



Full wwPDB X-ray Structure Validation Report

Mar 27, 2014 – 01:57 AM EDT

PDB ID : 4OJQ
Title : Crystal Structure of Hepatitis C Virus NS3 Helicase Inhibitor Co-complex with
Fragment 1 [(5-bromo-1H-indol-3-yl)aceticacid]
Authors : Padyana, A.K.
Deposited on : 2014-01-21
Resolution : 2.25 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

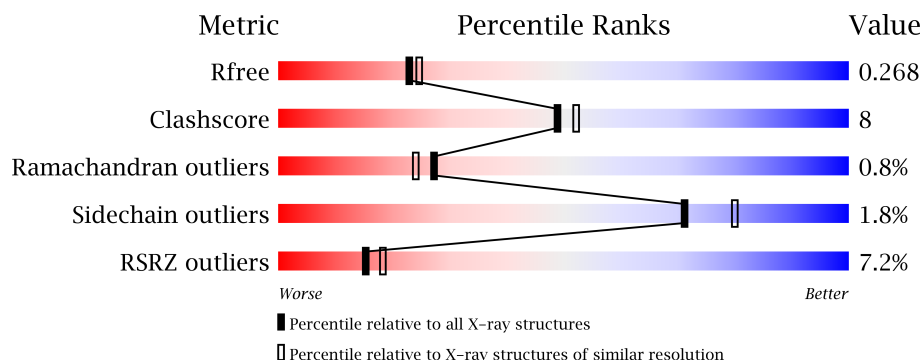
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.15 2013
Xtriage (Phenix)	:	dev-1439
EDS	:	stable22978
Percentile statistics	:	21963
Refmac	:	5.8.0049
CCP4	:	6.3.0 (Settle)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	stable22978

1 Overall quality at a glance

The reported resolution of this entry is 2.25 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}	66092	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	464	
1	B	464	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6714 atoms, of which 0 are hydrogen and 0 are deuterium.

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	440	Total	C	N	O	S	0	4	0
			3337	2115	560	637	25			
1	B	420	Total	C	N	O	S	0	1	0
			3176	2018	532	603	23			

There are 30 discrepancies between the modelled and reference sequences:

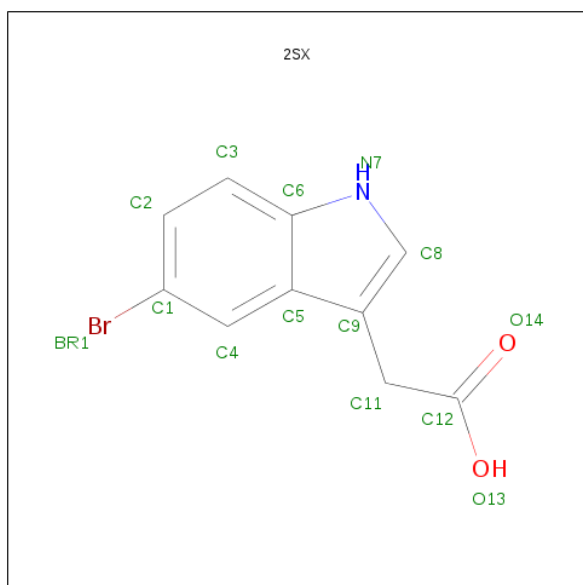
Chain	Residue	Modelled	Actual	Comment	Reference
A	167	MET	-	EXPRESSION TAG	UNP K4KA16
A	168	GLY	-	EXPRESSION TAG	UNP K4KA16
A	169	SER	-	EXPRESSION TAG	UNP K4KA16
A	170	SER	-	EXPRESSION TAG	UNP K4KA16
A	171	HIS	-	EXPRESSION TAG	UNP K4KA16
A	172	HIS	-	EXPRESSION TAG	UNP K4KA16
A	173	HIS	-	EXPRESSION TAG	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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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 (5-BROMO-1H-INDOL-3-YL)ACETICACID (three-letter code: 2SX) (formula: C₁₀H₈BrNO₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	0	0
			14	1	10	1	2		

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Ca	0	0
			2	2		

- Molecule 4 is water.

