



Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 08:52 pm BST

PDB ID : 4J08
Title : Crystal structure of hcv ns5b polymerase in complex with 2-[(4-METHYLPHENYL)SULFONYL]AMINO}-5-PHENOXYBENZOIC ACID
Authors : Coulombe, R.
Deposited on : 2013-01-30
Resolution : 2.10 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	:	2.11
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)	:	2.11

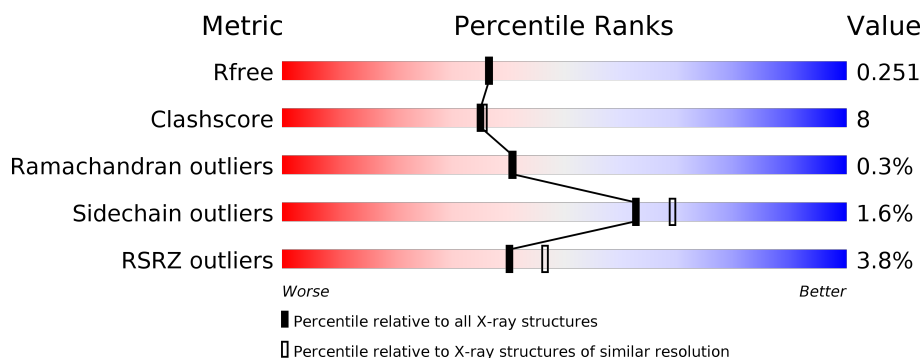
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	576	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>13%</div> <div>• •</div> </div> </div>
1	B	576	<div> <div>6%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>• •</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9027 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.

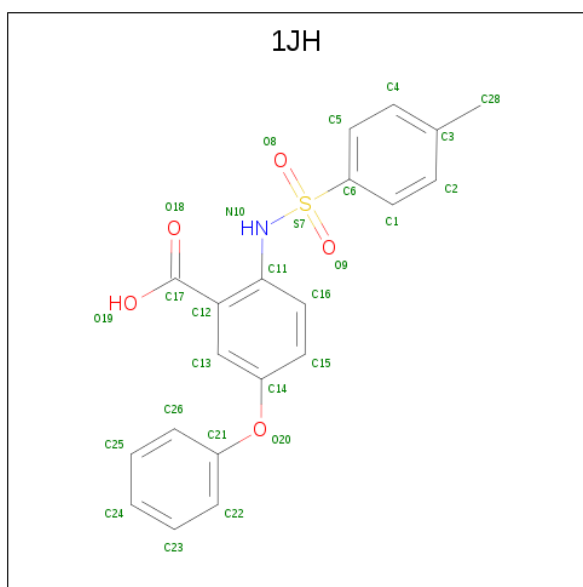
- Molecule 1 is a protein called Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	0	0
			4358	2745	770	811	32			
1	B	558	Total	C	N	O	S	0	0	0
			4346	2737	768	809	32			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	571	HIS	-	EXPRESSION TAG	UNP O92972
A	572	HIS	-	EXPRESSION TAG	UNP O92972
A	573	HIS	-	EXPRESSION TAG	UNP O92972
A	574	HIS	-	EXPRESSION TAG	UNP O92972
A	575	HIS	-	EXPRESSION TAG	UNP O92972
A	576	HIS	-	EXPRESSION TAG	UNP O92972
B	571	HIS	-	EXPRESSION TAG	UNP O92972
B	572	HIS	-	EXPRESSION TAG	UNP O92972
B	573	HIS	-	EXPRESSION TAG	UNP O92972
B	574	HIS	-	EXPRESSION TAG	UNP O92972
B	575	HIS	-	EXPRESSION TAG	UNP O92972
B	576	HIS	-	EXPRESSION TAG	UNP O92972

- Molecule 2 is 2-[[[(4-methylphenyl)sulfonyl]amino]-5-phenoxybenzoic acid (three-letter code: 1JH) (formula: C₂₀H₁₇NO₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			27	20	1	5	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	181	Total	O	0	0
			181	181		
3	B	115	Total	O	0	0
			115	115		

These plots are drawn for all protein, RNA and DNA 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 ($\text{RSRZ} > 2$). 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.

