



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:20 PM GMT

PDB ID : 4OK6
Title : Crystal Structure of Hepatitis C Virus NS3 Helicase Inhibitor Co-complex with
Compound 13 [[1-(2-methoxy-5-nitrobenzyl)-1H-indol-3-yl]acetic acid]
Authors : Padyana, A.K.
Deposited on : 2014-01-21
Resolution : 2.40 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

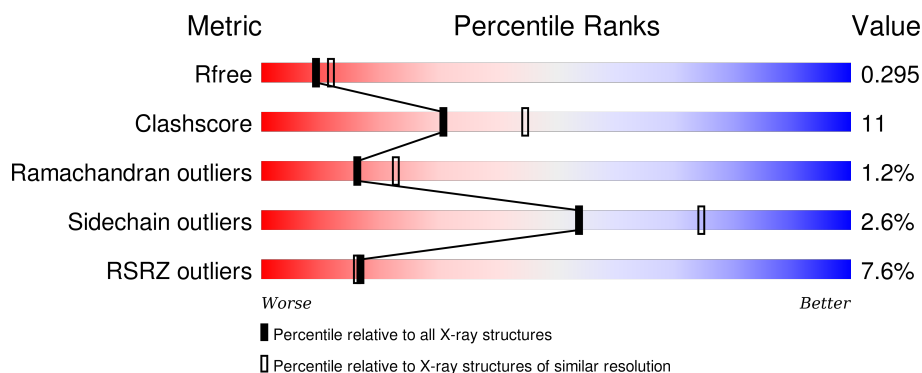
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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. 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	464	<div> <div>9%</div> <div>70%</div> <div>20%</div> <div>7%</div> </div>
1	B	464	<div> <div>5%</div> <div>73%</div> <div>15%</div> <div>11%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6746 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 Serine protease NS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	1	0
			3250	2058	549	620	23			
1	B	415	Total	C	N	O	S	0	1	0
			3137	1993	527	595	22			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	167	MET	-	EXPRESSION TAG	UNP K4KA16
A	168	GLY	-	EXPRESSION TAG	UNP K4KA16
A	169	SER	-	EXPRESSION TAG	UNP K4KA16
A	170	SER	-	EXPRESSION TAG	UNP K4KA16
A	171	HIS	-	EXPRESSION TAG	UNP K4KA16
A	172	HIS	-	EXPRESSION TAG	UNP K4KA16
A	173	HIS	-	EXPRESSION TAG	UNP K4KA16
A	174	HIS	-	EXPRESSION TAG	UNP K4KA16
A	175	HIS	-	EXPRESSION TAG	UNP K4KA16
A	176	HIS	-	EXPRESSION TAG	UNP K4KA16
A	177	SER	-	EXPRESSION TAG	UNP K4KA16
A	178	SER	-	EXPRESSION TAG	UNP K4KA16
A	179	GLY	-	EXPRESSION TAG	UNP K4KA16
A	403	ASN	SER	CONFLICT	UNP K4KA16
A	505	MET	THR	CONFLICT	UNP K4KA16
B	167	MET	-	EXPRESSION TAG	UNP K4KA16
B	168	GLY	-	EXPRESSION TAG	UNP K4KA16
B	169	SER	-	EXPRESSION TAG	UNP K4KA16
B	170	SER	-	EXPRESSION TAG	UNP K4KA16
B	171	HIS	-	EXPRESSION TAG	UNP K4KA16
B	172	HIS	-	EXPRESSION TAG	UNP K4KA16
B	173	HIS	-	EXPRESSION TAG	UNP K4KA16
B	174	HIS	-	EXPRESSION TAG	UNP K4KA16
B	175	HIS	-	EXPRESSION TAG	UNP K4KA16
B	176	HIS	-	EXPRESSION TAG	UNP K4KA16

