



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:15 PM UTC

PDB ID : 4JY1 / pdb_00004jy1
Title : CRYSTAL STRUCTURE OF HCV NS5B POLYMERASE IN COMPLEX
WITH COMPOUND 5
Authors : Coulombe, R.
Deposited on : 2013-03-28
Resolution : 2.60 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

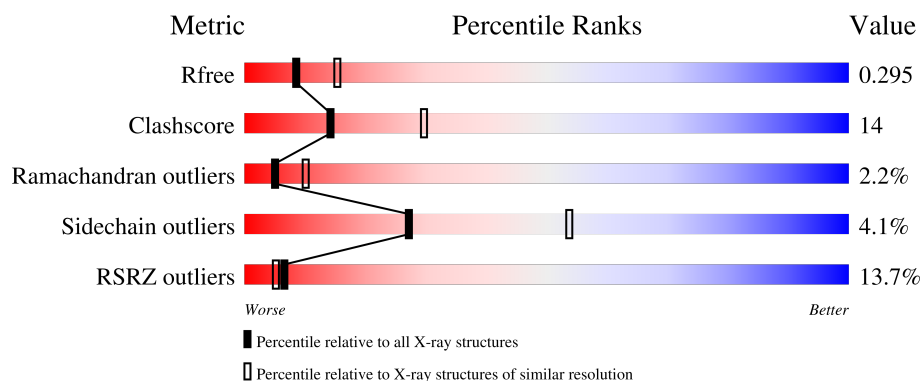
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	73% 22% • •
1	B	576	25% 59% 32% 6% •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8731 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.

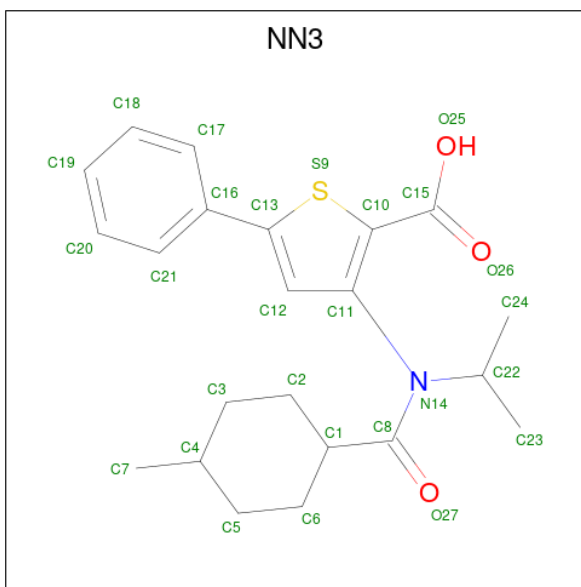
- Molecule 1 is a protein called Genome polyprotein.

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 3-{ISOPROPYL[(TRANS-4-METHYLCYCLOHEXYL)CARBONYL]AMINO}-5-PHENYLTHIOPHENE-2-CARBOXYLIC ACID (CCD ID: NN3) (formula: C₂₂H₂₇NO₃S).

