



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:53 PM UTC

PDB ID : 2ZNO / pdb_00002zno
Title : Human PPAR gamma ligand binding domain in complex with a synthetic agonist TIPP703
Authors : Oyama, T.; Waku, T.; Kasuga, J.; Miyachi, H.; Morikawa, K.
Deposited on : 2008-04-30
Resolution : 2.40 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

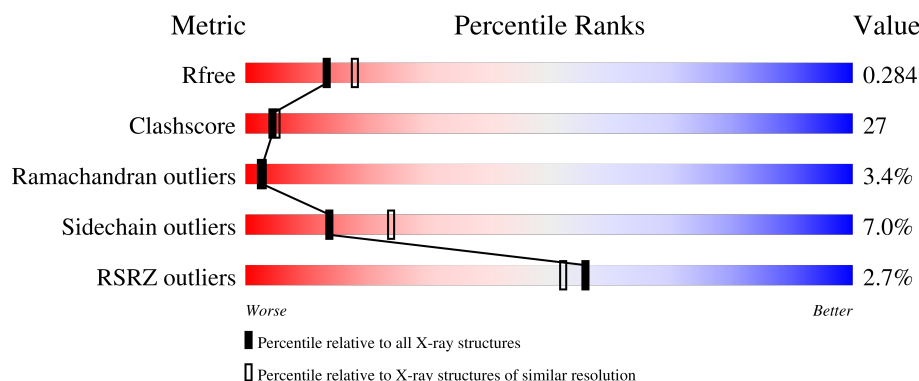
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	286	
1	B	286	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4222 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.

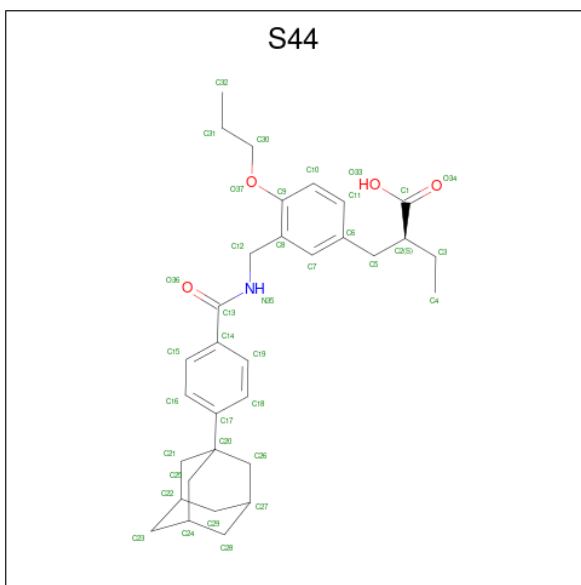
- Molecule 1 is a protein called Peroxisome proliferator-activated receptor gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	266	Total	C	N	O	S	0	0	0
			2110	1358	345	397	10			
1	B	251	Total	C	N	O	S	0	0	0
			2000	1292	327	372	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	191	GLY	-	expression tag	UNP P37231
A	192	SER	-	expression tag	UNP P37231
A	193	HIS	-	expression tag	UNP P37231
A	194	MET	-	expression tag	UNP P37231
B	191	GLY	-	expression tag	UNP P37231
B	192	SER	-	expression tag	UNP P37231
B	193	HIS	-	expression tag	UNP P37231
B	194	MET	-	expression tag	UNP P37231

- Molecule 2 is (2S)-2-(4-propoxy-3-({4-[(3S,5S,7S)-tricyclo[3.3.1.1^{3,7}]dec-1-yl]phenyl}carbonyl)amino)methyl)benzyl)butanoic acid (CCD ID: S44) (formula: C₃₂H₄₁NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 33	C 29	N 1	O 3	0	0
2	B	1	Total 33	C 29	N 1	O 3	0	0

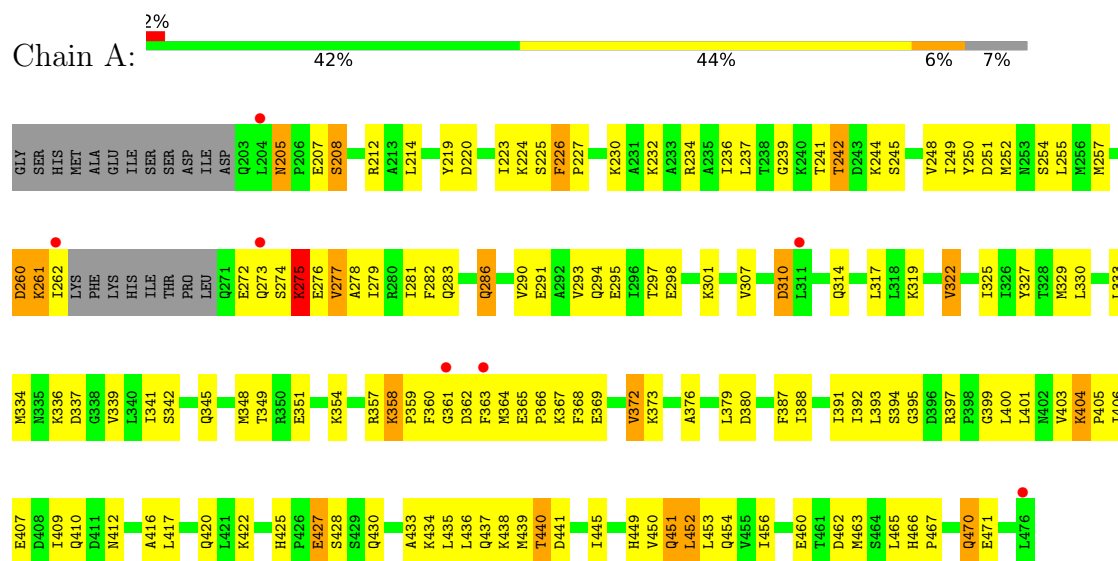
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	29	Total O 29 29	0	0
3	B	17	Total O 17 17	0	0

