



# wwPDB X-ray Structure Validation Summary Report

Oct 6, 2022 – 01:11 PM EDT

PDB ID : 5XVP  
Title : E. fae Cas1-Cas2/prespacer/target ternary complex revealing the fully integrated states  
Authors : Xiao, Y.; Ng, S.; Nam, K.H.; Ke, A.  
Deposited on : 2017-06-28  
Resolution : 3.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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 : 2.31.2  
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) : 2.31.2

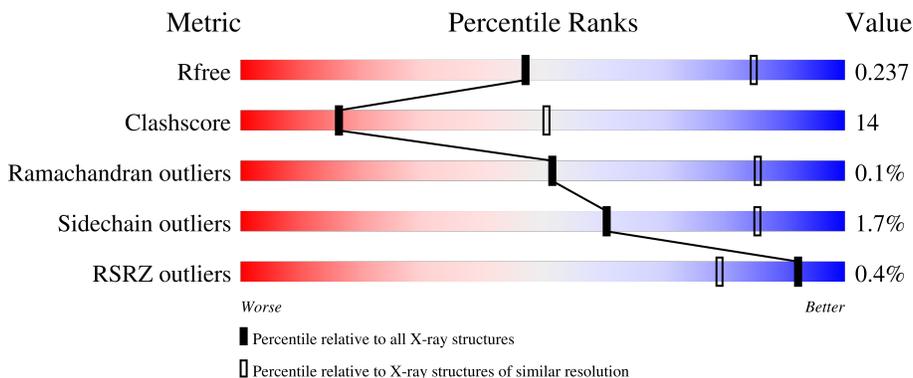
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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  $\geq 3$ , 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	288	 66% 32% ..
1	B	288	 82% 17% .
1	C	288	 77% 22% .
1	D	288	 82% 17% .
2	E	109	 59% 35% . 5%

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Mol	Chain	Length	Quality of chain
2	F	109	
3	G	73	
4	H	73	
5	I	9	
5	J	9	

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 14393 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 CRISPR-associated endonuclease Cas1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	286	Total	C	N	O	S	0	0	0
			2346	1507	407	422	10			
1	B	288	Total	C	N	O	S	0	0	0
			2359	1515	409	425	10			
1	C	288	Total	C	N	O	S	0	0	0
			2358	1515	409	424	10			
1	D	288	Total	C	N	O	S	0	0	0
			2359	1515	409	425	10			

- Molecule 2 is a protein called CRISPR-associated endoribonuclease Cas2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	E	104	Total	C	N	O	S	0	0	0
			864	549	158	151	6			
2	F	102	Total	C	N	O	S	0	0	0
			852	541	156	149	6			

- Molecule 3 is a DNA chain called DNA (73-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	G	71	Total	C	N	O	P	0	0	0
			1448	691	260	426	71			

- Molecule 4 is a DNA chain called DNA (73-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
4	H	71	Total	C	N	O	P	0	0	0
			1459	695	265	428	71			

- Molecule 5 is a DNA chain called DNA (5'-D(P\*TP\*TP\*CP\*TP\*CP\*CP\*GP\*AP\*G)-3').

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace	
5	I	9	Total	C	N	O	P	0	0	0
			182	87	30	56	9			
5	J	8	Total	C	N	O	P	0	0	0
			162	77	28	49	8			

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	1	Total	Mg	0	0
			1	1		
6	F	1	Total	Mg	0	0
			1	1		

