



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 12, 2025 – 12:22 PM JST

PDB ID : 8YND  
Title : ATP-grasp peptide ligase from Streptomyces  
Authors : Xu, M.J.; Yan, Y.Q.  
Deposited on : 2024-03-11  
Resolution : 2.19 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)

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<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)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

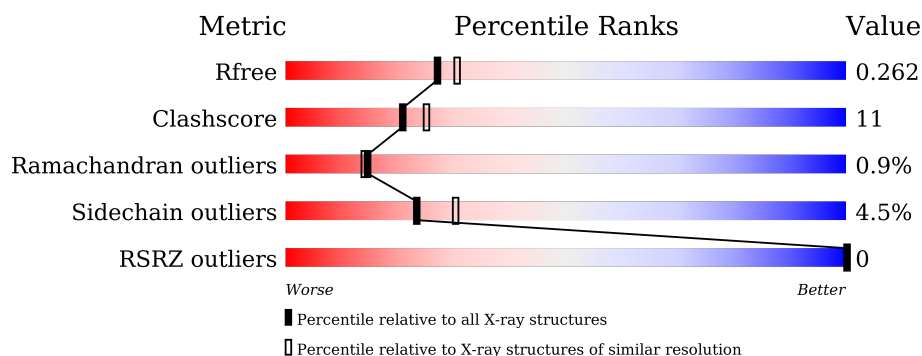
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.19 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))
$R_{free}$	164625	5791 (2.20-2.20)
Clashscore	180529	6634 (2.20-2.20)
Ramachandran outliers	177936	6560 (2.20-2.20)
Sidechain outliers	177891	6561 (2.20-2.20)
RSRZ outliers	164620	5791 (2.20-2.20)

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	448	
1	B	448	
1	C	448	
1	D	448	
1	E	448	
1	F	448	

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Mol	Chain	Length	Quality of chain
1	G	448	 69%21%8%
1	H	448	 75%16%8%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 27004 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 ATP-grasp peptide ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	414	Total	C	N	O	S	0	0	0
			3197	2014	553	622	8			
1	B	413	Total	C	N	O	S	0	0	0
			3183	2003	551	622	7			
1	C	408	Total	C	N	O	S	0	0	0
			3155	1988	544	615	8			
1	D	417	Total	C	N	O	S	0	0	0
			3217	2025	559	625	8			
1	E	415	Total	C	N	O	S	0	0	0
			3206	2018	556	625	7			
1	F	413	Total	C	N	O	S	0	0	0
			3191	2011	552	620	8			
1	G	414	Total	C	N	O	S	0	0	0
			3198	2013	555	623	7			
1	H	414	Total	C	N	O	S	0	0	0
			3202	2016	556	623	7			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	190	Total	O	0	0
			190	190		
2	B	167	Total	O	0	0
			167	167		
2	C	160	Total	O	0	0
			160	160		
2	D	159	Total	O	0	0
			159	159		
2	E	200	Total	O	0	0
			200	200		
2	F	190	Total	O	0	0
			190	190		

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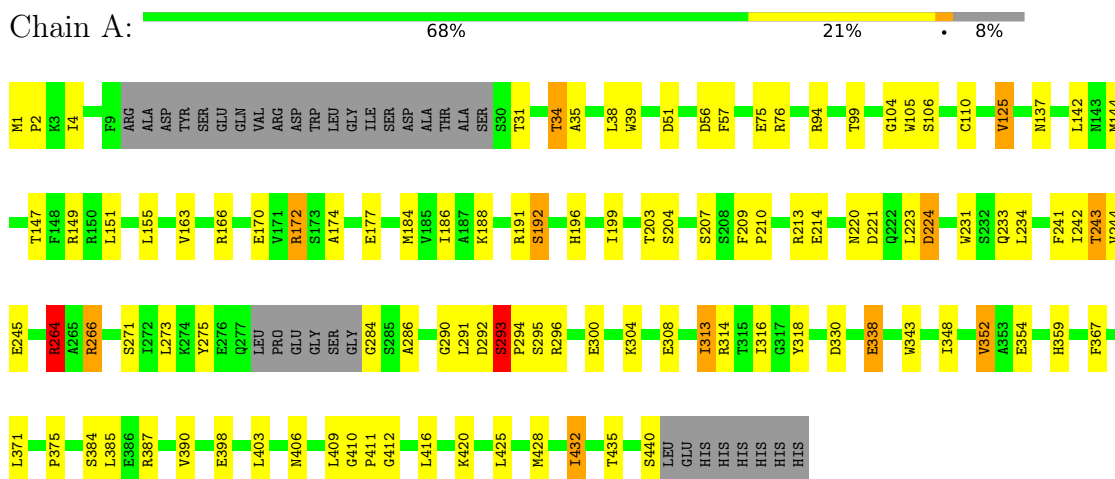
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	191	Total 191	O 191	0	0
2	H	198	Total 198	O 198	0	0

