



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 05:06 PM UTC

PDB ID : 2C2V / pdb_00002c2v
Title : Crystal structure of the CHIP-UBC13-UEV1a complex
Authors : Zhang, M.; Roe, S.M.; Pearl, L.H.
Deposited on : 2005-09-30
Resolution : 2.90 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 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
Xtrriage (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

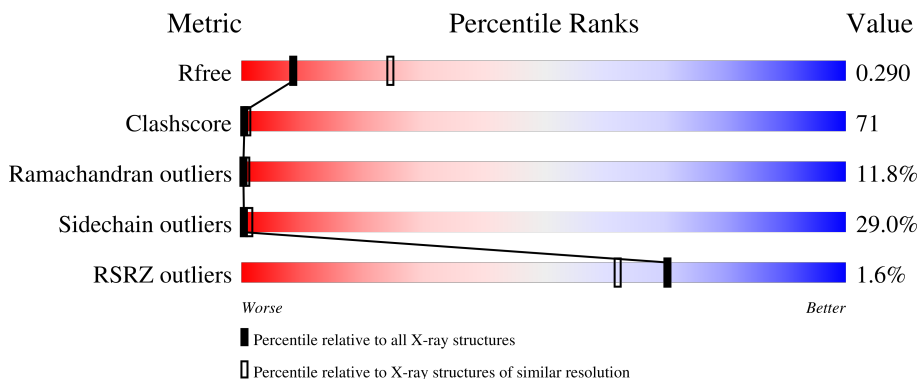
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	B	154	 2% 29% 47% 21%
1	E	154	 3% 8% 23% 45% 20%
1	H	154	 1% 21% 53% 19%
1	K	154	 3% 25% 43% 27%
2	C	142	 4% 36% 45% 18%

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Mol	Chain	Length	Quality of chain
2	F	142	<p>% 6% 30% 42% 20% .</p>
2	I	142	<p>. 31% 35% 29% .</p>
2	L	142	<p>% 7% 28% 40% 23% .</p>
3	S	78	<p>. 13% 46% 33% .</p>
3	T	78	<p>3% . 24% 44% 29%</p>
3	U	78	<p>. 19% 54% 19% 6%</p>
3	V	78	<p>. 19% 31% 40% 9%</p>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11636 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 Ubiquitin-conjugating enzyme E2 N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	152	1202	769	208	221	4	0	0	0
1	E	149	1187	761	205	217	4	0	0	0
1	H	149	1187	761	205	217	4	0	0	0
1	K	152	1202	769	208	221	4	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	3	ALA	-	expression tag	UNP P61088
B	4	GLY	-	expression tag	UNP P61088
B	5	SER	-	expression tag	UNP P61088
E	3	ALA	-	expression tag	UNP P61088
E	4	GLY	-	expression tag	UNP P61088
E	5	SER	-	expression tag	UNP P61088
H	3	ALA	-	expression tag	UNP P61088
H	4	GLY	-	expression tag	UNP P61088
H	5	SER	-	expression tag	UNP P61088
K	3	ALA	-	expression tag	UNP P61088
K	4	GLY	-	expression tag	UNP P61088
K	5	SER	-	expression tag	UNP P61088

- Molecule 2 is a protein called Ubiquitin-conjugating enzyme E2 variant 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	142	1123	709	195	211	8	0	0	0
2	F	139	1109	701	192	208	8	0	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	139	Total	C	N	O	S	0	0	0
			1109	701	192	208	8			
2	L	139	Total	C	N	O	S	0	0	0
			1109	701	192	208	8			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	80	LEU	ILE	conflict	UNP Q13404
F	80	LEU	ILE	conflict	UNP Q13404
I	80	LEU	ILE	conflict	UNP Q13404
L	80	LEU	ILE	conflict	UNP Q13404

- Molecule 3 is a protein called STIP1 homology and U box-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	75	Total	C	N	O	S	0	0	1
			598	379	101	114	4			
3	T	78	Total	C	N	O	S	0	0	0
			634	402	104	124	4			
3	U	73	Total	C	N	O	S	0	0	1
			577	365	98	110	4			
3	V	71	Total	C	N	O	S	0	0	1
			564	356	96	108	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	269	ASN	ASP	conflict	UNP Q9WUD1
T	269	ASN	ASP	conflict	UNP Q9WUD1
U	269	ASN	ASP	conflict	UNP Q9WUD1
V	269	ASN	ASP	conflict	UNP Q9WUD1

