



wwPDB X-ray Structure Validation Summary Report ⓘ

May 17, 2020 – 02:10 am BST

PDB ID : 4LO7
Title : HA70(D3)-HA17-HA33
Authors : Lee, K.; Gu, S.; Jin, L.; Le, T.T.; Cheng, L.W.; Strotmeier, J.; Kruel, A.M.;
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Deposited on : 2013-07-12
Resolution : 3.73 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

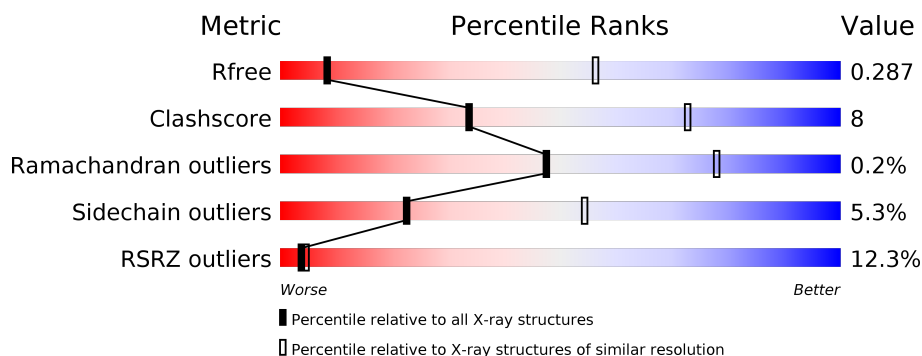
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.73 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	1001 (3.90-3.58)
Clashscore	141614	1063 (3.90-3.58)
Ramachandran outliers	138981	1027 (3.90-3.58)
Sidechain outliers	138945	1023 (3.90-3.58)
RSRZ outliers	127900	1006 (3.92-3.56)

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	254	<div> <div>14%</div> <div>72%</div> <div>15%</div> <div>•</div> <div>10%</div> </div>
1	E	254	<div> <div>4%</div> <div>76%</div> <div>13%</div> <div>•</div> <div>10%</div> </div>
2	B	296	<div> <div>5%</div> <div>84%</div> <div>11%</div> <div>• •</div> </div>
2	D	296	<div> <div>22%</div> <div>78%</div> <div>16%</div> <div>• •</div> </div>
2	F	296	<div> <div>11%</div> <div>85%</div> <div>10%</div> <div>• •</div> </div>
2	H	296	<div> <div>23%</div> <div>76%</div> <div>18%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	147	<div> <div> <div></div> <div>2%</div> </div> <div> <div></div> <div>79%</div> </div> <div> <div></div> <div>15%</div> </div> <div> <div></div> <div>5%</div> </div> </div>
3	G	147	<div> <div> <div></div> <div>%</div> </div> <div> <div></div> <div>80%</div> </div> <div> <div></div> <div>14%</div> </div> <div> <div></div> <div>5%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15326 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 HA-70.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	228	Total	C	N	O	S	12	0	0
			1852	1171	315	365	1			
1	E	229	Total	C	N	O	S	12	0	0
			1860	1177	316	366	1			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	373	GLY	-	EXPRESSION TAG	UNP Q8KHU9
A	374	PRO	-	EXPRESSION TAG	UNP Q8KHU9
A	375	LEU	-	EXPRESSION TAG	UNP Q8KHU9
A	376	GLY	-	EXPRESSION TAG	UNP Q8KHU9
A	377	SER	-	EXPRESSION TAG	UNP Q8KHU9
E	373	GLY	-	EXPRESSION TAG	UNP Q8KHU9
E	374	PRO	-	EXPRESSION TAG	UNP Q8KHU9
E	375	LEU	-	EXPRESSION TAG	UNP Q8KHU9
E	376	GLY	-	EXPRESSION TAG	UNP Q8KHU9
E	377	SER	-	EXPRESSION TAG	UNP Q8KHU9

