



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 04:20 am GMT

PDB ID : 2P1I  
Title : Plasmodium yoelii Ribonucleotide Reductase Subunit R2 (PY03671)  
Authors : Wernimont, A.K.; Dong, A.; Choe, J.; Gao, M.; Walker, J.; Lew, J.; Alam, Z.; Zhao, Y.; Nordlund, P.; Arrowsmith, C.H.; Edwards, A.M.; Weigelt, J.; Sundstrom, M.; Bochkarev, A.; Hui, R.; Artz, J.D.; Structural Genomics Consortium (SGC)  
Deposited on : 2007-03-05  
Resolution : 2.70 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
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

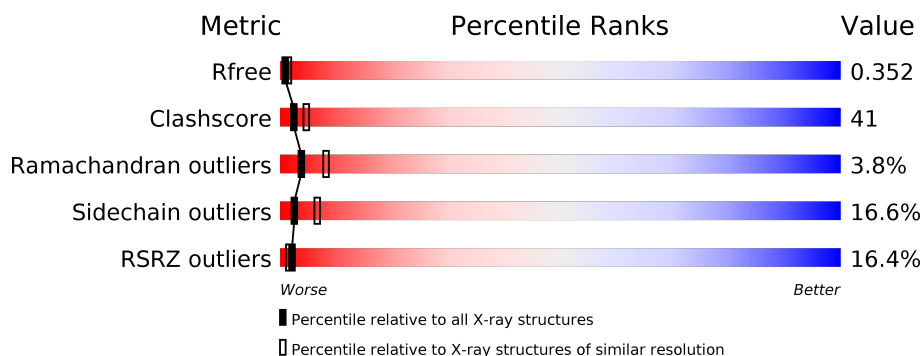
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2259 (2.70-2.70)
Clashscore	112137	2590 (2.70-2.70)
Ramachandran outliers	110173	2550 (2.70-2.70)
Sidechain outliers	110143	2550 (2.70-2.70)
RSRZ outliers	101464	2275 (2.70-2.70)

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	349	<div> <div>7%</div> <div> <div>30%</div> <div>35%</div> <div>8%</div> <div>26%</div> </div> </div>
1	B	349	<div> <div>14%</div> <div> <div>28%</div> <div>32%</div> <div>10%</div> <div>28%</div> </div> </div>
1	C	349	<div> <div>16%</div> <div> <div>24%</div> <div>38%</div> <div>10%</div> <div>27%</div> </div> </div>
1	D	349	<div> <div>6%</div> <div> <div>31%</div> <div>34%</div> <div>8%</div> <div>26%</div> </div> </div>
1	E	349	<div> <div>13%</div> <div> <div>27%</div> <div>37%</div> <div>8%</div> <div>26%</div> </div> </div>
1	F	349	<div> <div>12%</div> <div> <div>33%</div> <div>33%</div> <div>7%</div> <div>26%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	349	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>15%27%34%9%28%</div></div>
1	H	349	<div><div><div></div><div></div><div></div><div></div><div></div></div><div>13%28%34%10%26%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16904 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 Ribonucleotide reductase, small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total	C	N	O	S	0	0	0
			2104	1364	343	387	10			
1	B	252	Total	C	N	O	S	0	0	0
			2056	1332	335	379	10			
1	C	256	Total	C	N	O	S	0	0	0
			2099	1361	343	385	10			
1	D	258	Total	C	N	O	S	0	0	0
			2116	1372	345	389	10			
1	E	258	Total	C	N	O	S	0	0	0
			2109	1367	344	388	10			
1	F	258	Total	C	N	O	S	0	0	0
			2116	1372	345	389	10			
1	G	252	Total	C	N	O	S	0	0	0
			2059	1340	333	376	10			
1	H	258	Total	C	N	O	S	0	0	0
			2116	1372	345	389	10			

- Molecule 2 is FE (III) ION (three-letter code: FE) (formula: Fe).

