1	B	467	PRO
1	B	475	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	220	ASN
1	A	227	ASN
1	A	286	GLN
1	A	312	ASN
1	A	422	GLN
1	A	437	GLN
1	B	220	ASN
1	B	243	HIS
1	B	250	HIS
1	B	312	ASN
1	B	429	GLN
1	B	437	GLN
1	B	470	GLN

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	$\# Z > 2$
3	K55	B	923	-	31,34,34	1.41	6 (19%)	44,47,47	1.45	6 (13%)
2	B7G	A	921	-	19,19,19	0.78	0	24,24,24	1.40	1 (4%)
2	B7G	B	920	-	19,19,19	0.74	1 (5%)	24,24,24	1.52	3 (12%)
3	K55	A	922	-	31,34,34	1.40	7 (22%)	44,47,47	1.33	5 (11%)

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	K55	B	923	-	-	8/26/30/30	0/2/2/2
2	B7G	A	921	-	-	0/10/30/30	0/1/1/1
2	B7G	B	920	-	-	0/10/30/30	0/1/1/1
3	K55	A	922	-	-	8/26/30/30	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	923	K55	C7-C8	3.86	1.46	1.39
3	A	922	K55	C14-C13	-3.54	1.43	1.50
3	B	923	K55	C7-C6	3.07	1.44	1.39
3	A	922	K55	C13-N27	3.06	1.40	1.33
3	B	923	K55	C13-N27	2.98	1.40	1.33
3	A	922	K55	C16-C17	2.67	1.43	1.39
3	B	923	K55	C16-C15	2.61	1.42	1.37
3	A	922	K55	C16-C15	2.50	1.41	1.37
3	A	922	K55	O33-C9	-2.38	1.32	1.37
3	B	923	K55	C16-C17	2.37	1.43	1.39
3	A	922	K55	C7-C6	2.14	1.42	1.39
3	B	923	K55	C14-C13	-2.08	1.45	1.50
2	B	920	B7G	O1-C1	2.04	1.43	1.40
3	A	922	K55	C7-C8	2.01	1.42	1.39

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	920	B7G	C7-O1-C1	-5.63	104.50	113.84
2	A	921	B7G	C7-O1-C1	-5.18	105.25	113.84
3	B	923	K55	C6-C5-C2	4.86	120.09	113.81
3	A	922	K55	C16-C15-C14	-3.87	119.40	123.53
3	B	923	K55	C16-C15-C14	-3.79	119.49	123.53
3	A	922	K55	C19-C14-C15	3.69	120.86	116.67
3	B	923	K55	C3-C2-C1	-3.26	104.38	112.45
3	A	922	K55	C6-C5-C2	2.99	117.68	113.81
3	B	923	K55	C19-C14-C15	2.73	119.77	116.67
3	B	923	K55	C5-C6-C7	2.71	125.09	120.44
3	A	922	K55	C8-C12-N27	2.28	117.83	113.03
2	B	920	B7G	C9-C8-C7	-2.23	103.58	113.49
3	A	922	K55	C15-C14-C13	-2.17	120.08	125.09
2	B	920	B7G	C11-C10-C9	-2.07	103.91	114.42
3	B	923	K55	C5-C6-C11	-2.04	116.86	120.91

There are no chirality outliers.

All (16) torsion outliers are listed below:

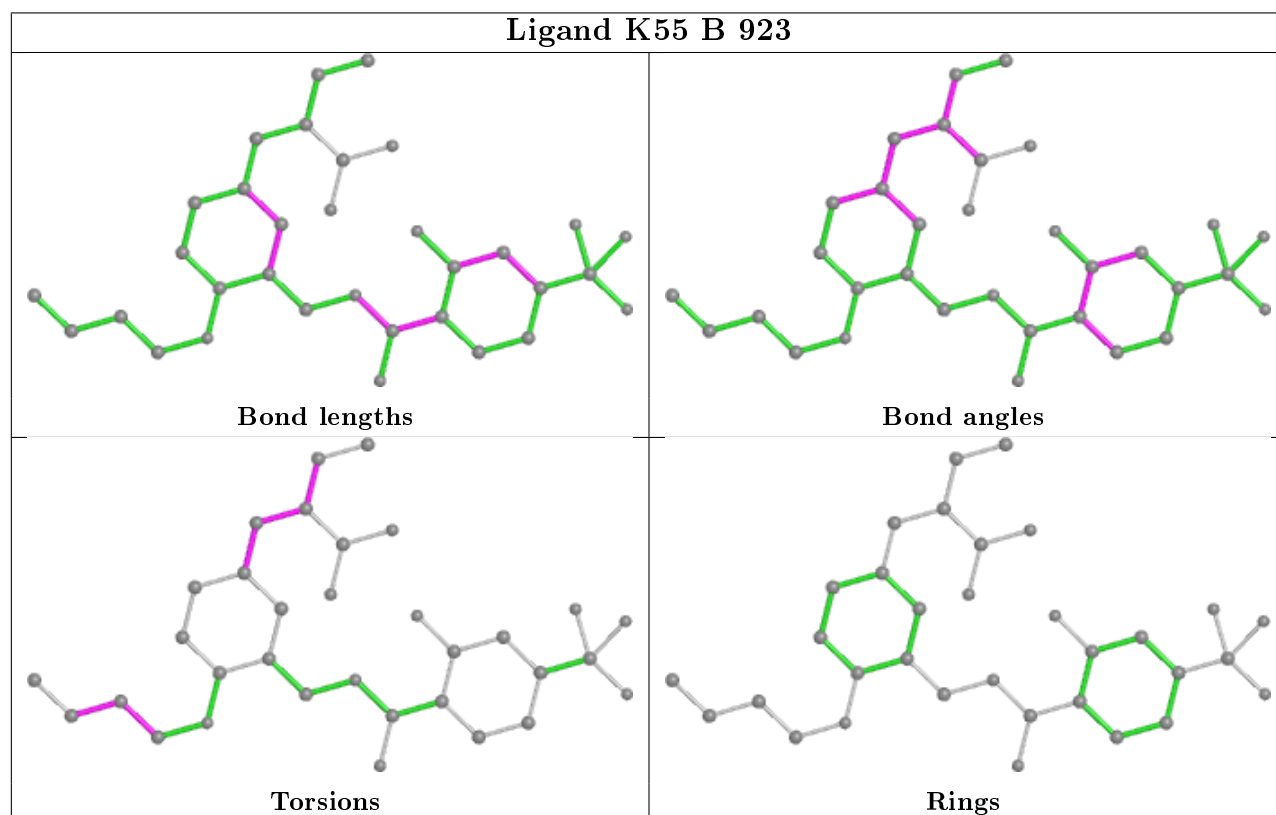
Mol	Chain	Res	Type	Atoms
3	B	923	K55	C1-C2-C3-C4
3	B	923	K55	C5-C2-C3-C4
3	B	923	K55	C3-C2-C5-C6
3	A	922	K55	C1-C2-C3-C4
3	A	922	K55	C5-C2-C3-C4
3	A	922	K55	C1-C2-C5-C6
3	A	922	K55	C3-C2-C5-C6
3	B	923	K55	C2-C5-C6-C11
3	A	922	K55	C2-C5-C6-C11
3	B	923	K55	C2-C5-C6-C7
3	A	922	K55	C2-C5-C6-C7
3	A	922	K55	O33-C21-C22-C23
3	B	923	K55	O33-C21-C22-C23
3	A	922	K55	C21-C22-C23-C24
3	B	923	K55	C21-C22-C23-C24
3	B	923	K55	C1-C2-C5-C6

