



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 18, 2026 – 07:56 PM UTC

PDB ID : 8W3Q / pdb_00008w3q
Title : Crystal structure of prefusion-stabilized hMPV F protein UFCM1-P2-iSS
Authors : Lee, Y.Z.; Stanfield, R.L.; Wilson, I.A.; Zhu, J.
Deposited on : 2024-02-22
Resolution : 5.99 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

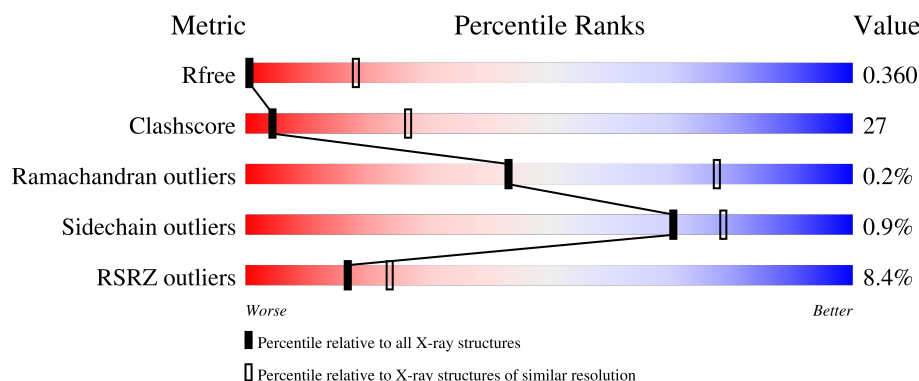
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.99 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}	180053	1143 (8.00-4.00)
Clashscore	190562	1210 (8.00-4.00)
Ramachandran outliers	187476	1034 (8.00-4.00)
Sidechain outliers	187428	1000 (8.00-4.00)
RSRZ outliers	180081	1136 (8.00-4.00)

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	F	514	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 3149 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.

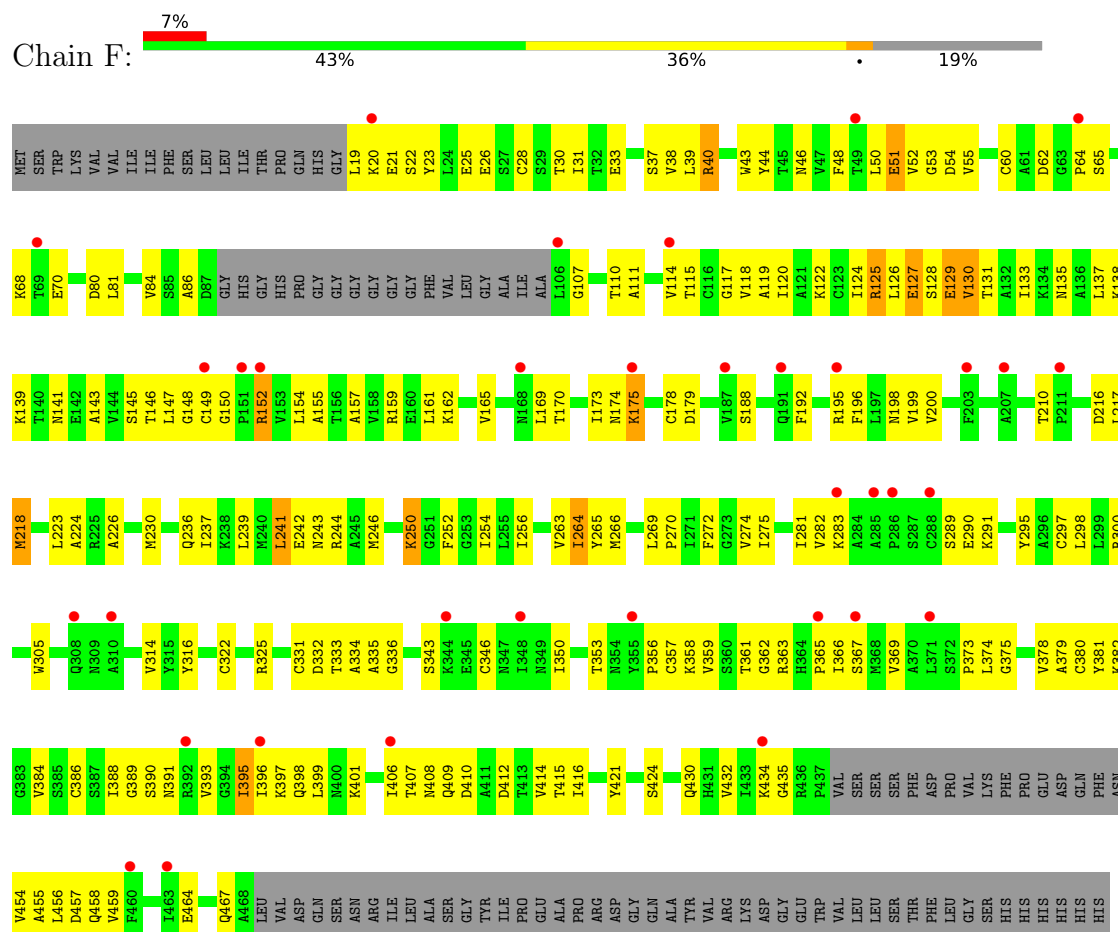
- Molecule 1 is a protein called prefusion-stabilized hMPV F protein UFCM1-P2-iSS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	F	416	3149	1967	543	614	25	0	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: prefusion-stabilized hMPV F protein UFCM1-P2-iSS