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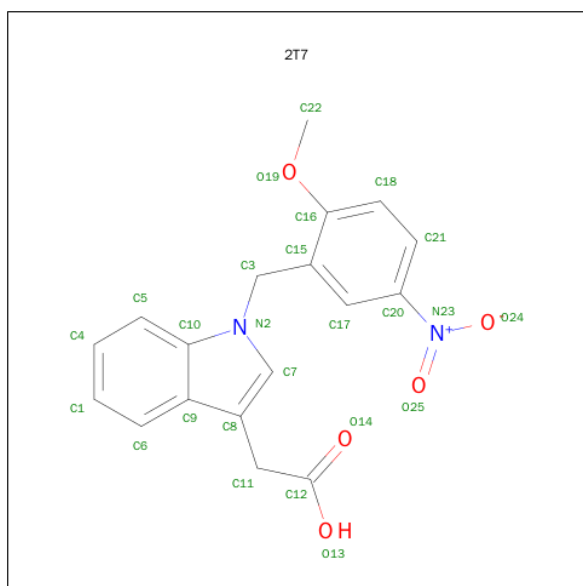
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Chain	Residue	Modelled	Actual	Comment	Reference
B	177	SER	-	EXPRESSION TAG	UNP K4KA16
B	178	SER	-	EXPRESSION TAG	UNP K4KA16
B	179	GLY	-	EXPRESSION TAG	UNP K4KA16
B	403	ASN	SER	CONFLICT	UNP K4KA16
B	505	MET	THR	CONFLICT	UNP K4KA16

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Ca 2 2	0	0

- Molecule 3 is [1-(2-METHOXY-5-NITROBENZYL)-1H-INDOL-3-YL]ACETIC ACID (three-letter code: 2T7) (formula: C₁₈H₁₆N₂O₅).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 25 18 2 5	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	153	Total O 153 153	0	0
4	B	179	Total O 179 179	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.15Å 103.32Å 118.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.08 – 2.40 64.30 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.3 (33.08-2.40) 94.5 (64.30-2.40)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.77 (at 2.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.239 , 0.300 0.247 , 0.295	Depositor DCC
R_{free} test set	2004 reflections (5.55%)	DCC
Wilson B-factor (Å ²)	42.9	Xtriage
Anisotropy	0.097	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Outliers	0 of 39953 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6746	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, 2T7

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	1/3326 (0.0%)	0.70	6/4539 (0.1%)
1	B	0.47	0/3213	0.65	1/4388 (0.0%)
All	All	0.49	1/6539 (0.0%)	0.68	7/8927 (0.1%)

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	2
1	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	600	TYR	CD1-CE1	-6.54	1.29	1.39

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	392	TYR	N-CA-C	-6.50	93.44	111.00
1	B	588	LEU	CA-CB-CG	6.11	129.35	115.30
1	A	392	TYR	C-N-CA	-5.85	107.07	121.70
1	A	393	ARG	NE-CZ-NH1	-5.67	117.46	120.30
1	A	600	TYR	CB-CG-CD1	-5.48	117.71	121.00
1	A	588	LEU	CA-CB-CG	5.09	127.02	115.30
1	A	394	GLY	N-CA-C	-5.00	100.59	113.10