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	5	Total	O	0	0
			5	5		
4	C	5	Total	O	0	0
			5	5		
4	E	3	Total	O	0	0
			3	3		

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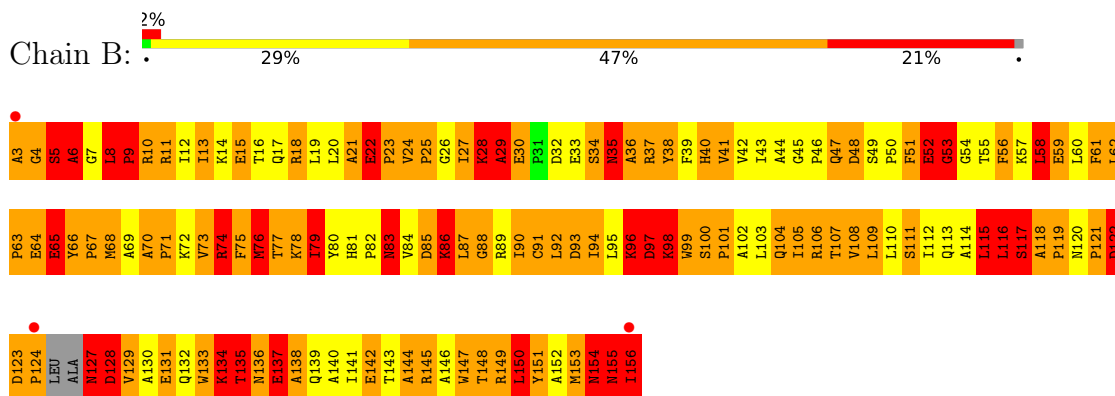
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	7	Total O 7 7	0	0
4	H	1	Total O 1 1	0	0
4	I	1	Total O 1 1	0	0
4	L	1	Total O 1 1	0	0
4	S	6	Total O 6 6	0	0
4	T	2	Total O 2 2	0	0
4	U	1	Total O 1 1	0	0
4	V	3	Total O 3 3	0	0

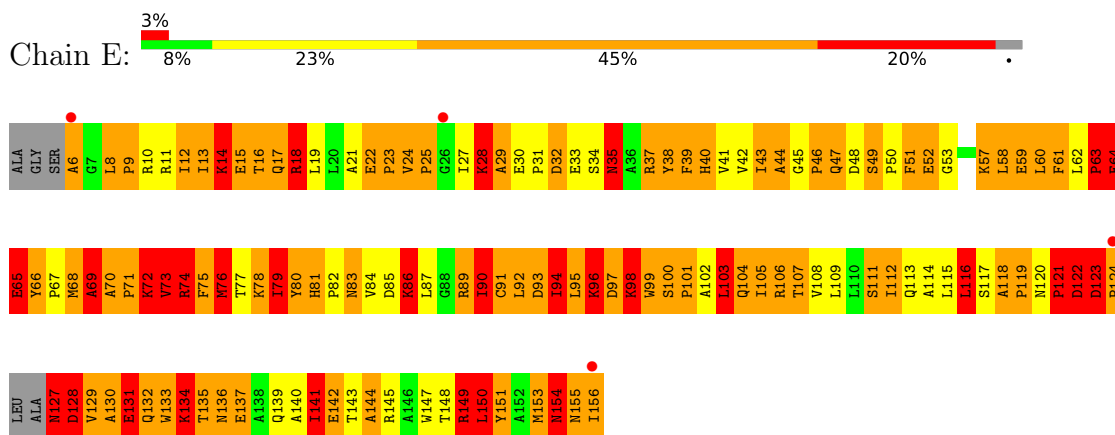
3 Residue-property plots [i](#)

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.

