



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 07:56 AM EDT

PDB ID : 7BBF
Title : Crystal structure of ubiquitin charged Ube2N (Ube2N Ub) in complex with Ube2V2
Authors : Kiss, L.; Neuhaus, D.; James, L.C.
Deposited on : 2020-12-17
Resolution : 2.54 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	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

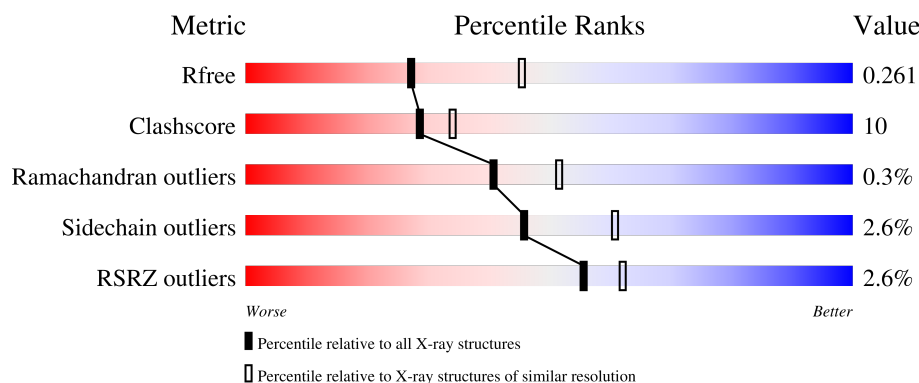
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	150	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 73%, yellow 73%, yellow 91%, grey 91%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> % 73% 20% • 6% </div> </div>
1	E	150	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 4%, green 4%, green 72%, yellow 72%, yellow 94%, grey 94%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 4% 72% 22% 6% </div> </div>
1	H	150	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 72%, yellow 72%, yellow 97%, grey 97%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> % 72% 22% • 5% </div> </div>
2	A	153	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 1%, green 1%, green 86%, yellow 86%, yellow 97%, grey 97%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> % 86% 11% •• </div> </div>
2	D	153	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 0%, red 6%, green 6%, green 69%, yellow 69%, yellow 96%, grey 96%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 6% 69% 27% •• </div> </div>

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Mol	Chain	Length	Quality of chain
2	G	153	<div><div></div><div>4%</div><div>81%</div><div>17%</div><div>••</div></div>
3	C	76	<div><div></div><div>4%</div><div>59%</div><div>37%</div><div>•</div></div>
3	F	76	<div><div></div><div>%</div><div>67%</div><div>28%</div><div>••</div></div>
3	I	76	<div><div></div><div></div><div>63%</div><div>34%</div><div>•</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8651 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 variant 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	142	Total	C	N	O	S	0	0	0
			1105	692	192	213	8			
1	B	141	Total	C	N	O	S	0	0	0
			1115	698	195	214	8			
1	E	141	Total	C	N	O	S	0	0	0
			1111	695	194	214	8			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-4	GLY	-	expression tag	UNP Q15819
H	-3	SER	-	expression tag	UNP Q15819
H	-2	GLN	-	expression tag	UNP Q15819
H	-1	GLU	-	expression tag	UNP Q15819
H	0	PHE	-	expression tag	UNP Q15819
B	-4	GLY	-	expression tag	UNP Q15819
B	-3	SER	-	expression tag	UNP Q15819
B	-2	GLN	-	expression tag	UNP Q15819
B	-1	GLU	-	expression tag	UNP Q15819
B	0	PHE	-	expression tag	UNP Q15819
E	-4	GLY	-	expression tag	UNP Q15819
E	-3	SER	-	expression tag	UNP Q15819
E	-2	GLN	-	expression tag	UNP Q15819
E	-1	GLU	-	expression tag	UNP Q15819
E	0	PHE	-	expression tag	UNP Q15819

