



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 12:18 am BST

PDB ID : 6DQW
Title : Flavobacterium johnsoniae class Id ribonucleotide reductase alpha subunit
Authors : Maggiolo, A.O.; Boal, A.K.
Deposited on : 2018-06-11
Resolution : 2.60 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 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	:	2.11
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)	:	2.11

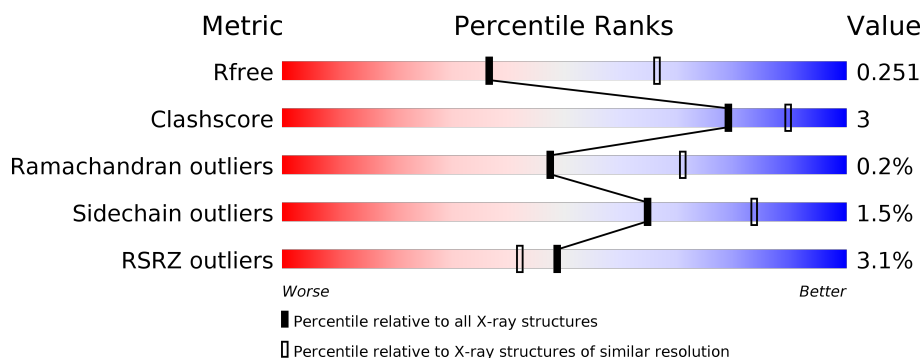
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 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	585	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; bottom: 0; left: 82%; width: 14%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; bottom: 0; left: 96%; width: 4%; height: 10px; background-color: grey;"></div> </div> <div> % 82% • 14% </div> </div>
1	B	585	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; bottom: 0; left: 79%; width: 7%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; bottom: 0; left: 86%; width: 14%; height: 10px; background-color: grey;"></div> </div> <div> % 79% 7% • 14% </div> </div>
1	C	585	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; bottom: 0; left: 79%; width: 6%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; bottom: 0; left: 85%; width: 15%; height: 10px; background-color: grey;"></div> </div> <div> 2% 79% 6% • 15% </div> </div>
1	D	585	<div> <div style="width: 100%; height: 10px; position: relative;"> <div style="position: absolute; top: -10px; left: 0; width: 100%; height: 10px; background-color: red;"></div> <div style="position: absolute; bottom: 0; left: 0; width: 100%; height: 10px; background-color: green;"></div> <div style="position: absolute; bottom: 0; left: 60%; width: 6%; height: 10px; background-color: yellow;"></div> <div style="position: absolute; bottom: 0; left: 66%; width: 33%; height: 10px; background-color: grey;"></div> </div> <div> 5% 60% 6% • 33% </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15313 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 Ribonucleoside-diphosphate reductase, alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	0	0
			4034	2565	684	760	25			
1	B	504	Total	C	N	O	S	0	0	0
			4026	2560	683	759	24			
1	C	499	Total	C	N	O	S	0	0	0
			3992	2542	675	750	25			
1	D	392	Total	C	N	O	S	0	0	0
			3127	2006	525	578	18			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP A5FCJ4
A	-18	GLY	-	expression tag	UNP A5FCJ4
A	-17	SER	-	expression tag	UNP A5FCJ4
A	-16	SER	-	expression tag	UNP A5FCJ4
A	-15	HIS	-	expression tag	UNP A5FCJ4
A	-14	HIS	-	expression tag	UNP A5FCJ4
A	-13	HIS	-	expression tag	UNP A5FCJ4
A	-12	HIS	-	expression tag	UNP A5FCJ4
A	-11	HIS	-	expression tag	UNP A5FCJ4
A	-10	HIS	-	expression tag	UNP A5FCJ4
A	-9	SER	-	expression tag	UNP A5FCJ4
A	-8	SER	-	expression tag	UNP A5FCJ4
A	-7	GLY	-	expression tag	UNP A5FCJ4
A	-6	LEU	-	expression tag	UNP A5FCJ4
A	-5	VAL	-	expression tag	UNP A5FCJ4
A	-4	PRO	-	expression tag	UNP A5FCJ4
A	-3	ARG	-	expression tag	UNP A5FCJ4
A	-2	GLY	-	expression tag	UNP A5FCJ4
A	-1	SER	-	expression tag	UNP A5FCJ4
A	0	HIS	-	expression tag	UNP A5FCJ4
B	-19	MET	-	initiating methionine	UNP A5FCJ4