Chain A:

82% 13%

%

S1 P22 I23 N24 S27 L31 R32 Y36 R48 L57 A73 S76 A80 K81 L82 L83 S84 I85 E86 E87 P93 P94 G102 R114 I119 V144 P145 C146 P149 GLU LYS GLY GLY R154 I160 L165 V169 K172 M173 P182 Q184 I233 R234 L245 E248 Q251 R254 T257 Y261 I262 M268 Q272 K273 C274 C289 T300 K307 K313 L314 V321 L336 Y346 S347 G351 P356 P356 R374 D375 V381 T390 P391 R394 R401 H402 L434 D444

Y452 R465 L474 V485 L489 Q493 R501 H502 R503 A504 R505 S506 V507 R508 L512 R523 R531 L534 K535 A542 S543 Q544 L545 D546 L547 I560 V561 H562 S563 LEU SER ARG ALA ARG ARG PRO ARG HIS HIS HIS HIS HIS HIS HIS

Chain B:

Item	Category
S1	Green
T7	Green
I11	Green
C14	Red
A15	Red
E18	Green
S19	Green
P20	Green
I21	Green
P22	Green
I23	Green
N24	Green
P25	Green
I26	Green
S27	Green
N28	Green
L31	Green
H34	Red
K51	Green
L57	Red
L83	Green
S84	Green
I85	Green
P93	Green
G102	Green
R114	Green
A115	Green
V116	Green
N117	Green
H118	Green
I119	Green
V122	Green
T137	Green
V144	Green
V147	Green
GLN	Green
PRO	Green
GLU	Green
LYS	Green
GLY	Green
G153	Red
R158	Green
T159	Green
I160	Green
V161	Green
V169	Green
K172	Green
M173	Green
L182	Green
P183	Green
V205	Green
W208	Red
S210	Green
K211	Green
K212	Red
C213	Red
Y219	Green
R222	Green
C223	Green
I233	Green
P247	Green
Q251	Green
R254	Green
Y261	Green
N268	Green
Q272	Green
N273	Green
C274	Green
G275	Green
S282	Green
C289	Green
T300	Green
Q309	Red
D310	Green
M313	Red
L314	Green
L320	Green
V321	Green
I322	Green
I323	Green
C324	Green
Q330	Red
E331	Red
L336	Green
Y346	Green
S347	Green
G351	Green
P356	Green
E361	Green
V370	Green
S371	Green
V372	Green
A373	Green
H374	Green
D375	Green
A376	Red
K379	Red
T385	Green
R386	Green
D387	Green
P388	Green
T389	Green
T390	Green
P391	Green
R394	Green
A395	Green
A396	Green
T399	Green
A400	Green
R401	Green
H402	Red
W408	Green
I412	Green
A416	Green
P417	Green
T418	Green
L419	Green
W420	Green
A421	Green
R422	Green
S431	Green
L434	Green
L439	Green
H562	Red
S563	Green
L564	Green
L547	Green
D546	Green
L545	Green
Q544	Green
S543	Green
A542	Green
A541	Green
P540	Green
T539	Green
P538	Green
L536	Green
T537	Green
L534	Green
K533	Green
T532	Green
R531	Green
S530	Green
R523	Red
G522	Green
A519	Green
G515	Red
O514	Green
S513	Green
L512	Green
L511	Green
A509	Green
R508	Green
V507	Red
S506	Green
R503	Green
V494	Green
L489	Green
I482	Green
S478	Green
L474	Green
R465	Red
E464	Green
I463	Green
V462	Green
Q461	Green
ALA	Green
P460	Green
L459	Green

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.83Å 107.68Å 135.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.10 41.54 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.10) 99.6 (41.54-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.71 (at 2.10Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.225 , 0.255 0.220 , 0.251	Depositor DCC
R_{free} test set	9100 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	32.5	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9027	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% 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: 1JH

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	0.34	0/4453	0.62	2/6044 (0.0%)
1	B	0.35	0/4440	0.60	1/6025 (0.0%)
All	All	0.34	0/8893	0.61	3/12069 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	LEU	CA-CB-CG	5.52	127.99	115.30
1	B	351	GLY	N-CA-C	-5.22	100.04	113.10
1	A	351	GLY	N-CA-C	-5.13	100.27	113.10

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	4358	0	4371	60	0
1	B	4346	0	4359	86	0
2	A	27	0	16	0	0
3	A	181	0	0	4	0
3	B	115	0	0	0	0
All	All	9027	0	8746	143	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 8.

