



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:13 PM UTC

PDB ID : 6DUP / pdb_00006dup
Title : CRYSTAL STRUCTURE OF PXR IN COMPLEX WITH COMPOUND 7
Authors : Chen, X.; Zhang, Y.; Mclean, L.R.
Deposited on : 2018-06-21
Resolution : 2.30 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

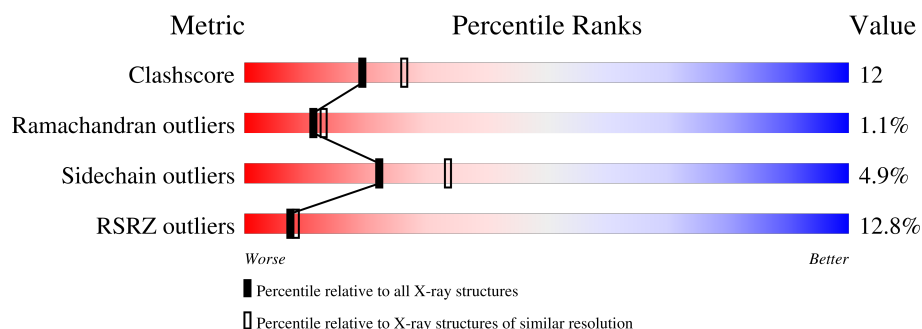
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	344	11% 62% 16% • • 18%
1	B	344	10% 63% 17% • 19%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4720 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Nuclear receptor subfamily 1 group I member 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	282	Total	C	N	O	S	0	1	0
			2315	1486	400	410	19			
1	B	280	Total	C	N	O	S	0	1	0
			2299	1479	395	406	19			

There are 94 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	119	MET	-	expression tag	UNP O75469
A	120	LYS	-	expression tag	UNP O75469
A	121	LYS	-	expression tag	UNP O75469
A	122	GLY	-	expression tag	UNP O75469
A	123	HIS	-	expression tag	UNP O75469
A	124	HIS	-	expression tag	UNP O75469
A	125	HIS	-	expression tag	UNP O75469
A	126	HIS	-	expression tag	UNP O75469
A	127	HIS	-	expression tag	UNP O75469
A	128	HIS	-	expression tag	UNP O75469
A	129	GLY	-	expression tag	UNP O75469
A	427	GLU	-	expression tag	UNP O75469
A	428	LEU	-	expression tag	UNP O75469
A	429	PHE	-	expression tag	UNP O75469
A	430	GLY	-	expression tag	UNP O75469
A	431	ILE	-	expression tag	UNP O75469
A	432	THR	-	expression tag	UNP O75469
A	433	GLY	-	expression tag	UNP O75469
A	434	SER	-	expression tag	UNP O75469
A	435	GLY	-	expression tag	UNP O75469
A	436	GLY	-	expression tag	UNP O75469
A	437	SER	-	expression tag	UNP O75469
A	438	GLY	-	expression tag	UNP O75469
A	439	GLY	-	expression tag	UNP O75469
A	440	SER	-	expression tag	UNP O75469

Continued on next page...

Continued from previous page...

