



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2021 – 08:07 AM JST

PDB ID : 7F9N
Title : Crystal structure of the variable region of Plasmodium RIFIN #4 (PF3D7_1000500) in complex with LAIR1
Authors : Xie, Y.; Song, H.; Li, X.; Qi, J.; Gao, G.F.
Deposited on : 2021-07-04
Resolution : 3.00 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

<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 : 2.23.1
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) : 2.23.1

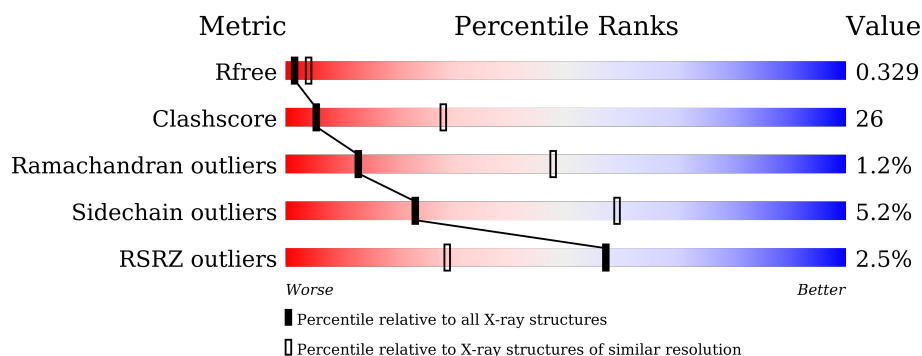
1 Overall quality at a glance

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))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 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	175	 9% 52% 34% •• 10%
1	B	175	 54% 33% • 10%
2	C	112	 54% 30% •• 12%
2	D	112	 9% 42% 39% •• 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3875 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 Rifin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	0	0	0
			1169	730	207	226	6			
1	B	158	Total	C	N	O	S	0	0	0
			1169	730	207	226	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	149	HIS	-	expression tag	UNP A0A143ZWD5
A	150	MET	-	expression tag	UNP A0A143ZWD5
A	151	HIS	-	expression tag	UNP A0A143ZWD5
A	152	HIS	-	expression tag	UNP A0A143ZWD5
A	153	HIS	-	expression tag	UNP A0A143ZWD5
A	154	HIS	-	expression tag	UNP A0A143ZWD5
A	155	HIS	-	expression tag	UNP A0A143ZWD5
A	156	HIS	-	expression tag	UNP A0A143ZWD5
B	149	HIS	-	expression tag	UNP A0A143ZWD5
B	150	MET	-	expression tag	UNP A0A143ZWD5
B	151	HIS	-	expression tag	UNP A0A143ZWD5
B	152	HIS	-	expression tag	UNP A0A143ZWD5
B	153	HIS	-	expression tag	UNP A0A143ZWD5
B	154	HIS	-	expression tag	UNP A0A143ZWD5
B	155	HIS	-	expression tag	UNP A0A143ZWD5
B	156	HIS	-	expression tag	UNP A0A143ZWD5

- Molecule 2 is a protein called Leukocyte-associated immunoglobulin-like receptor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	98	Total	C	N	O	S	0	0	0
			773	482	133	156	2			
2	D	97	Total	C	N	O	S	0	0	0
			764	477	132	153	2			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	14	HIS	-	expression tag	UNP Q6GTX8
C	15	MET	-	expression tag	UNP Q6GTX8
C	16	HIS	-	expression tag	UNP Q6GTX8
C	17	HIS	-	expression tag	UNP Q6GTX8
C	18	HIS	-	expression tag	UNP Q6GTX8
C	19	HIS	-	expression tag	UNP Q6GTX8
C	20	HIS	-	expression tag	UNP Q6GTX8
C	21	HIS	-	expression tag	UNP Q6GTX8
C	123	ALA	-	expression tag	UNP Q6GTX8
C	124	ALA	-	expression tag	UNP Q6GTX8
C	125	ALA	-	expression tag	UNP Q6GTX8
D	14	HIS	-	expression tag	UNP Q6GTX8
D	15	MET	-	expression tag	UNP Q6GTX8
D	16	HIS	-	expression tag	UNP Q6GTX8
D	17	HIS	-	expression tag	UNP Q6GTX8
D	18	HIS	-	expression tag	UNP Q6GTX8
D	19	HIS	-	expression tag	UNP Q6GTX8
D	20	HIS	-	expression tag	UNP Q6GTX8
D	21	HIS	-	expression tag	UNP Q6GTX8
D	123	ALA	-	expression tag	UNP Q6GTX8
D	124	ALA	-	expression tag	UNP Q6GTX8
D	125	ALA	-	expression tag	UNP Q6GTX8