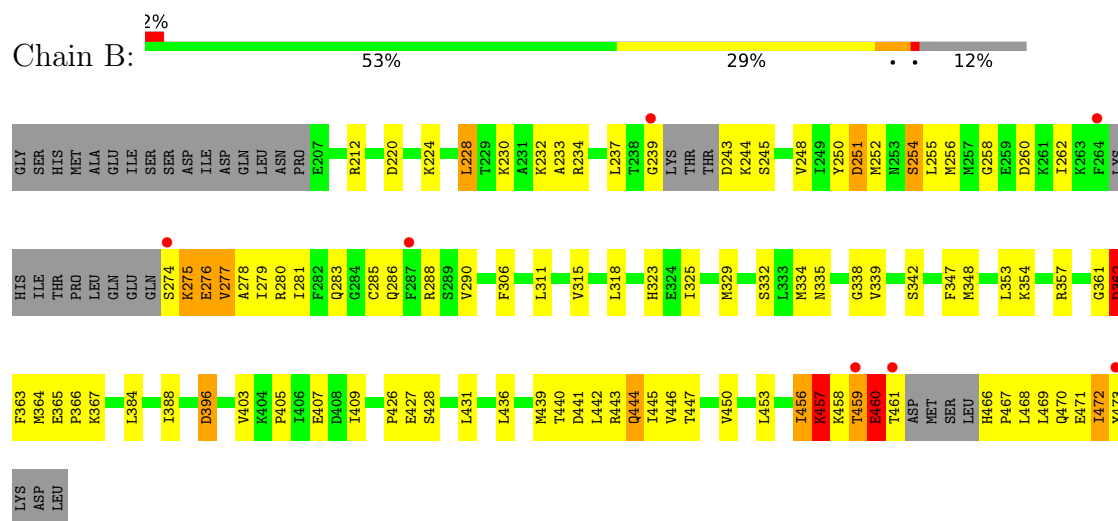
3 Residue-property plots

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: Peroxisome proliferator-activated receptor gamma



- Molecule 1: Peroxisome proliferator-activated receptor gamma



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	93.31Å 61.60Å 118.97Å 90.00° 103.64° 90.00°	Depositor
Resolution (Å)	49.09 – 2.40 49.09 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.1 (49.09-2.40) 93.1 (49.09-2.40)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.240 , 0.286 0.238 , 0.284	Depositor DCC
R_{free} test set	1217 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	41.0	Xtriage
Anisotropy	0.617	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4222	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: S44

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	0.55	0/2144	1.03	11/2889 (0.4%)
1	B	0.56	0/2031	0.93	7/2734 (0.3%)
All	All	0.55	0/4175	0.98	18/5623 (0.3%)

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	254	SER	N-CA-C	-6.60	103.91	112.23
1	A	248	VAL	N-CA-C	6.08	116.91	108.89
1	A	252	MET	N-CA-C	6.02	117.51	111.07
1	B	362	ASP	N-CA-C	-5.89	104.95	114.09
1	B	252	MET	N-CA-C	-5.89	104.77	111.07
1	A	242	THR	N-CA-C	-5.80	98.45	110.80
1	A	337	ASP	N-CA-C	5.79	120.50	113.38
1	B	444	GLN	N-CA-C	-5.78	104.89	111.07
1	B	306	PHE	N-CA-C	5.69	117.16	111.07
1	A	226	PHE	CA-C-N	5.69	124.88	118.97
1	A	226	PHE	C-N-CA	5.69	124.88	118.97
1	A	322	VAL	N-CA-C	5.60	116.24	110.36
1	B	335	ASN	N-CA-C	-5.36	101.16	109.14
1	A	310	ASP	N-CA-C	-5.30	103.36	110.24
1	A	237	LEU	N-CA-C	5.24	117.07	111.36
1	A	245	SER	CA-C-N	5.23	125.43	120.31
1	A	245	SER	C-N-CA	5.23	125.43	120.31
1	B	403	VAL	N-CA-C	5.21	117.60	111.09

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2110	0	2154	132	0
1	B	2000	0	2046	97	0
2	A	33	0	33	6	0
2	B	33	0	33	6	0
3	A	29	0	0	3	0
3	B	17	0	0	0	0
All	All	4222	0	4266	224	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 27.