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

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

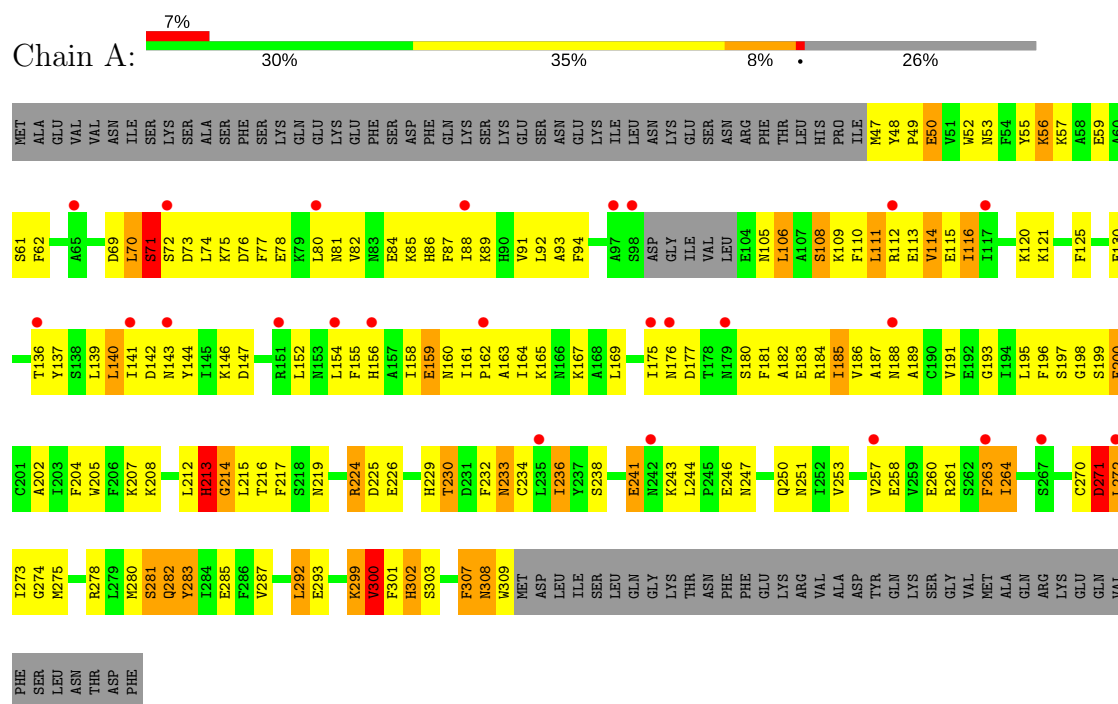
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total 19	O 19	0	0
3	B	11	Total 11	O 11	0	0
3	C	13	Total 13	O 13	0	0
3	D	18	Total 18	O 18	0	0
3	E	15	Total 15	O 15	0	0
3	F	15	Total 15	O 15	0	0
3	G	19	Total 19	O 19	0	0
3	H	11	Total 11	O 11	0	0

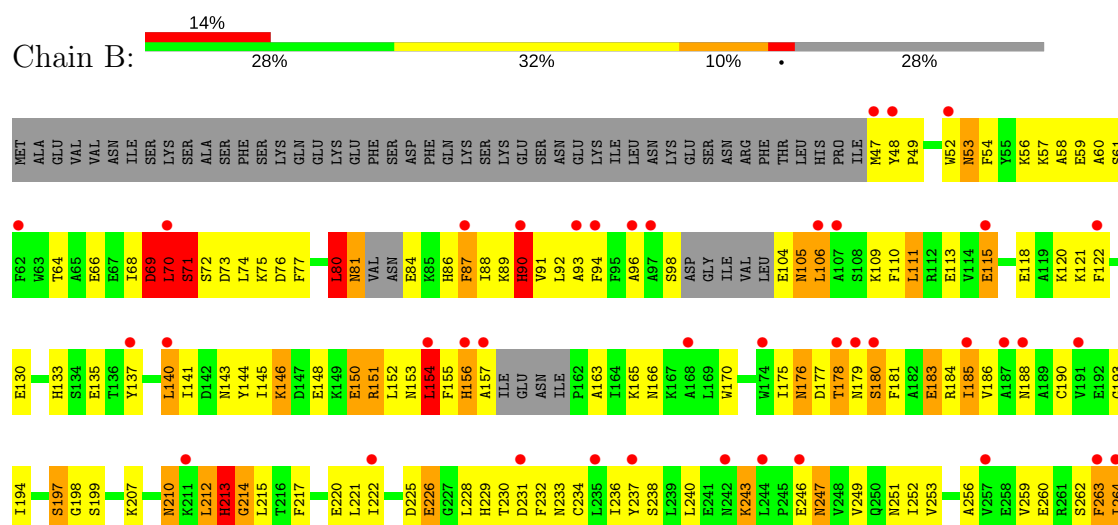
### 3 Residue-property plots

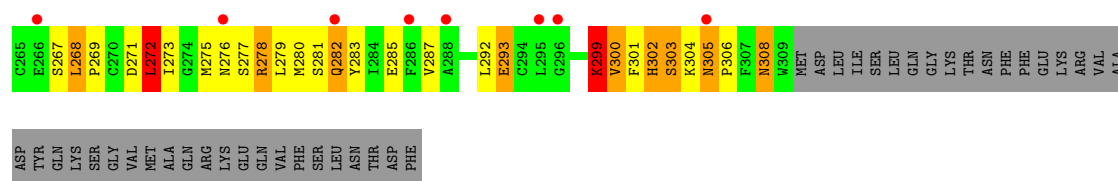
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Ribonucleotide reductase, small chain

