



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 11:29 am BST

PDB ID : 3IPD  
Title : Helical extension of the neuronal SNARE complex into the membrane, space-group I 21 21 21  
Authors : Stein, A.; Weber, G.; Wahl, M.C.; Jahn, R.  
Deposited on : 2009-08-17  
Resolution : 4.80 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.

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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

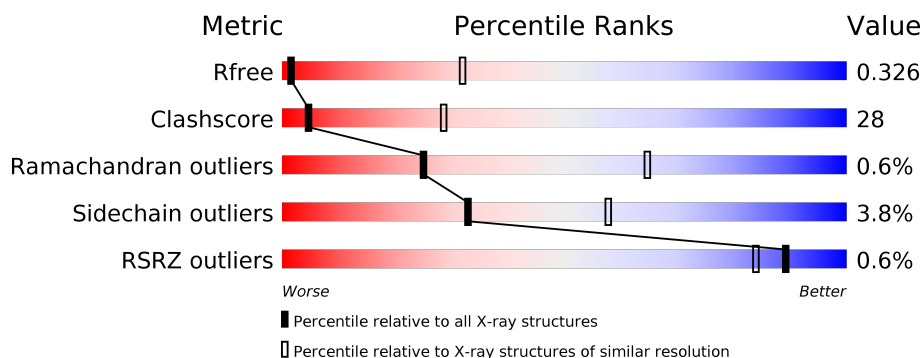
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.80 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	1096 (5.80-3.80)
Clashscore	141614	1170 (5.80-3.80)
Ramachandran outliers	138981	1105 (5.80-3.80)
Sidechain outliers	138945	1085 (5.80-3.80)
RSRZ outliers	127900	1126 (5.90-3.70)

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  $\geq 3$ , 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	91	<div> <div>%</div> <div> <div></div> <div>55%</div> <div>40%</div> <div>5%</div> </div> </div>
1	E	91	<div> <div>49%</div> <div>45%</div> <div>5%</div> </div>
2	B	109	<div> <div>51%</div> <div>35%</div> <div>• 10%</div> </div>
2	F	109	<div> <div>47%</div> <div>39%</div> <div>• 10%</div> </div>
3	C	80	<div> <div>%</div> <div>63%</div> <div>30%</div> <div>• 6%</div> </div>
3	G	80	<div> <div>50%</div> <div>43%</div> <div>• 6%</div> </div>

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Mol	Chain	Length	Quality of chain
4	D	68	<div><div><div></div><div></div><div></div></div><div>3%71%22%7%</div></div>
4	H	68	<div><div><div></div><div></div><div></div></div><div>54%38%7%</div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5242 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 Vesicle-associated membrane protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	91	Total	C	N	O	S	0	0	0
			733	467	129	132	5			
1	E	91	Total	C	N	O	S	0	0	0
			733	467	129	132	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	EXPRESSION TAG	UNP P63045
A	27	SER	-	EXPRESSION TAG	UNP P63045
A	28	HIS	-	EXPRESSION TAG	UNP P63045
A	29	MET	-	EXPRESSION TAG	UNP P63045
E	26	GLY	-	EXPRESSION TAG	UNP P63045
E	27	SER	-	EXPRESSION TAG	UNP P63045
E	28	HIS	-	EXPRESSION TAG	UNP P63045
E	29	MET	-	EXPRESSION TAG	UNP P63045

- Molecule 2 is a protein called Syntaxin-1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	98	Total	C	N	O	S	0	0	0
			779	490	135	146	8			
2	F	98	Total	C	N	O	S	0	0	0
			779	490	135	146	8			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	180	GLY	-	EXPRESSION TAG	UNP P32851
B	181	SER	-	EXPRESSION TAG	UNP P32851
B	182	HIS	-	EXPRESSION TAG	UNP P32851
F	180	GLY	-	EXPRESSION TAG	UNP P32851

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Chain	Residue	Modelled	Actual	Comment	Reference
F	181	SER	-	EXPRESSION TAG	UNP P32851
F	182	HIS	-	EXPRESSION TAG	UNP P32851

- Molecule 3 is a protein called Synaptosomal-associated protein 25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	75	Total	C	N	O	S	0	0	0
			607	360	112	130	5			
3	G	75	Total	C	N	O	S	0	0	0
			607	360	112	130	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	4	GLY	-	EXPRESSION TAG	UNP P60881
C	5	SER	-	EXPRESSION TAG	UNP P60881
C	6	HIS	-	EXPRESSION TAG	UNP P60881
G	4	GLY	-	EXPRESSION TAG	UNP P60881
G	5	SER	-	EXPRESSION TAG	UNP P60881
G	6	HIS	-	EXPRESSION TAG	UNP P60881

- Molecule 4 is a protein called Synaptosomal-associated protein 25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	63	Total	C	N	O	S	0	0	0
			502	293	98	106	5			
4	H	63	Total	C	N	O	S	0	0	0
			502	293	98	106	5			

