



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:58 PM UTC

PDB ID : 8XO7 / pdb\_00008xo7  
Title : Crystal structure of measles virus fusion inhibitor MEK35GE complexed with F protein HR1 (HR1-42) (P2 space group)  
Authors : Oishi, S.; Takahara, A.; Nakatsu, T.  
Deposited on : 2023-12-31  
Resolution : 2.17 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](mailto: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>.

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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

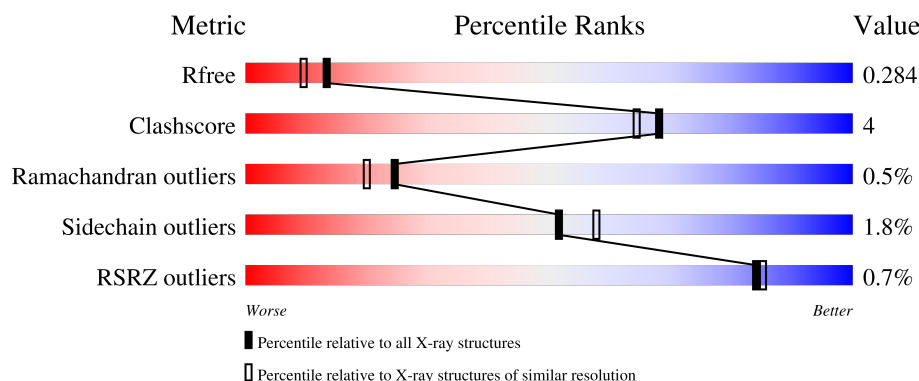
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.17 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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  $\geq 3$ , 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	<div> <div>2%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>
1	C	44	<div> <div>93%</div> <div>7%</div> </div>
1	E	44	<div> <div>93%</div> <div>7%</div> </div>
1	G	44	<div> <div>89%</div> <div>11%</div> </div>
1	I	44	<div> <div>91%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
1	K	44	<div><div></div><div>89%</div><div>11%</div></div>
2	B	37	<div><div></div><div>70%</div><div>19%</div><div>11%</div></div>
2	D	37	<div><div></div><div>89%</div><div>11%</div></div>
2	F	37	<div><div></div><div>81%</div><div>8%</div><div>11%</div></div>
2	H	37	<div><div>5%</div><div></div><div>86%</div><div>5%</div><div>8%</div></div>
2	J	37	<div><div></div><div>70%</div><div>14%</div><div>5%</div><div>11%</div></div>
2	L	37	<div><div></div><div>84%</div><div>5%</div><div>11%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 3835 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	199	60	69	2			
1	C	44	Total	C	N	O	S	0	1	1
			330	199	60	69	2			
1	E	44	Total	C	N	O	S	0	2	1
			338	204	63	69	2			
1	G	44	Total	C	N	O	S	0	2	1
			336	203	61	70	2			
1	I	44	Total	C	N	O	S	0	2	1
			336	203	60	71	2			
1	K	44	Total	C	N	O	S	0	3	1
			341	206	62	71	2			

There are 12 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
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

- Molecule 2 is a protein called Measles virus fusion inhibitor MEK35GE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	33	Total	C	N	O	0	2	1
			282	181	49	52			
2	D	37	Total	C	N	O	0	1	1
			295	187	49	59			
2	F	33	Total	C	N	O	0	2	1
			276	175	47	54			
2	H	34	Total	C	N	O	0	1	1
			278	176	47	55			
2	J	33	Total	C	N	O	0	1	1
			270	170	46	54			
2	L	33	Total	C	N	O	0	1	1
			270	171	47	52			

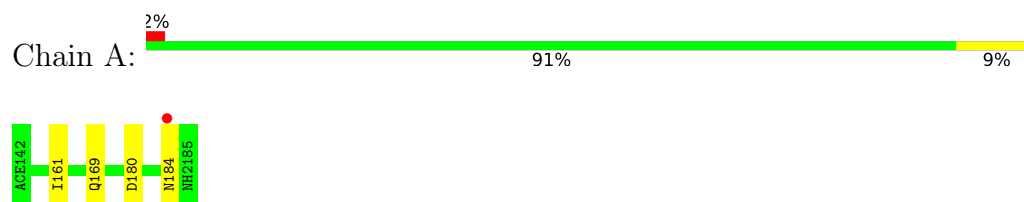
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	1
			16	16		
3	B	14	Total	O	0	0
			14	14		
3	C	22	Total	O	0	0
			22	22		
3	D	17	Total	O	0	0
			17	17		
3	E	19	Total	O	0	0
			19	19		
3	F	9	Total	O	0	0
			9	9		
3	G	8	Total	O	0	0
			8	8		
3	H	6	Total	O	0	0
			6	6		
3	I	10	Total	O	0	0
			10	10		
3	J	8	Total	O	0	0
			8	8		
3	K	15	Total	O	0	0
			15	15		
3	L	9	Total	O	0	0
			9	9		