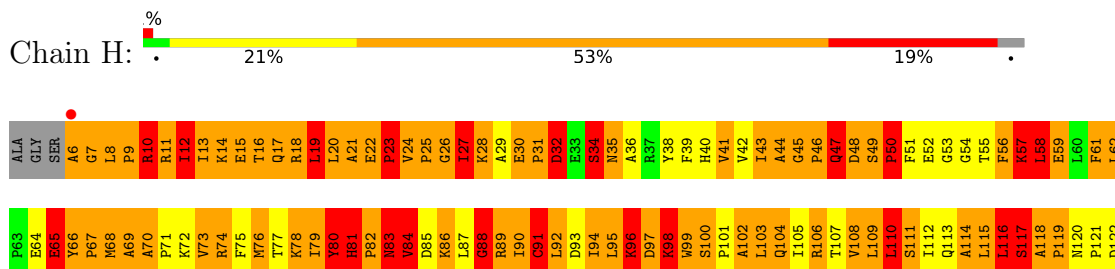
- Molecule 1: Ubiquitin-conjugating enzyme E2 N



- Molecule 1: Ubiquitin-conjugating enzyme E2 N

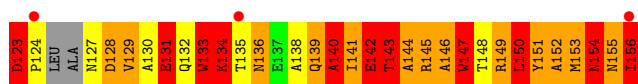


- Molecule 1: Ubiquitin-conjugating enzyme E2 N

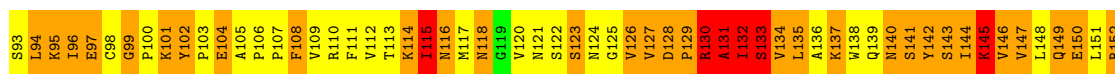




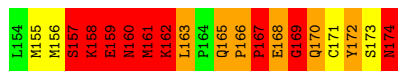
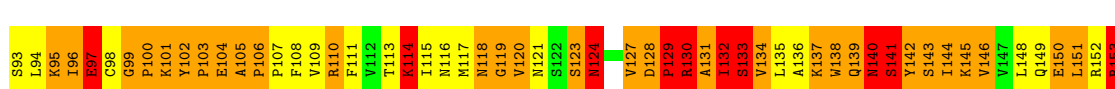
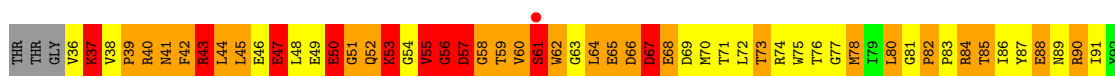
- Molecule 1: Ubiquitin-conjugating enzyme E2 N