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP A5FCJ4
B	-17	SER	-	expression tag	UNP A5FCJ4
B	-16	SER	-	expression tag	UNP A5FCJ4
B	-15	HIS	-	expression tag	UNP A5FCJ4
B	-14	HIS	-	expression tag	UNP A5FCJ4
B	-13	HIS	-	expression tag	UNP A5FCJ4
B	-12	HIS	-	expression tag	UNP A5FCJ4
B	-11	HIS	-	expression tag	UNP A5FCJ4
B	-10	HIS	-	expression tag	UNP A5FCJ4
B	-9	SER	-	expression tag	UNP A5FCJ4
B	-8	SER	-	expression tag	UNP A5FCJ4
B	-7	GLY	-	expression tag	UNP A5FCJ4
B	-6	LEU	-	expression tag	UNP A5FCJ4
B	-5	VAL	-	expression tag	UNP A5FCJ4
B	-4	PRO	-	expression tag	UNP A5FCJ4
B	-3	ARG	-	expression tag	UNP A5FCJ4
B	-2	GLY	-	expression tag	UNP A5FCJ4
B	-1	SER	-	expression tag	UNP A5FCJ4
B	0	HIS	-	expression tag	UNP A5FCJ4
C	-19	MET	-	initiating methionine	UNP A5FCJ4
C	-18	GLY	-	expression tag	UNP A5FCJ4
C	-17	SER	-	expression tag	UNP A5FCJ4
C	-16	SER	-	expression tag	UNP A5FCJ4
C	-15	HIS	-	expression tag	UNP A5FCJ4
C	-14	HIS	-	expression tag	UNP A5FCJ4
C	-13	HIS	-	expression tag	UNP A5FCJ4
C	-12	HIS	-	expression tag	UNP A5FCJ4
C	-11	HIS	-	expression tag	UNP A5FCJ4
C	-10	HIS	-	expression tag	UNP A5FCJ4
C	-9	SER	-	expression tag	UNP A5FCJ4
C	-8	SER	-	expression tag	UNP A5FCJ4
C	-7	GLY	-	expression tag	UNP A5FCJ4
C	-6	LEU	-	expression tag	UNP A5FCJ4
C	-5	VAL	-	expression tag	UNP A5FCJ4
C	-4	PRO	-	expression tag	UNP A5FCJ4
C	-3	ARG	-	expression tag	UNP A5FCJ4
C	-2	GLY	-	expression tag	UNP A5FCJ4
C	-1	SER	-	expression tag	UNP A5FCJ4
C	0	HIS	-	expression tag	UNP A5FCJ4
D	-19	MET	-	initiating methionine	UNP A5FCJ4
D	-18	GLY	-	expression tag	UNP A5FCJ4
D	-17	SER	-	expression tag	UNP A5FCJ4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP A5FCJ4
D	-15	HIS	-	expression tag	UNP A5FCJ4
D	-14	HIS	-	expression tag	UNP A5FCJ4
D	-13	HIS	-	expression tag	UNP A5FCJ4
D	-12	HIS	-	expression tag	UNP A5FCJ4
D	-11	HIS	-	expression tag	UNP A5FCJ4
D	-10	HIS	-	expression tag	UNP A5FCJ4
D	-9	SER	-	expression tag	UNP A5FCJ4
D	-8	SER	-	expression tag	UNP A5FCJ4
D	-7	GLY	-	expression tag	UNP A5FCJ4
D	-6	LEU	-	expression tag	UNP A5FCJ4
D	-5	VAL	-	expression tag	UNP A5FCJ4
D	-4	PRO	-	expression tag	UNP A5FCJ4
D	-3	ARG	-	expression tag	UNP A5FCJ4
D	-2	GLY	-	expression tag	UNP A5FCJ4
D	-1	SER	-	expression tag	UNP A5FCJ4
D	0	HIS	-	expression tag	UNP A5FCJ4

