



# Full wwPDB X-ray Structure Validation Report

Oct 9, 2014 – 07:10 AM EDT

PDB ID : 4PJW  
Title : crystal structure of human Stromal Antigen 2 (SA2) in complex with Sister Chromatid Cohesion protein 1 (Scc1), with bound MES  
Authors : Hara, K.; Chen, Z.; Tomchick, D.R.; Yu, H.  
Deposited on : 2014-05-12  
Resolution : 2.85 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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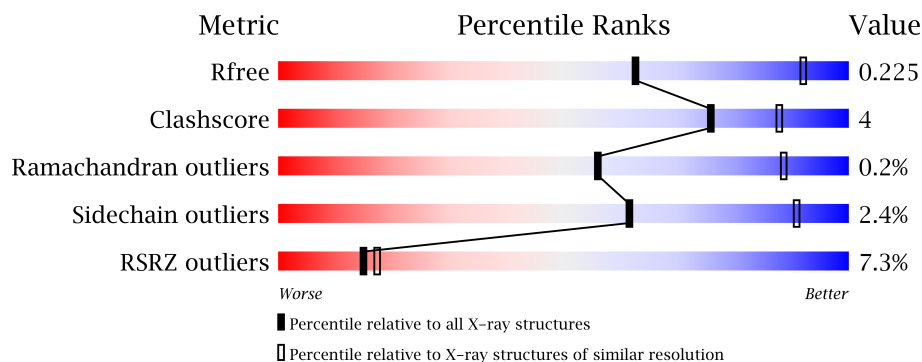
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.16 November 2013  
Xtriage (Phenix) : dev-1439  
EDS : stable23828  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable23828

# 1 Overall quality at a glance

The reported resolution of this entry is 2.85 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))
$R_{free}$	66092	1524 (2.90-2.82)
Clashscore	79885	1879 (2.90-2.82)
Ramachandran outliers	78287	1824 (2.90-2.82)
Sidechain outliers	78261	1827 (2.90-2.82)
RSRZ outliers	66119	1526 (2.90-2.82)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	981	
2	B	140	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MES	A	1101	-	X

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 15768 atoms, of which 7768 are hydrogens and 0 are deuterium.

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.

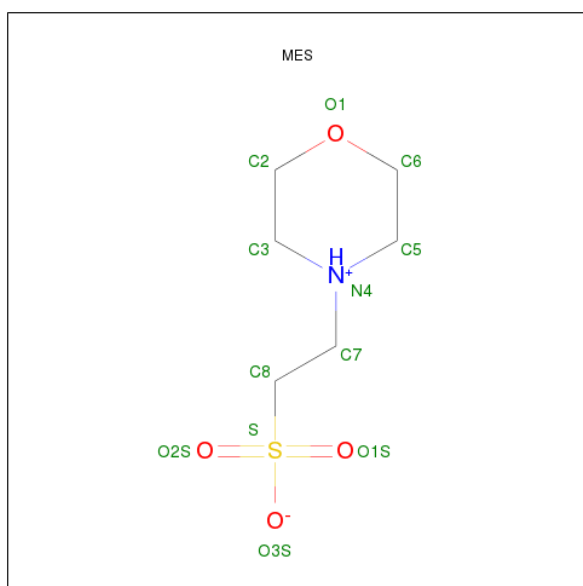
- Molecule 1 is a protein called Cohesin subunit SA-2.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
1	A	905	Total	C	H	N	O	S	Se		0	0	0
			14487	4705	7116	1228	1384	20	34				

- Molecule 2 is a protein called Double-strand-break repair protein rad21 homolog.