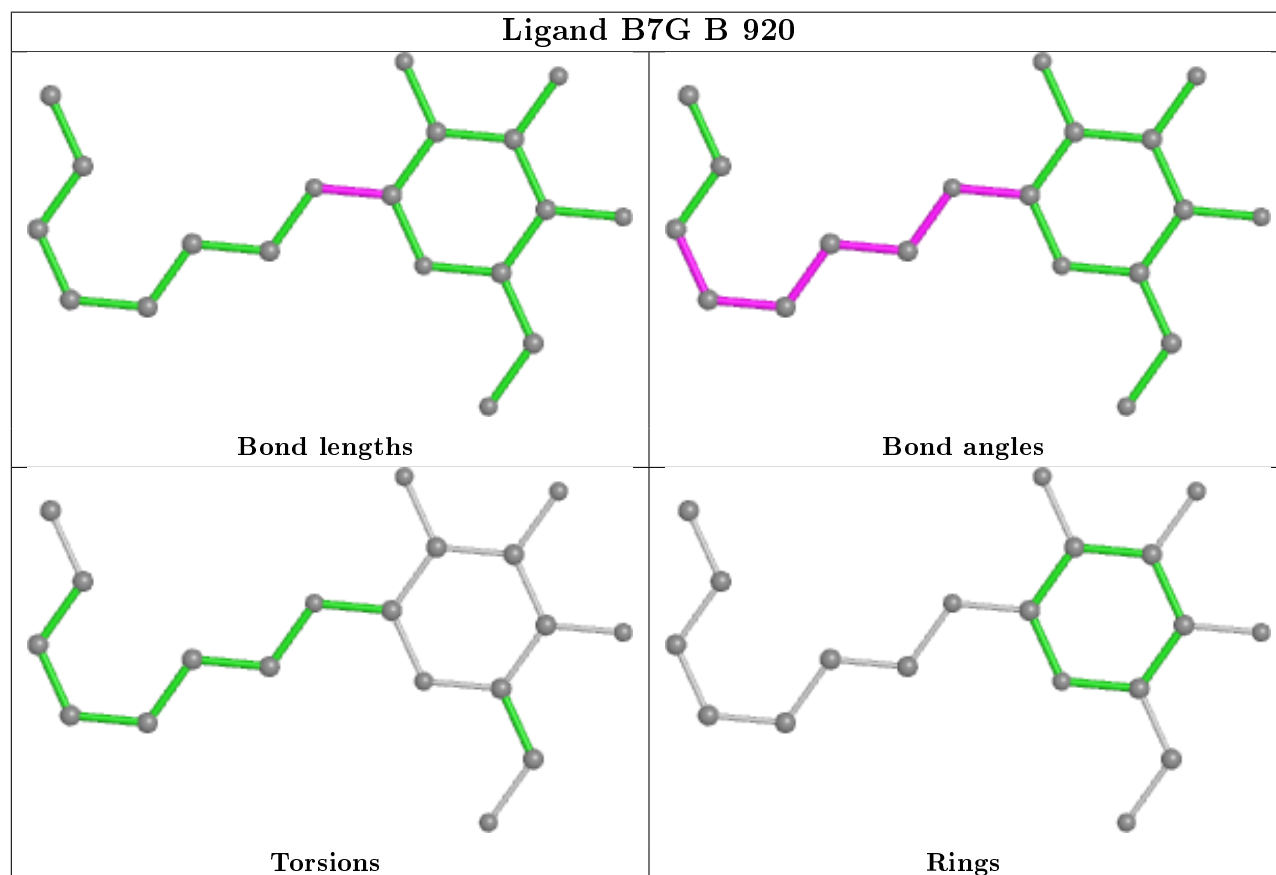
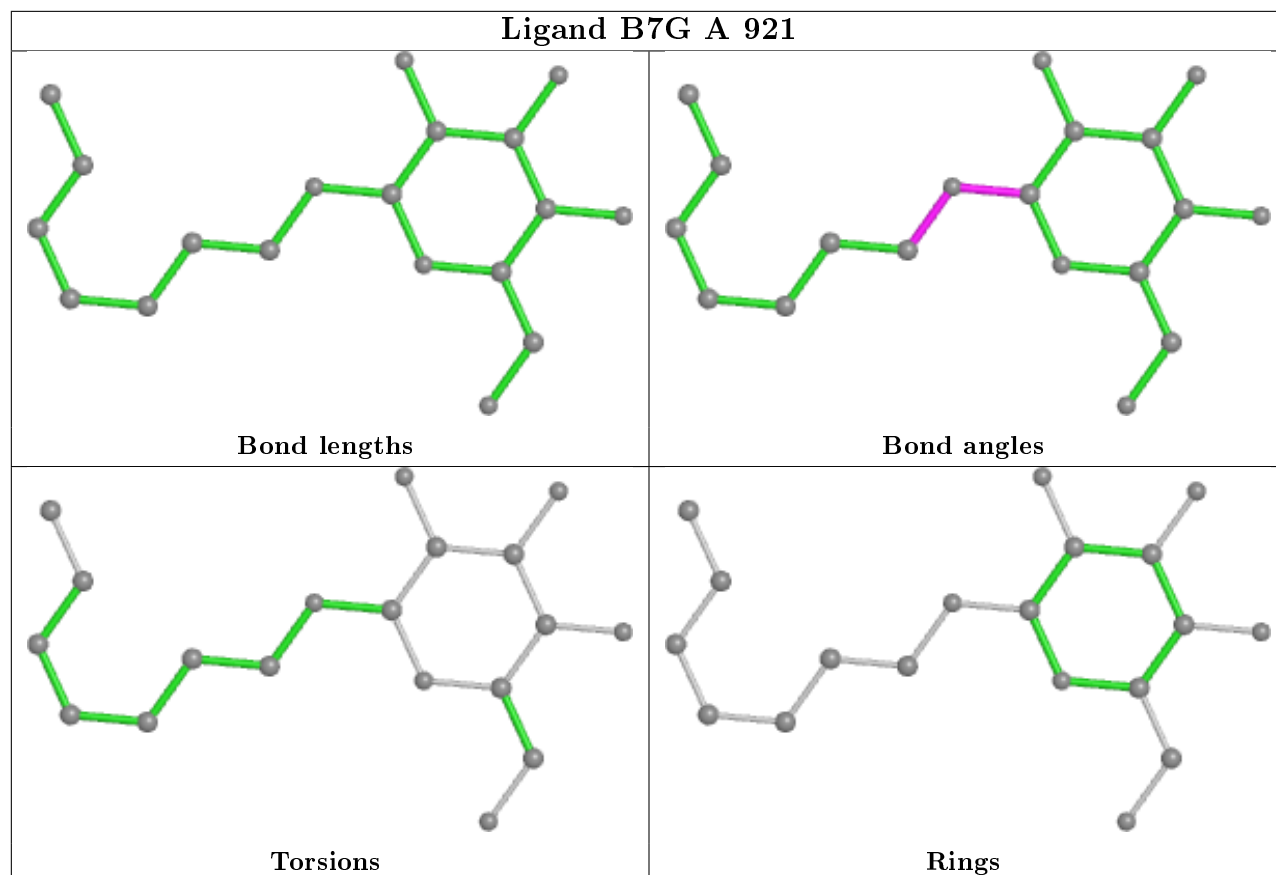
There are no ring outliers.