- Molecule 2: Ubiquitin-conjugating enzyme E2 variant 1



- Molecule 2: Ubiquitin-conjugating enzyme E2 variant 1



- Molecule 2: Ubiquitin-conjugating enzyme E2 variant 1

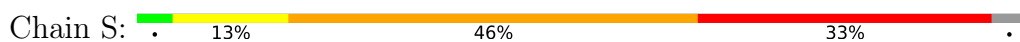




- Molecule 2: Ubiquitin-conjugating enzyme E2 variant 1



- Molecule 3: STIP1 homology and U box-containing protein 1



- Molecule 3: STIP1 homology and U box-containing protein 1



- Molecule 3: STIP1 homology and U box-containing protein 1



- Molecule 3: STIP1 homology and U box-containing protein 1



ASP	K287
ILE	K288
P229	E289
D230	V290
Y231	I291
L232	D292
C233	A293
G234	F294
K235	I295
I236	S296
S237	E297
F238	N298
E239	G299
L240	TRP
M241	VAL
R242	GLU
E243	ASP
P244	TYR
P244	
G245	
L246	
I247	
S248	
S249	
Q250	
I251	
T252	
Y253	
D254	
R255	
K256	
D257	
L258	
E259	
E260	
H261	
L262	
Q263	
R264	
V265	
G266	
H267	
F268	
N269	
P270	
V271	
T272	
R273	
S274	
P275	
L276	
I277	
Q278	
E279	
Q280	
L281	
I282	
P283	
N284	
L285	
A286	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	180.31Å 69.99Å 204.48Å 90.00° 106.95° 90.00°	Depositor
Resolution (Å)	196.12 – 2.90 195.59 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.3 (196.12-2.90) 95.3 (195.59-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 2.90Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.214 , 0.297 0.214 , 0.290	Depositor DCC
R_{free} test set	2621 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	64.0	Xtrriage
Anisotropy	0.605	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 57.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11636	wwPDB-VP
Average B, all atoms (Å ²)	4.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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	B	4.01	230/1231 (18.7%)	3.28	179/1673 (10.7%)
1	E	3.64	199/1216 (16.4%)	2.79	122/1653 (7.4%)
1	H	3.36	143/1216 (11.8%)	2.79	122/1653 (7.4%)
1	K	3.54	176/1231 (14.3%)	2.79	114/1673 (6.8%)
2	C	4.15	213/1147 (18.6%)	3.25	187/1551 (12.1%)
2	F	3.76	176/1133 (15.5%)	3.15	168/1532 (11.0%)
2	I	3.12	118/1133 (10.4%)	2.55	81/1532 (5.3%)
2	L	3.26	140/1133 (12.4%)	2.88	124/1532 (8.1%)
3	S	4.01	118/612 (19.3%)	3.61	123/831 (14.8%)
3	T	3.89	108/649 (16.6%)	2.92	74/880 (8.4%)
3	U	3.68	99/589 (16.8%)	3.31	89/799 (11.1%)
3	V	3.77	100/576 (17.4%)	3.21	90/780 (11.5%)
All	All	3.67	1820/11866 (15.3%)	3.01	1473/16089 (9.2%)

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	B	0	7
1	E	0	6
1	H	0	7
1	K	0	17
2	C	0	6
2	F	0	4
2	I	0	13
2	L	0	3
3	S	0	4
3	T	0	1
3	U	0	3
3	V	0	2
All	All	0	73

The worst 5 of 1820 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	131	ALA	CA-CB	37.51	2.16	1.53
2	F	55	VAL	CA-CB	27.92	1.85	1.54
2	C	34	THR	CA-CB	23.58	1.93	1.53
3	U	295	ILE	CA-CB	19.12	1.75	1.54
3	S	236	ILE	CA-CB	-18.51	1.29	1.54

The worst 5 of 1473 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	70	ALA	CA-C-N	-17.55	103.36	120.21
1	B	70	ALA	C-N-CA	-17.55	103.36	120.21
3	S	266	GLY	N-CA-C	17.09	133.16	112.48
1	B	7	GLY	N-CA-C	-16.95	95.45	113.58
2	F	38	VAL	CA-C-N	-16.85	103.79	120.31

There are no chirality outliers.

5 of 73 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	29	ALA	Peptide
1	B	5	SER	Peptide
1	B	6	ALA	Peptide
1	B	76	MET	Peptide
1	B	97	ASP	Peptide

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	B	1202	0	1209	147	1
1	E	1187	0	1196	153	1
1	H	1187	0	1196	195	1
1	K	1202	0	1209	221	1
2	C	1123	0	1121	133	1
2	F	1109	0	1114	143	0
2	I	1109	0	1114	159	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	L	1109	0	1114	132	1
3	S	598	0	584	91	0
3	T	634	0	612	92	0
3	U	577	0	569	142	0
3	V	564	0	557	116	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	E	3	0	0	0	0
4	F	7	0	0	1	0
4	H	1	0	0	0	0
4	I	1	0	0	0	0
4	L	1	0	0	0	0
4	S	6	0	0	0	0
4	T	2	0	0	1	0
4	U	1	0	0	0	0
4	V	3	0	0	1	0
All	All	11636	0	11595	1649	3

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 71.

The worst 5 of 1649 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:96:LYS:CD	1:E:96:LYS:CE	1.74	1.65
3:U:228:ILE:CG2	3:U:228:ILE:CB	1.74	1.64
3:V:288:LYS:CD	3:V:288:LYS:CG	1.74	1.63
1:E:8:LEU:CD1	1:E:8:LEU:CG	1.75	1.63
1:H:110:LEU:CD2	1:H:110:LEU:CG	1.77	1.62

All (3) 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:B:3:ALA:O	2:C:142:TYR:OH[2_555]	2.08	0.12
1:E:65:GLU:OE1	2:L:158:LYS:NZ[2_556]	2.16	0.04
1:H:142:GLU:OE2	1:K:145:ARG:NH1[3_434]	2.17	0.03