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	152	Total	C	N	O	S	0	0	0
			1162	750	198	211	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	149	Total	C	N	O	S	0	1	0
			1182	758	205	216	3			
2	A	150	Total	C	N	O	S	0	1	0
			1192	768	207	214	3			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	0	GLY	-	expression tag	UNP P61088
G	87	LYS	CYS	engineered mutation	UNP P61088
G	92	ALA	LYS	engineered mutation	UNP P61088
D	0	GLY	-	expression tag	UNP P61088
D	87	LYS	CYS	engineered mutation	UNP P61088
D	92	ALA	LYS	engineered mutation	UNP P61088
A	0	GLY	-	expression tag	UNP P61088
A	87	LYS	CYS	engineered mutation	UNP P61088
A	92	ALA	LYS	engineered mutation	UNP P61088

- Molecule 3 is a protein called Polyubiquitin-C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	74	Total	C	N	O	S	0	1	0
			592	372	102	117	1			
3	C	76	Total	C	N	O	S	0	0	0
			579	365	99	114	1			
3	F	73	Total	C	N	O	S	0	0	0
			573	362	96	114	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	4	Total	O	0	0
			4	4		
4	B	3	Total	O	0	0
			3	3		
4	E	8	Total	O	0	0
			8	8		
4	G	3	Total	O	0	0
			3	3		
4	D	3	Total	O	0	0
			3	3		

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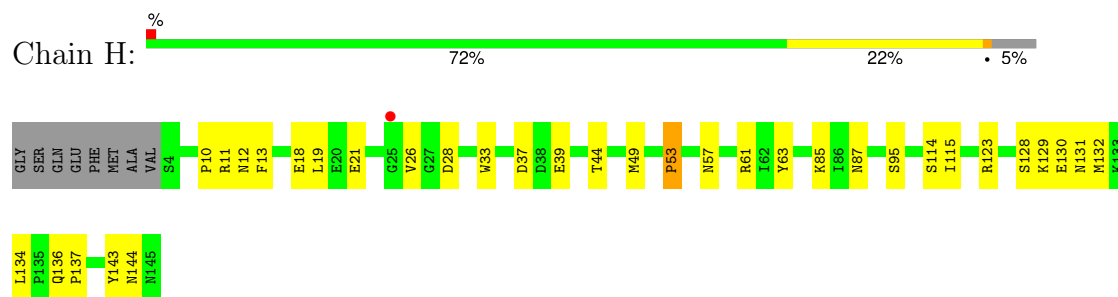
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	16	Total	O	0	0
			16	16		
4	I	3	Total	O	0	0
			3	3		

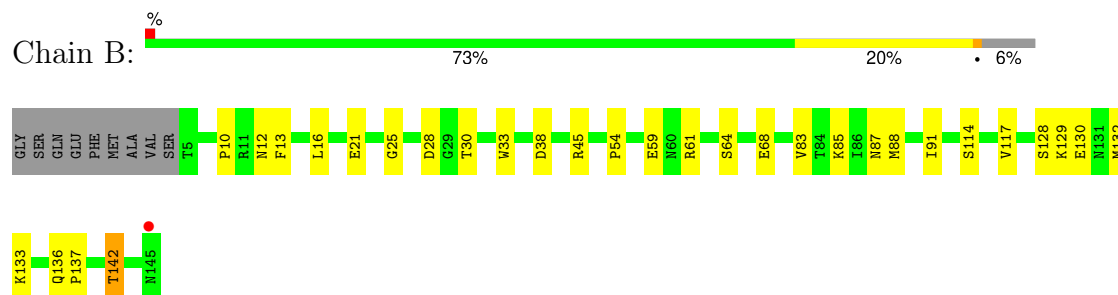
3 Residue-property plots [i](#)

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.