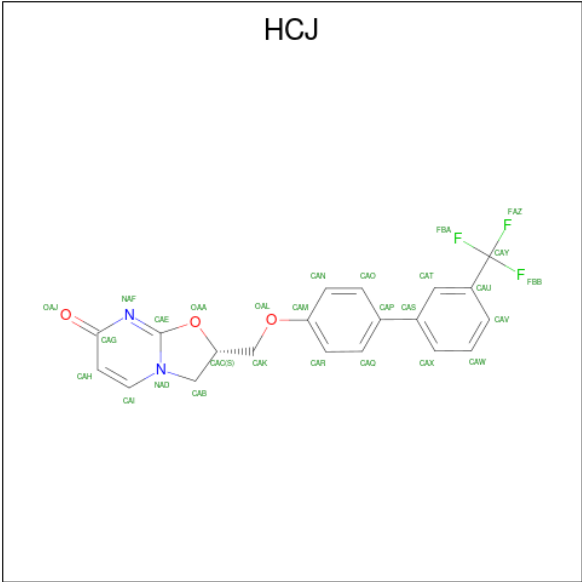
Chain	Residue	Modelled	Actual	Comment	Reference
A	441	SER	-	expression tag	UNP O75469
A	442	HIS	-	expression tag	UNP O75469
A	443	SER	-	expression tag	UNP O75469
A	444	SER	-	expression tag	UNP O75469
A	445	LEU	-	expression tag	UNP O75469
A	446	THR	-	expression tag	UNP O75469
A	447	GLU	-	expression tag	UNP O75469
A	448	ARG	-	expression tag	UNP O75469
A	449	HIS	-	expression tag	UNP O75469
A	450	LYS	-	expression tag	UNP O75469
A	451	ILE	-	expression tag	UNP O75469
A	452	LEU	-	expression tag	UNP O75469
A	453	HIS	-	expression tag	UNP O75469
A	454	ARG	-	expression tag	UNP O75469
A	455	LEU	-	expression tag	UNP O75469
A	456	LEU	-	expression tag	UNP O75469
A	457	GLN	-	expression tag	UNP O75469
A	458	GLU	-	expression tag	UNP O75469
A	459	GLY	-	expression tag	UNP O75469
A	460	SER	-	expression tag	UNP O75469
A	461	PRO	-	expression tag	UNP O75469
A	462	SER	-	expression tag	UNP O75469
B	119	MET	-	expression tag	UNP O75469
B	120	LYS	-	expression tag	UNP O75469
B	121	LYS	-	expression tag	UNP O75469
B	122	GLY	-	expression tag	UNP O75469
B	123	HIS	-	expression tag	UNP O75469
B	124	HIS	-	expression tag	UNP O75469
B	125	HIS	-	expression tag	UNP O75469
B	126	HIS	-	expression tag	UNP O75469
B	127	HIS	-	expression tag	UNP O75469
B	128	HIS	-	expression tag	UNP O75469
B	129	GLY	-	expression tag	UNP O75469
B	427	GLU	-	expression tag	UNP O75469
B	428	LEU	-	expression tag	UNP O75469
B	429	PHE	-	expression tag	UNP O75469
B	430	GLY	-	expression tag	UNP O75469
B	431	ILE	-	expression tag	UNP O75469
B	432	THR	-	expression tag	UNP O75469
B	433	GLY	-	expression tag	UNP O75469
B	434	SER	-	expression tag	UNP O75469
B	435	GLY	-	expression tag	UNP O75469

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	436	GLY	-	expression tag	UNP O75469
B	437	SER	-	expression tag	UNP O75469
B	438	GLY	-	expression tag	UNP O75469
B	439	GLY	-	expression tag	UNP O75469
B	440	SER	-	expression tag	UNP O75469
B	441	SER	-	expression tag	UNP O75469
B	442	HIS	-	expression tag	UNP O75469
B	443	SER	-	expression tag	UNP O75469
B	444	SER	-	expression tag	UNP O75469
B	445	LEU	-	expression tag	UNP O75469
B	446	THR	-	expression tag	UNP O75469
B	447	GLU	-	expression tag	UNP O75469
B	448	ARG	-	expression tag	UNP O75469
B	449	HIS	-	expression tag	UNP O75469
B	450	LYS	-	expression tag	UNP O75469
B	451	ILE	-	expression tag	UNP O75469
B	452	LEU	-	expression tag	UNP O75469
B	453	HIS	-	expression tag	UNP O75469
B	454	ARG	-	expression tag	UNP O75469
B	455	LEU	-	expression tag	UNP O75469
B	456	LEU	-	expression tag	UNP O75469
B	457	GLN	-	expression tag	UNP O75469
B	458	GLU	-	expression tag	UNP O75469
B	459	GLY	-	expression tag	UNP O75469
B	460	SER	-	expression tag	UNP O75469
B	461	PRO	-	expression tag	UNP O75469
B	462	SER	-	expression tag	UNP O75469

