



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 02:01 PM GMT

PDB ID : 3VS8  
Title : Crystal structure of type III PKS ArsC  
Authors : Satou, R.; Miyanaga, A.; Ozawa, H.; Funa, N.; Miyazono, K.; Tanokura, M.;  
Ohnishi, Y.; Horinouchi, S.  
Deposited on : 2012-04-23  
Resolution : 1.76 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  
<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  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865



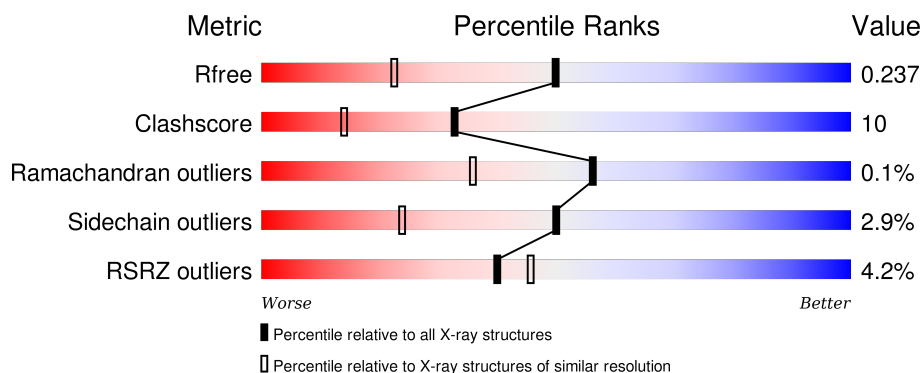
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.76 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))
$R_{free}$	91344	1609 (1.76-1.76)
Clashscore	102246	1730 (1.76-1.76)
Ramachandran outliers	100387	1711 (1.76-1.76)
Sidechain outliers	100360	1711 (1.76-1.76)
RSRZ outliers	91569	1610 (1.76-1.76)

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	A	410	<div> <div>5%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>
1	B	410	<div> <div>5%</div> <div>77%</div> <div>19%</div> <div>..</div> </div>
1	C	410	<div> <div>4%</div> <div>81%</div> <div>16%</div> <div>..</div> </div>
1	D	410	<div> <div>4%</div> <div>82%</div> <div>14%</div> <div>..</div> </div>
1	E	410	<div> <div>2%</div> <div>83%</div> <div>13%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	410	<div><div></div><div>2%</div><div>82%</div><div>15%</div><div>••</div></div>
1	G	410	<div><div></div><div>5%</div><div>79%</div><div>15%</div><div>••</div></div>
1	H	410	<div><div></div><div>10%</div><div>74%</div><div>16%</div><div>•6%</div></div>



## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 27375 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 Type III polyketide synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3123	1984	542	582	15			
1	B	399	Total	C	N	O	S	0	0	0
			3084	1961	537	571	15			
1	C	402	Total	C	N	O	S	0	0	0
			3108	1973	540	580	15			
1	D	401	Total	C	N	O	S	0	0	0
			3100	1969	539	577	15			
1	E	401	Total	C	N	O	S	0	0	0
			3107	1976	539	577	15			
1	F	404	Total	C	N	O	S	0	0	0
			3123	1984	542	582	15			
1	G	398	Total	C	N	O	S	0	0	0
			3078	1958	536	569	15			
1	H	384	Total	C	N	O	S	0	0	0
			2968	1891	518	544	15			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		
2	E	1	Total	Na	0	0
			1	1		
2	H	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		
2	C	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Na 1	0	0
2	F	1	Total 1	Na 1	0	0

- Molecule 3 is water.