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	B	148/154 (96%)	114 (77%)	28 (19%)	6 (4%)	2	9
1	E	145/154 (94%)	122 (84%)	13 (9%)	10 (7%)	1	2
1	H	145/154 (94%)	103 (71%)	23 (16%)	19 (13%)	0	0
1	K	148/154 (96%)	92 (62%)	27 (18%)	29 (20%)	0	0
2	C	140/142 (99%)	114 (81%)	12 (9%)	14 (10%)	0	1
2	F	137/142 (96%)	113 (82%)	12 (9%)	12 (9%)	0	1
2	I	137/142 (96%)	94 (69%)	20 (15%)	23 (17%)	0	0
2	L	137/142 (96%)	106 (77%)	17 (12%)	14 (10%)	0	1
3	S	73/78 (94%)	47 (64%)	15 (20%)	11 (15%)	0	0
3	T	76/78 (97%)	52 (68%)	14 (18%)	10 (13%)	0	0
3	U	71/78 (91%)	49 (69%)	14 (20%)	8 (11%)	0	1
3	V	69/78 (88%)	47 (68%)	10 (14%)	12 (17%)	0	0
All	All	1426/1496 (95%)	1053 (74%)	205 (14%)	168 (12%)	0	1

5 of 168 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	5	SER
1	B	137	GLU
2	C	34	THR
2	C	54	GLY
2	C	55	VAL

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	B	128/129 (99%)	89 (70%)	39 (30%)	0	1
1	E	127/129 (98%)	92 (72%)	35 (28%)	0	1
1	H	127/129 (98%)	92 (72%)	35 (28%)	0	1
1	K	128/129 (99%)	90 (70%)	38 (30%)	0	1
2	C	125/127 (98%)	95 (76%)	30 (24%)	1	2
2	F	125/127 (98%)	96 (77%)	29 (23%)	1	3
2	I	125/127 (98%)	79 (63%)	46 (37%)	0	0
2	L	125/127 (98%)	89 (71%)	36 (29%)	0	1
3	S	68/72 (94%)	48 (71%)	20 (29%)	0	1
3	T	72/72 (100%)	52 (72%)	20 (28%)	0	1
3	U	66/72 (92%)	53 (80%)	13 (20%)	1	5
3	V	65/72 (90%)	35 (54%)	30 (46%)	0	0
All	All	1281/1312 (98%)	910 (71%)	371 (29%)	0	1

5 of 371 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	74	ARG
2	L	171	CYS
1	K	98	LYS
2	L	55	VAL
3	S	278	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 56 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	83	ASN
3	V	298	ASN
1	K	35	ASN
3	V	263	GLN
3	T	269	ASN

5.3.3 RNA

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 [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, 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	B	152/154 (98%)	-0.01	3 (1%) 65 56	2, 2, 12, 28	0
1	E	149/154 (96%)	0.17	4 (2%) 56 47	2, 2, 18, 32	0
1	H	149/154 (96%)	-0.40	2 (1%) 75 67	2, 2, 20, 27	0
1	K	152/154 (98%)	0.15	4 (2%) 57 48	2, 3, 29, 38	0
2	C	142/142 (100%)	0.54	6 (4%) 40 32	2, 2, 10, 28	0
2	F	139/142 (97%)	-0.50	1 (0%) 84 79	2, 2, 10, 20	0
2	I	139/142 (97%)	-0.33	0 100 100	2, 2, 10, 17	0
2	L	139/142 (97%)	-0.02	1 (0%) 84 79	2, 2, 10, 13	0
3	S	75/78 (96%)	-0.57	0 100 100	2, 2, 17, 21	0
3	T	78/78 (100%)	-0.54	2 (2%) 57 48	2, 2, 50, 59	0
3	U	73/78 (93%)	-0.55	0 100 100	2, 2, 11, 17	0
3	V	71/78 (91%)	-0.48	0 100 100	2, 3, 14, 27	0
All	All	1458/1496 (97%)	-0.15	23 (1%) 70 62	2, 2, 18, 59	0

The worst 5 of 23 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	34	THR	5.5
1	B	124	PRO	5.0
2	C	58	GLY	3.8
1	H	6	ALA	3.7
1	E	6	ALA	3.2

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.