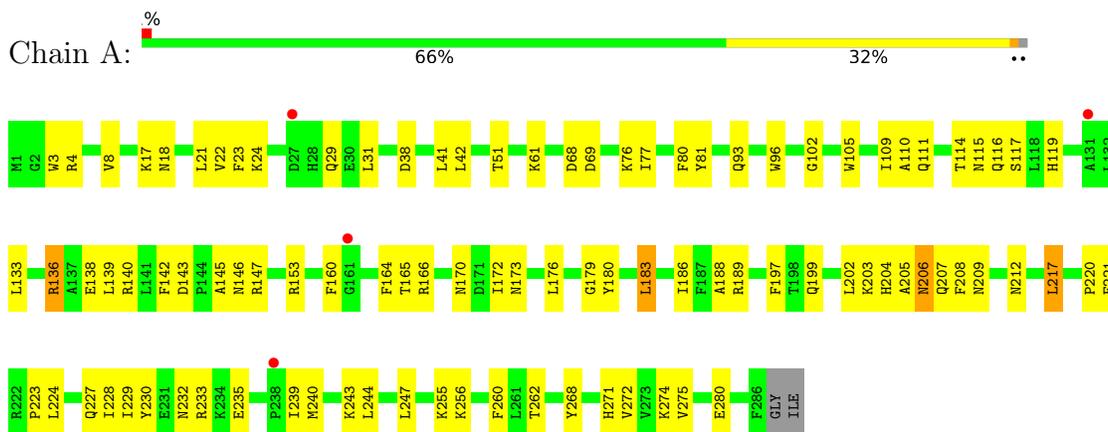
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	1	Total	O	0	0
			1	1		
7	I	1	Total	O	0	0
			1	1		

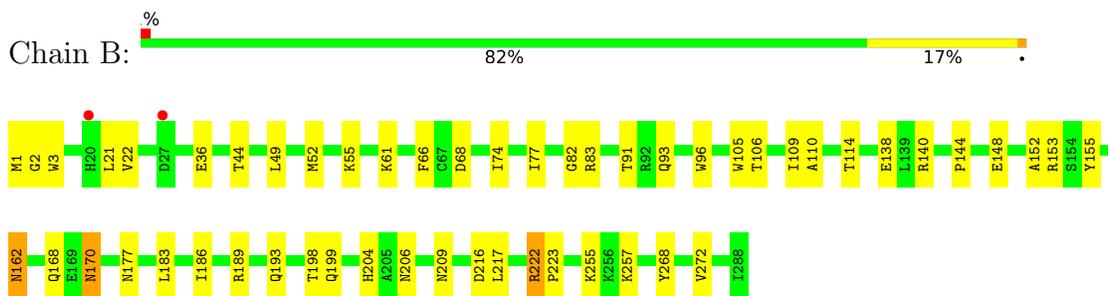
### 3 Residue-property plots

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.

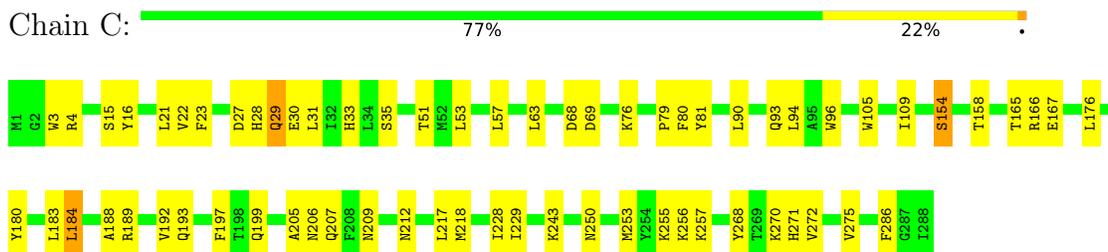
- Molecule 1: CRISPR-associated endonuclease Cas1



- Molecule 1: CRISPR-associated endonuclease Cas1

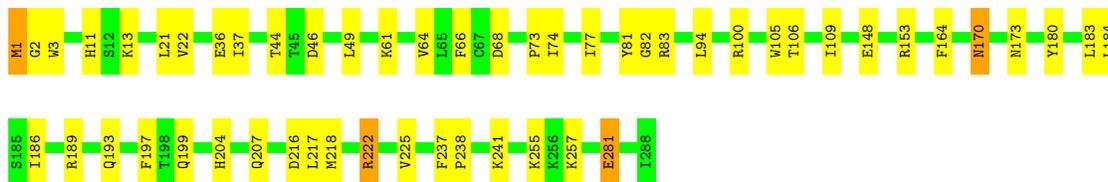


- Molecule 1: CRISPR-associated endonuclease Cas1



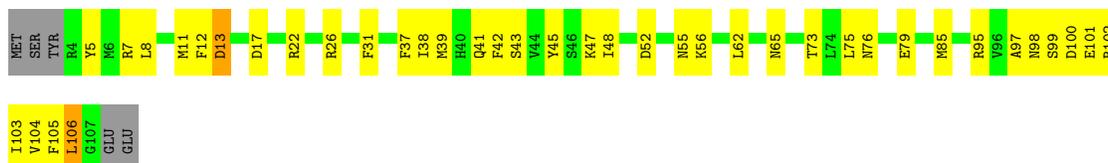
- Molecule 1: CRISPR-associated endonuclease Cas1