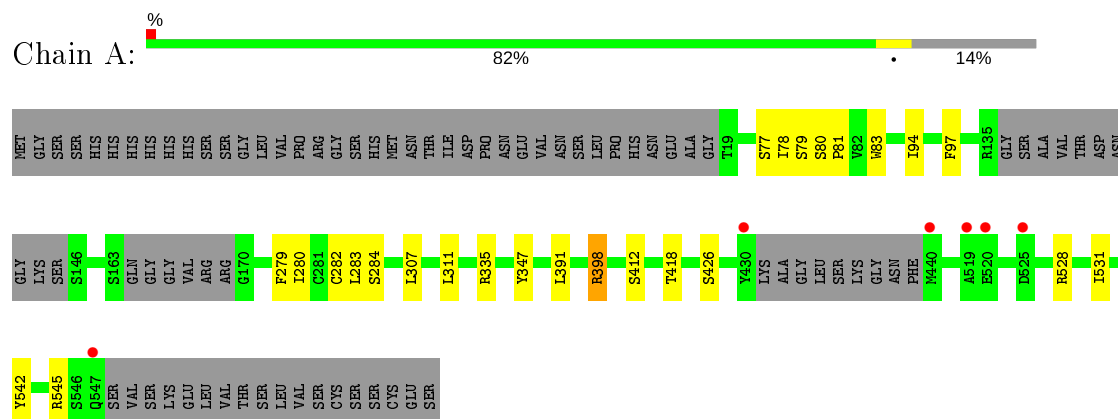
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	60	Total O 60 60	0	0
2	B	43	Total O 43 43	0	0
2	C	26	Total O 26 26	0	0
2	D	5	Total O 5 5	0	0

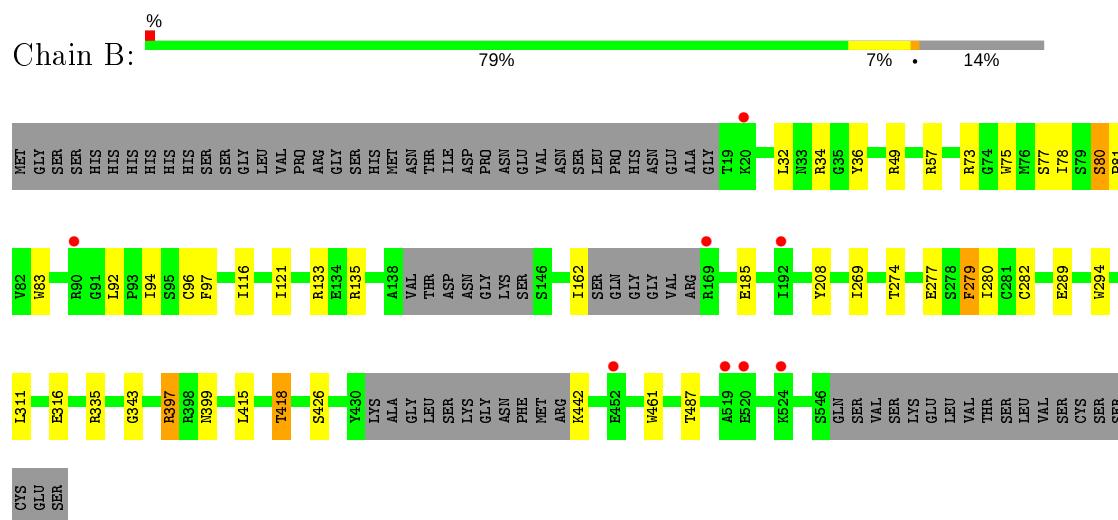
3 Residue-property plots [i](#)