- Molecule 2 is (2S)-2-({[3'-(trifluoromethyl)[1,1'-biphenyl]-4-yl]oxy}methyl)-2,3-dihydro-7H-[1,3]oxazolo[3,2-a]pyrimidin-7-one (CCD ID: HCJ) (formula: C₂₀H₁₅F₃N₂O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			28	20	3	2	3		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	B	31	Total	O	0	0
			31	31		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.03Å 88.93Å 106.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.08 – 2.30 39.08 – 2.31	Depositor EDS
% Data completeness (in resolution range)	94.0 (39.08-2.30) 94.1 (39.08-2.31)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 2.32Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.226 , 0.266 0.225 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	46.7	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 32.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4720	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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: H CJ

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	0/2364	0.71	1/3178 (0.0%)
1	B	0.38	0/2348	0.69	2/3158 (0.1%)
All	All	0.39	0/4712	0.70	3/6336 (0.0%)

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	A	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	320	LEU	N-CA-C	-6.33	106.09	113.88
1	B	381	ARG	CA-C-N	5.09	124.59	119.19
1	B	381	ARG	C-N-CA	5.09	124.59	119.19

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	383	GLN	Peptide

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	2315	0	2335	62	0
1	B	2299	0	2321	45	0
2	A	28	0	0	4	0
3	A	47	0	0	0	0
3	B	31	0	0	0	0
All	All	4720	0	4656	108	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 12.