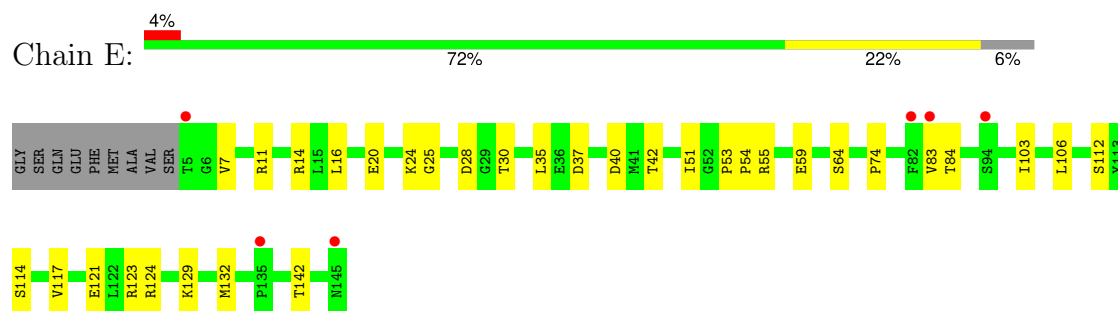
- Molecule 1: Ubiquitin-conjugating enzyme E2 variant 2



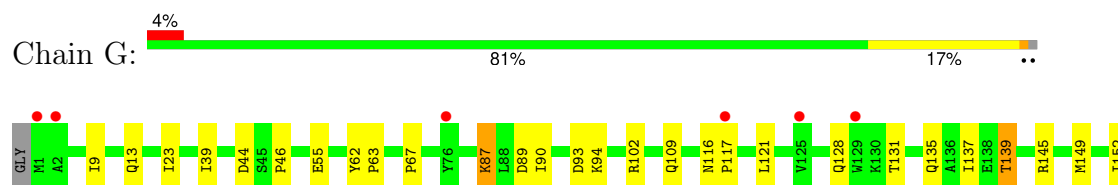
- Molecule 1: Ubiquitin-conjugating enzyme E2 variant 2



- Molecule 1: Ubiquitin-conjugating enzyme E2 variant 2

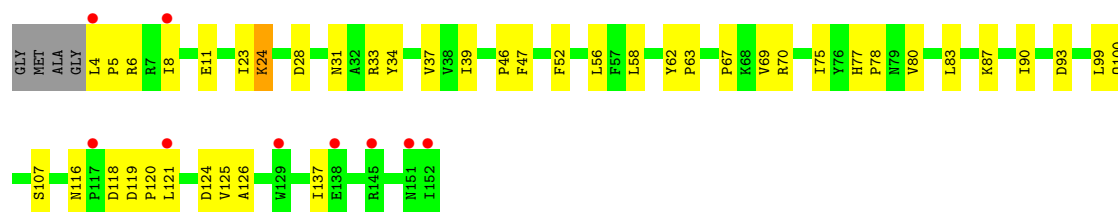


- Molecule 2: Ubiquitin-conjugating enzyme E2 N




- Molecule 2: Ubiquitin-conjugating enzyme E2 N

Chain D:  6% 69% 27% ..



- Molecule 2: Ubiquitin-conjugating enzyme E2 N

Chain A:  86% 11% ..



- Molecule 3: Polyubiquitin-C

Chain I:  63% 34% .



- Molecule 3: Polyubiquitin-C

Chain C:  4% 59% 37% .



- Molecule 3: Polyubiquitin-C

Chain F:  67% 28% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	145.84Å 145.84Å 49.23Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.74 – 2.54 47.74 – 2.54	Depositor EDS
% Data completeness (in resolution range)	99.9 (47.74-2.54) 100.0 (47.74-2.54)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.206 , 0.253 0.214 , 0.261	Depositor DCC
R_{free} test set	2019 reflections (5.24%)	wwPDB-VP
Wilson B-factor (Å ²)	79.1	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 66.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.026 for h,-h-k,-l 0.000 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8651	wwPDB-VP
Average B, all atoms (Å ²)	109.0	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 35.09 % 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 6.1639e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	0.29	0/1138	0.51	0/1540
1	E	0.30	0/1134	0.54	0/1536
1	H	0.28	0/1128	0.53	0/1529
2	A	0.27	0/1222	0.50	0/1665
2	D	0.28	0/1212	0.49	0/1655
2	G	0.28	0/1192	0.53	0/1631
3	C	0.31	0/585	0.62	1/791 (0.1%)
3	F	0.30	0/579	0.58	0/781
3	I	0.27	0/598	0.57	0/806
All	All	0.29	0/8788	0.53	1/11934 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	8	LEU	CA-CB-CG	5.53	128.02	115.30

