



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 27, 2026 – 05:34 PM EDT

PDB ID : 3GD7 / pdb_00003gd7
Title : Crystal structure of human NBD2 complexed with N6-Phenylethyl-ATP (P-ATP)
Authors : Atwell, S.; Antonysamy, S.; Conners, K.; Emtage, S.; Gheyi, T.; Lewis, H.A.; Lu, F.; Sauder, J.M.; Wasserman, S.R.; Zhao, X.
Deposited on : 2009-02-23
Resolution : 2.70 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

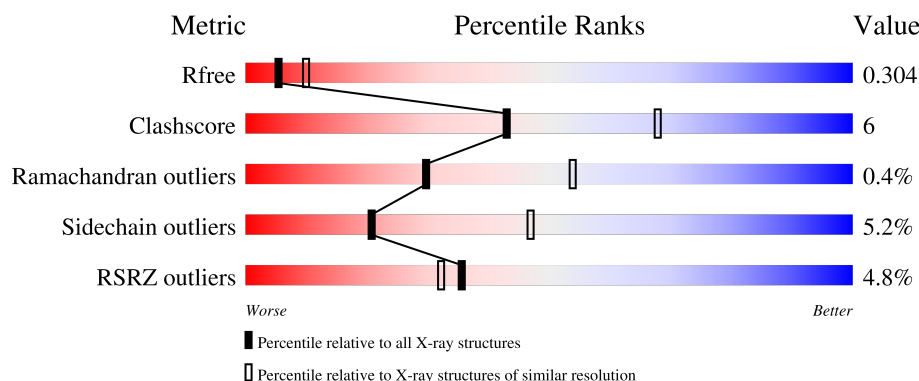
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	390	3% 78% 19% ..
1	B	390	2% 82% 14% ..
1	C	390	5% 81% 13% ..
1	D	390	9% 74% 21% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11834 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 Fusion complex of Cystic fibrosis transmembrane conductance regulator, residues 1193-1427 and Maltose/maltodextrin import ATP-binding protein malK, residues 219-371.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	378	Total	C	N	O	S	0	0	0
			2898	1844	506	535	13			
1	B	377	Total	C	N	O	S	0	0	0
			2907	1851	505	538	13			
1	C	376	Total	C	N	O	S	0	0	0
			2813	1798	482	520	13			
1	D	375	Total	C	N	O	S	0	0	0
			2806	1788	487	519	12			

There are 36 discrepancies between the modelled and reference sequences:

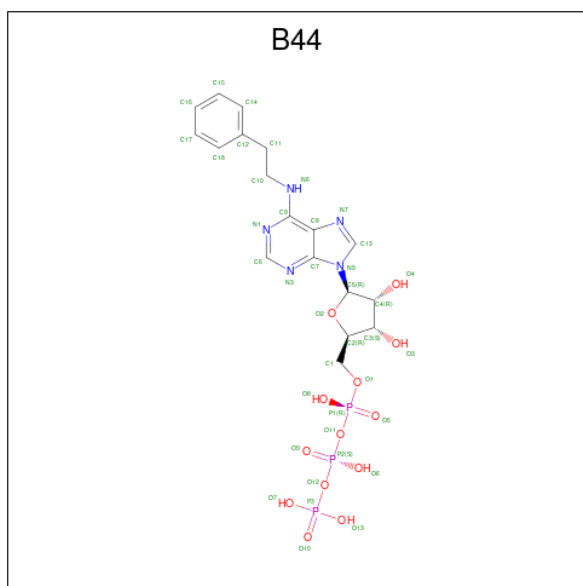
Chain	Residue	Modelled	Actual	Comment	Reference
A	1191	SER	-	expression tag	UNP P13569
A	1192	LEU	-	expression tag	UNP P13569
A	1280	GLU	GLN	engineered mutation	UNP P13569
A	1307	ASN	TYR	engineered mutation	UNP P13569
A	1308	ALA	GLU	engineered mutation	UNP P13569
A	1309	ALA	GLN	engineered mutation	UNP P13569
A	1310	HIS	TRP	engineered mutation	UNP P13569
A	1402	ALA	HIS	engineered mutation	UNP P13569
A	1411	ASP	GLN	engineered mutation	UNP P13569
B	1191	SER	-	expression tag	UNP P13569
B	1192	LEU	-	expression tag	UNP P13569
B	1280	GLU	GLN	engineered mutation	UNP P13569
B	1307	ASN	TYR	engineered mutation	UNP P13569
B	1308	ALA	GLU	engineered mutation	UNP P13569
B	1309	ALA	GLN	engineered mutation	UNP P13569
B	1310	HIS	TRP	engineered mutation	UNP P13569
B	1402	ALA	HIS	engineered mutation	UNP P13569
B	1411	ASP	GLN	engineered mutation	UNP P13569
C	1191	SER	-	expression tag	UNP P13569

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1192	LEU	-	expression tag	UNP P13569
C	1280	GLU	GLN	engineered mutation	UNP P13569
C	1307	ASN	TYR	engineered mutation	UNP P13569
C	1308	ALA	GLU	engineered mutation	UNP P13569
C	1309	ALA	GLN	engineered mutation	UNP P13569
C	1310	HIS	TRP	engineered mutation	UNP P13569
C	1402	ALA	HIS	engineered mutation	UNP P13569
C	1411	ASP	GLN	engineered mutation	UNP P13569
D	1191	SER	-	expression tag	UNP P13569
D	1192	LEU	-	expression tag	UNP P13569
D	1280	GLU	GLN	engineered mutation	UNP P13569
D	1307	ASN	TYR	engineered mutation	UNP P13569
D	1308	ALA	GLU	engineered mutation	UNP P13569
D	1309	ALA	GLN	engineered mutation	UNP P13569
D	1310	HIS	TRP	engineered mutation	UNP P13569
D	1402	ALA	HIS	engineered mutation	UNP P13569
D	1411	ASP	GLN	engineered mutation	UNP P13569

- Molecule 2 is N-(2-phenylethyl)adenosine 5'-(tetrahydrogen triphosphate) (CCD ID: B44) (formula: $C_{18}H_{24}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			39	18	5	13	3		
2	B	1	Total	C	N	O	P	0	0
			39	18	5	13	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			39	18	5	13	3		
2	D	1	Total	C	N	O	P	0	0
			39	18	5	13	3		

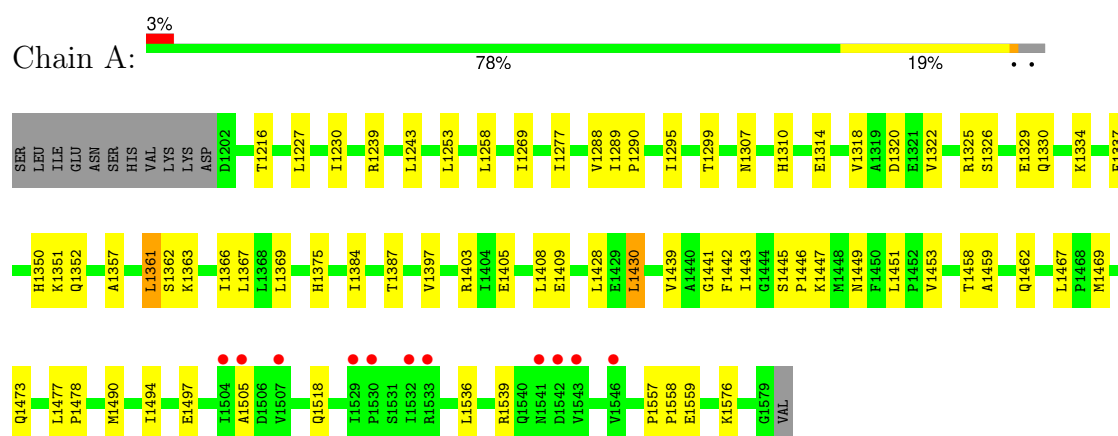
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	75	Total	O	0	0
			75	75		
3	B	80	Total	O	0	0
			80	80		
3	C	60	Total	O	0	0
			60	60		
3	D	39	Total	O	0	0
			39	39		

