



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:06 PM UTC

PDB ID : 8XO4 / pdb_00008xo4
Title : Crystal structure of measles virus fusion inhibitor M1EK complexed with F protein HR1 (HR1-42) (P21 space group)
Authors : Oishi, S.; Takahara, A.; Nakatsu, T.
Deposited on : 2023-12-31
Resolution : 2.36 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

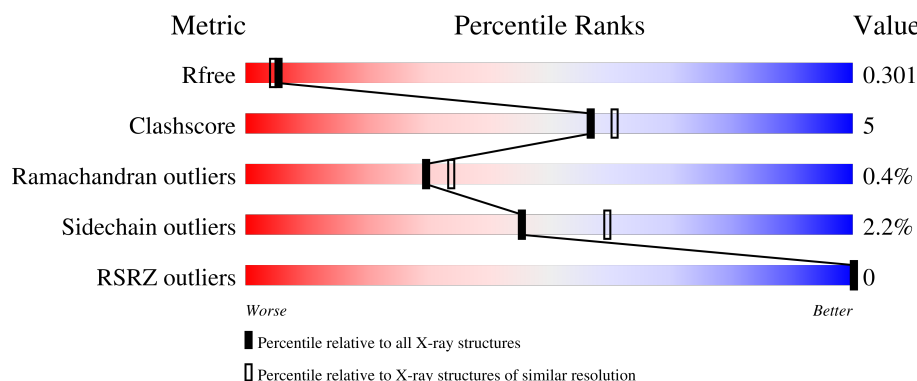
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 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.



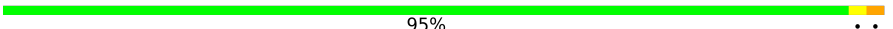
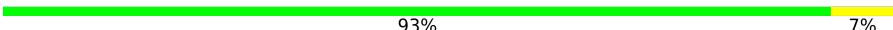
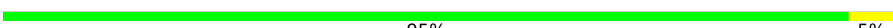
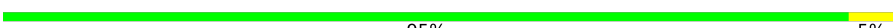
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	44	84% 16%
1	C	44	73% 27%
1	E	44	86% 11% .
1	G	44	82% 18%
1	I	44	93% 7%

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Mol	Chain	Length	Quality of chain
1	K	44	 82% 18%
1	M	44	 89% 11%
1	O	44	 91% 9%
1	Q	44	 95% . .
1	S	44	 93% 7%
1	U	44	 77% 23%
1	W	44	 91% 9%
2	B	37	 84% 16%
2	D	37	 81% 19%
2	F	37	 84% 16%
2	H	37	 89% 11%
2	J	37	 86% 14%
2	L	37	 68% 32%
2	N	37	 84% 14% .
2	P	37	 81% 19%
2	R	37	 86% 14%
2	T	37	 95% 5%
2	V	37	 81% 19%
2	X	37	 95% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7732 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 Fusion glycoprotein F1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	44	Total	C	N	O	S	0	1	1
			330	198	61	70	1			
1	C	44	Total	C	N	O	S	0	1	1
			331	199	61	70	1			
1	E	44	Total	C	N	O	S	0	0	1
			325	195	60	69	1			
1	G	44	Total	C	N	O	S	0	0	1
			325	195	60	69	1			
1	I	44	Total	C	N	O	S	0	0	1
			325	195	60	69	1			
1	K	44	Total	C	N	O	S	0	1	1
			330	198	61	70	1			
1	M	44	Total	C	N	O	S	0	1	1
			331	199	61	70	1			
1	O	44	Total	C	N	O	S	0	0	1
			325	195	60	69	1			
1	Q	44	Total	C	N	O	S	0	0	1
			325	195	60	69	1			
1	S	44	Total	C	N	O	S	0	0	1
			325	195	60	69	1			
1	U	44	Total	C	N	O	S	0	0	1
			325	195	60	69	1			
1	W	44	Total	C	N	O	S	0	1	1
			331	199	61	70	1			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	142	ACE	-	acetylation	UNP P69353
A	185	NH2	-	amidation	UNP P69353
C	142	ACE	-	acetylation	UNP P69353
C	185	NH2	-	amidation	UNP P69353
E	142	ACE	-	acetylation	UNP P69353

