



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 24, 2022 – 01:00 PM JST

PDB ID : 7YDG
Title : Crystal structure of human SARS2 catalytic domain with a disease related mutation
Authors : Wu, S.; Li, P.; Zhou, X.L.; Fang, P.
Deposited on : 2022-07-04
Resolution : 3.20 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

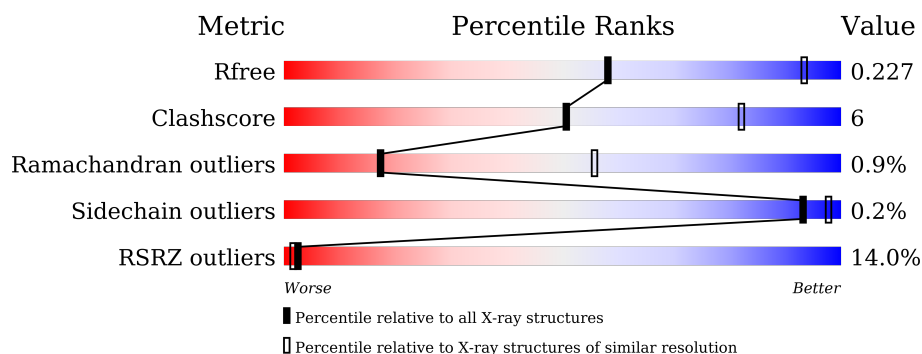
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	355	<div> <div>63%</div> <div>8%</div> <div>29%</div> </div>
1	B	355	<div> <div>62%</div> <div>8%</div> <div>29%</div> </div>
1	C	355	<div> <div>10%</div> <div>61%</div> <div>10%</div> <div>29%</div> </div>
1	D	355	<div> <div>27%</div> <div>59%</div> <div>11%</div> <div>29%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7952 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-tRNA ligase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			1988	1268	350	357	13			
1	B	252	Total	C	N	O	S	0	0	0
			1988	1268	350	357	13			
1	C	252	Total	C	N	O	S	0	0	0
			1988	1268	350	357	13			
1	D	252	Total	C	N	O	S	0	0	0
			1988	1268	350	357	13			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	168	MET	-	initiating methionine	UNP Q9NP81
A	169	GLY	-	expression tag	UNP Q9NP81
A	170	SER	-	expression tag	UNP Q9NP81
A	171	SER	-	expression tag	UNP Q9NP81
A	172	HIS	-	expression tag	UNP Q9NP81
A	173	HIS	-	expression tag	UNP Q9NP81
A	174	HIS	-	expression tag	UNP Q9NP81
A	175	HIS	-	expression tag	UNP Q9NP81
A	176	HIS	-	expression tag	UNP Q9NP81
A	177	HIS	-	expression tag	UNP Q9NP81
A	178	SER	-	expression tag	UNP Q9NP81
A	179	SER	-	expression tag	UNP Q9NP81
A	180	GLY	-	expression tag	UNP Q9NP81
A	218	ASN	-	insertion	UNP Q9NP81
A	219	LEU	-	insertion	UNP Q9NP81
A	220	SER	-	insertion	UNP Q9NP81
A	221	PRO	-	insertion	UNP Q9NP81
A	222	ARG	LYS	engineered mutation	UNP Q9NP81
B	168	MET	-	initiating methionine	UNP Q9NP81
B	169	GLY	-	expression tag	UNP Q9NP81
B	170	SER	-	expression tag	UNP Q9NP81

