



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 11:17 pm GMT

PDB ID : 3O8C
Title : Visualizing ATP-dependent RNA Translocation by the NS3 Helicase from HCV
Authors : Appleby, T.C.; Somoza, J.R.
Deposited on : 2010-08-02
Resolution : 2.00 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

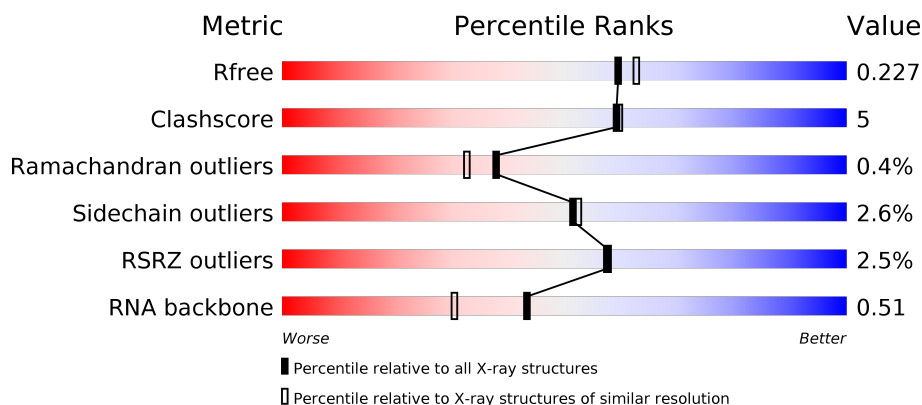
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)
RNA backbone	2435	1011 (2.66-1.34)

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	666	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>.</div> </div> </div>
1	B	666	<div> <div>2%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>..</div> </div> </div>
2	C	6	<div> <div>67%</div> <div>17%</div> <div>17%</div> </div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10544 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 HCV NS3 protease/helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	645	Total	C	N	O	S	0	0	0
			4807	3026	834	917	30			
1	B	645	Total	C	N	O	S	0	0	0
			4807	3026	834	917	30			