All (108) 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:202:VAL:HG21	1:B:417:ILE:HD12	1.59	0.82
1:B:431:ILE:H	1:B:431:ILE:HD13	1.46	0.81
1:A:214:GLN:HE21	1:A:216:ARG:HH11	1.32	0.78
1:A:383:GLN:HB2	1:A:384:PRO:HD3	1.70	0.74
1:A:277:LYS:HD2	1:A:449:HIS:CE1	2.24	0.73
1:A:175:PRO:HG3	1:A:239:LEU:HD13	1.72	0.71
1:A:443:SER:O	1:A:444:SER:HB3	1.91	0.70
1:B:213:LEU:HD23	1:B:214:GLN:N	2.07	0.69
1:A:320:LEU:HD23	1:A:320:LEU:N	2.07	0.69
1:A:415:GLN:HG2	1:A:431:ILE:HD13	1.76	0.68
1:A:324:LEU:HD22	1:A:324:LEU:O	1.94	0.67
1:B:233:GLY:O	1:B:234:LYS:HB3	1.95	0.67
2:A:501:HCJ:CAN	2:A:501:HCJ:CAE	2.74	0.66
1:A:383:GLN:CB	1:A:384:PRO:HD3	2.26	0.65
1:B:431:ILE:HD13	1:B:431:ILE:N	2.11	0.65
1:B:360:ARG:O	1:B:364:GLN:HG2	1.97	0.64
1:A:383:GLN:HB2	1:A:384:PRO:CD	2.24	0.64
1:B:317:GLN:HG2	1:B:318:LEU:N	2.13	0.64
1:A:289:ASN:HD22	1:A:327:HIS:HD1	1.44	0.63
1:B:202:VAL:HG21	1:B:417:ILE:CD1	2.29	0.63
1:A:445:LEU:O	1:A:449:HIS:HD2	1.82	0.62
1:A:254:ILE:HD11	1:A:287:ARG:HD2	1.81	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:GLN:HE21	1:A:216:ARG:NH1	1.98	0.61
1:B:317:GLN:N	1:B:320:LEU:HD23	2.16	0.61
1:B:424:LEU:O	1:B:424:LEU:HD12	2.02	0.59
1:B:217:GLY:C	1:B:219:ASP:H	2.10	0.59
1:A:259:LYS:HD2	1:A:456:LEU:HA	1.86	0.58
1:A:324:LEU:HD21	1:A:328:TYR:CE1	2.38	0.58
1:B:206:LEU:HD12	1:B:236:ILE:HD12	1.85	0.58
1:B:254:ILE:HD11	1:B:287:ARG:HD2	1.85	0.58
1:A:213:LEU:HD21	1:A:215:LEU:HD23	1.86	0.57
1:B:384:PRO:HA	1:B:387:ARG:HG3	1.86	0.57
1:B:303:ARG:HG3	1:B:304:LEU:HD12	1.87	0.56
1:A:443:SER:O	1:A:444:SER:CB	2.54	0.55
1:A:381:ARG:HB3	1:A:386:HIS:CD2	2.41	0.55
1:A:202:VAL:HG11	1:A:417:ILE:HD11	1.88	0.55
1:B:213:LEU:HD23	1:B:213:LEU:C	2.31	0.55
1:A:145:GLU:OE2	1:A:149:MET:HE2	2.08	0.54
1:A:383:GLN:CG	1:A:384:PRO:HD3	2.38	0.54
1:A:399:GLU:O	1:A:403:ILE:HG13	2.08	0.54
1:B:298:THR:HG22	1:B:307:CYS:HA	1.91	0.53
1:B:159:MET:O	1:B:159:MET:HE2	2.08	0.53
1:A:319:LEU:HA	1:A:324:LEU:HD12	1.91	0.53
1:A:206:LEU:HD12	1:A:236:ILE:HD13	1.91	0.52
1:B:278:GLY:HA3	1:B:353:ARG:HD2	1.92	0.52
1:A:383:GLN:O	1:A:385:ALA:N	2.42	0.52
1:A:202:VAL:HG21	1:A:417:ILE:CD1	2.40	0.52
1:B:298:THR:HG22	1:B:307:CYS:SG	2.49	0.51
1:A:213:LEU:C	1:A:213:LEU:HD23	2.36	0.51
1:A:299:TRP:CE2	2:A:501:HCJ:CAB	2.94	0.51
1:B:270:GLU:HB3	1:B:445:LEU:HD12	1.92	0.50
1:A:324:LEU:HD11	1:A:328:TYR:CE1	2.47	0.50
1:A:320:LEU:N	1:A:320:LEU:CD2	2.73	0.49
1:A:329:MET:HB3	1:A:396:MET:HE1	1.94	0.49
1:A:214:GLN:HB3	1:A:305:SER:HB2	1.95	0.49
1:A:445:LEU:O	1:A:449:HIS:CD2	2.64	0.49