All (143) 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:81:LYS:O	1:A:82:LEU:HB3	1.74	0.87
1:B:515:GLY:HA2	1:B:519:ALA:HB2	1.57	0.85
1:B:531:ARG:H	1:B:531:ARG:HH11	1.29	0.80
1:B:158:ARG:HG3	1:B:158:ARG:HH11	1.49	0.78
1:A:465:ARG:NH1	1:A:545:LEU:O	2.17	0.78
1:A:545:LEU:HB3	1:A:547:LEU:HD13	1.67	0.76
1:B:85:ILE:HD13	1:B:116:VAL:HG13	1.69	0.73
1:B:144:VAL:HB	1:B:394:ARG:HG2	1.70	0.72
1:A:531:ARG:HH11	1:A:531:ARG:HB2	1.55	0.70
1:B:506:SER:O	1:B:510:LYS:HG3	1.92	0.69
1:B:119:ILE:HD13	1:B:169:VAL:HG11	1.75	0.68
1:B:51:LYS:HE2	1:B:223:CYS:SG	2.34	0.67
1:B:503:ARG:O	1:B:507:VAL:HG23	1.94	0.67
1:A:336:LEU:HD12	1:A:356:PRO:HD3	1.77	0.66
1:A:503:ARG:O	1:A:507:VAL:HG23	1.97	0.65
1:A:501:ARG:HD3	3:A:843:HOH:O	1.98	0.64
1:B:27:SER:OG	1:B:399:THR:HB	1.98	0.64
1:B:205:VAL:HG13	1:B:209:LYS:HE2	1.81	0.62
1:B:434:LEU:HD23	1:B:439:LEU:HD11	1.81	0.62
1:B:465:ARG:HG3	1:B:545:LEU:HB3	1.81	0.61
1:A:268:ASN:HB3	1:A:274:CYS:SG	2.41	0.61
1:B:313:MET:SD	1:B:322:VAL:HG22	2.41	0.60
1:B:314:LEU:HB3	1:B:321:VAL:CG1	2.31	0.60
1:A:81:LYS:O	1:A:82:LEU:CB	2.46	0.60
1:A:381:VAL:HG11	1:A:474:LEU:CD2	2.32	0.59
1:A:531:ARG:HB2	1:A:531:ARG:NH1	2.19	0.57
1:A:434:LEU:HD12	1:A:507:VAL:HG13	1.86	0.57
1:B:515:GLY:CA	1:B:519:ALA:HB2	2.33	0.56
1:B:361:GLU:HG2	1:B:370:VAL:O	2.05	0.56
1:B:531:ARG:HD2	1:B:532:THR:H	1.71	0.55
1:A:390:THR:HB	1:A:391:PRO:HD3	1.88	0.55
1:A:512:LEU:HD21	1:A:523:ARG:HG2	1.89	0.55
1:B:478:SER:O	1:B:482:ILE:HG13	2.06	0.55
1:B:336:LEU:HD23	1:B:356:PRO:HD3	1.89	0.55
1:B:31:LEU:HD12	1:B:31:LEU:O	2.07	0.54
1:B:118:HIS:O	1:B:122:VAL:HG23	2.07	0.54
1:B:27:SER:OG	1:B:396:ALA:O	2.24	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:HIS:O	1:B:474:LEU:HA	2.07	0.54
1:B:531:ARG:HD3	1:B:532:THR:HG23	1.90	0.54
1:A:314:LEU:HB3	1:A:321:VAL:CG1	2.39	0.53
1:B:531:ARG:HD2	1:B:532:THR:N	2.24	0.53
1:B:22:PRO:HD2	1:B:400:ALA:HB1	1.91	0.52
1:A:508:ARG:HH11	1:A:508:ARG:HG2	1.75	0.51
1:A:523:ARG:HD3	1:A:534:LEU:HD13	1.92	0.51
1:B:172:LYS:HE3	1:B:560:ILE:HD13	1.93	0.51
1:A:234:ARG:HD3	1:B:247:PRO:HG3	1.93	0.51
1:A:80:ALA:HB3	1:A:245:LEU:HD23	1.92	0.51
1:B:158:ARG:HG3	1:B:158:ARG:NH1	2.23	0.51
1:B:205:VAL:O	1:B:209:LYS:HG2	2.11	0.51