There are 74 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-36	MET	-	EXPRESSION TAG	UNP Q99AU2
A	-35	GLY	-	EXPRESSION TAG	UNP Q99AU2
A	-34	SER	-	EXPRESSION TAG	UNP Q99AU2
A	-33	SER	-	EXPRESSION TAG	UNP Q99AU2
A	-32	HIS	-	EXPRESSION TAG	UNP Q99AU2
A	-31	HIS	-	EXPRESSION TAG	UNP Q99AU2
A	-30	HIS	-	EXPRESSION TAG	UNP Q99AU2
A	-29	HIS	-	EXPRESSION TAG	UNP Q99AU2
A	-28	HIS	-	EXPRESSION TAG	UNP Q99AU2
A	-27	HIS	-	EXPRESSION TAG	UNP Q99AU2
A	-26	SER	-	EXPRESSION TAG	UNP Q99AU2
A	-25	SER	-	EXPRESSION TAG	UNP Q99AU2
A	-24	GLY	-	EXPRESSION TAG	UNP Q99AU2
A	-23	LEU	-	EXPRESSION TAG	UNP Q99AU2
A	-22	VAL	-	EXPRESSION TAG	UNP Q99AU2
A	-21	PRO	-	EXPRESSION TAG	UNP Q99AU2
A	-20	ARG	-	EXPRESSION TAG	UNP Q99AU2
A	-19	GLY	-	EXPRESSION TAG	UNP Q99AU2
A	-18	SER	-	EXPRESSION TAG	UNP Q99AU2
A	-17	HIS	-	EXPRESSION TAG	UNP Q99AU2
A	-16	MET	-	EXPRESSION TAG	UNP Q99AU2
A	-15	GLY	-	EXPRESSION TAG	UNP Q99AU2
A	-14	SER	-	EXPRESSION TAG	UNP Q99AU2
A	-13	VAL	-	EXPRESSION TAG	UNP Q99AU2
A	-12	VAL	-	EXPRESSION TAG	UNP Q99AU2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	ILE	-	EXPRESSION TAG	UNP Q99AU2
A	-10	VAL	-	EXPRESSION TAG	UNP Q99AU2
A	-9	GLY	-	EXPRESSION TAG	UNP Q99AU2
A	-8	ARG	-	EXPRESSION TAG	UNP Q99AU2
A	-7	ILE	-	EXPRESSION TAG	UNP Q99AU2
A	-6	ILE	-	EXPRESSION TAG	UNP Q99AU2
A	-5	LEU	-	EXPRESSION TAG	UNP Q99AU2
A	-4	SER	-	EXPRESSION TAG	UNP Q99AU2
A	-3	GLY	-	EXPRESSION TAG	UNP Q99AU2
A	-2	SER	-	EXPRESSION TAG	UNP Q99AU2
A	-1	GLY	-	EXPRESSION TAG	UNP Q99AU2
A	0	SER	-	EXPRESSION TAG	UNP Q99AU2
B	-36	MET	-	EXPRESSION TAG	UNP Q99AU2
B	-35	GLY	-	EXPRESSION TAG	UNP Q99AU2
B	-34	SER	-	EXPRESSION TAG	UNP Q99AU2
B	-33	SER	-	EXPRESSION TAG	UNP Q99AU2
B	-32	HIS	-	EXPRESSION TAG	UNP Q99AU2
B	-31	HIS	-	EXPRESSION TAG	UNP Q99AU2
B	-30	HIS	-	EXPRESSION TAG	UNP Q99AU2
B	-29	HIS	-	EXPRESSION TAG	UNP Q99AU2
B	-28	HIS	-	EXPRESSION TAG	UNP Q99AU2
B	-27	HIS	-	EXPRESSION TAG	UNP Q99AU2
B	-26	SER	-	EXPRESSION TAG	UNP Q99AU2
B	-25	SER	-	EXPRESSION TAG	UNP Q99AU2
B	-24	GLY	-	EXPRESSION TAG	UNP Q99AU2
B	-23	LEU	-	EXPRESSION TAG	UNP Q99AU2
B	-22	VAL	-	EXPRESSION TAG	UNP Q99AU2
B	-21	PRO	-	EXPRESSION TAG	UNP Q99AU2
B	-20	ARG	-	EXPRESSION TAG	UNP Q99AU2
B	-19	GLY	-	EXPRESSION TAG	UNP Q99AU2
B	-18	SER	-	EXPRESSION TAG	UNP Q99AU2
B	-17	HIS	-	EXPRESSION TAG	UNP Q99AU2
B	-16	MET	-	EXPRESSION TAG	UNP Q99AU2
B	-15	GLY	-	EXPRESSION TAG	UNP Q99AU2
B	-14	SER	-	EXPRESSION TAG	UNP Q99AU2
B	-13	VAL	-	EXPRESSION TAG	UNP Q99AU2
B	-12	VAL	-	EXPRESSION TAG	UNP Q99AU2
B	-11	ILE	-	EXPRESSION TAG	UNP Q99AU2
B	-10	VAL	-	EXPRESSION TAG	UNP Q99AU2
B	-9	GLY	-	EXPRESSION TAG	UNP Q99AU2
B	-8	ARG	-	EXPRESSION TAG	UNP Q99AU2
B	-7	ILE	-	EXPRESSION TAG	UNP Q99AU2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	ILE	-	EXPRESSION TAG	UNP Q99AU2
B	-5	LEU	-	EXPRESSION TAG	UNP Q99AU2
B	-4	SER	-	EXPRESSION TAG	UNP Q99AU2
B	-3	GLY	-	EXPRESSION TAG	UNP Q99AU2
B	-2	SER	-	EXPRESSION TAG	UNP Q99AU2
B	-1	GLY	-	EXPRESSION TAG	UNP Q99AU2
B	0	SER	-	EXPRESSION TAG	UNP Q99AU2