All (224) 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:205:ASN:HD21	1:A:207:GLU:HB2	1.07	1.15
1:A:325:ILE:HG23	1:A:388:ILE:HD12	1.47	0.95
1:A:205:ASN:HD21	1:A:207:GLU:CB	1.82	0.93
1:A:261:LYS:H	1:A:261:LYS:HZ2	1.19	0.90
1:A:239:GLY:C	1:A:241:THR:H	1.79	0.89
1:B:325:ILE:HG22	1:B:329:MET:HE2	1.54	0.87
1:B:456:ILE:O	1:B:458:LYS:N	2.06	0.86
1:A:205:ASN:ND2	1:A:207:GLU:HB2	1.90	0.85
1:A:437:GLN:HE21	1:B:439:MET:HE1	1.43	0.82
1:A:260:ASP:HB2	1:A:261:LYS:NZ	1.94	0.82
1:A:261:LYS:H	1:A:261:LYS:NZ	1.77	0.81
1:B:274:SER:N	1:B:280:ARG:HD3	1.96	0.80
1:B:255:LEU:HD11	2:B:902:S44:H22	1.64	0.79
1:B:426:PRO:HG2	1:B:427:GLU:OE2	1.84	0.77
1:A:417:LEU:HD21	1:A:435:LEU:HD23	1.65	0.77
1:A:437:GLN:NE2	1:B:439:MET:HE1	2.02	0.75
1:B:220:ASP:O	1:B:224:LYS:HD3	1.89	0.73
1:B:275:LYS:NZ	1:B:460:GLU:HB3	2.03	0.73
1:A:404:LYS:HA	1:A:404:LYS:HE3	1.71	0.73
1:B:239:GLY:O	1:B:243:ASP:HA	1.91	0.71
1:A:275:LYS:HG2	1:A:276:GLU:H	1.54	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLY:C	1:A:241:THR:N	2.48	0.71
1:A:325:ILE:HD11	1:A:392:ILE:HG13	1.72	0.70
1:A:436:LEU:HD12	1:B:436:LEU:HD12	1.72	0.70
1:B:250:TYR:CE1	1:B:251:ASP:HB2	2.26	0.70
1:A:449:HIS:CD2	1:A:453:LEU:HD21	2.28	0.69
1:B:443:ARG:O	1:B:447:THR:HG23	1.92	0.69
1:A:261:LYS:HZ2	1:A:261:LYS:N	1.90	0.67
1:A:441:ASP:O	1:A:445:ILE:HG12	1.94	0.67
1:B:384:LEU:O	1:B:388:ILE:HG12	1.94	0.66
1:A:226:PHE:CD1	1:A:329:MET:HE1	2.30	0.66
1:B:290:VAL:HG21	1:B:473:TYR:CD1	2.31	0.65
1:B:459:THR:HG22	1:B:460:GLU:N	2.10	0.65
1:B:251:ASP:H	1:B:254:SER:HB3	1.61	0.65
1:B:357:ARG:HD2	1:B:357:ARG:O	1.97	0.64
1:A:260:ASP:HB2	1:A:261:LYS:HZ2	1.62	0.64
1:A:205:ASN:ND2	1:A:208:SER:H	1.95	0.64
1:A:261:LYS:H	1:A:261:LYS:CE	2.10	0.64
1:A:363:PHE:HE1	1:A:456:ILE:HD11	1.62	0.63
1:B:467:PRO:O	1:B:470:GLN:HG2	1.98	0.63
1:B:290:VAL:HG21	1:B:473:TYR:HD1	1.62	0.62
1:A:393:LEU:O	1:A:410:GLN:HB2	1.99	0.62
1:B:456:ILE:C	1:B:458:LYS:H	2.04	0.61
1:A:360:PHE:C	1:A:362:ASP:H	2.07	0.61
1:A:379:LEU:HD11	1:A:435:LEU:HD13	1.82	0.61
1:A:449:HIS:NE2	1:A:453:LEU:HD21	2.15	0.61
1:A:358:LYS:HB2	1:A:359:PRO:CD	2.31	0.61
1:B:275:LYS:HG2	1:B:279:ILE:HD12	1.83	0.60
1:B:459:THR:HG22	1:B:460:GLU:H	1.66	0.60
1:A:368:PHE:O	1:A:372:VAL:HG23	2.01	0.60
1:A:364:MET:SD	2:A:901:S44:H10	2.41	0.59
1:A:437:GLN:HE21	1:B:439:MET:CE	2.15	0.59
1:B:365:GLU:N	1:B:366:PRO:HD2	2.17	0.59
1:B:441:ASP:O	1:B:445:ILE:HG12	2.03	0.59
1:A:220:ASP:O	1:A:224:LYS:HG3	2.02	0.59
1:B:325:ILE:CG2	1:B:329:MET:HE2	2.29	0.59
1:B:446:VAL:O	1:B:450:VAL:HG23	2.02	0.59
1:A:451:GLN:O	1:A:451:GLN:HG2	2.01	0.59
1:A:317:LEU:HD21	1:A:406:ILE:HD13	1.84	0.58
1:A:241:THR:HG22	1:A:244:LYS:HB2	1.85	0.58
1:B:453:LEU:O	1:B:456:ILE:HG22	2.04	0.58
1:A:334:MET:HE2	1:A:368:PHE:CE1	2.39	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:LYS:HB2	1:A:359:PRO:HD3	1.85	0.58
1:A:276:GLU:OE2	1:A:357:ARG:NH2	2.37	0.57
1:A:364:MET:CE	2:A:901:S44:H10	2.34	0.57
1:B:348:MET:SD	1:B:353:LEU:HD21	2.45	0.57
1:A:363:PHE:CE2	1:A:452:LEU:HB3	2.39	0.57
1:A:307:VAL:HA	1:A:314:GLN:OE1	2.04	0.57
1:B:329:MET:O	1:B:332:SER:HB2	2.05	0.56
1:B:363:PHE:CE2	1:B:364:MET:HE3	2.41	0.56
1:A:236:ILE:HG23	1:A:244:LYS:O	2.06	0.56
1:B:275:LYS:HZ1	1:B:460:GLU:HB3	1.70	0.56
1:B:396:ASP:C	1:B:396:ASP:OD2	2.49	0.56
1:A:219:TYR:CZ	1:A:223:ILE:HD11	2.41	0.55
