



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 12:59 am GMT

PDB ID : 2A2F  
Title : Crystal Structure of Sec15 C-terminal domain  
Authors : Wu, S.; Mehta, S.Q.; Pichaud, F.; Bellen, H.J.; Quiocho, F.A.  
Deposited on : 2005-06-22  
Resolution : 2.50 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

<http://wwpdb.org/validation/2016/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) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

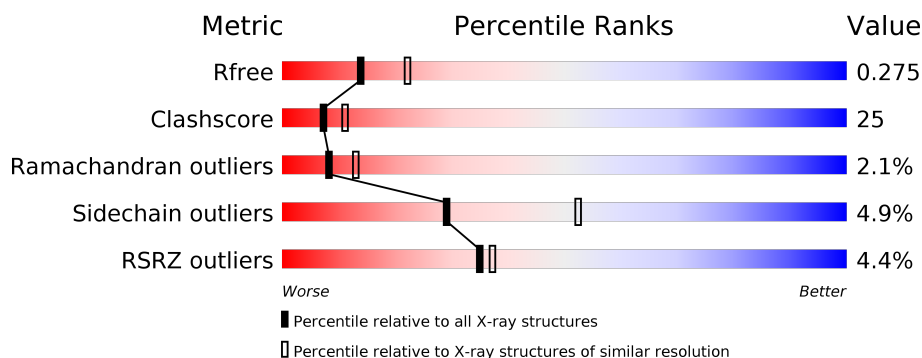
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	100719	3846 (2.50-2.50)
Clashscore	112137	4554 (2.50-2.50)
Ramachandran outliers	110173	4463 (2.50-2.50)
Sidechain outliers	110143	4465 (2.50-2.50)
RSRZ outliers	101464	3876 (2.50-2.50)

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. 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	X	325	<div> <div>4%</div> <div>54%</div> <div>33%</div> <div>• • 9%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2511 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 Exocyst complex component Sec15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	296	Total	C	N	O	S	0	0	0
			2424	1569	397	440	18			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	1	MET	-	CLONING ARTIFACT	UNP Q9VDE6
X	320	HIS	-	EXPRESSION TAG	UNP Q9VDE6
X	321	HIS	-	EXPRESSION TAG	UNP Q9VDE6
X	322	HIS	-	EXPRESSION TAG	UNP Q9VDE6
X	323	HIS	-	EXPRESSION TAG	UNP Q9VDE6
X	324	HIS	-	EXPRESSION TAG	UNP Q9VDE6
X	325	HIS	-	EXPRESSION TAG	UNP Q9VDE6

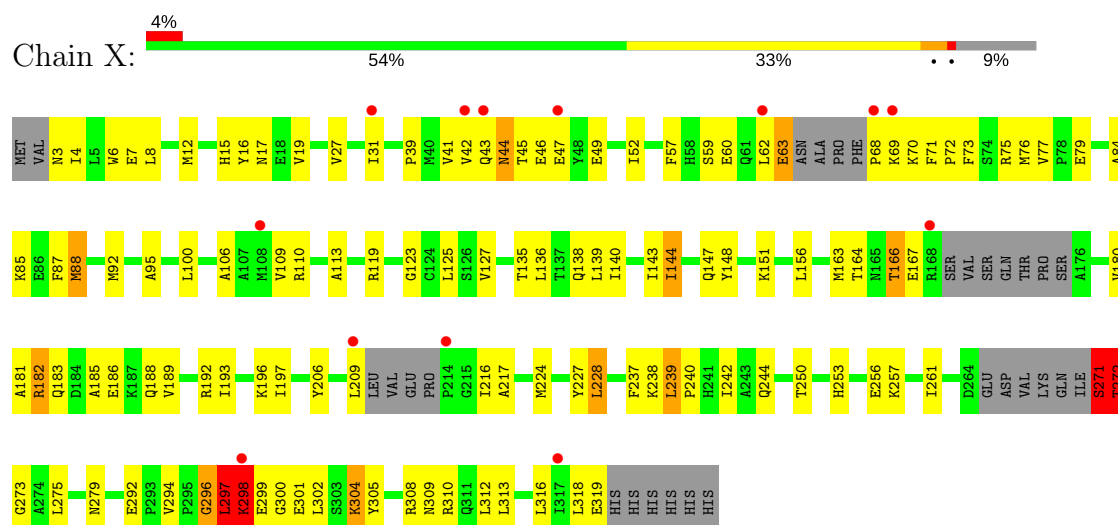
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	87	Total	O	0	0
			87	87		