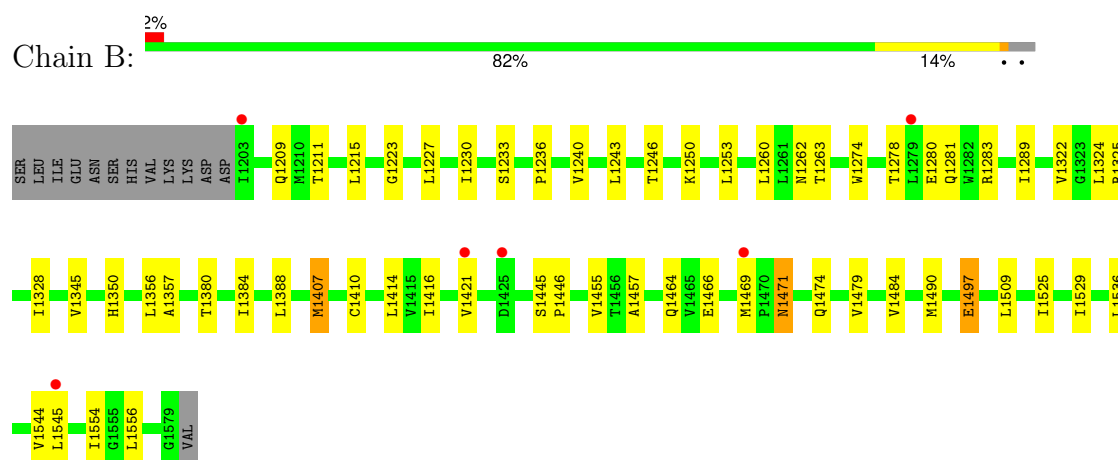
3 Residue-property plots

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.

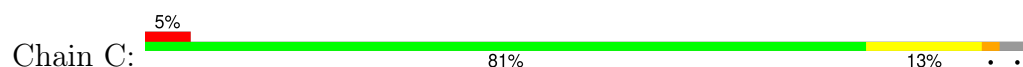
- Molecule 1: Fusion complex of Cystic fibrosis transmembrane conductance regulator, residues 1193-1427 and Maltose/maltodextrin import ATP-binding protein malK, residues 219-371

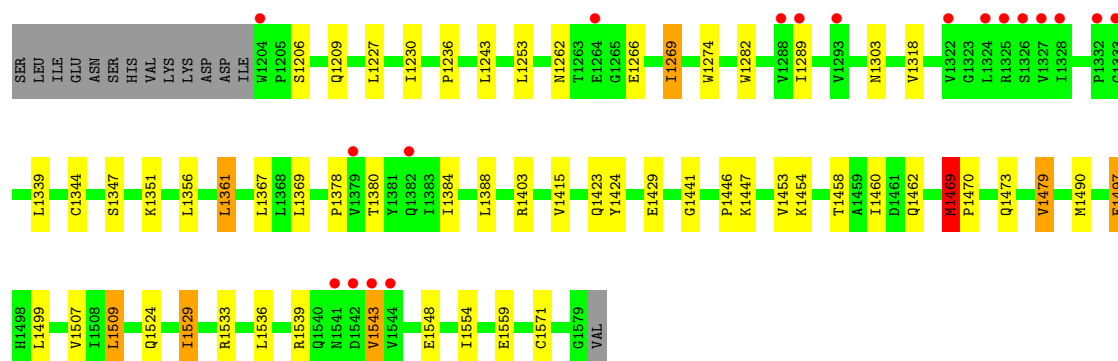


- Molecule 1: Fusion complex of Cystic fibrosis transmembrane conductance regulator, residues 1193-1427 and Maltose/maltodextrin import ATP-binding protein malK, residues 219-371

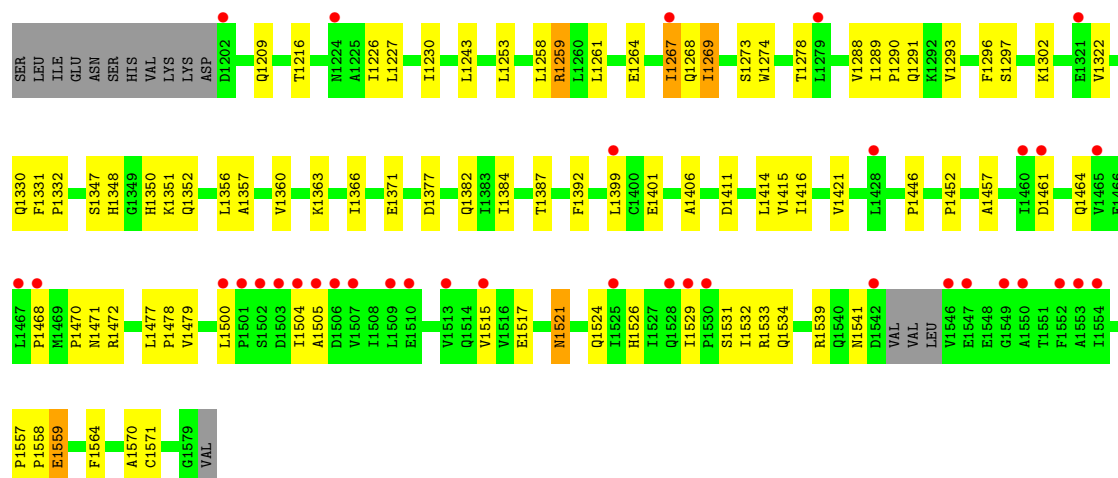
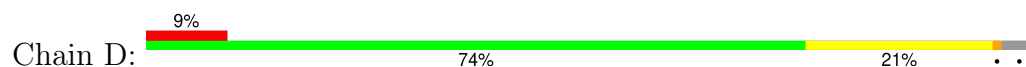


- Molecule 1: Fusion complex of Cystic fibrosis transmembrane conductance regulator, residues 1193-1427 and Maltose/maltodextrin import ATP-binding protein malK, residues 219-371





- Molecule 1: Fusion complex of Cystic fibrosis transmembrane conductance regulator, residues 1193-1427 and Maltose/maltodextrin import ATP-binding protein malK, residues 219-371



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	137.84Å 173.72Å 82.57Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	54.00 – 2.70 54.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (54.00-2.70) 99.9 (54.00-2.70)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.69Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.247 , 0.308 0.245 , 0.304	Depositor DCC
R_{free} test set	2768 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	53.4	Xtriage
Anisotropy	0.328	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11834	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: B44

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	0.40	0/2956	0.76	1/4018 (0.0%)
1	B	0.41	0/2965	0.75	0/4031
1	C	0.42	0/2871	0.78	2/3918 (0.1%)
1	D	0.42	0/2863	0.78	3/3903 (0.1%)
All	All	0.41	0/11655	0.77	6/15870 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1331	PHE	CA-C-N	5.87	127.17	119.84
1	D	1331	PHE	C-N-CA	5.87	127.17	119.84
1	A	1505	ALA	N-CA-C	5.64	115.86	108.07
1	C	1469	MET	CA-C-N	5.45	126.65	119.84
1	C	1469	MET	C-N-CA	5.45	126.65	119.84
1	D	1504	ILE	N-CA-C	5.23	116.31	111.45

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	2898	0	2866	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2907	0	2896	35	0
1	C	2813	0	2724	30	0
1	D	2806	0	2710	43	0
2	A	39	0	20	0	0
2	B	39	0	20	1	0
2	C	39	0	20	0	0
2	D	39	0	20	0	0
3	A	75	0	0	1	0
3	B	80	0	0	3	0
3	C	60	0	0	2	0
3	D	39	0	0	1	0
All	All	11834	0	11276	142	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 6.