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	245	ALA	Peptide
1	A	393	ARG	Peptide
1	B	587	ARG	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	3250	0	3208	83	0
1	B	3137	0	3093	60	0
2	A	2	0	0	0	0
3	A	25	0	15	0	0
4	A	153	0	0	4	0
4	B	179	0	0	1	0
All	All	6746	0	6316	139	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 (139) 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:363:ARG:NH2	1:B:400:ILE:O	2.05	0.89
1:A:587:ARG:NH2	4:A:1138:HOH:O	2.14	0.80
1:B:574:PRO:HG3	1:B:592:LEU:HA	1.63	0.80
1:A:358:VAL:HB	1:A:474:ARG:HH12	1.46	0.79
1:A:358:VAL:HB	1:A:474:ARG:NH1	1.98	0.79
1:A:337:GLU:HB2	1:A:472:ILE:HA	1.67	0.76
1:A:236:LEU:HD22	1:A:257:ARG:HH21	1.51	0.75
1:B:595:PRO:HA	1:B:608:GLU:HG3	1.71	0.72
1:A:481:ARG:HG2	1:B:485:MET:HE3	1.71	0.72
1:B:330:THR:HG23	1:B:480:GLU:OE1	1.90	0.72
1:A:616:THR:HG22	1:A:620:MET:HE2	1.70	0.71
1:A:378:ALA:HA	1:A:381:LEU:HD12	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ARG:HH22	1:A:399:VAL:HG13	1.59	0.67
1:A:246:HIS:HE1	4:A:1183:HOH:O	1.77	0.67
1:A:245:ALA:O	1:A:246:HIS:CD2	2.47	0.67
1:A:240:ALA:O	1:A:244:LYS:HG2	1.95	0.67
1:A:393:ARG:HG2	1:A:394:GLY:H	1.60	0.66
1:A:245:ALA:O	1:A:246:HIS:HD2	1.77	0.66
1:A:350:TYR:HB2	1:A:476:VAL:HG21	1.77	0.65
1:B:381:LEU:HD13	1:B:407:VAL:HG21	1.80	0.64
1:A:341:LEU:HD11	1:A:353:ALA:O	1.98	0.64
1:B:590:PRO:O	1:B:593:HIS:ND1	2.30	0.63
1:A:560:LEU:O	1:A:600:TYR:OH	2.18	0.62
1:A:574:PRO:HG3	1:A:592:LEU:HA	1.82	0.61
1:A:587:ARG:HG2	1:A:587:ARG:O	2.01	0.60
1:A:347:ILE:CG2	1:A:354:ILE:HG13	2.32	0.60
1:B:364:HIS:HB2	1:B:407:VAL:HG12	1.84	0.60
1:A:330:THR:HG22	1:A:459:THR:OG1	2.02	0.60
1:A:337:GLU:HG3	1:A:472:ILE:HG13	1.84	0.59
1:A:358:VAL:HG23	1:A:359:ILE:HG23	1.84	0.59
1:A:366:ILE:HG12	1:A:426:ILE:HB	1.85	0.59
1:A:337:GLU:CG	1:A:472:ILE:HG13	2.34	0.58
1:A:579:ASP:OD1	1:A:580:GLN:N	2.36	0.58
1:B:593:HIS:NE2	4:B:878:HOH:O	2.32	0.57
1:B:325:PRO:O	1:B:328:SER:OG	2.22	0.56
1:A:347:ILE:HG21	1:A:354:ILE:HG13	1.87	0.56
1:B:371:LYS:HG3	1:B:372:LYS:N	2.20	0.56
1:A:236:LEU:HD22	1:A:257:ARG:NH2	2.20	0.56
1:B:187:ASN:O	1:B:203:HIS:N	2.38	0.55
1:B:574:PRO:HB3	1:B:592:LEU:HG	1.88	0.55
1:B:519:THR:HB	1:B:522:LEU:HD12	1.89	0.54
1:B:578:TRP:HZ2	1:B:588:LEU:HD23	1.72	0.54