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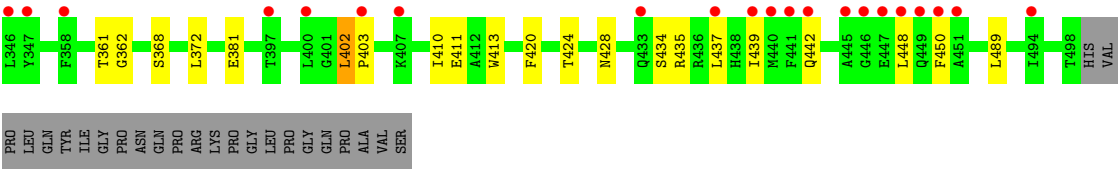
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Chain	Residue	Modelled	Actual	Comment	Reference
B	171	SER	-	expression tag	UNP Q9NP81
B	172	HIS	-	expression tag	UNP Q9NP81
B	173	HIS	-	expression tag	UNP Q9NP81
B	174	HIS	-	expression tag	UNP Q9NP81
B	175	HIS	-	expression tag	UNP Q9NP81
B	176	HIS	-	expression tag	UNP Q9NP81
B	177	HIS	-	expression tag	UNP Q9NP81
B	178	SER	-	expression tag	UNP Q9NP81
B	179	SER	-	expression tag	UNP Q9NP81
B	180	GLY	-	expression tag	UNP Q9NP81
B	218	ASN	-	insertion	UNP Q9NP81
B	219	LEU	-	insertion	UNP Q9NP81
B	220	SER	-	insertion	UNP Q9NP81
B	221	PRO	-	insertion	UNP Q9NP81
B	222	ARG	LYS	engineered mutation	UNP Q9NP81
C	168	MET	-	initiating methionine	UNP Q9NP81
C	169	GLY	-	expression tag	UNP Q9NP81
C	170	SER	-	expression tag	UNP Q9NP81
C	171	SER	-	expression tag	UNP Q9NP81
C	172	HIS	-	expression tag	UNP Q9NP81
C	173	HIS	-	expression tag	UNP Q9NP81
C	174	HIS	-	expression tag	UNP Q9NP81
C	175	HIS	-	expression tag	UNP Q9NP81
C	176	HIS	-	expression tag	UNP Q9NP81
C	177	HIS	-	expression tag	UNP Q9NP81
C	178	SER	-	expression tag	UNP Q9NP81
C	179	SER	-	expression tag	UNP Q9NP81
C	180	GLY	-	expression tag	UNP Q9NP81
C	218	ASN	-	insertion	UNP Q9NP81
C	219	LEU	-	insertion	UNP Q9NP81
C	220	SER	-	insertion	UNP Q9NP81
C	221	PRO	-	insertion	UNP Q9NP81
C	222	ARG	LYS	engineered mutation	UNP Q9NP81
D	168	MET	-	initiating methionine	UNP Q9NP81
D	169	GLY	-	expression tag	UNP Q9NP81
D	170	SER	-	expression tag	UNP Q9NP81
D	171	SER	-	expression tag	UNP Q9NP81
D	172	HIS	-	expression tag	UNP Q9NP81
D	173	HIS	-	expression tag	UNP Q9NP81
D	174	HIS	-	expression tag	UNP Q9NP81
D	175	HIS	-	expression tag	UNP Q9NP81
D	176	HIS	-	expression tag	UNP Q9NP81

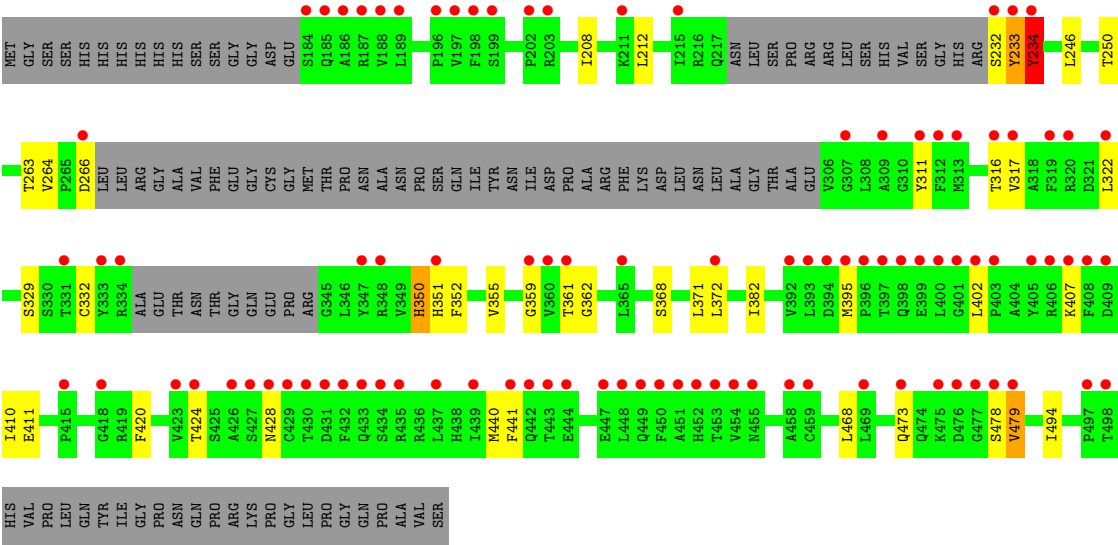
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Chain	Residue	Modelled	Actual	Comment	Reference
D	177	HIS	-	expression tag	UNP Q9NP81
D	178	SER	-	expression tag	UNP Q9NP81
D	179	SER	-	expression tag	UNP Q9NP81
D	180	GLY	-	expression tag	UNP Q9NP81
D	218	ASN	-	insertion	UNP Q9NP81
D	219	LEU	-	insertion	UNP Q9NP81
D	220	SER	-	insertion	UNP Q9NP81
D	221	PRO	-	insertion	UNP Q9NP81
D	222	ARG	LYS	engineered mutation	UNP Q9NP81