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	185.75Å 185.75Å 185.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.64 – 5.99 49.64 – 5.99	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.64-5.99) 99.6 (49.64-5.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 6.15Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.224 , 0.355 0.222 , 0.360	Depositor DCC
R_{free} test set	131 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	308.1	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 266.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.077 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	3149	wwPDB-VP
Average B, all atoms (Å ²)	252.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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	F	0.87	2/3191 (0.1%)	1.43	30/4322 (0.7%)

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	F	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	143	ALA	C-N	9.41	1.52	1.33
1	F	126	LEU	C-N	6.14	1.42	1.33

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	143	ALA	O-C-N	10.63	133.99	123.46
1	F	51	GLU	CA-CB-CG	7.89	129.87	114.10
1	F	363	ARG	N-CA-C	7.52	122.65	113.17
1	F	218	MET	CB-CG-SD	-7.33	90.69	112.70
1	F	86	ALA	N-CA-C	-6.94	99.04	109.94
1	F	107	GLY	CA-C-N	6.75	134.11	121.97
1	F	107	GLY	C-N-CA	6.75	134.11	121.97
1	F	343	SER	CA-C-N	-6.27	110.16	121.14
1	F	343	SER	C-N-CA	-6.27	110.16	121.14
1	F	363	ARG	N-CA-CB	-6.22	101.29	110.49
1	F	421	TYR	CA-C-N	-5.95	110.77	122.02
1	F	421	TYR	C-N-CA	-5.95	110.77	122.02
1	F	395	ILE	N-CA-CB	5.93	117.60	110.31
1	F	175	LYS	N-CA-CB	-5.90	103.14	112.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	70	GLU	CA-CB-CG	5.88	125.86	114.10
1	F	169	LEU	CA-CB-CG	5.72	136.33	116.30
1	F	264	ILE	N-CA-C	5.68	116.04	107.75
1	F	362	GLY	CA-C-N	5.64	131.85	122.54
1	F	362	GLY	C-N-CA	5.64	131.85	122.54
1	F	398	GLN	CA-CB-CG	5.50	125.11	114.10
1	F	40	ARG	CG-CD-NE	5.33	123.72	112.00
1	F	241	LEU	CA-CB-CG	-5.25	97.92	116.30
1	F	250	LYS	CA-CB-CG	5.20	124.51	114.10
1	F	129	GLU	O-C-N	5.20	128.13	122.20
1	F	467	GLN	N-CA-C	5.19	119.69	112.90
1	F	54	ASP	CB-CA-C	5.17	119.94	111.41
1	F	28	CYS	CA-CB-SG	5.08	126.09	114.40
1	F	38	VAL	N-CA-C	-5.07	98.77	106.42
1	F	464	GLU	CA-CB-CG	5.05	124.20	114.10
1	F	138	LYS	N-CA-C	-5.02	105.88	111.36

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	125	ARG	Sidechain
1	F	152	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	F	3149	0	3167	168	0
All	All	3149	0	3167	168	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 27.