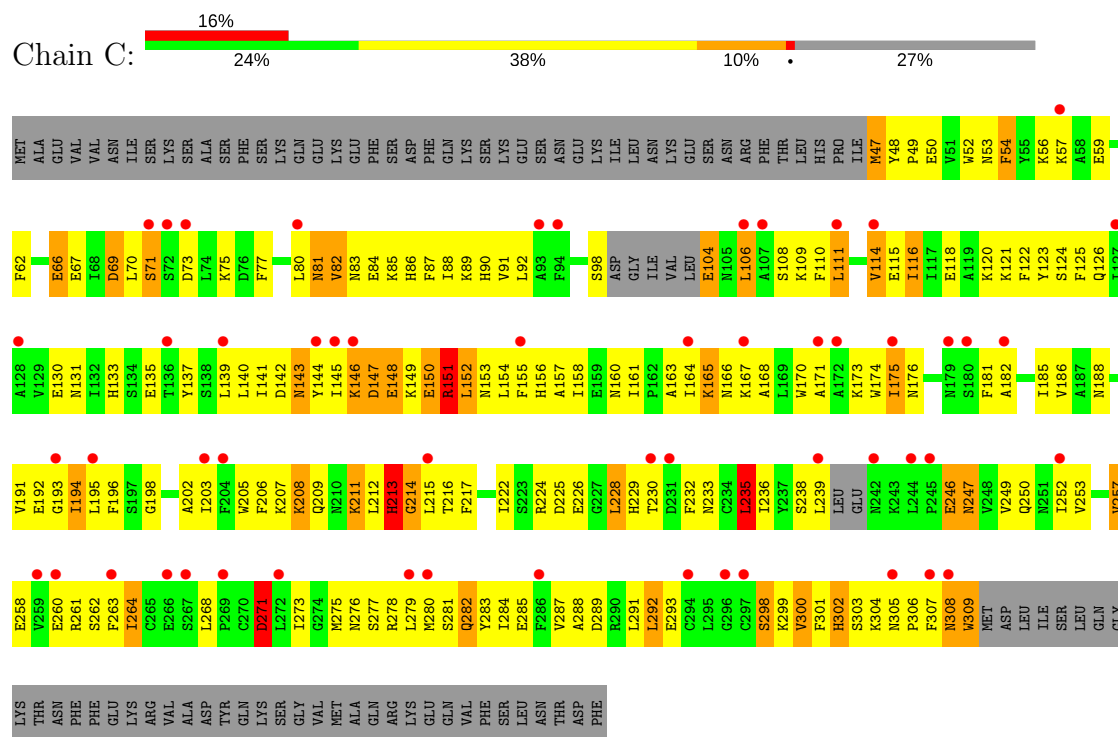


- Molecule 1: Ribonucleotide reductase, small chain

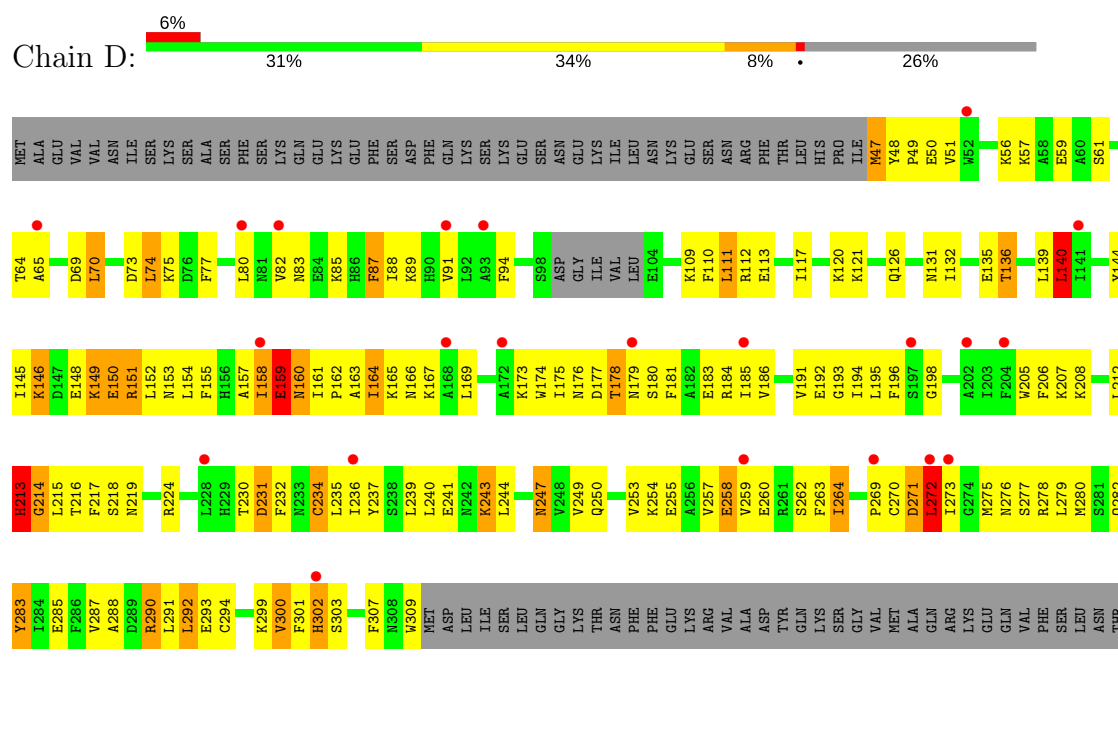




• Molecule 1: Ribonucleotide reductase, small chain

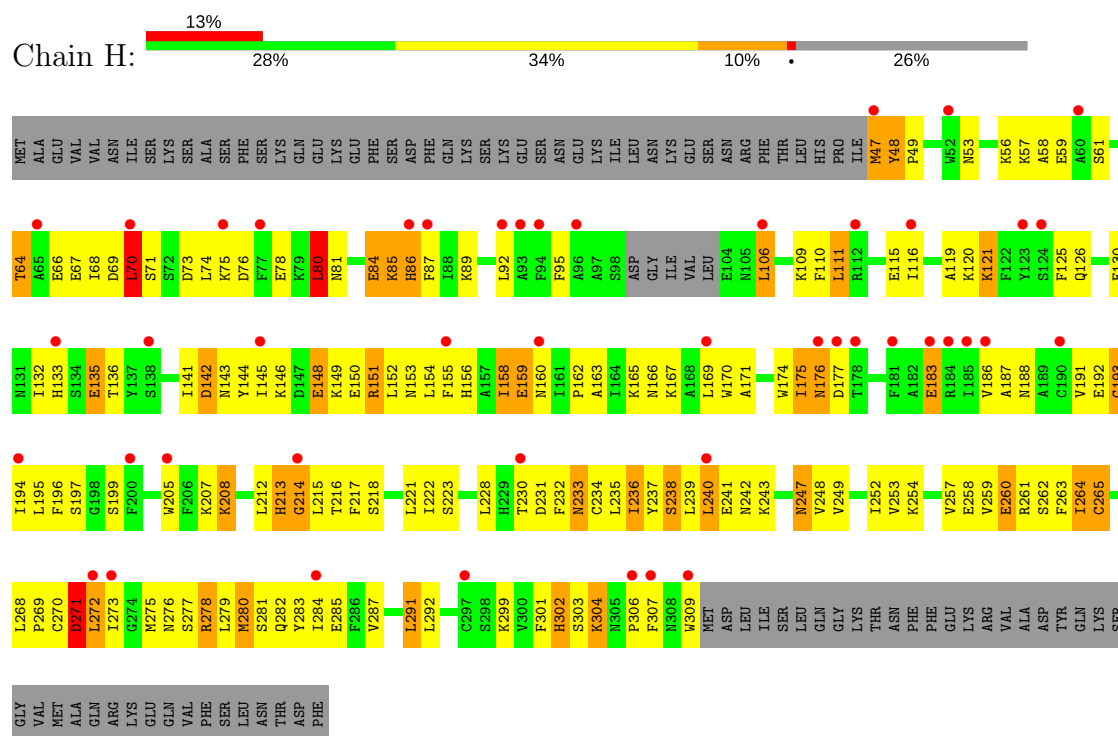
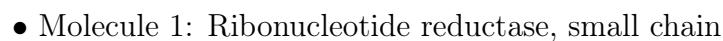


• Molecule 1: Ribonucleotide reductase, small chain









## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	192.04Å 153.46Å 143.36Å 90.00° 132.00° 90.00°	Depositor
Resolution (Å)	19.99 – 2.70 19.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.99-2.70) 87.6 (19.99-2.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.17 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.304 , 0.368 0.297 , 0.352	Depositor DCC
$R_{free}$ test set	3552 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.5	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 33.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.180 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	16904	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	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 20.83 % 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 7.9897e-03. 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, 0.333 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: FE

