



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:35 pm BST

PDB ID : 5V8W  
Title : Crystal structure of human Integrator IntS9-IntS11 CTD complex  
Authors : Wu, Y.; Tong, L.  
Deposited on : 2017-03-22  
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](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.

---

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Xtrriage (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

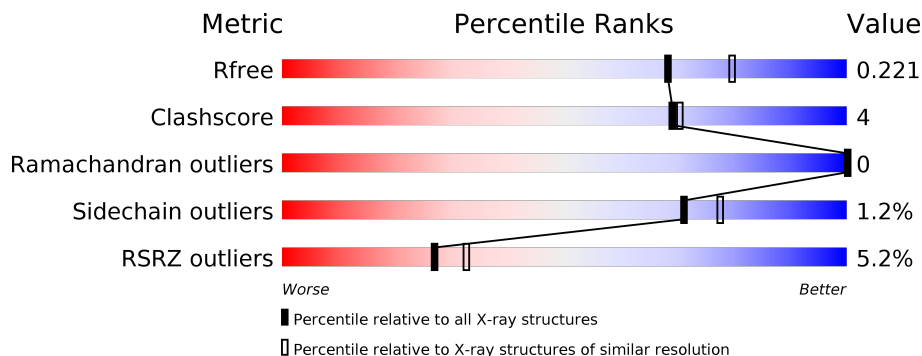
# 1 Overall quality at a glance

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.



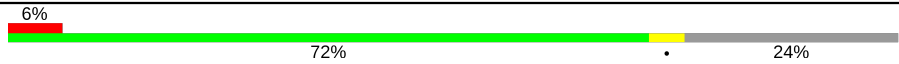

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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  $\geq 3$ , 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	78	
1	C	78	
1	E	78	
1	G	78	
2	B	114	
2	D	114	

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
2	F	114	
2	H	114	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6055 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 Integrator complex subunit 9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	77	622	397	104	119	2	0	0	0
1	C	77	622	397	104	119	2	0	0	0
1	E	77	622	397	104	119	2	0	0	0
1	G	77	622	397	104	119	2	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	581	MET	-	initiating methionine	UNP Q9NV88
C	581	MET	-	initiating methionine	UNP Q9NV88
E	581	MET	-	initiating methionine	UNP Q9NV88
G	581	MET	-	initiating methionine	UNP Q9NV88

- Molecule 2 is a protein called Integrator complex subunit 11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	104	815	514	143	156	2	0	0	0
2	D	104	815	514	142	157	2	0	0	0
2	F	87	694	442	123	127	2	0	0	0
2	H	105	824	519	144	159	2	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	487	GLY	-	expression tag	UNP Q5TA45
B	488	SER	-	expression tag	UNP Q5TA45
B	489	HIS	-	expression tag	UNP Q5TA45
B	490	MET	-	expression tag	UNP Q5TA45
D	487	GLY	-	expression tag	UNP Q5TA45
D	488	SER	-	expression tag	UNP Q5TA45
D	489	HIS	-	expression tag	UNP Q5TA45
D	490	MET	-	expression tag	UNP Q5TA45
F	487	GLY	-	expression tag	UNP Q5TA45
F	488	SER	-	expression tag	UNP Q5TA45
F	489	HIS	-	expression tag	UNP Q5TA45
F	490	MET	-	expression tag	UNP Q5TA45
H	487	GLY	-	expression tag	UNP Q5TA45
H	488	SER	-	expression tag	UNP Q5TA45
H	489	HIS	-	expression tag	UNP Q5TA45
H	490	MET	-	expression tag	UNP Q5TA45

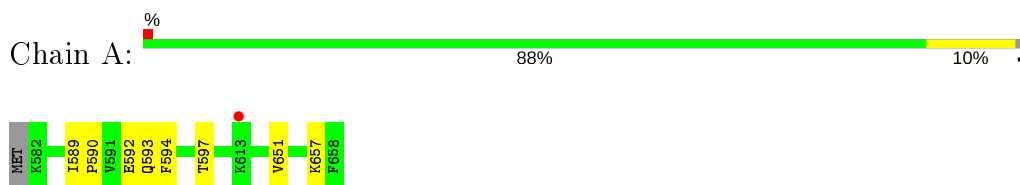
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	62	Total O 62 62	0	0
3	B	58	Total O 58 58	0	0
3	C	21	Total O 21 21	0	0
3	D	49	Total O 49 49	0	0
3	E	56	Total O 56 56	0	0
3	F	60	Total O 60 60	0	0
3	G	30	Total O 30 30	0	0
3	H	83	Total O 83 83	0	0