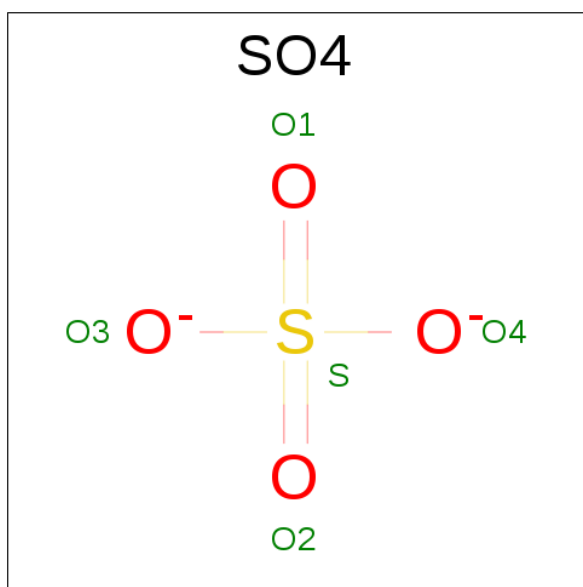
- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*(5BU)P*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	C	6	Total	Br	C	N	O	P	0	0	0
			122	1	54	12	49	6			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

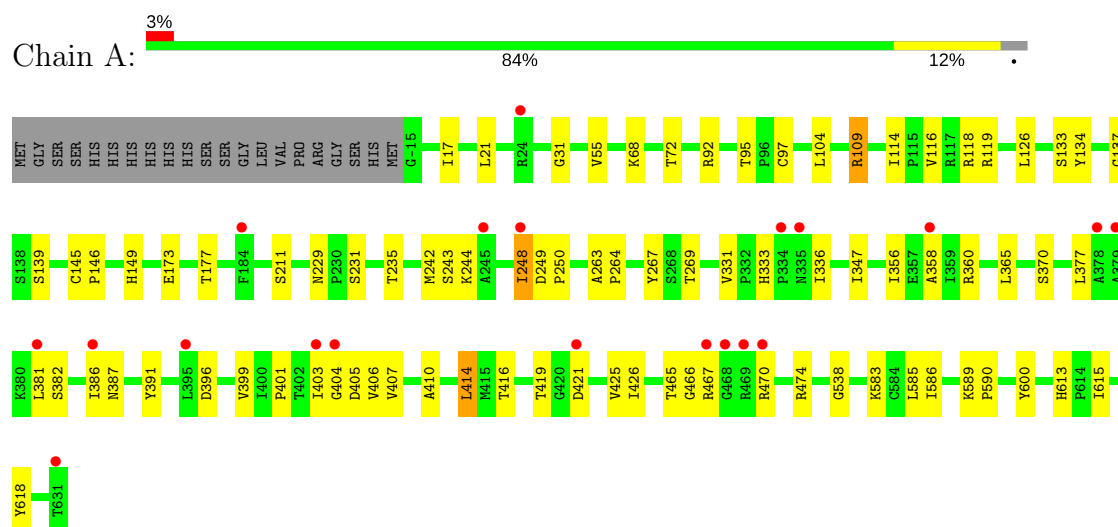
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	402	Total	O	0	0
			402	402		
5	C	17	Total	O	0	0
			17	17		
5	B	377	Total	O	0	0
			377	377		