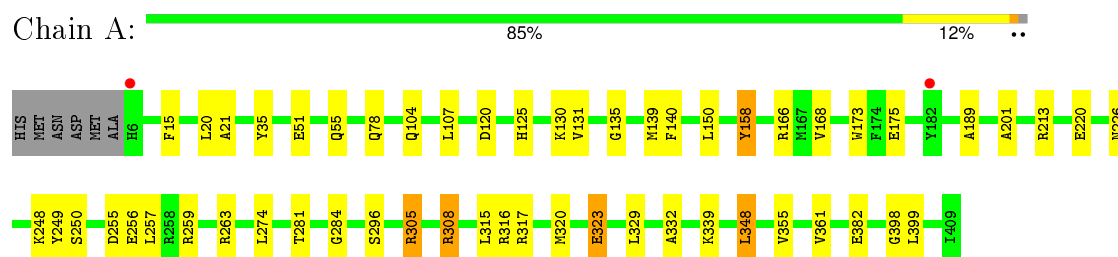
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	437	Total 437	O 437	0	0
3	B	258	Total 258	O 258	0	0
3	C	361	Total 361	O 361	0	0
3	D	356	Total 356	O 356	0	0
3	E	417	Total 417	O 417	0	0
3	F	330	Total 330	O 330	0	0
3	G	283	Total 283	O 283	0	0
3	H	234	Total 234	O 234	0	0



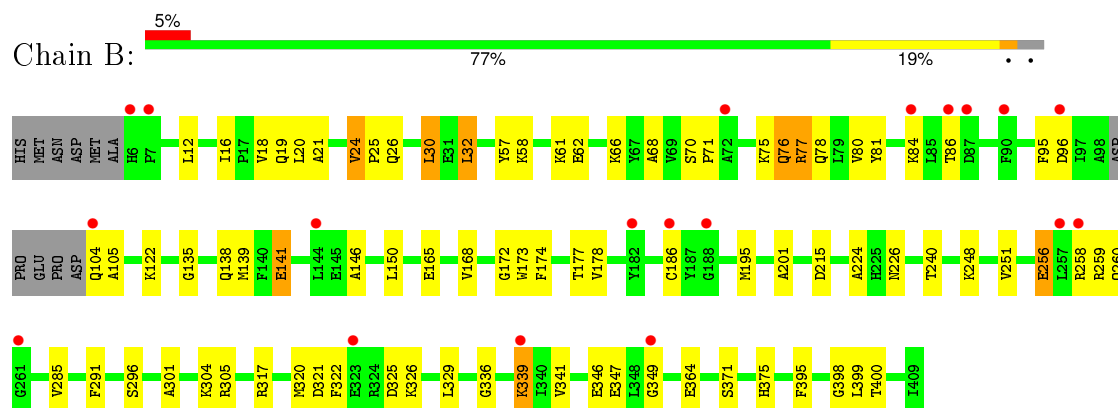
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

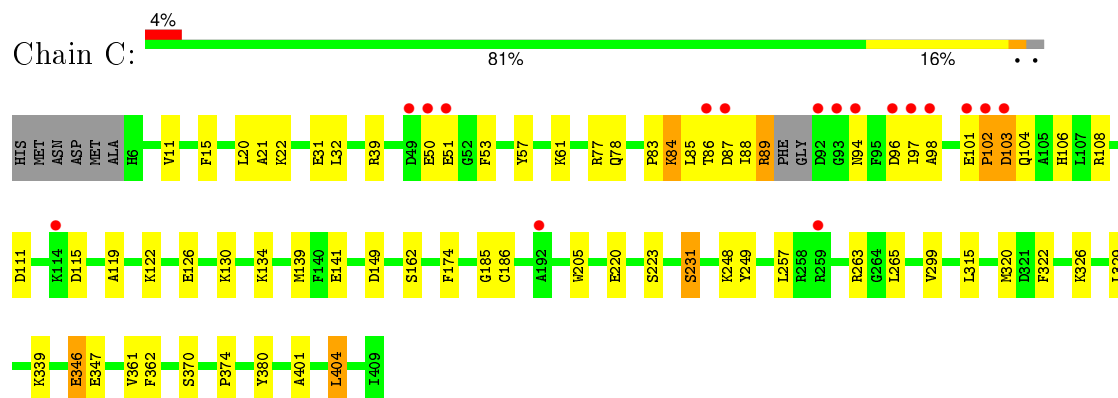
- Molecule 1: Type III polyketide synthase