1:A:434:LEU:CD1	1:A:507:VAL:HG13	2.42	0.50
1:A:485:VAL:O	1:A:489:LEU:HG	2.12	0.50
1:B:531:ARG:CD	1:B:532:THR:HG23	2.42	0.50
1:A:268:ASN:ND2	1:A:272:GLN:HB2	2.27	0.50
1:A:381:VAL:HG11	1:A:474:LEU:HD21	1.94	0.50
1:A:465:ARG:HG2	1:A:542:ALA:O	2.12	0.50
1:B:158:ARG:CG	1:B:158:ARG:HH11	2.21	0.50
1:A:24:ASN:HB3	1:A:27:SER:OG	2.12	0.49
1:A:165:LEU:O	1:A:169:VAL:HG23	2.12	0.49
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.94	0.49
1:A:144:VAL:HB	1:A:394:ARG:HG2	1.94	0.49
1:B:183:PRO:HG3	1:B:289:CYS:SG	2.53	0.49
1:A:452:TYR:OH	1:A:562:HIS:HD2	1.96	0.49
1:A:254:ARG:HG2	1:B:251:GLN:NE2	2.28	0.49
1:A:73:ALA:O	1:A:76:SER:HB2	2.13	0.48
1:B:273:ASN:ND2	1:B:275:GLY:H	2.10	0.48
1:B:160:ILE:HA	1:B:282:SER:OG	2.13	0.48
1:B:461:GLN:HG2	1:B:541:ALA:HB3	1.94	0.48
1:B:431:SER:HB2	1:B:507:VAL:HG21	1.96	0.48
1:B:268:ASN:HD21	1:B:272:GLN:HB2	1.78	0.48
1:A:251:GLN:NE2	1:B:254:ARG:HG2	2.29	0.48
1:A:172:LYS:HE3	1:A:560:ILE:HD13	1.96	0.47
1:B:390:THR:HB	1:B:391:PRO:HD3	1.95	0.47
1:A:119:ILE:HD13	1:A:169:VAL:HG11	1.97	0.47
1:A:268:ASN:HD21	1:A:272:GLN:HB2	1.80	0.47
1:B:11:ILE:HD13	1:B:159:LEU:HD22	1.96	0.47
1:B:459:LEU:O	1:B:463:ILE:HG13	2.14	0.46
1:B:512:LEU:O	1:B:515:GLY:N	2.33	0.46
1:B:83:LEU:HB2	1:B:173:MET:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ASN:ND2	1:B:272:GLN:HB2	2.30	0.46
1:B:459:LEU:N	1:B:460:PRO:CD	2.78	0.46
1:B:546:ASP:C	1:B:547:LEU:HD23	2.36	0.46
1:A:248:GLU:HG3	3:A:747:HOH:O	2.14	0.46
1:B:489:LEU:HD22	1:B:494:VAL:HG11	1.97	0.46
1:A:523:ARG:HD3	1:A:534:LEU:CD1	2.46	0.46
1:A:32:ARG:HD3	1:A:493:GLY:O	2.16	0.46
1:B:314:LEU:HB3	1:B:321:VAL:HG13	1.98	0.46
1:A:508:ARG:HG2	1:A:508:ARG:NH1	2.30	0.45
1:B:346:TYR:O	1:B:347:SER:HB3	2.16	0.45
1:B:233:ILE:HD13	1:B:261:TYR:O	2.16	0.45
1:B:51:LYS:HG2	1:B:223:CYS:SG	2.56	0.45
1:A:444:ASP:HA	1:A:452:TYR:O	2.16	0.45
1:B:416:ALA:HB3	1:B:417:PRO:HD3	1.99	0.45
1:A:346:TYR:O	1:A:347:SER:HB3	2.16	0.45
1:B:22:PRO:O	1:B:25:PRO:HG3	2.17	0.45
1:A:184:GLN:HG3	3:A:880:HOH:O	2.16	0.45
1:B:211:LYS:HE3	1:B:323:ILE:HG22	1.98	0.44
1:A:183:PRO:HG3	1:A:289:CYS:SG	2.58	0.44
1:B:372:VAL:HG22	1:B:373:ALA:N	2.33	0.44
1:A:545:LEU:HD22	1:A:547:LEU:HD11	2.00	0.44