All (168) 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:F:60:CYS:HB2	1:F:68:LYS:HG3	1.36	1.04
1:F:217:LEU:O	1:F:265:TYR:OH	1.85	0.95
1:F:137:LEU:HD11	1:F:155:ALA:HB1	1.51	0.93
1:F:407:THR:HG22	1:F:409:GLN:H	1.38	0.89
1:F:218:MET:HE2	1:F:223:LEU:HA	1.56	0.88
1:F:81:LEU:HD22	1:F:200:VAL:HG22	1.58	0.86
1:F:356:PRO:HB2	1:F:455:ALA:HB1	1.58	0.84
1:F:23:TYR:HD2	1:F:432:VAL:HG22	1.41	0.83
1:F:388:ILE:HG22	1:F:414:VAL:HG22	1.60	0.82
1:F:390:SER:HB3	1:F:393:VAL:HG22	1.64	0.80
1:F:358:LYS:HA	1:F:455:ALA:HA	1.64	0.79
1:F:366:ILE:HG22	1:F:367:SER:H	1.47	0.79
1:F:146:THR:HA	1:F:152:ARG:H	1.51	0.76
1:F:369:VAL:HG23	1:F:416:ILE:HD11	1.67	0.75
1:F:55:VAL:HG12	1:F:165:VAL:HG11	1.69	0.75
1:F:165:VAL:O	1:F:170:THR:OG1	2.03	0.73
1:F:37:SER:HB2	1:F:39:LEU:HG	1.71	0.73
1:F:359:VAL:HG22	1:F:456:LEU:HA	1.70	0.72
1:F:455:ALA:HB3	1:F:458:GLN:HG3	1.72	0.71
1:F:250:LYS:HB2	1:F:270:PRO:HG3	1.72	0.71
1:F:39:LEU:HB2	1:F:274:VAL:HB	1.71	0.70
1:F:366:ILE:HG22	1:F:367:SER:N	2.08	0.69
1:F:243:ASN:HB3	1:F:246:MET:CE	2.23	0.69
1:F:295:TYR:CD2	1:F:365:PRO:HB3	2.28	0.68
1:F:147:LEU:HB3	1:F:150:GLY:HA3	1.74	0.67
1:F:369:VAL:HG22	1:F:378:VAL:HG22	1.76	0.67
1:F:357:CYS:O	1:F:456:LEU:N	2.21	0.66
1:F:243:ASN:HB3	1:F:246:MET:HE3	1.76	0.65
1:F:256:ILE:HB	1:F:264:ILE:HG22	1.81	0.63
1:F:39:LEU:HB3	1:F:333:THR:CG2	2.29	0.63
1:F:146:THR:HA	1:F:152:ARG:N	2.14	0.63
1:F:369:VAL:HG23	1:F:416:ILE:CD1	2.29	0.62
1:F:39:LEU:HD12	1:F:274:VAL:HG11	1.81	0.62
1:F:359:VAL:HG13	1:F:456:LEU:HB2	1.82	0.62
1:F:30:THR:HG22	1:F:283:LYS:HB2	1.81	0.62
1:F:374:LEU:HA	1:F:408:ASN:ND2	2.14	0.61
1:F:350:ILE:HG13	1:F:357:CYS:SG	2.41	0.61
1:F:282:VAL:O	1:F:283:LYS:NZ	2.33	0.60
1:F:50:LEU:HB3	1:F:263:VAL:HB	1.83	0.60
1:F:396:ILE:O	1:F:397:LYS:HG3	2.02	0.60
1:F:300:ARG:NH2	1:F:346:CYS:HB3	2.18	0.59
1:F:31:ILE:HD12	1:F:281:ILE:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:124:ILE:HG21	1:F:256:ILE:HG21	1.85	0.58
1:F:356:PRO:HB3	1:F:457:ASP:HB3	1.85	0.58
1:F:135:ASN:O	1:F:139:LYS:HE3	2.03	0.58
1:F:174:ASN:O	1:F:175:LYS:HB2	2.02	0.58
1:F:53:GLY:HA2	1:F:162:LYS:HD2	1.86	0.58
1:F:55:VAL:CG1	1:F:165:VAL:HG11	2.34	0.58
1:F:281:ILE:HD12	1:F:305:TRP:CE2	2.38	0.58
1:F:250:LYS:CB	1:F:270:PRO:HG3	2.34	0.57
1:F:39:LEU:HB3	1:F:333:THR:HG23	1.86	0.57
1:F:379:ALA:HB1	1:F:381:TYR:CE2	2.40	0.56
1:F:246:MET:SD	1:F:325:ARG:NE	2.78	0.56
1:F:62:ASP:OD2	1:F:179:ASP:N	2.37	0.56
1:F:147:LEU:HB3	1:F:150:GLY:CA	2.36	0.56
1:F:40:ARG:HB3	1:F:332:ASP:HA	1.89	0.55