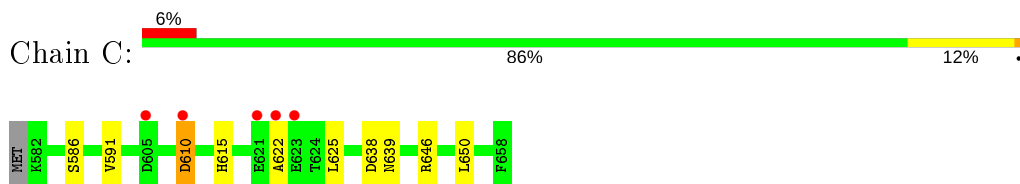
### 3 Residue-property plots [i](#)

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.

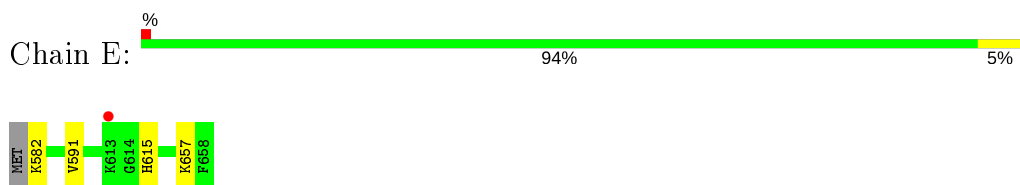
- Molecule 1: Integrator complex subunit 9



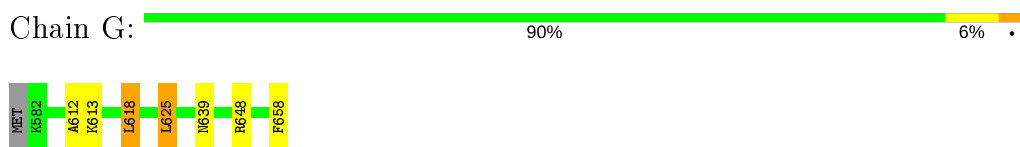
- Molecule 1: Integrator complex subunit 9



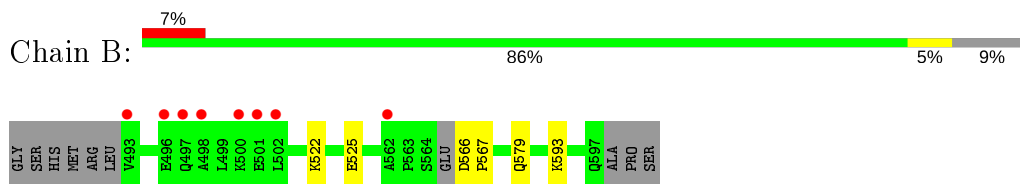
- Molecule 1: Integrator complex subunit 9



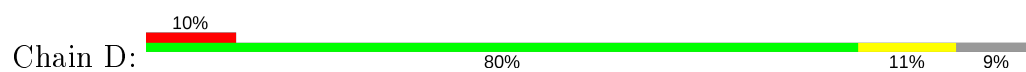
- Molecule 1: Integrator complex subunit 9



- Molecule 2: Integrator complex subunit 11



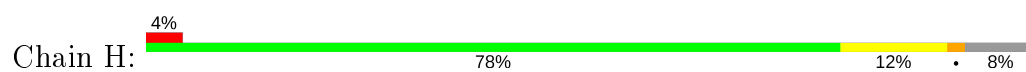
- Molecule 2: Integrator complex subunit 11



