



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:07 AM UTC

PDB ID : 4JU7 / pdb_00004ju7
Title : Crystal structure of hcv ns5b polymerase in complex with compound 24
Authors : Coulombe, R.
Deposited on : 2013-03-24
Resolution : 2.20 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

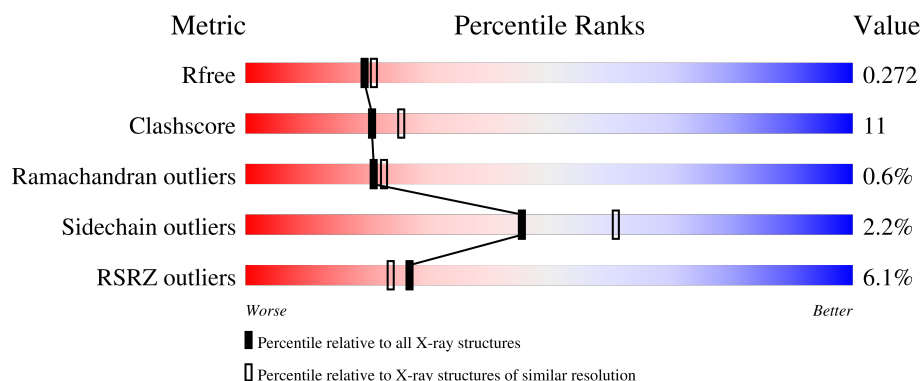
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	576	4% 75% 20% ..
1	B	576	8% 67% 27% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8989 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.

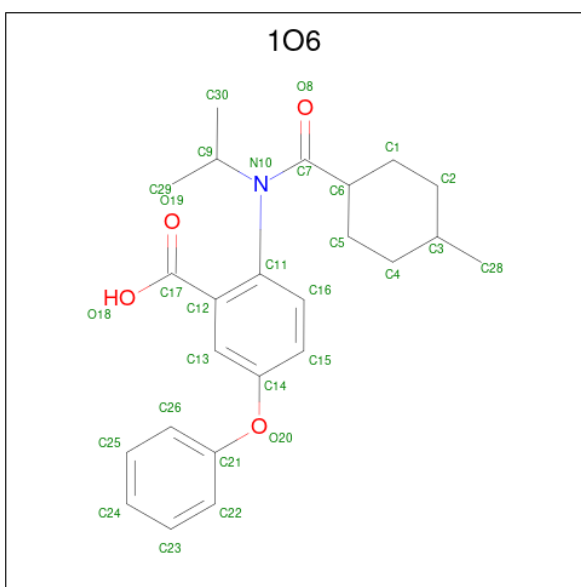
- Molecule 1 is a protein called Genome polyprotein.

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-[[[(trans-4-methylcyclohexyl)carbonyl](propan-2-yl)amino]-5-phenoxybenzoic acid (CCD ID: 1O6) (formula: C₂₄H₂₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			29	24	1	4		

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	157	Total	O	0	0
			157	157		
4	B	97	Total	O	0	0
			97	97		

L545	L546	L547	S548	G549	W550	S556	I560	S563	LEU	SER	ARG	ALA	ARG	PRO	ARG	HIS	HIS	HIS	HIS	HIS

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.84Å 108.07Å 135.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.20) 98.5 (50.00-2.20)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 2.20Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.246 , 0.274 0.245 , 0.272	Depositor DCC
R_{free} test set	7925 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å ²)	36.0	Xtriage
Anisotropy	0.354	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.012 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8989	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.07% 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: 1O6, MG

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	0.50	0/4453	0.96	15/6044 (0.2%)
1	B	0.49	0/4440	0.97	19/6025 (0.3%)
All	All	0.50	0/8893	0.97	34/12069 (0.3%)