1:B:300:THR:HA	1:B:313:MET:HE2	2.00	0.44
1:B:458:ASP:OD1	1:B:461:GLN:OE1	2.36	0.44
1:A:102:GLY:HA3	1:A:114:ARG:HE	1.82	0.44
1:B:408:TRP:O	1:B:412:ILE:HG13	2.18	0.44
1:A:314:LEU:HB3	1:A:321:VAL:HG13	2.00	0.43
1:A:93:PRO:HA	1:A:94:PRO:HD3	1.94	0.43
1:B:508:ARG:HG3	1:B:522:GLY:O	2.19	0.43
1:B:418:THR:O	1:B:422:ARG:HG3	2.18	0.43
1:B:7:THR:HG23	1:B:275:GLY:HA2	2.01	0.43
1:B:309:GLN:HA	1:B:309:GLN:HE21	1.83	0.43
1:B:31:LEU:HD12	1:B:31:LEU:C	2.39	0.43
1:B:531:ARG:HG3	1:B:531:ARG:HH11	1.83	0.43
1:A:85:ILE:HG12	1:A:173:MET:SD	2.59	0.43
1:B:309:GLN:O	1:B:324:CYS:HB2	2.19	0.43
1:B:309:GLN:CA	1:B:309:GLN:HE21	2.33	0.42
1:A:22:PRO:HG3	1:A:401:ARG:NH2	2.34	0.42
1:B:158:ARG:CG	1:B:158:ARG:NH1	2.79	0.42
1:A:531:ARG:HH11	1:A:531:ARG:CB	2.29	0.42
1:B:388:PRO:HB3	1:B:420:TRP:CD2	2.54	0.42
1:B:434:LEU:CD2	1:B:439:LEU:HD11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:ARG:NH1	1:B:531:ARG:HG3	2.34	0.42
1:B:102:GLY:O	1:B:114:ARG:HD3	2.18	0.42
1:B:434:LEU:HD12	1:B:507:VAL:HG13	2.01	0.42
1:A:535:LYS:HD3	1:A:535:LYS:HA	1.89	0.42
1:B:222:ARG:O	1:B:223:CYS:C	2.58	0.42
1:A:48:ARG:NH1	3:A:825:HOH:O	2.51	0.42
1:B:18:GLU:HA	1:B:18:GLU:OE2	2.19	0.42
1:B:431:SER:HB2	1:B:507:VAL:CG2	2.49	0.42
1:A:300:THR:HA	1:A:313:MET:CE	2.49	0.41
1:A:36:MET:O	1:A:146:CYS:HA	2.20	0.41
1:A:84:SER:OG	1:A:87:GLU:HG3	2.20	0.41
1:A:257:THR:O	1:A:262:ILE:HG23	2.21	0.41
1:B:85:ILE:CD1	1:B:116:VAL:HG13	2.43	0.41
1:B:489:LEU:HD22	1:B:494:VAL:CG1	2.51	0.41
1:B:530:VAL:O	1:B:533:LYS:NZ	2.45	0.41
1:A:57:LEU:HD23	1:A:57:LEU:C	2.41	0.41
1:B:137:THR:O	1:B:161:VAL:HA	2.21	0.41
1:B:512:LEU:O	1:B:513:SER:C	2.59	0.41
1:A:233:ILE:HD13	1:A:261:TYR:O	2.20	0.41
1:B:385:THR:OG1	1:B:386:ARG:N	2.53	0.41
1:B:93:PRO:HG3	1:B:561:TYR:HB2	2.03	0.41
1:A:375:ASP:OD1	1:A:375:ASP:C	2.60	0.41
1:A:374:HIS:O	1:A:474:LEU:HA	2.22	0.40
1:A:501:ARG:O	1:A:505:ARG:HG3	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	555/576 (96%)	538 (97%)	16 (3%)	1 (0%)	47 49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	554/576 (96%)	528 (95%)	24 (4%)	2 (0%)	34	32
All	All	1109/1152 (96%)	1066 (96%)	40 (4%)	3 (0%)	41	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	LEU
1	B	541	ALA
1	B	515	GLY

