



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 02:48 pm BST

PDB ID : 6KMU
Title : P22/P10 complex of caspase-11 mutant C254A
Authors : Ding, J.; Sun, Q.
Deposited on : 2019-08-01
Resolution : 2.10 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 : 2.11
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

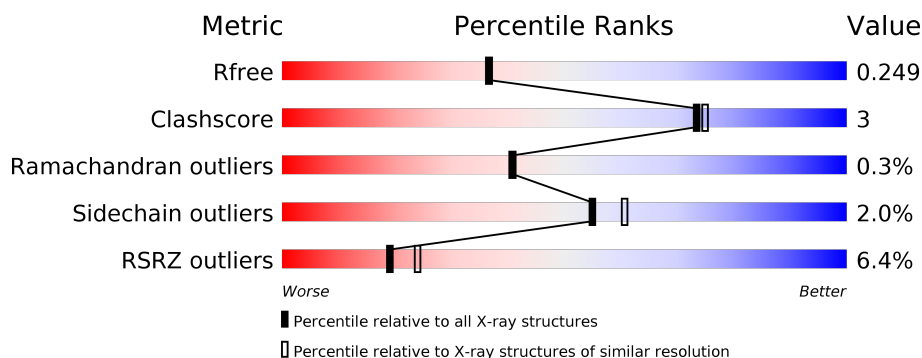
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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	184	<div> <div>8%</div> <div>83%</div> <div>11%</div> <div>7%</div> </div>
1	E	184	<div> <div>8%</div> <div>83%</div> <div>10%</div> <div>7%</div> </div>
2	B	86	<div> <div>94%</div> <div>6%</div> </div>
2	F	86	<div> <div>8%</div> <div>84%</div> <div>13%</div> <div>•</div> </div>
2	H	86	<div> <div>13%</div> <div>77%</div> <div>13%</div> <div>10%</div> </div>
3	C	185	<div> <div>5%</div> <div>83%</div> <div>10%</div> <div>7%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	87	 87% 13%
5	G	154	 5% 89% 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8405 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 Caspase-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	172	Total	C	N	O	S	0	0	0
			1359	851	235	260	13			
1	E	171	Total	C	N	O	S	0	0	0
			1348	845	231	259	13			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	ALA	CYS	engineered mutation	UNP P70343
E	254	ALA	CYS	engineered mutation	UNP P70343

- Molecule 2 is a protein called Caspase-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	86	Total	C	N	O	S	0	0	0
			714	463	123	124	4			
2	F	83	Total	C	N	O	S	0	0	0
			691	448	119	120	4			
2	H	77	Total	C	N	O	S	0	0	0
			639	417	108	110	4			

- Molecule 3 is a protein called Caspase-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	172	Total	C	N	O	S	0	0	0
			1355	849	232	261	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	254	ALA	CYS	engineered mutation	UNP P70343

- Molecule 4 is a protein called Caspase-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	87	Total	C	N	O	S	0	0	0
			721	468	124	125	4			

- Molecule 5 is a protein called Caspase-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	154	Total	C	N	O	S	0	0	0
			1214	765	205	233	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	254	ALA	CYS	engineered mutation	UNP P70343

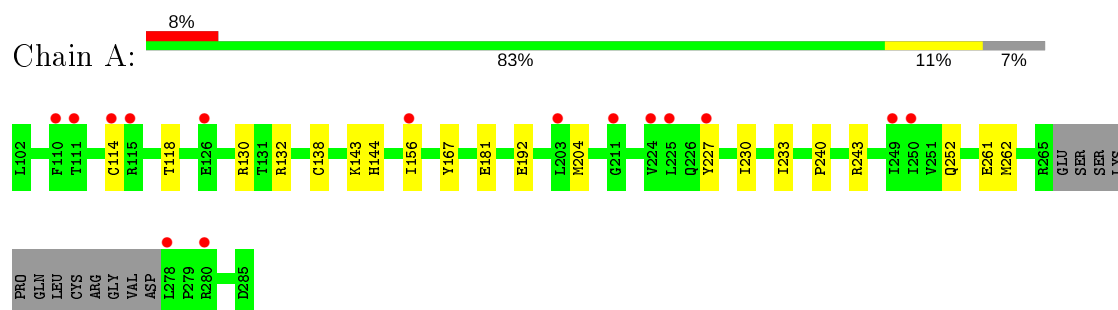
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	70	Total	O	0	0
			70	70		
6	B	40	Total	O	0	0
			40	40		
6	C	79	Total	O	0	0
			79	79		
6	D	41	Total	O	0	0
			41	41		
6	E	61	Total	O	0	0
			61	61		
6	F	21	Total	O	0	0
			21	21		
6	G	37	Total	O	0	0
			37	37		
6	H	15	Total	O	0	0
			15	15		