All (142) 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:1529:ILE:HD11	1:C:1536:LEU:HB2	1.48	0.96
1:B:1525:ILE:HD11	1:B:1544:VAL:HG11	1.63	0.81
1:D:1521:ASN:H	1:D:1521:ASN:HD22	1.28	0.78
1:B:1263:THR:HG21	1:B:1274:TRP:CH2	2.18	0.78
1:D:1356:LEU:HD21	1:D:1387:THR:HG21	1.72	0.71
1:D:1471:ASN:HD22	1:D:1531:SER:HB3	1.53	0.71
1:B:1466:GLU:HG2	3:B:258:HOH:O	1.90	0.71
1:C:1469:MET:HE1	1:C:1509:LEU:HD22	1.71	0.70
1:A:1227:LEU:HB3	1:A:1230:ILE:HD12	1.73	0.69
1:B:1278:THR:H	1:B:1281:GLN:HE21	1.40	0.69
1:D:1267:ILE:H	1:D:1274:TRP:CD1	2.11	0.67
1:B:1209:GLN:HB3	1:B:1236:PRO:HD3	1.77	0.66
1:A:1318:VAL:HG21	1:A:1361:LEU:HD13	1.80	0.64
1:B:1469:MET:HE3	1:B:1529:ILE:HG21	1.81	0.63
1:C:1227:LEU:HB3	1:C:1230:ILE:HD12	1.81	0.63
1:D:1259:ARG:HH21	1:D:1259:ARG:HG3	1.63	0.63
1:D:1259:ARG:HH21	1:D:1259:ARG:CG	2.12	0.63
1:D:1293:VAL:HG11	1:D:1351:LYS:HB3	1.83	0.59
1:B:1250:LYS:HE3	2:B:2:B44:O6	2.04	0.58
1:C:1536:LEU:HD23	1:C:1554:ILE:HD11	1.86	0.57
1:D:1216:THR:HB	1:D:1264:GLU:HB3	1.87	0.57
1:D:1471:ASN:ND2	1:D:1531:SER:HB3	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1258:LEU:HD11	1:D:1288:VAL:HG21	1.87	0.57
1:D:1457:ALA:HB3	1:D:1464:GLN:HE21	1.69	0.57
1:A:1239:ARG:HH11	1:A:1409:GLU:HB3	1.69	0.56
1:A:1289:ILE:HB	1:A:1369:LEU:HD13	1.87	0.56
1:B:1416:ILE:HG12	1:B:1421:VAL:HG12	1.87	0.56
1:C:1497:GLU:HG3	1:C:1539:ARG:HD3	1.88	0.56
1:A:1446:PRO:HD2	1:A:1539:ARG:HD2	1.87	0.56
1:C:1453:VAL:HG23	1:C:1490:MET:HB2	1.88	0.55
1:C:1446:PRO:HD2	1:C:1539:ARG:HD2	1.89	0.55
1:C:1499:LEU:HD13	1:C:1554:ILE:HD12	1.90	0.53
1:A:1430:LEU:HD13	1:A:1439:VAL:HG13	1.90	0.53
1:D:1416:ILE:HA	1:D:1421:VAL:HG12	1.91	0.53
1:B:1262:ASN:HB3	3:B:181:HOH:O	2.08	0.53
1:B:1536:LEU:HD23	1:B:1554:ILE:HD11	1.91	0.53
1:C:1289:ILE:HD11	1:C:1356:LEU:HD13	1.91	0.52
1:A:1322:VAL:HG21	1:A:1357:ALA:HB2	1.91	0.52
1:A:1445:SER:HA	1:A:1446:PRO:C	2.36	0.51
1:B:1466:GLU:HG3	1:B:1474:GLN:HG2	1.92	0.51
1:B:1322:VAL:HG21	1:B:1357:ALA:HB2	1.92	0.50
1:A:1350:HIS:HD2	1:D:1330:GLN:OE1	1.94	0.50
1:A:1430:LEU:HD13	1:A:1439:VAL:CG1	2.42	0.49
1:A:1384:ILE:O	1:A:1387:THR:HG22	2.14	0.48
1:A:1216:THR:HA	1:A:1227:LEU:O	2.13	0.48
1:A:1295:ILE:HD11	1:A:1351:LYS:HG2	1.95	0.48
1:B:1263:THR:HG21	1:B:1274:TRP:CZ2	2.47	0.48
1:B:1509:LEU:HD11	1:B:1556:LEU:HD13	1.94	0.48
1:D:1288:VAL:O	1:D:1291:GLN:HB2	2.14	0.48
1:D:1297:SER:HA	3:D:62:HOH:O	2.13	0.48
1:C:1543:VAL:HA	3:C:237:HOH:O	2.13	0.48
1:D:1259:ARG:CG	1:D:1259:ARG:NH2	2.75	0.48
1:D:1227:LEU:HB3	1:D:1230:ILE:HD12	1.96	0.47
1:C:1473:GLN:HE22	1:C:1507:VAL:HA	1.78	0.47
1:B:1227:LEU:HB3	1:B:1230:ILE:CD1	2.45	0.47
1:B:1350:HIS:HE1	1:C:1344:CYS:O	1.97	0.47
1:D:1269:ILE:HD13	1:D:1366:ILE:HD11	1.95	0.47
1:C:1243:LEU:HB2	1:C:1415:VAL:HG22	1.97	0.47
1:B:1380:THR:O	1:B:1384:ILE:HG12	2.14	0.46
1:A:1459:ALA:HB3	1:A:1462:GLN:HB2	1.96	0.46
1:C:1367:LEU:HD22	1:C:1388:LEU:HD11	1.96	0.46
1:A:1320:ASP:HA	1:A:1325:ARG:HB2	1.97	0.46
1:D:1500:LEU:HD12	1:D:1505:ALA:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1322:VAL:HG21	1:D:1357:ALA:HB2	1.97	0.46
1:B:1278:THR:HG22	1:B:1280:GLU:H	1.81	0.45
1:D:1468:PRO:HG2	1:D:1532:ILE:HG23	1.97	0.45
1:A:1290:PRO:HG3	1:A:1375:HIS:HB3	1.98	0.45
1:D:1515:VAL:HB	1:D:1526:HIS:HB2	1.98	0.45
1:D:1348:HIS:O	1:D:1352:GLN:HG2	2.17	0.45
1:B:1445:SER:HA	1:B:1446:PRO:C	2.41	0.45
1:B:1324:LEU:O	1:B:1328:ILE:HG12	2.16	0.45
1:B:1350:HIS:CE1	1:C:1344:CYS:O	2.70	0.44
1:D:1564:PHE:CE2	1:D:1570:ALA:HB2	2.52	0.44