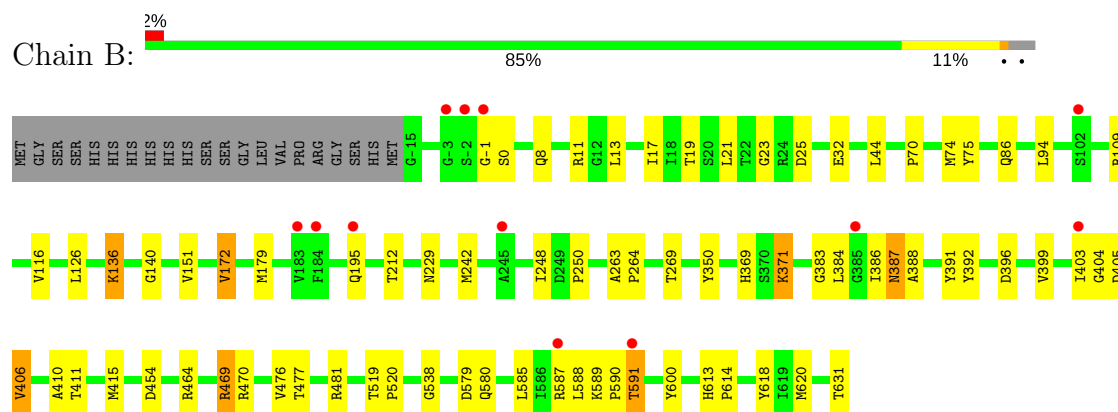
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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.

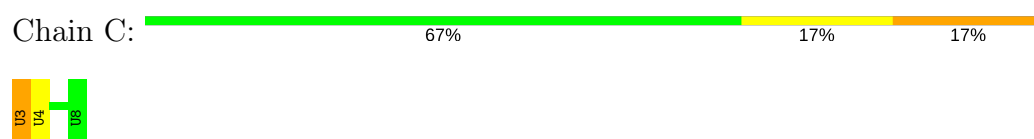
- Molecule 1: HCV NS3 protease/helicase



- Molecule 1: HCV NS3 protease/helicase



- Molecule 2: RNA (5'-R(P*UP*(5BU)P*UP*UP*UP*U)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	91.70Å 110.17Å 142.94Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.22 – 2.00 47.22 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.6 (47.22-2.00) 93.9 (47.22-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.41 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.200 , 0.232 0.195 , 0.227	Depositor DCC
R_{free} test set	1940 reflections (2.09%)	DCC
Wilson B-factor (Å ²)	30.1	Xtriage
Anisotropy	0.142	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10544	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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, 0.333 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: 5BU, ZN, SO4

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	0.39	0/4916	0.54	0/6714
1	B	0.39	0/4916	0.56	1/6714 (0.0%)
2	C	1.13	1/110 (0.9%)	1.02	0/166
All	All	0.41	1/9942 (0.0%)	0.56	1/13594 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	U	OP3-P	-9.94	1.49	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	371	LYS	CD-CE-NZ	5.08	123.38	111.70

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	4807	0	4784	58	0
1	B	4807	0	4784	46	0
2	C	122	0	60	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
5	A	402	0	0	9	0
5	B	377	0	0	0	0
5	C	17	0	0	0	0
All	All	10544	0	9628	105	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 5.