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	477/491 (97%)	468 (98%)	9 (2%)	57	63
1	B	475/491 (97%)	469 (99%)	6 (1%)	69	75
All	All	952/982 (97%)	937 (98%)	15 (2%)	62	69

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	32	ARG
1	A	160	ILE
1	A	184	GLN
1	A	307	LYS
1	A	336	LEU
1	A	381	VAL
1	A	402	HIS
1	A	465	ARG
1	B	182	LEU
1	B	309	GLN
1	B	310	ASP
1	B	313	MET

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Mol	Chain	Res	Type
1	B	465	ARG
1	B	531	ARG

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	251	GLN
1	A	273	ASN
1	A	374	HIS
1	A	438	GLN
1	A	514	GLN
1	A	544	GLN
1	A	562	HIS
1	B	24	ASN
1	B	251	GLN
1	B	273	ASN
1	B	309	GLN
1	B	411	ASN
1	B	461	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 carbohydrates 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	1JH	A	601	-	27,29,29	2.71	19 (70%)	36,41,41	1.07	3 (8%)

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	1JH	A	601	-	-	0/15/19/19	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	1JH	S7-N10	6.72	1.74	1.63
2	A	601	1JH	C22-C21	3.54	1.45	1.38
2	A	601	1JH	C12-C11	3.52	1.45	1.40
2	A	601	1JH	O20-C21	3.36	1.47	1.39
2	A	601	1JH	C26-C21	3.22	1.45	1.38
2	A	601	1JH	C5-C6	3.05	1.43	1.38
2	A	601	1JH	C11-N10	3.05	1.47	1.42
2	A	601	1JH	O9-S7	2.82	1.46	1.43
2	A	601	1JH	O8-S7	2.63	1.46	1.43
2	A	601	1JH	C24-C23	2.62	1.45	1.38
2	A	601	1JH	C5-C4	2.47	1.43	1.38
2	A	601	1JH	C15-C14	2.42	1.43	1.38
2	A	601	1JH	C25-C26	2.40	1.44	1.38
2	A	601	1JH	C1-C6	2.40	1.42	1.38
2	A	601	1JH	C25-C24	2.40	1.44	1.38
2	A	601	1JH	C23-C22	2.30	1.43	1.38
2	A	601	1JH	C2-C1	2.18	1.42	1.38
2	A	601	1JH	C6-S7	2.13	1.79	1.76
2	A	601	1JH	C16-C15	2.10	1.42	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	1JH	O9-S7-C6	-2.69	104.66	107.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	1JH	O8-S7-N10	2.47	112.92	106.73
2	A	601	1JH	O20-C14-C15	2.43	127.93	119.38

