



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 03:29 PM GMT

PDB ID : 4CBI
Title : Pestivirus NS3 helicase
Authors : Tortorici, M.A.; Duquerroy, S.; Kwok, J.; Vonnrhein, C.; Perez, J.; Lamp, B.;
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Deposited on : 2013-10-14
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

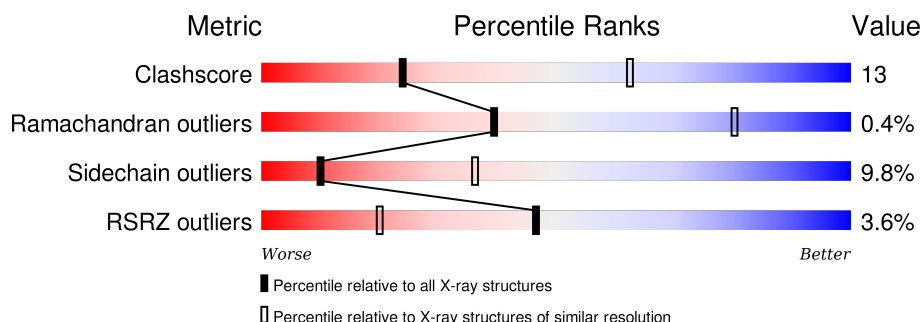
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	516	<div> <div>4%</div> <div>53% 19% • 24%</div> </div>
1	B	516	<div> <div>4%</div> <div>57% 20% 5% 19%</div> </div>
1	C	516	<div> <div>2%</div> <div>63% 21% • 12%</div> </div>
1	D	516	<div> <div>%</div> <div>63% 20% 5% 12%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13727 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	393	Total	C	N	O	S	0	0	0
			3135	1991	532	590	22			
1	B	419	Total	C	N	O	S	0	0	0
			3339	2123	575	620	21			
1	C	453	Total	C	N	O	S	0	0	0
			3603	2286	614	682	21			
1	D	456	Total	C	N	O	S	0	0	0
			3633	2309	617	686	21			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	176	MET	-	EXPRESSION TAG	UNP P19712
A	177	ALA	-	EXPRESSION TAG	UNP P19712
A	178	SER	-	EXPRESSION TAG	UNP P19712
A	179	HIS	-	EXPRESSION TAG	UNP P19712
A	180	HIS	-	EXPRESSION TAG	UNP P19712
A	181	HIS	-	EXPRESSION TAG	UNP P19712
A	182	HIS	-	EXPRESSION TAG	UNP P19712
A	183	HIS	-	EXPRESSION TAG	UNP P19712
A	184	HIS	-	EXPRESSION TAG	UNP P19712
A	185	HIS	-	EXPRESSION TAG	UNP P19712
A	186	GLU	-	EXPRESSION TAG	UNP P19712
A	187	ASN	-	EXPRESSION TAG	UNP P19712
A	188	LEU	-	EXPRESSION TAG	UNP P19712
A	189	TYR	-	EXPRESSION TAG	UNP P19712
A	190	PHE	-	EXPRESSION TAG	UNP P19712
A	191	GLN	-	EXPRESSION TAG	UNP P19712
A	192	GLY	-	EXPRESSION TAG	UNP P19712
B	176	MET	-	EXPRESSION TAG	UNP P19712
B	177	ALA	-	EXPRESSION TAG	UNP P19712
B	178	SER	-	EXPRESSION TAG	UNP P19712
B	179	HIS	-	EXPRESSION TAG	UNP P19712