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	26	LEU	N-CA-C	-10.40	100.59	113.18
1	A	352	ASP	CA-C-N	-8.57	113.41	119.66
1	A	352	ASP	C-N-CA	-8.57	113.41	119.66
1	A	78	VAL	N-CA-C	8.10	120.23	109.21
1	A	81	LYS	N-CA-C	7.52	122.86	112.04
1	A	196	SER	N-CA-C	-7.22	99.53	110.07
1	B	24	ASN	CA-C-N	6.70	126.62	119.85
1	B	24	ASN	C-N-CA	6.70	126.62	119.85
1	B	196	SER	N-CA-C	-6.62	102.52	110.13
1	B	403	THR	CA-C-N	6.26	127.67	119.84
1	B	403	THR	C-N-CA	6.26	127.67	119.84
1	A	192	GLY	N-CA-C	5.96	121.04	113.24
1	A	351	GLY	N-CA-C	-5.81	99.41	113.18
1	A	287	THR	N-CA-C	5.80	118.07	111.11
1	B	244	ASP	N-CA-C	-5.80	100.54	109.76
1	A	131	GLU	N-CA-C	5.77	119.85	112.12
1	A	315	VAL	N-CA-C	5.52	115.84	108.11
1	B	261	TYR	N-CA-C	5.52	117.38	111.36
1	B	131	GLU	N-CA-C	5.51	122.53	110.80
1	A	244	ASP	N-CA-C	-5.45	100.91	109.25
1	B	200	ARG	N-CA-C	-5.45	105.25	111.14
1	B	264	GLY	CA-C-N	5.43	125.19	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	264	GLY	C-N-CA	5.43	125.19	119.76
1	B	235	VAL	N-CA-C	-5.40	105.27	110.72
1	A	372	VAL	N-CA-C	5.37	117.61	108.86
1	A	261	TYR	N-CA-C	5.29	117.96	111.82
1	A	523	ARG	N-CA-C	5.27	116.71	111.07
1	B	230	GLU	N-CA-C	-5.24	105.47	111.07
1	B	171	GLU	N-CA-C	-5.13	105.58	111.07
1	B	37	VAL	N-CA-C	5.10	115.43	107.99
1	B	348	ALA	CA-C-N	5.08	123.37	119.66
1	B	348	ALA	C-N-CA	5.08	123.37	119.66
1	B	420	TRP	N-CA-C	5.07	116.88	111.36
1	A	424	ILE	N-CA-C	5.04	119.81	109.34

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	4358	0	4371	75	0
1	B	4346	0	4359	122	0
2	A	29	0	28	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	157	0	0	2	0
4	B	97	0	0	2	0
All	All	8989	0	8758	194	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 11.