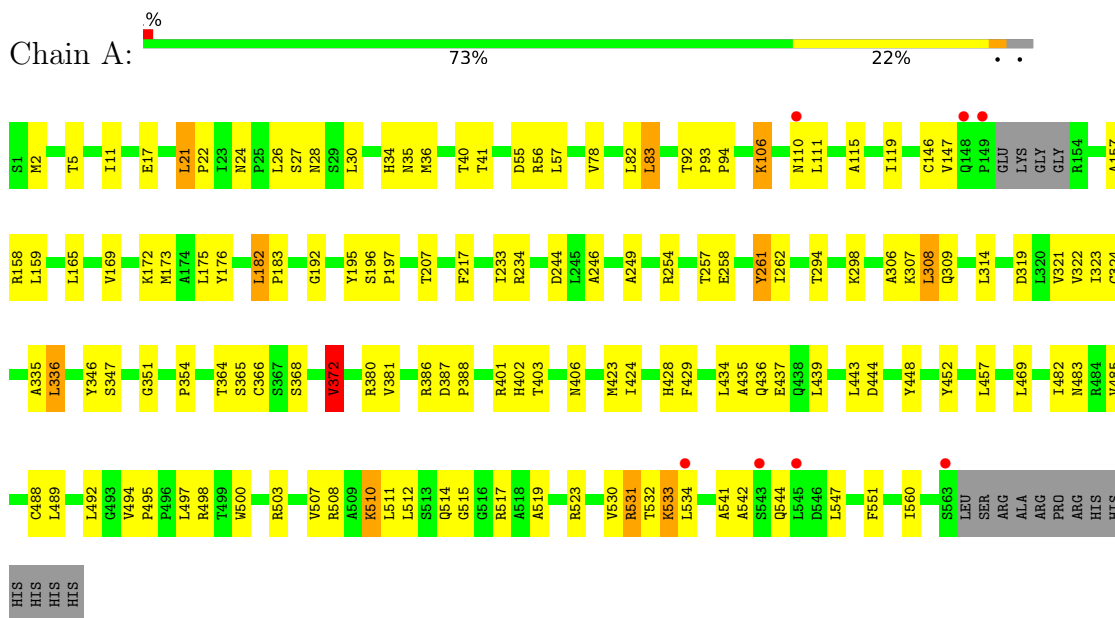


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			27	22	1	3	1		

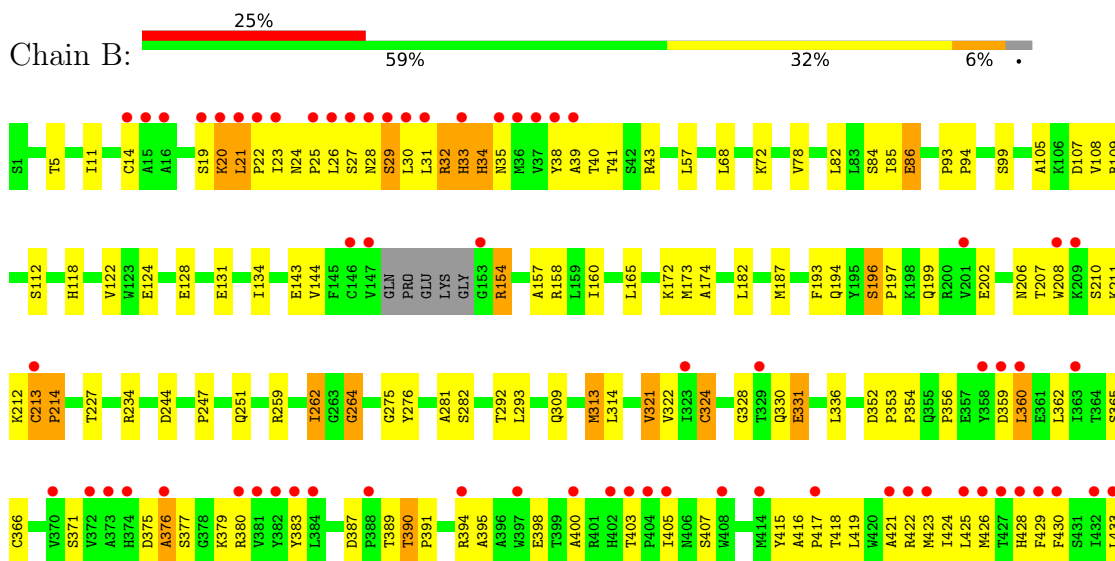
3 Residue-property plots

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: Genome polyprotein



• Molecule 1: Genome polyprotein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.26Å 108.03Å 135.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.60 40.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (40.00-2.60) 99.6 (40.00-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.92 (at 2.61Å)	Xtriage
Refinement program	CNX 2002	Depositor
R, R_{free}	0.252 , 0.299 0.249 , 0.295	Depositor DCC
R_{free} test set	4875 reflections (10.08%)	wwPDB-VP
Wilson B-factor (Å ²)	48.0	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for k,h,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8731	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% 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: NN3

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	0.48	0/4453	0.99	19/6044 (0.3%)
1	B	0.44	0/4440	1.03	30/6025 (0.5%)
All	All	0.46	0/8893	1.01	49/12069 (0.4%)

There are no bond length outliers.

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	213	CYS	CA-C-N	9.71	131.98	119.84
1	B	213	CYS	C-N-CA	9.71	131.98	119.84
1	B	29	SER	N-CA-C	-9.19	96.91	110.52
1	B	376	ALA	N-CA-C	-8.77	101.84	112.54
1	B	439	LEU	N-CA-C	-8.28	103.19	113.38
1	B	494	VAL	CA-C-N	7.82	128.43	120.38
1	B	494	VAL	C-N-CA	7.82	128.43	120.38
1	A	192	GLY	N-CA-C	7.81	121.56	112.50
1	A	403	THR	CA-C-N	7.65	126.92	118.97
1	A	403	THR	C-N-CA	7.65	126.92	118.97
1	A	429	PHE	N-CA-C	7.55	119.15	111.07
1	A	196	SER	N-CA-C	-7.13	99.70	110.39
1	A	514	GLN	N-CA-C	7.08	119.89	111.33
1	B	28	ASN	N-CA-C	-6.93	104.90	113.15
1	B	244	ASP	N-CA-C	-6.73	99.06	109.76
1	B	428	HIS	N-CA-C	6.24	118.88	111.33
1	A	261	TYR	N-CA-C	6.15	118.78	111.33
1	A	11	ILE	N-CA-C	-6.09	98.91	108.23
1	B	131	GLU	N-CA-C	6.08	120.51	112.72
1	B	463	ILE	N-CA-C	6.02	116.76	110.62
1	B	387	ASP	CA-C-N	5.99	126.77	120.12
1	B	387	ASP	C-N-CA	5.99	126.77	120.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	503	ARG	N-CA-C	-5.94	105.12	112.90
1	B	78	VAL	N-CA-C	5.93	117.27	109.21
1	B	512	LEU	N-CA-C	-5.80	106.05	113.01
1	B	196	SER	N-CA-C	-5.79	103.37	110.31
1	A	78	VAL	N-CA-C	5.74	117.01	109.21
1	B	528	TRP	N-CA-C	-5.70	106.00	113.12
1	A	175	LEU	N-CA-C	5.67	122.01	114.12
1	B	485	VAL	N-CA-C	5.61	115.81	110.42
1	B	466	LEU	N-CA-C	5.59	117.18	111.14
1	B	541	ALA	N-CA-C	-5.48	104.58	111.92
1	B	430	PHE	N-CA-C	-5.47	105.22	111.07
1	A	244	ASP	N-CA-C	-5.41	100.97	109.25
1	B	438	GLN	N-CA-C	5.33	122.16	110.80
1	B	324	CYS	N-CA-C	5.32	115.31	108.34
1	B	513	SER	N-CA-C	-5.28	106.81	113.20
1	A	351	GLY	N-CA-C	-5.28	100.68	113.18
1	A	246	ALA	N-CA-C	-5.27	102.55	110.24
1	B	174	ALA	N-CA-C	5.18	119.69	112.90
1	A	21	LEU	CA-C-N	5.13	125.04	119.85
1	A	21	LEU	C-N-CA	5.13	125.04	119.85
1	A	372	VAL	N-CA-C	5.11	116.88	108.97
1	A	195	TYR	N-CA-C	5.10	117.80	109.59
1	B	264	GLY	CA-C-N	5.10	125.09	119.89
1	B	264	GLY	C-N-CA	5.10	125.09	119.89
1	A	495	PRO	CA-C-N	5.01	125.28	119.92
1	A	495	PRO	C-N-CA	5.01	125.28	119.92
1	B	281	ALA	N-CA-C	-5.00	101.55	109.96

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	4369	85	0
1	B	4346	0	4357	165	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	27	0	26	2	0
All	All	8731	0	8752	248	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 14.