1:A:1307:ASN:ND2	1:B:1223:GLY:HA2	2.33	0.44
1:C:1209:GLN:HB2	1:C:1236:PRO:HD3	1.98	0.44
1:A:1449:ASN:HB2	1:A:1494:ILE:O	2.17	0.44
1:B:1484:VAL:HG13	1:B:1490:MET:HE3	2.00	0.44
1:A:1477:LEU:HA	1:A:1478:PRO:HD3	1.86	0.44
1:D:1521:ASN:HD22	1:D:1521:ASN:N	2.04	0.44
1:A:1361:LEU:C	1:A:1363:LYS:H	2.24	0.44
1:B:1211:THR:HG23	1:B:1233:SER:HB3	2.00	0.44
1:B:1227:LEU:HB3	1:B:1230:ILE:HD12	2.00	0.44
1:B:1455:VAL:HG23	1:B:1490:MET:HG3	2.00	0.44
1:A:1326:SER:O	1:A:1330:GLN:HG2	2.18	0.44
1:C:1318:VAL:HG21	1:C:1361:LEU:HD12	2.00	0.44
1:A:1384:ILE:HA	1:A:1387:THR:HG22	2.00	0.44
1:A:1557:PRO:HA	1:A:1558:PRO:HD3	1.86	0.44
1:C:1441:GLY:HA3	1:C:1447:LYS:HE3	1.99	0.44
1:A:1269:ILE:HD13	1:A:1366:ILE:HD12	1.99	0.43
1:A:1299:THR:HA	1:A:1337:PHE:O	2.17	0.43
1:B:1529:ILE:HD11	1:B:1536:LEU:HD22	2.00	0.43
1:D:1452:PRO:HD3	1:D:1534:GLN:HE22	1.83	0.43
1:A:1362:SER:HB2	3:A:80:HOH:O	2.18	0.43
1:D:1477:LEU:HA	1:D:1478:PRO:HD3	1.87	0.43
1:C:1266:GLU:HA	1:C:1274:TRP:HE1	1.83	0.43
1:A:1467:LEU:HD12	1:A:1473:GLN:HB2	2.01	0.43
1:A:1430:LEU:HD12	1:A:1443:ILE:CG1	2.48	0.43
1:B:1457:ALA:HB3	1:B:1464:GLN:HB3	2.01	0.43
1:D:1559:GLU:H	1:D:1559:GLU:HG3	1.64	0.43
1:C:1424:TYR:HD1	1:C:1429:GLU:HG3	1.84	0.43
1:D:1470:PRO:HD2	1:D:1531:SER:O	2.19	0.43
1:A:1310:HIS:HB3	1:A:1314:GLU:HG3	2.01	0.43
1:A:1329:GLU:HA	1:A:1334:LYS:HG2	2.01	0.43
1:A:1451:LEU:HD11	1:A:1536:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1303:ASN:HD22	1:C:1339:LEU:HD23	1.84	0.43
1:D:1446:PRO:HD2	1:D:1539:ARG:HD3	2.01	0.43
1:D:1347:SER:H	1:D:1350:HIS:CD2	2.37	0.42
1:D:1356:LEU:HD22	1:D:1384:ILE:HD13	2.00	0.42
1:A:1295:ILE:CD1	1:A:1351:LYS:HG2	2.50	0.42
1:B:1246:THR:HG22	3:B:116:HOH:O	2.19	0.42
1:D:1401:GLU:OE1	1:D:1406:ALA:HB3	2.19	0.42
1:B:1289:ILE:HD11	1:B:1356:LEU:HD13	2.01	0.42
1:C:1269:ILE:HG23	1:C:1282:TRP:CH2	2.54	0.42
1:D:1541:ASN:HD22	1:D:1541:ASN:HA	1.70	0.42
1:D:1268:GLN:HG2	1:D:1273:SER:HA	2.02	0.42
1:D:1517:GLU:HB3	1:D:1524:GLN:HB2	2.01	0.42
1:A:1441:GLY:HA3	1:A:1447:LYS:HE3	2.01	0.41
1:B:1345:VAL:O	1:C:1347:SER:HB2	2.20	0.41
1:B:1407:MET:HB2	1:B:1410:CYS:SG	2.59	0.41
1:D:1360:VAL:HG22	1:D:1392:PHE:CE1	2.55	0.41
1:C:1524:GLN:HG2	1:C:1539:ARG:HG2	2.03	0.41
1:A:1258:LEU:HD11	1:A:1288:VAL:HG21	2.03	0.41
1:A:1559:GLU:H	1:A:1559:GLU:CD	2.27	0.41
1:D:1529:ILE:O	1:D:1532:ILE:O	2.38	0.41
1:A:1367:LEU:HB2	1:A:1397:VAL:HG22	2.02	0.41
1:A:1453:VAL:HG23	1:A:1490:MET:HB2	2.03	0.41
1:C:1347:SER:O	1:C:1351:LYS:HG3	2.19	0.41
1:A:1430:LEU:CD1	1:A:1439:VAL:HG13	2.51	0.41
1:C:1289:ILE:HB	1:C:1369:LEU:HD13	2.03	0.41
1:C:1403:ARG:HG2	3:C:223:HOH:O	2.21	0.41
1:D:1289:ILE:HA	1:D:1290:PRO:C	2.45	0.41
1:D:1371:GLU:HG2	1:D:1401:GLU:HA	2.02	0.41
1:B:1240:VAL:HG11	1:B:1414:LEU:HD12	2.03	0.41
1:C:1380:THR:O	1:C:1384:ILE:HG12	2.21	0.41
1:C:1460:ILE:HD12	1:C:1460:ILE:H	1.86	0.41
1:B:1497:GLU:H	1:B:1497:GLU:CD	2.29	0.40
1:D:1243:LEU:HB2	1:D:1415:VAL:HG22	2.02	0.40
1:B:1471:ASN:H	1:B:1471:ASN:ND2	2.18	0.40
1:C:1479:VAL:HG13	1:C:1571:CYS:HB2	2.04	0.40
1:D:1479:VAL:CG1	1:D:1571:CYS:HB2	2.51	0.40
1:D:1557:PRO:HA	1:D:1558:PRO:HD2	1.89	0.40
1:A:1243:LEU:HD22	1:A:1442:PHE:CE2	2.57	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	376/390 (96%)	353 (94%)	23 (6%)	0	100	100
1	B	375/390 (96%)	361 (96%)	14 (4%)	0	100	100
1	C	374/390 (96%)	342 (91%)	29 (8%)	3 (1%)	16	37
1	D	371/390 (95%)	345 (93%)	23 (6%)	3 (1%)	16	37
All	All	1496/1560 (96%)	1401 (94%)	89 (6%)	6 (0%)	30	54