All (194) 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	1.70	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:VAL:HB	1:B:394:ARG:HG2	1.58	0.85
1:B:531:ARG:HH11	1:B:531:ARG:H	1.24	0.85
1:B:506:SER:O	1:B:510:LYS:HG3	1.78	0.82
1:B:187:MET:HE3	1:B:296:TYR:HB2	1.67	0.76
1:A:465:ARG:NH1	1:A:545:LEU:O	2.19	0.75
1:B:515:GLY:HA2	1:B:519:ALA:HB2	1.70	0.72
1:B:461:GLN:HG2	1:B:541:ALA:HB3	1.72	0.71
1:B:376:ALA:C	1:B:378:GLY:H	1.98	0.70
1:A:248:GLU:HG3	4:A:738:HOH:O	1.94	0.68
1:A:108:VAL:HG21	1:A:165:LEU:HD21	1.75	0.67
1:A:336:LEU:HD12	1:A:356:PRO:HD3	1.77	0.67
1:A:40:THR:HB	1:A:157:ALA:HB2	1.76	0.67
1:A:381:VAL:HG11	1:A:474:LEU:CD2	2.24	0.66
1:B:158:ARG:HH11	1:B:158:ARG:HG3	1.59	0.66
1:A:34:HIS:HB3	4:A:840:HOH:O	1.96	0.65
1:B:201:VAL:HG13	1:B:370:VAL:HG13	1.78	0.65
1:B:22:PRO:HD2	1:B:400:ALA:HB1	1.76	0.65
1:B:434:LEU:HG	1:B:439:LEU:HD11	1.78	0.65
1:A:73:ALA:O	1:A:76:SER:HB2	1.97	0.64
1:B:27:SER:OG	1:B:399:THR:HB	1.98	0.64
1:A:521:CYS:HB3	1:A:525:LEU:HD12	1.80	0.63
1:B:99:SER:HB2	1:B:165:LEU:HB3	1.81	0.63
1:A:72:LYS:HD2	1:A:242:CYS:SG	2.39	0.63
1:A:81:LYS:O	1:A:82:LEU:CB	2.43	0.62
1:B:408:TRP:O	1:B:412:ILE:HG13	2.00	0.62
1:B:66:ASP:O	1:B:70:GLU:HG3	1.99	0.62
1:B:23:ILE:O	1:B:24:ASN:HB2	2.00	0.62
1:B:205:VAL:CG1	1:B:209:LYS:HE3	2.29	0.62
1:B:314:LEU:HB3	1:B:321:VAL:CG1	2.30	0.62
1:B:370:VAL:HG23	4:B:780:HOH:O	2.00	0.61
1:A:503:ARG:O	1:A:507:VAL:HG23	2.00	0.61
1:A:461:GLN:HG2	1:A:541:ALA:HB3	1.81	0.61
1:B:478:SER:O	1:B:482:ILE:HG13	2.00	0.61
1:B:434:LEU:HD11	1:B:511:LEU:CD2	2.31	0.60
1:B:22:PRO:CD	1:B:400:ALA:HB1	2.31	0.60
1:B:508:ARG:HD2	1:B:526:PHE:O	2.02	0.60
1:B:506:SER:OG	1:B:510:LYS:HE3	2.01	0.60
1:B:512:LEU:C	1:B:514:GLN:H	2.09	0.60
1:A:14:CYS:O	1:A:15:ALA:HB2	2.01	0.60
1:B:158:ARG:HG3	1:B:158:ARG:NH1	2.14	0.58
1:A:144:VAL:HB	1:A:394:ARG:HG2	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:SER:OG	1:B:87:GLU:HG3	2.05	0.56
1:B:531:ARG:HH11	1:B:531:ARG:N	2.01	0.56
1:B:170:CYS:HA	1:B:173:MET:HE3	1.88	0.56
1:A:419:LEU:HD21	2:A:601:IO6:H20	1.87	0.55
1:A:531:ARG:HB2	1:A:531:ARG:NH1	2.22	0.55
1:B:38:TYR:CZ	1:B:145:PHE:HB2	2.41	0.55
1:B:119:ILE:HD13	1:B:169:VAL:HG11	1.88	0.55
1:B:336:LEU:HD23	1:B:356:PRO:HD3	1.89	0.55
1:B:376:ALA:C	1:B:378:GLY:N	2.64	0.55
1:A:85:ILE:HG12	1:A:173:MET:SD	2.47	0.55
1:B:31:LEU:HD12	1:B:31:LEU:O	2.07	0.55
1:B:300:THR:HA	1:B:313:MET:HE2	1.89	0.54
1:A:300:THR:HA	1:A:313:MET:CE	2.37	0.54
1:B:539:ILE:HG23	1:B:540:PRO:HD2	1.89	0.54
1:A:381:VAL:HG11	1:A:474:LEU:HD21	1.89	0.54
1:B:458:ASP:OD1	1:B:461:GLN:OE1	2.27	0.53
1:B:115:ALA:O	1:B:119:ILE:HG13	2.09	0.52
1:B:187:MET:HE3	1:B:296:TYR:CB	2.39	0.52
1:B:187:MET:HE1	1:B:292:THR:HG22	1.91	0.52
1:B:376:ALA:O	1:B:378:GLY:N	2.43	0.52
1:A:268:ASN:ND2	1:A:272:GLN:HB2	2.25	0.52
1:B:374:HIS:HA	1:B:379:LYS:O	2.10	0.51
1:B:233:ILE:HD13	1:B:261:TYR:O	2.10	0.51
1:B:428:HIS:O	1:B:432:ILE:HG13	2.10	0.51