1:F:21:GLU:OE1	1:F:373:PRO:HB2	2.07	0.54
1:F:119:ALA:HA	1:F:122:LYS:HE2	1.89	0.54
1:F:19:LEU:C	1:F:20:LYS:HD3	2.33	0.54
1:F:366:ILE:CG2	1:F:367:SER:H	2.19	0.54
1:F:407:THR:HB	1:F:410:ASP:CG	2.32	0.54
1:F:224:ALA:HB2	1:F:244:ARG:HH12	1.73	0.54
1:F:114:VAL:O	1:F:118:VAL:HG23	2.08	0.53
1:F:218:MET:HE1	1:F:269:LEU:HD11	1.90	0.53
1:F:236:GLN:HG3	1:F:275:ILE:HG23	1.89	0.53
1:F:146:THR:HA	1:F:152:ARG:HA	1.90	0.53
1:F:195:ARG:O	1:F:199:VAL:HG23	2.09	0.53
1:F:53:GLY:HA2	1:F:162:LYS:HG3	1.91	0.52
1:F:65:SER:HB3	1:F:68:LYS:HB2	1.91	0.52
1:F:37:SER:O	1:F:275:ILE:HA	2.09	0.52
1:F:454:VAL:HB	1:F:458:GLN:NE2	2.24	0.52
1:F:145:SER:C	1:F:152:ARG:HA	2.35	0.52
1:F:146:THR:HA	1:F:152:ARG:CA	2.40	0.52
1:F:254:ILE:HB	1:F:266:MET:HG3	1.92	0.51
1:F:48:PHE:CZ	1:F:218:MET:HG3	2.45	0.51
1:F:375:GLY:HA3	1:F:406:ILE:O	2.10	0.51
1:F:137:LEU:O	1:F:159:ARG:NH2	2.43	0.51
1:F:407:THR:O	1:F:410:ASP:HB2	2.09	0.51
1:F:305:TRP:HB2	1:F:316:TYR:HB2	1.93	0.51
1:F:256:ILE:HD11	1:F:266:MET:SD	2.51	0.50
1:F:147:LEU:HB3	1:F:150:GLY:H	1.76	0.50
1:F:369:VAL:CG2	1:F:378:VAL:HG13	2.42	0.50
1:F:25:GLU:CD	1:F:434:LYS:HA	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:ALA:O	1:F:115:THR:HG23	2.11	0.50
1:F:210:THR:O	1:F:252:PHE:HB2	2.10	0.50
1:F:117:GLY:HA2	1:F:120:ILE:HD12	1.92	0.50
1:F:53:GLY:HA2	1:F:162:LYS:CG	2.42	0.50
1:F:305:TRP:CD1	1:F:322:CYS:HB2	2.47	0.49
1:F:350:ILE:O	1:F:353:THR:HG22	2.13	0.49
1:F:62:ASP:CG	1:F:178:CYS:H	2.21	0.49
1:F:141:ASN:HA	1:F:157:ALA:HB3	1.95	0.49
1:F:188:SER:O	1:F:192:PHE:HD2	1.95	0.48
1:F:379:ALA:HB1	1:F:381:TYR:HE2	1.78	0.48
1:F:44:TYR:OH	1:F:154:LEU:HB2	2.13	0.48
1:F:46:ASN:OD1	1:F:226:ALA:HB2	2.12	0.48
1:F:118:VAL:O	1:F:122:LYS:HG3	2.13	0.48
1:F:359:VAL:CG1	1:F:456:LEU:HB2	2.43	0.48
1:F:373:PRO:O	1:F:374:LEU:HD23	2.14	0.48
1:F:300:ARG:HH22	1:F:346:CYS:HB3	1.78	0.48
1:F:316:TYR:OH	1:F:333:THR:HG22	2.13	0.48
1:F:384:VAL:O	1:F:401:LYS:NZ	2.41	0.47
1:F:23:TYR:CD2	1:F:432:VAL:HG22	2.33	0.47
1:F:128:SER:C	1:F:130:VAL:N	2.72	0.47
1:F:146:THR:N	1:F:152:ARG:HA	2.29	0.47
1:F:39:LEU:HD12	1:F:274:VAL:CG1	2.45	0.47
1:F:241:LEU:HA	1:F:241:LEU:HD23	1.39	0.47
1:F:290:GLU:C	1:F:291:LYS:HZ3	2.22	0.47
1:F:389:GLY:HA2	1:F:395:ILE:HA	1.96	0.47
1:F:26:GLU:HB3	1:F:435:GLY:HA3	1.97	0.46
1:F:129:GLU:HG2	1:F:147:LEU:CD1	2.44	0.46
1:F:110:THR:O	1:F:114:VAL:HG23	2.16	0.46
1:F:147:LEU:HB3	1:F:150:GLY:N	2.31	0.46
1:F:408:ASN:HB2	1:F:424:SER:O	2.16	0.46
1:F:19:LEU:N	1:F:33:GLU:O	2.49	0.46