All (248) 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:423:MET:HE2	1:A:497:LEU:HD13	1.43	1.00
1:B:531:ARG:H	1:B:531:ARG:HD3	1.28	0.98
1:B:423:MET:HE2	1:B:424:ILE:HG12	1.56	0.86
1:B:461:GLN:HB3	1:B:545:LEU:HD11	1.60	0.84
1:B:31:LEU:HB3	1:B:494:VAL:HG22	1.61	0.83
1:A:485:VAL:O	1:A:489:LEU:HG	1.80	0.81
1:B:31:LEU:HD12	1:B:31:LEU:O	1.81	0.79
1:B:520:THR:HG21	1:B:539:ILE:HD12	1.63	0.79
1:A:40:THR:HB	1:A:157:ALA:HB2	1.65	0.78
1:A:423:MET:HE1	2:A:601:NN3:H17	1.66	0.78
1:B:30:LEU:O	1:B:494:VAL:HG22	1.84	0.77
1:A:314:LEU:HB3	1:A:321:VAL:HG12	1.64	0.76
1:B:489:LEU:HD22	1:B:494:VAL:HB	1.66	0.76
1:B:30:LEU:O	1:B:494:VAL:HG13	1.86	0.75
1:B:531:ARG:H	1:B:531:ARG:CD	2.00	0.75
1:B:419:LEU:HD13	1:B:477:TYR:CE1	2.23	0.74
1:B:309:GLN:O	1:B:324:CYS:HB2	1.89	0.73
1:B:423:MET:HE3	1:B:500:TRP:CD1	2.24	0.72
1:B:531:ARG:HD3	1:B:531:ARG:N	2.04	0.72
1:B:314:LEU:HB3	1:B:321:VAL:HG13	1.72	0.72
1:B:336:LEU:HD23	1:B:356:PRO:HD3	1.72	0.71
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.73	0.71
1:B:423:MET:HE3	1:B:500:TRP:HD1	1.56	0.69
1:B:29:SER:O	1:B:30:LEU:HB3	1.90	0.69
1:A:30:LEU:O	1:A:494:VAL:HG13	1.93	0.69
1:A:308:LEU:HD13	1:A:335:ALA:HB1	1.75	0.69
1:B:416:ALA:HB3	1:B:417:PRO:HD3	1.76	0.68
1:B:459:LEU:O	1:B:463:ILE:HG13	1.95	0.66
1:B:27:SER:C	1:B:29:SER:H	2.02	0.66
1:A:34:HIS:HD2	1:A:35:ASN:H	1.44	0.64
1:A:423:MET:HE2	1:A:497:LEU:CD1	2.25	0.64
1:B:489:LEU:CD2	1:B:494:VAL:HB	2.28	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ASN:ND2	1:A:443:LEU:HB3	2.13	0.63
1:B:434:LEU:HG	1:B:439:LEU:HD11	1.79	0.63
1:B:436:GLN:O	1:B:437:GLU:HB3	1.98	0.63
1:B:21:LEU:HG	1:B:22:PRO:HD2	1.82	0.62
1:B:22:PRO:O	1:B:24:ASN:N	2.32	0.62
1:B:208:TRP:CE3	1:B:360:LEU:HD13	2.35	0.62
1:B:93:PRO:HG3	1:B:561:TYR:HB2	1.81	0.61
1:B:376:ALA:HB2	1:B:473:THR:HB	1.80	0.61
1:A:503:ARG:O	1:A:507:VAL:HG23	2.01	0.61
1:A:233:ILE:HD13	1:A:261:TYR:O	2.00	0.61
1:A:309:GLN:O	1:A:324:CYS:HB2	2.01	0.60
1:B:85:ILE:HD13	1:B:173:MET:SD	2.40	0.60
1:A:30:LEU:HB2	1:A:428:HIS:CE1	2.35	0.60
1:B:479:PRO:O	1:B:482:ILE:HG22	2.01	0.60
1:A:119:ILE:HD13	1:A:169:VAL:HG11	1.82	0.60
1:B:124:GLU:O	1:B:128:GLU:HG2	2.01	0.59
1:B:30:LEU:HA	1:B:500:TRP:HZ2	1.66	0.59
1:B:40:THR:HB	1:B:157:ALA:HB2	1.83	0.59
1:B:505:ARG:HD3	1:B:531:ARG:HH12	1.66	0.59
1:B:196:SER:H	1:B:199:GLN:HB2	1.67	0.59
1:B:520:THR:HG21	1:B:539:ILE:CD1	2.32	0.59
1:B:375:ASP:CB	1:B:379:LYS:H	2.16	0.58
1:A:24:ASN:HB3	1:A:27:SER:OG	2.03	0.58
1:B:331:GLU:CD	1:B:331:GLU:H	2.12	0.58
1:B:359:ASP:HB3	1:B:362:LEU:CD1	2.34	0.58
1:B:470:SER:HB2	1:B:474:LEU:HD21	1.85	0.58
1:B:86:GLU:H	1:B:86:GLU:CD	2.08	0.58
1:B:434:LEU:CD1	1:B:507:VAL:HG13	2.34	0.58
1:A:257:THR:O	1:A:262:ILE:HG23	2.04	0.58
1:B:234:ARG:HG3	1:B:262:ILE:HD11	1.85	0.58
1:B:211:LYS:HB2	1:B:214:PRO:HB3	1.85	0.57
1:B:84:SER:OG	1:B:86:GLU:HG2	2.05	0.56
1:B:439:LEU:HB3	1:B:457:LEU:HD21	1.88	0.56
1:B:488:CYS:HA	1:B:491:LYS:HD3	1.87	0.56
1:A:83:LEU:HD22	1:A:176:TYR:HB3	1.87	0.56
1:A:533:LYS:H	1:A:533:LYS:HD2	1.71	0.56
1:A:22:PRO:HG3	1:A:401:ARG:NH2	2.20	0.56
1:B:469:LEU:HD11	1:B:538:PRO:HG3	1.88	0.56
1:A:57:LEU:HD23	1:A:57:LEU:C	2.30	0.56
1:B:383:TYR:CE2	1:B:418:THR:HA	2.41	0.56
1:B:505:ARG:HD3	1:B:531:ARG:NH1	2.22	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:HIS:CD2	1:A:35:ASN:N	2.75	0.55
1:B:313:MET:SD	1:B:322:VAL:HG22	2.47	0.54
1:B:20:LYS:O	1:B:21:LEU:HB2	2.07	0.54
1:B:359:ASP:HB3	1:B:362:LEU:HD12	1.89	0.54
1:B:380:ARG:HH11	1:B:380:ARG:HB3	1.71	0.54
1:A:34:HIS:HD2	1:A:35:ASN:N	2.06	0.54
1:A:541:ALA:O	1:A:544:GLN:HB3	2.08	0.54
1:B:434:LEU:HD12	1:B:507:VAL:HG13	1.89	0.54
1:A:336:LEU:HD11	1:A:354:PRO:HG2	1.89	0.53