1:A:249:ILE:HD13	1:A:255:LEU:HD12	1.87	0.55
1:B:311:LEU:O	1:B:315:VAL:HG23	2.07	0.55
1:B:275:LYS:CE	1:B:460:GLU:HB3	2.36	0.55
1:A:404:LYS:N	1:A:405:PRO:HD2	2.22	0.55
1:B:230:LYS:O	1:B:234:ARG:HG2	2.07	0.55
1:B:353:LEU:HD13	1:B:364:MET:HG3	1.89	0.55
1:B:466:HIS:HA	1:B:469:LEU:HD13	1.88	0.55
1:A:436:LEU:O	1:A:439:MET:HB2	2.07	0.54
1:B:283:GLN:HA	1:B:286:GLN:HG3	1.89	0.54
1:A:251:ASP:OD1	1:A:254:SER:HB2	2.08	0.54
1:B:470:GLN:HG3	1:B:471:GLU:N	2.21	0.54
1:A:394:SER:O	1:A:397:ARG:HG2	2.08	0.54
1:A:293:VAL:HG22	1:A:322:VAL:HG11	1.89	0.54
1:A:450:VAL:HA	1:A:453:LEU:HD23	1.90	0.54
1:B:277:VAL:HG13	1:B:278:ALA:N	2.23	0.53
1:B:456:ILE:CG2	1:B:457:LYS:N	2.71	0.53
1:A:291:GLU:HA	1:A:294:GLN:OE1	2.09	0.53
1:A:360:PHE:O	1:A:362:ASP:N	2.40	0.53
1:B:251:ASP:H	1:B:254:SER:CB	2.20	0.53
1:A:275:LYS:HG2	1:A:276:GLU:N	2.23	0.53
1:B:275:LYS:CG	1:B:276:GLU:H	2.21	0.53
1:B:285:CYS:HA	2:B:902:S44:HN35	1.74	0.53
1:B:250:TYR:CD1	1:B:251:ASP:HB2	2.43	0.53
1:A:325:ILE:HD13	1:A:388:ILE:HG23	1.91	0.53
1:B:456:ILE:O	1:B:456:ILE:HD13	2.09	0.53
1:A:357:ARG:HH12	1:A:460:GLU:CD	2.16	0.52
1:A:260:ASP:HB2	1:A:261:LYS:CE	2.38	0.52
1:A:351:GLU:HA	1:A:351:GLU:OE2	2.09	0.52
1:B:275:LYS:HG3	1:B:276:GLU:H	1.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:PHE:CE1	1:A:452:LEU:HD22	2.45	0.52
1:A:363:PHE:CE1	1:A:456:ILE:HD11	2.44	0.52
1:A:366:PRO:O	1:A:369:GLU:HB3	2.09	0.52
1:A:440:THR:HG22	1:B:440:THR:OG1	2.10	0.52
1:A:262:ILE:HG23	1:A:342:SER:CB	2.39	0.52
1:A:286:GLN:O	1:A:290:VAL:HG23	2.10	0.52
1:A:341:ILE:HD13	1:A:348:MET:HE3	1.92	0.52
1:B:472:ILE:HG22	1:B:473:TYR:CE1	2.45	0.52
1:B:275:LYS:HE2	1:B:460:GLU:HB3	1.91	0.52
1:B:457:LYS:HZ2	1:B:457:LYS:HA	1.76	0.51
1:A:307:VAL:HG22	3:A:1006:HOH:O	2.10	0.51
1:B:258:GLY:O	1:B:262:ILE:HB	2.11	0.51
1:A:373:LYS:O	1:A:376:ALA:HB3	2.11	0.51
1:A:399:GLY:O	1:A:401:LEU:HD12	2.10	0.51
1:A:282:PHE:CE2	1:A:463:MET:HE1	2.47	0.50
1:A:262:ILE:HG23	1:A:342:SER:HB2	1.93	0.50
1:A:330:LEU:O	1:A:334:MET:HG3	2.11	0.50
1:A:348:MET:HE1	2:A:901:S44:H21A	1.94	0.50
1:A:364:MET:HE1	2:A:901:S44:H10	1.93	0.50
1:B:283:GLN:HA	1:B:286:GLN:CG	2.41	0.50
1:A:230:LYS:O	1:A:234:ARG:HB2	2.13	0.49
1:B:466:HIS:O	1:B:467:PRO:C	2.55	0.49
1:B:363:PHE:CZ	1:B:364:MET:HE3	2.47	0.49
1:B:456:ILE:C	1:B:458:LYS:N	2.65	0.49
1:B:354:LYS:HE3	1:B:365:GLU:HG3	1.93	0.49
1:A:279:ILE:O	1:A:283:GLN:HG2	2.13	0.49
1:A:290:VAL:HG11	1:A:466:HIS:NE2	2.28	0.49
1:B:212:ARG:HE	1:B:212:ARG:HA	1.77	0.49
1:B:275:LYS:HG3	1:B:276:GLU:N	2.28	0.49
1:A:212:ARG:HA	1:A:212:ARG:NE	2.28	0.49
1:A:400:LEU:HD22	1:A:406:ILE:CD1	2.43	0.49
1:B:456:ILE:HG23	1:B:457:LYS:N	2.28	0.48
1:A:251:ASP:OD1	1:A:254:SER:CB	2.62	0.48
1:A:387:PHE:CE2	1:A:391:ILE:HD11	2.49	0.48
1:B:466:HIS:O	1:B:469:LEU:N	2.46	0.48
1:A:351:GLU:OE2	1:A:354:LYS:HE2	2.12	0.48
1:A:360:PHE:C	1:A:362:ASP:N	2.72	0.48
1:A:212:ARG:HA	1:A:212:ARG:HE	1.78	0.47
1:A:365:GLU:HB3	1:A:366:PRO:HD3	1.96	0.47
1:B:338:GLY:HA3	1:B:347:PHE:CZ	2.49	0.47
1:B:457:LYS:O	1:B:458:LYS:HD2	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:THR:HB	3:A:1028:HOH:O	2.13	0.47
1:A:214:LEU:HD23	1:A:416:ALA:HB2	1.97	0.47
1:B:364:MET:SD	2:B:902:S44:H10	2.54	0.47
1:A:230:LYS:NZ	1:A:379:LEU:O	2.39	0.47
1:A:281:ILE:HA	2:A:901:S44:H25	1.97	0.47
1:A:435:LEU:O	1:A:438:LYS:HB2	2.15	0.47
1:A:451:GLN:O	1:A:451:GLN:CG	2.62	0.47