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	73.44Å 73.44Å 341.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.67 – 3.00 49.67 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.67-3.00) 99.6 (49.67-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.14 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.264 , 0.330 0.264 , 0.329	Depositor DCC
R_{free} test set	996 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	108.3	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 72.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	3875	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.03% 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	0.52	0/1180	0.74	3/1596 (0.2%)
1	B	0.43	0/1180	0.65	0/1596
2	C	0.65	1/792 (0.1%)	0.98	6/1077 (0.6%)
2	D	0.44	0/783	0.73	1/1065 (0.1%)
All	All	0.51	1/3935 (0.0%)	0.77	10/5334 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	50	ARG	CZ-NH2	5.56	1.40	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	50	ARG	NE-CZ-NH2	-12.39	114.10	120.30
2	C	50	ARG	NE-CZ-NH1	-11.05	114.78	120.30
2	C	50	ARG	NH1-CZ-NH2	8.43	128.68	119.40
1	A	266	LEU	CA-CB-CG	7.28	132.03	115.30
1	A	260	ILE	CG1-CB-CG2	-6.40	97.33	111.40
2	C	102	ILE	CG1-CB-CG2	-5.93	98.35	111.40
2	C	50	ARG	CB-CG-CD	-5.62	97.00	111.60
1	A	273	LEU	CB-CG-CD1	-5.27	102.03	111.00
2	D	105	LYS	CD-CE-NZ	-5.25	99.64	111.70
2	C	25	ASP	C-N-CA	-5.15	108.83	121.70

There are no chirality outliers.

There are no planarity outliers.

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	1169	0	1216	59	0
1	B	1169	0	1216	63	2
2	C	773	0	738	32	0
2	D	764	0	734	52	2
All	All	3875	0	3904	202	2

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 26.