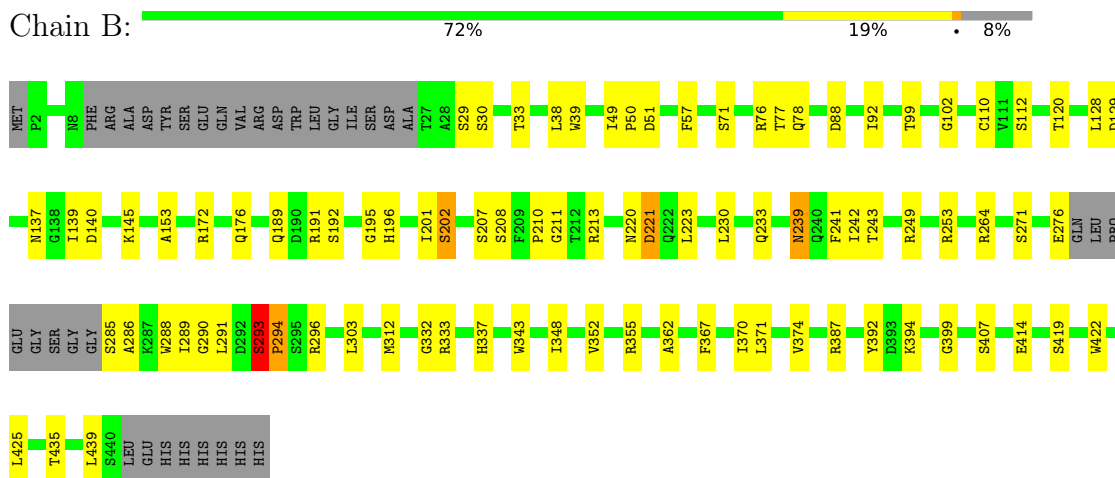
### 3 Residue-property plots [i](#)