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Chain	Residue	Modelled	Actual	Comment	Reference
E	185	NH2	-	amidation	UNP P69353
G	142	ACE	-	acetylation	UNP P69353
G	185	NH2	-	amidation	UNP P69353
I	142	ACE	-	acetylation	UNP P69353
I	185	NH2	-	amidation	UNP P69353
K	142	ACE	-	acetylation	UNP P69353
K	185	NH2	-	amidation	UNP P69353
M	142	ACE	-	acetylation	UNP P69353
M	185	NH2	-	amidation	UNP P69353
O	142	ACE	-	acetylation	UNP P69353
O	185	NH2	-	amidation	UNP P69353
Q	142	ACE	-	acetylation	UNP P69353
Q	185	NH2	-	amidation	UNP P69353
S	142	ACE	-	acetylation	UNP P69353
S	185	NH2	-	amidation	UNP P69353
U	142	ACE	-	acetylation	UNP P69353
U	185	NH2	-	amidation	UNP P69353
W	142	ACE	-	acetylation	UNP P69353
W	185	NH2	-	amidation	UNP P69353

- Molecule 2 is a protein called Measles virus fusion inhibitor M1EK.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	37	Total	C	N	O	0	1	1
			306	193	51	62			
2	D	37	Total	C	N	O	0	0	1
			300	189	51	60			
2	F	37	Total	C	N	O	0	2	1
			312	197	51	64			
2	H	37	Total	C	N	O	0	2	1
			314	198	54	62			
2	J	37	Total	C	N	O	0	0	1
			300	189	51	60			
2	L	37	Total	C	N	O	0	1	1
			306	194	52	60			
2	N	37	Total	C	N	O	0	3	1
			318	201	51	66			
2	P	37	Total	C	N	O	0	0	1
			300	189	51	60			
2	R	37	Total	C	N	O	0	1	1
			306	193	51	62			
2	T	37	Total	C	N	O	0	1	1
			305	194	51	60			

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	V	37	Total	C	N	O	0	2	1
			312	197	51	64			
2	X	37	Total	C	N	O	0	2	1
			314	198	54	62			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total	O	0	0
			10	10		
3	B	8	Total	O	0	0
			8	8		
3	C	5	Total	O	0	0
			5	5		
3	D	6	Total	O	0	0
			6	6		
3	E	5	Total	O	0	0
			5	5		
3	F	7	Total	O	0	1
			7	7		
3	G	1	Total	O	0	0
			1	1		
3	H	3	Total	O	0	0
			3	3		
3	I	5	Total	O	0	0
			5	5		
3	J	4	Total	O	0	0
			4	4		
3	K	3	Total	O	0	0
			3	3		
3	L	3	Total	O	0	0
			3	3		
3	M	4	Total	O	0	0
			4	4		
3	N	8	Total	O	0	0
			8	8		
3	O	2	Total	O	0	0
			2	2		
3	P	4	Total	O	0	0
			4	4		
3	Q	2	Total	O	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	R	4	Total 4	O 4	0	0
3	S	6	Total 6	O 6	0	0
3	T	6	Total 6	O 6	0	0
3	U	4	Total 4	O 4	0	0
3	V	3	Total 3	O 3	0	0
3	W	2	Total 2	O 2	0	0
3	X	6	Total 6	O 6	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: Fusion glycoprotein F1

Chain A:  84% 16%



- Molecule 1: Fusion glycoprotein F1

Chain C:  73% 27%



- Molecule 1: Fusion glycoprotein F1

Chain E:  86% 11% .