1:B:33:HIS:C	1:B:35:ASN:H	2.16	0.53
1:A:531:ARG:H	1:A:531:ARG:HE	1.55	0.53
1:B:197:PRO:HB2	1:B:467:HIS:HE1	1.73	0.53
1:B:390:THR:HB	1:B:391:PRO:HD3	1.90	0.53
1:A:336:LEU:HD11	1:A:354:PRO:HB2	1.91	0.53
1:A:457:LEU:HD12	1:A:517:ARG:HH21	1.74	0.52
1:A:182:LEU:HB3	1:A:183:PRO:HD3	1.89	0.52
1:B:526:PHE:HA	1:B:528:TRP:CD1	2.45	0.52
1:B:520:THR:CG2	1:B:539:ILE:HD12	2.39	0.52
1:B:107:ASP:HB3	1:B:112:SER:OG	2.09	0.52
1:B:160:ILE:O	1:B:160:ILE:HG13	2.08	0.52
1:A:388:PRO:HG2	1:A:488:CYS:SG	2.50	0.52
1:A:515:GLY:O	1:A:519:ALA:HB2	2.10	0.51
1:A:531:ARG:O	1:A:533:LYS:HD2	2.11	0.51
1:B:172:LYS:HE3	1:B:560:ILE:HD13	1.91	0.51
1:A:531:ARG:H	1:A:531:ARG:NE	2.08	0.51
1:A:533:LYS:H	1:A:533:LYS:CD	2.23	0.51
1:B:383:TYR:HE2	1:B:418:THR:HA	1.75	0.51
1:B:197:PRO:HB2	1:B:467:HIS:CE1	2.45	0.51
1:A:542:ALA:C	1:A:544:GLN:H	2.16	0.51
1:B:500:TRP:C	1:B:502:HIS:H	2.18	0.51
1:B:33:HIS:HB2	1:B:492:LEU:O	2.11	0.51
1:B:487:SER:O	1:B:491:LYS:HG3	2.11	0.51
1:B:105:ALA:O	1:B:109:ARG:HG3	2.11	0.51
1:B:371:SER:HB3	1:B:383:TYR:CE1	2.46	0.51
1:B:433:LEU:HB3	1:B:438:GLN:O	2.11	0.51
1:B:504:ALA:C	1:B:506:SER:N	2.68	0.51
1:A:2:MET:SD	1:A:55:ASP:HB2	2.51	0.50
1:A:423:MET:HE1	2:A:601:NN3:C17	2.39	0.50
1:B:375:ASP:HB2	1:B:379:LYS:HB2	1.93	0.50
1:B:526:PHE:HA	1:B:528:TRP:NE1	2.26	0.50
1:B:506:SER:OG	1:B:510:LYS:HE3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ARG:HD3	1:A:56:ARG:N	2.26	0.50
1:B:455:GLU:HB2	1:B:458:ASP:OD2	2.12	0.50
1:A:24:ASN:OD1	1:A:26:LEU:N	2.45	0.49
1:B:11:ILE:O	1:B:11:ILE:HG22	2.12	0.49
1:B:395:ALA:HB1	1:B:429:PHE:HZ	1.76	0.49
1:A:106:LYS:HE2	1:A:106:LYS:HA	1.95	0.49
1:B:496:PRO:O	1:B:498:ARG:N	2.43	0.49
1:A:234:ARG:HD3	1:B:247:PRO:HG3	1.93	0.49
1:B:202:GLU:O	1:B:206:ASN:ND2	2.46	0.49
1:A:444:ASP:HA	1:A:452:TYR:O	2.12	0.49
1:B:144:VAL:HB	1:B:394:ARG:HG2	1.95	0.49
1:B:511:LEU:HD13	1:B:521:CYS:HB2	1.93	0.49
1:B:27:SER:C	1:B:29:SER:N	2.66	0.49
1:B:118:HIS:O	1:B:122:VAL:HG23	2.13	0.48
1:B:202:GLU:HG2	1:B:206:ASN:HD21	1.77	0.48
1:A:254:ARG:HG2	1:B:251:GLN:NE2	2.29	0.48
1:A:510:LYS:NZ	1:A:510:LYS:HB2	2.27	0.48
1:B:26:LEU:O	1:B:27:SER:HB3	2.12	0.48
1:B:444:ASP:HA	1:B:452:TYR:O	2.13	0.48
1:B:445:CYS:O	1:B:452:TYR:HB2	2.12	0.48
1:B:464:GLU:OE1	1:B:539:ILE:HG22	2.12	0.48
1:A:531:ARG:HG2	1:A:532:THR:N	2.28	0.48
1:B:134:ILE:HG13	1:B:259:ARG:HB3	1.96	0.48
1:B:328:GLY:HA3	1:B:331:GLU:OE2	2.14	0.48
1:B:506:SER:O	1:B:510:LYS:HG3	2.13	0.48
1:A:336:LEU:CD1	1:A:354:PRO:HG2	2.43	0.48
1:B:196:SER:O	1:B:197:PRO:C	2.57	0.48
1:A:482:ILE:HG13	1:A:483:ASN:N	2.28	0.48
1:A:294:THR:CG2	1:A:298:LYS:HE3	2.44	0.47
1:A:372:VAL:HG11	1:A:380:ARG:NH2	2.28	0.47
1:A:423:MET:CE	1:A:497:LEU:HD13	2.30	0.47
1:A:364:THR:HA	1:A:368:SER:O	2.14	0.47
1:A:523:ARG:HG3	1:A:534:LEU:HD12	1.95	0.47
1:B:365:SER:O	1:B:366:CYS:HB2	2.12	0.47
1:B:68:LEU:O	1:B:72:LYS:HG3	2.14	0.47
1:A:434:LEU:C	1:A:436:GLN:H	2.23	0.47
1:B:202:GLU:CG	1:B:206:ASN:HD21	2.28	0.47
1:B:517:ARG:HG3	1:B:517:ARG:HH11	1.80	0.47
1:B:187:MET:HE1	1:B:292:THR:HG22	1.97	0.47
1:B:202:GLU:HG2	1:B:206:ASN:ND2	2.30	0.47
1:A:336:LEU:HD11	1:A:354:PRO:CG	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:SER:C	1:B:31:LEU:H	2.22	0.46
1:B:383:TYR:OH	1:B:481:GLU:HG2	2.15	0.46
1:B:160:ILE:HA	1:B:282:SER:OG	2.15	0.46
1:B:375:ASP:HB2	1:B:379:LYS:H	1.80	0.46
1:A:319:ASP:CG	1:A:366:CYS:H	2.23	0.46
1:B:94:PRO:HD3	1:B:561:TYR:CD2	2.51	0.46
1:A:314:LEU:HB3	1:A:321:VAL:CG1	2.39	0.46
1:B:31:LEU:HA	1:B:493:GLY:O	2.15	0.46
1:B:504:ALA:C	1:B:506:SER:H	2.24	0.46
1:B:539:ILE:O	1:B:542:ALA:HB2	2.16	0.46
1:B:418:THR:OG1	1:B:421:ALA:HB2	2.16	0.46
1:A:83:LEU:HD12	1:A:83:LEU:HA	1.73	0.45