All (105) 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:212:THR:HG22	1:B:242:MET:HE1	1.48	0.95
1:A:114:ILE:HD11	1:A:134:TYR:HE1	1.29	0.93
1:A:401:PRO:HG2	1:A:406:VAL:HG21	1.55	0.88
1:A:370:SER:HA	2:C:3:U:H5'	1.60	0.83
1:A:331:VAL:HG22	5:A:854:HOH:O	1.85	0.76
1:A:116:VAL:HG22	1:A:126:LEU:HD23	1.70	0.73
1:A:243:SER:HA	1:A:248:ILE:O	1.90	0.71
1:A:396:ASP:O	1:A:399:VAL:HG13	1.92	0.70
1:B:350:TYR:OH	1:B:369:HIS:HD2	1.75	0.69
1:A:17:ILE:O	1:A:21:LEU:HG	1.95	0.67
1:A:365:LEU:HD21	1:A:414:LEU:HD22	1.78	0.66
1:A:97:CYS:HB2	1:A:149:HIS:HB2	1.78	0.65
1:A:403:ILE:HD12	1:A:404:GLY:H	1.62	0.65
1:A:401:PRO:CG	1:A:406:VAL:HG21	2.26	0.65
1:A:589:LYS:HB3	1:A:590:PRO:HD3	1.77	0.64
1:B:371:LYS:HE3	1:B:392:TYR:HB2	1.79	0.63
1:A:104:LEU:HD11	1:A:118:ARG:HB2	1.80	0.63
1:B:32:GLU:HG3	1:B:94:LEU:HD21	1.80	0.63
1:A:387:ASN:ND2	1:A:406:VAL:HG22	2.15	0.62
1:B:212:THR:CG2	1:B:242:MET:HE1	2.27	0.62
1:B:371:LYS:HD2	1:B:411:THR:HG21	1.81	0.62
1:A:114:ILE:HD11	1:A:134:TYR:CE1	2.22	0.61
1:B:371:LYS:HG3	1:B:392:TYR:CG	2.36	0.61
1:B:13:LEU:O	1:B:17:ILE:HD13	2.04	0.56
1:B:396:ASP:O	1:B:399:VAL:HG12	2.03	0.56
1:B:538:GLY:HA3	1:B:618:TYR:CE2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:GLU:HG3	1:B:94:LEU:CD2	2.37	0.55
1:B:588:LEU:O	1:B:591:THR:HG23	2.07	0.55
1:A:399:VAL:O	1:A:401:PRO:HD3	2.07	0.54
1:A:421:ASP:OD1	1:A:467:ARG:HB2	2.08	0.54
1:B:580:GLN:CD	1:B:580:GLN:H	2.11	0.54
1:B:580:GLN:CD	1:B:580:GLN:N	2.62	0.53
1:A:416:THR:HG23	5:A:733:HOH:O	2.07	0.53
1:A:263:ALA:HB1	1:A:264:PRO:HD2	1.90	0.53
1:B:242:MET:CA	1:B:242:MET:HE2	2.38	0.53
1:A:95:THR:HG22	5:A:853:HOH:O	2.07	0.53
1:A:347:ILE:HD13	1:A:381:LEU:HD21	1.91	0.52
1:B:589:LYS:N	1:B:590:PRO:HD2	2.24	0.52
1:B:469:ARG:HG3	1:B:470:ARG:N	2.25	0.52
1:A:538:GLY:HA3	1:A:618:TYR:CE2	2.44	0.52
1:B:387:ASN:O	1:B:406:VAL:HA	2.10	0.52
1:A:72:THR:HG23	5:A:1015:HOH:O	2.10	0.51
1:B:405:ASP:O	1:B:406:VAL:HB	2.10	0.51
1:A:173:GLU:O	1:A:177:THR:HG23	2.11	0.51
1:A:336:ILE:HD11	1:A:465:THR:O	2.11	0.50
1:A:235:THR:HG23	1:A:267:TYR:HB3	1.93	0.50
1:B:74:MET:CE	1:B:86:GLN:HB2	2.42	0.50
1:B:383:GLY:C	1:B:384:LEU:HD23	2.33	0.49
1:A:583:LYS:HA	1:A:586:ILE:HG13	1.94	0.49
1:B:476:VAL:HG12	1:B:477:THR:HG23	1.93	0.49
1:B:44:LEU:O	1:B:140:GLY:HA3	2.13	0.49
1:B:151:VAL:O	1:B:172:VAL:HG22	2.12	0.49
1:B:136:LYS:HA	1:B:631:THR:HB	1.95	0.49
1:B:248:ILE:O	1:B:250:PRO:HD3	2.13	0.49