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

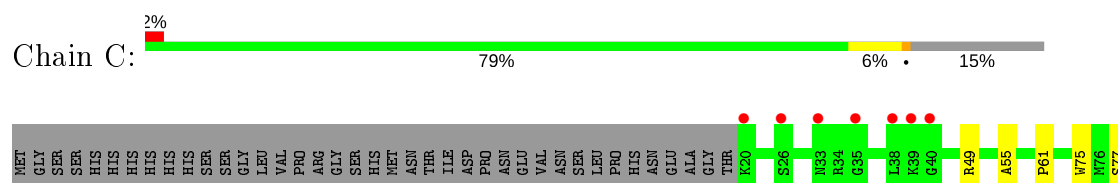
- Molecule 1: Ribonucleoside-diphosphate reductase, alpha chain



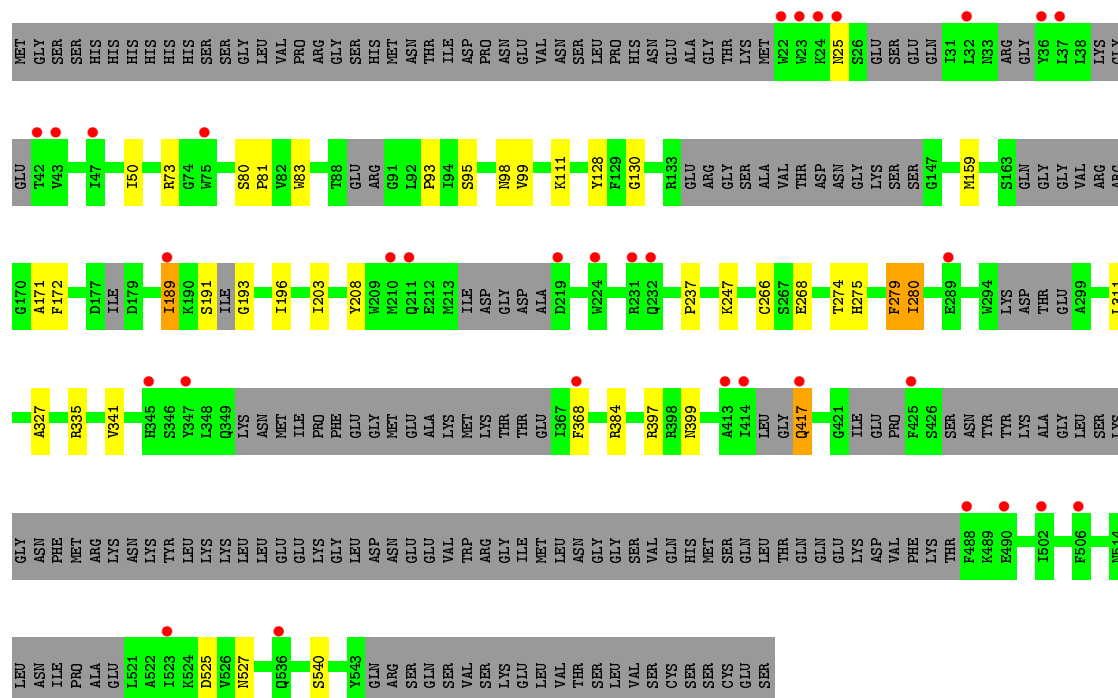
- Molecule 1: Ribonucleoside-diphosphate reductase, alpha chain



- Molecule 1: Ribonucleoside-diphosphate reductase, alpha chain



Chain D:  5% 60% 6% 33%



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	161.03Å 161.03Å 187.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.53 – 2.60 46.49 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.53-2.60) 99.8 (46.49-2.60)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.33 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.8.0222	Depositor
R, R_{free}	0.206 , 0.251 0.209 , 0.251	Depositor DCC
R_{free} test set	4248 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	39.2	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.021 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	15313	wwPDB-VP
Average B, all atoms (Å ²)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.53% 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	0.42	0/4113	0.56	0/5534
1	B	0.39	0/4105	0.56	0/5524
1	C	0.38	0/4070	0.54	0/5475
1	D	0.35	0/3183	0.52	0/4275
All	All	0.39	0/15471	0.55	0/20808