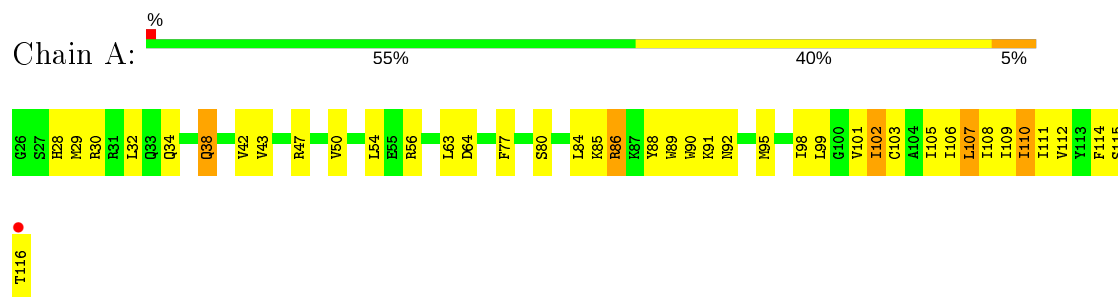
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	137	GLY	-	EXPRESSION TAG	UNP P60881
D	138	SER	-	EXPRESSION TAG	UNP P60881
D	139	HIS	-	EXPRESSION TAG	UNP P60881
D	140	MET	-	EXPRESSION TAG	UNP P60881
H	137	GLY	-	EXPRESSION TAG	UNP P60881
H	138	SER	-	EXPRESSION TAG	UNP P60881
H	139	HIS	-	EXPRESSION TAG	UNP P60881
H	140	MET	-	EXPRESSION TAG	UNP P60881

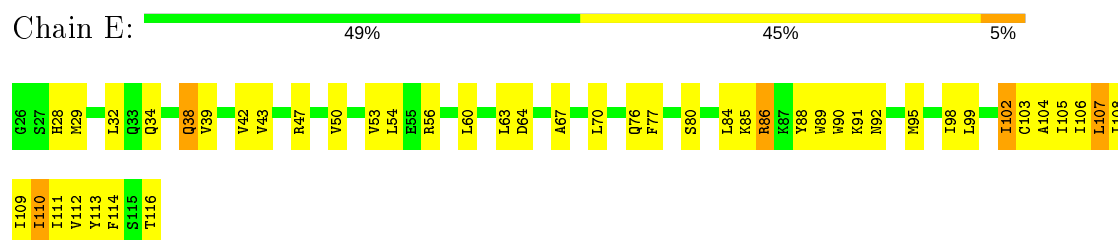
### 3 Residue-property plots [i](#)

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.

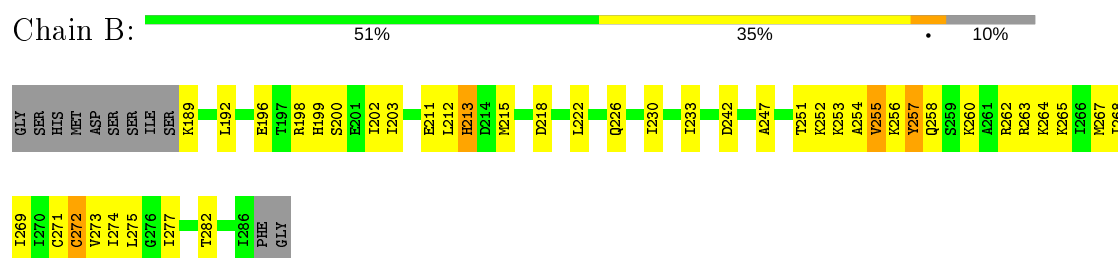
- Molecule 1: Vesicle-associated membrane protein 2



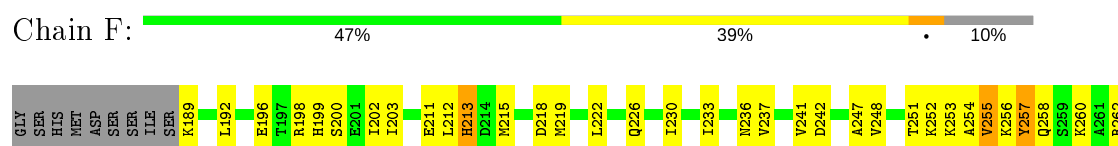
- Molecule 1: Vesicle-associated membrane protein 2