All (202) 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)
2:D:100:ARG:NH2	2:D:115:TYR:CE2	2.05	1.22
2:D:100:ARG:NH2	2:D:115:TYR:HE2	1.42	1.16
2:C:102:ILE:HD11	2:C:112:GLN:HA	1.46	0.97
1:A:179:ALA:HA	1:A:309:ILE:HD11	1.44	0.97
2:C:32:SER:OG	2:C:50:ARG:NH1	1.98	0.96
1:B:235:ILE:HD11	1:B:279:VAL:HG11	1.47	0.95
1:B:260:ILE:HD12	1:B:261:ASN:N	1.85	0.92
1:B:264:THR:HG23	1:B:265:VAL:HG23	1.53	0.90
1:A:295:ASN:O	1:A:299:LYS:HE2	1.70	0.89
2:C:102:ILE:HD11	2:C:112:GLN:HG2	1.55	0.86
1:B:198:ILE:HD11	1:B:290:ALA:HA	1.57	0.86
1:B:260:ILE:HD12	1:B:261:ASN:H	1.42	0.83
2:D:46:THR:HA	2:D:87:ARG:HB2	1.61	0.82
2:D:100:ARG:HD2	2:D:112:GLN:NE2	1.97	0.80
1:B:235:ILE:HD11	1:B:279:VAL:CG1	2.11	0.79
2:D:93:GLU:HB2	2:D:120:VAL:HG11	1.65	0.78
2:D:49:CYS:HG	2:D:101:CYS:HG	1.27	0.78
1:B:179:ALA:HA	1:B:309:ILE:HD11	1.66	0.78
1:A:227:ARG:HA	1:A:227:ARG:HE	1.48	0.77
2:C:62:ARG:NH1	2:C:96:ALA:O	2.14	0.77
2:D:49:CYS:HB3	2:D:101:CYS:SG	2.25	0.76
2:D:55:VAL:HA	2:D:105:LYS:HG3	1.66	0.76
1:A:295:ASN:O	1:A:299:LYS:CE	2.34	0.74
1:B:232:SER:O	1:B:236:ILE:HG13	1.88	0.73
2:D:104:TYR:HB2	2:D:109:TRP:CD2	2.24	0.73
1:B:168:LYS:H	1:B:168:LYS:HD3	1.54	0.72
1:A:295:ASN:HB3	1:A:299:LYS:NZ	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LEU:HB2	1:A:272:ASN:HB2	1.71	0.72
2:D:50:ARG:HE	2:D:81:GLU:HG3	1.55	0.71
1:B:179:ALA:CA	1:B:309:ILE:HD11	2.20	0.71
1:B:219:VAL:O	1:B:222:THR:HG22	1.91	0.71
1:A:267:ARG:HG2	1:A:268:ASN:N	2.06	0.70
1:B:179:ALA:CB	1:B:309:ILE:HD11	2.22	0.69
2:D:100:ARG:NH2	2:D:115:TYR:CZ	2.60	0.69
2:D:53:VAL:O	2:D:105:LYS:NZ	2.27	0.68
1:A:206:LEU:HD12	1:A:261:ASN:HB3	1.75	0.66
2:C:102:ILE:CD1	2:C:112:GLN:HA	2.25	0.66
1:A:295:ASN:HB3	1:A:299:LYS:HZ1	1.58	0.66
1:A:180:LEU:HD12	1:B:307:VAL:HG12	1.77	0.66
2:C:102:ILE:HD11	2:C:112:GLN:CA	2.25	0.66
2:D:60:LEU:HD23	2:D:86:PHE:CD2	2.32	0.65
1:A:239:ARG:C	1:A:239:ARG:HH21	2.00	0.65
1:A:263:GLY:O	1:A:272:ASN:ND2	2.31	0.64
1:A:307:VAL:HG23	1:B:172:ILE:HB	1.79	0.64
2:D:93:GLU:N	2:D:93:GLU:OE1	2.30	0.64
1:A:295:ASN:CA	1:A:299:LYS:HZ3	2.12	0.63
2:D:49:CYS:CB	2:D:101:CYS:HG	2.11	0.63
2:D:88:ILE:HD12	2:D:89:ASP:H	1.63	0.63
1:A:295:ASN:O	1:A:299:LYS:NZ	2.32	0.62
2:C:102:ILE:HG22	2:C:109:TRP:CE3	2.34	0.62
2:D:38:VAL:C	2:D:39:ILE:HD12	2.20	0.62
2:D:50:ARG:HH21	2:D:83:GLU:HB3	1.65	0.62
2:D:100:ARG:HB2	2:D:112:GLN:OE1	2.01	0.61
1:B:179:ALA:HB2	1:B:309:ILE:HD11	1.81	0.61
1:B:196:MET:HE1	1:B:223:GLY:O	2.00	0.61
1:A:264:THR:OG1	1:A:265:VAL:HG23	2.02	0.60
2:C:102:ILE:HG22	2:C:109:TRP:HE3	1.66	0.60
2:D:49:CYS:CB	2:D:101:CYS:SG	2.90	0.59
1:B:253:ASP:N	1:B:253:ASP:OD1	2.30	0.59
2:C:102:ILE:CD1	2:C:112:GLN:HG2	2.32	0.59
1:A:183:GLY:HA2	1:A:305:VAL:CG1	2.33	0.58
1:B:210:LYS:HE3	1:B:210:LYS:HA	1.84	0.58
2:D:100:ARG:HH22	2:D:115:TYR:HE2	1.46	0.58
2:C:38:VAL:C	2:C:39:ILE:HD12	2.24	0.58
1:A:267:ARG:HG2	1:A:268:ASN:H	1.68	0.58
1:A:224:ASP:OD2	1:A:227:ARG:HG2	2.04	0.57