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: ATP-grasp peptide ligase

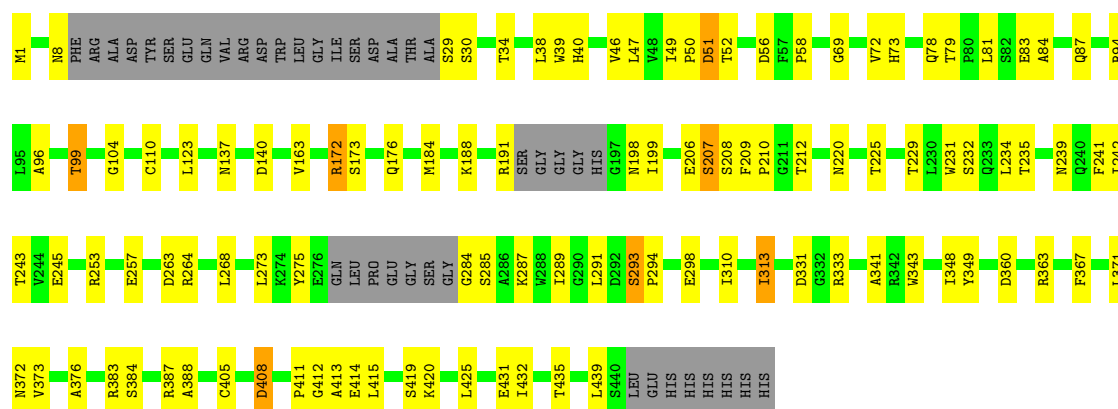


- Molecule 1: ATP-grasp peptide ligase



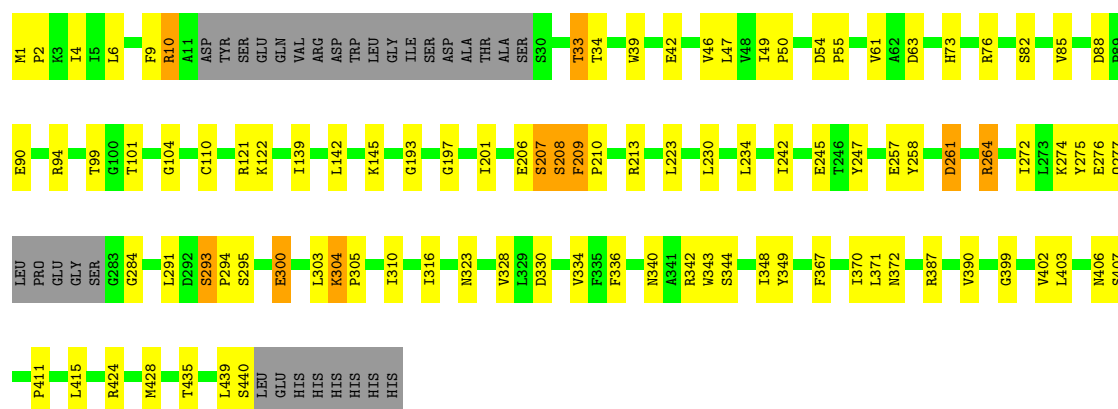
- Molecule 1: ATP-grasp peptide ligase





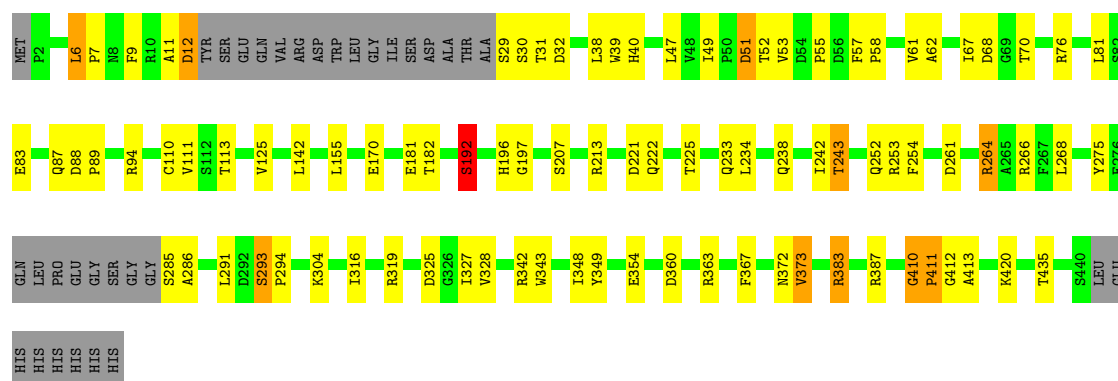
- Molecule 1: ATP-grasp peptide ligase

Chain D: 71% 20% 7%



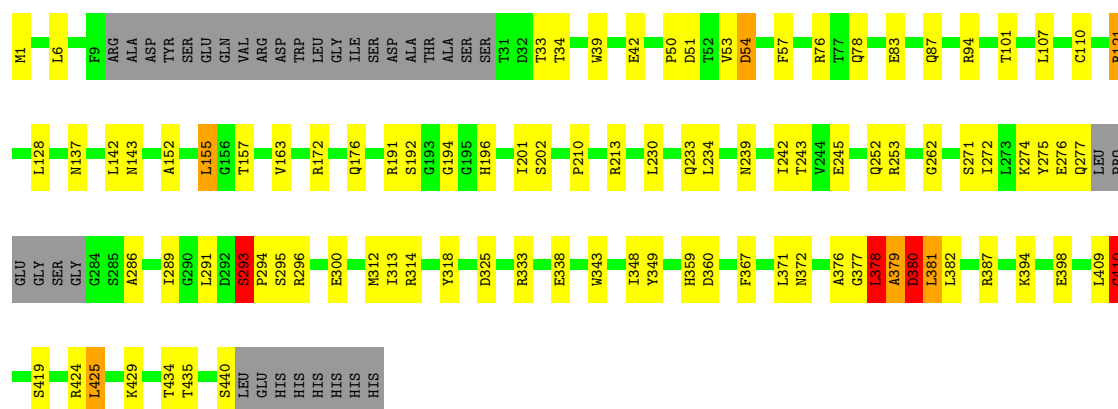
- Molecule 1: ATP-grasp peptide ligase

Chain E: 72% 18% 7%



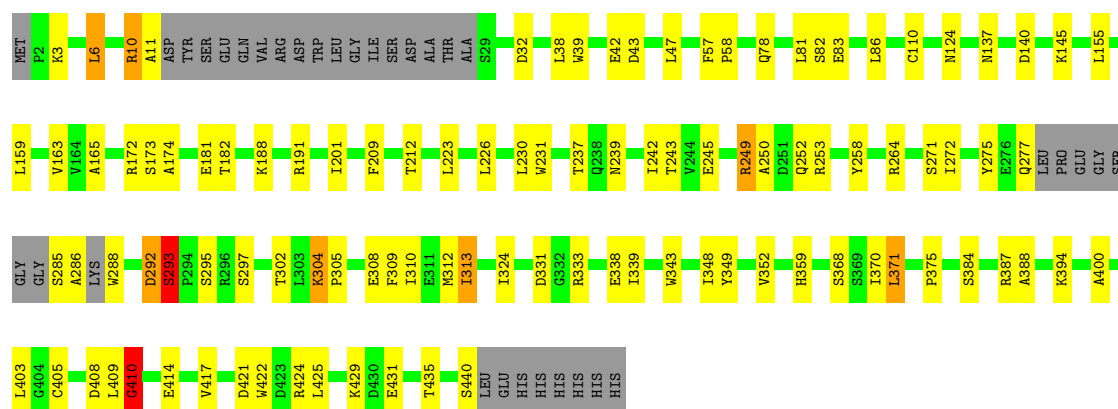
- Molecule 1: ATP-grasp peptide ligase

Chain F: 71% 19% 8%



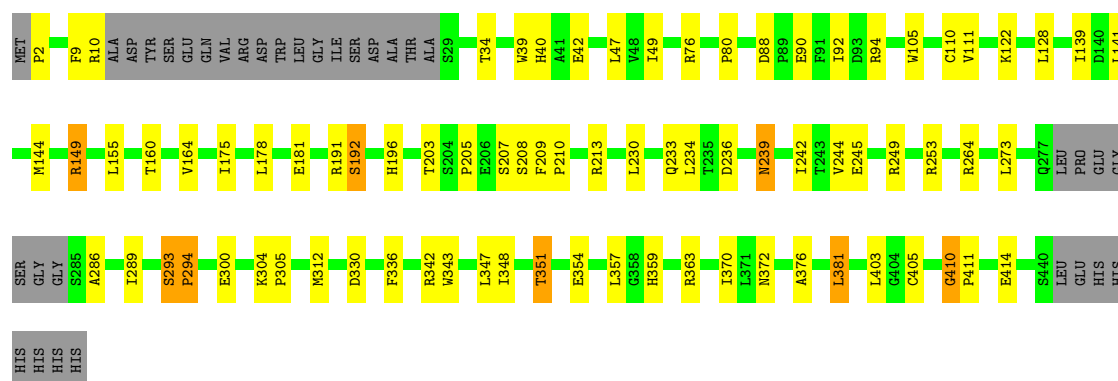
• Molecule 1: ATP-grasp peptide ligase

Chain G: 69% 21% 8%



• Molecule 1: ATP-grasp peptide ligase

Chain H: 75% 16% 8%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.93Å 100.64Å 131.56Å 99.54° 101.88° 115.94°	Depositor
Resolution (Å)	50.00 – 2.19 50.00 – 2.19	Depositor EDS
% Data completeness (in resolution range)	92.0 (50.00-2.19) 92.0 (50.00-2.19)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.77 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, $R_{free}$	0.211 , 0.263 0.213 , 0.262	Depositor DCC