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
1	B	0	4
1	C	0	1
1	D	0	1
All	All	0	7

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	545	ARG	Sidechain
1	B	133	ARG	Sidechain
1	B	397	ARG	Sidechain
1	B	49	ARG	Sidechain
1	B	73	ARG	Sidechain
1	C	49	ARG	Sidechain
1	D	384	ARG	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	4034	0	4015	13	0
1	B	4026	0	4006	30	0
1	C	3992	0	3975	19	0
1	D	3127	0	3096	22	0
2	A	60	0	0	0	0
2	B	43	0	0	1	0
2	C	26	0	0	1	0
2	D	5	0	0	1	0
All	All	15313	0	15092	84	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 3.

All (84) 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:57:ARG:NH1	1:B:316:GLU:OE1	2.11	0.83
1:B:94:ILE:HG21	1:B:280:ILE:HD11	1.70	0.73
1:B:94:ILE:CG2	1:B:280:ILE:HD11	2.20	0.72
1:B:97:PHE:CE1	1:B:280:ILE:HD13	2.25	0.70
1:B:397:ARG:NH2	2:B:601:HOH:O	2.06	0.69
1:B:96:CYS:O	1:B:280:ILE:HD12	1.93	0.69
1:D:417:GLN:N	1:D:417:GLN:HE21	1.91	0.68
1:C:116:ILE:HG23	1:C:162:ILE:HD13	1.75	0.68
1:A:311:LEU:HD21	1:A:335:ARG:HA	1.79	0.64
1:D:203:ILE:HD13	1:D:237:PRO:CG	2.30	0.62
1:A:79:SER:OG	1:A:283:LEU:O	2.18	0.62
1:B:97:PHE:CD1	1:B:280:ILE:HD13	2.34	0.62
1:A:80:SER:N	1:A:81:PRO:HD2	2.15	0.61
1:B:94:ILE:HG21	1:B:280:ILE:CD1	2.31	0.61
1:D:191:SER:O	1:D:193:GLY:N	2.34	0.61
1:B:80:SER:N	1:B:81:PRO:HD2	2.16	0.61
1:A:97:PHE:CD1	1:A:280:ILE:HG22	2.37	0.59
1:C:397:ARG:NH1	2:C:601:HOH:O	2.38	0.57
1:D:266:CYS:HB2	1:D:268:GLU:OE2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:ARG:HH11	1:A:531:ILE:HG21	1.73	0.54
1:B:94:ILE:CD1	1:B:282:CYS:HB3	2.37	0.54
1:B:311:LEU:HD21	1:B:335:ARG:HA	1.91	0.53
1:D:203:ILE:HD13	1:D:237:PRO:HG3	1.89	0.53
1:B:78:ILE:HG13	1:B:83:TRP:CD1	2.44	0.53
1:B:34:ARG:O	1:B:34:ARG:HG3	2.10	0.52
1:D:280:ILE:HG21	1:D:327:ALA:HB1	1.92	0.51
1:D:99:VAL:HG11	1:D:111:LYS:HB3	1.93	0.51
1:C:77:SER:OG	1:C:411:SER:HB3	2.11	0.50
1:A:94:ILE:CD1	1:A:282:CYS:HB3	2.41	0.49
1:D:189:ILE:O	1:D:196:ILE:O	2.32	0.47
1:D:203:ILE:HD12	1:D:203:ILE:N	2.29	0.47
1:C:78:ILE:HG13	1:C:83:TRP:CD1	2.49	0.47
1:B:77:SER:HB3	1:B:415:LEU:HD22	1.96	0.47
1:A:412:SER:HB2	1:A:418:THR:O	2.15	0.47
1:B:116:ILE:HG12	1:B:162:ILE:CD1	2.44	0.47
1:C:311:LEU:HD21	1:C:335:ARG:HA	1.95	0.47