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	B	1115	0	1107	22	0
1	E	1111	0	1096	22	0
1	H	1105	0	1081	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	1192	0	1202	11	0
2	D	1182	0	1175	28	0
2	G	1162	0	1145	19	0
3	C	579	0	586	20	0
3	F	573	0	590	18	0
3	I	592	0	608	14	0
4	A	16	0	0	0	0
4	B	3	0	0	0	0
4	D	3	0	0	0	0
4	E	8	0	0	1	0
4	G	3	0	0	1	0
4	H	4	0	0	0	0
4	I	3	0	0	0	0
All	All	8651	0	8590	167	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 10.

All (167) 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)
2:G:89:ASP:HB2	2:G:94:LYS:HD2	1.46	0.98
3:C:2:GLN:HG2	3:C:14:THR:HG22	1.61	0.80
2:D:116:ASN:ND2	2:D:118:ASP:OD2	2.15	0.80
3:C:2:GLN:HB2	3:C:16:GLU:OE2	1.87	0.74
2:D:75:ILE:HG23	2:D:80:VAL:HG11	1.69	0.74
2:D:77:HIS:HB3	2:D:80:VAL:HG12	1.71	0.72
1:B:45:ARG:NH1	1:B:68:GLU:OE2	2.25	0.69
3:F:6:LYS:NZ	3:F:12:THR:OG1	2.26	0.68
3:F:17:VAL:HA	3:F:29:LYS:HZ1	1.61	0.66
1:H:61:ARG:NH1	1:H:137:PRO:O	2.20	0.66
3:F:23:ILE:HA	3:F:26:VAL:HG22	1.78	0.65
2:A:15:LEU:HD21	2:A:25:ALA:HB3	1.77	0.65
3:F:2:GLN:HG3	3:F:16:GLU:OE2	1.97	0.65
2:G:135:GLN:O	2:G:139:THR:OG1	2.14	0.65
1:B:132:MET:HG3	1:B:133:LYS:HG3	1.80	0.63
2:G:23:ILE:HG12	2:G:39:ILE:HG12	1.80	0.63
1:E:16:LEU:HD11	2:D:70:ARG:HD3	1.82	0.61
1:E:7:VAL:HG21	2:D:33:ARG:HD2	1.83	0.60
1:E:11:ARG:NH2	1:E:42:THR:O	2.34	0.60
3:C:1:MET:HE3	3:C:63:LYS:HA	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:23:ILE:HG12	2:A:39:ILE:HG12	1.84	0.60
2:G:46:PRO:HB3	2:G:137:ILE:HG23	1.83	0.59
3:C:44:ILE:HG23	3:C:68:HIS:HB2	1.85	0.59
2:D:46:PRO:HG3	2:D:137:ILE:HG23	1.86	0.58
3:C:4:PHE:HE1	3:C:66:THR:HG1	1.51	0.58
3:F:50:LEU:HD11	3:F:67:LEU:HD23	1.86	0.57
3:C:26:VAL:O	3:C:30:ILE:HG23	2.04	0.57
3:F:17:VAL:HA	3:F:29:LYS:NZ	2.20	0.57
1:H:26:VAL:HG11	1:H:33:TRP:CH2	2.39	0.57
1:H:33:TRP:CD1	1:H:115:ILE:HD11	2.40	0.57
3:I:26:VAL:O	3:I:30:ILE:HG23	2.05	0.57
1:H:21:GLU:HG3	1:H:33:TRP:HZ2	1.69	0.57
2:D:52:PHE:CE1	2:D:75:ILE:HD13	2.41	0.56
1:B:28:ASP:OD2	1:B:30:THR:OG1	2.24	0.55
1:B:61:ARG:NH1	1:B:137:PRO:O	2.28	0.55
1:B:54:PRO:HA	1:B:59:GLU:HG3	1.89	0.55
3:F:14:THR:O	3:F:33:LYS:NZ	2.39	0.55
1:E:129:LYS:HA	1:E:132:MET:HG2	1.88	0.55
1:B:114:SER:H	1:B:117:VAL:HG22	1.71	0.54
1:B:21:GLU:HG3	1:B:33:TRP:HZ2	1.72	0.54
1:H:131:ASN:HA	1:H:134:LEU:HD13	1.89	0.53
3:C:15:LEU:HD12	3:C:29:LYS:HE2	1.90	0.53
2:D:70:ARG:NH1	2:D:83:LEU:O	2.41	0.53
1:H:10:PRO:HG2	1:H:13:PHE:HD2	1.73	0.53
1:E:53:PRO:HA	1:E:123:ARG:NH2	2.24	0.52
1:H:26:VAL:HG11	1:H:33:TRP:HH2	1.74	0.52
1:B:28:ASP:HB2	1:B:30:THR:HG23	1.90	0.52
3:C:8:LEU:HD11	3:C:70:VAL:HA	1.91	0.52
2:D:47:PHE:CD1	2:D:75:ILE:HD11	2.45	0.51
1:H:85:LYS:HA	1:H:143:TYR:CE2	2.45	0.51
1:E:54:PRO:HA	1:E:59:GLU:HG3	1.93	0.51