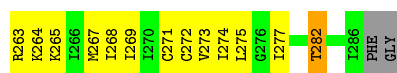


- Molecule 2: Syntaxin-1A



- Molecule 2: Syntaxin-1A

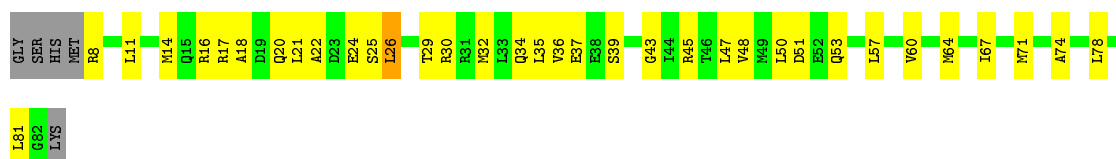




- Molecule 3: Synaptosomal-associated protein 25



- Molecule 3: Synaptosomal-associated protein 25



- Molecule 4: Synaptosomal-associated protein 25



- Molecule 4: Synaptosomal-associated protein 25



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.85Å 215.68Å 262.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.88 – 4.80 49.88 – 4.80	Depositor EDS
% Data completeness (in resolution range)	84.2 (49.88-4.80) 99.9 (49.88-4.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.11	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.10 (at 4.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.4_4)	Depositor
R, $R_{free}$	0.304 , 0.332 0.302 , 0.326	Depositor DCC
$R_{free}$ test set	783 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	202.5	Xtriage
Anisotropy	0.759	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.24 , 201.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.40$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	5242	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	289.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.77% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [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	0.30	0/741	0.45	0/996
1	E	0.29	0/741	0.45	0/996
2	B	0.25	0/785	0.44	0/1049
2	F	0.26	0/785	0.45	0/1049
3	C	0.22	0/607	0.40	0/807
3	G	0.24	0/607	0.41	0/807
4	D	0.23	0/503	0.40	0/671
4	H	0.23	0/503	0.41	0/671
All	All	0.26	0/5272	0.43	0/7046

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 [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	733	0	768	70	0
1	E	733	0	768	90	0
2	B	779	0	815	64	0
2	F	779	0	815	87	0
3	C	607	0	592	22	0
3	G	607	0	592	44	0
4	D	502	0	480	20	0
4	H	502	0	480	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5242	0	5310	296	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 28.