● Molecule 1: Serine–tRNA ligase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	144.18Å 144.18Å 245.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.45 – 3.20 49.91 – 3.20	Depositor EDS
% Data completeness (in resolution range)	85.6 (25.45-3.20) 85.6 (49.91-3.20)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.91 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.13	Depositor
R, R_{free}	0.203 , 0.228 0.205 , 0.227	Depositor DCC
R_{free} test set	2000 reflections (5.39%)	wwPDB-VP
Wilson B-factor (Å ²)	100.7	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 81.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7952	wwPDB-VP
Average B, all atoms (Å ²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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

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	0/2031	0.69	1/2744 (0.0%)
1	B	0.36	0/2031	0.71	0/2744
1	C	0.36	1/2031 (0.0%)	0.65	2/2744 (0.1%)
1	D	0.31	0/2031	0.68	5/2744 (0.2%)
All	All	0.35	1/8124 (0.0%)	0.68	8/10976 (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	D	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	311	TYR	CB-CG	-5.65	1.43	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	234	TYR	CA-CB-CG	11.28	134.84	113.40
1	D	234	TYR	CB-CG-CD2	-8.50	115.90	121.00
1	D	234	TYR	CB-CG-CD1	8.22	125.93	121.00
1	A	378	LEU	CB-CG-CD2	-6.87	99.32	111.00
1	D	234	TYR	N-CA-CB	-6.51	98.88	110.60
1	C	311	TYR	CB-CG-CD1	-6.31	117.21	121.00
1	D	234	TYR	CB-CA-C	5.51	121.42	110.40
1	C	311	TYR	CA-CB-CG	-5.48	102.99	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	233	TYR	Peptide
1	D	234	TYR	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	1988	0	1980	23	0
1	B	1988	0	1980	23	0
1	C	1988	0	1980	29	0
1	D	1988	0	1980	30	0
All	All	7952	0	7920	90	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 6.