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Chain	Residue	Modelled	Actual	Comment	Reference
B	180	HIS	-	EXPRESSION TAG	UNP P19712
B	181	HIS	-	EXPRESSION TAG	UNP P19712
B	182	HIS	-	EXPRESSION TAG	UNP P19712
B	183	HIS	-	EXPRESSION TAG	UNP P19712
B	184	HIS	-	EXPRESSION TAG	UNP P19712
B	185	HIS	-	EXPRESSION TAG	UNP P19712
B	186	GLU	-	EXPRESSION TAG	UNP P19712
B	187	ASN	-	EXPRESSION TAG	UNP P19712
B	188	LEU	-	EXPRESSION TAG	UNP P19712
B	189	TYR	-	EXPRESSION TAG	UNP P19712
B	190	PHE	-	EXPRESSION TAG	UNP P19712
B	191	GLN	-	EXPRESSION TAG	UNP P19712
B	192	GLY	-	EXPRESSION TAG	UNP P19712
C	176	MET	-	EXPRESSION TAG	UNP P19712
C	177	ALA	-	EXPRESSION TAG	UNP P19712
C	178	SER	-	EXPRESSION TAG	UNP P19712
C	179	HIS	-	EXPRESSION TAG	UNP P19712
C	180	HIS	-	EXPRESSION TAG	UNP P19712
C	181	HIS	-	EXPRESSION TAG	UNP P19712
C	182	HIS	-	EXPRESSION TAG	UNP P19712
C	183	HIS	-	EXPRESSION TAG	UNP P19712
C	184	HIS	-	EXPRESSION TAG	UNP P19712
C	185	HIS	-	EXPRESSION TAG	UNP P19712
C	186	GLU	-	EXPRESSION TAG	UNP P19712
C	187	ASN	-	EXPRESSION TAG	UNP P19712
C	188	LEU	-	EXPRESSION TAG	UNP P19712
C	189	TYR	-	EXPRESSION TAG	UNP P19712
C	190	PHE	-	EXPRESSION TAG	UNP P19712
C	191	GLN	-	EXPRESSION TAG	UNP P19712
C	192	GLY	-	EXPRESSION TAG	UNP P19712
D	176	MET	-	EXPRESSION TAG	UNP P19712
D	177	ALA	-	EXPRESSION TAG	UNP P19712
D	178	SER	-	EXPRESSION TAG	UNP P19712
D	179	HIS	-	EXPRESSION TAG	UNP P19712
D	180	HIS	-	EXPRESSION TAG	UNP P19712
D	181	HIS	-	EXPRESSION TAG	UNP P19712
D	182	HIS	-	EXPRESSION TAG	UNP P19712
D	183	HIS	-	EXPRESSION TAG	UNP P19712
D	184	HIS	-	EXPRESSION TAG	UNP P19712
D	185	HIS	-	EXPRESSION TAG	UNP P19712
D	186	GLU	-	EXPRESSION TAG	UNP P19712
D	187	ASN	-	EXPRESSION TAG	UNP P19712

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Chain	Residue	Modelled	Actual	Comment	Reference
D	188	LEU	-	EXPRESSION TAG	UNP P19712
D	189	TYR	-	EXPRESSION TAG	UNP P19712
D	190	PHE	-	EXPRESSION TAG	UNP P19712
D	191	GLN	-	EXPRESSION TAG	UNP P19712
D	192	GLY	-	EXPRESSION TAG	UNP P19712

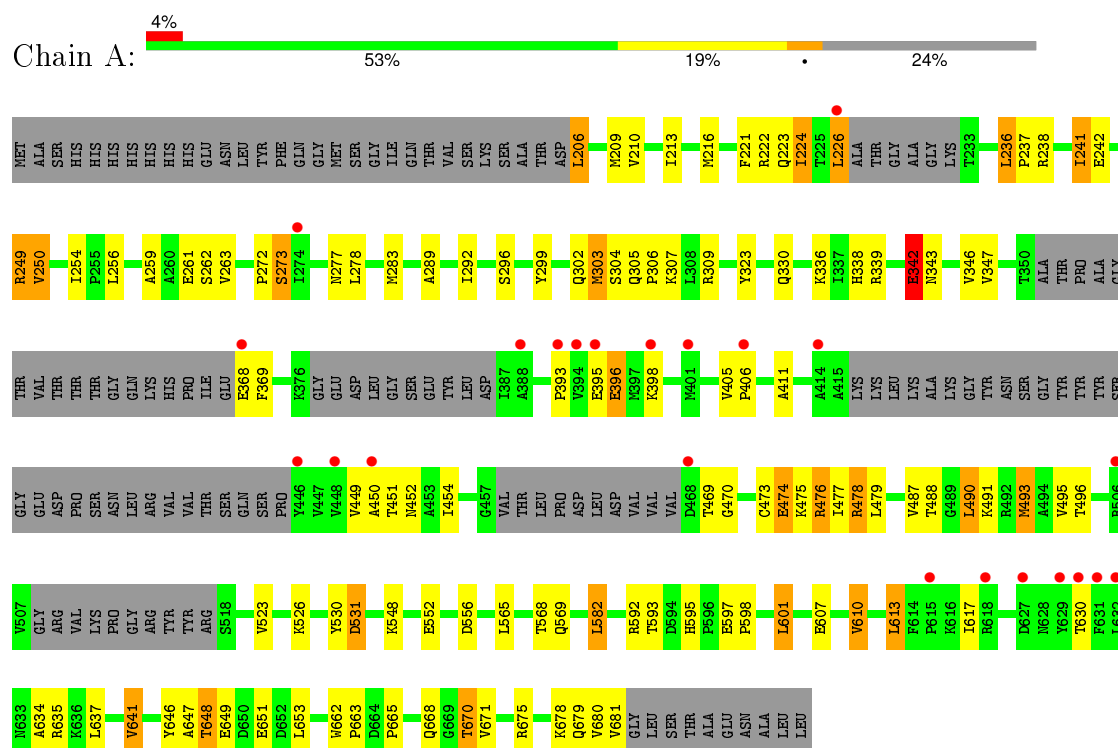
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O 1 1	0	0
2	B	4	Total O 4 4	0	0
2	C	7	Total O 7 7	0	0
2	D	5	Total O 5 5	0	0