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1206	SER
1	C	1378	PRO
1	D	1533	ARG
1	D	1332	PRO
1	D	1472	ARG
1	C	1470	PRO

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	308/339 (91%)	294 (96%)	14 (4%)	24	52
1	B	314/339 (93%)	302 (96%)	12 (4%)	29	58
1	C	290/339 (86%)	273 (94%)	17 (6%)	18	42
1	D	289/339 (85%)	270 (93%)	19 (7%)	15	36

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1201/1356 (89%)	1139 (95%)	62 (5%)	21	47

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1253	LEU
1	A	1277	ILE
1	A	1352	GLN
1	A	1361	LEU
1	A	1403	ARG
1	A	1405	GLU
1	A	1408	LEU
1	A	1428	LEU
1	A	1430	LEU
1	A	1458	THR
1	A	1469	MET
1	A	1497	GLU
1	A	1518	GLN
1	A	1576	LYS
1	B	1215	LEU
1	B	1243	LEU
1	B	1253	LEU
1	B	1260	LEU
1	B	1283	ARG
1	B	1325	ARG
1	B	1388	LEU
1	B	1407	MET
1	B	1471	ASN
1	B	1479	VAL
1	B	1497	GLU
1	B	1545	LEU
1	C	1253	LEU
1	C	1262	ASN
1	C	1269	ILE
1	C	1361	LEU
1	C	1423	GLN
1	C	1454	LYS
1	C	1458	THR
1	C	1462	GLN
1	C	1469	MET
1	C	1479	VAL
1	C	1497	GLU

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Mol	Chain	Res	Type
1	C	1509	LEU
1	C	1529	ILE
1	C	1533	ARG
1	C	1543	VAL
1	C	1548	GLU
1	C	1559	GLU
1	D	1209	GLN
1	D	1226	ILE
1	D	1253	LEU
1	D	1259	ARG
1	D	1261	LEU
1	D	1267	ILE
1	D	1269	ILE
1	D	1278	THR
1	D	1296	PHE
1	D	1302	LYS
1	D	1363	LYS
1	D	1377	ASP
1	D	1382	GLN
1	D	1399	LEU
1	D	1411	ASP
1	D	1414	LEU
1	D	1461	ASP
1	D	1521	ASN
1	D	1559	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1307	ASN
1	A	1348	HIS
1	A	1350	HIS
1	A	1464	GLN
1	B	1262	ASN
1	B	1281	GLN
1	B	1303	ASN
1	B	1350	HIS
1	B	1464	GLN
1	B	1471	ASN
1	B	1473	GLN
1	B	1518	GLN
1	B	1562	HIS

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Mol	Chain	Res	Type
1	C	1209	GLN
1	C	1262	ASN
1	C	1307	ASN
1	C	1423	GLN
1	C	1462	GLN
1	C	1464	GLN
1	C	1471	ASN
1	C	1473	GLN
1	C	1518	GLN
1	C	1535	ASN
1	C	1575	HIS
1	D	1350	HIS
1	D	1375	HIS
1	D	1464	GLN
1	D	1473	GLN
1	D	1474	GLN
1	D	1521	ASN
1	D	1534	GLN
1	D	1540	GLN
1	D	1541	ASN
1	D	1562	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	B44	C	3	-	41,42,42	0.90	2 (4%)	59,63,63	0.99	2 (3%)
2	B44	D	4	-	41,42,42	0.86	1 (2%)	59,63,63	0.87	2 (3%)
2	B44	B	2	-	41,42,42	0.93	2 (4%)	59,63,63	0.88	2 (3%)
2	B44	A	1	-	41,42,42	0.88	1 (2%)	59,63,63	0.87	2 (3%)

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	B44	C	3	-	-	8/28/44/44	0/4/4/4
2	B44	D	4	-	-	4/28/44/44	0/4/4/4
2	B44	B	2	-	-	3/28/44/44	0/4/4/4
2	B44	A	1	-	-	3/28/44/44	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	B44	C9-N6	3.05	1.39	1.34
2	C	3	B44	C9-N6	2.97	1.39	1.34
2	D	4	B44	C9-N6	2.86	1.39	1.34
2	A	1	B44	C9-N6	2.77	1.38	1.34
2	B	2	B44	P2-O12	2.14	1.61	1.59
2	C	3	B44	P2-O12	2.09	1.61	1.59

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	3	B44	C10-C11-C12	3.41	120.52	112.83
2	A	1	B44	C10-C11-C12	3.01	119.61	112.83
2	B	2	B44	N6-C9-N1	2.76	122.90	118.47
2	D	4	B44	C10-C11-C12	2.35	118.13	112.83
2	C	3	B44	C11-C10-N6	2.21	115.40	111.72
2	B	2	B44	C10-C11-C12	2.13	117.63	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	B44	N6-C9-N1	2.12	121.89	118.47
2	D	4	B44	N6-C9-N1	2.02	121.72	118.47

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	3	B44	C1-O1-P1-O8
2	C	3	B44	N6-C10-C11-C12
2	C	3	B44	C10-C11-C12-C18
2	C	3	B44	C10-C11-C12-C14
2	C	3	B44	C1-O1-P1-O11
2	C	3	B44	C1-O1-P1-O5
2	D	4	B44	P2-O12-P3-O10
2	A	1	B44	O1-C1-C2-C3
2	D	4	B44	P3-O12-P2-O9
2	C	3	B44	O1-C1-C2-O2
2	D	4	B44	P3-O12-P2-O6
2	B	2	B44	N6-C10-C11-C12
2	A	1	B44	O1-C1-C2-O2
2	A	1	B44	P1-O11-P2-O6
2	B	2	B44	P1-O11-P2-O6
2	B	2	B44	P1-O11-P2-O9
2	C	3	B44	P3-O12-P2-O6
2	D	4	B44	P1-O11-P2-O6