2:D:75:SER:O	2:D:83:GLU:HG2	2.04	0.57
2:D:95:ASN:O	2:D:99:TYR:OH	2.09	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:52:PRO:O	2:D:82:SER:OG	2.15	0.57
1:B:226:THR:O	1:B:229:ILE:HG22	2.04	0.57
1:B:212:VAL:CG2	1:B:235:ILE:HG22	2.35	0.57
2:D:50:ARG:NH1	2:D:81:GLU:O	2.38	0.57
2:D:50:ARG:HH12	2:D:77:ALA:H	1.51	0.56
1:B:259:ASN:O	1:B:264:THR:HG22	2.05	0.56
1:A:212:VAL:HG13	1:A:215:ILE:HB	1.86	0.56
1:B:310:THR:O	1:B:314:THR:HG22	2.05	0.56
2:D:50:ARG:NH2	2:D:83:GLU:OE2	2.39	0.56
2:C:29:PRO:HG3	2:C:103:TYR:CD1	2.42	0.54
1:A:314:THR:HA	1:A:317:ILE:HD12	1.89	0.54
1:B:235:ILE:HD12	1:B:236:ILE:N	2.21	0.54
1:A:179:ALA:CA	1:A:309:ILE:HD11	2.29	0.54
1:A:211:LEU:HA	1:A:242:MET:HE1	1.89	0.54
1:A:265:VAL:HG12	1:A:265:VAL:O	2.09	0.53
1:A:252:LYS:NZ	1:A:253:ASP:OD2	2.41	0.53
1:B:211:LEU:HA	1:B:242:MET:HE2	1.90	0.53
1:B:309:ILE:C	1:B:309:ILE:HD12	2.29	0.52
1:A:263:GLY:C	1:A:272:ASN:HD22	2.13	0.52
1:B:212:VAL:HG23	1:B:235:ILE:HG22	1.90	0.52
1:B:235:ILE:HA	1:B:238:LYS:HB2	1.91	0.51
2:D:112:GLN:NE2	2:D:113:SER:O	2.43	0.51
1:A:266:LEU:HB3	1:A:270:LYS:O	2.09	0.51
1:A:274:PRO:O	1:A:276:LYS:N	2.43	0.51
1:B:273:LEU:O	1:B:275:ASP:N	2.42	0.51
2:D:62:ARG:NH1	2:D:96:ALA:O	2.45	0.50
2:C:88:ILE:HD12	2:C:89:ASP:H	1.77	0.49
1:A:232:SER:HB2	1:A:279:VAL:HG12	1.95	0.49
2:C:32:SER:HG	2:C:50:ARG:HH11	1.60	0.49
1:A:250:LEU:HB3	1:A:254:MET:HE3	1.93	0.49
2:C:28:ARG:NH2	2:C:114:ASP:OD1	2.43	0.49
2:C:61:GLU:OE1	2:C:112:GLN:NE2	2.46	0.49
1:A:187:GLY:HA2	1:A:301:THR:OG1	2.12	0.48
1:A:274:PRO:C	1:A:276:LYS:H	2.16	0.48
1:B:276:LYS:HG3	1:B:277:GLU:OE1	2.13	0.48
2:D:88:ILE:CD1	2:D:89:ASP:H	2.26	0.48
1:A:295:ASN:C	1:A:299:LYS:HZ3	2.16	0.48
2:C:39:ILE:HG23	2:C:43:SER:HB2	1.96	0.48
2:C:63:GLU:OE1	2:C:65:ARG:HB2	2.13	0.48
2:D:30:SER:O	2:D:49:CYS:HA	2.13	0.48
2:D:87:ARG:HG2	2:D:88:ILE:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:305:VAL:HG23	1:A:308:LYS:NZ	2.29	0.47
1:B:168:LYS:O	1:B:172:ILE:HG12	2.14	0.47
2:D:104:TYR:HB2	2:D:109:TRP:CG	2.50	0.47
1:B:236:ILE:HD13	1:B:276:LYS:HA	1.95	0.47
2:C:100:ARG:HD3	2:C:115:TYR:CE1	2.50	0.47
1:A:239:ARG:O	1:A:239:ARG:NH2	2.48	0.47
1:A:200:ILE:O	1:A:204:LYS:HG3	2.15	0.47
1:B:183:GLY:HA2	1:B:305:VAL:CG2	2.45	0.47
2:C:27:PRO:HG2	2:C:52:PRO:HD3	1.97	0.46
2:D:50:ARG:NH2	2:D:83:GLU:HB3	2.31	0.46
1:A:259:ASN:HB3	1:A:265:VAL:CG2	2.46	0.46
1:A:295:ASN:CB	1:A:299:LYS:NZ	2.77	0.46
1:B:211:LEU:HA	1:B:211:LEU:HD12	1.82	0.46
2:D:62:ARG:O	2:D:67:THR:OG1	2.29	0.46
2:D:88:ILE:HD12	2:D:89:ASP:N	2.29	0.46
1:A:309:ILE:O	1:A:313:GLN:HG2	2.16	0.46
1:B:238:LYS:O	1:B:242:MET:HG3	2.15	0.46
1:B:222:THR:HG23	1:B:223:GLY:O	2.16	0.46
1:A:217:LYS:HE3	1:A:221:SER:HB3	1.98	0.46
2:D:27:PRO:HG2	2:D:52:PRO:HD3	1.98	0.46
2:D:36:GLY:O	2:D:39:ILE:HD11	2.16	0.45
1:A:242:MET:HE3	1:A:250:LEU:HD11	1.98	0.45
1:B:233:LYS:H	1:B:233:LYS:HD3	1.81	0.45
2:D:50:ARG:HE	2:D:81:GLU:CG	2.26	0.45
1:A:300:ASP:O	1:A:303:GLN:HG2	2.16	0.45