1:A:293:HIS:HE1	4:A:1127:HOH:O	1.89	0.54
1:A:450:THR:O	1:B:526:GLN:NE2	2.41	0.53
1:B:458:ARG:NH2	1:B:477:ALA:O	2.36	0.53
1:B:535:VAL:O	1:B:539:LEU:HD13	2.08	0.53
1:B:400:ILE:HG22	1:B:402:THR:CG2	2.39	0.52
1:A:481:ARG:CG	1:B:485:MET:HE3	2.39	0.52
1:A:393:ARG:HB3	1:A:393:ARG:NH1	2.24	0.52
1:A:351:GLY:C	1:A:352:LYS:HD2	2.29	0.52
1:B:403:ASN:OD1	1:B:403:ASN:O	2.27	0.52
1:A:333:HIS:ND1	1:A:336:ILE:HG13	2.24	0.52
1:B:486:PHE:CZ	1:B:525:CYS:HB2	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ASP:CG	1:A:397:VAL:H	2.12	0.51
1:B:587:ARG:HD3	1:B:587:ARG:N	2.25	0.51
1:A:351:GLY:O	1:A:352:LYS:HD2	2.10	0.51
1:B:588:LEU:CD2	1:B:592:LEU:HB2	2.41	0.51
1:A:354:ILE:C	1:A:354:ILE:HD12	2.31	0.51
1:B:425:VAL:HG23	1:B:465:THR:HB	1.92	0.51
1:A:354:ILE:O	1:A:354:ILE:HD12	2.11	0.51
1:A:239:GLY:HA2	1:A:250:PRO:HG2	1.93	0.51
1:A:393:ARG:HG2	1:A:394:GLY:N	2.26	0.50
1:A:240:ALA:HB1	1:A:244:LYS:HE2	1.92	0.50
1:A:545:HIS:O	1:A:549:GLN:HG3	2.11	0.50
1:B:460:GLN:OE1	1:B:464:ARG:NH2	2.41	0.49
1:A:333:HIS:HB3	1:A:336:ILE:HB	1.95	0.49
1:B:588:LEU:HA	1:B:591:THR:CG2	2.43	0.48
1:A:525[A]:CYS:SG	1:A:526:GLN:N	2.85	0.48
1:B:229:ASN:O	1:B:269:THR:HA	2.13	0.48
1:A:587:ARG:O	1:A:590:PRO:HD2	2.14	0.48
1:A:425:VAL:HG23	1:A:465:THR:HB	1.96	0.48
1:A:572:GLN:O	1:A:593:HIS:HB3	2.14	0.48
1:B:268:SER:OG	1:B:269:THR:N	2.46	0.48
1:A:364:HIS:HB2	1:A:407:VAL:HG22	1.96	0.47
1:A:441:ASP:O	1:A:601:ARG:NH1	2.45	0.47
1:B:588:LEU:HD21	1:B:592:LEU:HB2	1.96	0.47
1:B:574:PRO:HD3	1:B:593:HIS:H	1.78	0.47
1:A:616:THR:HG22	1:A:620:MET:CE	2.40	0.47
1:A:474:ARG:NH2	4:A:1204:HOH:O	2.44	0.46
1:A:462:ARG:HG3	1:A:473:TYR:CG	2.49	0.46
1:B:194:PRO:O	1:B:316:ARG:NH2	2.44	0.46
1:B:400:ILE:HG22	1:B:402:THR:HG22	1.97	0.46
1:B:588:LEU:O	1:B:588:LEU:HD22	2.16	0.46
1:A:212:THR:C	1:A:215:PRO:HD2	2.36	0.46
1:B:574:PRO:CG	1:B:592:LEU:HA	2.41	0.46
1:B:485:MET:HE1	1:B:524:VAL:HG12	1.98	0.46
1:A:254:THR:C	1:A:272:LYS:HG3	2.36	0.45
1:B:518:ASN:O	1:B:520:PRO:HD3	2.17	0.45
1:B:598:LEU:HD21	1:B:601:ARG:HG2	1.98	0.45
1:B:462:ARG:O	1:B:465:THR:HG22	2.16	0.45
1:B:347:ILE:HD13	1:B:381:LEU:HD21	1.99	0.45
1:A:341:LEU:HD12	1:A:342:SER:N	2.32	0.45
1:B:402:THR:O	1:B:404:GLY:N	2.50	0.45