All (296) 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:A:109:ILE:HD12	2:B:275:LEU:HD22	1.40	1.03
1:A:28:HIS:HB2	2:B:198:ARG:CZ	1.98	0.94
1:E:106:ILE:HG12	2:F:275:LEU:HD21	1.47	0.93
1:A:91:LYS:O	1:A:95:MET:HG2	1.75	0.86
1:E:91:LYS:O	1:E:95:MET:HG2	1.76	0.86
1:A:95:MET:O	2:B:264:LYS:HB3	1.79	0.82
1:E:43:VAL:HG22	2:F:212:LEU:HD13	1.61	0.81
1:E:106:ILE:HG12	2:F:275:LEU:CD2	2.08	0.81
1:A:88:TYR:HE2	2:B:258:GLN:HB2	1.47	0.80
1:A:28:HIS:HB2	2:B:198:ARG:NH2	1.96	0.80
1:A:88:TYR:CE2	2:B:258:GLN:HB2	2.18	0.79
4:H:146:MET:O	4:H:150:LEU:HB2	1.83	0.79
4:D:146:MET:O	4:D:150:LEU:HB2	1.83	0.79
3:G:22:ALA:HB1	4:H:142:ARG:HD3	1.64	0.78
1:E:88:TYR:OH	2:F:258:GLN:N	2.16	0.78
1:E:109:ILE:HD12	2:F:275:LEU:HD22	1.66	0.78
1:E:39:VAL:CG2	4:H:157:ILE:HD13	2.14	0.76
1:A:34:GLN:HE22	4:H:163:MET:HA	1.51	0.75
1:A:106:ILE:HG12	2:B:275:LEU:HD21	1.71	0.73
1:E:89:TRP:CE3	1:E:90:TRP:HD1	2.08	0.72
1:A:89:TRP:CE3	1:A:90:TRP:HD1	2.06	0.72
1:A:89:TRP:CE3	1:A:90:TRP:CD1	2.78	0.72
1:E:39:VAL:HG23	4:H:157:ILE:HD13	1.72	0.72
3:G:26:LEU:HD22	4:H:146:MET:HB3	1.72	0.72
1:E:89:TRP:CE3	1:E:90:TRP:CD1	2.78	0.71
1:E:63:LEU:HD23	2:F:233:ILE:HG21	1.70	0.71
2:F:257:TYR:HD2	2:F:257:TYR:H	1.39	0.71
1:A:88:TYR:OH	2:B:258:GLN:N	2.21	0.71
1:E:108:ILE:HA	1:E:111:ILE:HD12	1.73	0.71
1:E:95:MET:O	2:F:264:LYS:HB3	1.91	0.71
4:D:162:HIS:HE1	1:E:34:GLN:HE22	1.38	0.71
2:B:199:HIS:HE2	2:B:203:ILE:HD11	1.56	0.70
1:A:38:GLN:HG2	4:H:162:HIS:CD2	2.26	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:64:MET:HE2	4:H:185:ALA:HA	1.73	0.70
2:F:199:HIS:HE1	3:G:24:GLU:OE1	1.75	0.69
1:E:63:LEU:CD1	4:H:182:MET:HG3	2.23	0.69
2:F:199:HIS:HE2	2:F:203:ILE:HD11	1.58	0.69
1:E:88:TYR:HH	2:F:258:GLN:HB2	1.58	0.68
1:E:63:LEU:HD13	4:H:182:MET:HG3	1.75	0.68
1:A:109:ILE:HD12	2:B:275:LEU:CD2	2.21	0.68
2:F:211:GLU:O	2:F:215:MET:HG2	1.93	0.68
2:B:211:GLU:O	2:B:215:MET:HG2	1.92	0.68
3:G:64:MET:CE	4:H:185:ALA:HA	2.24	0.68
2:B:257:TYR:H	2:B:257:TYR:HD2	1.40	0.67
1:A:108:ILE:HA	1:A:111:ILE:HD12	1.77	0.67
1:A:88:TYR:OH	2:B:255:VAL:C	2.32	0.67
4:D:162:HIS:CE1	1:E:34:GLN:NE2	2.63	0.67
4:D:162:HIS:HE1	1:E:34:GLN:NE2	1.94	0.66
1:A:89:TRP:HE3	1:A:90:TRP:HD1	1.43	0.66
3:C:26:LEU:HD22	4:D:146:MET:HB3	1.76	0.66
1:A:106:ILE:HD11	2:B:271:CYS:HB3	1.77	0.65
2:F:196:GLU:O	2:F:200:SER:HB2	1.95	0.65
1:A:42:VAL:HG11	2:B:212:LEU:HD21	1.78	0.64
2:B:196:GLU:O	2:B:200:SER:HB2	1.98	0.64
1:A:107:LEU:O	1:A:111:ILE:HG13	1.98	0.63
3:C:26:LEU:O	3:C:29:THR:HG22	1.99	0.63
2:F:192:LEU:HD13	3:G:14:MET:HG2	1.81	0.63
2:F:230:ILE:HD13	3:G:57:LEU:HD11	1.80	0.63
1:E:56:ARG:HH21	1:E:56:ARG:HG2	1.64	0.63
1:E:85:LYS:HE2	2:F:253:LYS:CB	2.27	0.63
1:E:88:TYR:OH	2:F:258:GLN:HB2	1.98	0.62
2:F:258:GLN:HG2	2:F:262:ARG:HH11	1.64	0.62
1:A:56:ARG:HG2	1:A:56:ARG:HH21	1.64	0.62
3:G:26:LEU:O	3:G:29:THR:HG22	1.99	0.62
3:G:71:MET:HB3	4:H:191:ARG:HD2	1.81	0.62
4:D:162:HIS:CD2	1:E:38:GLN:OE1	2.53	0.62
1:E:102:ILE:O	1:E:106:ILE:HG13	2.00	0.61
1:E:89:TRP:HE3	1:E:90:TRP:HD1	1.44	0.61
2:F:198:ARG:O	2:F:202:ILE:HG13	2.00	0.61
1:A:89:TRP:HE3	1:A:90:TRP:CD1	2.17	0.61
1:E:99:LEU:HD13	2:F:268:ILE:CG1	2.30	0.61
2:F:199:HIS:CE1	3:G:24:GLU:HB2	2.35	0.61
2:B:258:GLN:HG2	2:B:262:ARG:HH11	1.63	0.61
2:B:198:ARG:O	2:B:202:ILE:HG13	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:213:HIS:HD2	3:G:35:LEU:HD23	1.66	0.60