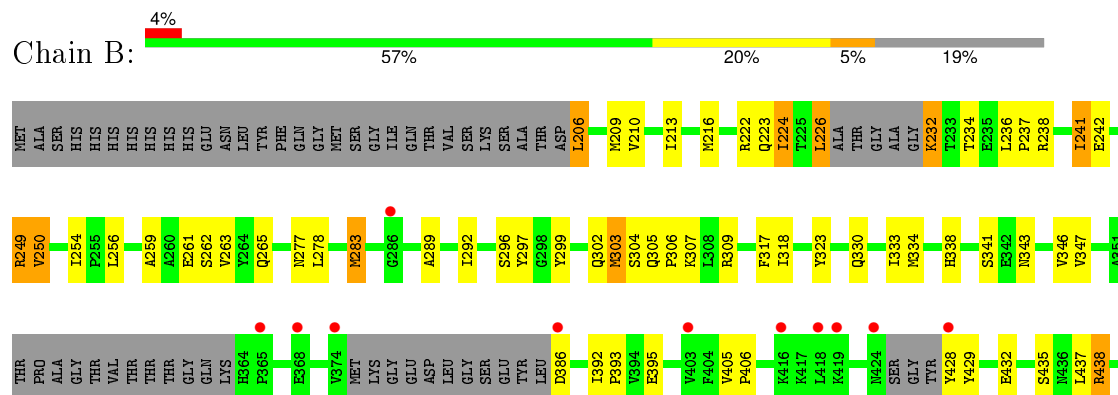
3 Residue-property plots [i](#)

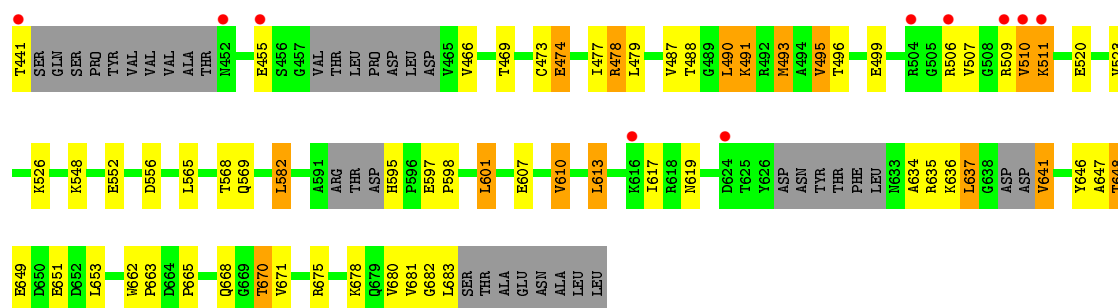
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