1:B:515:GLY:CA	1:B:519:ALA:HB2	2.39	0.51
1:B:187:MET:HE3	1:B:296:TYR:CD2	2.46	0.51
1:B:227:THR:HB	1:B:347:SER:O	2.10	0.51
1:B:489:LEU:HD22	1:B:494:VAL:HB	1.91	0.51
1:A:108:VAL:CG2	1:A:165:LEU:HD21	2.41	0.50
1:B:24:ASN:N	1:B:25:PRO:HD3	2.26	0.50
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.94	0.50
1:A:254:ARG:HG2	1:B:251:GLN:NE2	2.27	0.49
1:A:465:ARG:HG2	1:A:542:ALA:O	2.12	0.49
1:B:361:GLU:HG3	1:B:370:VAL:O	2.13	0.49
1:B:359:ASP:HB3	1:B:362:LEU:CD1	2.43	0.49
1:A:461:GLN:HG2	1:A:541:ALA:CB	2.43	0.49
1:B:328:GLY:HA3	1:B:331:GLU:OE1	2.13	0.49
1:A:14:CYS:O	1:A:14:CYS:SG	2.70	0.49
1:B:390:THR:HB	1:B:391:PRO:HD3	1.95	0.48
1:A:175:LEU:HD21	1:A:253:ILE:HG12	1.95	0.48
1:B:434:LEU:HD11	1:B:511:LEU:HD21	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:LEU:C	1:B:514:GLN:N	2.70	0.48
1:B:359:ASP:HB3	1:B:362:LEU:HD12	1.94	0.48
1:A:434:LEU:HD11	1:A:511:LEU:HG	1.95	0.48
1:A:555:TYR:CD1	1:A:560:ILE:HG13	2.49	0.48
1:B:30:LEU:HD22	1:B:428:HIS:CD2	2.48	0.48
1:B:508:ARG:HG3	1:B:522:GLY:O	2.13	0.48
1:A:57:LEU:C	1:A:57:LEU:HD23	2.39	0.48
1:B:183:PRO:HG3	1:B:289:CYS:SG	2.53	0.48
1:B:273:ASN:ND2	1:B:275:GLY:H	2.11	0.48
1:B:196:SER:O	1:B:197:PRO:C	2.57	0.48
1:A:93:PRO:HG3	1:A:561:TYR:HB2	1.96	0.47
1:A:14:CYS:O	1:A:15:ALA:CB	2.60	0.47
1:B:7:THR:HG23	1:B:275:GLY:HA2	1.94	0.47
1:B:388:PRO:HB3	1:B:420:TRP:CD2	2.49	0.47
1:B:40:THR:HB	1:B:157:ALA:HB2	1.97	0.47
1:B:299:ALA:C	1:B:313:MET:HE1	2.40	0.47
1:A:268:ASN:HD21	1:A:272:GLN:HB2	1.80	0.47
1:A:237:GLU:HG3	1:A:257:THR:OG1	2.14	0.47
1:A:300:THR:HA	1:A:313:MET:HE3	1.97	0.47
1:A:390:THR:HB	1:A:391:PRO:HD3	1.96	0.47
1:B:211:LYS:NZ	1:B:310:ASP:O	2.44	0.47
1:B:416:ALA:HB3	1:B:417:PRO:HD3	1.97	0.47
1:B:527:ASN:O	1:B:530:VAL:HG22	2.14	0.47
1:B:201:VAL:HG13	1:B:370:VAL:CG1	2.45	0.46
1:B:403:THR:HA	1:B:404:PRO:HD3	1.78	0.46
1:A:21:LEU:HD12	1:A:22:PRO:HD2	1.98	0.46
1:A:512:LEU:HD21	1:A:523:ARG:HG2	1.98	0.46
1:B:172:LYS:HE3	1:B:560:ILE:HD13	1.97	0.46
1:B:481:GLU:O	1:B:485:VAL:HG23	2.16	0.46
1:B:201:VAL:O	1:B:205:VAL:HG23	2.14	0.46
1:B:205:VAL:HG13	1:B:209:LYS:HE3	1.98	0.46
1:A:233:ILE:HD13	1:A:261:TYR:O	2.16	0.46
1:A:416:ALA:HB3	1:A:417:PRO:HD3	1.98	0.46
1:B:336:LEU:CD2	1:B:356:PRO:HD3	2.46	0.46
1:B:314:LEU:HB3	1:B:321:VAL:HG13	1.97	0.46
1:B:346:TYR:O	1:B:347:SER:HB3	2.16	0.46
1:B:112:SER:O	1:B:116:VAL:HG23	2.15	0.45
1:B:205:VAL:O	1:B:206:ASN:C	2.58	0.45
1:B:556:SER:HB2	4:B:746:HOH:O	2.16	0.45
1:B:48:ARG:HG2	1:B:159:LEU:HG	1.99	0.45
1:B:268:ASN:HD21	1:B:272:GLN:HB2	1.82	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:HIS:O	1:B:67:VAL:HG23	2.17	0.45
1:B:197:PRO:O	1:B:201:VAL:HG23	2.16	0.45
1:B:547:LEU:O	1:B:550:TRP:HB2	2.16	0.45
1:A:306:ALA:O	1:A:307:LYS:HB2	2.17	0.45
1:A:227:THR:HB	1:A:347:SER:O	2.17	0.44
1:A:314:LEU:HB3	1:A:321:VAL:CG1	2.47	0.44
1:B:211:LYS:HB2	1:B:214:PRO:HB3	1.99	0.44