- Molecule 2 is a protein called HA-33.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	286	Total	C	N	O	S	0	1	0
			2334	1477	399	455	3			
2	D	286	Total	C	N	O	S	0	1	0
			2334	1477	399	455	3			
2	F	286	Total	C	N	O	S	0	1	0
			2334	1477	399	455	3			
2	H	286	Total	C	N	O	S	0	1	0
			2334	1477	399	455	3			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	294	PRO	-	EXPRESSION TAG	UNP Q45871
B	295	GLY	-	EXPRESSION TAG	UNP Q45871
B	296	SER	-	EXPRESSION TAG	UNP Q45871
B	297	ALA	-	EXPRESSION TAG	UNP Q45871
D	294	PRO	-	EXPRESSION TAG	UNP Q45871
D	295	GLY	-	EXPRESSION TAG	UNP Q45871
D	296	SER	-	EXPRESSION TAG	UNP Q45871
D	297	ALA	-	EXPRESSION TAG	UNP Q45871
F	294	PRO	-	EXPRESSION TAG	UNP Q45871
F	295	GLY	-	EXPRESSION TAG	UNP Q45871
F	296	SER	-	EXPRESSION TAG	UNP Q45871
F	297	ALA	-	EXPRESSION TAG	UNP Q45871
H	294	PRO	-	EXPRESSION TAG	UNP Q45871
H	295	GLY	-	EXPRESSION TAG	UNP Q45871
H	296	SER	-	EXPRESSION TAG	UNP Q45871
H	297	ALA	-	EXPRESSION TAG	UNP Q45871

- Molecule 3 is a protein called HA-17.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	139	Total	C	N	O	S	0	0	0
			1139	735	181	218	5			
3	G	139	Total	C	N	O	S	0	0	0
			1139	735	181	218	5			

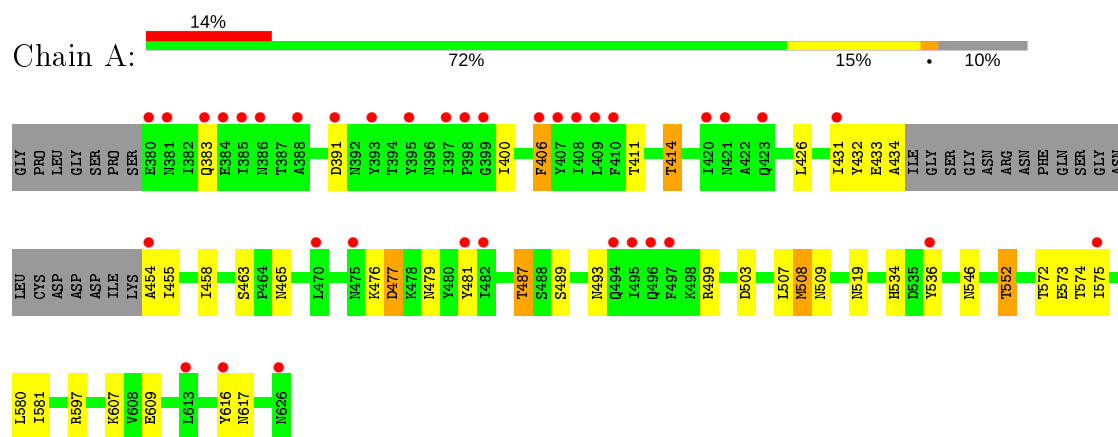
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	GLY	-	EXPRESSION TAG	UNP Q45878
C	1	PRO	-	EXPRESSION TAG	UNP Q45878
G	0	GLY	-	EXPRESSION TAG	UNP Q45878
G	1	PRO	-	EXPRESSION TAG	UNP Q45878

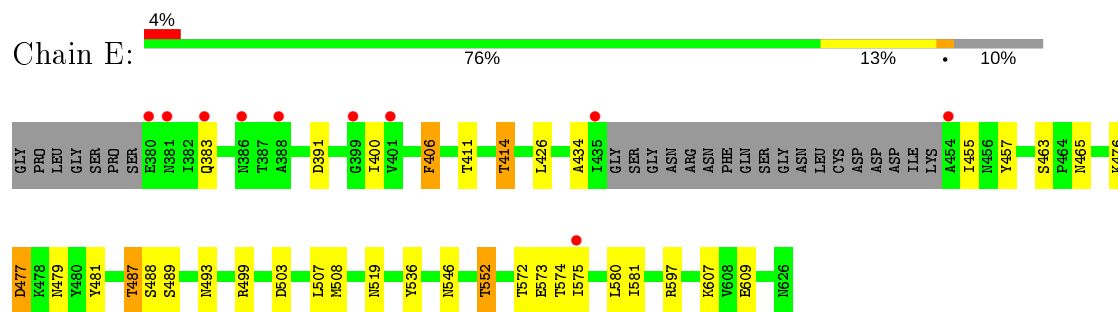
3 Residue-property plots [i](#)

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.