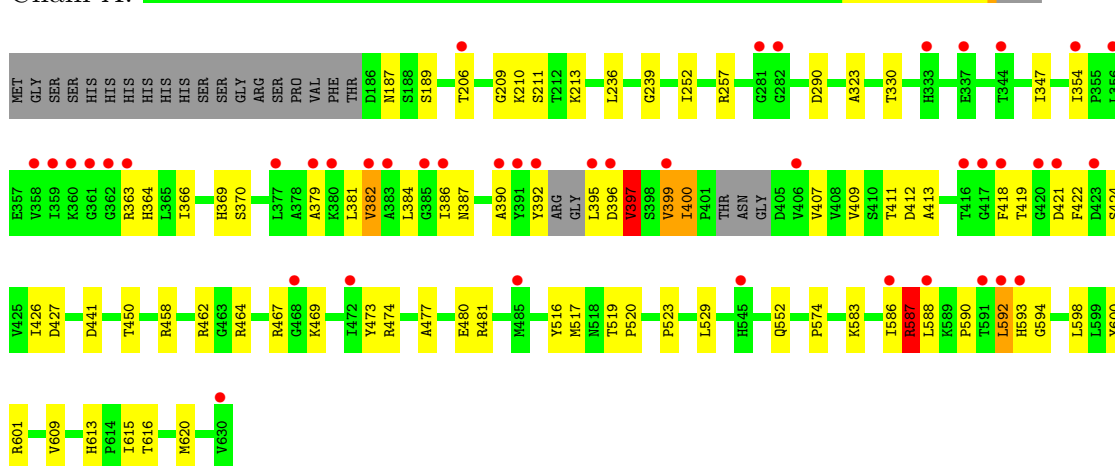
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	85	Total	O	0	0
			85	85		
4	B	100	Total	O	0	0
			100	100		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

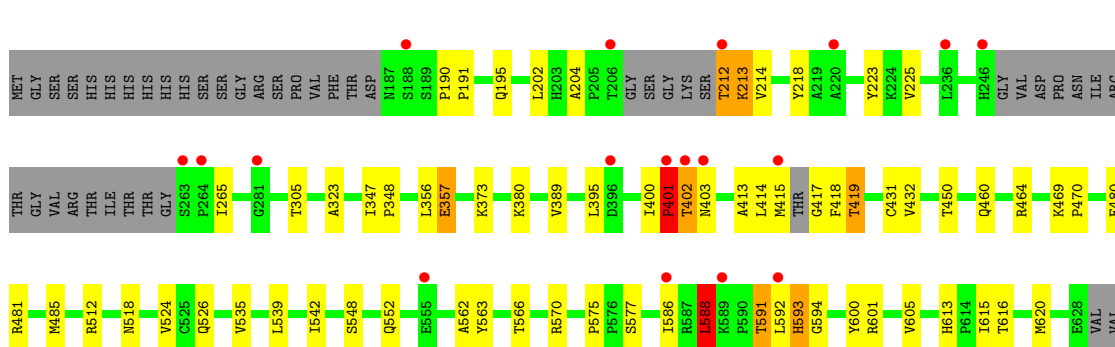
• Molecule 1: Serine protease NS3

Chain A:



• Molecule 1: Serine protease NS3

Chain B:



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.14Å 103.53Å 119.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.10 – 2.25 39.10 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.10-2.25) 96.9 (39.10-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.67 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.217 , 0.270 0.216 , 0.268	Depositor DCC
R_{free} test set	2391 reflections (5.05%)	DCC
Wilson B-factor (Å ²)	50.4	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Outliers	1 of 48646 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6714	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, 2SX

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	0.45	0/3416	0.64	3/4666 (0.1%)
1	B	0.46	0/3253	0.62	1/4441 (0.0%)
All	All	0.46	0/6669	0.63	4/9107 (0.0%)

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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	588	LEU	CA-CB-CG	8.26	134.31	115.30
1	A	588	LEU	CB-CG-CD2	6.59	122.20	111.00
1	B	588	LEU	CA-CB-CG	5.75	128.54	115.30
1	A	592	LEU	CA-CB-CG	5.65	128.29	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	397	VAL	Peptide
1	A	399	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	B	401	PRO	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3337	0	3292	56	1
1	B	3176	0	3127	46	1
2	A	14	0	0	0	0
3	B	2	0	0	0	0
4	A	85	0	0	1	0
4	B	100	0	0	3	0
All	All	6714	0	6419	100	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 8.