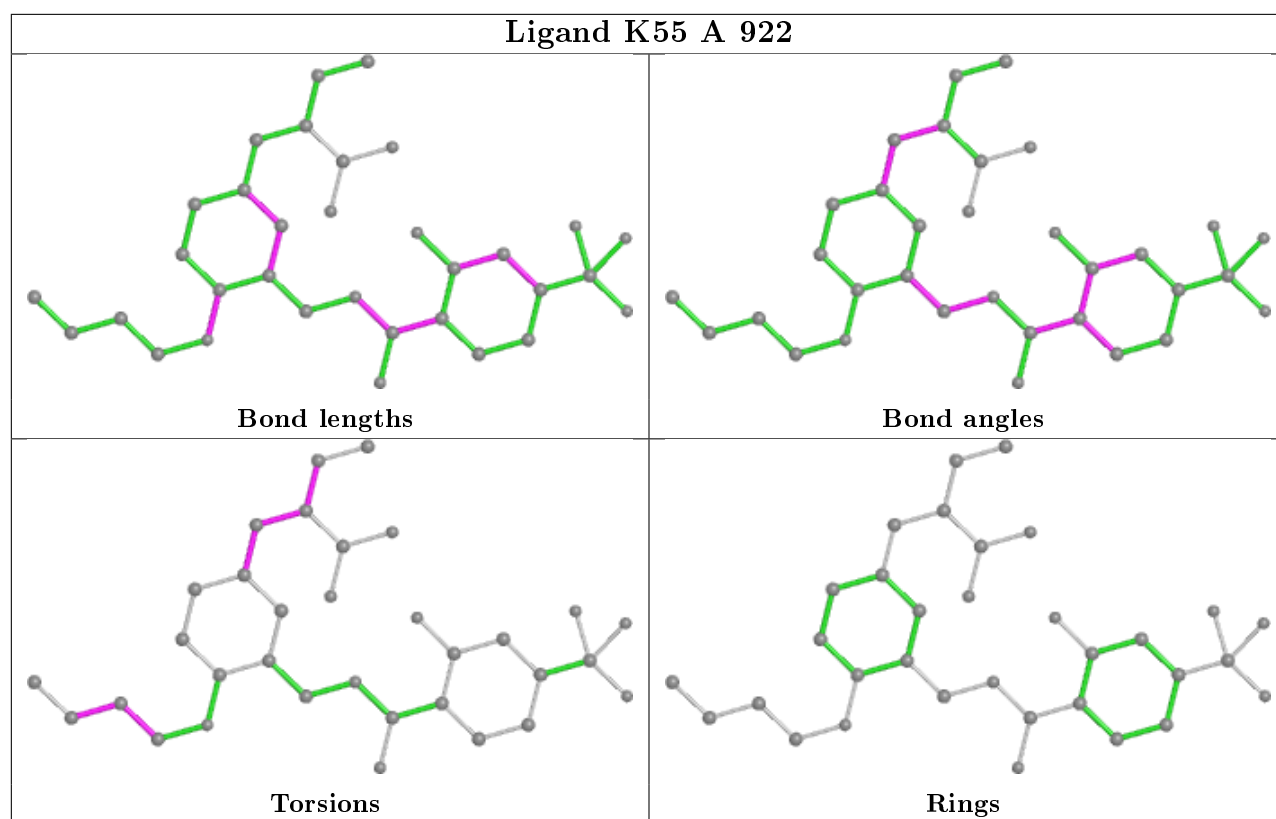
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	923	K55	5	0
2	A	921	B7G	1	0
2	B	920	B7G	4	0
3	A	922	K55	2	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	259/276 (93%)	-0.29	0	100 100	27, 44, 60, 75	0
1	B	262/276 (94%)	-0.38	1 (0%)	92 79	23, 39, 57, 77	0
All	All	521/552 (94%)	-0.33	1 (0%)	95 87	23, 41, 60, 77	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	206	PRO	2.7