1:B:359:ASP:HB3	1:B:362:LEU:HG	1.99	0.44
1:B:83:LEU:HB2	1:B:173:MET:HA	2.00	0.44
1:A:93:PRO:HA	1:A:94:PRO:HD3	1.87	0.44
1:A:434:LEU:CD1	1:A:507:VAL:HG13	2.47	0.44
1:B:327:ALA:O	1:B:331:GLU:HB2	2.17	0.44
1:A:517:ARG:O	1:A:520:THR:HB	2.18	0.44
1:B:22:PRO:O	1:B:25:PRO:HG3	2.18	0.44
1:A:247:PRO:HG3	1:B:234:ARG:HD3	1.99	0.44
1:A:309:GLN:O	1:A:324:CYS:HB2	2.17	0.44
1:A:80:ALA:HB3	1:A:245:LEU:HD23	2.00	0.44
1:A:466:LEU:HD22	1:A:551:PHE:HE2	1.83	0.44
1:B:160:ILE:HA	1:B:282:SER:OG	2.17	0.43
1:B:431:SER:HB2	1:B:507:VAL:HG21	1.99	0.43
1:B:485:VAL:O	1:B:489:LEU:HG	2.18	0.43
1:B:155:LYS:HB3	1:B:155:LYS:HE2	1.82	0.43
1:B:309:GLN:O	1:B:324:CYS:HB2	2.17	0.43
1:A:385:THR:HG21	1:A:481:GLU:OE1	2.19	0.43
1:B:464:GLU:O	1:B:468:GLY:N	2.52	0.43
1:A:113:SER:O	1:A:117:ASN:ND2	2.52	0.43
1:B:422:ARG:HA	1:B:426:MET:HE3	2.01	0.43
1:B:18:GLU:OE2	1:B:18:GLU:HA	2.18	0.43
1:B:268:ASN:ND2	1:B:272:GLN:HB2	2.33	0.43
1:A:409:LEU:O	1:A:413:ILE:HG13	2.18	0.43
1:B:434:LEU:HD11	1:B:511:LEU:HG	2.00	0.43
1:A:72:LYS:HB3	1:B:76:SER:HB2	2.00	0.42
1:A:422:ARG:HA	1:A:426:MET:SD	2.59	0.42
1:A:160:ILE:HA	1:A:282:SER:OG	2.19	0.42
1:A:394:ARG:O	1:A:398:GLU:HG3	2.20	0.42
1:A:445:CYS:SG	1:A:454:ILE:HD12	2.59	0.42
1:B:137:THR:HA	1:B:267:THR:O	2.19	0.42
1:B:108:VAL:HG21	1:B:165:LEU:HD21	2.01	0.42
1:B:187:MET:HE3	1:B:296:TYR:CG	2.54	0.42
1:A:544:GLN:O	1:A:544:GLN:HG2	2.19	0.42
1:B:65:ARG:O	1:B:69:LYS:HG3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:416:ALA:CB	1:B:463:ILE:HG23	2.50	0.42
1:A:388:PRO:C	1:A:391:PRO:HD2	2.45	0.42
1:B:512:LEU:O	1:B:514:GLN:N	2.53	0.42
1:A:545:LEU:HD22	1:A:547:LEU:CD1	2.50	0.42
1:B:531:ARG:H	1:B:531:ARG:NH1	2.04	0.41
1:A:18:GLU:HG3	1:A:401:ARG:NH1	2.35	0.41
1:B:459:LEU:N	1:B:460:PRO:CD	2.83	0.41
1:A:452:TYR:OH	1:A:562:HIS:HD2	2.03	0.41
1:B:515:GLY:HA2	1:B:519:ALA:CB	2.46	0.41
1:A:40:THR:HB	1:A:157:ALA:CB	2.47	0.41
1:B:120:ARG:HG3	1:B:120:ARG:NH1	2.35	0.41
1:A:508:ARG:CZ	1:A:530:VAL:HG11	2.51	0.41
1:B:138:ILE:O	1:B:139:MET:HG2	2.20	0.41
1:B:175:LEU:HD21	1:B:253:ILE:HG12	2.02	0.41
1:A:435:ALA:C	1:A:437:GLU:H	2.29	0.41
1:B:434:LEU:CD1	1:B:507:VAL:HG13	2.51	0.41
1:B:464:GLU:HG3	1:B:469:LEU:HD23	2.02	0.41
1:A:182:LEU:N	1:A:183:PRO:CD	2.83	0.41
1:A:21:LEU:HA	1:A:22:PRO:HD3	1.92	0.40
1:A:508:ARG:NH1	1:A:530:VAL:HG11	2.36	0.40
1:B:191:TYR:O	1:B:194:GLN:HG2	2.22	0.40
1:B:548:SER:C	1:B:550:TRP:H	2.30	0.40
1:A:432:ILE:O	1:A:436:GLN:HG3	2.21	0.40
1:B:431:SER:HB2	1:B:507:VAL:CG2	2.51	0.40
1:A:421:ALA:O	1:A:426:MET:HG3	2.20	0.40
1:A:420:TRP:CD1	1:A:420:TRP:H	2.39	0.40
1:B:518:ALA:O	1:B:521:CYS:HB2	2.20	0.40
1:A:374:HIS:O	1:A:474:LEU:HA	2.22	0.40
1:A:423:MET:HE3	1:A:500:TRP:CD1	2.56	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	555/576 (96%)	534 (96%)	19 (3%)	2 (0%)	30	34
1	B	554/576 (96%)	518 (94%)	31 (6%)	5 (1%)	14	14
All	All	1109/1152 (96%)	1052 (95%)	50 (4%)	7 (1%)	21	23