- Molecule 1: Type III polyketide synthase

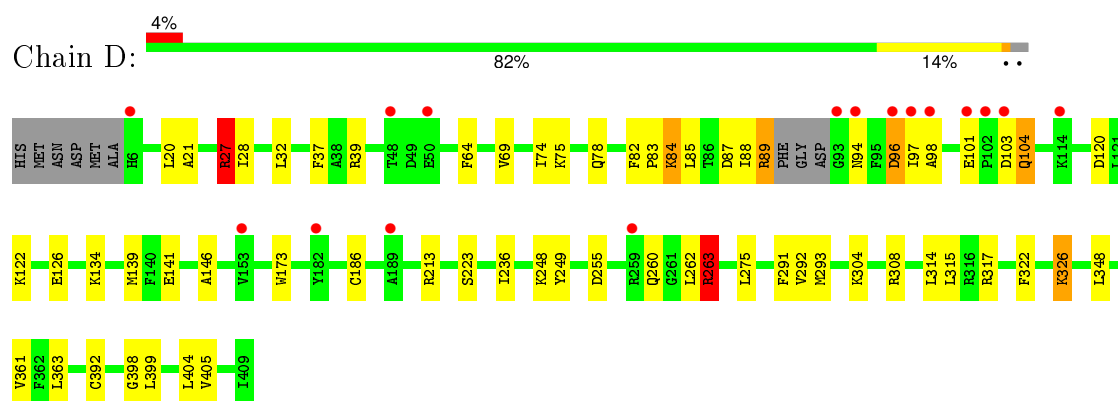


- Molecule 1: Type III polyketide synthase

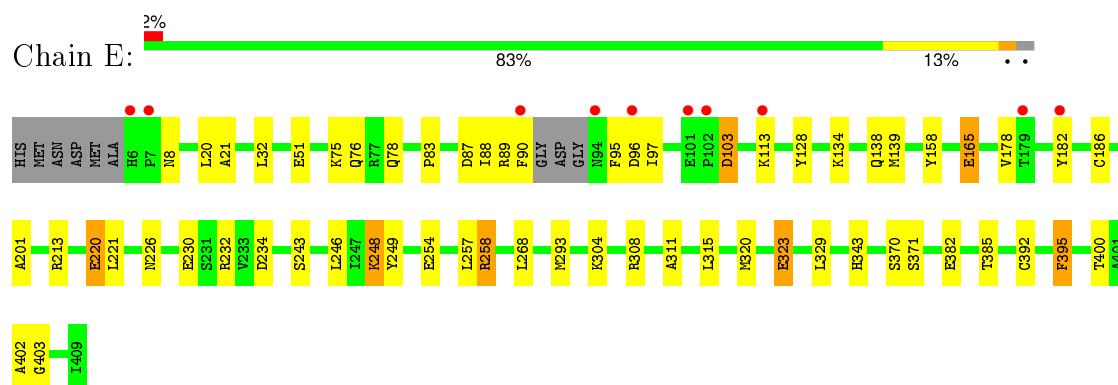


- Molecule 1: Type III polyketide synthase

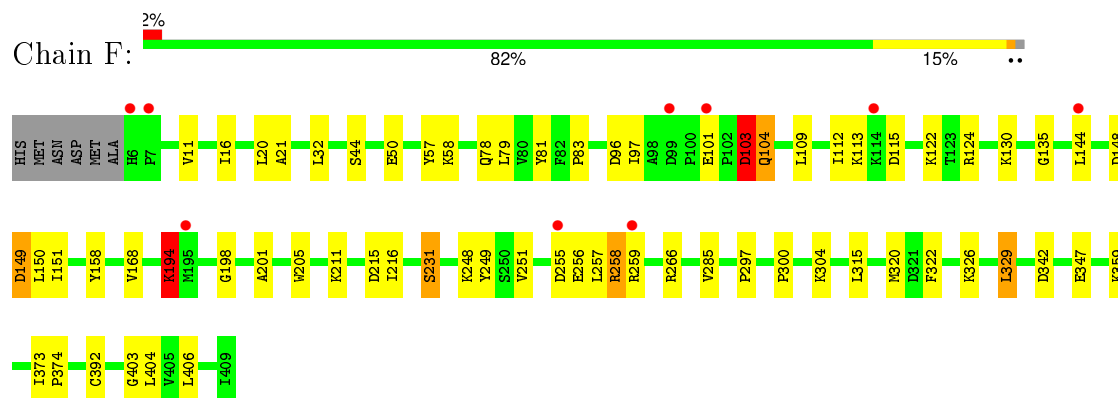