1:B:459:THR:O	1:B:461:THR:N	2.46	0.46
1:A:394:SER:OG	1:A:397:ARG:NE	2.48	0.46
1:A:433:ALA:O	1:A:437:GLN:HG3	2.14	0.46
1:A:453:LEU:O	1:A:454:GLN:C	2.58	0.46
1:A:319:LYS:HE2	1:A:471:GLU:O	2.15	0.46
1:A:334:MET:HG2	1:A:339:VAL:HG23	1.98	0.46
1:A:425:HIS:HB3	1:A:428:SER:HB3	1.98	0.46
1:B:459:THR:CG2	1:B:460:GLU:H	2.27	0.46
1:B:466:HIS:N	1:B:467:PRO:CD	2.79	0.46
1:A:239:GLY:O	1:A:241:THR:N	2.41	0.45
1:A:274:SER:C	1:A:275:LYS:HD2	2.42	0.45
1:B:457:LYS:C	1:B:458:LYS:HD2	2.41	0.45
1:B:325:ILE:HD13	1:B:388:ILE:CG2	2.46	0.45
1:A:453:LEU:N	1:A:453:LEU:HD22	2.32	0.45
1:B:233:ALA:O	1:B:237:LEU:HG	2.17	0.45
1:B:255:LEU:CD1	2:B:902:S44:H22	2.39	0.45
1:B:364:MET:HE1	2:B:902:S44:H11	1.99	0.45
1:A:277:VAL:O	1:A:278:ALA:C	2.60	0.44
1:B:250:TYR:CD1	1:B:250:TYR:C	2.95	0.44
1:A:297:THR:O	1:A:301:LYS:HG3	2.17	0.44
1:A:430:GLN:O	1:A:434:LYS:HG3	2.18	0.44
1:A:225:SER:O	1:A:295:GLU:HG2	2.18	0.44
1:B:472:ILE:HG22	1:B:472:ILE:O	2.18	0.44
1:A:286:GLN:HE22	1:A:465:LEU:HA	1.83	0.44
1:A:465:LEU:HB2	1:A:470:GLN:HE21	1.83	0.44
1:A:354:LYS:O	1:A:354:LYS:HG2	2.19	0.43
1:A:275:LYS:HD2	1:A:275:LYS:N	2.33	0.43
1:A:403:VAL:O	1:A:407:GLU:HG3	2.18	0.43
1:A:462:ASP:OD2	1:A:462:ASP:N	2.50	0.43
1:B:279:ILE:O	1:B:283:GLN:HG3	2.18	0.43
1:A:295:GLU:O	1:A:298:GLU:HB3	2.19	0.43
1:B:428:SER:HB3	1:B:431:LEU:HB2	2.00	0.43
1:B:470:GLN:CG	1:B:471:GLU:N	2.82	0.43
1:B:248:VAL:HG12	1:B:250:TYR:HD2	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:LEU:HD23	1:B:232:LYS:HE3	2.01	0.43
1:B:427:GLU:OE2	1:B:427:GLU:N	2.52	0.43
1:A:212:ARG:NH2	1:A:420:GLN:OE1	2.39	0.43
1:A:275:LYS:CG	1:A:276:GLU:H	2.17	0.43
1:A:325:ILE:CD1	1:A:388:ILE:HG23	2.49	0.43
1:B:277:VAL:O	1:B:281:ILE:HG13	2.19	0.43
1:B:405:PRO:O	1:B:409:ILE:HG13	2.19	0.42
1:A:450:VAL:C	1:A:452:LEU:H	2.28	0.42
1:A:249:ILE:HD13	1:A:255:LEU:CD1	2.49	0.42
1:B:251:ASP:CB	1:B:254:SER:HB2	2.49	0.42
1:B:364:MET:HE2	1:B:364:MET:HA	2.01	0.42
1:B:334:MET:HG2	1:B:339:VAL:HB	2.00	0.42
1:A:395:GLY:O	1:A:400:LEU:HD12	2.20	0.42
1:A:380:ASP:HB2	3:A:1014:HOH:O	2.19	0.42
1:A:232:LYS:O	1:A:236:ILE:HG13	2.19	0.42
1:B:472:ILE:O	1:B:472:ILE:CG2	2.68	0.42
1:B:243:ASP:O	1:B:245:SER:N	2.53	0.42
1:A:342:SER:O	1:A:345:GLN:HG3	2.20	0.41
1:A:363:PHE:CZ	1:A:452:LEU:HD22	2.54	0.41
1:A:427:GLU:H	1:A:427:GLU:CD	2.25	0.41
1:B:281:ILE:HA	2:B:902:S44:H25	2.01	0.41
1:A:205:ASN:CG	1:A:207:GLU:H	2.28	0.41
1:A:358:LYS:H	1:A:358:LYS:HD3	1.84	0.41
1:A:341:ILE:HD12	2:A:901:S44:H21	2.03	0.41
1:B:466:HIS:HB3	1:B:467:PRO:HD3	2.02	0.41
1:A:250:TYR:HB3	1:A:349:THR:HG21	2.03	0.41
1:A:363:PHE:O	1:A:367:LYS:NZ	2.54	0.41
1:A:467:PRO:O	1:A:470:GLN:N	2.54	0.41
1:B:275:LYS:CG	1:B:276:GLU:N	2.84	0.41
1:B:361:GLY:C	1:B:362:ASP:OD2	2.63	0.41
1:A:261:LYS:H	1:A:261:LYS:HE3	1.86	0.40
1:A:393:LEU:HD12	1:A:409:ILE:HB	2.02	0.40
1:B:276:GLU:HB2	1:B:277:VAL:H	1.57	0.40
1:A:327:TYR:CE1	1:A:367:LYS:HE2	2.56	0.40
1:B:366:PRO:HG2	1:B:367:LYS:HD2	2.03	0.40
1:B:442:LEU:O	1:B:445:ILE:HB	2.21	0.40
1:B:467:PRO:HA	1:B:470:GLN:HE21	1.86	0.40
1:A:226:PHE:HA	1:A:227:PRO:HD3	1.81	0.40
1:A:310:ASP:O	1:A:314:GLN:HG3	2.22	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	262/286 (92%)	236 (90%)	17 (6%)	9 (3%)	3	2
1	B	243/286 (85%)	216 (89%)	19 (8%)	8 (3%)	3	2
All	All	505/572 (88%)	452 (90%)	36 (7%)	17 (3%)	3	2