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	ALA
1	B	377	SER
1	B	515	GLY
1	A	82	LEU
1	B	513	SER
1	B	540	PRO
1	B	541	ALA

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%)	466 (98%)	11 (2%)	44	59
1	B	475/491 (97%)	465 (98%)	10 (2%)	47	63
All	All	952/982 (97%)	931 (98%)	21 (2%)	45	61

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	86	GLU
1	A	184	GLN
1	A	336	LEU
1	A	337	ARG
1	A	381	VAL
1	A	402	HIS
1	A	431	SER
1	A	434	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	461	GLN
1	A	548	SER
1	B	83	LEU
1	B	139	MET
1	B	220	ASP
1	B	310	ASP
1	B	313	MET
1	B	315	VAL
1	B	434	LEU
1	B	473	THR
1	B	514	GLN
1	B	531	ARG

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	117	ASN
1	A	184	GLN
1	A	251	GLN
1	A	273	ASN
1	A	330	GLN
1	A	374	HIS
1	A	406	ASN
1	A	436	GLN
1	A	438	GLN
1	A	483	ASN
1	A	544	GLN
1	A	562	HIS
1	B	117	ASN
1	B	251	GLN
1	B	273	ASN
1	B	309	GLN
1	B	406	ASN
1	B	428	HIS
1	B	436	GLN
1	B	438	GLN

5.3.3 RNA ⓘ

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](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

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	1O6	A	601	-	31,31,31	2.17	12 (38%)	41,43,43	1.06	1 (2%)

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	1O6	A	601	-	-	2/24/34/34	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	1O6	C7-N10	6.64	1.44	1.36
2	A	601	1O6	C9-N10	3.23	1.53	1.48
2	A	601	1O6	C12-C11	2.94	1.45	1.41
2	A	601	1O6	C6-C7	2.89	1.56	1.51
2	A	601	1O6	C26-C21	2.76	1.43	1.38
2	A	601	1O6	C25-C26	2.50	1.43	1.38
2	A	601	1O6	C16-C11	2.47	1.43	1.39
2	A	601	1O6	C15-C14	2.40	1.43	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	1O6	C16-C15	2.33	1.42	1.38
2	A	601	1O6	C22-C21	2.27	1.43	1.38
2	A	601	1O6	C11-N10	2.20	1.46	1.43
2	A	601	1O6	C25-C24	2.17	1.43	1.38

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	1O6	C29-C9-N10	4.31	117.19	111.11

There are no chirality outliers.