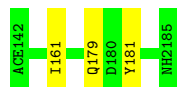
- Molecule 1: Fusion glycoprotein F1

Chain G:  82% 18%



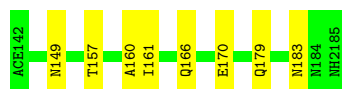
- Molecule 1: Fusion glycoprotein F1

Chain I:  93% 7%



- Molecule 1: Fusion glycoprotein F1

Chain K:  82% 18%



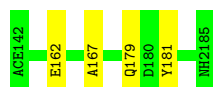
- Molecule 1: Fusion glycoprotein F1

Chain M:  89% 11%



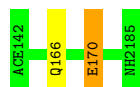
- Molecule 1: Fusion glycoprotein F1

Chain O:  91% 9%



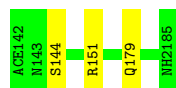
- Molecule 1: Fusion glycoprotein F1

Chain Q:  95% ..



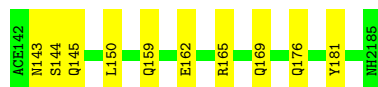
- Molecule 1: Fusion glycoprotein F1

Chain S:  93% 7%



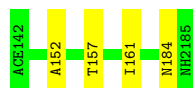
- Molecule 1: Fusion glycoprotein F1

Chain U:  77% 23%



- Molecule 1: Fusion glycoprotein F1

Chain W:  91% 9%



- Molecule 2: Measles virus fusion inhibitor M1EK

Chain B:  84% 16%



- Molecule 2: Measles virus fusion inhibitor M1EK

Chain D:  81% 19%



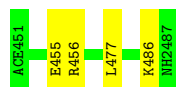
- Molecule 2: Measles virus fusion inhibitor M1EK

Chain F:  84% 16%



- Molecule 2: Measles virus fusion inhibitor M1EK

Chain H:  89% 11%



- Molecule 2: Measles virus fusion inhibitor M1EK

Chain J:  86% 14%



- Molecule 2: Measles virus fusion inhibitor M1EK

Chain L:  68% 32%



- Molecule 2: Measles virus fusion inhibitor M1EK

Chain N:  84% 14%



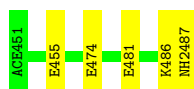
- Molecule 2: Measles virus fusion inhibitor M1EK

Chain P: 81% 19%



- Molecule 2: Measles virus fusion inhibitor M1EK

Chain R: 86% 14%



- Molecule 2: Measles virus fusion inhibitor M1EK

Chain T: 95% 5%



- Molecule 2: Measles virus fusion inhibitor M1EK

Chain V: 81% 19%



- Molecule 2: Measles virus fusion inhibitor M1EK

Chain X: 95% 5%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.84Å 35.58Å 237.65Å 90.00° 93.98° 90.00°	Depositor
Resolution (Å)	49.10 – 2.36 49.10 – 2.36	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.10-2.36) 99.5 (49.10-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.42 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.215 , 0.301 0.223 , 0.301	Depositor DCC
R_{free} test set	1953 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	55.1	Xtriage
Anisotropy	0.694	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.026 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7732	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.29% 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

Bond lengths and bond angles in the following residue types are not validated in this section: NH2, ACE

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	1.14	0/330	1.60	1/447 (0.2%)
1	C	1.16	0/331	1.72	0/448
1	E	1.15	0/322	1.63	2/436 (0.5%)
1	G	1.08	0/322	1.69	4/436 (0.9%)
1	I	1.05	0/322	1.71	0/436
1	K	1.05	0/330	1.78	0/447
1	M	1.03	0/331	1.68	0/448
1	O	1.07	0/322	1.74	0/436
1	Q	1.03	0/322	1.73	1/436 (0.2%)
1	S	1.06	0/322	1.68	0/436
1	U	1.08	0/322	1.66	2/436 (0.5%)
1	W	1.02	0/331	1.62	2/448 (0.4%)
2	B	1.07	0/305	1.73	2/398 (0.5%)
2	D	1.08	0/296	1.72	0/386
2	F	1.06	0/314	1.72	0/410
2	H	0.99	0/316	1.59	0/412
2	J	1.00	0/296	1.74	0/386
2	L	0.98	0/305	1.64	0/397
2	N	0.99	0/323	1.64	0/422
2	P	0.99	0/296	1.68	0/386
2	R	1.01	0/305	1.60	0/398
2	T	0.96	0/304	1.57	0/397
2	V	1.06	0/314	1.56	0/410
2	X	1.02	0/316	1.66	0/412
All	All	1.05	0/7597	1.67	14/10104 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	475	GLU	CB-CA-C	-6.90	99.78	110.81
1	G	148	ASP	CA-C-N	5.91	128.66	120.63
1	G	148	ASP	C-N-CA	5.91	128.66	120.63
1	G	167	ALA	CA-C-N	5.63	126.36	119.99
1	G	167	ALA	C-N-CA	5.63	126.36	119.99
1	W	152	ALA	CA-C-N	5.42	127.98	120.29
1	W	152	ALA	C-N-CA	5.42	127.98	120.29
2	B	475	GLU	N-CA-CB	5.29	117.82	109.94
1	A	158	ASN	CB-CA-C	5.28	119.83	110.85
1	U	176	GLN	CA-C-N	5.19	125.84	120.03
1	U	176	GLN	C-N-CA	5.19	125.84	120.03
1	E	155	GLU	CA-C-N	5.17	127.17	120.44
1	E	155	GLU	C-N-CA	5.17	127.17	120.44
1	Q	170	GLU	CB-CG-CD	5.13	121.33	112.60