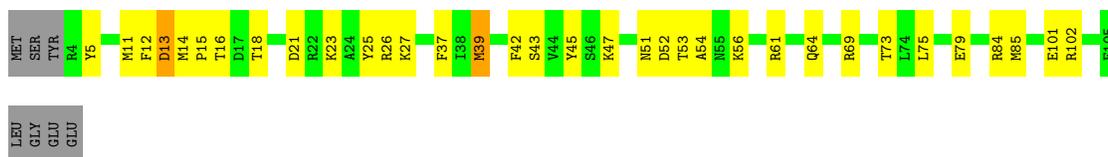
- Molecule 2: CRISPR-associated endoribonuclease Cas2

Chain E: 59% 35% 5%



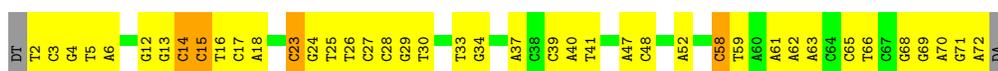
- Molecule 2: CRISPR-associated endoribonuclease Cas2

Chain F: 62% 29% 6%



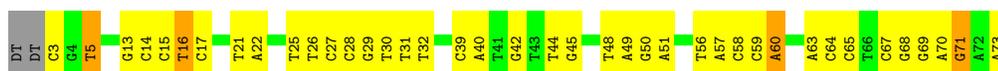
- Molecule 3: DNA (73-MER)

Chain G: 41% 51% 5%



- Molecule 4: DNA (73-MER)

Chain H: 42% 49% 5%



- Molecule 5: DNA (5'-D(P\*TP\*TP\*CP\*TP\*CP\*CP\*GP\*AP\*G)-3')

Chain I: 22% 67% 11%



- Molecule 5: DNA (5'-D(P\*TP\*TP\*CP\*TP\*CP\*CP\*GP\*AP\*G)-3')

Chain J: 22% 67% 11%

DT	T2	C3	T4	C5	C6	T7	A8	O9
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## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.87Å 212.29Å 512.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.03 – 3.00 49.03 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.03-3.00) 99.8 (49.03-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 3.01Å)	Xtrriage
Refinement program	REFMAC 5.8.0158	Depositor
R, $R_{free}$	0.194 , 0.233 0.199 , 0.237	Depositor DCC
$R_{free}$ test set	3549 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	68.4	Xtrriage
Anisotropy	0.578	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 66.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.39$ , $\langle L^2 \rangle = 0.22$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	14393	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	72.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.33% 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

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

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	0.78	1/2394 (0.0%)	0.91	2/3231 (0.1%)
1	B	0.76	0/2407	0.85	2/3247 (0.1%)
1	C	0.71	0/2406	0.86	1/3247 (0.0%)
1	D	0.73	1/2407 (0.0%)	0.83	1/3247 (0.0%)
2	E	0.85	0/878	1.00	3/1175 (0.3%)
2	F	0.95	1/866 (0.1%)	1.02	1/1159 (0.1%)
3	G	0.66	0/1622	0.95	7/2499 (0.3%)
4	H	0.70	4/1636 (0.2%)	0.95	6/2524 (0.2%)
5	I	0.64	1/202 (0.5%)	0.85	0/309
5	J	0.97	1/180 (0.6%)	0.81	0/275
All	All	0.75	9/14998 (0.1%)	0.90	23/20913 (0.1%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	2	DT	P-OP1	7.97	1.62	1.49
4	H	71	DG	O3'-P	-6.08	1.53	1.61
5	I	5	DC	O3'-P	-5.65	1.54	1.61
4	H	3	DC	P-OP2	5.62	1.58	1.49
1	A	136	ARG	CZ-NH1	-5.53	1.25	1.33