1:A:115:ALA:O	1:A:119:ILE:HG13	2.16	0.45
1:B:421:ALA:HA	1:B:425:LEU:HD12	1.99	0.45
1:B:437:GLU:HG2	1:B:438:GLN:N	2.20	0.45
1:B:30:LEU:O	1:B:494:VAL:CG2	2.61	0.45
1:B:144:VAL:HB	1:B:394:ARG:CG	2.47	0.45
1:A:439:LEU:O	1:A:457:LEU:HG	2.17	0.45
1:B:32:ARG:O	1:B:34:HIS:N	2.45	0.45
1:B:422:ARG:HA	1:B:426:MET:SD	2.57	0.45
1:B:522:GLY:HA2	1:B:526:PHE:HD2	1.82	0.45
1:B:5:THR:O	1:B:275:GLY:HA3	2.17	0.44
1:B:29:SER:O	1:B:30:LEU:CB	2.62	0.44
1:B:533:LYS:O	1:B:534:LEU:HB2	2.17	0.44
1:A:34:HIS:C	1:A:36:MET:H	2.25	0.44
1:A:83:LEU:HB2	1:A:173:MET:HA	1.99	0.44
1:A:448:TYR:CE2	1:A:551:PHE:HD1	2.36	0.44
1:B:415:TYR:HB3	1:B:418:THR:HG21	1.99	0.44
1:A:17:GLU:OE1	1:A:41:THR:HB	2.18	0.44
1:B:540:PRO:O	1:B:541:ALA:HB3	2.17	0.44
1:A:217:PHE:CE1	1:A:322:VAL:HB	2.53	0.44
1:B:41:THR:C	1:B:43:ARG:H	2.26	0.44
1:B:93:PRO:HA	1:B:94:PRO:HD3	1.85	0.44
1:A:172:LYS:HE3	1:A:560:ILE:HD13	2.00	0.43
1:A:336:LEU:HD11	1:A:354:PRO:CB	2.48	0.43
1:A:110:ASN:O	1:A:111:LEU:HB2	2.17	0.43
1:B:143:GLU:OE1	1:B:158:ARG:NH1	2.51	0.43
1:B:194:GLN:O	1:B:551:PHE:O	2.37	0.43
1:B:353:PRO:HA	1:B:354:PRO:HD2	1.90	0.43
1:B:518:ALA:O	1:B:521:CYS:HB2	2.19	0.43
1:A:508:ARG:CZ	1:A:530:VAL:HG11	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ALA:HA	1:B:143:GLU:O	2.18	0.42
1:B:196:SER:OG	1:B:199:GLN:HG3	2.18	0.42
1:B:172:LYS:HE3	1:B:560:ILE:CD1	2.50	0.42
1:B:465:ARG:NH1	1:B:545:LEU:HB2	2.34	0.42
1:B:524:TYR:CE2	1:B:536:LEU:HB3	2.53	0.42
1:B:22:PRO:HG2	1:B:400:ALA:HB1	2.01	0.42
1:B:439:LEU:O	1:B:457:LEU:HG	2.19	0.42
1:B:510:LYS:O	1:B:514:GLN:HG2	2.19	0.42
1:A:386:ARG:O	1:A:387:ASP:C	2.63	0.42
1:A:531:ARG:HE	1:A:531:ARG:N	2.17	0.42
1:B:33:HIS:C	1:B:35:ASN:N	2.77	0.42
1:A:254:ARG:HH12	1:A:258:GLU:CG	2.32	0.42
1:B:398:GLU:OE2	1:B:407:SER:HB3	2.19	0.42
1:B:19:SER:CB	1:B:43:ARG:HH22	2.33	0.42
1:A:207:THR:HG22	1:A:323:ILE:HG21	2.02	0.42
1:B:517:ARG:O	1:B:518:ALA:C	2.62	0.42
1:A:434:LEU:HD22	1:A:510:LYS:HD2	2.02	0.41
1:A:508:ARG:O	1:A:511:LEU:HB2	2.19	0.41
1:B:82:LEU:HD12	1:B:173:MET:O	2.21	0.41
1:B:108:VAL:HG21	1:B:165:LEU:HD21	2.02	0.41
1:B:445:CYS:HB3	1:B:454:ILE:HD12	2.02	0.41
1:A:92:THR:HA	1:A:93:PRO:HD3	1.98	0.41
1:B:423:MET:CE	1:B:500:TRP:CD1	3.00	0.41
1:B:418:THR:OG1	1:B:421:ALA:CB	2.68	0.41
1:B:419:LEU:HB2	1:B:477:TYR:CZ	2.55	0.41
1:B:490:ARG:O	1:B:491:LYS:C	2.62	0.41
1:B:541:ALA:HA	1:B:544:GLN:OE1	2.20	0.41
1:A:346:TYR:O	1:A:347:SER:HB3	2.19	0.41
1:B:264:GLY:HA2	1:B:276:TYR:CZ	2.55	0.41
1:B:182:LEU:CD2	1:B:293:LEU:HD11	2.51	0.41
1:A:21:LEU:HA	1:A:22:PRO:HD3	1.86	0.41
1:B:30:LEU:O	1:B:494:VAL:CG1	2.62	0.41
1:B:99:SER:HB2	1:B:165:LEU:HB3	2.02	0.41
1:B:375:ASP:C	1:B:377:SER:N	2.74	0.41
1:A:106:LYS:HA	1:A:106:LYS:CE	2.51	0.41
1:B:213:CYS:HA	1:B:214:PRO:HD2	1.78	0.41
1:B:389:THR:HG23	1:B:492:LEU:HD11	2.02	0.41
1:B:459:LEU:N	1:B:460:PRO:CD	2.83	0.41
1:B:497:LEU:O	1:B:497:LEU:HG	2.21	0.41
1:B:504:ALA:O	1:B:507:VAL:N	2.53	0.41
1:B:537:THR:O	1:B:539:ILE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:512:LEU:HA	1:A:519:ALA:HA	2.03	0.41
1:B:416:ALA:N	1:B:417:PRO:CD	2.84	0.41
1:B:436:GLN:O	1:B:437:GLU:CB	2.67	0.41
1:B:499:THR:O	1:B:503:ARG:HG3	2.21	0.41
1:B:207:THR:O	1:B:210:SER:OG	2.23	0.40
1:A:146:CYS:SG	1:A:492:LEU:HD11	2.61	0.40
1:A:165:LEU:O	1:A:169:VAL:HG23	2.21	0.40
1:A:306:ALA:O	1:A:307:LYS:HB2	2.21	0.40
1:A:365:SER:O	1:A:366:CYS:HB2	2.21	0.40
1:A:424:ILE:HG23	1:A:500:TRP:CZ2	2.56	0.40
1:B:38:TYR:CE2	1:B:154:ARG:HG3	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	555/576 (96%)	526 (95%)	25 (4%)	4 (1%)	18	38
1	B	554/576 (96%)	482 (87%)	52 (9%)	20 (4%)	2	4
All	All	1109/1152 (96%)	1008 (91%)	77 (7%)	24 (2%)	5	10