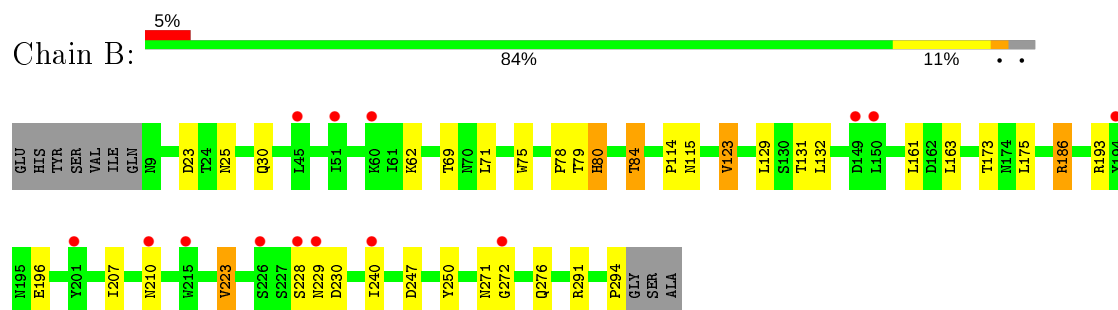
• Molecule 1: HA-70



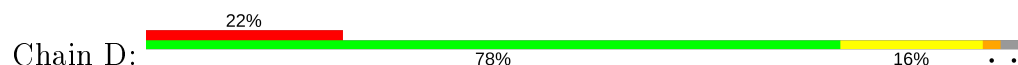
• Molecule 1: HA-70

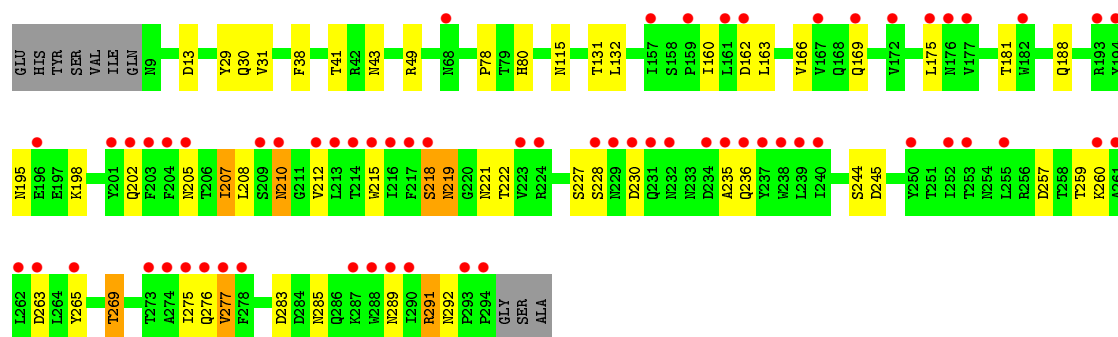


• Molecule 2: HA-33

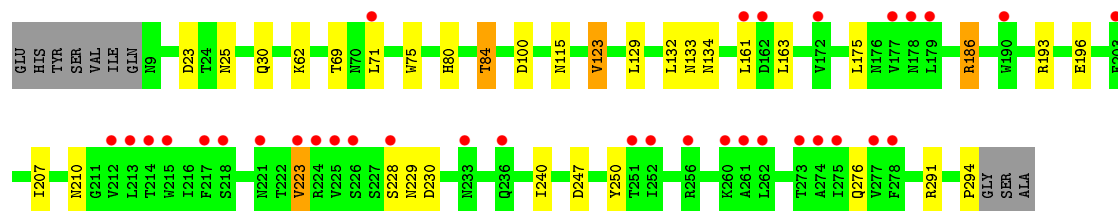
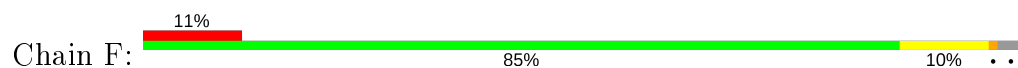