1:C:236:LEU:HB3	1:C:237:PRO:HA	1.97	0.47
1:C:98:ASN:HB2	1:C:279:PHE:CZ	2.50	0.46
1:D:99:VAL:HG13	1:D:111:LYS:HD2	1.97	0.46
1:D:128:TYR:CZ	1:D:130:GLY:HA3	2.50	0.46
1:A:311:LEU:CD2	1:A:335:ARG:HA	2.44	0.46
1:B:92:LEU:HD12	1:B:121:ILE:HD13	1.97	0.45
1:A:78:ILE:HG13	1:A:83:TRP:CD1	2.52	0.45
1:D:80:SER:N	1:D:81:PRO:CD	2.78	0.45
1:B:397:ARG:HD2	1:B:399:ASN:O	2.16	0.45
1:D:159:MET:SD	1:D:172:PHE:HB2	2.56	0.45
1:B:426:SER:O	1:B:487:THR:HB	2.15	0.45
1:A:398:ARG:HG3	1:A:398:ARG:O	2.17	0.45
1:C:80:SER:HB2	1:C:81:PRO:HD3	1.99	0.45
1:C:341:VAL:HG21	1:C:368:PHE:HZ	1.82	0.45
1:C:427:SER:HA	1:C:487:THR:HG21	1.99	0.44
1:B:135:ARG:NH1	1:B:185:GLU:OE1	2.51	0.44
1:B:75:TRP:CD2	1:B:294:TRP:HB3	2.52	0.44
1:C:459:GLU:HG3	1:C:462:ARG:HH22	1.82	0.44
1:D:397:ARG:HD2	1:D:399:ASN:O	2.18	0.43
1:B:116:ILE:HG23	1:B:162:ILE:HD13	1.99	0.43
1:D:341:VAL:HG21	1:D:368:PHE:HZ	1.83	0.43
1:B:279:PHE:CD1	1:B:279:PHE:C	2.92	0.43
1:C:101:VAL:HG12	1:C:132:LEU:HD11	2.01	0.43
1:B:94:ILE:HG22	1:B:280:ILE:HD11	1.98	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:208:TYR:C	1:C:208:TYR:CD1	2.92	0.43
1:D:397:ARG:NH2	2:D:601:HOH:O	2.50	0.43
1:B:289:GLU:OE1	1:B:418:THR:HG23	2.18	0.42
1:C:532:GLU:OE2	1:C:536:GLN:NE2	2.52	0.42
1:B:442:LYS:HE2	1:B:461:TRP:CD2	2.54	0.42
1:A:284:SER:HB2	1:A:307:LEU:HD21	2.01	0.42
1:C:128:TYR:CZ	1:C:130:GLY:HA3	2.53	0.42
1:B:96:CYS:SG	1:B:269:ILE:HG13	2.60	0.42
1:B:343:GLY:HA2	1:B:418:THR:HG22	2.01	0.42
1:D:274:THR:HG22	1:D:275:HIS:N	2.35	0.41
1:D:50:ILE:HD11	1:D:83:TRP:HA	2.02	0.41
1:B:274:THR:OG1	1:B:277:GLU:HB2	2.20	0.41
1:D:311:LEU:HD21	1:D:335:ARG:HA	2.02	0.41
1:B:415:LEU:HA	1:B:415:LEU:HD12	1.96	0.41
1:C:209:TRP:CE2	1:C:220:LYS:HG3	2.55	0.41
1:C:55:ALA:HB1	1:C:61:PRO:HA	2.03	0.41
1:C:75:TRP:CD2	1:C:294:TRP:HB3	2.56	0.41
1:D:159:MET:CE	1:D:171:ALA:N	2.83	0.41
1:A:347:TYR:CD2	1:A:347:TYR:C	2.94	0.41
1:B:32:LEU:O	1:B:36:TYR:HB2	2.20	0.41
1:C:280:ILE:HD13	1:C:314:PHE:CE2	2.55	0.41
1:D:247:LYS:HE2	1:D:247:LYS:HA	2.03	0.41
1:A:391:LEU:HA	1:A:391:LEU:HD23	1.86	0.41
1:D:98:ASN:CB	1:D:279:PHE:CZ	3.04	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	496/585 (85%)	479 (97%)	16 (3%)	1 (0%)	47 71