- Molecule 2: Integrator complex subunit 11



- Molecule 2: Integrator complex subunit 11



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.01Å 67.78Å 98.58Å 90.00° 100.65° 90.00°	Depositor
Resolution (Å)	24.83 – 2.10 24.83 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (24.83-2.10) 99.6 (24.83-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.93 (at 2.10Å)	Xtrriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.167 , 0.220 0.168 , 0.221	Depositor DCC
$R_{free}$ test set	1861 reflections (3.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtrriage
Anisotropy	0.064	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 47.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6055	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.04 % 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 4.1458e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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	0.61	0/630	0.64	0/848
1	C	0.50	0/630	0.60	0/848
1	E	0.56	0/630	0.64	0/848
1	G	0.58	0/630	0.71	2/848 (0.2%)
2	B	0.58	0/829	0.62	0/1122
2	D	0.53	0/830	0.63	0/1125
2	F	0.61	0/707	0.62	0/957
2	H	0.63	0/839	0.67	0/1137
All	All	0.58	0/5725	0.64	2/7733 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	648	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	G	625	LEU	CA-CB-CG	5.18	127.22	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	622	0	638	4	0
1	C	622	0	638	9	0
1	E	622	0	638	2	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	622	0	638	5	0
2	B	815	0	822	5	0
2	D	815	0	821	9	0
2	F	694	0	706	3	0
2	H	824	0	829	12	0
3	A	62	0	0	1	0
3	B	58	0	0	3	0
3	C	21	0	0	0	0
3	D	49	0	0	0	0
3	E	56	0	0	0	0
3	F	60	0	0	1	0
3	G	30	0	0	1	0
3	H	83	0	0	0	0
All	All	6055	0	5730	42	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 4.

All (42) 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:G:618:LEU:HD23	1:G:625:LEU:HD22	1.78	0.65
1:A:589:ILE:HD11	1:A:651:VAL:HG13	1.78	0.64
2:F:523:GLU:HA	2:F:570:LYS:HD3	1.81	0.62
2:H:550:SER:HB3	2:H:559:GLN:HG2	1.83	0.60
1:C:610:ASP:N	1:C:610:ASP:OD1	2.36	0.59
1:A:594:PHE:O	1:A:597:THR:HG22	2.04	0.57
1:C:591:VAL:HG21	1:C:615:HIS:CD2	2.41	0.56
1:C:646:ARG:O	1:C:650:LEU:HG	2.08	0.54
1:C:639:ASN:ND2	2:D:592:LYS:HB2	2.24	0.52
2:D:584:GLY:O	2:D:588:THR:HG23	2.08	0.52
2:B:579:GLN:HG2	3:B:732:HOH:O	2.09	0.51
1:G:612:ALA:O	1:G:613:LYS:HG2	2.10	0.51
2:H:521:ARG:NH1	2:H:529:ARG:HD3	2.26	0.51
2:H:538:LEU:HD11	2:H:587:LEU:HD21	1.92	0.50
2:D:566:ASP:OD2	2:D:569:THR:OG1	2.19	0.50
1:C:586:SER:HB3	2:D:499:LEU:HD11	1.94	0.50
2:B:525:GLU:OE1	3:B:701:HOH:O	2.20	0.48
1:E:582:LYS:HB2	3:F:702:HOH:O	2.12	0.48
2:B:522:LYS:NZ	3:B:704:HOH:O	2.47	0.48
1:G:639:ASN:ND2	2:H:592:LYS:HB2	2.29	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:591:VAL:HG21	1:E:615:HIS:ND1	2.29	0.47
1:C:639:ASN:HD21	2:D:592:LYS:HB2	1.79	0.47
1:C:622:ALA:HB1	1:C:638:ASP:HB2	1.96	0.47
2:F:519:ASP:HB2	2:F:570:LYS:CE	2.45	0.46
2:F:525:GLU:O	2:F:529:ARG:HG3	2.15	0.46
2:D:538:LEU:HD11	2:D:587:LEU:HD21	1.98	0.45
2:H:521:ARG:CZ	2:H:529:ARG:HD3	2.46	0.45
2:H:561:ALA:HB3	2:H:571:VAL:HB	1.97	0.45
2:D:565:GLU:N	2:D:565:GLU:OE1	2.39	0.45
1:C:586:SER:HA	2:D:507:HIS:HB2	1.98	0.44
2:H:538:LEU:HD11	2:H:587:LEU:CD2	2.48	0.44
2:B:566:ASP:HA	2:B:567:PRO:HD3	1.63	0.43
1:G:658:PHE:CD2	2:H:499:LEU:HD21	2.53	0.43
1:C:610:ASP:HB3	1:C:615:HIS:ND1	2.34	0.43
1:G:639:ASN:HA	2:H:513:CYS:SG	2.59	0.42
1:A:590:PRO:HG2	1:A:593:GLN:HB2	2.01	0.41
2:B:593:LYS:N	2:B:593:LYS:HD2	2.36	0.41
2:D:550:SER:HB2	2:D:559:GLN:HG2	2.03	0.41
2:H:576:TRP:CD1	2:H:581:GLU:HA	2.55	0.41
3:G:724:HOH:O	2:H:516:HIS:HD2	2.04	0.40
1:A:592:GLU:HG2	3:A:743:HOH:O	2.21	0.40
2:H:519:ASP:O	2:H:570:LYS:NZ	2.54	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	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
1	C	75/78 (96%)	70 (93%)	5 (7%)	0	100	100
1	E	75/78 (96%)	75 (100%)	0	0	100	100