All (90) 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:264:VAL:HG12	1:D:234:TYR:HE1	1.39	0.86
1:A:262:MET:HG3	1:B:234:TYR:HE1	1.49	0.78
1:A:262:MET:SD	1:B:234:TYR:CE1	2.79	0.76
1:A:262:MET:CG	1:B:234:TYR:HE1	1.99	0.74
1:C:322:LEU:HD13	1:C:362:GLY:HA2	1.71	0.72
1:A:262:MET:HG3	1:B:234:TYR:CE1	2.25	0.72
1:B:212:LEU:HD22	1:B:494:ILE:HG22	1.73	0.68
1:B:322:LEU:HD13	1:B:362:GLY:HA2	1.74	0.68
1:B:243:GLN:HG3	1:B:461:VAL:HG11	1.78	0.64
1:A:322:LEU:HD13	1:A:362:GLY:HA2	1.79	0.64
1:C:264:VAL:HG12	1:D:234:TYR:CE1	2.28	0.64
1:D:372:LEU:HD22	1:D:428:ASN:HB2	1.81	0.63
1:A:257:ARG:NH2	1:A:381:GLU:OE2	2.33	0.62
1:C:402:LEU:H	1:C:403:PRO:CD	2.13	0.60
1:A:402:LEU:H	1:A:403:PRO:HD2	1.67	0.60
1:C:264:VAL:HG13	1:C:328:CYS:SG	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:LEU:HD13	1:D:362:GLY:HA2	1.85	0.57
1:A:262:MET:SD	1:B:234:TYR:HE1	2.25	0.57
1:C:264:VAL:HA	1:D:234:TYR:CE1	2.39	0.57
1:C:411:GLU:HB3	1:C:420:PHE:HB3	1.86	0.57
1:C:216:ARG:HD2	1:C:234:TYR:CE2	2.39	0.57
1:C:257:ARG:NH2	1:C:381:GLU:OE2	2.39	0.55
1:A:262:MET:CG	1:B:234:TYR:CE1	2.84	0.55
1:A:411:GLU:HB3	1:A:420:PHE:HB3	1.89	0.54
1:C:372:LEU:HD22	1:C:428:ASN:HB2	1.90	0.54
1:C:216:ARG:O	1:C:217:GLN:HG2	2.08	0.54
1:D:232:SER:OG	1:D:233:TYR:N	2.41	0.54
1:D:411:GLU:HB3	1:D:420:PHE:HB3	1.89	0.54
1:C:402:LEU:H	1:C:403:PRO:HD2	1.71	0.53
1:D:317:VAL:O	1:D:441:PHE:HA	2.09	0.53
1:B:212:LEU:HD23	1:B:496:ALA:HB2	1.90	0.52
1:D:473:GLN:HA	1:D:479:VAL:HG22	1.92	0.52
1:B:184:SER:HA	1:B:399:GLU:HG3	1.92	0.51
1:B:347:TYR:OH	1:B:417:ARG:HG3	2.11	0.51
1:D:332:CYS:O	1:D:351:HIS:HA	2.11	0.50
1:A:392:VAL:HG22	1:A:410:ILE:HG12	1.93	0.49
1:D:395:MET:HB2	1:D:407:LYS:HB3	1.93	0.49
1:A:243:GLN:HG3	1:A:461:VAL:HG11	1.94	0.49
1:C:313:MET:HA	1:C:437:LEU:O	2.12	0.49
1:B:478:SER:O	1:B:479:VAL:HB	2.13	0.48
1:C:361:THR:HG21	1:C:368:SER:HA	1.95	0.48
1:C:265:PRO:HD2	1:D:234:TYR:CD1	2.48	0.48
1:A:361:THR:HG21	1:A:368:SER:HA	1.96	0.48
1:D:250:THR:HG23	1:D:382:ILE:HD13	1.95	0.48
1:C:234:TYR:HB2	1:D:311:TYR:CE1	2.49	0.48
1:D:212:LEU:HD22	1:D:494:ILE:HG22	1.95	0.48
1:A:324:VAL:O	1:A:359:GLY:HA2	2.14	0.48
1:A:184:SER:HA	1:A:399:GLU:OE1	2.14	0.47