1:E:105:ILE:O	1:E:109:ILE:HG13	2.01	0.60
1:E:107:LEU:O	1:E:111:ILE:HG13	2.01	0.60
1:E:89:TRP:HE3	1:E:90:TRP:CD1	2.17	0.60
1:A:105:ILE:O	1:A:109:ILE:HG13	2.01	0.60
1:A:106:ILE:HG12	2:B:275:LEU:CD2	2.32	0.59
1:E:67:ALA:HB1	2:F:236:ASN:CB	2.32	0.59
2:F:257:TYR:N	2:F:257:TYR:CD2	2.70	0.59
1:E:103:CYS:O	1:E:107:LEU:HD23	2.02	0.59
1:E:88:TYR:CE2	2:F:258:GLN:HB2	2.38	0.59
2:F:213:HIS:HA	3:G:39:SER:OG	2.03	0.59
2:F:255:VAL:HG12	3:G:81:LEU:CD1	2.32	0.59
2:F:254:ALA:O	3:G:81:LEU:HD21	2.03	0.58
2:F:263:ARG:O	2:F:267:MET:HG2	2.03	0.58
2:F:271:CYS:HA	2:F:274:ILE:HB	1.86	0.58
2:B:263:ARG:O	2:B:267:MET:HG2	2.04	0.57
3:C:74:ALA:O	3:C:78:LEU:HD13	2.04	0.57
2:B:271:CYS:HA	2:B:274:ILE:HB	1.85	0.57
2:B:257:TYR:CD2	2:B:257:TYR:N	2.71	0.57
2:F:248:VAL:HG23	3:G:74:ALA:HB2	1.86	0.57
3:G:22:ALA:O	3:G:26:LEU:HB2	2.04	0.57
3:C:22:ALA:O	3:C:26:LEU:HB2	2.05	0.56
1:A:103:CYS:O	1:A:107:LEU:HD23	2.05	0.56
1:E:99:LEU:HD13	2:F:268:ILE:HG13	1.87	0.56
3:C:43:GLY:HA3	4:D:163:MET:HE1	1.88	0.56
1:A:109:ILE:CD1	2:B:275:LEU:HD22	2.26	0.56
1:A:109:ILE:HG22	1:A:109:ILE:O	2.06	0.56
2:F:189:LYS:HA	2:F:192:LEU:HD12	1.87	0.56
1:E:53:VAL:HG21	2:F:219:MET:SD	2.46	0.55
1:A:92:ASN:HD21	2:B:264:LYS:NZ	2.04	0.55
3:G:43:GLY:HA3	4:H:163:MET:HE1	1.88	0.55
2:B:189:LYS:HA	2:B:192:LEU:HD12	1.87	0.55
3:C:17:ARG:HA	3:C:20:GLN:HB3	1.88	0.55
3:G:8:ARG:HG2	3:G:11:LEU:HD12	1.89	0.55
3:G:74:ALA:O	3:G:78:LEU:HD13	2.07	0.55
3:G:17:ARG:HA	3:G:20:GLN:HB3	1.87	0.55
1:A:102:ILE:O	1:A:106:ILE:HG13	2.07	0.54
3:G:36:VAL:HG11	4:H:156:ILE:HB	1.89	0.54
1:A:115:SER:O	1:A:116:THR:CB	2.55	0.54
2:B:213:HIS:HA	3:C:39:SER:OG	2.07	0.54
1:E:109:ILE:O	1:E:109:ILE:HG22	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ARG:HH11	3:G:51:ASP:HB2	1.71	0.54
3:C:8:ARG:HG2	3:C:11:LEU:HD12	1.88	0.54
2:B:258:GLN:HG2	2:B:262:ARG:NH1	2.23	0.53
2:B:213:HIS:HD2	3:C:35:LEU:HD23	1.74	0.53
2:F:273:VAL:O	2:F:277:ILE:HG13	2.07	0.53
2:F:241:VAL:HA	3:G:67:ILE:HD11	1.91	0.53
1:A:102:ILE:HD12	2:B:268:ILE:HG23	1.90	0.53
3:G:32:MET:O	3:G:36:VAL:HG23	2.09	0.53
2:F:255:VAL:HG12	3:G:81:LEU:HD13	1.89	0.53
2:B:273:VAL:O	2:B:277:ILE:HG13	2.09	0.52
2:F:199:HIS:CE1	3:G:24:GLU:OE1	2.61	0.52
3:G:64:MET:HE2	4:H:185:ALA:CA	2.40	0.52
4:D:152:GLN:O	4:D:156:ILE:HG13	2.10	0.52
2:F:258:GLN:HG2	2:F:262:ARG:NH1	2.23	0.52
1:A:56:ARG:HD3	2:B:226:GLN:OE1	2.10	0.52
1:E:106:ILE:HG12	2:F:275:LEU:CG	2.39	0.52
1:E:67:ALA:HB1	2:F:236:ASN:HB2	1.90	0.52
3:C:32:MET:O	3:C:36:VAL:HG23	2.09	0.52
4:H:152:GLN:O	4:H:156:ILE:HG13	2.10	0.52
3:G:26:LEU:HD23	4:H:142:ARG:HG3	1.92	0.52
1:E:28:HIS:HB2	2:F:198:ARG:NH2	2.25	0.52
1:A:98:ILE:O	1:A:98:ILE:HG22	2.09	0.51
1:E:85:LYS:HE2	2:F:253:LYS:HB3	1.91	0.51
1:E:60:LEU:HD21	2:F:230:ILE:HG13	1.92	0.51
1:E:98:ILE:O	1:E:98:ILE:HG22	2.10	0.51
2:F:257:TYR:HA	2:F:260:LYS:HB2	1.92	0.51
1:E:56:ARG:HD3	2:F:226:GLN:OE1	2.10	0.51
1:A:64:ASP:HB2	2:B:233:ILE:HD11	1.93	0.51
1:A:88:TYR:CZ	2:B:258:GLN:N	2.79	0.50
2:B:265:LYS:O	2:B:269:ILE:HG13	2.12	0.50
1:A:99:LEU:HD13	2:B:268:ILE:HG13	1.92	0.49
3:G:16:ARG:O	3:G:20:GLN:HB2	2.13	0.49
4:D:150:LEU:HD12	4:D:153:VAL:HG21	1.94	0.49
1:E:106:ILE:HD11	2:F:271:CYS:HB3	1.94	0.49
3:G:29:THR:CG2	4:H:149:ASN:HD21	2.26	0.49
1:A:88:TYR:HH	2:B:258:GLN:HB2	1.77	0.49
1:A:92:ASN:ND2	2:B:260:LYS:HB3	2.28	0.49