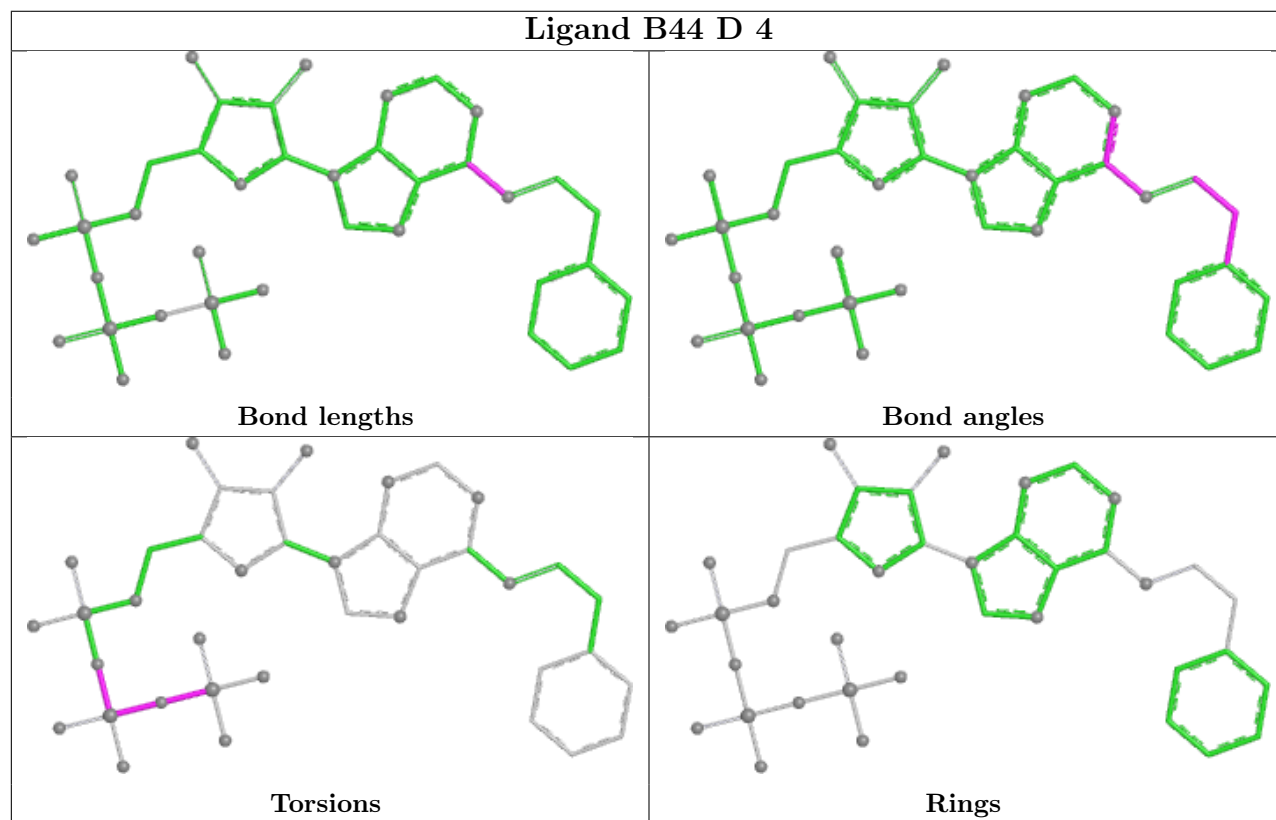
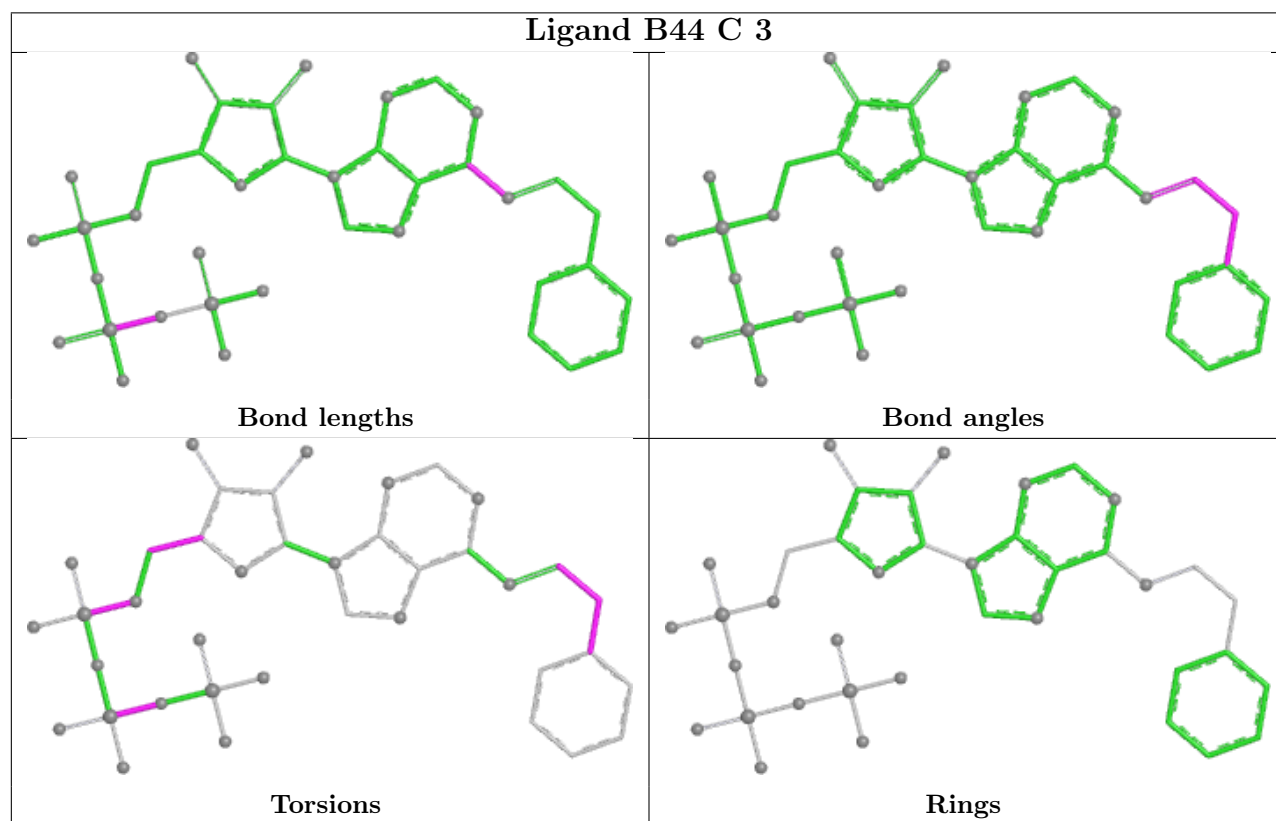
There are no ring outliers.

1 monomer is involved in 1 short contact:

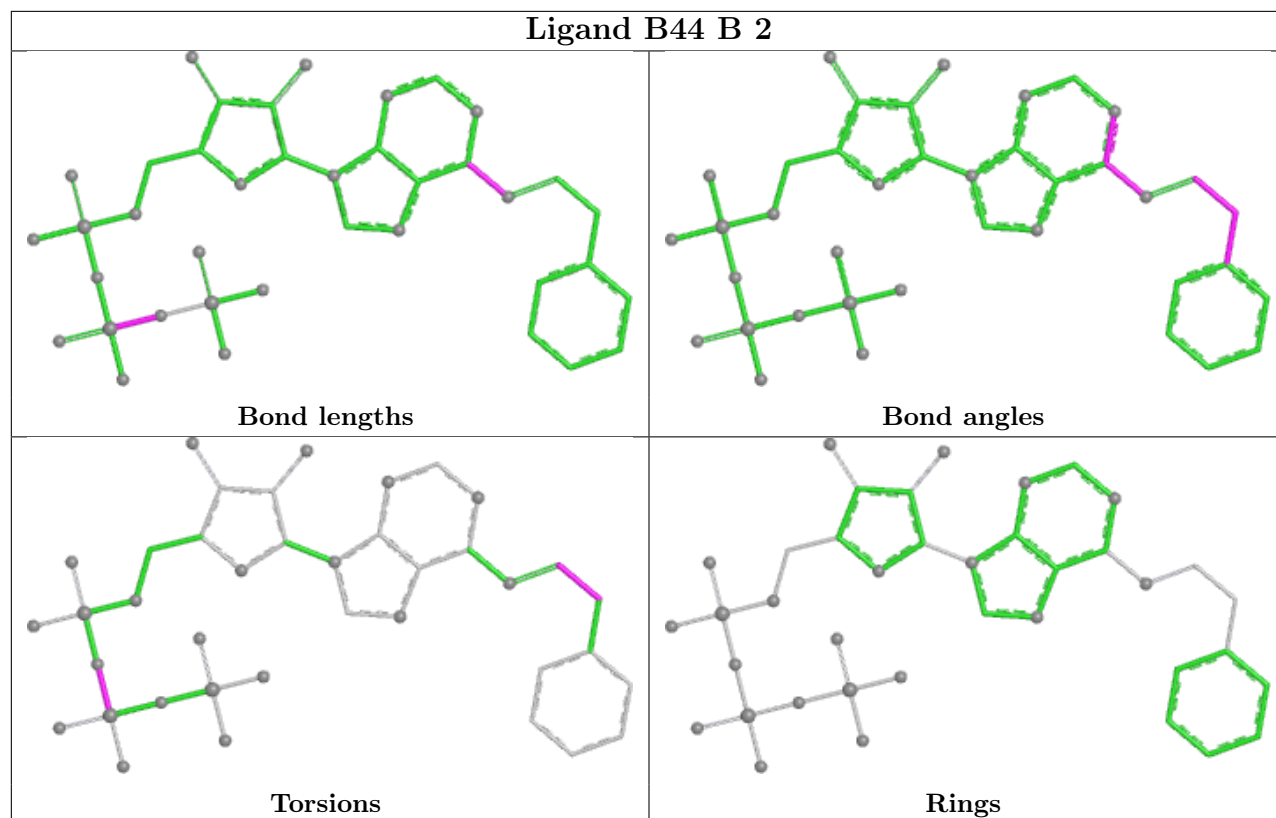
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2	B44	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier.