All (2) torsion outliers are listed below:

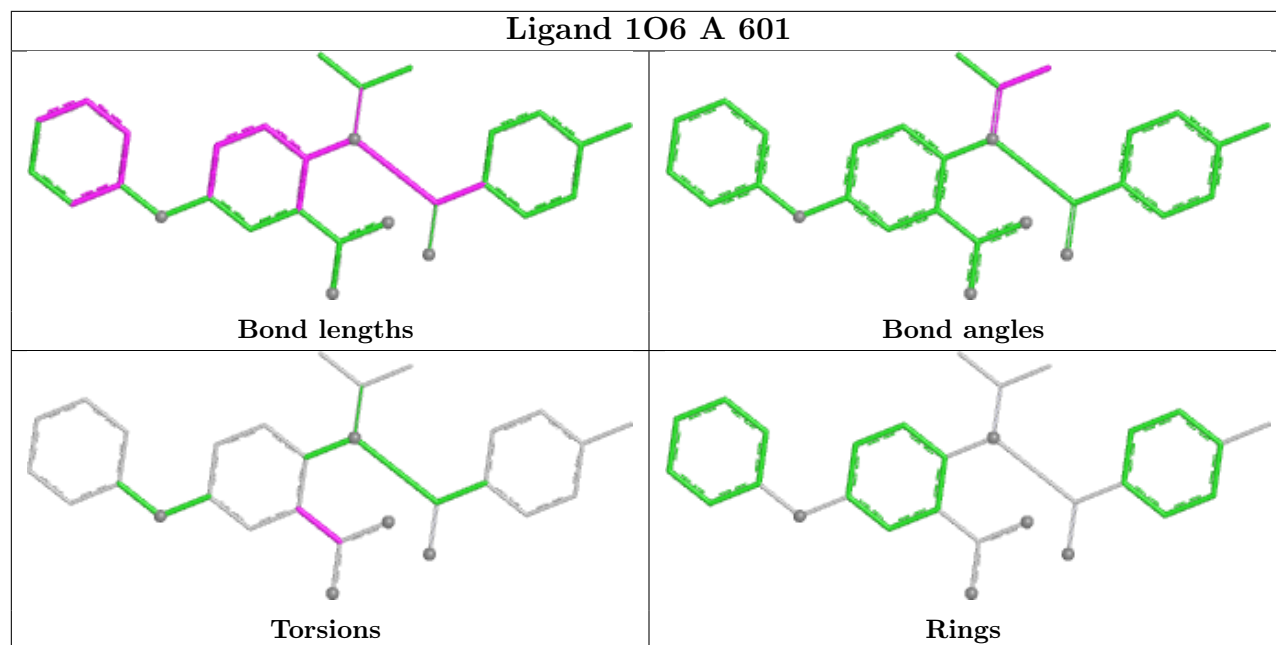
Mol	Chain	Res	Type	Atoms
2	A	601	1O6	C11-C12-C17-O18
2	A	601	1O6	C11-C12-C17-O19

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	1O6	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.