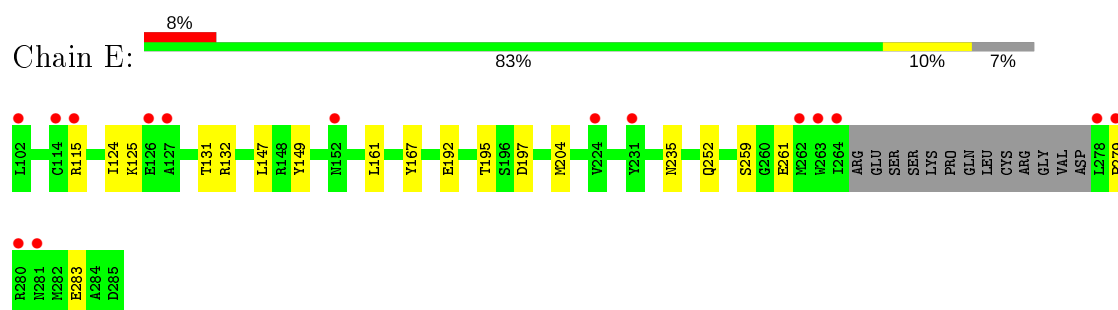
3 Residue-property plots [i](#)

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.

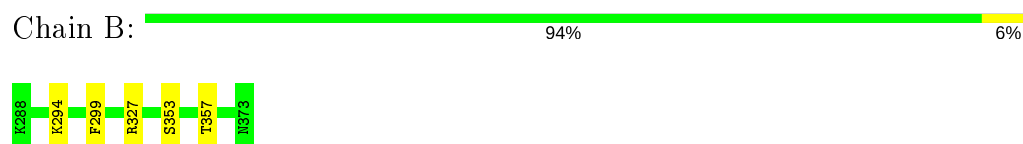
• Molecule 1: Caspase-4



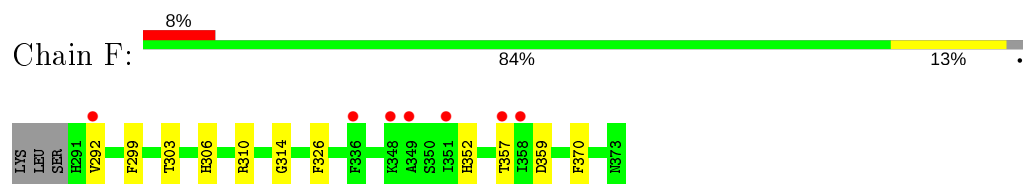
• Molecule 1: Caspase-4



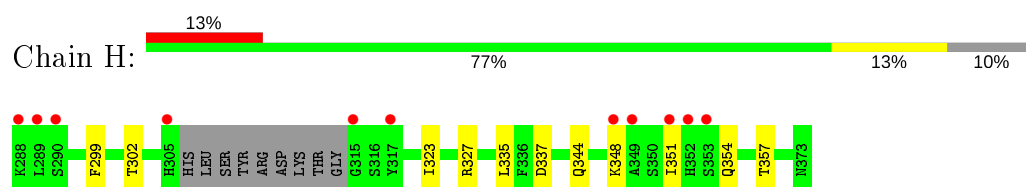
• Molecule 2: Caspase-4



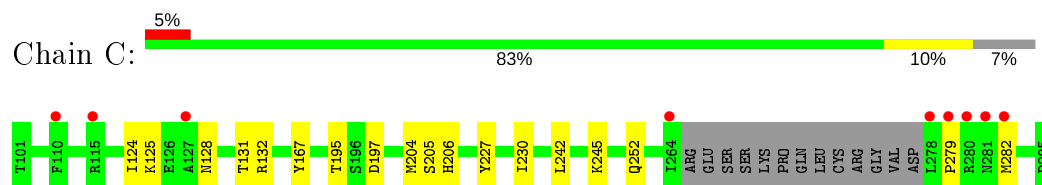
• Molecule 2: Caspase-4



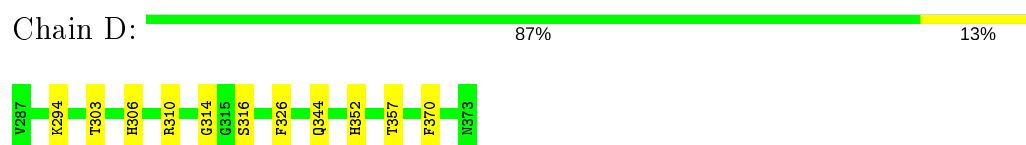
• Molecule 2: Caspase-4



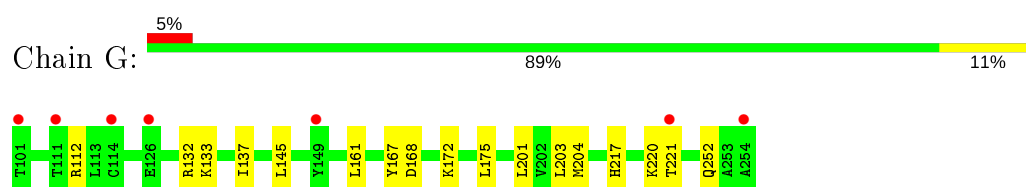
- Molecule 3: Caspase-4



- Molecule 4: Caspase-4



- Molecule 5: Caspase-4



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	61.97Å 102.00Å 99.74Å 90.00° 93.52° 90.00°	Depositor
Resolution (Å)	49.78 – 2.10 49.78 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.78-2.10) 98.9 (49.78-2.10)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 2.10Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.210 , 0.251 0.210 , 0.249	Depositor DCC
R_{free} test set	2020 reflections (2.82%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.562	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8405	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% 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	0.24	0/1382	0.42	0/1857
1	E	0.24	0/1371	0.41	0/1843
2	B	0.24	0/736	0.43	0/990
2	F	0.24	0/713	0.41	0/960
2	H	0.28	0/658	0.40	0/884
3	C	0.23	0/1378	0.42	0/1853
4	D	0.25	0/743	0.42	0/1000
5	G	0.23	0/1235	0.42	0/1664
All	All	0.24	0/8216	0.42	0/11051

There are no bond length outliers.

There are no bond angle outliers.

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	1359	0	1346	12	0
1	E	1348	0	1333	11	0
2	B	714	0	697	2	0
2	F	691	0	668	6	0
2	H	639	0	624	7	0
3	C	1355	0	1340	10	0
4	D	721	0	706	5	0
5	G	1214	0	1211	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	70	0	0	1	0
6	B	40	0	0	1	0
6	C	79	0	0	1	0
6	D	41	0	0	0	0
6	E	61	0	0	0	0
6	F	21	0	0	0	0
6	G	37	0	0	0	0
6	H	15	0	0	1	0
All	All	8405	0	7925	52	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 3.