1:A:324:LEU:HD22	1:A:324:LEU:C	2.36	0.49
1:A:202:VAL:HG21	1:A:417:ILE:HD13	1.95	0.48
1:A:219:ASP:HB2	1:B:235:GLU:HB2	1.95	0.48
1:A:260:VAL:O	1:A:260:VAL:HG23	2.12	0.48
1:A:324:LEU:HD11	1:A:328:TYR:HE1	1.78	0.48
1:A:383:GLN:CB	1:A:384:PRO:CD	2.89	0.48
1:A:234:LYS:HD3	1:A:237:PHE:CE1	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:LYS:HD2	1:B:449:HIS:NE2	2.29	0.48
1:B:251:PHE:CD2	1:B:284[A]:CYS:SG	3.05	0.47
1:A:259:LYS:O	1:A:265:ARG:HG3	2.14	0.47
1:A:299:TRP:CD2	2:A:501:HCJ:CAB	2.98	0.46
1:A:384:PRO:O	1:A:387:ARG:HB2	2.15	0.46
1:A:319:LEU:C	1:A:320:LEU:HD23	2.40	0.46
1:B:213:LEU:C	1:B:213:LEU:CD2	2.88	0.46
1:B:239:LEU:O	1:B:243:MET:HG2	2.16	0.46
1:B:431:ILE:N	1:B:431:ILE:CD1	2.79	0.45
1:A:201:GLN:HA	1:A:204:LYS:HD2	1.99	0.45
1:B:216:ARG:HG3	1:B:216:ARG:HH11	1.81	0.45
1:B:214:GLN:HB3	1:B:305:SER:HB2	1.99	0.45
1:A:235:GLU:H	1:A:235:GLU:CD	2.25	0.44
1:B:317:GLN:HG2	1:B:318:LEU:H	1.81	0.44
2:A:501:HCJ:CAE	2:A:501:HCJ:CAM	2.96	0.43
1:B:202:VAL:HG13	1:B:414:ILE:HG12	2.00	0.43
1:B:217:GLY:C	1:B:219:ASP:N	2.76	0.43
1:B:321:GLU:HA	1:B:322:PRO:HD3	1.90	0.43
1:A:324:LEU:HD21	1:A:328:TYR:HE1	1.80	0.43
1:B:407:HIS:CE1	1:B:411:LEU:HD13	2.54	0.43
1:A:323:MET:HA	1:A:403:ILE:HD13	2.00	0.43
1:A:411:LEU:C	1:A:411:LEU:HD23	2.44	0.42
1:B:216:ARG:HG3	1:B:216:ARG:NH1	2.34	0.42
1:B:339:GLU:OE2	1:B:381:ARG:HD2	2.19	0.42
1:A:382:PRO:O	1:A:383:GLN:O	2.38	0.42
1:B:206:LEU:HD11	1:B:237:PHE:CE2	2.54	0.42
1:A:277:LYS:HB3	1:A:277:LYS:HE3	1.89	0.42
1:B:317:GLN:CG	1:B:318:LEU:N	2.82	0.42
1:A:209:LEU:HD12	1:A:209:LEU:HA	1.91	0.41
1:B:318:LEU:C	1:B:320:LEU:N	2.79	0.41
1:A:251:PHE:CD2	1:A:284[A]:CYS:SG	3.13	0.41
1:B:201:GLN:NE2	1:B:413:ARG:NH1	2.67	0.41
1:B:360:ARG:HE	1:B:360:ARG:HB2	1.70	0.41
1:B:402:SER:O	1:B:406:GLN:HG3	2.21	0.41
1:A:269:ILE:HG23	1:A:270:GLU:N	2.35	0.41
1:A:349:PHE:O	1:A:366:GLN:HB2	2.21	0.41
1:A:148:ARG:HE	1:A:148:ARG:HB2	1.60	0.41
1:A:215:LEU:HD22	1:A:304:LEU:CD2	2.51	0.41
1:B:155:MET:HE1	1:B:337:GLU:CB	2.51	0.41
1:B:342:LEU:HD13	1:B:373:LEU:HA	2.01	0.41
1:A:157:ALA:HA	1:A:260:VAL:HG21	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LYS:HA	1:A:237:PHE:CD1	2.56	0.40
1:A:319:LEU:O	1:A:319:LEU:HG	2.21	0.40
1:A:324:LEU:C	1:A:324:LEU:HD13	2.47	0.40
1:B:210:LYS:HG2	1:B:309:GLU:HG3	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	275/344 (80%)	260 (94%)	11 (4%)	4 (2%)	8	8
1	B	273/344 (79%)	262 (96%)	9 (3%)	2 (1%)	18	23
All	All	548/688 (80%)	522 (95%)	20 (4%)	6 (1%)	11	13