Mol	Chain	Residues	Atoms								ZeroOcc	AltConf	Trace
2	B	75	Total	C	H	N	O	S	Se		0	0	0
			1242	390	639	102	108	1	2				

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	S			0	0
			25	6	13	1	4	1				

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	11	Total 11	O 11	0	0
4	B	3	Total 3	O 3	0	0

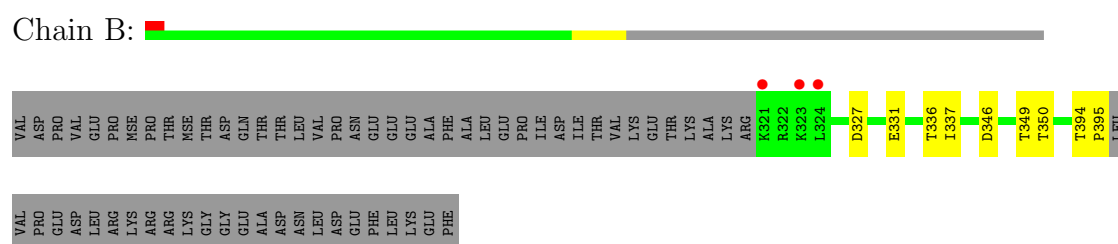
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Cohesin subunit SA-2



#### • Molecule 2: Double-strand-break repair protein rad21 homolog



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.73Å 108.05Å 180.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.70 – 2.85 41.71 – 2.77	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.70-2.85) 98.8 (41.71-2.77)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.37 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, $R_{free}$	0.210 , 0.225 0.209 , 0.225	Depositor DCC
$R_{free}$ test set	1836 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.9	Xtriage
Anisotropy	0.430	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 9.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 39571 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15768	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MES

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	0.27	0/7463	0.47	0/9997
2	B	0.28	0/612	0.51	0/824
All	All	0.27	0/8075	0.47	0/10821

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7371	7116	280	60	0
2	B	603	639	7	5	0
3	A	12	13	0	0	0
4	A	11	0	0	1	0
4	B	3	0	0	0	0
All	All	8000	7768	287	62	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 4.