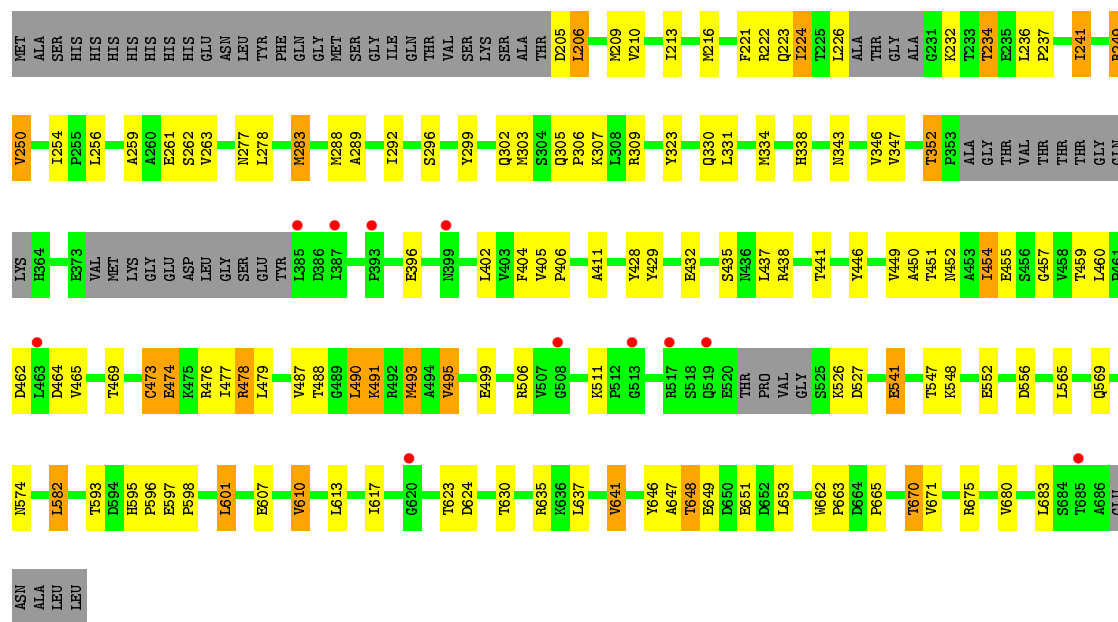


• Molecule 1: SERINE PROTEASE NS3

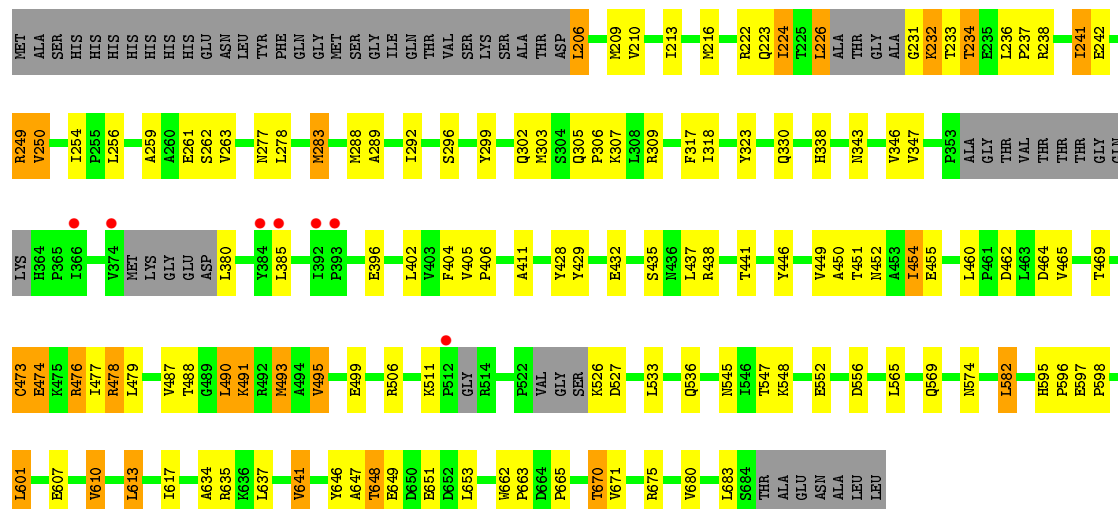




• Molecule 1: SERINE PROTEASE NS3



• Molecule 1: SERINE PROTEASE NS3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.63Å 96.30Å 97.61Å 91.23° 110.86° 107.62°	Depositor
Resolution (Å)	15.00 – 3.00 14.99 – 3.00	Depositor EDS
% Data completeness (in resolution range)	89.8 (15.00-3.00) 86.4 (14.99-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.11.4	Depositor
R, R_{free}	0.210 , 0.242 (Not available) , (Not available)	Depositor DCC
R_{free} test set	NotAvailable	DCC
Wilson B-factor (Å ²)	60.9	Xtriage
Anisotropy	0.752	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 63.0	EDS
Estimated twinning fraction	0.020 for -h,-l,-k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 39850 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13727	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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