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	358	LYS
1	B	276	GLU
1	B	457	LYS
1	B	244	LYS
1	B	460	GLU
1	A	242	THR
1	A	260	ASP
1	A	273	GLN
1	B	275	LYS
1	B	342	SER
1	A	272	GLU
1	A	275	LYS
1	B	459	THR
1	A	277	VAL
1	A	336	LYS
1	A	361	GLY
1	B	277	VAL

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	234/257 (91%)	218 (93%)	16 (7%)	14	25
1	B	221/257 (86%)	205 (93%)	16 (7%)	13	23
All	All	455/514 (88%)	423 (93%)	32 (7%)	14	24

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	208	SER
1	A	257	MET
1	A	261	LYS
1	A	275	LYS
1	A	286	GLN
1	A	333	LEU
1	A	372	VAL
1	A	404	LYS
1	A	412	ASN
1	A	422	LYS
1	A	427	GLU
1	A	440	THR
1	A	451	GLN
1	A	452	LEU
1	A	470	GLN
1	B	228	LEU
1	B	251	ASP
1	B	256	MET
1	B	260	ASP
1	B	288	ARG
1	B	318	LEU
1	B	323	HIS
1	B	362	ASP
1	B	396	ASP
1	B	407	GLU
1	B	444	GLN
1	B	456	ILE
1	B	457	LYS
1	B	460	GLU
1	B	468	LEU
1	B	472	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	ASN
1	A	283	GLN
1	A	286	GLN
1	A	308	ASN
1	A	312	ASN
1	A	345	GLN
1	A	415	GLN
1	A	424	ASN
1	A	430	GLN
1	A	437	GLN
1	A	444	GLN
1	A	451	GLN
1	A	470	GLN
1	B	253	ASN
1	B	286	GLN
1	B	308	ASN
1	B	323	HIS
1	B	410	GLN
1	B	424	ASN
1	B	430	GLN
1	B	451	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	S44	A	901	-	37,37,41	2.67	16 (43%)	53,54,59	0.74	1 (1%)
2	S44	B	902	-	37,37,41	2.71	16 (43%)	53,54,59	0.71	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
2	S44	A	901	-	-	2/25/52/56	0/6/5/5
2	S44	B	902	-	-	4/25/52/56	0/6/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	S44	C2-C1	-6.89	1.39	1.51
2	B	902	S44	C2-C1	-6.76	1.39	1.51
2	A	901	S44	C14-C13	-5.62	1.37	1.50
2	B	902	S44	C14-C13	-5.34	1.38	1.50
2	A	901	S44	C7-C8	4.80	1.47	1.39
2	A	901	S44	C7-C6	4.75	1.47	1.39
2	B	902	S44	C7-C8	4.61	1.47	1.39
2	B	902	S44	C7-C6	4.37	1.46	1.39
2	B	902	S44	C18-C17	4.35	1.46	1.39
2	B	902	S44	C10-C11	4.29	1.46	1.38
2	A	901	S44	C16-C15	4.14	1.45	1.38
2	B	902	S44	C19-C14	4.09	1.45	1.39
2	B	902	S44	C19-C18	3.93	1.45	1.38
2	B	902	S44	C16-C17	3.83	1.45	1.39
2	A	901	S44	C18-C17	3.74	1.45	1.39
2	A	901	S44	C16-C17	3.59	1.45	1.39
2	B	902	S44	C15-C14	3.47	1.44	1.39
2	A	901	S44	C19-C18	3.38	1.44	1.38
2	A	901	S44	C15-C14	3.35	1.44	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	902	S44	C9-C8	3.33	1.45	1.38
2	A	901	S44	C10-C11	3.32	1.44	1.38
2	B	902	S44	C10-C9	3.21	1.44	1.38
2	A	901	S44	C10-C9	3.16	1.44	1.38
2	A	901	S44	C13-N35	3.11	1.40	1.33
2	B	902	S44	C16-C15	2.97	1.43	1.38
2	A	901	S44	C11-C6	2.89	1.44	1.38
2	A	901	S44	C19-C14	2.88	1.43	1.39
2	B	902	S44	C11-C6	2.85	1.44	1.38
2	A	901	S44	C9-C8	2.80	1.44	1.38
2	B	902	S44	C12-C8	-2.72	1.45	1.51
2	A	901	S44	C12-C8	-2.02	1.47	1.51
2	B	902	S44	C13-N35	2.01	1.38	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	901	S44	O34-C1-C2	2.16	128.59	122.86

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	S44	C1-C2-C5-C6
2	A	901	S44	C3-C2-C5-C6
2	B	902	S44	N35-C13-C14-C15
2	B	902	S44	O36-C13-C14-C15
2	B	902	S44	N35-C13-C14-C19
2	B	902	S44	O36-C13-C14-C19