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	330	0	323	5	0
1	C	331	0	325	9	0
1	E	325	0	317	7	0
1	G	325	0	317	3	0
1	I	325	0	317	3	0
1	K	330	0	323	7	0
1	M	331	0	325	4	0
1	O	325	0	317	4	0
1	Q	325	0	317	1	0
1	S	325	0	317	2	0
1	U	325	0	317	7	0
1	W	331	0	325	2	0
2	B	306	0	338	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	300	0	332	6	0
2	F	312	0	344	7	0
2	H	314	0	351	4	0
2	J	300	0	332	4	0
2	L	306	0	345	9	0
2	N	318	0	350	3	0
2	P	300	0	332	6	0
2	R	306	0	338	3	0
2	T	305	0	343	1	0
2	V	312	0	344	4	0
2	X	314	0	351	3	0
3	A	10	0	0	1	0
3	B	8	0	0	0	0
3	C	5	0	0	0	0
3	D	6	0	0	0	0
3	E	5	0	0	0	0
3	F	7	0	0	0	0
3	G	1	0	0	0	0
3	H	3	0	0	0	0
3	I	5	0	0	0	0
3	J	4	0	0	1	0
3	K	3	0	0	0	0
3	L	3	0	0	0	0
3	M	4	0	0	0	0
3	N	8	0	0	0	0
3	O	2	0	0	0	0
3	P	4	0	0	1	0
3	Q	2	0	0	0	0
3	R	4	0	0	0	0
3	S	6	0	0	0	0
3	T	6	0	0	0	0
3	U	4	0	0	0	0
3	V	3	0	0	0	0
3	W	2	0	0	0	0
3	X	6	0	0	0	0
All	All	7732	0	7940	71	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 5.