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	23	ILE
1	B	441	LYS
1	B	495	PRO
1	A	469	LEU
1	B	25	PRO
1	B	193	PHE
1	B	438	GLN

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Mol	Chain	Res	Type
1	B	477	TYR
1	B	534	LEU
1	A	437	GLU
1	B	33	HIS
1	B	34	HIS
1	B	154	ARG
1	B	360	LEU
1	B	497	LEU
1	B	20	LYS
1	B	212	LYS
1	B	330	GLN
1	B	538	PRO
1	A	435	ALA
1	B	21	LEU
1	A	147	VAL
1	B	214	PRO
1	B	496	PRO

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%)	458 (96%)	19 (4%)	28	55
1	B	475/491 (97%)	455 (96%)	20 (4%)	26	52
All	All	952/982 (97%)	913 (96%)	39 (4%)	27	54

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	THR
1	A	28	ASN
1	A	83	LEU
1	A	94	PRO
1	A	106	LYS
1	A	158	ARG

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Mol	Chain	Res	Type
1	A	159	LEU
1	A	182	LEU
1	A	197	PRO
1	A	308	LEU
1	A	336	LEU
1	A	372	VAL
1	A	381	VAL
1	A	402	HIS
1	A	498	ARG
1	A	510	LYS
1	A	531	ARG
1	A	533	LYS
1	A	547	LEU
1	B	14	CYS
1	B	32	ARG
1	B	57	LEU
1	B	86	GLU
1	B	227	THR
1	B	262	ILE
1	B	313	MET
1	B	321	VAL
1	B	331	GLU
1	B	352	ASP
1	B	390	THR
1	B	403	THR
1	B	405	ILE
1	B	434	LEU
1	B	437	GLU
1	B	443	LEU
1	B	485	VAL
1	B	495	PRO
1	B	539	ILE
1	B	550	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	34	HIS
1	A	251	GLN
1	A	273	ASN
1	A	309	GLN

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Mol	Chain	Res	Type
1	A	406	ASN
1	A	428	HIS
1	A	502	HIS
1	A	514	GLN
1	A	544	GLN
1	A	562	HIS
1	B	24	ASN
1	B	206	ASN
1	B	251	GLN
1	B	374	HIS
1	B	411	ASN
1	B	467	HIS
1	B	527	ASN

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	NN3	A	601	-	28,29,29	1.57	7 (25%)	36,41,41	1.40	5 (13%)

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	NN3	A	601	-	-	4/23/34/34	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	NN3	C22-N14	2.74	1.52	1.48
2	A	601	NN3	C21-C16	2.72	1.43	1.39
2	A	601	NN3	C17-C16	2.63	1.43	1.39
2	A	601	NN3	C8-N14	2.62	1.44	1.40
2	A	601	NN3	C1-C8	2.58	1.55	1.51
2	A	601	NN3	C18-C17	2.16	1.42	1.38
2	A	601	NN3	C20-C21	2.09	1.42	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	NN3	C1-C8-N14	4.06	123.99	119.17
2	A	601	NN3	O27-C8-C1	-3.74	115.37	120.86
2	A	601	NN3	C6-C1-C8	3.30	115.52	109.96
2	A	601	NN3	C11-C12-C13	2.07	113.32	111.57
2	A	601	NN3	C13-S9-C10	2.05	93.39	91.75

There are no chirality outliers.