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	383	GLN
1	A	444	SER
1	B	218	GLU
1	B	234	LYS
1	A	208	SER
1	A	235	GLU

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	256/302 (85%)	241 (94%)	15 (6%)	18	26
1	B	255/302 (84%)	245 (96%)	10 (4%)	28	43
All	All	511/604 (85%)	486 (95%)	25 (5%)	22	34

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	TRP
1	A	207	CYS
1	A	209	LEU
1	A	215	LEU
1	A	236	ILE
1	A	239	LEU
1	A	260	VAL
1	A	308	LEU
1	A	320	LEU
1	A	324	LEU
1	A	325	LYS
1	A	329	MET
1	A	383	GLN
1	A	443	SER
1	A	452	LEU
1	B	159	MET
1	B	199	TRP
1	B	201	GLN
1	B	265	ARG
1	B	323	MET
1	B	324	LEU
1	B	332	LYS
1	B	358	GLN
1	B	411	LEU
1	B	431	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	214	GLN
1	A	224	ASN
1	A	272	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	285	GLN
1	A	289	ASN
1	A	359	HIS
1	A	368	GLN
1	A	386	HIS
1	A	407	HIS
1	A	449	HIS
1	B	201	GLN
1	B	214	GLN
1	B	224	ASN
1	B	272	GLN
1	B	289	ASN
1	B	317	GLN
1	B	383	GLN
1	B	407	HIS
1	B	453	HIS
1	B	457	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](#)

1 ligand is 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	HCJ	A	501	-	30,31,31	1.60	5 (16%)	41,45,45	2.48	8 (19%)

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	HCJ	A	501	-	-	1/15/23/23	0/4/4/4

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HCJ	CAE-NAF	5.62	1.40	1.30
2	A	501	HCJ	CAS-CAP	-3.93	1.39	1.49
2	A	501	HCJ	CAI-NAD	2.62	1.40	1.37
2	A	501	HCJ	CAH-CAG	-2.35	1.39	1.44
2	A	501	HCJ	CAY-CAU	2.09	1.54	1.49

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	HCJ	NAD-CAE-NAF	-9.83	118.64	127.05
2	A	501	HCJ	OAA-CAE-NAF	7.42	131.95	121.24
2	A	501	HCJ	OAA-CAC-CAK	4.39	118.11	109.10
2	A	501	HCJ	OAA-CAC-CAB	-4.34	100.29	104.50
2	A	501	HCJ	CAE-NAF-CAG	3.78	120.50	116.66
2	A	501	HCJ	OAA-CAE-NAD	-3.04	109.39	111.81
2	A	501	HCJ	OAL-CAK-CAC	2.84	114.32	107.79
2	A	501	HCJ	CAH-CAI-NAD	-2.12	120.26	122.39

There are no chirality outliers.

All (1) torsion outliers are listed below:

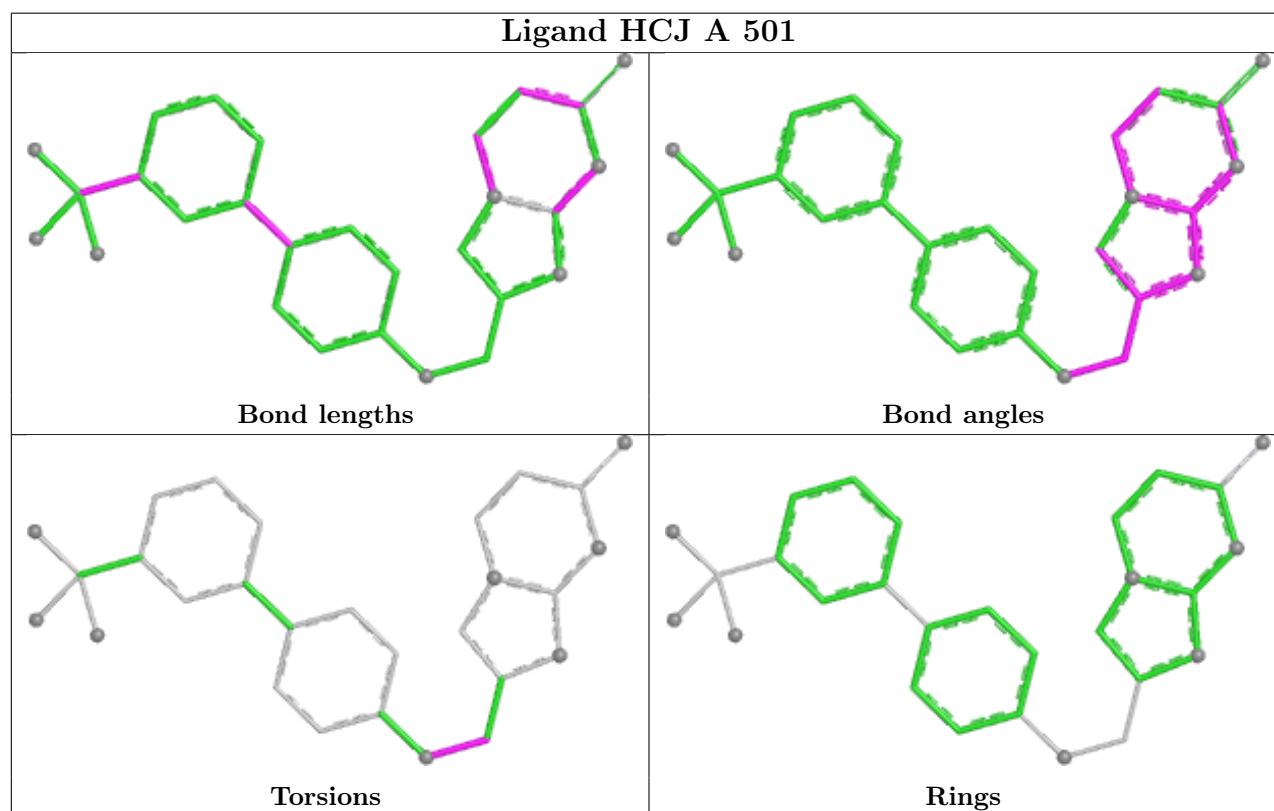
Mol	Chain	Res	Type	Atoms
2	A	501	HCJ	CAC-CAK-OAL-CAM