3:F:23:ILE:HD12	3:F:54:ARG:O	2.10	0.51
2:D:31:ASN:HB3	2:D:34:TYR:HB3	1.92	0.51
1:H:129:LYS:HA	1:H:132:MET:HG2	1.92	0.51
3:C:45:PHE:HB2	3:C:67:LEU:HD22	1.93	0.50
1:E:28:ASP:N	1:E:28:ASP:OD1	2.44	0.50
1:H:87:ASN:HB3	1:H:136:GLN:HE22	1.77	0.50
3:F:4:PHE:HD1	3:F:14:THR:HG22	1.77	0.50
2:D:58:LEU:HD23	2:D:67:PRO:HB3	1.94	0.50
2:D:23:ILE:HG12	2:D:39:ILE:HG12	1.94	0.50
1:B:83:VAL:O	1:B:142:THR:OG1	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:145:ARG:O	2:G:149:MET:HG3	2.12	0.49
1:E:83:VAL:O	1:E:142:THR:HB	2.13	0.49
2:D:93:ASP:N	2:D:93:ASP:OD1	2.46	0.49
2:G:87:LYS:HB2	2:G:121:LEU:HD22	1.94	0.49
2:G:9:ILE:O	2:G:13:GLN:HG2	2.14	0.48
3:F:5:VAL:HA	3:F:67:LEU:O	2.13	0.48
1:E:20:GLU:O	1:E:24:LYS:HD3	2.14	0.48
2:G:128:GLN:HA	2:G:131:THR:HB	1.95	0.48
1:B:85:LYS:H	1:B:142:THR:HA	1.77	0.48
3:I:4:PHE:HD1	3:I:14:THR:HG22	1.79	0.48
1:B:28:ASP:OD1	1:B:28:ASP:N	2.44	0.48
3:I:15:LEU:HD11	3:I:30:ILE:HG22	1.95	0.48
3:C:22:THR:HA	3:C:55:THR:HA	1.95	0.47
3:F:26:VAL:HA	3:F:29:LYS:HB2	1.96	0.47
1:B:142:THR:HG21	2:G:152:ILE:HA	1.96	0.47
2:G:44:ASP:N	4:G:201:HOH:O	2.45	0.47
3:I:23:ILE:HG13	3:I:50:LEU:HB3	1.96	0.47
3:C:4:PHE:HA	3:C:13:ILE:O	2.13	0.47
2:D:4:LEU:HD12	2:D:5:PRO:HD2	1.96	0.47
3:I:43:LEU:O	3:I:44:ILE:HD13	2.15	0.47
3:C:23:ILE:HD12	3:C:54:ARG:O	2.15	0.47
1:H:28:ASP:N	1:H:28:ASP:OD1	2.48	0.47
1:E:14:ARG:HD3	1:E:74:PRO:HG3	1.97	0.46
2:A:93:ASP:OD1	2:A:93:ASP:N	2.45	0.46
1:B:64:SER:O	1:B:83:VAL:HG12	2.15	0.46
3:I:51:GLU:HG2	3:I:59:TYR:OH	2.16	0.46
3:I:14:THR:O	3:I:33:LYS:NZ	2.47	0.46
3:C:2:GLN:HG3	3:C:15:LEU:C	2.36	0.46
1:E:54:PRO:HB2	1:E:55:ARG:HD3	1.98	0.46
2:G:23:ILE:HD11	2:G:109:GLN:HB2	1.97	0.46
2:D:78:PRO:HB3	2:D:126:ALA:HB2	1.97	0.46
2:D:87:LYS:HB2	2:D:121:LEU:HD13	1.97	0.46
1:H:53:PRO:HA	1:H:123:ARG:NH2	2.31	0.46
3:F:24:GLU:HG2	3:F:25:ASN:N	2.29	0.46
3:I:6:LYS:NZ	3:I:10:GLY:HA2	2.31	0.45
3:I:51:GLU:OE2	3:I:54:ARG:HG3	2.17	0.45
2:D:47:PHE:CE1	2:D:75:ILE:HD11	2.51	0.45
2:A:146:LEU:HD13	2:A:147:TYR:CZ	2.52	0.45
1:E:30:THR:HA	1:E:51:ILE:HG12	1.97	0.45
3:C:31:GLN:OE1	3:C:38:PRO:HD3	2.17	0.45
3:C:41:GLN:HB3	3:C:69:LEU:HD11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:57:ASN:ND2	1:H:134:LEU:O	2.50	0.45
3:F:4:PHE:CD1	3:F:14:THR:HG22	2.52	0.45
1:B:10:PRO:HG2	1:B:13:PHE:HD2	1.81	0.44
1:H:87:ASN:HB3	1:H:136:GLN:NE2	2.33	0.44
1:H:11:ARG:NH2	1:H:44:THR:HG22	2.32	0.44
1:B:128:SER:OG	1:B:130:GLU:HG2	2.17	0.44
1:E:114:SER:O	1:E:117:VAL:HG12	2.18	0.44
1:E:54:PRO:HD3	1:E:123:ARG:HH22	1.83	0.44
1:B:142:THR:CG2	2:G:152:ILE:HA	2.48	0.44
1:H:12:ASN:HD22	2:G:55:GLU:CD	2.21	0.44
3:F:44:ILE:CG2	3:F:68:HIS:HB2	2.47	0.44
1:H:128:SER:OG	1:H:130:GLU:HG2	2.18	0.43
2:D:62:TYR:CD1	2:D:63:PRO:HA	2.53	0.43
3:I:22:THR:HA	3:I:55:THR:HA	1.99	0.43