All (4) torsion outliers are listed below:

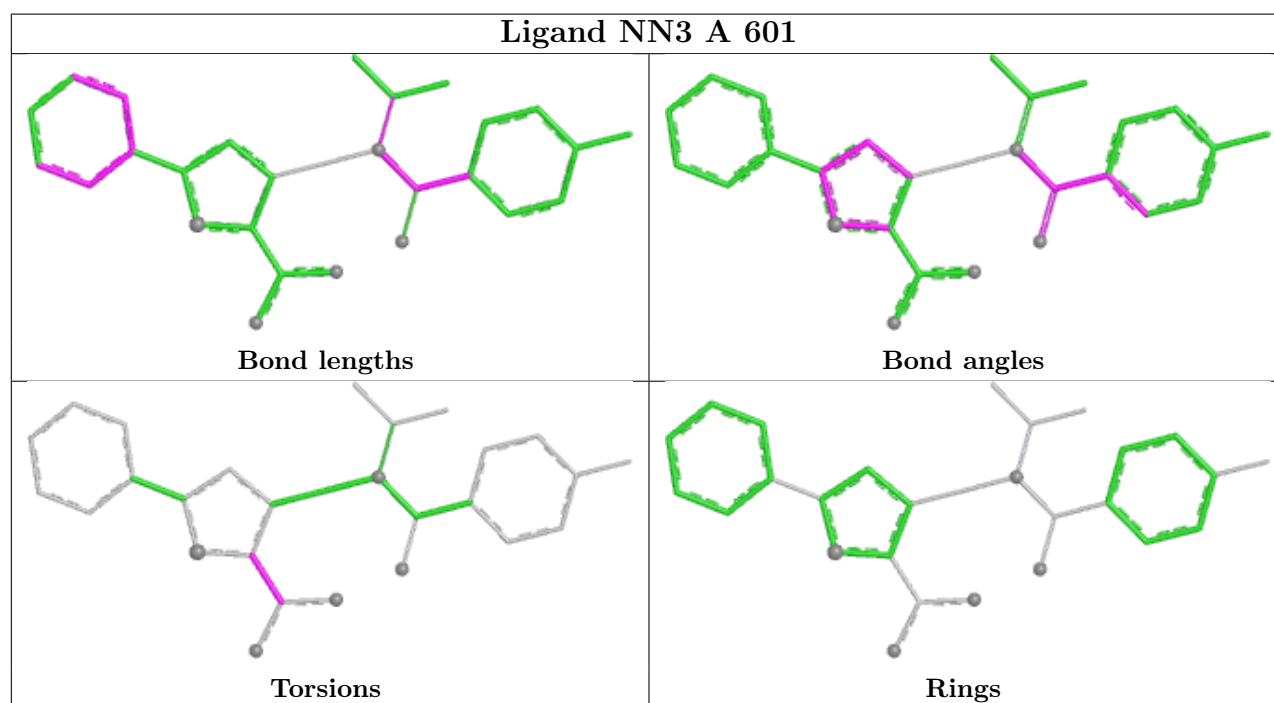
Mol	Chain	Res	Type	Atoms
2	A	601	NN3	S9-C10-C15-O26
2	A	601	NN3	S9-C10-C15-O25
2	A	601	NN3	C11-C10-C15-O26
2	A	601	NN3	C11-C10-C15-O25

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	NN3	2	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%)	0.00	7 (1%) 75 71	21, 38, 64, 89	0
1	B	558/576 (96%)	1.05	146 (26%) 1 1	24, 57, 92, 106	0
All	All	1117/1152 (96%)	0.53	153 (13%) 6 5	21, 44, 88, 106	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	528	TRP	5.6
1	B	511	LEU	5.5
1	B	541	ALA	4.9
1	A	149	PRO	4.7
1	B	425	LEU	4.5
1	B	525	LEU	4.5
1	B	529	ALA	4.5
1	B	26	LEU	4.4
1	B	469	LEU	4.2
1	B	30	LEU	4.1
1	B	500	TRP	4.1
1	B	468	GLY	4.1
1	B	472	PHE	4.1
1	B	430	PHE	4.0
1	B	370	VAL	3.9
1	B	486	ALA	3.9
1	B	497	LEU	3.9
1	B	153	GLY	3.9
1	B	37	VAL	3.8
1	B	477	TYR	3.8
1	B	540	PRO	3.8
1	B	360	LEU	3.8
1	B	492	LEU	3.8
1	B	429	PHE	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	502	HIS	3.7
1	B	16	ALA	3.7
1	B	27	SER	3.6
1	B	493	GLY	3.6
1	B	23	ILE	3.6
1	B	524	TYR	3.6
1	B	532	THR	3.5
1	B	508	ARG	3.5
1	B	523	ARG	3.5
1	B	501	ARG	3.4
1	B	373	ALA	3.4
1	B	499	THR	3.4
1	B	494	VAL	3.4
1	B	471	ALA	3.3
1	B	496	PRO	3.3
1	B	509	ALA	3.3
1	B	147	VAL	3.3
1	B	405	ILE	3.3
1	B	545	LEU	3.3
1	B	533	LYS	3.3
1	B	21	LEU	3.2
1	B	480	GLY	3.2
1	B	372	VAL	3.2
1	B	512	LEU	3.2
1	B	534	LEU	3.2
1	B	402	HIS	3.2
1	B	19	SER	3.2
1	B	489	LEU	3.2
1	B	507	VAL	3.2
1	B	441	LYS	3.2
1	B	520	THR	3.2
1	B	542	ALA	3.2
1	B	539	ILE	3.1
1	B	442	ALA	3.1
1	B	491	LYS	3.1
1	B	414	MET	3.1
1	B	403	THR	3.1
1	B	39	ALA	3.1
1	B	543	SER	3.1
1	B	518	ALA	3.0
1	A	563	SER	3.0
1	B	29	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	20	LYS	3.0
1	A	534	LEU	3.0
1	B	25	PRO	3.0
1	B	388	PRO	2.9
1	B	433	LEU	2.9
1	B	439	LEU	2.9
1	B	526	PHE	2.9
1	B	481	GLU	2.9
1	B	426	MET	2.9
1	B	28	ASN	2.9
1	B	466	LEU	2.9
1	B	535	LYS	2.9
1	B	495	PRO	2.8
1	B	498	ARG	2.8
1	B	454	ILE	2.8
1	B	482	ILE	2.8
1	B	504	ALA	2.8
1	B	22	PRO	2.7
1	B	544	GLN	2.7
1	B	423	MET	2.7
1	B	427	THR	2.7
1	B	530	VAL	2.7
1	B	536	LEU	2.7
1	B	374	HIS	2.7
1	B	384	LEU	2.7
1	B	503	ARG	2.7
1	B	31	LEU	2.6
1	B	435	ALA	2.6
1	B	474	LEU	2.6
1	B	522	GLY	2.6
1	B	422	ARG	2.6
1	B	428	HIS	2.6
1	B	505	ARG	2.5
1	B	376	ALA	2.5
1	B	549	GLY	2.5
1	B	563	SER	2.5
1	B	382	TYR	2.5
1	A	545	LEU	2.4
1	B	443	LEU	2.4
1	B	488	CYS	2.4
1	B	434	LEU	2.4
1	B	404	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	421	ALA	2.4
1	B	538	PRO	2.4
1	B	381	VAL	2.4
1	B	15	ALA	2.4
1	B	146	CYS	2.3
1	B	213	CYS	2.3
1	B	363	ILE	2.3
1	B	383	TYR	2.3
1	B	464	GLU	2.3
1	B	476	SER	2.3
1	B	514	GLN	2.3
1	B	33	HIS	2.3
1	B	201	VAL	2.3
1	B	475	HIS	2.2
1	B	209	LYS	2.2
1	B	510	LYS	2.2
1	B	517	ARG	2.2
1	B	531	ARG	2.2
1	B	36	MET	2.2
1	B	358	TYR	2.2
1	B	208	TRP	2.2
1	B	562	HIS	2.2
1	B	38	TYR	2.2
1	B	490	ARG	2.2
1	B	485	VAL	2.2
1	B	400	ALA	2.1
1	B	457	LEU	2.1
1	B	359	ASP	2.1
1	B	432	ILE	2.1
1	B	380	ARG	2.1
1	B	456	PRO	2.1
1	A	148	GLN	2.1
1	B	14	CYS	2.1
1	B	323	ILE	2.1
1	B	463	ILE	2.1
1	B	329	THR	2.0
1	B	479	PRO	2.0
1	B	516	GLY	2.0
1	A	543	SER	2.0
1	B	397	TRP	2.0
1	B	408	TRP	2.0
1	B	417	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	110	ASN	2.0
1	B	35	ASN	2.0
1	B	394	ARG	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](#)