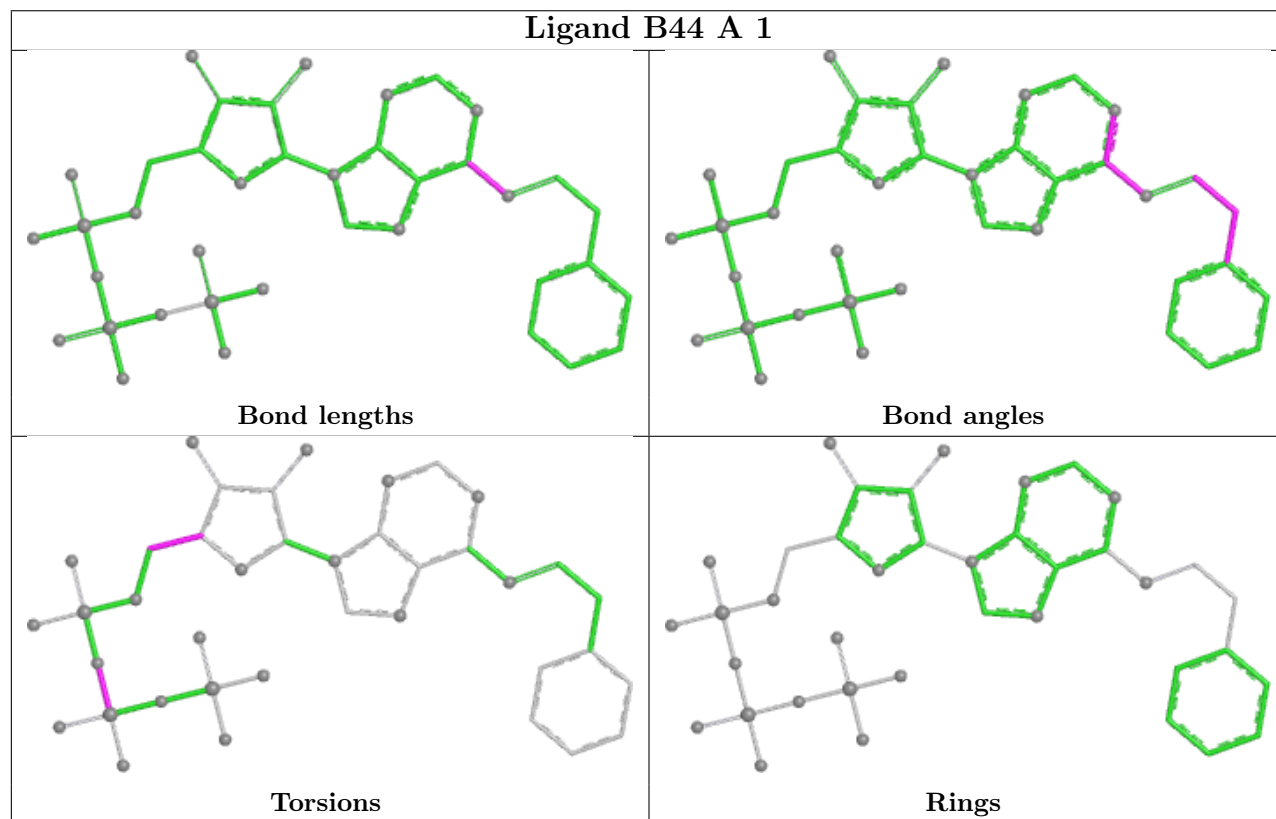
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



Ligand B44 B 2



Ligand B44 A 1



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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	378/390 (96%)	0.28	11 (2%) 53 50	26, 51, 78, 89	0
1	B	377/390 (96%)	0.36	6 (1%) 70 68	27, 53, 73, 80	0
1	C	376/390 (96%)	0.66	19 (5%) 33 29	33, 66, 96, 102	0
1	D	375/390 (96%)	0.84	36 (9%) 13 11	36, 67, 91, 99	0
All	All	1506/1560 (96%)	0.53	72 (4%) 35 32	26, 59, 89, 102	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1546	VAL	3.9
1	D	1503	ASP	3.6
1	D	1505	ALA	3.5
1	D	1224	ASN	3.3
1	A	1542	ASP	3.2
1	C	1293	VAL	3.1
1	C	1541	ASN	3.1
1	B	1203	ILE	3.1
1	D	1550	ALA	3.1
1	B	1421	VAL	3.0
1	D	1525	ILE	3.0
1	D	1502	SER	3.0
1	D	1506	ASP	3.0
1	B	1469	MET	3.0
1	C	1543	VAL	3.0
1	D	1547	GLU	2.9
1	C	1322	VAL	2.9
1	A	1504	ILE	2.9
1	D	1267	ILE	2.9
1	D	1507	VAL	2.9
1	C	1264	GLU	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	1542	ASP	2.8
1	A	1505	ALA	2.7
1	D	1202	ASP	2.7
1	D	1552	PHE	2.7
1	C	1379	VAL	2.7
1	D	1530	PRO	2.7
1	D	1460	ILE	2.6
1	C	1333	GLY	2.6
1	D	1510	GLU	2.6
1	D	1504	ILE	2.6
1	C	1289	ILE	2.5
1	A	1541	ASN	2.5
1	A	1546	VAL	2.5
1	C	1382	GLN	2.5
1	B	1545	LEU	2.5
1	D	1467	LEU	2.5
1	D	1549	GLY	2.4
1	C	1542	ASP	2.4
1	C	1288	VAL	2.4
1	A	1532	ILE	2.3
1	C	1544	VAL	2.3
1	D	1279	LEU	2.3
1	D	1399	LEU	2.3
1	C	1332	PRO	2.3
1	C	1324	LEU	2.3
1	C	1325	ARG	2.3
1	D	1468	PRO	2.3
1	D	1461	ASP	2.2
1	A	1507	VAL	2.2
1	B	1279	LEU	2.2
1	D	1553	ALA	2.2
1	D	1428	LEU	2.2
1	D	1501	PRO	2.2
1	D	1528	GLN	2.2
1	A	1543	VAL	2.2
1	C	1327	VAL	2.2
1	C	1328	ILE	2.2
1	D	1513	VAL	2.2
1	D	1500	LEU	2.1
1	B	1425	ASP	2.1
1	C	1204	TRP	2.1
1	D	1509	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	1515	VAL	2.1
1	C	1326	SER	2.1
1	D	1321	GLU	2.1
1	D	1465	VAL	2.1
1	D	1529	ILE	2.1
1	A	1533	ARG	2.0
1	A	1530	PRO	2.0
1	A	1529	ILE	2.0
1	D	1554	ILE	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 [i](#)