### 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: Exocyst complex component Sec15



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.50Å 93.90Å 123.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	500.00 – 2.50 43.44 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (500.00-2.50) 92.6 (43.44-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.92 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.243 , 0.276 0.244 , 0.275	Depositor DCC
$R_{free}$ test set	740 reflections (4.89%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.8	Xtriage
Anisotropy	0.594	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 73.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	2511	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.79% 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

### 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	X	0.66	5/2478 (0.2%)	0.89	12/3343 (0.4%)

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	X	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	272	THR	C-N	-15.94	1.04	1.33
1	X	298	LYS	C-N	-13.21	1.03	1.34
1	X	275	LEU	C-N	-8.94	1.13	1.34
1	X	297	LEU	CB-CG	8.34	1.76	1.52
1	X	271	SER	C-N	-7.90	1.15	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	298	LYS	O-C-N	-20.21	90.37	122.70
1	X	298	LYS	CA-C-N	16.42	153.33	117.20
1	X	298	LYS	C-N-CA	14.56	158.11	121.70
1	X	271	SER	O-C-N	-13.29	101.44	122.70
1	X	272	THR	CA-C-N	8.71	133.62	116.20
1	X	297	LEU	O-C-N	-7.74	110.32	122.70
1	X	275	LEU	CA-C-O	-6.43	106.61	120.10
1	X	275	LEU	CA-C-N	6.23	130.91	117.20
1	X	296	GLY	O-C-N	-6.14	112.87	122.70
1	X	272	THR	C-N-CA	5.99	134.88	122.30
1	X	272	THR	CA-C-O	-5.36	108.84	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	297	LEU	CB-CG-CD2	-5.13	102.28	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	271	SER	Mainchain,Peptide
1	X	296	GLY	Mainchain
1	X	297	LEU	Mainchain
1	X	298	LYS	Peptide

## 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	X	2424	0	2387	120	0
2	X	87	0	0	2	0
All	All	2511	0	2387	120	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 25.