3:C:1:MET:HE2	3:C:1:MET:HB2	1.91	0.43
3:F:17:VAL:HG12	3:F:29:LYS:HZ3	1.84	0.43
1:E:35:LEU:N	4:E:201:HOH:O	2.33	0.43
1:E:64:SER:O	1:E:83:VAL:HG12	2.17	0.43
1:E:114:SER:H	1:E:117:VAL:HG12	1.83	0.43
2:D:62:TYR:CE1	2:D:67:PRO:HG3	2.53	0.43
2:D:118:ASP:O	2:D:120:PRO:HD3	2.18	0.43
2:A:120:PRO:HB3	2:A:126:ALA:CB	2.49	0.43
1:B:114:SER:H	1:B:117:VAL:CG2	2.31	0.43
3:C:2:GLN:HA	3:C:16:GLU:HA	2.01	0.43
2:G:93:ASP:N	2:G:93:ASP:OD1	2.45	0.42
2:A:96:SER:H	2:A:99:LEU:HD12	1.85	0.42
2:G:62:TYR:CD1	2:G:63:PRO:HA	2.53	0.42
2:G:89:ASP:OD1	2:G:90:ILE:N	2.53	0.42
2:G:116:ASN:HA	2:G:117:PRO:HD3	1.85	0.42
1:B:87:ASN:HB3	1:B:136:GLN:NE2	2.34	0.42
2:D:28:ASP:N	2:D:34:TYR:O	2.46	0.42
1:B:129:LYS:HA	1:B:132:MET:HG2	2.01	0.42
1:B:16:LEU:HD11	2:A:70:ARG:HD3	2.01	0.42
1:E:84:THR:HA	1:E:142:THR:HG22	2.00	0.42
2:A:53:LYS:HE3	2:A:72:MET:HE3	2.00	0.42
3:C:5:VAL:HG12	3:C:13:ILE:HD11	2.02	0.42
1:H:18:GLU:OE1	1:H:114:SER:HB2	2.19	0.42
2:A:87:LYS:HB2	2:A:121:LEU:HB2	2.01	0.42
3:C:22:THR:O	3:C:26:VAL:HG23	2.20	0.41
3:F:6:LYS:HG2	3:F:12:THR:OG1	2.20	0.41
1:E:121:GLU:CD	1:E:124:ARG:HH21	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:56:LEU:HG	2:D:69:VAL:HG12	2.02	0.41
2:D:5:PRO:HD2	2:D:8:ILE:HD12	2.02	0.41
1:H:37:ASP:C	1:H:39:GLU:H	2.23	0.41
1:B:88:MET:HB3	1:B:91:ILE:HD13	2.03	0.41
1:E:37:ASP:HB3	1:E:40:ASP:HB2	2.02	0.41
2:D:11:GLU:OE1	2:D:100:GLN:HB2	2.20	0.41
3:F:37:PRO:HA	3:F:38:PRO:HD3	1.97	0.41
3:F:43:LEU:HD23	3:F:43:LEU:HA	1.93	0.41
2:G:62:TYR:CE1	2:G:67:PRO:HG3	2.56	0.41
3:I:63:LYS:O	3:I:64:GLU:HG2	2.21	0.41
1:H:49:MET:HG3	1:H:63:TYR:O	2.20	0.41
2:A:83:LEU:HD12	2:A:85:ARG:NH2	2.35	0.41
1:H:136:GLN:HA	1:H:137:PRO:HD3	1.92	0.41
1:B:12:ASN:HD22	2:A:55:GLU:CD	2.24	0.41
1:E:7:VAL:HG21	2:D:33:ARG:CD	2.48	0.41
2:D:24:LYS:O	2:D:37:VAL:HA	2.21	0.41
3:I:19:PRO:HB3	3:I:57:SER:OG	2.21	0.41
2:G:62:TYR:CG	2:G:63:PRO:HA	2.56	0.40
3:I:37:PRO:HA	3:I:38:PRO:HD3	1.95	0.40
1:E:103:ILE:HG22	1:E:106:LEU:H	1.85	0.40
3:C:28:ALA:O	3:C:32:ASP:OD1	2.39	0.40
2:D:90:ILE:HG23	2:D:99:LEU:HD13	2.04	0.40
2:D:78:PRO:HA	2:D:125:VAL:HG23	2.03	0.40
3:I:4:PHE:CD1	3:I:14:THR:HG22	2.56	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	B	139/150 (93%)	134 (96%)	4 (3%)	1 (1%)	22 30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	139/150 (93%)	136 (98%)	2 (1%)	1 (1%)	22	30
1	H	140/150 (93%)	136 (97%)	4 (3%)	0	100	100
2	A	149/153 (97%)	145 (97%)	3 (2%)	1 (1%)	22	30
2	D	148/153 (97%)	142 (96%)	6 (4%)	0	100	100
2	G	150/153 (98%)	145 (97%)	5 (3%)	0	100	100
3	C	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
3	F	71/76 (93%)	70 (99%)	1 (1%)	0	100	100
3	I	73/76 (96%)	73 (100%)	0	0	100	100
All	All	1083/1137 (95%)	1053 (97%)	27 (2%)	3 (0%)	41	51