All (100) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:363:ARG:HG3	1:A:422:PHE:HA	1.55	0.87
1:B:402:THR:HG22	1:B:403:ASN:H	1.42	0.84
1:A:397:VAL:HG21	1:A:418:PHE:HE2	1.46	0.81
1:A:399:VAL:HG12	1:A:400:ILE:HB	1.68	0.75
1:B:417:GLY:N	4:B:1199:HOH:O	2.20	0.74
1:B:460:GLN:HE21	1:B:464:ARG:HH11	1.36	0.72
1:A:397:VAL:HG21	1:A:418:PHE:CE2	2.22	0.72
1:B:402:THR:CG2	1:B:403:ASN:H	2.03	0.72
1:A:381:LEU:HA	1:A:384:LEU:HB2	1.72	0.71
1:A:392:TYR:O	1:A:395:LEU:N	2.25	0.69
1:A:396:ASP:OD1	1:A:397:VAL:N	2.22	0.69
1:A:364:HIS:HB2	1:A:407:VAL:HG22	1.80	0.64
1:A:363:ARG:CZ	1:A:400:ILE:HD11	2.29	0.63
1:A:366:ILE:HG12	1:A:426:ILE:HB	1.81	0.62
1:B:389:VAL:HG21	1:B:400:ILE:HD13	1.81	0.61
1:A:411:THR:HG23	1:A:413:ALA:H	1.65	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:587:ARG:O	1:A:590:PRO:HD2	2.02	0.60
1:A:517:MET:HE3	1:A:529:LEU:HD21	1.84	0.60
1:A:587:ARG:HG2	1:A:587:ARG:O	2.02	0.59
1:A:206:THR:HG23	1:A:323:ALA:HB2	1.84	0.59
1:A:481:ARG:HD3	1:B:485:MET:SD	2.43	0.59
1:A:363:ARG:NE	1:A:400:ILE:HD11	2.19	0.58
1:B:348:PRO:HD2	1:B:380:LYS:HE2	1.86	0.57
1:B:460:GLN:NE2	1:B:464:ARG:HH11	2.02	0.56
1:B:347:ILE:HD11	1:B:356:LEU:HD13	1.88	0.56
1:A:381:LEU:HD13	1:A:386:ILE:HB	1.88	0.55
1:B:402:THR:CG2	1:B:403:ASN:N	2.69	0.55
1:B:432:VAL:HG22	1:B:450:THR:HG22	1.89	0.55
1:A:381:LEU:HB2	1:A:386:ILE:HD13	1.88	0.54
1:A:239:GLY:HA3	1:A:252:ILE:HD11	1.90	0.54
1:A:363:ARG:NH2	1:A:421:ASP:OD2	2.42	0.53
1:A:209:GLY:HA2	4:A:866:HOH:O	2.09	0.52
1:A:552:GLN:H	1:A:552:GLN:CD	2.13	0.52
1:B:592:LEU:O	1:B:594:GLY:N	2.43	0.52
1:A:364:HIS:HD2	1:A:424:SER:OG	1.93	0.51
1:A:426:ILE:HG12	1:A:474:ARG:HB2	1.92	0.51
1:B:413:ALA:O	1:B:414:LEU:HB3	2.10	0.51
1:B:213:LYS:HD3	1:B:213:LYS:H	1.74	0.51
1:A:598:LEU:HD22	1:A:609:VAL:HG11	1.92	0.51
1:B:418:PHE:CG	1:B:419:THR:N	2.79	0.51
1:B:601:ARG:HH21	1:B:605:VAL:HB	1.75	0.51
1:A:583:LYS:O	1:A:586:ILE:HG12	2.11	0.50
1:A:441:ASP:O	1:A:601:ARG:NH1	2.42	0.50
1:A:613:HIS:HE1	1:A:615:ILE:HD12	1.75	0.50
1:B:202:LEU:HD21	1:B:214:VAL:HG21	1.95	0.49
1:A:592:LEU:O	1:A:594:GLY:N	2.46	0.48
1:B:548:SER:O	1:B:552:GLN:HG3	2.14	0.48
1:A:400:ILE:HG21	1:A:419:THR:HG21	1.96	0.48
1:B:575:PRO:HB2	1:B:577:SER:O	2.14	0.47
1:A:411:THR:OG1	1:A:412:ASP:N	2.46	0.47