• Molecule 2: HA-33

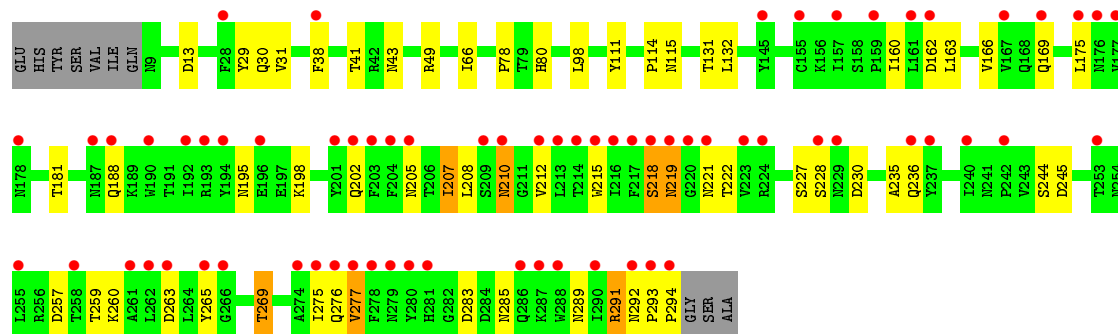
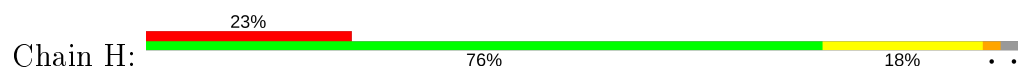




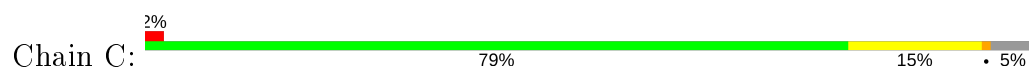
• Molecule 2: HA-33



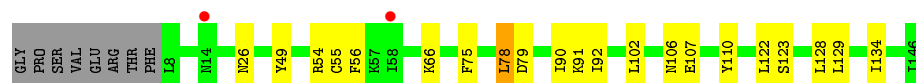
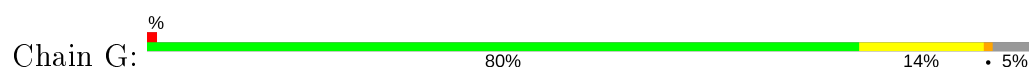
• Molecule 2: HA-33



• Molecule 3: HA-17



• Molecule 3: HA-17



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	159.59 Å 187.49 Å 120.43 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.20 – 3.73 49.20 – 3.73	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.20-3.73) 99.5 (49.20-3.73)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.77 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.268 , 0.293 0.263 , 0.287	Depositor DCC
R_{free} test set	1907 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	111.9	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 97.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	15326	wwPDB-VP
Average B, all atoms (Å ²)	169.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.24	0/1886	0.45	0/2570
1	E	0.24	0/1894	0.45	0/2581
2	B	0.49	0/2393	0.59	1/3267 (0.0%)
2	D	0.46	0/2393	0.61	1/3267 (0.0%)
2	F	0.49	0/2393	0.59	1/3267 (0.0%)
2	H	0.47	0/2393	0.61	1/3267 (0.0%)
3	C	0.50	0/1168	0.62	0/1587
3	G	0.50	0/1168	0.62	0/1587
All	All	0.44	0/15688	0.57	4/21393 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	230	ASP	CB-CG-OD2	5.20	122.98	118.30
2	F	230	ASP	CB-CG-OD2	5.20	122.97	118.30
2	D	230	ASP	CB-CG-OD2	5.18	122.97	118.30
2	B	230	ASP	CB-CG-OD2	5.16	122.94	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1852	0	1807	61	9

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1860	0	1818	59	4
2	B	2334	0	2250	46	7
2	D	2334	0	2250	35	3
2	F	2334	0	2250	41	0
2	H	2334	0	2250	42	3
3	C	1139	0	1097	57	0
3	G	1139	0	1097	50	0
All	All	15326	0	14819	255	13

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 8.