All (62) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:986:ASN:HD22	1:A:994:PRO:HB3	1.49	0.78
1:A:678:GLU:HB3	1:A:679:PRO:C	2.16	0.66
1:A:989:GLY:N	1:A:990:GLU:HA	2.09	0.65
1:A:1015:LYS:HD3	1:A:1048:LEU:HA	1.77	0.65
1:A:802:ILE:HG12	1:A:810:LEU:HB3	1.78	0.65
1:A:1011:LEU:O	1:A:1015:LYS:N	2.29	0.65
1:A:803:MSE:HA	1:A:807:ARG:HB2	1.79	0.64
1:A:316:MSE:HE1	1:A:329:LEU:HG	1.80	0.63
1:A:756:GLU:N	1:A:756:GLU:OE2	2.33	0.62
1:A:225:LYS:NZ	1:A:311:GLU:OE2	2.33	0.61
1:A:950:GLU:OE2	1:A:953:ARG:NH2	2.34	0.60
1:A:917:LYS:NZ	1:A:976:ASP:OD2	2.37	0.57
1:A:937:ASN:O	1:A:939:ASP:N	2.39	0.56
1:A:807:ARG:HG3	1:A:810:LEU:HD12	1.87	0.55
1:A:224:MSE:HB3	1:A:311:GLU:HG3	1.89	0.55
1:A:990:GLU:OE2	1:A:1033:ARG:NH2	2.40	0.54
1:A:227:MSE:HG2	1:A:315:TRP:CZ2	2.43	0.54
1:A:316:MSE:HE1	1:A:329:LEU:CG	2.40	0.51
1:A:811:GLU:N	1:A:812:PRO:CD	2.74	0.51
1:A:676:GLY:O	1:A:677:GLU:HG3	2.12	0.50
1:A:374:ARG:HG3	1:A:378:MSE:HE2	1.95	0.48
1:A:693:ARG:NH2	4:A:1201:HOH:O	2.45	0.48
1:A:122:ILE:HG21	1:A:148:MSE:CE	2.43	0.48
1:A:197:MSE:HE2	1:A:284:MSE:HE3	1.94	0.48
1:A:213:ARG:NH2	2:B:327:ASP:OD1	2.43	0.48
1:A:183:VAL:HG21	1:A:226:LEU:HD12	1.96	0.48
1:A:862:ARG:NH2	1:A:898:ASP:OD1	2.47	0.47
1:A:989:GLY:H	1:A:990:GLU:HA	1.80	0.47
1:A:243:ASN:OD1	1:A:246:ARG:NH2	2.45	0.46
1:A:90:MSE:O	1:A:91:GLY:C	2.54	0.46
1:A:609:LEU:HD21	1:A:646:ILE:HG23	1.97	0.46
1:A:919:LEU:HD21	1:A:955:PHE:HB3	1.97	0.46
2:B:349:THR:OG1	2:B:350:THR:N	2.49	0.45
1:A:591:LEU:HB2	1:A:592:PRO:HD3	1.97	0.45
1:A:898:ASP:OD1	1:A:898:ASP:N	2.49	0.45
1:A:329:LEU:HD13	1:A:367:PHE:CG	2.52	0.44
1:A:382:LYS:NZ	2:B:346:ASP:O	2.50	0.44
1:A:958:THR:O	1:A:958:THR:HG22	2.18	0.44
1:A:987:PRO:O	1:A:991:SER:OG	2.36	0.43
1:A:753:SER:N	1:A:809:MSE:HE1	2.32	0.43
1:A:807:ARG:CG	1:A:810:LEU:HD12	2.47	0.43
1:A:359:GLU:HB3	1:A:360:LEU:CA	2.49	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:316:MSE:HE1	1:A:329:LEU:CD2	2.49	0.43
1:A:231:VAL:HG22	1:A:285:MSE:HE3	2.00	0.42
1:A:335:THR:HG22	1:A:343:VAL:HG12	2.00	0.42
2:B:394:THR:HG21	2:B:395:PRO:HD2	2.01	0.42
1:A:359:GLU:HB3	1:A:360:LEU:HA	2.01	0.42
1:A:1039:LEU:N	1:A:1040:PRO:CD	2.83	0.42
1:A:298:ARG:NH2	2:B:331:GLU:OE1	2.50	0.42
1:A:1010:LEU:HD23	1:A:1011:LEU:HB2	2.01	0.42
1:A:678:GLU:HB3	1:A:680:ASP:N	2.35	0.41
1:A:309:ILE:HG13	1:A:335:THR:HG21	2.01	0.41
1:A:890:MSE:HE2	1:A:950:GLU:HG3	2.01	0.41
1:A:1026:MSE:HE2	1:A:1031:SER:HB2	2.02	0.41
1:A:129:GLY:C	1:A:148:MSE:HE1	2.41	0.41
1:A:678:GLU:N	1:A:679:PRO:HA	2.35	0.41
1:A:803:MSE:CA	1:A:807:ARG:HB2	2.50	0.41
1:A:807:ARG:HD2	1:A:810:LEU:CD1	2.51	0.41
1:A:643:GLU:HG2	1:A:643:GLU:O	2.22	0.40
1:A:677:GLU:OE1	1:A:677:GLU:N	2.54	0.40
1:A:1010:LEU:HB3	1:A:1011:LEU:HB2	2.04	0.40
1:A:727:GLU:O	1:A:731:ILE:HG12	2.20	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	883/981 (90%)	856 (97%)	25 (3%)	2 (0%)	56	88
2	B	73/140 (52%)	72 (99%)	1 (1%)	0	100	100
All	All	956/1121 (85%)	928 (97%)	26 (3%)	2 (0%)	56	88

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	938	PHE
1	A	727	GLU

### 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	819/843 (97%)	800 (98%)	19 (2%)	63	91
2	B	70/125 (56%)	68 (97%)	2 (3%)	55	88
All	All	889/968 (92%)	868 (98%)	21 (2%)	61	91