All (71) 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:181:TYR:HB2	2:D:455:GLU:HG3	1.73	0.69
1:O:162:GLU:OE2	2:R:474:GLU:OE1	2.11	0.69
2:B:474[A]:GLU:OE1	1:E:165:ARG:NE	2.31	0.63
1:W:157:THR:O	1:W:161:ILE:HG13	2.00	0.62
2:D:459:VAL:O	2:D:463:LEU:HG	2.00	0.61
1:C:168:GLY:HA2	1:C:171:MET:HE3	1.86	0.57
1:G:165:ARG:NE	2:J:474:GLU:OE1	2.42	0.52
1:U:162:GLU:OE1	2:X:474:GLU:OE2	2.28	0.52
2:N:452:ILE:O	2:N:455[B]:GLU:HG3	2.10	0.52
1:O:179:GLN:OE1	2:R:455:GLU:OE2	2.27	0.52
1:C:165:ARG:NH1	1:C:169[B]:GLN:OE1	2.43	0.51
2:B:452:ILE:CG1	2:B:452:ILE:O	2.58	0.51
1:C:155:GLU:OE1	2:F:481[A]:GLU:OE1	2.29	0.51
1:M:168:GLY:HA2	1:M:171:MET:HE3	1.92	0.51
2:P:453:GLU:OE2	2:X:456[B]:ARG:NH2	2.46	0.48
2:H:455[A]:GLU:OE2	1:K:179:GLN:OE1	2.30	0.48
2:H:477:LEU:HD11	1:K:161:ILE:HG22	1.95	0.48
2:L:454:GLU:O	2:L:458[B]:LYS:HG2	2.14	0.48
1:C:181:TYR:CB	2:D:455:GLU:HG3	2.42	0.48
1:E:181:TYR:CB	2:F:455:GLU:HG3	2.43	0.48
1:G:162:GLU:HG3	1:G:166:GLN:HE21	1.78	0.47
2:B:474[A]:GLU:OE1	1:E:162:GLU:OE1	2.33	0.47
1:U:181:TYR:HB2	2:V:455[B]:GLU:HG3	1.97	0.47
1:K:166:GLN:O	1:K:170:GLU:HG2	2.15	0.46
1:G:146:ALA:O	1:G:149:ASN:HB3	2.16	0.46
1:O:181:TYR:CB	2:P:455:GLU:HG3	2.45	0.46
1:C:142:ACE:O	1:C:145:GLN:HG2	2.16	0.46
1:C:166:GLN:O	1:C:170:GLU:HG2	2.15	0.46
2:T:453:GLU:HA	2:T:453:GLU:OE1	2.16	0.46
2:H:456[B]:ARG:HE	1:K:183:ASN:ND2	2.13	0.45
2:R:486:LYS:HG3	2:R:487:NH2:N	2.32	0.45
2:L:459:VAL:O	2:L:463:LEU:HG	2.17	0.45
1:S:179:GLN:NE2	2:V:456:ARG:HA	2.31	0.44
1:Q:166:GLN:O	1:Q:170:GLU:HG2	2.18	0.44
1:U:165:ARG:NE	2:X:474:GLU:OE1	2.49	0.44
2:B:455:GLU:OE2	2:B:459:VAL:HG21	2.17	0.44
1:C:172:ILE:HD11	2:F:466:ALA:HB1	1.99	0.44
1:S:151:ARG:HG2	1:U:150:LEU:HD21	2.00	0.44
1:C:163:ALA:HB3	2:D:473:ALA:HB2	1.98	0.44
2:J:456:ARG:HD3	3:J:501:HOH:O	2.18	0.44
2:L:457:LYS:O	2:L:461:GLU:HB3	2.18	0.44
1:I:179:GLN:OE1	2:L:455:GLU:OE2	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:ILE:HG22	2:D:477:LEU:HD22	2.00	0.43
1:U:165:ARG:NH1	1:U:169:GLN:OE1	2.49	0.43
1:A:153:SER:OG	1:E:154:LEU:HD21	2.17	0.43
2:B:452:ILE:O	2:B:452:ILE:HG12	2.19	0.43
2:V:458:LYS:O	2:V:462:ASN:ND2	2.47	0.43
1:M:176[B]:GLN:HG3	2:P:463:LEU:HD13	1.99	0.43
1:A:166:GLN:O	1:A:170:GLU:HG2	2.18	0.43
1:I:181:TYR:HB2	2:J:455:GLU:HG3	2.01	0.42
2:B:484:LEU:HD13	1:E:155:GLU:HG3	2.01	0.42
1:O:167:ALA:HB2	2:P:469:LYS:HB2	2.01	0.42
2:L:457:LYS:O	2:L:461:GLU:CB	2.68	0.42
2:F:452:ILE:HG21	2:J:456:ARG:HH21	1.84	0.42
1:U:143:ASN:N	1:U:143:ASN:HD22	2.16	0.42
1:U:159:GLN:HB3	2:V:476:LEU:HD13	2.02	0.42
1:E:181:TYR:HB2	2:F:455:GLU:HG3	2.02	0.41
1:K:149[A]:ASN:ND2	2:L:486:LYS:O	2.54	0.41
2:P:474:GLU:OE2	2:P:474:GLU:HA	2.19	0.41
2:P:478:LYS:NZ	3:P:501:HOH:O	2.48	0.41
1:A:148:ASP:HB2	3:A:206:HOH:O	2.20	0.41
1:I:161:ILE:HG22	2:L:477:LEU:HD11	2.03	0.41
1:K:160:ALA:HB2	2:L:476:LEU:HB3	2.03	0.41
2:F:477:LEU:HD23	2:F:477:LEU:HA	1.89	0.40
2:H:456[B]:ARG:HE	1:K:183:ASN:CG	2.29	0.40
1:E:181:TYR:HB2	2:F:455:GLU:CG	2.51	0.40
1:M:156:THR:HG21	2:N:479:LYS:HB3	2.03	0.40
1:M:156:THR:HG22	2:N:476:LEU:O	2.22	0.40
1:A:162:GLU:OE1	2:D:474:GLU:OE1	2.40	0.40
2:L:477:LEU:HD23	2:L:477:LEU:HA	1.84	0.40
1:W:184:ASN:HD22	1:W:184:ASN:HA	1.75	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	43/44 (98%)	43 (100%)	0	0	100	100
1	C	43/44 (98%)	42 (98%)	1 (2%)	0	100	100
1	E	42/44 (96%)	39 (93%)	2 (5%)	1 (2%)	4	3
1	G	42/44 (96%)	42 (100%)	0	0	100	100
1	I	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
1	K	43/44 (98%)	41 (95%)	2 (5%)	0	100	100
1	M	43/44 (98%)	42 (98%)	1 (2%)	0	100	100
1	O	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
1	Q	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
1	S	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
1	U	42/44 (96%)	41 (98%)	0	1 (2%)	4	3
1	W	43/44 (98%)	42 (98%)	1 (2%)	0	100	100
2	B	36/37 (97%)	36 (100%)	0	0	100	100
2	D	35/37 (95%)	35 (100%)	0	0	100	100
2	F	37/37 (100%)	35 (95%)	1 (3%)	1 (3%)	4	2
2	H	37/37 (100%)	33 (89%)	3 (8%)	1 (3%)	4	2
2	J	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
2	L	36/37 (97%)	35 (97%)	1 (3%)	0	100	100
2	N	38/37 (103%)	37 (97%)	1 (3%)	0	100	100
2	P	35/37 (95%)	35 (100%)	0	0	100	100
2	R	36/37 (97%)	31 (86%)	5 (14%)	0	100	100
2	T	36/37 (97%)	35 (97%)	1 (3%)	0	100	100
2	V	37/37 (100%)	32 (86%)	5 (14%)	0	100	100
2	X	37/37 (100%)	34 (92%)	3 (8%)	0	100	100
All	All	944/972 (97%)	907 (96%)	33 (4%)	4 (0%)	30	34