All (52) 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:204:MET:HG2	1:E:252:GLN:HB3	1.70	0.74
1:A:204:MET:HG2	1:A:252:GLN:HB3	1.74	0.69
3:C:204:MET:HG2	3:C:252:GLN:HB3	1.72	0.69
3:C:131:THR:HG1	3:C:195:THR:HG1	1.41	0.64
5:G:204:MET:HG2	5:G:252:GLN:HB3	1.81	0.60
5:G:133:LYS:NZ	5:G:168:ASP:OD2	2.34	0.60
2:H:327:ARG:NH1	6:H:401:HOH:O	2.33	0.60
1:A:227:TYR:HA	1:A:230:ILE:HD12	1.84	0.59
2:H:351:ILE:O	2:H:351:ILE:HG22	2.02	0.59
1:E:259:SER:OG	1:E:261:GLU:OE1	2.23	0.57
3:C:279:PRO:HD3	4:D:352:HIS:CE1	2.42	0.55
5:G:137:ILE:HB	5:G:203:LEU:HD23	1.89	0.54
1:A:114:CYS:O	1:A:118:THR:OG1	2.23	0.54
2:B:294:LYS:NZ	6:B:402:HOH:O	2.41	0.54
1:A:192:GLU:N	1:A:192:GLU:OE1	2.43	0.52
1:E:147:LEU:HD23	1:E:149:TYR:CZ	2.46	0.50
3:C:125:LYS:HG3	3:C:197:ASP:HB3	1.93	0.49
1:E:131:THR:HG1	1:E:195:THR:HG1	1.57	0.49
5:G:145:LEU:HD11	5:G:217:HIS:HD2	1.77	0.49
6:C:303:HOH:O	4:D:294:LYS:NZ	2.46	0.49
3:C:227:TYR:HA	3:C:230:ILE:HD12	1.96	0.47
3:C:132:ARG:HB3	3:C:167:TYR:CD2	2.49	0.47
5:G:220:LYS:HG3	5:G:221:THR:HG23	1.96	0.46
1:A:261:GLU:HB3	2:B:353:SER:HB2	1.97	0.46
2:F:303:THR:OG1	2:F:306:HIS:ND1	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:172:LYS:HB3	5:G:175:LEU:HD11	1.98	0.46
1:A:181:GLU:HG3	1:A:233:ILE:HD11	1.98	0.46
1:A:130:ARG:HD3	1:A:132:ARG:HG3	1.98	0.45
5:G:132:ARG:HB3	5:G:167:TYR:CD2	2.52	0.45
2:H:344:GLN:O	2:H:348:LYS:HG3	2.17	0.45
1:E:125:LYS:HG3	1:E:197:ASP:HB3	1.99	0.44
3:C:124:ILE:HG13	4:D:370:PHE:HD2	1.82	0.44
1:E:283:GLU:OE1	2:F:310:ARG:NH1	2.40	0.44
2:H:344:GLN:HB3	2:H:348:LYS:NZ	2.32	0.44
1:A:240:PRO:HA	1:A:243:ARG:HG3	2.00	0.44
2:H:344:GLN:HB3	2:H:348:LYS:HZ3	1.82	0.44
1:E:279:PRO:HD3	2:F:352:HIS:NE2	2.32	0.44
5:G:161:LEU:HD22	2:H:323:ILE:HA	2.00	0.43
1:A:156:ILE:N	6:A:301:HOH:O	2.50	0.43
3:C:279:PRO:HD2	3:C:282:MET:HB3	2.01	0.42
4:D:303:THR:OG1	4:D:306:HIS:ND1	2.41	0.42
3:C:242:LEU:HA	3:C:245:LYS:HD2	2.00	0.42
1:E:124:ILE:HG13	2:F:370:PHE:HD2	1.83	0.42
1:E:132:ARG:HB3	1:E:167:TYR:CD2	2.54	0.42
1:A:143:LYS:HE3	1:A:144:HIS:NE2	2.35	0.42
2:H:302:THR:HG22	2:H:354:GLN:HG3	2.01	0.42
1:A:132:ARG:HB3	1:A:167:TYR:CD2	2.55	0.41
4:D:310:ARG:HA	4:D:316:SER:HA	2.02	0.41
1:E:235:ASN:HB2	2:F:292:VAL:O	2.21	0.41
1:A:138:CYS:HA	1:A:204:MET:O	2.21	0.40
3:C:205:SER:OG	3:C:206:HIS:N	2.54	0.40
1:E:161:LEU:HD11	2:F:326:PHE:HB3	2.03	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	168/184 (91%)	163 (97%)	5 (3%)	0	100	100
1	E	167/184 (91%)	162 (97%)	5 (3%)	0	100	100
2	B	84/86 (98%)	82 (98%)	2 (2%)	0	100	100
2	F	81/86 (94%)	78 (96%)	2 (2%)	1 (1%)	13	8
2	H	73/86 (85%)	72 (99%)	1 (1%)	0	100	100
3	C	168/185 (91%)	161 (96%)	6 (4%)	1 (1%)	25	21
4	D	85/87 (98%)	83 (98%)	1 (1%)	1 (1%)	13	8
5	G	152/154 (99%)	144 (95%)	8 (5%)	0	100	100
All	All	978/1052 (93%)	945 (97%)	30 (3%)	3 (0%)	41	41

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	128	ASN
4	D	314	GLY
2	F	314	GLY