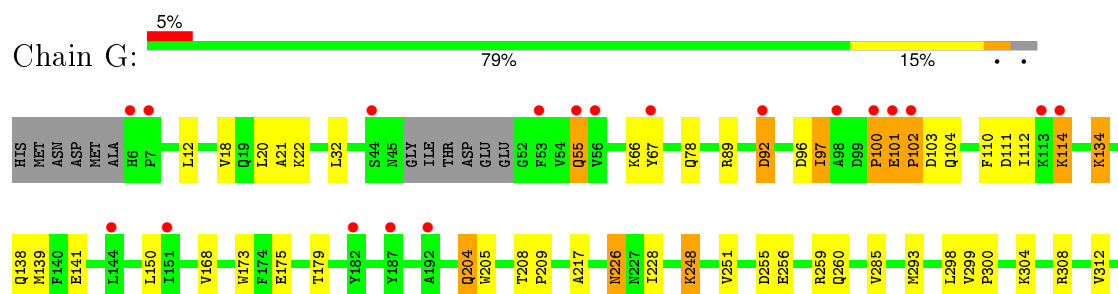
- Molecule 1: Type III polyketide synthase



- Molecule 1: Type III polyketide synthase



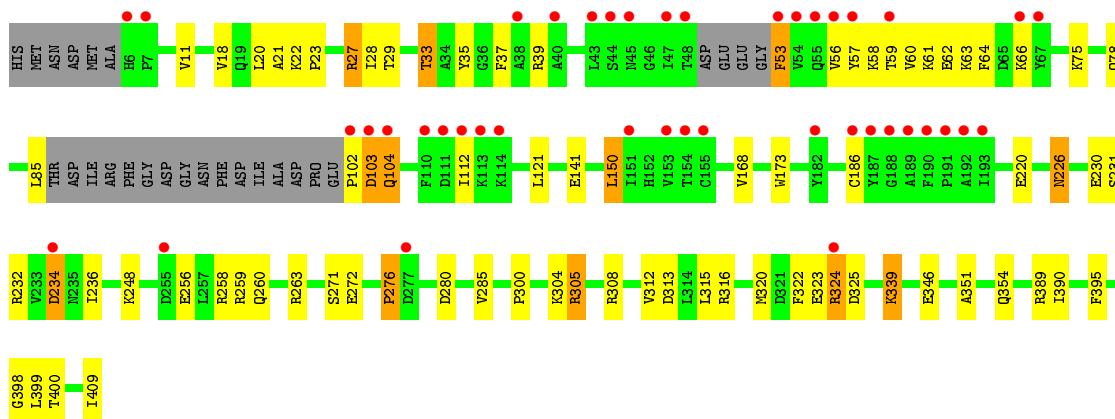
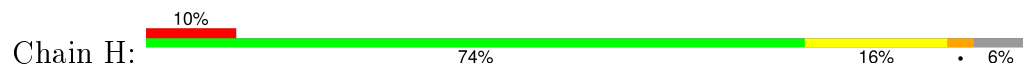
- Molecule 1: Type III polyketide synthase