3:G:45:ARG:HA	3:G:48:VAL:HG12	1.94	0.49
1:E:113:TYR:CE1	2:F:282:THR:HG21	2.48	0.49
2:B:230:ILE:HD13	3:C:57:LEU:HD11	1.93	0.49
1:A:63:LEU:HD11	4:D:181:ILE:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:88:TYR:CE1	2:F:257:TYR:HB2	2.48	0.48
1:A:43:VAL:HG22	2:B:212:LEU:HD13	1.95	0.48
1:E:92:ASN:HD21	2:F:264:LYS:NZ	2.11	0.48
1:A:108:ILE:C	1:A:110:ILE:N	2.67	0.48
3:C:45:ARG:HA	3:C:48:VAL:HG12	1.95	0.48
1:E:77:PHE:HA	4:H:196:ASN:OD1	2.13	0.48
1:E:99:LEU:HD13	2:F:268:ILE:HA	1.96	0.48
1:E:92:ASN:OD1	2:F:264:LYS:NZ	2.46	0.48
2:B:247:ALA:O	2:B:251:THR:HG23	2.13	0.48
3:C:16:ARG:O	3:C:20:GLN:HB2	2.13	0.48
2:F:192:LEU:HD22	3:G:18:ALA:HB2	1.95	0.48
1:A:85:LYS:HE2	2:B:253:LYS:CB	2.43	0.48
2:F:269:ILE:O	2:F:273:VAL:HG23	2.14	0.48
4:H:150:LEU:HD12	4:H:153:VAL:HG21	1.95	0.48
1:A:38:GLN:O	1:A:42:VAL:HG23	2.14	0.48
2:F:265:LYS:O	2:F:269:ILE:HG13	2.14	0.48
2:B:269:ILE:O	2:B:273:VAL:HG23	2.13	0.47
1:E:38:GLN:O	1:E:42:VAL:HG23	2.13	0.47
2:F:252:LYS:O	2:F:255:VAL:HG22	2.14	0.47
3:G:25:SER:O	4:H:146:MET:HE3	2.15	0.47
1:E:63:LEU:HD12	4:H:182:MET:CG	2.45	0.47
2:F:213:HIS:C	2:F:213:HIS:HD1	2.18	0.47
2:B:257:TYR:HA	2:B:260:LYS:HB2	1.97	0.47
1:E:88:TYR:CZ	2:F:258:GLN:HB2	2.49	0.47
2:F:265:LYS:O	2:F:268:ILE:HB	2.15	0.47
2:B:252:LYS:O	2:B:255:VAL:HG22	2.15	0.47
1:E:89:TRP:CD1	2:F:257:TYR:CE1	3.02	0.47
1:E:56:ARG:CG	1:E:56:ARG:HH21	2.26	0.46
4:H:144:ASN:O	4:H:148:GLU:HB2	2.16	0.46
1:E:63:LEU:HD12	4:H:182:MET:HG3	1.97	0.46
1:A:92:ASN:HD21	2:B:264:LYS:HZ1	1.63	0.46
1:E:60:LEU:HD11	2:F:230:ILE:HG12	1.98	0.46
1:E:88:TYR:OH	2:F:258:GLN:CB	2.64	0.46
1:E:113:TYR:CZ	2:F:282:THR:HG21	2.50	0.46
3:G:60:VAL:HG12	4:H:181:ILE:HD13	1.96	0.46
1:E:108:ILE:C	1:E:110:ILE:N	2.68	0.46
3:C:17:ARG:O	3:C:21:LEU:HG	2.15	0.46
2:B:213:HIS:C	2:B:213:HIS:HD1	2.18	0.46
1:A:86:ARG:O	1:A:89:TRP:N	2.49	0.46
1:E:92:ASN:ND2	2:F:260:LYS:HB3	2.30	0.46
1:E:88:TYR:HE2	2:F:258:GLN:HB2	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ARG:CG	1:A:56:ARG:HH21	2.26	0.45
1:A:108:ILE:C	1:A:110:ILE:H	2.20	0.45
1:A:88:TYR:HH	2:B:255:VAL:C	2.20	0.45
1:E:67:ALA:HB1	2:F:236:ASN:HB3	1.97	0.45
2:F:247:ALA:O	2:F:251:THR:HG23	2.16	0.45
2:B:199:HIS:O	2:B:199:HIS:HD2	2.00	0.45
3:G:17:ARG:O	3:G:21:LEU:HG	2.16	0.45
1:E:86:ARG:O	1:E:89:TRP:N	2.49	0.45
1:A:29:MET:SD	1:A:32:LEU:HD12	2.57	0.45
4:D:144:ASN:O	4:D:148:GLU:HB2	2.16	0.45
1:E:85:LYS:HE2	2:F:253:LYS:HB2	1.96	0.45
2:F:218:ASP:O	2:F:222:LEU:HD13	2.16	0.45
1:E:64:ASP:HB2	2:F:233:ILE:HD11	2.00	0.44
4:D:192:ILE:O	4:D:196:ASN:HB2	2.17	0.44
3:C:36:VAL:HG11	4:D:156:ILE:HB	2.00	0.44
1:E:77:PHE:O	1:E:77:PHE:CD2	2.70	0.44
4:H:161:ARG:O	4:H:164:ALA:HB3	2.17	0.44
3:G:71:MET:CB	4:H:191:ARG:HD2	2.47	0.44
2:B:265:LYS:O	2:B:268:ILE:HB	2.17	0.44
1:E:108:ILE:C	1:E:110:ILE:H	2.21	0.44
1:E:89:TRP:CE3	1:E:90:TRP:HA	2.52	0.44
1:A:88:TYR:CE1	2:B:257:TYR:HB2	2.53	0.44
1:A:99:LEU:HD13	2:B:268:ILE:CG1	2.47	0.44
3:G:67:ILE:HG22	4:H:188:ASN:ND2	2.33	0.44
4:H:192:ILE:O	4:H:196:ASN:HB2	2.18	0.43
1:A:89:TRP:CE3	1:A:90:TRP:HA	2.52	0.43
1:E:88:TYR:CZ	2:F:258:GLN:N	2.86	0.43
1:E:99:LEU:HD13	2:F:268:ILE:CA	2.48	0.43
1:A:34:GLN:HE22	4:H:163:MET:CA	2.25	0.43
2:B:253:LYS:O	2:B:257:TYR:CD2	2.71	0.43
2:F:256:LYS:HE2	2:F:260:LYS:NZ	2.33	0.43
2:F:273:VAL:HG12	2:F:277:ILE:HD11	2.00	0.43
1:A:80:SER:O	1:A:84:LEU:HG	2.18	0.43