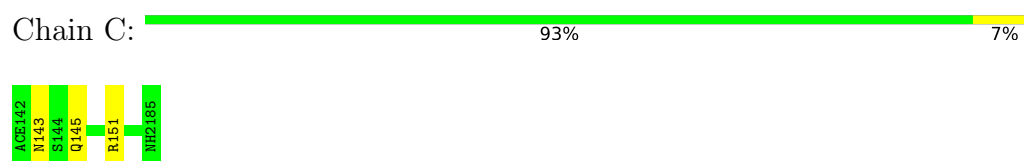
### 3 Residue-property plots [i](#)

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.

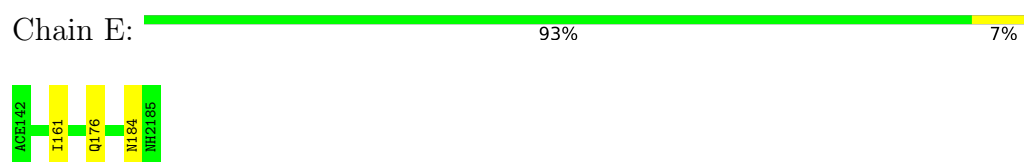
- Molecule 1: Fusion glycoprotein F1



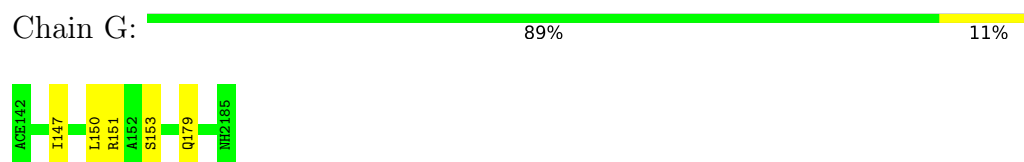
- Molecule 1: Fusion glycoprotein F1



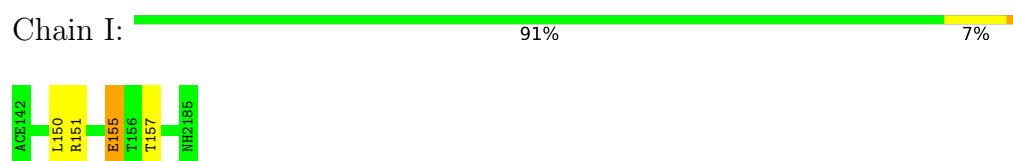
- Molecule 1: Fusion glycoprotein F1




- Molecule 1: Fusion glycoprotein F1

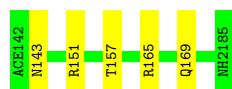


- Molecule 1: Fusion glycoprotein F1



- Molecule 1: Fusion glycoprotein F1

Chain K:  89% 11%



- Molecule 2: Measles virus fusion inhibitor MEK35GE

Chain B:  70% 19% 11%




- Molecule 2: Measles virus fusion inhibitor MEK35GE

Chain D:  89% 11%




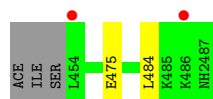
- Molecule 2: Measles virus fusion inhibitor MEK35GE

Chain F:  81% 8% 11%



- Molecule 2: Measles virus fusion inhibitor MEK35GE

Chain H:  5% 86% 5% 8%




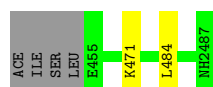
- Molecule 2: Measles virus fusion inhibitor MEK35GE