• Molecule 1: Type III polyketide synthase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	102.32Å 143.39Å 129.62Å 90.00° 110.33° 90.00°	Depositor
Resolution (Å)	37.57 – 1.76 35.27 – 1.76	Depositor EDS
% Data completeness (in resolution range)	97.4 (37.57-1.76) 97.4 (35.27-1.76)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.75 (at 1.76Å)	Xtriage
Refinement program	REFMAC 5.5.0066	Depositor
R, $R_{free}$	0.183 , 0.230 0.194 , 0.237	Depositor DCC
$R_{free}$ test set	16976 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	22.9	Xtriage
Anisotropy	0.179	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.8	EDS
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 335793 reflections (0.000%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	27375	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 72.42 % 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 2.2090e-06. 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.



## 5 Model quality

### 5.1 Standard geometry

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

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	1.36	14/3194 (0.4%)	1.17	13/4331 (0.3%)
1	B	1.18	6/3152 (0.2%)	1.07	8/4270 (0.2%)
1	C	1.25	16/3177 (0.5%)	1.08	6/4307 (0.1%)
1	D	1.25	6/3169 (0.2%)	1.11	13/4296 (0.3%)
1	E	1.32	14/3177 (0.4%)	1.11	13/4307 (0.3%)
1	F	1.22	11/3194 (0.3%)	1.04	5/4331 (0.1%)
1	G	1.05	0/3148	0.98	2/4267 (0.0%)
1	H	1.08	3/3034 (0.1%)	0.99	5/4110 (0.1%)
All	All	1.22	70/25245 (0.3%)	1.07	65/34219 (0.2%)

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	F	0	1
1	G	0	2
All	All	0	3

The worst 5 of 70 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	186	CYS	CB-SG	9.00	1.97	1.82
1	E	182	TYR	CD1-CE1	8.70	1.52	1.39
1	A	220	GLU	CB-CG	8.15	1.67	1.52
1	B	186	CYS	CB-SG	-8.04	1.68	1.82
1	E	186	CYS	CA-CB	7.44	1.70	1.53

The worst 5 of 65 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	27	ARG	NE-CZ-NH2	-15.83	112.38	120.30
1	B	77	ARG	NE-CZ-NH2	-12.60	114.00	120.30
1	D	27	ARG	NE-CZ-NH1	12.47	126.53	120.30
1	E	186	CYS	CA-CB-SG	-12.02	92.37	114.00
1	A	305	ARG	NE-CZ-NH1	11.49	126.05	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	103	ASP	Peptide
1	G	100	PRO	Peptide
1	G	92	ASP	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	A	3123	0	3112	30	0
1	B	3084	0	3083	86	0
1	C	3108	0	3099	72	0
1	D	3100	0	3095	55	0
1	E	3107	0	3101	42	0
1	F	3123	0	3112	66	0
1	G	3078	0	3074	77	0
1	H	2968	0	2986	97	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	437	0	0	8	1
3	B	258	0	0	13	0
3	C	361	0	0	8	1
3	D	356	0	0	13	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	417	0	0	9	0
3	F	330	0	0	13	0
3	G	283	0	0	11	0
3	H	234	0	0	7	0
All	All	27375	0	24662	514	2

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 10.