1:A:481:ARG:HG2	1:B:485:MET:CE	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:360:LYS:HA	1:A:361:GLY:HA2	1.70	0.45
1:B:492:CYS:HB2	1:B:532:TRP:CZ2	2.52	0.45
1:A:207:GLY:O	1:A:209:GLY:N	2.48	0.45
1:A:391:TYR:HE2	1:A:414:LEU:HA	1.82	0.44
1:A:599:LEU:HB2	1:A:600:TYR:CD2	2.53	0.44
1:A:340:ALA:HA	1:A:475:PHE:CZ	2.52	0.44
1:B:442:PRO:HB3	1:B:611:LEU:HG	2.00	0.44
1:A:587:ARG:O	1:A:587:ARG:CG	2.65	0.44
1:A:364:HIS:ND1	1:A:424:SER:OG	2.40	0.44
1:A:616:THR:O	1:A:620:MET:HG3	2.18	0.44
1:B:324:THR:HG23	1:B:328:SER:HB2	2.00	0.43
1:B:563:TYR:HE1	1:B:615:ILE:HD13	1.82	0.43
1:A:391:TYR:CZ	1:A:393:ARG:HG3	2.53	0.43
1:B:307:LEU:HD13	1:B:519:THR:OG1	2.18	0.43
1:A:491:LEU:HD13	1:A:529:LEU:HD23	2.01	0.43
1:B:400:ILE:N	1:B:400:ILE:HD13	2.33	0.43
1:A:354:ILE:HA	1:A:355:PRO:HD3	1.86	0.43
1:A:458:ARG:HD2	1:A:480:GLU:OE1	2.19	0.43
1:B:194:PRO:HD3	1:B:317:LEU:HD13	2.01	0.43
1:B:574:PRO:HG3	1:B:592:LEU:CA	2.40	0.42
1:B:588:LEU:O	1:B:591:THR:N	2.52	0.42
1:B:599:LEU:HD22	1:B:615:ILE:HG22	2.01	0.42
1:B:616:THR:HG22	1:B:620:MET:CE	2.50	0.42
1:A:629:VAL:O	1:A:629:VAL:HG13	2.20	0.42
1:B:469:LYS:HG2	1:B:470:PRO:O	2.18	0.42
1:A:440:LEU:HA	1:A:440:LEU:HD23	1.85	0.42
1:A:388:ALA:HA	1:A:407:VAL:O	2.20	0.42
1:B:616:THR:HG22	1:B:620:MET:HE2	2.02	0.42
1:A:207:GLY:C	1:A:209:GLY:H	2.22	0.42
1:B:324:THR:HG21	1:B:456:VAL:HG13	2.02	0.42
1:A:346:GLU:OE2	1:A:356:LEU:HB2	2.20	0.42
1:A:229:ASN:O	1:A:269:THR:HA	2.20	0.42
1:A:363:ARG:NH2	1:A:399:VAL:HG13	2.31	0.41
1:A:393:ARG:HB3	1:A:393:ARG:HH11	1.85	0.41
1:A:589:LYS:H	1:A:589:LYS:HG2	1.44	0.41
1:A:391:TYR:CE1	1:A:393:ARG:HG3	2.54	0.41
1:A:517:MET:HE3	1:A:517:MET:HB3	1.89	0.41
1:B:441:ASP:O	1:B:601:ARG:NH1	2.46	0.41
1:B:485:MET:CE	1:B:524:VAL:HG12	2.50	0.41
1:A:600:TYR:CD1	1:A:600:TYR:C	2.94	0.41
1:B:516:TYR:OH	1:B:523:PRO:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:GLY:HA2	1:A:469:LYS:O	2.21	0.41
1:A:576:PRO:HD2	1:A:582:TRP:CE2	2.57	0.40
1:A:363:ARG:HG2	1:A:406:VAL:HG12	2.02	0.40
1:B:613:HIS:HE1	1:B:615:ILE:HD12	1.87	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	423/464 (91%)	394 (93%)	21 (5%)	8 (2%)	10	12
1	B	408/464 (88%)	384 (94%)	22 (5%)	2 (0%)	34	48
All	All	831/928 (90%)	778 (94%)	43 (5%)	10 (1%)	16	23