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	486	LYS
2	F	486	LYS
1	U	144	SER
1	E	144	SER

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	35/34 (103%)	35 (100%)	0	100	100
1	C	35/34 (103%)	35 (100%)	0	100	100
1	E	34/34 (100%)	34 (100%)	0	100	100
1	G	34/34 (100%)	33 (97%)	1 (3%)	37	49
1	I	34/34 (100%)	34 (100%)	0	100	100
1	K	35/34 (103%)	34 (97%)	1 (3%)	37	49
1	M	35/34 (103%)	34 (97%)	1 (3%)	37	49
1	O	34/34 (100%)	34 (100%)	0	100	100
1	Q	34/34 (100%)	34 (100%)	0	100	100
1	S	34/34 (100%)	33 (97%)	1 (3%)	37	49
1	U	34/34 (100%)	33 (97%)	1 (3%)	37	49
1	W	35/34 (103%)	35 (100%)	0	100	100
2	B	34/33 (103%)	34 (100%)	0	100	100
2	D	33/33 (100%)	32 (97%)	1 (3%)	36	48
2	F	35/33 (106%)	35 (100%)	0	100	100
2	H	35/33 (106%)	35 (100%)	0	100	100
2	J	33/33 (100%)	31 (94%)	2 (6%)	17	20
2	L	34/33 (103%)	32 (94%)	2 (6%)	18	22
2	N	36/33 (109%)	33 (92%)	3 (8%)	10	11
2	P	33/33 (100%)	32 (97%)	1 (3%)	36	48
2	R	34/33 (103%)	33 (97%)	1 (3%)	37	49
2	T	34/33 (103%)	33 (97%)	1 (3%)	37	49
2	V	35/33 (106%)	33 (94%)	2 (6%)	18	23
2	X	35/33 (106%)	35 (100%)	0	100	100
All	All	824/804 (102%)	806 (98%)	18 (2%)	45	59