1:B:386:ILE:O	1:B:388:ALA:N	2.46	0.49
1:A:365:LEU:HB3	1:A:425:VAL:HG22	1.93	0.48
5:A:689:HOH:O	1:B:620:MET:HE2	2.14	0.48
1:A:391:TYR:O	1:A:410:ALA:HA	2.14	0.48
1:A:109:ARG:HD2	1:A:137:GLY:HA3	1.96	0.47
1:A:613:HIS:CE1	1:A:615:ILE:HG12	2.49	0.47
1:B:263:ALA:HB1	1:B:264:PRO:HD2	1.96	0.47
1:A:336:ILE:HD11	1:A:466:GLY:HA3	1.96	0.47
2:C:3:U:H2'	2:C:4:5BU:H6	1.97	0.47
1:A:401:PRO:HG2	1:A:406:VAL:CG2	2.36	0.47
1:B:19:THR:CG2	1:B:25:ASP:HB2	2.45	0.47
1:B:613:HIS:ND1	1:B:614:PRO:HD2	2.30	0.47
1:A:470:ARG:NH2	5:A:726:HOH:O	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:TYR:CE1	1:B:179:MET:HA	2.51	0.46
1:A:365:LEU:CD2	1:A:414:LEU:HD22	2.44	0.46
1:A:358:ALA:HB1	1:A:474:ARG:CZ	2.46	0.46
1:A:133:SER:HB3	5:A:880:HOH:O	2.14	0.46
1:A:360:ARG:HA	1:A:386:ILE:HD11	1.98	0.45
1:A:97:CYS:HB2	1:A:149:HIS:CB	2.46	0.45
1:A:406:VAL:CG1	1:A:407:VAL:N	2.79	0.45
1:A:336:ILE:CD1	1:A:466:GLY:HA3	2.46	0.45
1:B:23:GLY:HA3	1:B:70:PRO:HG3	1.99	0.45
1:A:470:ARG:CZ	5:A:726:HOH:O	2.64	0.45
1:B:391:TYR:O	1:B:410:ALA:HA	2.16	0.45
1:B:229:ASN:O	1:B:269:THR:HA	2.17	0.44
5:A:688:HOH:O	1:B:8:GLN:HG2	2.16	0.44
1:B:116:VAL:HG22	1:B:126:LEU:HD23	2.00	0.44
2:C:3:U:H2'	2:C:4:5BU:C6	2.48	0.44
1:A:426:ILE:HG12	1:A:474:ARG:HB2	2.00	0.43
1:A:358:ALA:HB1	1:A:474:ARG:NH1	2.33	0.43
1:A:248:ILE:O	1:A:250:PRO:HD3	2.18	0.43
1:A:377:LEU:O	1:A:381:LEU:HG	2.19	0.43
1:B:384:LEU:HD23	1:B:384:LEU:N	2.35	0.42
1:A:382:SER:HA	1:A:386:ILE:O	2.20	0.42
1:B:403:ILE:CG2	1:B:404:GLY:N	2.83	0.42
1:B:19:THR:HG21	1:B:25:ASP:HB2	2.02	0.42
1:B:613:HIS:CG	1:B:614:PRO:HD2	2.55	0.41
1:A:17:ILE:HD13	1:B:13:LEU:HG	2.02	0.41
1:A:470:ARG:HA	1:A:470:ARG:NE	2.36	0.41
1:A:145:CYS:HB2	1:A:146:PRO:CD	2.50	0.41
1:A:356:ILE:O	1:A:360:ARG:HB2	2.20	0.41
1:A:31:GLY:H	1:A:92:ARG:HH11	1.67	0.41
1:B:74:MET:HB2	1:B:74:MET:HE3	1.73	0.41
1:A:55:VAL:HG21	1:A:139:SER:HB3	2.03	0.41
1:A:104:LEU:CD1	1:A:118:ARG:HB2	2.50	0.40
1:B:519:THR:HA	1:B:520:PRO:HD3	1.89	0.40
1:A:405:ASP:O	1:A:406:VAL:HG23	2.22	0.40
1:B:17:ILE:O	1:B:21:LEU:HD13	2.21	0.40
1:B:464:ARG:HA	1:B:464:ARG:HD3	1.76	0.40
1:A:229:ASN:O	1:A:269:THR:HA	2.21	0.40
1:A:470:ARG:HE	1:A:470:ARG:HA	1.86	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	643/666 (96%)	627 (98%)	16 (2%)	0	100	100
1	B	643/666 (96%)	627 (98%)	11 (2%)	5 (1%)	22	15
All	All	1286/1332 (96%)	1254 (98%)	27 (2%)	5 (0%)	38	33