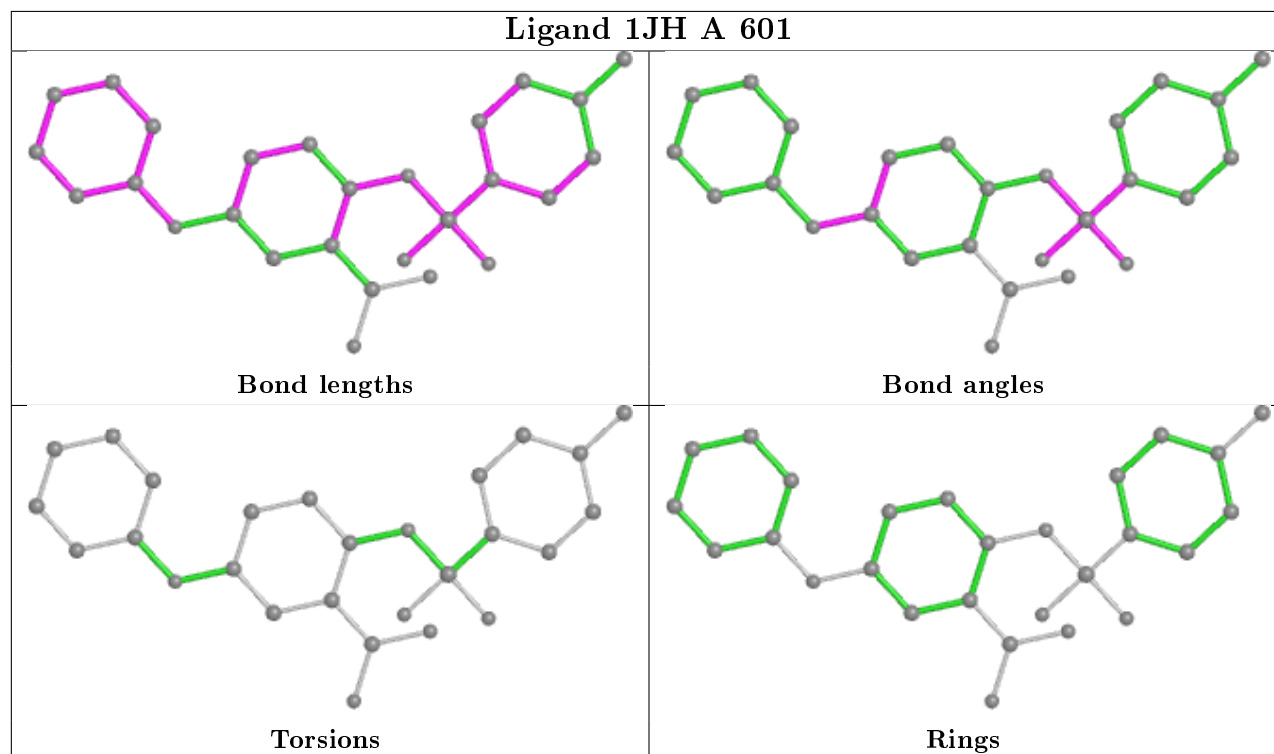
There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	559/576 (97%)	-0.12	7 (1%) 77 80	20, 31, 48, 57	0
1	B	558/576 (96%)	0.29	36 (6%) 18 23	22, 39, 54, 60	0
All	All	1117/1152 (96%)	0.08	43 (3%) 40 46	20, 35, 52, 60	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	23	ILE	5.9
1	B	24	ASN	5.5
1	B	542	ALA	4.6
1	B	543	SER	4.3
1	B	25	PRO	4.1
1	B	535	LYS	4.0
1	B	540	PRO	3.9
1	B	531	ARG	3.8
1	B	539	ILE	3.8
1	B	376	ALA	3.8
1	B	530	VAL	3.8
1	A	149	PRO	3.7
1	B	541	ALA	3.7
1	B	532	THR	3.7
1	B	153	GLY	3.7
1	B	27	SER	3.6
1	B	213	CYS	3.1
1	A	544	GLN	3.1
1	B	402	HIS	3.1
1	B	22	PRO	3.1
1	B	545	LEU	3.0
1	A	535	LYS	3.0
1	B	379	LYS	2.9
1	B	21	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	402	HIS	2.7
1	B	507	VAL	2.7
1	B	546	ASP	2.7
1	A	543	SER	2.6
1	B	212	LYS	2.6
1	B	330	GLN	2.5
1	B	14	CYS	2.4
1	A	546	ASP	2.3
1	B	19	SER	2.2
1	B	563	SER	2.2
1	B	208	TRP	2.2
1	A	86	GLU	2.1
1	B	34	HIS	2.1
1	B	331	GLU	2.1
1	B	28	ASN	2.1
1	B	57	LEU	2.1
1	B	523	ARG	2.1
1	B	15	ALA	2.0
1	B	537	THR	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 carbohydrates in this entry.