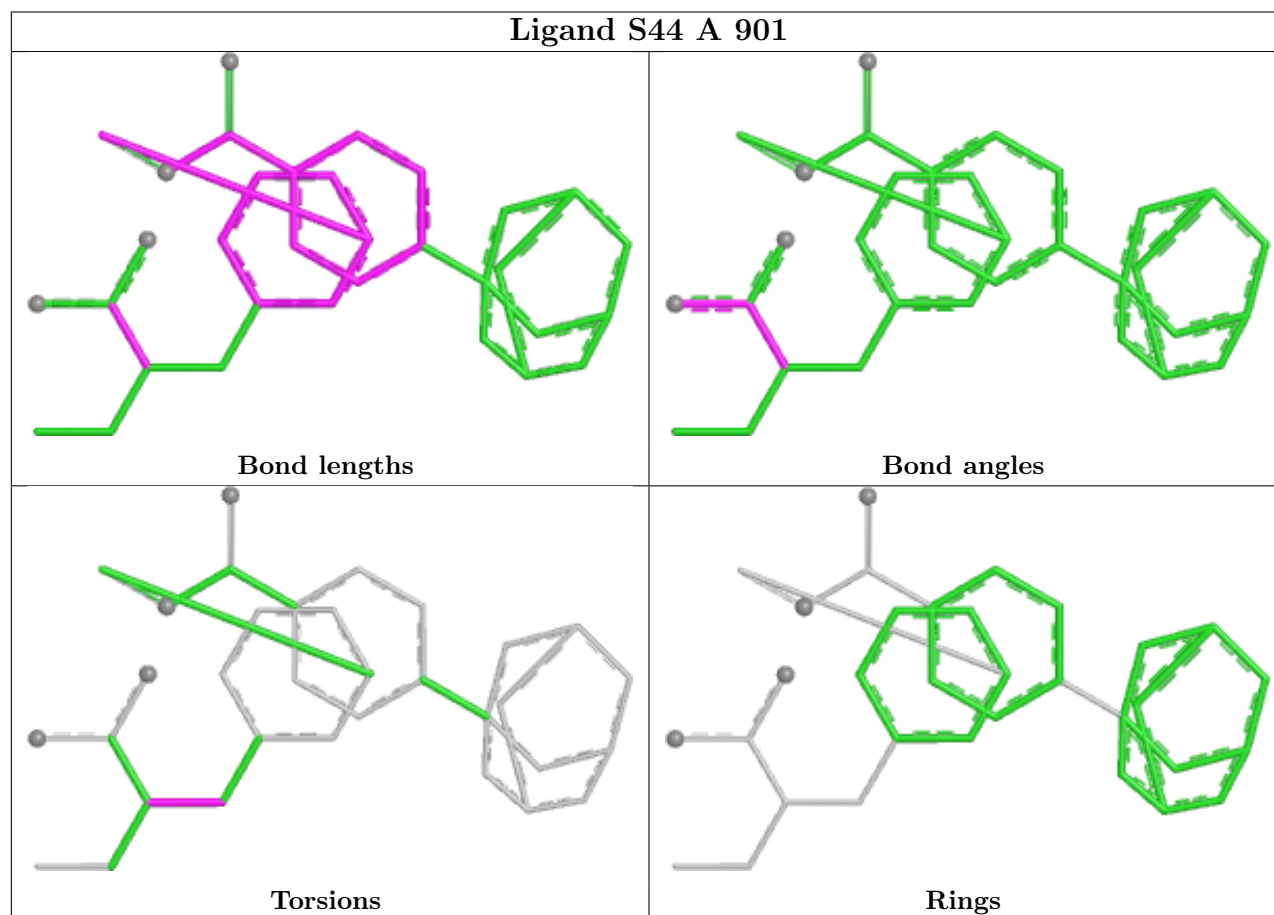
There are no ring outliers.

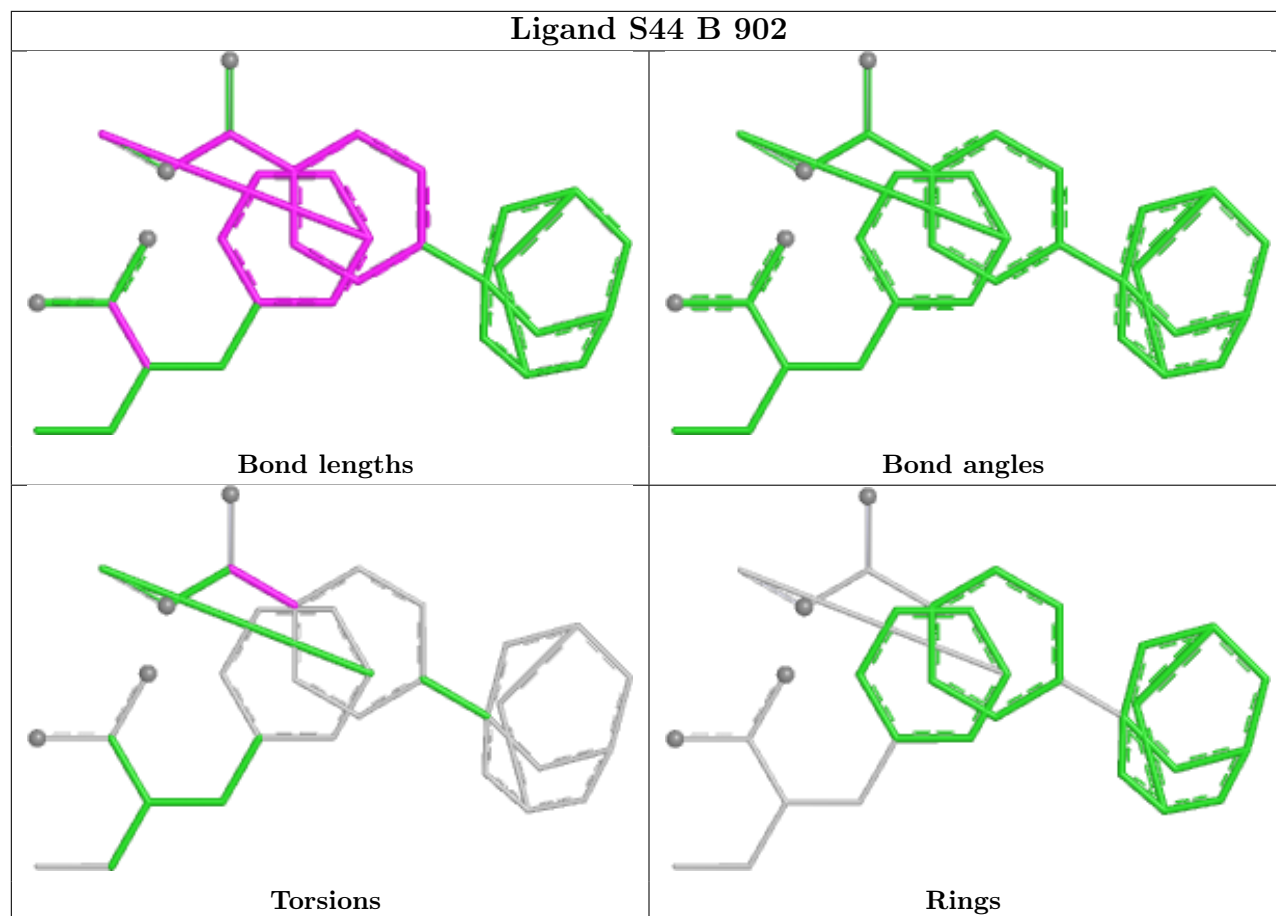
2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	S44	6	0
2	B	902	S44	6	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	266/286 (93%)	0.32	7 (2%) 57 53	31, 48, 69, 80	0
1	B	251/286 (87%)	0.26	7 (2%) 55 51	30, 47, 70, 84	0
All	All	517/572 (90%)	0.29	14 (2%) 56 52	30, 47, 70, 84	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	264	PHE	3.7
1	B	459	THR	3.3
1	A	363	PHE	3.1
1	B	473	TYR	2.8
1	A	262	ILE	2.7
1	B	461	THR	2.7
1	B	239	GLY	2.5
1	A	273	GLN	2.5
1	B	274	SER	2.4
1	A	476	LEU	2.4
1	A	204	LEU	2.3
1	B	287	PHE	2.3
1	A	311	LEU	2.1
1	A	361	GLY	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](#)