$R_{free}$ test set	8851 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.8	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 29.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	27004	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.65% 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	A	0.45	0/3263	0.70	4/4431 (0.1%)
1	B	0.41	0/3248	0.67	1/4412 (0.0%)
1	C	0.42	0/3218	0.67	2/4370 (0.0%)
1	D	0.40	0/3283	0.66	2/4457 (0.0%)
1	E	0.44	1/3272 (0.0%)	0.69	2/4443 (0.0%)
1	F	0.44	1/3257 (0.0%)	0.68	1/4423 (0.0%)
1	G	0.43	0/3263	0.66	0/4430
1	H	0.41	0/3268	0.69	2/4437 (0.0%)
All	All	0.42	2/26072 (0.0%)	0.68	14/35403 (0.0%)

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	A	0	4
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	2
1	F	0	3
1	G	0	4
1	H	0	2
All	All	0	19

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	383	ARG	CG-CD	-6.97	1.34	1.51
1	F	293	SER	C-N	5.16	1.44	1.34

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	383	ARG	CB-CG-CD	-11.38	82.02	111.60
1	D	293	SER	C-N-CD	-9.85	98.92	120.60
1	H	410	GLY	C-N-CD	-9.30	100.15	120.60
1	H	293	SER	C-N-CD	-8.24	102.48	120.60
1	A	266	ARG	CD-NE-CZ	7.42	134.00	123.60

There are no chirality outliers.