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	356	LEU
1	A	587	ARG
1	B	403	ASN
1	B	281	GLY
1	A	208	SER
1	A	246	HIS
1	A	357	GLU
1	A	355	PRO
1	A	590	PRO
1	A	190	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	356/382 (93%)	349 (98%)	7 (2%)	63	81
1	B	342/382 (90%)	331 (97%)	11 (3%)	46	68
All	All	698/764 (91%)	680 (97%)	18 (3%)	54	74

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	SER
1	A	213	LYS
1	A	244	LYS
1	A	356	LEU
1	A	371	LYS
1	A	393	ARG
1	A	395	LEU
1	B	235	THR
1	B	332	SER
1	B	371	LYS
1	B	403	ASN
1	B	449	THR
1	B	480	GLU
1	B	511	VAL
1	B	524	VAL
1	B	588	LEU
1	B	592	LEU
1	B	600	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	246	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
3	2T7	A	1003	-	19,27,27	0.75	0	25,38,38	1.11	3 (12%)

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
3	2T7	A	1003	-	-	0/11/14/14	0/3/3/3

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	2T7	O19-C16-C18	-2.07	120.87	124.35
3	A	1003	2T7	C21-C20-N23	2.10	121.18	119.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	2T7	O19-C16-C15	2.20	118.65	115.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	430/464 (92%)	0.65	42 (9%) 10 9	31, 46, 87, 109	0
1	B	415/464 (89%)	0.41	22 (5%) 30 30	30, 46, 75, 97	0
All	All	845/928 (91%)	0.53	64 (7%) 17 16	30, 46, 84, 109	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	591	THR	10.6
1	B	592	LEU	7.0
1	B	403	ASN	6.6
1	B	246	HIS	5.8
1	A	592	LEU	5.7
1	A	394	GLY	5.1
1	B	593	HIS	5.0
1	A	393	ARG	4.7
1	A	354	ILE	4.6
1	B	402	THR	4.0
1	A	359	ILE	4.0
1	B	281	GLY	4.0
1	A	356	LEU	3.9
1	A	281	GLY	3.9
1	A	397	VAL	3.8
1	A	405	ASP	3.7
1	A	207	GLY	3.7
1	A	244	LYS	3.5
1	B	189	SER	3.5
1	A	347	ILE	3.4
1	B	263	SER	3.2
1	A	206	THR	3.2
1	A	282	GLY	3.1
1	A	415	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	339	VAL	3.1
1	A	396	ASP	3.1
1	A	399	VAL	3.1
1	B	401	PRO	3.0
1	A	591	THR	3.0
1	A	353	ALA	2.9
1	B	213	LYS	2.9
1	A	357	GLU	2.9
1	A	358	VAL	2.9
1	A	186	ASP	2.8
1	A	406	VAL	2.6
1	B	220	ALA	2.6
1	B	236	LEU	2.6
1	A	467	ARG	2.6
1	A	390	ALA	2.5
1	A	362	GLY	2.5
1	A	386	ILE	2.4
1	B	242	MET	2.4
1	A	629	VAL	2.4
1	A	379	ALA	2.4
1	A	593	HIS	2.3
1	A	388	ALA	2.3
1	B	588	LEU	2.3
1	B	485	MET	2.3
1	A	545	HIS	2.3
1	A	252	ILE	2.2
1	B	316	ARG	2.1
1	B	431[A]	CYS	2.1
1	A	387	ASN	2.1
1	A	335	ASN	2.1
1	A	257	ARG	2.1
1	B	407	VAL	2.1
1	A	336	ILE	2.1
1	A	449	THR	2.1
1	A	472	ILE	2.1
1	B	264	PRO	2.1
1	B	466	GLY	2.0
1	B	235	THR	2.0
1	A	332	SER	2.0
1	A	375	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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	2T7	A	1003	25/25	0.91	0.19	0.74	41,48,65,69	0
2	CA	A	1001	1/1	0.92	0.16	-	65,65,65,65	0
2	CA	A	1002	1/1	0.83	0.10	-	60,60,60,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.