1:A:462:ARG:HG3	1:A:473:TYR:CG	2.50	0.47
1:A:613:HIS:CE1	1:A:615:ILE:HD12	2.50	0.46
1:A:236:LEU:HD23	1:A:252:ILE:HG21	1.96	0.46
1:A:379:ALA:HA	1:A:382:VAL:HG13	1.96	0.46
1:B:566:THR:O	1:B:570:ARG:HG3	2.16	0.46
1:A:464:ARG:HA	1:A:467:ARG:HH11	1.81	0.46
1:B:400:ILE:HA	1:B:401:PRO:HD2	1.45	0.46
1:A:213:LYS:HB2	1:A:213:LYS:HE3	1.55	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:330:THR:HG23	1:A:480:GLU:OE1	2.15	0.45
1:B:485:MET:HG3	1:B:524:VAL:HG23	1.96	0.45
1:A:206:THR:HG22	1:A:210:LYS:NZ	2.31	0.45
1:A:386:ILE:O	1:A:387:ASN:HB3	2.17	0.45
1:B:204:ALA:O	1:B:323:ALA:HA	2.17	0.45
1:B:373:LYS:NZ	4:B:1112:HOH:O	2.50	0.45
1:A:450:THR:O	1:B:526:GLN:NE2	2.47	0.45
1:A:210:LYS:NZ	1:A:290:ASP:OD1	2.42	0.44
1:A:347:ILE:HD12	1:A:354:ILE:O	2.17	0.44
1:A:616:THR:HG22	1:A:620:MET:HE3	1.98	0.44
1:A:616:THR:HG22	1:A:620:MET:CE	2.47	0.44
1:B:542:ILE:HD11	1:B:562:ALA:HB3	1.99	0.44
1:B:212:THR:OG1	1:B:213:LYS:N	2.49	0.44
1:A:427:ASP:OD2	1:A:473:TYR:OH	2.35	0.44
1:B:431:CYS:O	1:B:450:THR:HA	2.18	0.44
1:B:591:THR:O	1:B:593:HIS:N	2.50	0.44
1:B:357:GLU:H	1:B:357:GLU:HG3	1.43	0.43
1:B:535:VAL:O	1:B:539:LEU:HG	2.18	0.43
1:A:519:THR:HA	1:A:520:PRO:HD3	1.85	0.43
1:B:616:THR:O	1:B:620:MET:HG3	2.19	0.43
1:A:458:ARG:NH2	1:A:477:ALA:O	2.51	0.43
1:B:518:ASN:ND2	4:B:1110:HOH:O	2.40	0.42
1:A:390:ALA:HA	1:A:409:VAL:O	2.19	0.42
1:B:563:TYR:HE2	1:B:615:ILE:HD13	1.83	0.42
1:A:366:ILE:O	1:A:409:VAL:HA	2.20	0.42
1:A:574:PRO:HG3	1:A:592:LEU:HA	2.01	0.42
1:B:469:LYS:HG2	1:B:470:PRO:N	2.34	0.42
1:B:613:HIS:CE1	1:B:615:ILE:HD12	2.54	0.42
1:B:616:THR:HG22	1:B:620:MET:CE	2.49	0.42
1:B:380:LYS:HE3	1:B:380:LYS:HB3	1.77	0.42
1:B:218:TYR:O	1:B:223:TYR:HB2	2.19	0.42
1:B:305:THR:OG1	1:B:512:ARG:HD3	2.20	0.42
1:A:469:LYS:HE3	1:A:469:LYS:HB3	1.67	0.42
1:B:415:MET:HG2	1:B:464:ARG:HH12	1.85	0.41
1:B:480:GLU:H	1:B:480:GLU:HG2	1.68	0.41
1:B:190:PRO:HA	1:B:191:PRO:HD3	1.83	0.41
1:A:187:ASN:HB3	1:A:189:SER:O	2.21	0.41
1:B:415:MET:HG2	1:B:464:ARG:NH1	2.36	0.41
1:A:369:HIS:CD2	1:A:370:SER:HB3	2.56	0.41
1:A:516:TYR:OH	1:A:523:PRO:HD2	2.22	0.40
1:B:225:VAL:HG22	1:B:265:ILE:HG12	2.03	0.40
1:B:586:ILE:O	1:B:588:LEU:N	2.54	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:257:ARG:NH1	1:B:195:GLN:O[3_545]	2.19	0.01