5 of 19 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	MET	Peptide
1	A	293	SER	Peptide
1	A	371	LEU	Peptide
1	A	410	GLY	Peptide
1	B	293	SER	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	3197	0	3104	72	2
1	B	3183	0	3090	65	0
1	C	3155	0	3070	81	1
1	D	3217	0	3125	68	0
1	E	3206	0	3109	64	0
1	F	3191	0	3099	79	0
1	G	3198	0	3099	68	0
1	H	3202	0	3108	59	1
2	A	190	0	0	16	2
2	B	167	0	0	22	0
2	C	160	0	0	22	4
2	D	159	0	0	19	3
2	E	200	0	0	24	0
2	F	190	0	0	23	0
2	G	191	0	0	10	1
2	H	198	0	0	17	2
All	All	27004	0	24804	550	8

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 11.

The worst 5 of 550 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:E:213:ARG:NH1	2:E:501:HOH:O	1.86	1.09
1:E:383:ARG:NH2	2:E:502:HOH:O	1.87	1.06
1:F:176:GLN:NE2	2:F:504:HOH:O	1.93	0.99
1:G:181:GLU:OE1	2:G:501:HOH:O	1.81	0.96
1:D:49:ILE:HD11	1:D:76:ARG:HG2	1.47	0.94

The worst 5 of 8 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)
2:A:648:HOH:O	2:H:678:HOH:O[1_554]	1.91	0.29
1:A:304:LYS:NZ	1:C:263:ASP:OD2[1_455]	1.97	0.23
2:A:679:HOH:O	2:C:618:HOH:O[1_455]	2.07	0.13
2:C:572:HOH:O	2:D:579:HOH:O[1_545]	2.07	0.13
2:C:660:HOH:O	2:D:653:HOH:O[1_545]	2.08	0.12

## 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	408/448 (91%)	386 (95%)	18 (4%)	4 (1%)	13	12
1	B	407/448 (91%)	386 (95%)	18 (4%)	3 (1%)	19	19
1	C	400/448 (89%)	380 (95%)	18 (4%)	2 (0%)	25	28
1	D	411/448 (92%)	390 (95%)	16 (4%)	5 (1%)	11	9
1	E	409/448 (91%)	392 (96%)	13 (3%)	4 (1%)	13	12
1	F	407/448 (91%)	384 (94%)	18 (4%)	5 (1%)	11	9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	406/448 (91%)	392 (97%)	13 (3%)	1 (0%)	44	52
1	H	408/448 (91%)	392 (96%)	12 (3%)	4 (1%)	13	12
All	All	3256/3584 (91%)	3102 (95%)	126 (4%)	28 (1%)	14	14

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	192	SER
1	A	294	PRO
1	B	51	ASP
1	B	294	PRO
1	C	294	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	337/365 (92%)	319 (95%)	18 (5%)	19	24
1	B	336/365 (92%)	323 (96%)	13 (4%)	27	37
1	C	334/365 (92%)	321 (96%)	13 (4%)	27	37
1	D	338/365 (93%)	323 (96%)	15 (4%)	24	31
1	E	338/365 (93%)	325 (96%)	13 (4%)	28	37
1	F	336/365 (92%)	318 (95%)	18 (5%)	18	23
1	G	337/365 (92%)	319 (95%)	18 (5%)	19	24
1	H	338/365 (93%)	324 (96%)	14 (4%)	26	34
All	All	2694/2920 (92%)	2572 (96%)	122 (4%)	23	30

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	304	LYS
1	H	155	LEU

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Mol	Chain	Res	Type
1	E	373	VAL
1	H	149	ARG
1	H	330	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 11 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	189	GLN
1	F	323	ASN
1	H	372	ASN
1	H	359	HIS
1	B	239	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 oligosaccharides 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	A	414/448 (92%)	-1.52	0 100 100	19, 31, 56, 73	0
1	B	413/448 (92%)	-1.46	0 100 100	21, 34, 55, 78	0
1	C	408/448 (91%)	-1.49	0 100 100	20, 34, 54, 76	0
1	D	417/448 (93%)	-1.47	0 100 100	21, 34, 57, 78	0
1	E	415/448 (92%)	-1.47	0 100 100	19, 34, 58, 74	0
1	F	413/448 (92%)	-1.52	0 100 100	18, 31, 47, 63	0
1	G	414/448 (92%)	-1.49	0 100 100	21, 32, 55, 98	0
1	H	414/448 (92%)	-1.48	0 100 100	19, 32, 56, 73	0
All	All	3308/3584 (92%)	-1.49	0 100 100	18, 33, 55, 98	0

There are no RSRZ outliers to report.

### 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](#)

There are no ligands in this entry.

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

There are no such residues in this entry.