1:B:392:VAL:HG22	1:B:410:ILE:HG12	1.95	0.47
1:D:246:LEU:HD21	1:D:468:LEU:HD11	1.95	0.47
1:B:361:THR:HG21	1:B:368:SER:HA	1.97	0.47
1:C:235:LEU:HB2	1:D:263:THR:CG2	2.44	0.47
1:A:255:LEU:HD21	1:A:261:PRO:HB3	1.98	0.46
1:B:243:GLN:CG	1:B:461:VAL:HG11	2.44	0.46
1:C:319:PHE:HB2	1:C:442:GLN:O	2.16	0.46
1:D:361:THR:HB	1:D:371:LEU:HD22	1.99	0.45
1:D:264:VAL:HG23	1:D:266:ASP:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:PHE:HB2	1:A:442:GLN:O	2.17	0.44
1:B:232:SER:OG	1:B:233:TYR:N	2.50	0.44
1:A:388:LEU:HD21	1:A:468:LEU:HD23	1.99	0.44
1:D:329:SER:HB2	1:D:355:VAL:HG22	1.99	0.44
1:C:489:LEU:HD23	1:C:489:LEU:HA	1.85	0.44
1:C:311:TYR:HE2	1:D:234:TYR:CE2	2.36	0.44
1:C:196:PRO:HD2	1:C:413:TRP:CD1	2.53	0.43
1:C:434:SER:HA	1:C:439:ILE:HB	2.01	0.43
1:A:257:ARG:HH22	1:A:381:GLU:CD	2.21	0.43
1:B:319:PHE:HB2	1:B:442:GLN:O	2.18	0.43
1:C:257:ARG:HH22	1:C:381:GLU:CD	2.22	0.43
1:A:254:LEU:CD2	1:A:378:LEU:HD13	2.49	0.43
1:C:410:ILE:HB	1:C:424:THR:HG22	2.01	0.42
1:D:359:GLY:HA3	1:D:371:LEU:HD21	2.01	0.42
1:D:316:THR:HA	1:D:440:MET:O	2.20	0.42
1:C:264:VAL:HA	1:D:234:TYR:CD1	2.55	0.42
1:A:402:LEU:H	1:A:403:PRO:CD	2.32	0.42
1:B:357:MET:HG3	1:B:458:ALA:HB2	2.02	0.41
1:D:208:ILE:HG21	1:D:479:VAL:HG21	2.02	0.41
1:C:435:ARG:HA	1:C:450:PHE:CE1	2.55	0.41
1:D:361:THR:HG21	1:D:368:SER:HA	2.03	0.41
1:B:411:GLU:HB3	1:B:420:PHE:HB3	2.03	0.41
1:A:441:PHE:CE2	1:A:443:THR:HG22	2.56	0.41
1:C:311:TYR:CE2	1:D:234:TYR:CE2	3.09	0.41
1:D:410:ILE:HB	1:D:424:THR:HG22	2.03	0.41
1:A:184:SER:OG	1:A:185:GLN:N	2.53	0.41
1:D:478:SER:HA	1:D:494:ILE:O	2.21	0.41
1:D:350:HIS:O	1:D:352:PHE:HD1	2.05	0.40
1:B:480:LEU:HA	1:B:480:LEU:HD23	1.86	0.40
1:C:184:SER:OG	1:C:185:GLN:N	2.54	0.40
1:C:316:THR:HG21	1:C:448:LEU:HD22	2.03	0.40
1:B:372:LEU:HD22	1:B:428:ASN:HB2	2.04	0.40
1:B:464:LEU:HA	1:B:464:LEU:HD23	1.82	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	244/355 (69%)	238 (98%)	5 (2%)	1 (0%)	34	69
1	B	244/355 (69%)	233 (96%)	8 (3%)	3 (1%)	13	49
1	C	244/355 (69%)	238 (98%)	5 (2%)	1 (0%)	34	69
1	D	244/355 (69%)	231 (95%)	9 (4%)	4 (2%)	9	43
All	All	976/1420 (69%)	940 (96%)	27 (3%)	9 (1%)	17	56