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	438/464 (94%)	412 (94%)	23 (5%)	3 (1%)	30	29
1	B	413/464 (89%)	388 (94%)	21 (5%)	4 (1%)	22	17
All	All	851/928 (92%)	800 (94%)	44 (5%)	7 (1%)	27	24

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	587	ARG
1	B	213	LYS
1	B	401	PRO
1	B	419	THR
1	B	593	HIS
1	A	593	HIS
1	A	400	ILE

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	366/382 (96%)	361 (99%)	5 (1%)	78	87
1	B	346/382 (91%)	338 (98%)	8 (2%)	63	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	712/764 (93%)	699 (98%)	13 (2%)	71	80

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	211	SER
1	A	382	VAL
1	A	397	VAL
1	A	587	ARG
1	A	600	TYR
1	B	212	THR
1	B	357	GLU
1	B	395	LEU
1	B	402	THR
1	B	481	ARG
1	B	588	LEU
1	B	591	THR
1	B	600	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	364	HIS
1	A	526	GLN
1	B	198	GLN
1	B	460	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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	$\# Z > 2$
2	2SX	A	701	-	15,15,15	0.82	0	21,21,21	1.25	4 (19%)

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	2SX	A	701	-	-	0/4/4/4	0/0/2/2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	2SX	C2-C1-C4	-2.74	119.44	121.94
2	A	701	2SX	O13-C12-C11	2.24	119.41	113.80
2	A	701	2SX	BR1-C1-C2	2.04	122.68	119.27
2	A	701	2SX	C3-C2-C1	2.03	121.22	119.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	440/464 (94%)	0.55	44 (10%) 8 9	41, 59, 98, 114	0
1	B	420/464 (90%)	0.37	18 (4%) 34 39	39, 58, 94, 110	0
All	All	860/928 (92%)	0.46	62 (7%) 15 18	39, 59, 97, 114	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	420	GLY	7.0
1	A	592	LEU	6.7
1	A	383	ALA	6.5
1	B	592	LEU	6.4
1	B	263	SER	6.1
1	B	281	GLY	6.0
1	B	401	PRO	5.9
1	A	382	VAL	5.8
1	B	236	LEU	4.9
1	A	418	PHE	4.6
1	A	392	TYR	4.2
1	A	281	GLY	4.1
1	A	363	ARG	4.1
1	A	416	THR	3.8
1	A	385	GLY	3.8
1	A	356	LEU	3.7
1	A	358	VAL	3.7
1	B	402	THR	3.6
1	A	361	GLY	3.6
1	B	403	ASN	3.5
1	A	391	TYR	3.4
1	B	206	THR	3.4
1	A	354	ILE	3.3
1	A	282	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	220	ALA	3.2
1	A	423	ASP	3.2
1	A	395	LEU	3.1
1	A	377	LEU	3.1
1	A	380	LYS	3.1
1	A	421	ASP	3.0
1	A	206	THR	3.0
1	B	212	THR	3.0
1	A	379	ALA	2.9
1	B	188	SER	2.8
1	A	362	GLY	2.8
1	A	386	ILE	2.8
1	B	396	ASP	2.8
1	A	593	HIS	2.8
1	B	415	MET	2.7
1	A	406	VAL	2.7
1	A	472	ILE	2.7
1	A	591	THR	2.7
1	A	545	HIS	2.6
1	A	337	GLU	2.5
1	A	390	ALA	2.5
1	A	359	ILE	2.4
1	A	399	VAL	2.4
1	A	485[A]	MET	2.4
1	A	588	LEU	2.3
1	A	360	LYS	2.3
1	B	246	HIS	2.3
1	A	630	VAL	2.3
1	A	396	ASP	2.2
1	A	468	GLY	2.2
1	A	586	ILE	2.2
1	A	417	GLY	2.2
1	B	586	ILE	2.2
1	B	264	PRO	2.2
1	A	333	HIS	2.2
1	B	555	GLU	2.1
1	B	589	LYS	2.1
1	A	344	THR	2.0

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	2SX	A	701	14/14	0.12	-0.23	55,61,68,115	0
3	CA	B	1002	1/1	0.09	-1.31	81,81,81,81	0
3	CA	B	1001	1/1	0.09	-1.56	76,76,76,76	0

6.5 Other polymers

There are no such residues in this entry.