3:C:26:LEU:HD23	4:D:142:ARG:HG3	2.01	0.43
1:A:98:ILE:HG22	2:B:268:ILE:HD13	2.01	0.43
2:B:256:LYS:HE2	2:B:260:LYS:NZ	2.33	0.43
2:B:213:HIS:HD2	3:C:35:LEU:CD2	2.31	0.43
1:E:113:TYR:OH	2:F:282:THR:HG21	2.19	0.43
1:A:112:VAL:O	1:A:112:VAL:HG22	2.19	0.43
4:D:159:ASN:HD22	4:D:159:ASN:H	1.65	0.43
1:A:34:GLN:NE2	4:H:163:MET:HA	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:TYR:CD1	2:B:254:ALA:HA	2.54	0.42
1:E:76:GLN:HG2	4:H:196:ASN:HD21	1.84	0.42
1:A:43:VAL:O	1:A:47:ARG:HG3	2.19	0.42
4:D:159:ASN:HD21	4:H:155:GLY:HA3	1.83	0.42
2:B:218:ASP:O	2:B:222:LEU:HD13	2.19	0.42
1:A:102:ILE:HD11	2:B:272:CYS:SG	2.59	0.42
3:G:43:GLY:O	3:G:47:LEU:HG	2.20	0.42
2:B:273:VAL:HG12	2:B:277:ILE:HD11	2.01	0.42
3:G:34:GLN:HA	3:G:37:GLU:OE1	2.20	0.42
2:F:237:VAL:O	2:F:241:VAL:N	2.50	0.42
1:E:102:ILE:HD12	2:F:268:ILE:HG23	2.01	0.42
4:H:159:ASN:H	4:H:159:ASN:HD22	1.65	0.42
1:A:98:ILE:HB	2:B:268:ILE:CD1	2.50	0.42
1:E:43:VAL:O	1:E:47:ARG:HG3	2.20	0.42
3:G:29:THR:HG21	4:H:149:ASN:HD21	1.84	0.42
1:A:29:MET:HG3	1:A:29:MET:O	2.20	0.42
1:A:77:PHE:CD2	1:A:77:PHE:O	2.72	0.42
1:E:43:VAL:HG13	2:F:215:MET:HG3	2.02	0.42
1:E:80:SER:O	1:E:84:LEU:HG	2.19	0.42
2:B:222:LEU:O	2:B:226:GLN:HG3	2.20	0.41
1:E:29:MET:SD	1:E:32:LEU:HD12	2.60	0.41
2:F:258:GLN:OE1	3:G:81:LEU:CD1	2.68	0.41
1:E:50:VAL:O	1:E:54:LEU:HD13	2.20	0.41
3:G:53:GLN:O	3:G:57:LEU:HD13	2.20	0.41
1:E:56:ARG:NH1	4:H:174:GLN:OE1	2.53	0.41
1:E:113:TYR:HA	1:E:116:THR:OG1	2.20	0.41
2:F:199:HIS:HD2	2:F:199:HIS:O	2.02	0.41
2:F:222:LEU:O	2:F:226:GLN:HG3	2.20	0.41
1:A:92:ASN:HD21	2:B:260:LYS:HB3	1.86	0.41
1:E:112:VAL:HG22	1:E:112:VAL:O	2.19	0.41
1:E:70:LEU:HA	1:E:70:LEU:HD12	1.82	0.41
1:A:98:ILE:CG2	2:B:268:ILE:HD13	2.50	0.41
4:D:150:LEU:HD12	4:D:150:LEU:HA	1.88	0.41
1:E:43:VAL:HG22	2:F:212:LEU:CD1	2.42	0.41
1:E:104:ALA:HA	1:E:107:LEU:HB2	2.03	0.41
1:E:34:GLN:O	1:E:38:GLN:HG3	2.21	0.41
1:A:50:VAL:O	1:A:54:LEU:HD13	2.21	0.41
3:C:31:ARG:O	3:C:35:LEU:HG	2.21	0.41
1:E:42:VAL:HG11	2:F:212:LEU:HD21	2.02	0.41
1:E:88:TYR:OH	2:F:255:VAL:C	2.58	0.41
1:E:95:MET:N	1:E:95:MET:SD	2.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:VAL:HG23	1:A:102:ILE:N	2.36	0.41
3:C:26:LEU:O	3:C:30:ARG:HG3	2.20	0.41
3:C:47:LEU:HD11	4:D:163:MET:HE3	2.03	0.41
4:D:140:MET:O	4:D:144:ASN:HB2	2.21	0.41
4:D:156:ILE:O	4:D:159:ASN:HB2	2.21	0.41
1:E:43:VAL:HG22	2:F:212:LEU:HB2	2.03	0.41
3:C:34:GLN:HA	3:C:37:GLU:OE1	2.22	0.40
3:C:53:GLN:O	3:C:57:LEU:HD13	2.20	0.40
4:H:156:ILE:O	4:H:159:ASN:HB2	2.22	0.40
1:A:34:GLN:O	1:A:38:GLN:HG3	2.21	0.40
3:G:50:LEU:HA	3:G:50:LEU:HD23	1.89	0.40
1:A:88:TYR:CZ	2:B:258:GLN:HB2	2.55	0.40
3:G:26:LEU:O	3:G:30:ARG:HG3	2.21	0.40
4:H:157:ILE:O	4:H:157:ILE:HG22	2.22	0.40
1:E:88:TYR:HH	2:F:258:GLN:CB	2.31	0.40
2:F:253:LYS:O	2:F:257:TYR:CD2	2.74	0.40
4:H:177:GLN:O	4:H:180:ARG:HB3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	89/91 (98%)	83 (93%)	5 (6%)	1 (1%)	14	51
1	E	89/91 (98%)	84 (94%)	4 (4%)	1 (1%)	14	51
2	B	96/109 (88%)	88 (92%)	7 (7%)	1 (1%)	15	53
2	F	96/109 (88%)	88 (92%)	7 (7%)	1 (1%)	15	53
3	C	73/80 (91%)	72 (99%)	1 (1%)	0	100	100
3	G	73/80 (91%)	72 (99%)	1 (1%)	0	100	100
4	D	61/68 (90%)	59 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	H	61/68 (90%)	59 (97%)	2 (3%)	0	100	100
All	All	638/696 (92%)	605 (95%)	29 (4%)	4 (1%)	25	65