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HCJ	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 ⓘ

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	282/344 (81%)	0.71	38 (13%) 7 8	15, 54, 95, 123	1 (0%)
1	B	280/344 (81%)	0.70	34 (12%) 8 9	16, 55, 95, 99	1 (0%)
All	All	562/688 (81%)	0.71	72 (12%) 7 8	15, 54, 95, 123	2 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	431	ILE	6.6
1	B	178	LEU	6.6
1	A	209	LEU	6.5
1	A	320	LEU	5.9
1	A	192	SER	5.0
1	A	308	LEU	4.9
1	B	460	SER	4.9
1	A	229	ALA	4.3
1	B	385	ALA	4.3
1	B	234	LYS	4.2
1	A	215	LEU	4.1
1	A	177	VAL	3.9
1	B	384	PRO	3.9
1	B	317	GLN	3.7
1	B	318	LEU	3.7
1	B	229	ALA	3.6
1	A	431	ILE	3.6
1	A	202	VAL	3.4
1	B	177	VAL	3.4
1	A	383	GLN	3.4
1	B	446	THR	3.3
1	A	233	GLY	3.2
1	B	199	TRP	3.2
1	B	445	LEU	3.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	236	ILE	3.1
1	A	211	VAL	3.0
1	A	142	GLY	3.0
1	A	458	GLU	3.0
1	B	319	LEU	3.0
1	B	357	LEU	3.0
1	B	361	VAL	2.9
1	A	319	LEU	2.9
1	A	357	LEU	2.8
1	A	234	LYS	2.8
1	A	143	LEU	2.8
1	B	430	GLY	2.7
1	A	323	MET	2.7
1	B	429	PHE	2.7
1	B	444	SER	2.7
1	A	430	GLY	2.6
1	B	417	ILE	2.5
1	A	199	TRP	2.5
1	A	208	SER	2.5
1	B	201	GLN	2.5
1	A	196	ALA	2.4
1	B	208	SER	2.4
1	A	324	LEU	2.3
1	A	411	LEU	2.3
1	B	379	CYS	2.3
1	A	193	ARG	2.3
1	B	218	GLU	2.3
1	A	361	VAL	2.3
1	A	354	PRO	2.3
1	A	197	ALA	2.2
1	B	320	LEU	2.2
1	A	146	GLU	2.2
1	A	200	SER	2.2
1	B	206	LEU	2.2
1	A	210	LYS	2.2
1	B	202	VAL	2.1
1	B	263	TYR	2.1
1	A	445	LEU	2.1
1	B	207	CYS	2.1
1	B	209	LEU	2.1
1	B	355	GLY	2.1
1	A	206	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	359	HIS	2.1
1	B	235	GLU	2.0
1	B	309	GLU	2.0
1	A	236	ILE	2.0
1	A	144	THR	2.0
1	A	207	CYS	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](#)