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](#)

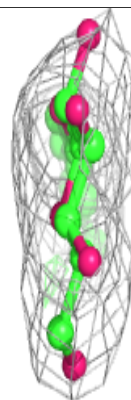
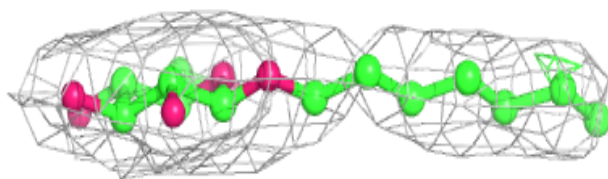
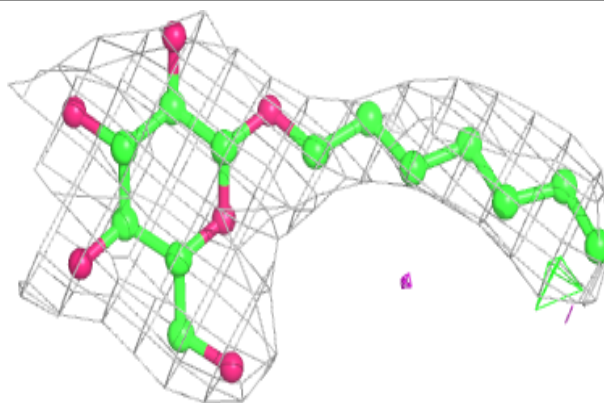
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	B7G	A	921	19/19	0.85	0.26	38,64,68,68	0
2	B7G	B	920	19/19	0.89	0.27	43,59,62,64	0
3	K55	B	923	33/33	0.94	0.27	25,36,42,43	0
3	K55	A	922	33/33	0.94	0.24	31,37,40,41	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.

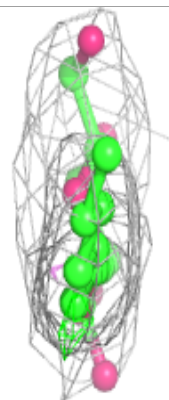
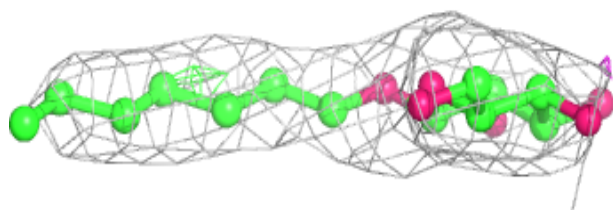
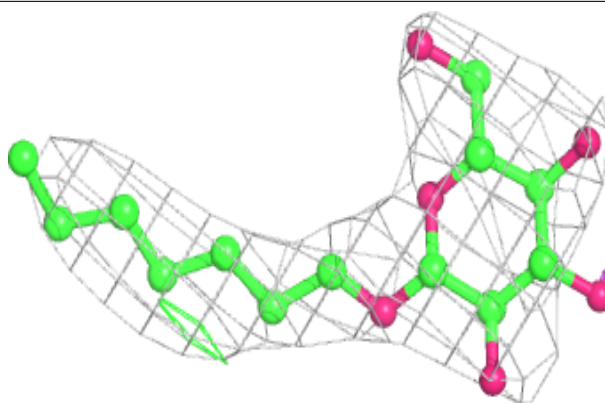
Electron density around B7G A 921:

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

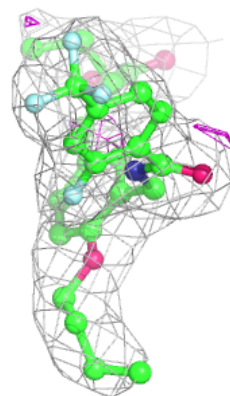
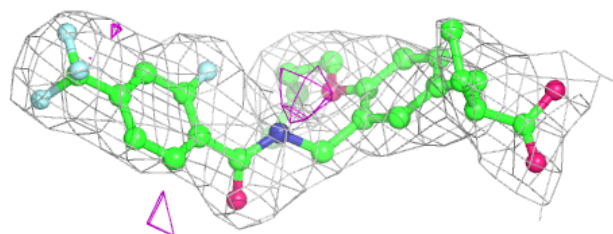
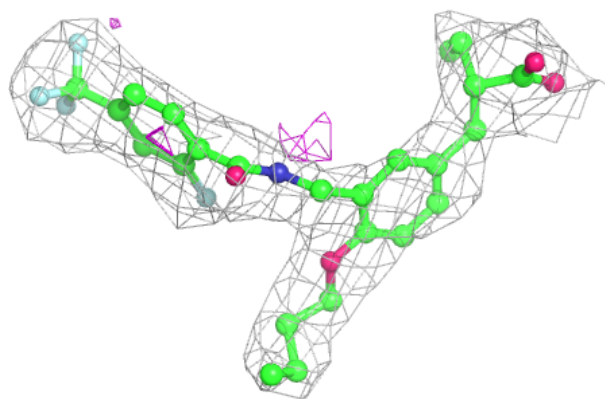


Electron density around B7G B 920:

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

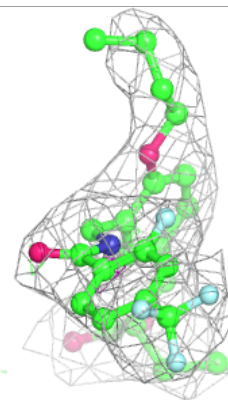
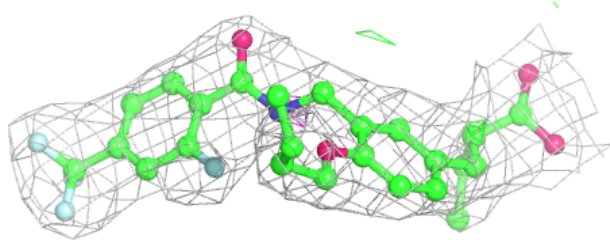
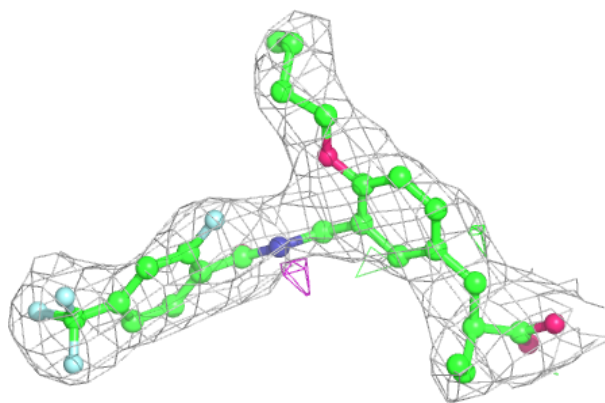
**Electron density around K55 B 923:**

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



Electron density around K55 A 922:

$2mF_o - DF_c$ (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.