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	496/585 (85%)	481 (97%)	15 (3%)	0	100	100
1	C	489/585 (84%)	474 (97%)	15 (3%)	0	100	100
1	D	360/585 (62%)	346 (96%)	12 (3%)	2 (1%)	25	47
All	All	1841/2340 (79%)	1780 (97%)	58 (3%)	3 (0%)	47	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	25	ASN
1	A	542	TYR
1	D	93	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	437/505 (86%)	433 (99%)	4 (1%)	78	91
1	B	435/505 (86%)	431 (99%)	4 (1%)	78	91
1	C	432/505 (86%)	426 (99%)	6 (1%)	67	85
1	D	337/505 (67%)	327 (97%)	10 (3%)	41	67
All	All	1641/2020 (81%)	1617 (98%)	24 (2%)	65	83

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	SER
1	A	279	PHE
1	A	398	ARG
1	A	426	SER
1	B	80	SER
1	B	208	TYR
1	B	279	PHE
1	B	418	THR

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Mol	Chain	Res	Type
1	C	134	GLU
1	C	135	ARG
1	C	208	TYR
1	C	279	PHE
1	C	397	ARG
1	C	411	SER
1	D	73	ARG
1	D	95	SER
1	D	189	ILE
1	D	208	TYR
1	D	279	PHE
1	D	280	ILE
1	D	417	GLN
1	D	525	ASP
1	D	527	ASN
1	D	540	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	233	GLN
1	D	527	ASN

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 ⓘ

There are no ligands in this entry.

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	504/585 (86%)	-0.09	6 (1%) 79 76	24, 36, 59, 87	0
1	B	504/585 (86%)	-0.07	8 (1%) 72 68	24, 37, 65, 89	0
1	C	499/585 (85%)	-0.00	12 (2%) 59 53	27, 43, 68, 83	0
1	D	392/585 (67%)	0.33	32 (8%) 11 8	40, 65, 95, 117	0
All	All	1899/2340 (81%)	0.02	58 (3%) 49 42	24, 43, 81, 117	0

All (58) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	523	ILE	4.3
1	D	345	HIS	3.8
1	A	547	GLN	3.8
1	D	506	PHE	3.7
1	D	490	GLU	3.5
1	B	169	ARG	3.3
1	C	20	LYS	3.3
1	C	26	SER	3.3
1	D	37	LEU	3.2
1	C	38	LEU	3.2
1	A	440	MET	3.0
1	D	425	PHE	3.0
1	D	23	TRP	2.9
1	D	536	GLN	2.9
1	A	525	ASP	2.8
1	D	289	GLU	2.8
1	C	133	ARG	2.8
1	D	232	GLN	2.8
1	B	520	GLU	2.7
1	D	211	GLN	2.7
1	D	413	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	192	ILE	2.5
1	D	189	ILE	2.5
1	D	219	ASP	2.5
1	A	520	GLU	2.4
1	C	33	ASN	2.4
1	D	25	ASN	2.4
1	D	488	PHE	2.4
1	D	75	TRP	2.3
1	C	40	GLY	2.3
1	C	462	ARG	2.3
1	D	22	TRP	2.3
1	D	417	GLN	2.3
1	D	47	ILE	2.3
1	C	91	GLY	2.3
1	D	32	LEU	2.3
1	A	430	TYR	2.3
1	D	502	ILE	2.3
1	C	146	SER	2.3
1	B	20	LYS	2.2
1	B	524	LYS	2.2
1	C	466	LEU	2.2
1	C	39	LYS	2.2
1	D	414	ILE	2.2
1	C	35	GLY	2.2
1	D	43	VAL	2.1
1	D	210	MET	2.1
1	D	224	TRP	2.1
1	D	368	PHE	2.1
1	B	519	ALA	2.1
1	D	231	ARG	2.1
1	A	519	ALA	2.1
1	B	90	ARG	2.1
1	D	42	THR	2.1
1	B	452	GLU	2.0
1	D	347	TYR	2.0
1	D	24	LYS	2.0
1	D	36	TYR	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 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.