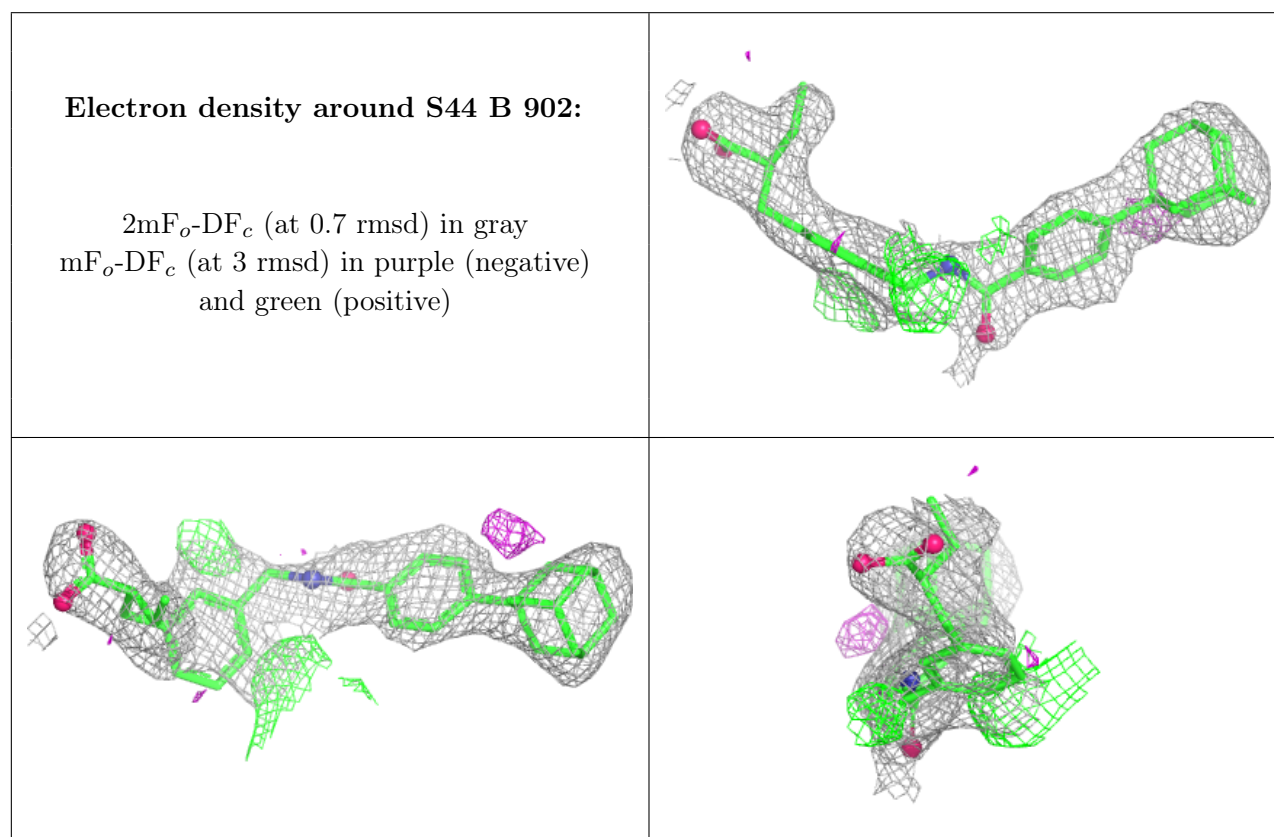
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

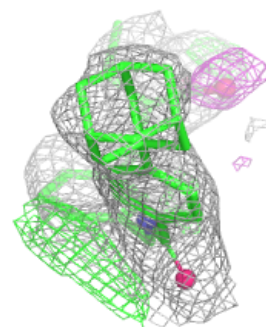
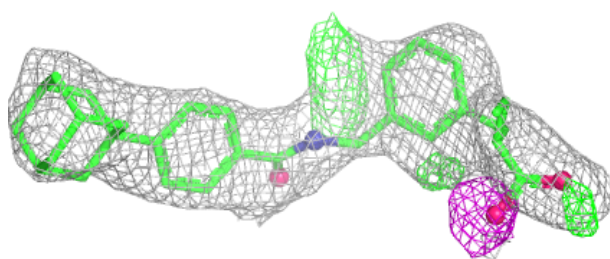
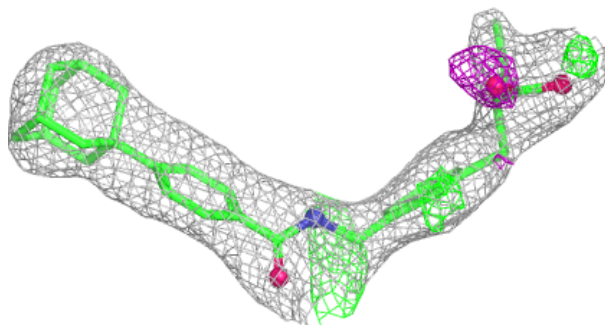
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	S44	B	902	33/37	0.79	0.17	59,64,68,69	0
2	S44	A	901	33/37	0.80	0.19	64,66,69,71	0

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 S44 A 901:

$2mF_o-DF_c$ (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.