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	16	DT	O5'-P-OP1	-8.72	97.86	105.70
1	A	136	ARG	NE-CZ-NH2	8.08	124.34	120.30
1	C	184	LEU	CA-CB-CG	7.50	132.56	115.30
4	H	5	DT	O5'-P-OP1	-6.92	99.47	105.70
3	G	39	DC	C1'-O4'-C4'	-6.78	103.32	110.10

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	A	2346	0	2372	118	0
1	B	2359	0	2386	51	0
1	C	2358	0	2386	59	0
1	D	2359	0	2386	42	0
2	E	864	0	883	41	0
2	F	852	0	869	39	0
3	G	1448	0	801	44	0
4	H	1459	0	802	40	0
5	I	182	0	103	12	0
5	J	162	0	91	8	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
7	D	1	0	0	0	0
7	I	1	0	0	0	0
All	All	14393	0	13079	395	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 14.

The worst 5 of 395 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:114:THR:HB	1:A:136:ARG:NH1	1.14	1.42
1:A:114:THR:CB	1:A:136:ARG:HH12	1.39	1.33
1:A:110:ALA:C	1:A:136:ARG:NH2	2.02	1.12
1:A:114:THR:CB	1:A:136:ARG:NH1	2.04	1.09
1:B:109:ILE:HD11	1:B:148:GLU:HB2	1.33	1.08

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	284/288 (99%)	262 (92%)	21 (7%)	1 (0%)	34	72
1	B	286/288 (99%)	265 (93%)	21 (7%)	0	100	100
1	C	286/288 (99%)	265 (93%)	21 (7%)	0	100	100
1	D	286/288 (99%)	270 (94%)	16 (6%)	0	100	100
2	E	102/109 (94%)	92 (90%)	10 (10%)	0	100	100
2	F	100/109 (92%)	93 (93%)	7 (7%)	0	100	100
All	All	1344/1370 (98%)	1247 (93%)	96 (7%)	1 (0%)	51	85

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	ASN

### 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	254/255 (100%)	251 (99%)	3 (1%)	71	90
1	B	255/255 (100%)	251 (98%)	4 (2%)	62	86
1	C	255/255 (100%)	251 (98%)	4 (2%)	62	86
1	D	255/255 (100%)	249 (98%)	6 (2%)	49	79
2	E	94/99 (95%)	91 (97%)	3 (3%)	39	74
2	F	93/99 (94%)	92 (99%)	1 (1%)	73	90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1206/1218 (99%)	1185 (98%)	21 (2%)	60 85

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	207	GLN
2	E	17	ASP
2	F	39	MET
2	E	48	ILE
1	D	241	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	250	ASN
1	D	258	GLN
1	D	212	ASN
2	E	65	ASN
1	B	162	ASN

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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 [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	286/288 (99%)	-0.06	4 (1%) 75 49	41, 92, 130, 160	0
1	B	288/288 (100%)	-0.37	2 (0%) 87 69	31, 76, 105, 151	0
1	C	288/288 (100%)	-0.51	0 100 100	31, 66, 93, 108	0
1	D	288/288 (100%)	-0.55	0 100 100	40, 64, 96, 136	0
2	E	104/109 (95%)	-0.63	0 100 100	26, 55, 75, 92	0
2	F	102/109 (93%)	-0.68	0 100 100	22, 54, 80, 96	0
3	G	71/73 (97%)	-0.56	0 100 100	37, 69, 114, 141	0
4	H	71/73 (97%)	-0.59	0 100 100	33, 66, 98, 110	0
5	I	9/9 (100%)	-0.36	0 100 100	52, 61, 82, 104	0
5	J	8/9 (88%)	-0.57	0 100 100	55, 75, 115, 118	0
All	All	1515/1534 (98%)	-0.43	6 (0%) 92 79	22, 69, 113, 160	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	27	ASP	3.0
1	B	20	HIS	2.8
1	A	238	PRO	2.3
1	A	131	ALA	2.1
1	A	161	GLY	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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

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. 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	MG	E	201	1/1	0.97	0.22	56,56,56,56	0
6	MG	F	201	1/1	0.98	0.10	32,32,32,32	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.