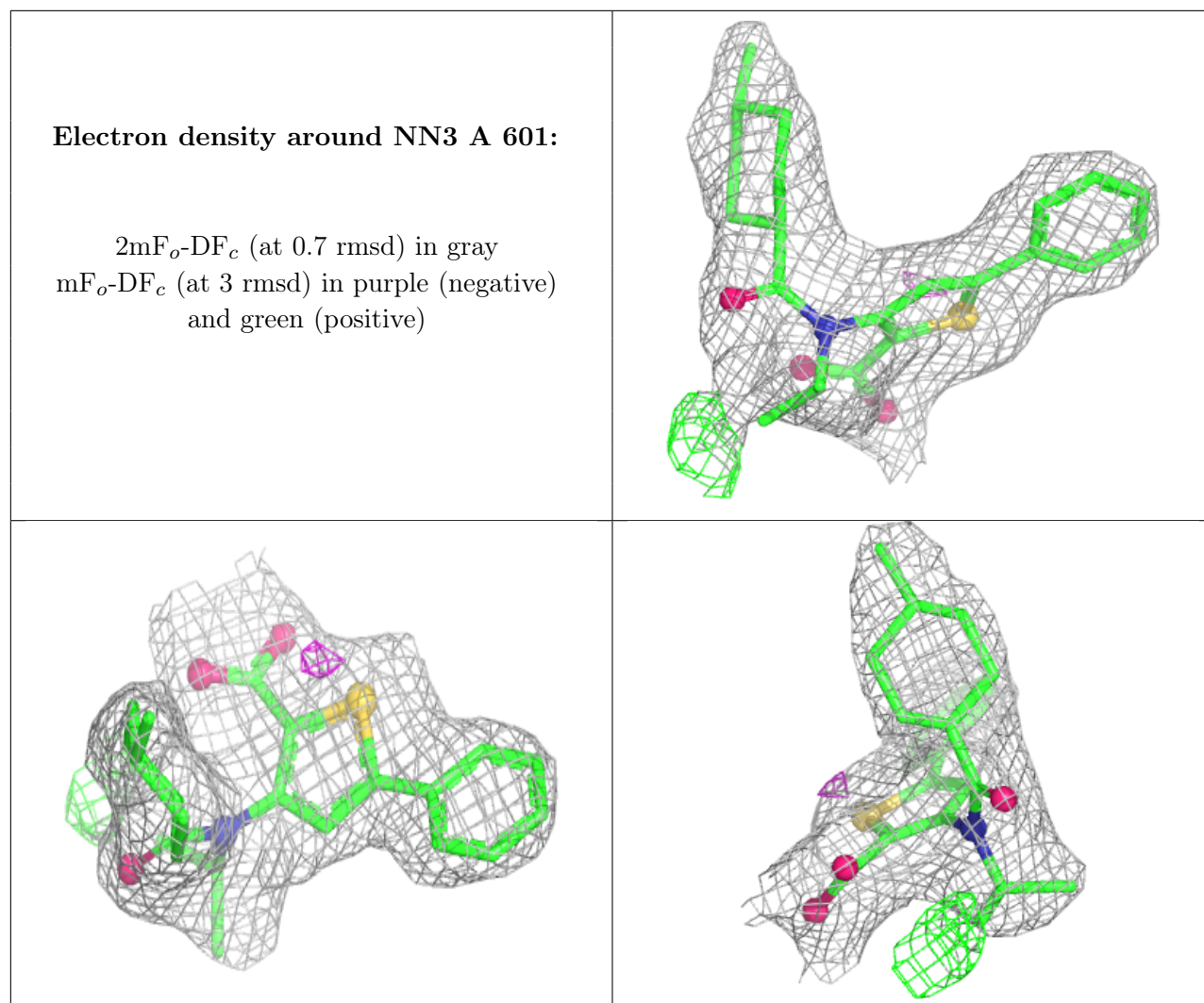
There are no oligosaccharides in this entry.

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	NN3	A	601	27/27	0.91	0.13	41,47,50,51	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.