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	150/161 (93%)	149 (99%)	1 (1%)	84	88
1	E	149/161 (92%)	147 (99%)	2 (1%)	69	75
2	B	79/79 (100%)	76 (96%)	3 (4%)	33	34
2	F	76/79 (96%)	73 (96%)	3 (4%)	32	33
2	H	71/79 (90%)	67 (94%)	4 (6%)	21	18
3	C	150/162 (93%)	150 (100%)	0	100	100
4	D	80/80 (100%)	77 (96%)	3 (4%)	33	34
5	G	136/136 (100%)	134 (98%)	2 (2%)	65	71
All	All	891/937 (95%)	873 (98%)	18 (2%)	55	60

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

Mol	Chain	Res	Type
1	A	262	MET
2	B	299	PHE
2	B	327	ARG
2	B	357	THR
4	D	326	PHE
4	D	344	GLN
4	D	357	THR
1	E	115	ARG
1	E	192	GLU
2	F	299	PHE
2	F	357	THR
2	F	359	ASP
5	G	112	ARG
5	G	201	LEU
2	H	299	PHE
2	H	335	LEU
2	H	337	ASP
2	H	357	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	354	GLN

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

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	172/184 (93%)	0.53	15 (8%) 10 13	32, 45, 81, 94	0
1	E	171/184 (92%)	0.67	15 (8%) 10 12	36, 52, 89, 108	0
2	B	86/86 (100%)	0.46	0 100 100	29, 41, 61, 79	0
2	F	83/86 (96%)	0.66	7 (8%) 11 14	37, 54, 81, 90	0
2	H	77/86 (89%)	0.81	11 (14%) 2 3	38, 59, 92, 95	0
3	C	172/185 (92%)	0.17	9 (5%) 27 32	31, 47, 79, 106	0
4	D	87/87 (100%)	0.31	0 100 100	29, 43, 67, 75	0
5	G	154/154 (100%)	0.40	7 (4%) 33 38	40, 54, 82, 96	0
All	All	1002/1052 (95%)	0.48	64 (6%) 19 24	29, 50, 82, 108	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	351	ILE	6.5
1	E	278	LEU	5.7
2	H	289	LEU	5.5
1	E	115	ARG	5.1
1	E	263	TRP	4.9
3	C	280	ARG	4.6
5	G	149	TYR	4.4
1	A	126	GLU	4.2
5	G	114	CYS	4.2
1	E	279	PRO	4.2
1	E	281	ASN	4.0
1	A	115	ARG	3.8
1	E	280	ARG	3.8
1	A	278	LEU	3.6
2	H	349	ALA	3.4
1	A	114	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
2	F	336	PHE	3.4
5	G	111	THR	3.3
1	E	114	CYS	3.2
1	E	264	ILE	3.1
3	C	279	PRO	3.1
2	H	288	LYS	3.0
2	H	352	HIS	2.9
1	A	110	PHE	2.8
5	G	254	ALA	2.8
1	A	224	VAL	2.8
2	F	292	VAL	2.7
1	A	249	ILE	2.7
2	H	348	LYS	2.7
5	G	221	THR	2.7
1	E	262	MET	2.7
1	A	280	ARG	2.6
3	C	281	ASN	2.6
1	A	156	ILE	2.6
1	E	127	ALA	2.6
1	A	225	LEU	2.5
2	H	351	ILE	2.5
1	E	102	LEU	2.5
1	E	152	ASN	2.5
2	H	315	GLY	2.4
3	C	278	LEU	2.4
5	G	126	GLU	2.3
3	C	264	ILE	2.3
2	H	353	SER	2.3
2	H	305	HIS	2.2
2	F	357	THR	2.2
1	E	224	VAL	2.2
3	C	110	PHE	2.2
3	C	127	ALA	2.2
2	F	358	ILE	2.1
3	C	115	ARG	2.1
1	A	203	LEU	2.1
1	E	126	GLU	2.1
1	A	227	TYR	2.1
1	A	111	THR	2.1
2	F	349	ALA	2.1
2	F	348	LYS	2.1
2	H	290	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	231	TYR	2.0
3	C	282	MET	2.0
5	G	101	THR	2.0
2	H	317	TYR	2.0
1	A	250	ILE	2.0
1	A	211	GLY	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 carbohydrates 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.