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	478	LYS
1	G	154	LEU
2	J	464	LYS
2	J	481	GLU
1	K	157	THR
2	L	464	LYS
2	L	471	LYS
1	M	145	GLN
2	N	468	GLU
2	N	477	LEU
2	N	479	LYS
2	P	458	LYS
2	R	481	GLU
1	S	144	SER
2	T	485	LYS
1	U	145	GLN
2	V	467	GLU
2	V	483	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	145	GLN
1	C	145	GLN
1	C	149	ASN
1	E	145	GLN
1	E	169	GLN
1	E	184	ASN
1	G	149	ASN
1	G	158	ASN
1	G	166	GLN
1	I	169	GLN
1	I	179	GLN
1	K	176	GLN
1	K	179	GLN
1	K	183	ASN
1	M	159	GLN
2	N	462	ASN
1	O	159	GLN
1	O	184	ASN
1	S	143	ASN
1	S	179	GLN
1	U	145	GLN

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Mol	Chain	Res	Type
1	U	184	ASN
1	W	166	GLN
1	W	184	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 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	A	42/44 (95%)	-0.32	0 100 100	37, 54, 82, 96	1 (2%)
1	C	42/44 (95%)	-0.26	0 100 100	31, 60, 74, 92	1 (2%)
1	E	42/44 (95%)	-0.38	0 100 100	38, 51, 75, 92	0
1	G	42/44 (95%)	-0.11	0 100 100	52, 70, 93, 114	0
1	I	42/44 (95%)	-0.12	0 100 100	56, 74, 115, 125	0
1	K	42/44 (95%)	0.04	0 100 100	59, 77, 119, 125	1 (2%)
1	M	42/44 (95%)	-0.18	0 100 100	28, 57, 83, 104	1 (2%)
1	O	42/44 (95%)	-0.23	0 100 100	52, 63, 97, 103	0
1	Q	42/44 (95%)	-0.24	0 100 100	43, 65, 85, 91	0
1	S	42/44 (95%)	-0.35	0 100 100	48, 64, 99, 116	0
1	U	42/44 (95%)	-0.27	0 100 100	44, 60, 88, 121	0
1	W	42/44 (95%)	-0.48	0 100 100	27, 56, 79, 105	1 (2%)
2	B	35/37 (94%)	-0.28	0 100 100	29, 59, 96, 99	1 (2%)
2	D	35/37 (94%)	-0.30	0 100 100	48, 66, 87, 101	0
2	F	35/37 (94%)	-0.31	0 100 100	33, 62, 89, 99	2 (5%)
2	H	35/37 (94%)	-0.07	0 100 100	34, 78, 105, 113	2 (5%)
2	J	35/37 (94%)	-0.19	0 100 100	64, 78, 97, 110	0
2	L	35/37 (94%)	0.09	0 100 100	50, 91, 114, 120	1 (2%)
2	N	35/37 (94%)	-0.24	0 100 100	28, 63, 89, 91	3 (8%)
2	P	35/37 (94%)	-0.21	0 100 100	55, 73, 92, 103	0
2	R	35/37 (94%)	-0.05	0 100 100	38, 74, 98, 103	1 (2%)
2	T	35/37 (94%)	-0.10	0 100 100	43, 70, 94, 106	1 (2%)
2	V	35/37 (94%)	-0.11	0 100 100	34, 72, 98, 100	2 (5%)
2	X	35/37 (94%)	-0.30	0 100 100	31, 66, 89, 94	2 (5%)

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
All	All	924/972 (95%)	-0.21	0 100 100	27, 67, 101, 125	20 (2%)

There are no RSRZ outliers to report.

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.