The worst 5 of 514 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:C:89:ARG:CB	1:C:96:ASP:HB3	1.55	1.35
1:C:89:ARG:HB2	1:C:96:ASP:CB	1.62	1.29
1:D:122:LYS:HD3	3:D:872:HOH:O	1.32	1.26
1:C:39:ARG:NH2	1:C:94:ASN:ND2	1.86	1.22
1:H:104:GLN:CA	1:H:104:GLN:HE21	1.51	1.22

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:864:HOH:O	3:D:864:HOH:O[1_655]	2.04	0.16
3:A:998:HOH:O	3:D:946:HOH:O[2_646]	2.16	0.04

## 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	402/410 (98%)	391 (97%)	11 (3%)	0	100	100
1	B	395/410 (96%)	381 (96%)	14 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	398/410 (97%)	386 (97%)	11 (3%)	1 (0%)	46	25
1	D	397/410 (97%)	385 (97%)	12 (3%)	0	100	100
1	E	397/410 (97%)	386 (97%)	11 (3%)	0	100	100
1	F	402/410 (98%)	389 (97%)	12 (3%)	1 (0%)	52	32
1	G	394/410 (96%)	376 (95%)	16 (4%)	2 (0%)	34	14
1	H	378/410 (92%)	360 (95%)	18 (5%)	0	100	100
All	All	3163/3280 (96%)	3054 (97%)	105 (3%)	4 (0%)	56	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	104	GLN
1	G	92	ASP
1	C	102	PRO
1	G	102	PRO

### 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	333/338 (98%)	328 (98%)	5 (2%)	72	55
1	B	328/338 (97%)	320 (98%)	8 (2%)	57	31
1	C	332/338 (98%)	320 (96%)	12 (4%)	42	16
1	D	331/338 (98%)	322 (97%)	9 (3%)	52	27
1	E	332/338 (98%)	323 (97%)	9 (3%)	52	27
1	F	333/338 (98%)	327 (98%)	6 (2%)	66	46
1	G	328/338 (97%)	315 (96%)	13 (4%)	38	14
1	H	317/338 (94%)	303 (96%)	14 (4%)	35	11
All	All	2634/2704 (97%)	2558 (97%)	76 (3%)	50	24

5 of 76 residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	E	32	LEU
1	E	385	THR
1	H	234	ASP
1	E	76	GLN
1	E	248	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	41	HIS
1	E	55	GLN
1	H	226	ASN
1	D	226	ASN
1	E	78	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](#)

Of 8 ligands modelled in this entry, 8 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 [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	404/410 (98%)	-0.19	2 (0%) 91 93	13, 21, 37, 48	0
1	B	399/410 (97%)	0.20	19 (4%) 34 39	21, 32, 52, 67	0
1	C	402/410 (98%)	0.08	17 (4%) 40 46	14, 23, 51, 79	0
1	D	401/410 (97%)	0.05	16 (3%) 42 48	14, 24, 53, 68	0
1	E	401/410 (97%)	-0.08	10 (2%) 61 67	13, 22, 46, 63	0
1	F	404/410 (98%)	-0.05	9 (2%) 65 72	18, 29, 45, 58	0
1	G	398/410 (97%)	0.17	19 (4%) 34 39	19, 31, 54, 68	0
1	H	384/410 (93%)	0.50	42 (10%) 7 9	19, 33, 63, 85	0
All	All	3193/3280 (97%)	0.08	134 (4%) 40 46	13, 27, 52, 85	0

The worst 5 of 134 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	102	PRO	7.0
1	D	102	PRO	6.5
1	H	53	PHE	5.5
1	F	144	LEU	5.4
1	H	56	VAL	5.4

### 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 [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. 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	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	NA	G	501	1/1	0.98	0.15	1.30	25,25,25,25	0
2	NA	F	501	1/1	0.99	0.15	0.95	27,27,27,27	0
2	NA	B	501	1/1	0.97	0.13	0.53	25,25,25,25	0
2	NA	H	501	1/1	0.98	0.14	0.53	28,28,28,28	0
2	NA	C	501	1/1	1.00	0.12	0.13	19,19,19,19	0
2	NA	E	501	1/1	1.00	0.12	-0.14	19,19,19,19	0
2	NA	D	501	1/1	1.00	0.11	-0.35	20,20,20,20	0
2	NA	A	501	1/1	0.99	0.09	-0.91	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.