1:F:380:CYS:O	1:F:401:LYS:HA	2.16	0.46
1:F:22:SER:HB3	1:F:31:ILE:CG2	2.46	0.46
1:F:51:GLU:HB3	1:F:162:LYS:HB2	1.97	0.46
1:F:391:ASN:ND2	1:F:412:ASP:HB3	2.31	0.45
1:F:122:LYS:C	1:F:124:ILE:H	2.24	0.45
1:F:173:ILE:HG22	1:F:173:ILE:O	2.16	0.45
1:F:239:LEU:HA	1:F:242:GLU:CD	2.42	0.45
1:F:146:THR:CA	1:F:152:ARG:HA	2.46	0.45
1:F:295:TYR:OH	1:F:382:LYS:NZ	2.41	0.45
1:F:359:VAL:HG21	1:F:456:LEU:HD13	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:147:LEU:O	1:F:148:GLY:C	2.58	0.45
1:F:39:LEU:CD2	1:F:331:CYS:HB2	2.46	0.45
1:F:40:ARG:NH2	1:F:334:ALA:HB3	2.32	0.45
1:F:39:LEU:O	1:F:272:PHE:HA	2.17	0.44
1:F:246:MET:SD	1:F:325:ARG:NH2	2.89	0.44
1:F:369:VAL:CG2	1:F:416:ILE:HD11	2.41	0.44
1:F:289:SER:CB	1:F:291:LYS:HZ1	2.31	0.44
1:F:388:ILE:CD1	1:F:396:ILE:HD12	2.48	0.44
1:F:130:VAL:HG23	1:F:131:THR:H	1.84	0.43
1:F:40:ARG:HB2	1:F:272:PHE:CE1	2.52	0.43
1:F:297:CYS:C	1:F:298:LEU:HD12	2.43	0.43
1:F:395:ILE:HD13	1:F:395:ILE:HG21	1.77	0.43
1:F:407:THR:HG21	1:F:430:GLN:NE2	2.34	0.43
1:F:254:ILE:HD12	1:F:266:MET:HE2	2.00	0.43
1:F:52:VAL:HA	1:F:161:LEU:HD23	1.99	0.43
1:F:386:CYS:HB2	1:F:399:LEU:HG	2.00	0.43
1:F:236:GLN:HG3	1:F:275:ILE:CG2	2.48	0.42
1:F:37:SER:HB2	1:F:39:LEU:CG	2.45	0.42
1:F:217:LEU:HA	1:F:217:LEU:HD23	1.75	0.42
1:F:130:VAL:O	1:F:133:ILE:HG13	2.19	0.42
1:F:39:LEU:HD23	1:F:331:CYS:HB2	2.02	0.42
1:F:40:ARG:N	1:F:272:PHE:HD1	2.18	0.42
1:F:127:GLU:O	1:F:128:SER:C	2.61	0.42
1:F:31:ILE:O	1:F:31:ILE:HG23	2.19	0.42
1:F:386:CYS:HA	1:F:415:THR:O	2.20	0.41
1:F:369:VAL:HG22	1:F:378:VAL:HG13	2.02	0.41
1:F:196:PHE:O	1:F:200:VAL:HG23	2.20	0.41
1:F:230:MET:O	1:F:237:ILE:HD11	2.20	0.41
1:F:48:PHE:HZ	1:F:218:MET:HG3	1.82	0.41
1:F:80:ASP:O	1:F:84:VAL:HG23	2.21	0.41
1:F:250:LYS:HG3	1:F:272:PHE:HZ	1.86	0.41
1:F:40:ARG:HD3	1:F:43:TRP:CZ2	2.55	0.41
1:F:390:SER:CB	1:F:393:VAL:HG22	2.43	0.41
1:F:198:ASN:HB2	1:F:216:ASP:OD2	2.21	0.41
1:F:333:THR:C	1:F:335:ALA:H	2.29	0.41
1:F:361:THR:CG2	1:F:459:VAL:HG21	2.50	0.41
1:F:256:ILE:HD11	1:F:266:MET:HG2	2.02	0.41
1:F:314:VAL:CG1	1:F:336:GLY:HA3	2.50	0.41
1:F:386:CYS:HB2	1:F:399:LEU:CD1	2.51	0.41
1:F:39:LEU:HB3	1:F:333:THR:HG21	2.02	0.41
1:F:53:GLY:HA2	1:F:162:LYS:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:64:PRO:HA	1:F:68:LYS:NZ	2.37	0.40
1:F:224:ALA:HB2	1:F:244:ARG:NH1	2.35	0.40
1:F:51:GLU:O	1:F:161:LEU:HB3	2.22	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	F	410/514 (80%)	387 (94%)	22 (5%)	1 (0%)	43 77