All (120) 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:X:297:LEU:CB	1:X:297:LEU:CG	1.76	1.57
1:X:42:VAL:HG11	1:X:47:GLU:HB2	1.41	1.03
1:X:292:GLU:OE2	1:X:298:LYS:HE2	1.71	0.90
1:X:88:MET:CE	1:X:156:LEU:HG	2.04	0.87
1:X:297:LEU:CD2	1:X:297:LEU:CB	2.55	0.83
1:X:92:MET:HG2	1:X:109:VAL:HG21	1.61	0.83
1:X:279:ASN:ND2	1:X:310:ARG:HH12	1.81	0.78
1:X:297:LEU:HB3	1:X:301:GLU:OE2	1.83	0.78
1:X:297:LEU:CG	1:X:297:LEU:CA	2.62	0.77
1:X:297:LEU:CB	1:X:297:LEU:CD1	2.63	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:292:GLU:OE2	1:X:298:LYS:CE	2.33	0.75
1:X:135:THR:H	1:X:138:GLN:NE2	1.84	0.74
1:X:88:MET:HE2	1:X:156:LEU:HG	1.68	0.74
1:X:42:VAL:O	1:X:70:LYS:HE2	1.86	0.74
1:X:181:ALA:C	1:X:183:GLN:H	1.90	0.74
1:X:41:VAL:HA	1:X:70:LYS:CB	2.18	0.73
1:X:297:LEU:N	1:X:297:LEU:CG	2.51	0.72
1:X:123:GLY:O	1:X:127:VAL:HG23	1.88	0.72
1:X:42:VAL:HG11	1:X:47:GLU:CB	2.19	0.72
1:X:41:VAL:HA	1:X:70:LYS:HB2	1.74	0.69
1:X:41:VAL:HG13	1:X:70:LYS:HB2	1.75	0.69
1:X:292:GLU:OE2	1:X:298:LYS:CD	2.42	0.67
1:X:271:SER:O	1:X:273:GLY:N	2.27	0.67
1:X:139:LEU:O	1:X:143:ILE:HG12	1.94	0.67
1:X:3:ASN:O	1:X:7:GLU:HG2	1.96	0.66
1:X:92:MET:CG	1:X:109:VAL:HG21	2.26	0.65
1:X:41:VAL:HG22	1:X:70:LYS:N	2.12	0.64
1:X:297:LEU:HG	1:X:297:LEU:N	2.13	0.64
1:X:135:THR:HG22	1:X:138:GLN:CD	2.19	0.63
1:X:182:ARG:C	1:X:182:ARG:HD2	2.18	0.63
1:X:299:GLU:O	1:X:301:GLU:N	2.32	0.63
1:X:279:ASN:HD21	1:X:310:ARG:HH12	1.44	0.62
1:X:206:TYR:HE1	1:X:261:ILE:HD13	1.66	0.60
1:X:125:LEU:HD13	1:X:180:VAL:HG22	1.82	0.60
1:X:60:GLU:OE1	1:X:60:GLU:HA	2.01	0.60
1:X:185:ALA:O	1:X:189:VAL:HG23	2.01	0.60
1:X:196:LYS:HG2	1:X:227:TYR:CZ	2.36	0.60
1:X:41:VAL:HG13	1:X:70:LYS:HD3	1.83	0.60
1:X:181:ALA:C	1:X:183:GLN:N	2.56	0.59
1:X:140:ILE:O	1:X:144:ILE:HG23	2.03	0.59
1:X:135:THR:HG23	1:X:138:GLN:H	1.67	0.59
1:X:42:VAL:CG1	1:X:47:GLU:HB2	2.27	0.57
1:X:135:THR:HG22	1:X:138:GLN:CG	2.35	0.56
1:X:181:ALA:O	1:X:183:GLN:N	2.38	0.56
1:X:297:LEU:H	1:X:297:LEU:HG	1.71	0.56
1:X:299:GLU:OE1	1:X:299:GLU:HA	2.05	0.56
1:X:182:ARG:O	1:X:182:ARG:HD2	2.06	0.56
1:X:41:VAL:HA	1:X:70:LYS:HB3	1.88	0.56
1:X:209:LEU:O	1:X:209:LEU:HG	2.06	0.55
1:X:41:VAL:HG21	1:X:69:LYS:N	2.22	0.55
1:X:8:LEU:O	1:X:12:MET:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:106:ALA:O	1:X:110:ARG:HB2	2.08	0.54
1:X:73:PHE:HB2	1:X:77:VAL:HG21	1.91	0.53
1:X:292:GLU:OE2	1:X:298:LYS:HD3	2.09	0.52
1:X:244:GLN:HG2	1:X:297:LEU:HD21	1.90	0.51
1:X:17:ASN:OD1	1:X:119:ARG:HD3	2.10	0.51
1:X:206:TYR:CE1	1:X:261:ILE:HD13	2.44	0.51
1:X:257:LYS:O	1:X:261:ILE:HG13	2.11	0.51
1:X:224:MET:HG2	1:X:228:LEU:HD22	1.93	0.50
1:X:49:GLU:HA	1:X:52:ILE:HB	1.95	0.49
1:X:45:THR:C	1:X:47:GLU:H	2.14	0.49
1:X:164:THR:OG1	1:X:166:THR:HB	2.12	0.49
1:X:43:GLN:HE22	1:X:63:GLU:C	2.15	0.48
1:X:271:SER:O	1:X:272:THR:C	2.48	0.48
1:X:135:THR:HG22	1:X:138:GLN:NE2	2.29	0.48
1:X:41:VAL:O	1:X:42:VAL:HG23	2.14	0.48
1:X:4:ILE:N	1:X:4:ILE:HD12	2.29	0.47
1:X:31:ILE:CD1	1:X:76:MET:HA	2.44	0.47
1:X:318:LEU:O	1:X:319:GLU:HG3	2.15	0.47
1:X:253:HIS:O	1:X:256:GLU:HG2	2.15	0.47
1:X:239:LEU:HB3	1:X:242:ILE:HB	1.95	0.47
1:X:238:LYS:C	1:X:240:PRO:HD3	2.34	0.47
1:X:87:PHE:HE2	1:X:113:ALA:HA	1.78	0.47
1:X:182:ARG:O	1:X:186:GLU:HG3	2.15	0.46
1:X:253:HIS:HA	1:X:256:GLU:HG2	1.96	0.46
1:X:88:MET:HE3	1:X:156:LEU:HG	1.94	0.46
1:X:92:MET:CE	1:X:163:MET:SD	3.04	0.45
1:X:308:ARG:HG3	1:X:309:ASN:N	2.32	0.45
1:X:301:GLU:O	1:X:304:LYS:CD	2.65	0.45
1:X:72:PRO:O	1:X:144:ILE:HD11	2.16	0.45
1:X:239:LEU:HG	1:X:242:ILE:HD12	1.99	0.45
1:X:72:PRO:HB2	1:X:148:TYR:CE2	2.51	0.45
1:X:84:ALA:O	1:X:88:MET:HG2	2.17	0.45
1:X:16:TYR:CE2	1:X:87:PHE:HE1	2.35	0.45
1:X:43:GLN:O	1:X:44:ASN:HB2	2.16	0.44
1:X:31:ILE:HD13	1:X:76:MET:N	2.32	0.44
1:X:62:LEU:HB3	1:X:63:GLU:OE2	2.18	0.44
1:X:3:ASN:HB3	1:X:6:TRP:HB3	1.99	0.44
1:X:147:GLN:O	1:X:151:LYS:HG3	2.17	0.44
1:X:166:THR:HG23	1:X:167:GLU:N	2.32	0.44
1:X:39:PRO:HB3	1:X:71:PHE:O	2.18	0.43
1:X:139:LEU:HD12	1:X:192:ARG:CZ	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:136:LEU:O	1:X:140:ILE:HD13	2.19	0.43
1:X:43:GLN:HA	1:X:43:GLN:OE1	2.19	0.43
1:X:139:LEU:HD12	1:X:192:ARG:NE	2.34	0.42
1:X:192:ARG:HH11	1:X:192:ARG:HG3	1.84	0.42
1:X:302:LEU:O	1:X:305:TYR:HD2	2.01	0.42
1:X:312:LEU:O	1:X:316:LEU:HD23	2.19	0.42
1:X:193:ILE:O	1:X:197:ILE:HG13	2.20	0.42
1:X:216:ILE:HG23	1:X:217:ALA:N	2.34	0.42
1:X:197:ILE:HD11	1:X:250:THR:HG23	2.01	0.42
1:X:297:LEU:O	1:X:298:LYS:C	2.57	0.42
1:X:41:VAL:HG22	1:X:70:LYS:HB2	2.02	0.42
1:X:294:VAL:O	1:X:294:VAL:HG23	2.18	0.42
1:X:63:GLU:HB3	2:X:386:HOH:O	2.19	0.42
1:X:42:VAL:CG1	1:X:43:GLN:N	2.82	0.42
1:X:43:GLN:NE2	1:X:63:GLU:O	2.53	0.42
1:X:301:GLU:O	1:X:304:LYS:HD2	2.20	0.42
1:X:75:ARG:HE	1:X:75:ARG:HB2	1.65	0.41
1:X:156:LEU:HA	1:X:156:LEU:HD12	1.94	0.41
1:X:41:VAL:CA	1:X:70:LYS:HB2	2.48	0.41
1:X:237:PHE:CE1	1:X:238:LYS:HG3	2.56	0.41
1:X:95:ALA:HB1	1:X:100:LEU:HD12	2.03	0.41
1:X:15:HIS:O	1:X:19:VAL:HG23	2.20	0.41
1:X:44:ASN:HB3	1:X:47:GLU:HG3	2.02	0.41
1:X:57:PHE:HD2	1:X:71:PHE:HE1	1.69	0.41
1:X:151:LYS:NZ	2:X:405:HOH:O	2.53	0.41
1:X:62:LEU:O	1:X:63:GLU:C	2.59	0.41
1:X:41:VAL:CG1	1:X:70:LYS:HB2	2.48	0.40
1:X:68:PRO:C	1:X:69:LYS:HG3	2.41	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	X	286/325 (88%)	263 (92%)	17 (6%)	6 (2%)	8	13