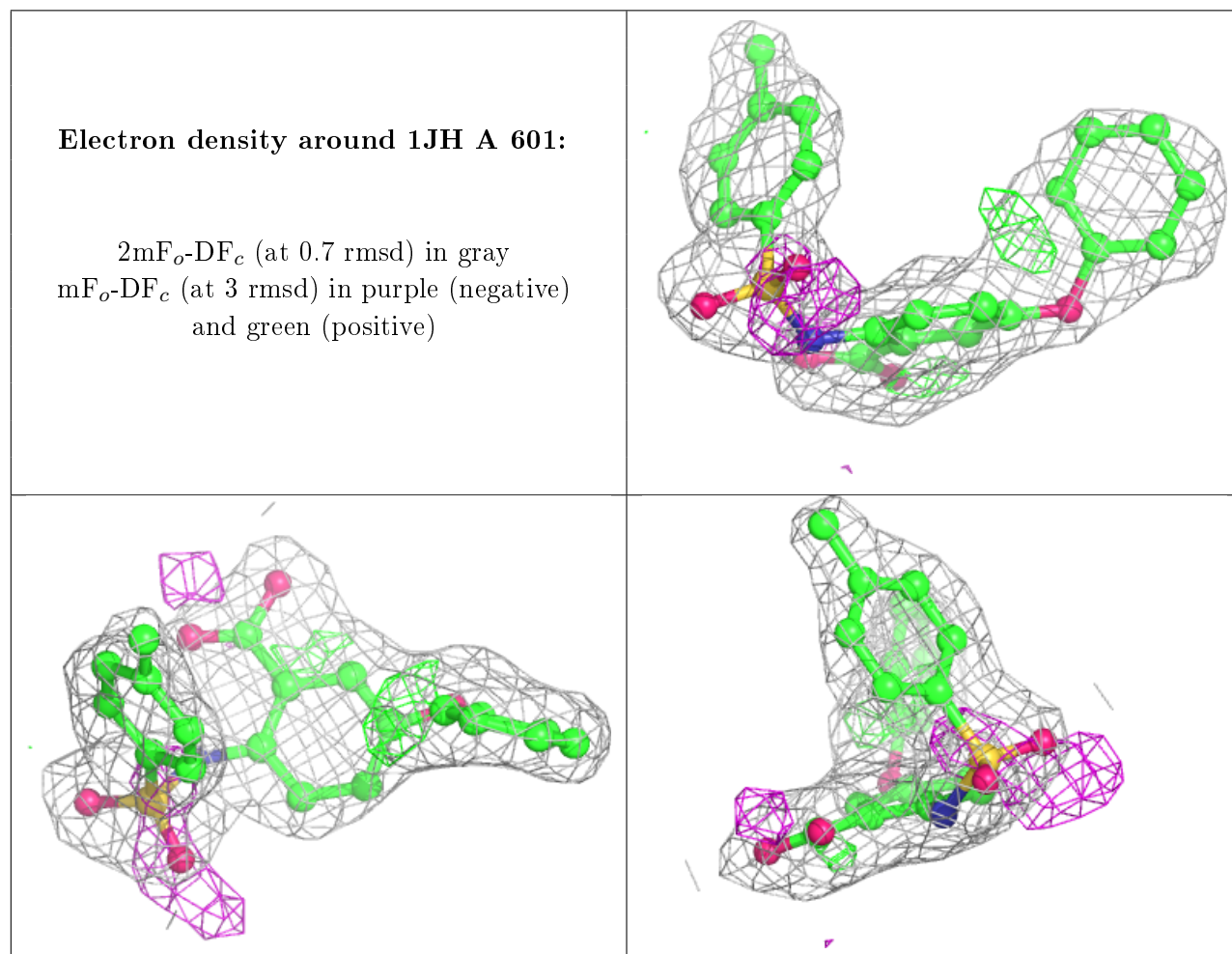
6.4 Ligands [i](#)

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(\AA^2)	Q<0.9
2	1JH	A	601	27/27	0.89	0.14	37,44,46,49	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 ⓘ

There are no such residues in this entry.