The worst 5 of 255 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:E:575:ILE:HG12	3:G:49:TYR:CE1	1.62	1.33
1:E:575:ILE:HD13	3:G:56:PHE:CZ	1.65	1.31
1:A:575:ILE:HG12	3:C:49:TYR:CE1	1.74	1.22
2:B:294:PRO:HB3	2:F:23:ASP:OD2	1.40	1.17
1:E:575:ILE:CG1	3:G:49:TYR:CE1	2.27	1.16

The worst 5 of 13 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:A:616:TYR:CB	2:B:272:GLY:O[3_456]	1.30	0.90
1:A:616:TYR:CD2	2:B:272:GLY:CA[3_456]	1.34	0.86
2:B:173:THR:O	1:E:481:TYR:OH[4_546]	1.55	0.65
1:A:455:ILE:O	1:E:455:ILE:O[2_455]	1.65	0.55
1:A:616:TYR:CB	2:B:272:GLY:C[3_456]	1.86	0.34

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	224/254 (88%)	212 (95%)	12 (5%)	0	100	100
1	E	225/254 (89%)	213 (95%)	11 (5%)	1 (0%)	34	69
2	B	285/296 (96%)	276 (97%)	9 (3%)	0	100	100
2	D	285/296 (96%)	269 (94%)	15 (5%)	1 (0%)	34	69
2	F	285/296 (96%)	277 (97%)	8 (3%)	0	100	100
2	H	285/296 (96%)	270 (95%)	14 (5%)	1 (0%)	34	69
3	C	137/147 (93%)	133 (97%)	4 (3%)	0	100	100
3	G	137/147 (93%)	133 (97%)	4 (3%)	0	100	100
All	All	1863/1986 (94%)	1783 (96%)	77 (4%)	3 (0%)	47	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	265	TYR
2	H	265	TYR
1	E	488	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	211/232 (91%)	197 (93%)	14 (7%)	16	48
1	E	212/232 (91%)	198 (93%)	14 (7%)	16	48
2	B	263/270 (97%)	253 (96%)	10 (4%)	33	61
2	D	263/270 (97%)	245 (93%)	18 (7%)	16	47
2	F	263/270 (97%)	253 (96%)	10 (4%)	33	61
2	H	263/270 (97%)	245 (93%)	18 (7%)	16	47
3	C	130/138 (94%)	126 (97%)	4 (3%)	40	65
3	G	130/138 (94%)	126 (97%)	4 (3%)	40	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1735/1820 (95%)	1643 (95%)	92 (5%)	22 54

5 of 92 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	277	VAL
1	E	465	ASN
2	H	269	THR
2	D	283	ASP
1	E	406	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
2	B	115	ASN
2	H	86	GLN
2	D	86	GLN
1	A	534	HIS
1	E	392	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 [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	228/254 (89%)	0.81	36 (15%) 2 2	99, 151, 222, 268	3 (1%)
1	E	229/254 (90%)	0.22	10 (4%) 34 29	101, 147, 213, 274	3 (1%)
2	B	286/296 (96%)	0.48	14 (4%) 29 26	85, 132, 183, 234	0
2	D	286/296 (96%)	1.15	64 (22%) 0 0	99, 207, 325, 398	0
2	F	286/296 (96%)	0.61	34 (11%) 4 5	93, 145, 203, 256	0
2	H	286/296 (96%)	1.09	69 (24%) 0 0	94, 195, 353, 422	0
3	C	139/147 (94%)	0.18	3 (2%) 62 55	107, 154, 194, 221	0
3	G	139/147 (94%)	0.19	2 (1%) 75 70	109, 147, 192, 208	0
All	All	1879/1986 (94%)	0.66	232 (12%) 4 4	85, 153, 303, 422	6 (0%)

The worst 5 of 232 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	202	GLN	15.5
2	D	215	TRP	8.5
2	D	237	TYR	7.6
1	A	381	ASN	7.6
2	H	169	GLN	7.6

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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.