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	300	GLY
1	X	44	ASN
1	X	182	ARG
1	X	46	GLU
1	X	59	SER
1	X	272	THR

### 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	X	265/295 (90%)	252 (95%)	13 (5%)	29	52

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	27	VAL
1	X	63	GLU
1	X	79	GLU
1	X	85	LYS
1	X	88	MET
1	X	144	ILE
1	X	166	THR
1	X	188	GLN
1	X	228	LEU
1	X	239	LEU
1	X	297	LEU
1	X	304	LYS
1	X	313	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	11	ASN
1	X	36	GLN
1	X	43	GLN
1	X	114	ASN
1	X	138	GLN
1	X	165	ASN
1	X	183	GLN
1	X	279	ASN
1	X	311	GLN

### 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 [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	X	296/325 (91%)	0.50	13 (4%) 35 37	53, 77, 117, 142	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	68	PRO	9.8
1	X	62	LEU	6.4
1	X	42	VAL	5.1
1	X	298	LYS	4.5
1	X	214	PRO	3.5
1	X	209	LEU	2.6
1	X	69	LYS	2.6
1	X	47	GLU	2.4
1	X	108	MET	2.3
1	X	31	ILE	2.2
1	X	168	ARG	2.2
1	X	317	ILE	2.1
1	X	43	GLN	2.0

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.