Chain J:  70% 14% 5% 11%



- Molecule 2: Measles virus fusion inhibitor MEK35GE

Chain L:  84% 5% 11%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	52.40Å 35.57Å 123.26Å 90.00° 91.26° 90.00°	Depositor
Resolution (Å)	48.60 – 2.17 48.60 – 2.17	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.60-2.17) 99.0 (48.60-2.17)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.68 (at 2.16Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.203 , 0.281 0.209 , 0.284	Depositor DCC
$R_{free}$ test set	1246 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.1	Xtriage
Anisotropy	0.537	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 34.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.020 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3835	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.85 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.4332e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: ACE, NH2

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	1.47	0/446
1	C	1.07	0/330	1.41	0/446
1	E	1.12	0/341	1.53	2/460 (0.4%)
1	G	1.03	0/339	1.56	0/458
1	I	1.05	0/339	1.72	0/458
1	K	1.10	0/347	1.51	1/469 (0.2%)
2	B	1.11	0/287	1.59	3/369 (0.8%)
2	D	1.05	0/294	1.48	1/386 (0.3%)
2	F	1.10	0/280	1.46	0/365
2	H	1.01	0/279	1.48	0/365
2	J	1.11	0/271	1.67	0/354
2	L	1.07	0/271	1.59	0/353
All	All	1.08	0/3708	1.54	7/4929 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	468	GLU	CB-CG-CD	5.67	122.23	112.60
2	B	459	VAL	CA-C-N	5.40	126.94	120.13
2	B	459	VAL	C-N-CA	5.40	126.94	120.13
1	E	176	GLN	CA-C-N	5.32	125.98	120.03
1	E	176	GLN	C-N-CA	5.32	125.98	120.03
2	B	459	VAL	N-CA-C	-5.28	106.28	111.77
1	K	157	THR	CB-CA-C	5.05	118.89	110.81

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	326	3	0
1	C	330	0	326	2	0
1	E	338	0	339	2	0
1	G	336	0	334	5	0
1	I	336	0	332	5	0
1	K	341	0	340	2	0
2	B	282	0	330	4	0
2	D	295	0	328	2	0
2	F	276	0	310	1	0
2	H	278	0	308	2	0
2	J	270	0	297	5	0
2	L	270	0	304	5	0
3	A	16	0	0	1	0
3	B	14	0	0	1	0
3	C	22	0	0	1	0
3	D	17	0	0	0	0
3	E	19	0	0	0	0
3	F	9	0	0	0	0
3	G	8	0	0	0	0
3	H	6	0	0	0	0
3	I	10	0	0	0	0
3	J	8	0	0	0	0
3	K	15	0	0	0	0
3	L	9	0	0	0	0
All	All	3835	0	3874	27	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 4.

All (27) 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:G:151:ARG:NH1	2:J:484:LEU:O	2.31	0.59
1:I:151:ARG:NH2	2:L:484:LEU:O	2.34	0.59
1:I:155[A]:GLU:HG2	2:L:484:LEU:HD23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:155[B]:GLU:HG3	2:L:484:LEU:HD23	1.88	0.55
2:B:477:LEU:HD11	1:E:161:ILE:HG22	1.91	0.53
1:A:180:ASP:O	1:A:184:ASN:N	2.37	0.52
1:A:161:ILE:HG22	2:D:477:LEU:HD11	1.91	0.52
1:G:151:ARG:HG2	1:I:150:LEU:HD21	1.92	0.51
2:J:472:LYS:O	2:J:475:GLU:HB2	2.12	0.50
1:C:151:ARG:HD3	3:C:222:HOH:O	2.11	0.49
2:D:465:LYS:O	2:D:469:LYS:HG2	2.13	0.49
2:B:478:LYS:O	2:B:482:GLU:HG2	2.13	0.48
2:F:482:GLU:HA	2:F:482:GLU:OE1	2.12	0.48
2:J:479:LYS:HA	2:J:482:GLU:OE1	2.13	0.48
2:H:475[B]:GLU:OE1	2:H:475[B]:GLU:HA	2.13	0.47
1:G:150:LEU:HD21	1:K:151:ARG:HG2	1.97	0.46
2:J:482:GLU:OE2	2:J:483:ILE:HG13	2.16	0.46
2:B:485[B]:LYS:NZ	3:B:502:HOH:O	2.49	0.45
2:L:471[B]:LYS:HB3	2:L:471[B]:LYS:HE2	1.41	0.45
1:G:179:GLN:OE1	2:J:459:VAL:HG22	2.18	0.43
1:C:143:ASN:OD1	1:C:145:GLN:HB2	2.19	0.42
1:E:184:ASN:HD22	1:E:184:ASN:HA	1.62	0.42
1:G:153:SER:OG	2:H:484:LEU:HG	2.20	0.41
1:I:155[B]:GLU:HG3	2:L:484:LEU:CD2	2.50	0.41
2:B:486[C]:LYS:HA	2:B:486[C]:LYS:HD3	1.86	0.41
1:A:169:GLN:HG2	3:A:215:HOH:O	2.21	0.40
1:K:165:ARG:HH12	1:K:169[A]:GLN:HE21	1.69	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	43/44 (98%)	42 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	43/44 (98%)	43 (100%)	0	0	100	100
1	E	44/44 (100%)	44 (100%)	0	0	100	100
1	G	44/44 (100%)	44 (100%)	0	0	100	100
1	I	44/44 (100%)	44 (100%)	0	0	100	100
1	K	45/44 (102%)	44 (98%)	1 (2%)	0	100	100
2	B	34/37 (92%)	31 (91%)	3 (9%)	0	100	100
2	D	36/37 (97%)	35 (97%)	1 (3%)	0	100	100
2	F	33/37 (89%)	31 (94%)	1 (3%)	1 (3%)	3	0
2	H	33/37 (89%)	32 (97%)	1 (3%)	0	100	100
2	J	32/37 (86%)	29 (91%)	2 (6%)	1 (3%)	3	0
2	L	32/37 (86%)	30 (94%)	2 (6%)	0	100	100
All	All	463/486 (95%)	449 (97%)	12 (3%)	2 (0%)	24	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	486	LYS
2	J	479	LYS