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	-1	GLY
1	B	0	SER
1	B	387	ASN
1	B	406	VAL
1	B	579	ASP

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	526/544 (97%)	512 (97%)	14 (3%)	50	51
1	B	526/544 (97%)	513 (98%)	13 (2%)	53	54
All	All	1052/1088 (97%)	1025 (97%)	27 (3%)	51	52

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	LYS

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Mol	Chain	Res	Type
1	A	109	ARG
1	A	119	ARG
1	A	211	SER
1	A	231	SER
1	A	242	MET
1	A	244	LYS
1	A	248	ILE
1	A	249	ASP
1	A	333	HIS
1	A	414	LEU
1	A	419	THR
1	A	585	LEU
1	A	600	TYR
1	B	11	ARG
1	B	109	ARG
1	B	136	LYS
1	B	172	VAL
1	B	195	GLN
1	B	415	MET
1	B	454	ASP
1	B	469	ARG
1	B	481	ARG
1	B	585	LEU
1	B	587	ARG
1	B	591	THR
1	B	600	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	149	HIS
1	B	195	GLN
1	B	369	HIS
1	B	434	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	5/6 (83%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue 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	5BU	C	4	2	14,22,23	2.63	3 (21%)	15,32,35	2.08	2 (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	5BU	C	4	2	-	0/3/25/26	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	4	5BU	O4-C4	-2.11	1.19	1.24
2	C	4	5BU	C4-N3	2.75	1.38	1.33
2	C	4	5BU	C4-C5	8.96	1.49	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	4	5BU	C5-C4-N3	-2.63	120.49	123.64
2	C	4	5BU	C4-N3-C2	7.40	121.63	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	4	5BU	2	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
4	SO4	A	850	-	4,4,4	0.17	0	6,6,6	0.19	0
4	SO4	B	850	-	4,4,4	0.19	0	6,6,6	0.17	0

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
4	SO4	A	850	-	-	0/0/0/0	0/0/0/0
4	SO4	B	850	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

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	645/666 (96%)	0.03	20 (3%) 49 49	17, 33, 59, 68	0
1	B	645/666 (96%)	-0.05	12 (1%) 67 66	19, 35, 52, 80	0
2	C	5/6 (83%)	-0.59	0 100 100	30, 35, 51, 53	0
All	All	1295/1338 (96%)	-0.01	32 (2%) 58 57	17, 34, 57, 80	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	ILE	5.0
1	A	404	GLY	4.9
1	B	183	VAL	4.2
1	A	381	LEU	4.1
1	A	334	PRO	3.9
1	B	184	PHE	3.7
1	B	-1	GLY	3.6
1	A	468	GLY	3.5
1	B	587	ARG	3.2
1	B	385	GLY	3.0
1	A	470	ARG	3.0
1	B	245	ALA	2.9
1	A	245	ALA	2.8
1	A	358	ALA	2.8
1	A	386	ILE	2.8
1	B	195	GLN	2.6
1	B	-3	GLY	2.6
1	B	-2	SER	2.5
1	A	631	THR	2.4
1	A	24	ARG	2.4
1	A	379	ALA	2.4
1	A	467	ARG	2.3
1	A	248	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	421	ASP	2.3
1	A	378	ALA	2.3
1	A	395	LEU	2.3
1	A	469	ARG	2.3
1	B	102	SER	2.2
1	A	184	PHE	2.0
1	A	335	ASN	2.0
1	B	403	ILE	2.0
1	B	591	THR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q < 0.9
2	5BU	C	4	21/22	0.94	0.10	-	42,47,52,82	0

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(Å ²)	Q < 0.9
4	SO4	B	850	5/5	0.98	0.12	0.98	34,36,38,44	0
4	SO4	A	850	5/5	0.97	0.08	-0.47	31,35,38,44	0
3	ZN	A	800	1/1	0.98	0.07	-1.50	46,46,46,46	0
3	ZN	B	800	1/1	0.98	0.06	-2.69	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.