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	120	PRO
1	B	25	GLY
1	E	25	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	B	125/133 (94%)	123 (98%)	2 (2%)	62	77
1	E	124/133 (93%)	123 (99%)	1 (1%)	81	88
1	H	122/133 (92%)	118 (97%)	4 (3%)	38	51
2	A	125/128 (98%)	124 (99%)	1 (1%)	81	88
2	D	124/128 (97%)	119 (96%)	5 (4%)	31	43
2	G	117/128 (91%)	114 (97%)	3 (3%)	46	61
3	C	63/68 (93%)	59 (94%)	4 (6%)	18	23
3	F	65/68 (96%)	64 (98%)	1 (2%)	65	77
3	I	67/68 (98%)	64 (96%)	3 (4%)	27	37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	932/987 (94%)	908 (97%)	24 (3%)	46 61

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	19	LEU
1	H	53	PRO
1	H	95	SER
1	H	144	ASN
1	B	38	ASP
1	B	142	THR
1	E	112	SER
2	G	87	LYS
2	G	102	ARG
2	G	139	THR
2	D	6	ARG
2	D	24	LYS
2	D	107	SER
2	D	119	ASP
2	D	124	ASP
2	A	146	LEU
3	I	16	GLU
3	I	20	SER
3	I	24	GLU
3	C	1	MET
3	C	4	PHE
3	C	52	ASP
3	C	57	SER
3	F	5	VAL