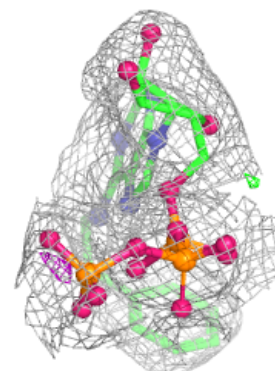
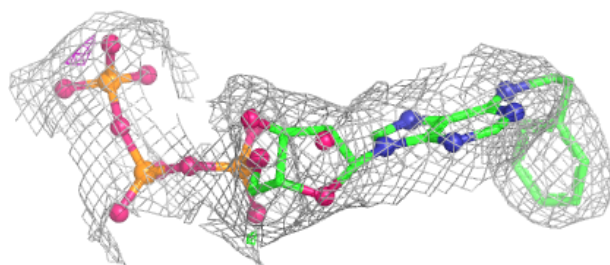
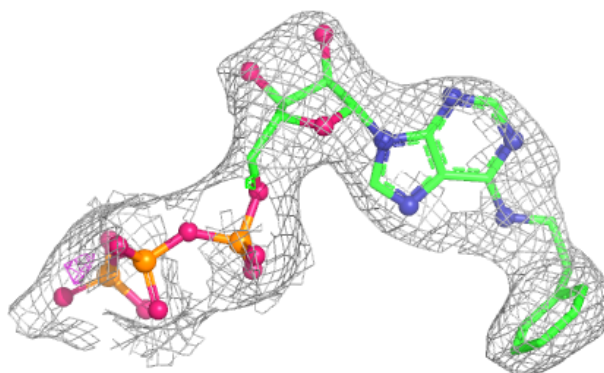
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	B44	D	4	39/39	0.93	0.09	67,72,76,76	0
2	B44	C	3	39/39	0.96	0.08	40,53,59,59	0
2	B44	A	1	39/39	0.97	0.07	36,47,51,52	0
2	B44	B	2	39/39	0.97	0.06	24,29,38,39	0

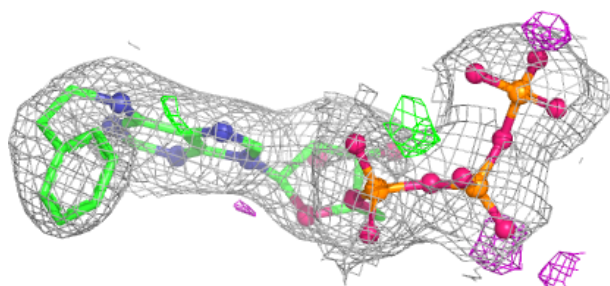
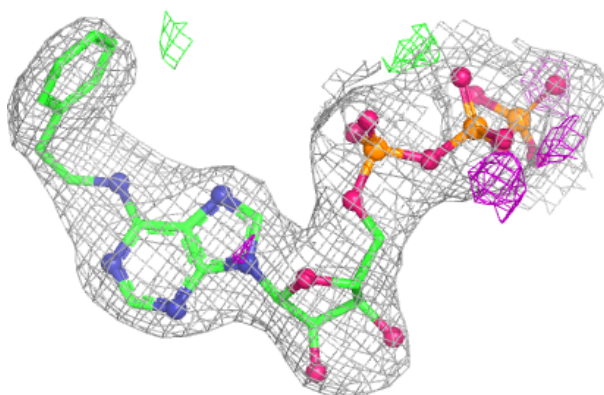
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around B44 D 4:

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

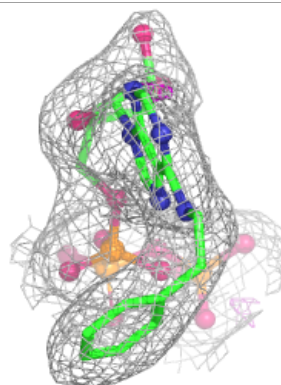
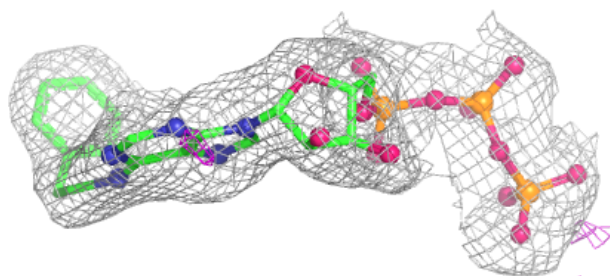
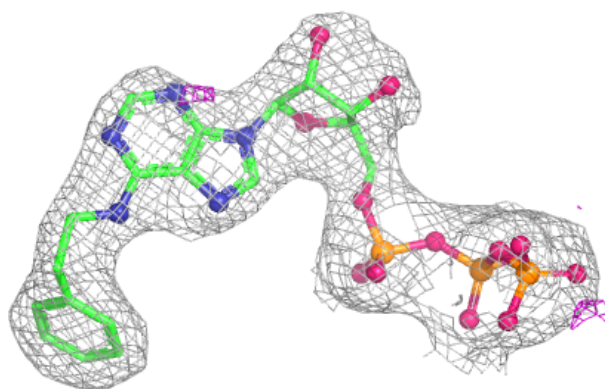
**Electron density around B44 C 3:**

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

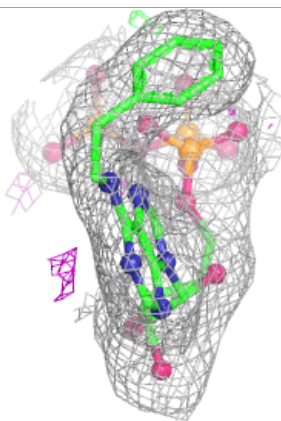
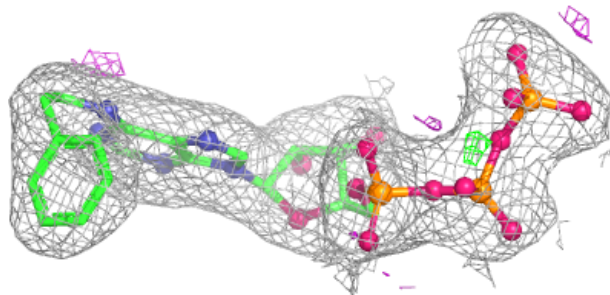
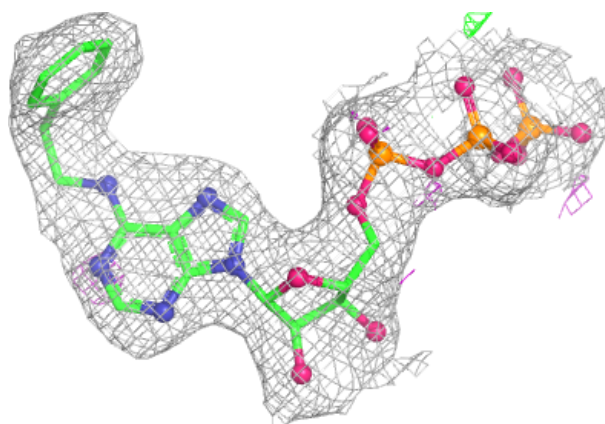


Electron density around B44 A 1:

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

**Electron density around B44 B 2:**

$2mF_o-DF_c$ (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.