### 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	36/34 (106%)	36 (100%)	0	100	100
1	G	36/34 (106%)	35 (97%)	1 (3%)	38	40
1	I	36/34 (106%)	33 (92%)	3 (8%)	10	6
1	K	37/34 (109%)	36 (97%)	1 (3%)	39	41
2	B	32/32 (100%)	31 (97%)	1 (3%)	35	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	33/32 (103%)	33 (100%)	0	100	100
2	F	31/32 (97%)	30 (97%)	1 (3%)	34	36
2	H	31/32 (97%)	31 (100%)	0	100	100
2	J	30/32 (94%)	29 (97%)	1 (3%)	33	34
2	L	30/32 (94%)	30 (100%)	0	100	100
All	All	402/396 (102%)	394 (98%)	8 (2%)	51	54

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	484	LEU
2	F	471	LYS
1	G	147	ILE
1	I	155[A]	GLU
1	I	155[B]	GLU
1	I	157	THR
2	J	482	GLU
1	K	143	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	149	ASN
1	E	169	GLN
1	E	184	ASN
1	G	149	ASN
1	G	166	GLN
2	H	462	ASN
1	K	143	ASN
2	L	462	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 [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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	42/44 (95%)	-0.12	1 (2%) 59 63	27, 43, 60, 86	1 (2%)
1	C	42/44 (95%)	-0.31	0 100 100	26, 39, 52, 59	1 (2%)
1	E	42/44 (95%)	-0.24	0 100 100	24, 43, 61, 67	2 (4%)
1	G	42/44 (95%)	0.17	0 100 100	28, 52, 71, 80	2 (4%)
1	I	42/44 (95%)	0.22	0 100 100	27, 52, 75, 76	2 (4%)
1	K	42/44 (95%)	-0.08	0 100 100	21, 41, 72, 96	3 (7%)
2	B	32/37 (86%)	0.12	0 100 100	22, 53, 68, 87	2 (6%)
2	D	35/37 (94%)	0.00	0 100 100	33, 52, 65, 80	1 (2%)
2	F	32/37 (86%)	-0.07	0 100 100	27, 50, 69, 82	2 (6%)
2	H	33/37 (89%)	0.41	2 (6%) 27 31	36, 55, 90, 106	1 (3%)
2	J	32/37 (86%)	0.67	0 100 100	36, 68, 94, 107	1 (3%)
2	L	32/37 (86%)	0.07	0 100 100	35, 58, 81, 91	1 (3%)
All	All	448/486 (92%)	0.05	3 (0%) 84 85	21, 50, 80, 107	19 (4%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	454	LEU	4.2
2	H	486	LYS	2.6
1	A	184	ASN	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.