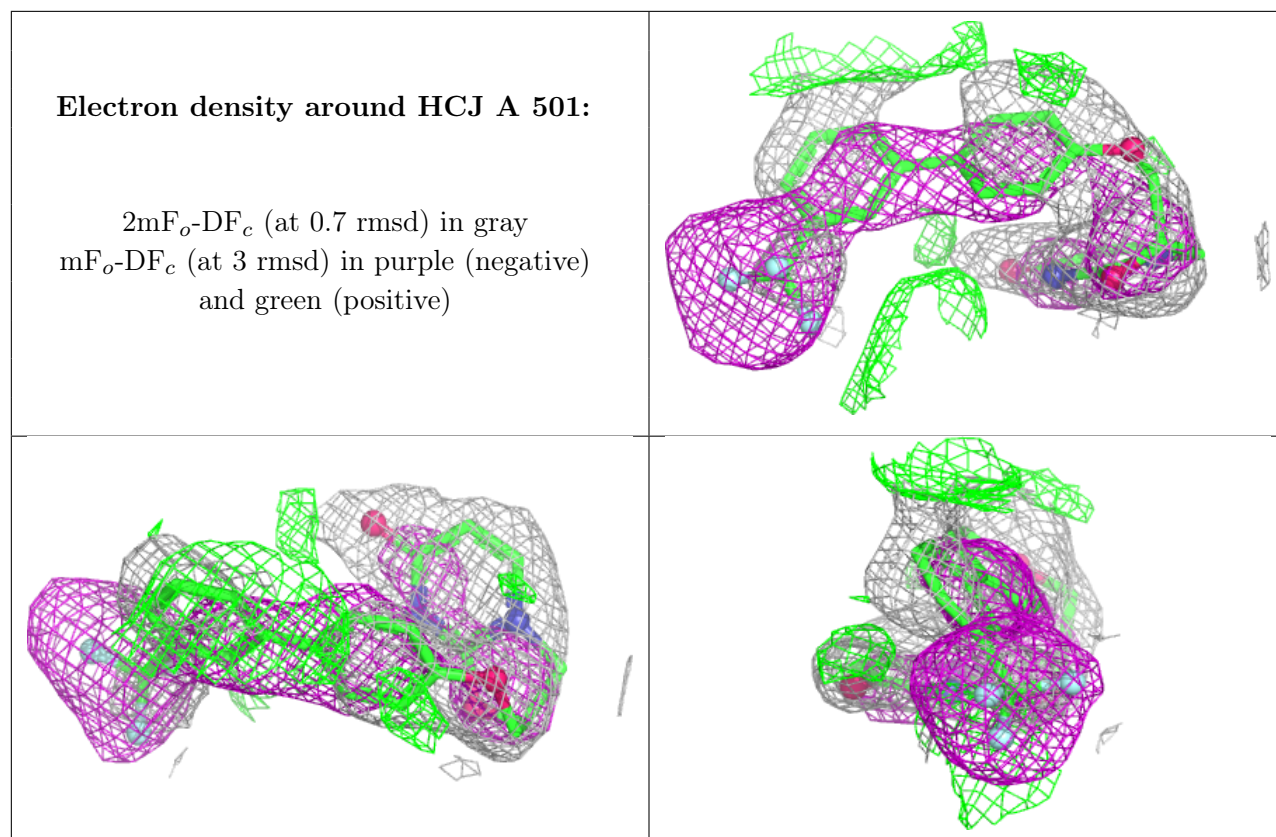
There are no oligosaccharides in this entry.

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	HCJ	A	501	28/28	0.39	0.25	58,62,69,70	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.