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	127	GLU

5.3.2 Protein sidechains [i](#)

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	F	352/431 (82%)	349 (99%)	3 (1%)	70 78

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	125	ARG
1	F	130	VAL
1	F	149	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	198	ASN
1	F	328	HIS
1	F	342	GLN
1	F	391	ASN
1	F	409	GLN
1	F	458	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 oligosaccharides 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	F	416/514 (80%)	0.63	35 (8%) 17 24	182, 242, 336, 409	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	286	PRO	4.1
1	F	106	LEU	3.3
1	F	434	LYS	3.2
1	F	49	THR	3.2
1	F	211	PRO	3.1
1	F	344	LYS	2.9
1	F	285	ALA	2.9
1	F	168	ASN	2.9
1	F	365	PRO	2.8
1	F	355	TYR	2.8
1	F	371	LEU	2.8
1	F	195	ARG	2.7
1	F	392	ARG	2.7
1	F	149	CYS	2.7
1	F	20	LYS	2.6
1	F	367	SER	2.6
1	F	187	VAL	2.6
1	F	460	PHE	2.5
1	F	463	ILE	2.4
1	F	310	ALA	2.4
1	F	152	ARG	2.4
1	F	69	THR	2.4
1	F	151	PRO	2.3
1	F	207	ALA	2.3
1	F	64	PRO	2.3
1	F	396	ILE	2.3
1	F	191	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	203	PHE	2.2
1	F	175	LYS	2.2
1	F	348	ILE	2.2
1	F	308	GLN	2.1
1	F	283	LYS	2.1
1	F	406	ILE	2.0
1	F	288	CYS	2.0
1	F	114	VAL	2.0

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 oligosaccharides 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.