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	1/3189 (0.0%)	0.68	4/4307 (0.1%)
1	B	0.46	0/3396	0.66	1/4578 (0.0%)
1	C	0.56	0/3671	0.71	3/4966 (0.1%)
1	D	0.53	0/3702	0.67	1/5008 (0.0%)
All	All	0.51	1/13958 (0.0%)	0.68	9/18859 (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	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	530	TYR	C-N	-5.28	1.21	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	530	TYR	N-CA-C	-10.60	82.38	111.00
1	C	623	THR	N-CA-C	6.88	129.59	111.00
1	A	530	TYR	C-N-CA	6.30	137.44	121.70
1	C	624	ASP	N-CA-CB	6.28	121.90	110.60
1	A	531	ASP	N-CA-CB	5.96	121.32	110.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	342	GLU	Sidechain

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	3135	0	3146	91	1
1	B	3339	0	3371	91	1
1	C	3603	0	3611	93	0
1	D	3633	0	3643	98	0
2	A	1	0	0	0	0
2	B	4	0	0	0	0
2	C	7	0	0	1	0
2	D	5	0	0	0	0
All	All	13727	0	13771	361	1

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 13.

The worst 5 of 361 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:C:450:ALA:CB	1:C:454:ILE:HG12	1.78	1.12
1:D:450:ALA:CB	1:D:454:ILE:HG12	1.79	1.12
1:D:665:PRO:HB3	1:D:670:THR:HG23	1.33	1.08
1:C:450:ALA:HB1	1:C:454:ILE:HG12	1.15	1.08
1:C:665:PRO:HB3	1:C:670:THR:HG23	1.34	1.08

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	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:ARG:O	1:B:265:GLN:OE1[1_565]	2.15	0.05

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	379/516 (73%)	370 (98%)	7 (2%)	2 (0%)	34	76
1	B	399/516 (77%)	388 (97%)	10 (2%)	1 (0%)	46	84
1	C	443/516 (86%)	426 (96%)	14 (3%)	3 (1%)	26	70
1	D	444/516 (86%)	430 (97%)	14 (3%)	0	100	100
All	All	1665/2064 (81%)	1614 (97%)	45 (3%)	6 (0%)	39	80

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	510	VAL
1	C	459	THR
1	A	273	SER
1	A	531	ASP
1	C	352	THR

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	342/442 (77%)	309 (90%)	33 (10%)	10	38
1	B	362/442 (82%)	322 (89%)	40 (11%)	8	30
1	C	393/442 (89%)	356 (91%)	37 (9%)	11	39
1	D	397/442 (90%)	361 (91%)	36 (9%)	12	41
All	All	1494/1768 (84%)	1348 (90%)	146 (10%)	10	36

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	637	LEU
1	C	249	ARG
1	D	495	VAL
1	B	641	VAL
1	C	206	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	324	HIS
1	C	574	ASN
1	D	588	ASN
1	C	338	HIS
1	C	343	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	393/516 (76%)	0.28	23 (5%)	26 10	45, 98, 155, 182	0
1	B	419/516 (81%)	0.24	21 (5%)	32 13	41, 98, 161, 188	0
1	C	453/516 (87%)	-0.01	11 (2%)	62 32	37, 73, 128, 163	0
1	D	456/516 (88%)	-0.00	7 (1%)	76 49	37, 73, 131, 158	0
All	All	1721/2064 (83%)	0.12	62 (3%)	46 20	37, 83, 148, 188	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	385	LEU	8.4
1	B	428	TYR	6.0
1	A	398	LYS	4.2
1	B	509	ARG	4.2
1	B	368	GLU	4.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.