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	402	LEU
1	B	402	LEU
1	C	402	LEU
1	D	402	LEU
1	D	234	TYR
1	D	479	VAL
1	B	479	VAL
1	D	350	HIS
1	B	496	ALA

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	215/299 (72%)	215 (100%)	0	100	100
1	B	215/299 (72%)	215 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	215/299 (72%)	214 (100%)	1 (0%)	88	95
1	D	215/299 (72%)	214 (100%)	1 (0%)	88	95
All	All	860/1196 (72%)	858 (100%)	2 (0%)	93	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	311	TYR
1	D	234	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides 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 [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	252/355 (70%)	0.28	4 (1%) 72 59	46, 75, 148, 209	0
1	B	252/355 (70%)	0.34	4 (1%) 72 59	50, 86, 152, 203	0
1	C	252/355 (70%)	0.81	37 (14%) 2 1	75, 115, 198, 291	0
1	D	252/355 (70%)	1.68	96 (38%) 0 0	112, 183, 243, 290	0
All	All	1008/1420 (70%)	0.78	141 (13%) 2 1	46, 108, 218, 291	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	403	PRO	9.4
1	D	408	PHE	9.3
1	D	426	ALA	8.4
1	D	184	SER	8.3
1	D	347	TYR	8.3
1	D	198	PHE	7.2
1	D	396	PRO	6.5
1	D	452	HIS	6.3
1	C	346	LEU	5.9
1	C	433	GLN	5.5
1	C	312	PHE	5.5
1	C	448	LEU	5.2
1	D	397	THR	5.2
1	D	234	TYR	5.1
1	D	312	PHE	5.1
1	D	427	SER	4.9
1	C	403	PRO	4.8
1	D	196	PRO	4.8
1	C	309	ALA	4.7
1	D	359	GLY	4.7
1	D	398	GLN	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	477	GLY	4.6
1	D	360	VAL	4.5
1	D	458	ALA	4.5
1	D	393	LEU	4.5
1	D	394	ASP	4.4
1	D	311	TYR	4.4
1	D	439	ILE	4.3
1	C	451	ALA	4.3
1	C	307	GLY	4.3
1	C	445	ALA	4.2
1	D	351	HIS	4.2
1	D	497	PRO	4.2
1	D	395	MET	4.1
1	D	185	GLN	4.1
1	D	319	PHE	4.0
1	D	232	SER	3.9
1	D	475	LYS	3.9
1	D	186	ALA	3.9
1	C	313	MET	3.9
1	D	406	ARG	3.8
1	C	347	TYR	3.8
1	D	188	VAL	3.8
1	A	400	LEU	3.8
1	D	451	ALA	3.8
1	D	320	ARG	3.8
1	C	450	PHE	3.8
1	C	266	ASP	3.7
1	D	450	PHE	3.7
1	D	405	TYR	3.7
1	D	402	LEU	3.7
1	C	442	GLN	3.6
1	C	439	ILE	3.6
1	D	407	LYS	3.6
1	D	309	ALA	3.5
1	D	453	THR	3.5
1	D	203	ARG	3.4
1	D	348	ARG	3.4
1	D	409	ASP	3.3
1	C	333	TYR	3.3
1	D	365	LEU	3.3
1	D	197	VAL	3.3
1	D	333	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	478	SER	3.2
1	C	447	GLU	3.2
1	D	202	PRO	3.2
1	C	233	TYR	3.2
1	D	392	VAL	3.2
1	D	442	GLN	3.1
1	C	400	LEU	3.1
1	D	399	GLU	3.1
1	C	441	PHE	3.0
1	D	199	SER	3.0
1	C	316	THR	3.0
1	D	428	ASN	3.0
1	C	397	THR	3.0
1	D	459	CYS	3.0
1	C	449	GLN	3.0
1	D	313	MET	3.0
1	D	441	PHE	2.9
1	C	437	LEU	2.8
1	D	430	THR	2.8
1	D	211	LYS	2.8
1	A	347	TYR	2.8
1	D	431	ASP	2.8
1	D	444	GLU	2.8
1	D	435	ARG	2.8
1	D	454	VAL	2.8
1	D	449	GLN	2.8
1	D	401	GLY	2.7
1	D	443	THR	2.7
1	D	400	LEU	2.7
1	D	266	ASP	2.7
1	D	317	VAL	2.7
1	B	437	LEU	2.6
1	D	479	VAL	2.6
1	B	312	PHE	2.6
1	D	423	VAL	2.6
1	D	187	ARG	2.6
1	D	476	ASP	2.6
1	D	429	CYS	2.6
1	D	433	GLN	2.5
1	A	333	TYR	2.5
1	C	494	ILE	2.5
1	C	215	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	334	ARG	2.5
1	D	437	LEU	2.5
1	D	331	THR	2.5
1	D	455	ASN	2.5
1	C	446	GLY	2.5
1	D	316	THR	2.4
1	D	448	LEU	2.4
1	C	329	SER	2.4
1	D	361	THR	2.4
1	D	469	LEU	2.4
1	D	447	GLU	2.3
1	C	317	VAL	2.3
1	D	424	THR	2.3
1	D	415	PRO	2.3
1	C	234	TYR	2.3
1	D	307	GLY	2.2
1	D	498	THR	2.2
1	D	322	LEU	2.2
1	C	306	VAL	2.2
1	C	310	GLY	2.2
1	A	350	HIS	2.2
1	D	473	GLN	2.2
1	D	233	TYR	2.2
1	D	215	ILE	2.2
1	C	440	MET	2.1
1	B	351	HIS	2.1
1	C	358	PHE	2.1
1	D	418	GLY	2.1
1	D	434	SER	2.1
1	D	334	ARG	2.1
1	D	372	LEU	2.1
1	D	432	PHE	2.0
1	C	314	ASP	2.0
1	B	306	VAL	2.0
1	D	189	LEU	2.0
1	C	407	LYS	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 [i](#)

There are no monosaccharides 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.