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	294	VAL
1	A	296	ARG
1	A	298	ARG
1	A	319	TYR
1	A	325	ASN
1	A	327	SER
1	A	474	HIS
1	A	535	CYS
1	A	636	TYR
1	A	669	LEU
1	A	699	ASN
1	A	708	LEU
1	A	724	ASP
1	A	737	THR
1	A	754	THR
1	A	809	MSE
1	A	818	ASP
1	A	827	SER
1	A	1019	TYR
2	B	336	THR
2	B	337	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	656	GLN
1	A	1046	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	MES	A	1101	-	12,12,12	2.14	1 (8%)	16,16,16	1.74	3 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	A	1101	-	-	0/6/14/14	1/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1101	MES	C8-S	-6.54	1.67	1.78

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1101	MES	C6-C5-N4	-3.91	104.99	109.97
3	A	1101	MES	C8-C7-N4	-2.81	107.33	112.53
3	A	1101	MES	C5-N4-C3	2.61	115.40	109.77

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1101	MES	C2-C3-C5-C6-N4-O1

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	905/981 (92%)	0.65	69 (7%) 14 16	12, 55, 116, 161	0
2	B	75/140 (53%)	0.41	3 (4%) 36 43	21, 41, 79, 112	0
All	All	980/1121 (87%)	0.63	72 (7%) 15 17	12, 54, 116, 161	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1010	LEU	7.9
1	A	967	ARG	6.3
1	A	965	LYS	5.9
1	A	809	MSE	5.5
1	A	673	LEU	5.5
1	A	810	LEU	4.9
1	A	808	ASP	4.8
1	A	966	THR	4.6
1	A	455	GLY	4.5
1	A	813	LEU	4.2
1	A	1012	ARG	4.2
1	A	597	LEU	4.2
1	A	261	ASN	4.1
1	A	854	LYS	4.0
1	A	674	GLN	3.9
1	A	676	GLY	3.8
1	A	675	GLU	3.7
1	A	936	TYR	3.6
2	B	321	LYS	3.5
1	A	167	GLN	3.5
1	A	678	GLU	3.4
1	A	1038	TRP	3.4
1	A	1011	LEU	3.3
1	A	835	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	404	VAL	3.2
1	A	982	PHE	3.1
1	A	308	CYS	3.1
1	A	969	ALA	3.1
1	A	938	PHE	3.1
1	A	599	ILE	2.9
1	A	912	LYS	2.9
1	A	600	TYR	2.9
1	A	758	LEU	2.9
1	A	913	ILE	2.9
1	A	970	ILE	2.9
1	A	792	CYS	2.9
1	A	694	ILE	2.8
1	A	769	CYS	2.8
1	A	262	GLU	2.8
1	A	89	LYS	2.8
2	B	323	LYS	2.6
1	A	1013	GLN	2.6
1	A	405	LEU	2.6
1	A	347	CYS	2.6
1	A	748	ILE	2.6
1	A	1014	ASP	2.5
1	A	959	PHE	2.5
1	A	855	ILE	2.4
1	A	341	GLY	2.4
1	A	1041	LEU	2.4
1	A	338	ASP	2.3
1	A	1032	LEU	2.3
1	A	987	PRO	2.3
1	A	971	ALA	2.3
1	A	1035	GLU	2.3
1	A	761	LEU	2.3
1	A	775	TYR	2.3
1	A	908	ARG	2.2
1	A	860	LYS	2.2
1	A	725	MSE	2.2
2	B	324	LEU	2.1
1	A	462	LYS	2.1
1	A	294	VAL	2.1
1	A	239	ILE	2.1
1	A	669	LEU	2.1
1	A	685	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	940	ARG	2.1
1	A	853	SER	2.1
1	A	303	GLU	2.0
1	A	244	THR	2.0
1	A	306	ALA	2.0
1	A	717	LYS	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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	MES	A	1101	12/12	0.52	4.67	40,52,83,97	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.