*Continued on next page...*

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	75/78 (96%)	74 (99%)	1 (1%)	0	100	100
2	B	100/114 (88%)	98 (98%)	2 (2%)	0	100	100
2	D	102/114 (90%)	101 (99%)	1 (1%)	0	100	100
2	F	83/114 (73%)	81 (98%)	2 (2%)	0	100	100
2	H	103/114 (90%)	102 (99%)	1 (1%)	0	100	100
All	All	688/768 (90%)	675 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	A	72/73 (99%)	71 (99%)	1 (1%)	67	73
1	C	72/73 (99%)	70 (97%)	2 (3%)	43	47
1	E	72/73 (99%)	71 (99%)	1 (1%)	67	73
1	G	72/73 (99%)	71 (99%)	1 (1%)	67	73
2	B	93/101 (92%)	93 (100%)	0	100	100
2	D	93/101 (92%)	92 (99%)	1 (1%)	73	79
2	F	79/101 (78%)	79 (100%)	0	100	100
2	H	94/101 (93%)	92 (98%)	2 (2%)	53	59
All	All	647/696 (93%)	639 (99%)	8 (1%)	71	77

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	657	LYS
1	C	610	ASP
1	C	625	LEU
2	D	496	GLU
1	E	657	LYS

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	618	LEU
2	H	513	CYS
2	H	550	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA [i](#)

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 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

### 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, 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	77/78 (98%)	-0.39	1 (1%) 77 80	17, 27, 55, 73	0
1	C	77/78 (98%)	0.29	5 (6%) 18 23	25, 49, 91, 115	0
1	E	77/78 (98%)	-0.28	1 (1%) 77 80	18, 30, 51, 64	0
1	G	77/78 (98%)	-0.34	0 100 100	18, 32, 52, 82	0
2	B	104/114 (91%)	-0.01	8 (7%) 13 17	18, 32, 87, 106	0
2	D	104/114 (91%)	0.26	11 (10%) 6 7	16, 35, 94, 110	0
2	F	87/114 (76%)	-0.10	7 (8%) 12 16	16, 27, 86, 97	0
2	H	105/114 (92%)	-0.13	4 (3%) 40 46	15, 29, 59, 103	0
All	All	708/768 (92%)	-0.07	37 (5%) 27 32	15, 32, 82, 115	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	524	GLN	4.8
2	D	520	THR	4.4
2	B	502	LEU	4.2
2	B	562	ALA	4.1
2	D	493	VAL	4.0
2	F	520	THR	3.8
2	B	501	GLU	3.7
2	F	522	LYS	3.6
2	D	523	GLU	3.4
2	D	519	ASP	3.3
2	B	493	VAL	3.3
2	D	524	GLN	3.2
1	A	613	LYS	3.2
2	F	562	ALA	3.2
2	F	563	PRO	3.0
2	H	565	GLU	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	622	ALA	2.8
2	H	494	SER	2.7
2	B	498	ALA	2.7
2	B	496	GLU	2.7
2	H	493	VAL	2.6
2	D	562	ALA	2.6
2	D	497	GLN	2.5
2	B	500	LYS	2.5
1	C	610	ASP	2.5
2	F	504	LEU	2.4
1	C	623	GLU	2.3
2	D	522	LYS	2.3
2	H	520	THR	2.3
2	D	563	PRO	2.3
1	C	621	GLU	2.2
1	C	605	ASP	2.2
2	D	565	GLU	2.2
2	F	521	ARG	2.1
2	B	497	GLN	2.1
2	D	500	LYS	2.1
1	E	613	LYS	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.