1:A:307:VAL:CG2	1:B:172:ILE:HB	2.44	0.45
2:C:39:ILE:CG2	2:C:43:SER:HB2	2.46	0.45
1:A:224:ASP:OD2	1:A:226:THR:HG23	2.17	0.45
2:D:55:VAL:HG21	2:D:103:TYR:HB2	1.97	0.45
1:A:250:LEU:HD13	1:A:254:MET:CE	2.47	0.45
1:B:268:ASN:OD1	1:B:269:GLY:N	2.49	0.45
1:B:279:VAL:O	1:B:283:LEU:HD12	2.16	0.45
2:D:34:GLU:OE2	2:D:35:PRO:HA	2.17	0.44
1:A:203:LEU:HD13	1:A:215:ILE:HG13	1.98	0.44
1:A:273:LEU:HB2	1:A:274:PRO:HD2	2.00	0.44
1:B:277:GLU:OE1	1:B:277:GLU:N	2.50	0.44
1:B:235:ILE:HD12	1:B:235:ILE:C	2.37	0.44
2:C:119:LEU:HD12	2:C:119:LEU:N	2.32	0.44
1:B:179:ALA:HB2	1:B:309:ILE:CD1	2.47	0.44
2:C:102:ILE:HD13	2:C:102:ILE:HA	1.63	0.44
2:D:76:GLN:HG2	2:D:81:GLU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:HIS:O	1:A:197:ASN:N	2.51	0.44
2:D:55:VAL:HG11	2:D:58:PHE:CE2	2.53	0.44
2:D:72:GLU:N	2:D:72:GLU:OE2	2.51	0.44
1:B:200:ILE:O	1:B:204:LYS:HG3	2.17	0.43
1:A:172:ILE:CD1	1:A:314:THR:HG22	2.48	0.43
2:C:63:GLU:HG3	2:C:66:SER:OG	2.18	0.43
1:B:223:GLY:O	1:B:224:ASP:C	2.56	0.43
1:B:265:VAL:HG12	1:B:265:VAL:O	2.18	0.43
1:A:313:GLN:O	1:A:316:ALA:N	2.50	0.43
1:B:259:ASN:HB3	1:B:265:VAL:CG2	2.48	0.43
1:B:195:GLY:O	1:B:199:VAL:HG13	2.19	0.43
2:C:111:GLU:H	2:C:111:GLU:HG2	1.66	0.43
1:B:217:LYS:HE3	1:B:221:SER:OG	2.19	0.43
2:C:59:ARG:HA	2:C:69:ASN:O	2.19	0.43
2:C:106:PRO:HA	2:C:107:PRO:HA	1.74	0.43
2:C:58:PHE:CE1	2:C:103:TYR:HB3	2.54	0.42
1:B:217:LYS:HD2	1:B:217:LYS:HA	1.63	0.42
2:D:50:ARG:HH11	2:D:81:GLU:HG2	1.84	0.42
2:D:58:PHE:CD1	2:D:103:TYR:HB3	2.53	0.42
1:A:274:PRO:HG3	2:C:104:TYR:CD2	2.54	0.42
1:B:198:ILE:HD11	1:B:290:ALA:CA	2.40	0.42
1:B:211:LEU:HD21	1:B:239:ARG:HB2	2.01	0.42
2:C:93:GLU:H	2:C:93:GLU:HG2	1.61	0.42
2:C:102:ILE:CG2	2:C:109:TRP:CE3	3.01	0.42
1:B:279:VAL:HB	1:B:280:PRO:HD3	2.01	0.42
1:B:227:ARG:HA	1:B:227:ARG:HD2	1.84	0.42
1:B:266:LEU:HB2	1:B:272:ASN:HB2	2.01	0.42
1:A:262:LEU:O	1:A:278:ALA:HB1	2.20	0.42
1:A:273:LEU:HD12	1:A:277:GLU:HB3	2.02	0.42
1:B:308:LYS:HZ2	1:B:312:GLN:HB3	1.83	0.42
1:A:219:VAL:O	1:A:222:THR:HG22	2.20	0.42
2:C:54:GLY:O	2:C:105:LYS:HD3	2.20	0.42
1:A:199:VAL:HG21	1:A:225:TYR:HB2	2.02	0.41
1:A:318:ASN:O	1:A:322:THR:HG23	2.20	0.41
1:B:228:VAL:HA	1:B:231:PHE:CE1	2.55	0.41
1:A:211:LEU:HA	1:A:242:MET:CE	2.49	0.41
2:C:28:ARG:HG3	2:C:28:ARG:HH21	1.85	0.41
1:B:212:VAL:HG21	1:B:235:ILE:HG22	2.03	0.41
1:B:217:LYS:NZ	1:B:220:SER:OG	2.33	0.41
1:B:233:LYS:HD3	1:B:233:LYS:N	2.35	0.41
1:B:171:ALA:HB1	1:B:317:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LYS:O	1:A:177:GLU:HG3	2.21	0.41
2:D:43:SER:OG	2:D:44:HIS:N	2.54	0.41
2:D:104:TYR:CE1	2:D:106:PRO:HA	2.56	0.41
1:B:172:ILE:O	1:B:176:THR:HG23	2.21	0.41
1:B:229:ILE:HD13	1:B:284:ASN:OD1	2.21	0.41
2:D:49:CYS:HB3	2:D:101:CYS:CB	2.51	0.41
2:D:29:PRO:O	2:D:113:SER:HB2	2.20	0.40
2:D:88:ILE:HD12	2:D:88:ILE:HA	1.85	0.40
1:A:199:VAL:HG22	1:A:286:LEU:CD2	2.51	0.40
2:D:56:GLN:HG3	2:D:104:TYR:O	2.21	0.40
1:B:279:VAL:O	1:B:280:PRO:C	2.60	0.40