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	255	VAL
1	A	86	ARG
1	E	86	ARG
2	F	255	VAL

### 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	80/80 (100%)	75 (94%)	5 (6%)	18	44
1	E	80/80 (100%)	75 (94%)	5 (6%)	18	44
2	B	87/96 (91%)	82 (94%)	5 (6%)	20	47
2	F	87/96 (91%)	82 (94%)	5 (6%)	20	47
3	C	67/71 (94%)	66 (98%)	1 (2%)	65	80
3	G	67/71 (94%)	66 (98%)	1 (2%)	65	80
4	D	55/58 (95%)	55 (100%)	0	100	100
4	H	55/58 (95%)	55 (100%)	0	100	100
All	All	578/610 (95%)	556 (96%)	22 (4%)	33	58

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	102	ILE
1	A	107	LEU
1	A	110	ILE

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Mol	Chain	Res	Type
1	A	114	PHE
2	B	213	HIS
2	B	242	ASP
2	B	257	TYR
2	B	272	CYS
2	B	282	THR
3	C	26	LEU
1	E	38	GLN
1	E	102	ILE
1	E	107	LEU
1	E	110	ILE
1	E	114	PHE
2	F	213	HIS
2	F	242	ASP
2	F	257	TYR
2	F	272	CYS
2	F	282	THR
3	G	26	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	92	ASN
4	D	159	ASN
4	D	162	HIS
1	E	34	GLN
2	F	199	HIS
2	F	213	HIS
4	H	149	ASN
4	H	162	HIS
4	H	188	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 carbohydrates 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	91/91 (100%)	-0.32	1 (1%) 80 73	175, 264, 308, 361	0
1	E	91/91 (100%)	-0.41	0 100 100	187, 264, 353, 387	0
2	B	98/109 (89%)	-0.52	0 100 100	181, 286, 355, 422	0
2	F	98/109 (89%)	-0.32	0 100 100	191, 281, 364, 503	0
3	C	75/80 (93%)	-0.42	1 (1%) 77 68	187, 314, 388, 395	0
3	G	75/80 (93%)	-0.18	0 100 100	205, 304, 377, 441	0
4	D	63/68 (92%)	-0.14	2 (3%) 47 38	222, 295, 380, 411	0
4	H	63/68 (92%)	-0.24	0 100 100	193, 290, 362, 426	0
All	All	654/696 (93%)	-0.33	4 (0%) 89 84	175, 284, 373, 503	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	8	ARG	3.3
4	D	138	SER	2.9
4	D	139	HIS	2.5
1	A	116	THR	2.1

### 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.