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	559/576 (97%)	0.43	22 (3%) 43 40	19, 34, 51, 63	0
1	B	558/576 (96%)	0.78	46 (8%) 17 15	22, 42, 60, 67	0
All	All	1117/1152 (96%)	0.61	68 (6%) 27 24	19, 37, 57, 67	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	529	ALA	3.8
1	A	149	PRO	3.7
1	B	530	VAL	3.7
1	B	26	LEU	3.6
1	A	14	CYS	3.5
1	B	542	ALA	3.5
1	B	153	GLY	3.4
1	B	27	SER	3.4
1	B	14	CYS	3.4
1	A	563	SER	3.3
1	B	539	ILE	3.3
1	B	563	SER	3.3
1	B	468	GLY	3.1
1	A	446	GLN	3.1
1	B	24	ASN	3.0
1	B	522	GLY	2.9
1	B	532	THR	2.9
1	B	39	ALA	2.8
1	B	147	VAL	2.8
1	B	362	LEU	2.8
1	B	541	ALA	2.8
1	B	446	GLN	2.8
1	B	545	LEU	2.8
1	B	440	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	540	PRO	2.7
1	A	434	LEU	2.7
1	B	311	CYS	2.6
1	B	534	LEU	2.6
1	A	376	ALA	2.6
1	B	15	ALA	2.6
1	A	309	GLN	2.5
1	B	405	ILE	2.5
1	B	158	ARG	2.4
1	B	507	VAL	2.4
1	B	366	CYS	2.4
1	A	547	LEU	2.4
1	B	319	ASP	2.4
1	A	435	ALA	2.4
1	B	531	ARG	2.4
1	B	25	PRO	2.3
1	B	502	HIS	2.3
1	A	402	HIS	2.3
1	B	303	CYS	2.3
1	B	431	SER	2.3
1	B	518	ALA	2.2
1	A	543	SER	2.2
1	A	352	ASP	2.2
1	A	541	ALA	2.2
1	B	364	THR	2.2
1	B	322	VAL	2.2
1	A	22	PRO	2.2
1	B	373	ALA	2.2
1	B	547	LEU	2.1
1	A	24	ASN	2.1
1	A	381	VAL	2.1
1	B	365	SER	2.1
1	A	524	TYR	2.1
1	B	382	TYR	2.1
1	A	519	ALA	2.1
1	B	548	SER	2.1
1	A	23	ILE	2.1
1	B	528	TRP	2.1
1	B	469	LEU	2.0
1	A	401	ARG	2.0
1	B	381	VAL	2.0
1	A	82	LEU	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	546	ASP	2.0
1	B	546	ASP	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](#)

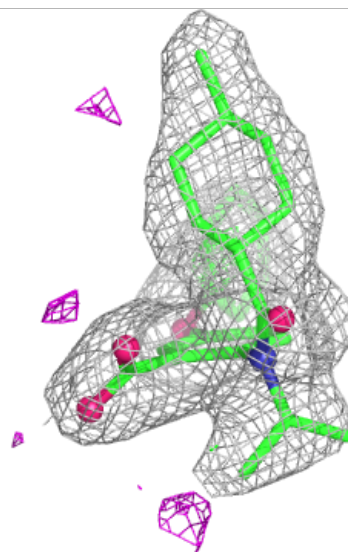
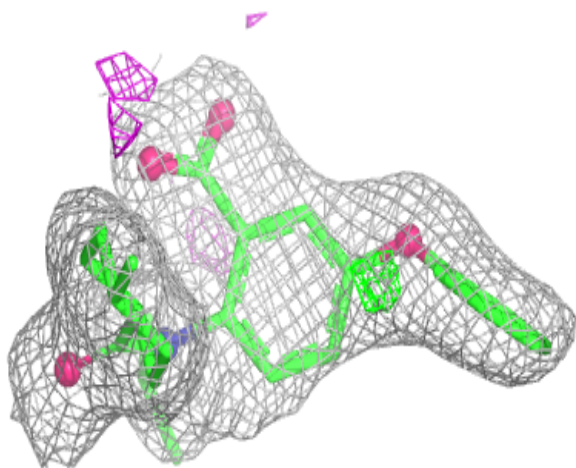
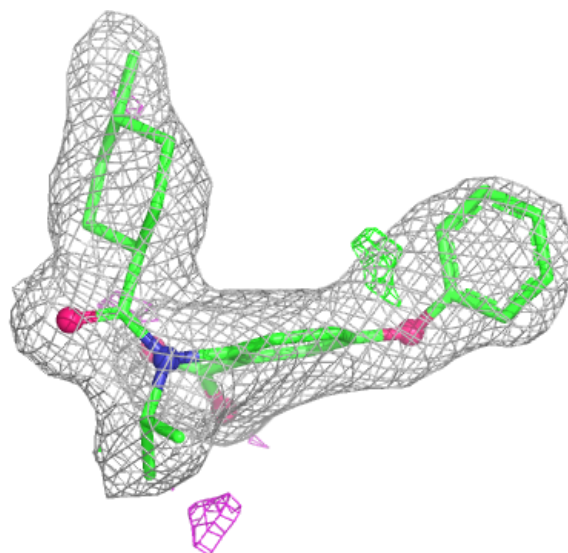
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	MG	B	601	1/1	0.57	0.28	75,75,75,75	0
3	MG	A	602	1/1	0.67	0.15	57,57,57,57	0
2	1O6	A	601	29/29	0.91	0.14	35,40,46,47	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 1O6 A 601:

$2mF_o-DF_c$ (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.