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

Mol	Chain	Res	Type
3	F	62	GLN

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 monosaccharides 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	B	141/150 (94%)	-0.11	1 (0%) 87 90	67, 90, 138, 234	0
1	E	141/150 (94%)	0.23	6 (4%) 35 42	94, 116, 161, 237	0
1	H	142/150 (94%)	-0.17	1 (0%) 87 90	77, 103, 150, 192	0
2	A	150/153 (98%)	0.02	2 (1%) 77 82	53, 77, 135, 158	0
2	D	149/153 (97%)	0.29	9 (6%) 21 25	88, 115, 176, 221	0
2	G	152/153 (99%)	0.12	6 (3%) 39 45	67, 103, 168, 213	0
3	C	76/76 (100%)	0.27	3 (3%) 39 45	97, 127, 168, 208	0
3	F	73/76 (96%)	0.21	1 (1%) 75 81	90, 118, 160, 178	0
3	I	74/76 (97%)	-0.13	0 100 100	74, 99, 143, 162	0
All	All	1098/1137 (96%)	0.08	29 (2%) 56 62	53, 107, 163, 237	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	5	THR	8.2
2	D	117	PRO	7.3
3	F	73	LEU	6.1
2	G	117	PRO	5.2
2	D	129	TRP	4.7
2	G	2	ALA	4.2
1	E	145	ASN	3.9
1	B	145	ASN	3.9
2	D	152	ILE	3.7
2	D	151	ASN	3.6
2	D	145	ARG	3.5
2	G	129	TRP	3.0
2	A	120	PRO	3.0
1	E	94	SER	2.8
1	E	135	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
2	G	1	MET	2.8
2	D	4	LEU	2.4
3	C	70	VAL	2.4
2	D	138	GLU	2.3
2	G	125	VAL	2.3
3	C	73	LEU	2.3
2	D	121	LEU	2.3
2	A	76	TYR	2.2
1	E	83	VAL	2.2
1	H	25	GLY	2.1
2	D	8	ILE	2.1
3	C	68	HIS	2.1
1	E	82	PHE	2.1
2	G	76	TYR	2.0

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 monosaccharides 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.