All (2) 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:B:178:TYR:OH	2:D:100:ARG:NH1[6_464]	2.06	0.14
1:B:178:TYR:OH	2:D:100:ARG:NH2[6_464]	2.17	0.03

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	156/175 (89%)	138 (88%)	17 (11%)	1 (1%)	25	64
1	B	156/175 (89%)	142 (91%)	11 (7%)	3 (2%)	8	36
2	C	96/112 (86%)	89 (93%)	6 (6%)	1 (1%)	15	53
2	D	95/112 (85%)	88 (93%)	6 (6%)	1 (1%)	14	50
All	All	503/574 (88%)	457 (91%)	40 (8%)	6 (1%)	13	48

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	267	ARG
1	A	267	ARG
2	D	73	ASP
1	B	224	ASP
1	B	266	LEU
2	C	63	GLU

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	124/137 (90%)	116 (94%)	8 (6%)	17	50
1	B	124/137 (90%)	120 (97%)	4 (3%)	39	74
2	C	88/99 (89%)	86 (98%)	2 (2%)	50	80
2	D	87/99 (88%)	79 (91%)	8 (9%)	9	34
All	All	423/472 (90%)	401 (95%)	22 (5%)	23	59

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	227	ARG
1	A	239	ARG
1	A	252	LYS
1	A	267	ARG
1	A	273	LEU
1	A	299	LYS
1	A	304	SER
1	A	308	LYS
1	B	168	LYS
1	B	233	LYS
1	B	267	ARG
1	B	312	GLN
2	C	50	ARG
2	C	75	SER
2	D	32	SER
2	D	49	CYS

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Mol	Chain	Res	Type
2	D	50	ARG
2	D	76	GLN
2	D	78	SER
2	D	87	ARG
2	D	105	LYS
2	D	112	GLN

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

Mol	Chain	Res	Type
1	A	214	ASN
1	A	272	ASN
1	B	192	ASN
1	B	312	GLN
2	C	112	GLN

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 ⓘ

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	158/175 (90%)	-0.11	1 (0%) 89 72	80, 98, 119, 135	0
1	B	158/175 (90%)	-0.10	1 (0%) 89 72	99, 117, 134, 169	0
2	C	98/112 (87%)	-0.02	1 (1%) 82 59	78, 99, 129, 152	0
2	D	97/112 (86%)	0.66	10 (10%) 6 2	111, 154, 201, 221	0
All	All	511/574 (89%)	0.06	13 (2%) 57 29	78, 111, 171, 221	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	166	VAL	4.5
2	D	58	PHE	4.4
2	D	54	GLY	3.2
2	D	81	GLU	2.8
2	D	26	LEU	2.8
2	D	55	VAL	2.8
2	D	47	PHE	2.6
2	C	25	ASP	2.5
2	D	109	TRP	2.3
1	B	166	VAL	2.3
2	D	56	GLN	2.2
2	D	75	SER	2.2
2	D	27	PRO	2.1

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.