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	1.22	10/2154 (0.5%)	1.06	5/2911 (0.2%)
1	B	1.03	3/2104 (0.1%)	0.98	6/2837 (0.2%)
1	C	0.99	3/2148 (0.1%)	0.95	6/2898 (0.2%)
1	D	1.26	11/2166 (0.5%)	1.11	10/2924 (0.3%)
1	E	1.02	4/2159 (0.2%)	1.04	10/2913 (0.3%)
1	F	1.03	8/2166 (0.4%)	0.97	3/2924 (0.1%)
1	G	1.08	9/2107 (0.4%)	0.95	1/2841 (0.0%)
1	H	0.83	1/2166 (0.0%)	0.88	5/2924 (0.2%)
All	All	1.06	49/17170 (0.3%)	1.00	46/23172 (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	A	0	3
1	B	0	4
1	C	0	3
1	D	0	3
1	E	0	2
1	F	0	2
1	G	0	4
1	H	0	1
All	All	0	22

The worst 5 of 49 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	241	GLU	CD-OE2	12.58	1.39	1.25
1	G	243	LYS	CE-NZ	7.88	1.68	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	146	LYS	CE-NZ	7.86	1.68	1.49
1	G	76	ASP	CG-OD2	7.60	1.42	1.25
1	G	241	GLU	CD-OE1	7.58	1.33	1.25

The worst 5 of 46 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	226	GLU	OE1-CD-OE2	10.35	135.72	123.30
1	E	139	LEU	CA-CB-CG	-8.86	94.93	115.30
1	B	140	LEU	CA-CB-CG	8.06	133.84	115.30
1	E	272	LEU	CB-CG-CD1	7.17	123.20	111.00
1	A	224	ARG	NE-CZ-NH2	-7.02	116.79	120.30

There are no chirality outliers.

5 of 22 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	212	LEU	Peptide
1	A	214	GLY	Peptide
1	A	71	SER	Peptide
1	B	212	LEU	Peptide
1	B	71	SER	Peptide

## 5.2 Too-close contacts [i](#)

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	2104	0	2048	160	0
1	B	2056	0	1992	194	7
1	C	2099	0	2056	185	0
1	D	2116	0	2074	150	0
1	E	2109	0	2061	193	2
1	F	2116	0	2074	151	0
1	G	2059	0	2019	170	3
1	H	2116	0	2074	172	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	19	0	0	5	0
3	B	11	0	0	5	0
3	C	13	0	0	6	0
3	D	18	0	0	5	0
3	E	15	0	0	5	0
3	F	15	0	0	4	0
3	G	19	0	0	5	0
3	H	11	0	0	7	0
All	All	16904	0	16398	1363	10

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 41.

The worst 5 of 1363 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:G:243:LYS:CE	1:G:243:LYS:NZ	1.68	1.55
1:B:146:LYS:NZ	1:B:146:LYS:CE	1.68	1.54
1:G:121:LYS:CE	1:G:121:LYS:NZ	1.67	1.52
1:B:163:ALA:HB1	1:B:263:PHE:CD2	1.65	1.30
1:E:279:LEU:HD13	1:E:307:PHE:CE1	1.66	1.28

The worst 5 of 10 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)
1:E:302:HIS:ND1	1:G:71:SER:O[3_444]	1.31	0.89
1:G:267:SER:O	1:G:267:SER:O[2_657]	1.60	0.60
1:B:267:SER:O	1:B:272:LEU:O[2_555]	1.87	0.33
1:B:267:SER:C	1:B:272:LEU:O[2_555]	2.06	0.14
1:B:276:ASN:OD1	1:B:278:ARG:NE[2_555]	2.11	0.09

## 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	254/349 (73%)	219 (86%)	25 (10%)	10 (4%)	3	8
1	B	244/349 (70%)	208 (85%)	26 (11%)	10 (4%)	3	7
1	C	250/349 (72%)	206 (82%)	35 (14%)	9 (4%)	4	9
1	D	254/349 (73%)	215 (85%)	27 (11%)	12 (5%)	3	5
1	E	254/349 (73%)	219 (86%)	25 (10%)	10 (4%)	3	8
1	F	254/349 (73%)	220 (87%)	26 (10%)	8 (3%)	5	11
1	G	244/349 (70%)	209 (86%)	27 (11%)	8 (3%)	4	10
1	H	254/349 (73%)	220 (87%)	24 (9%)	10 (4%)	3	8
All	All	2008/2792 (72%)	1716 (86%)	215 (11%)	77 (4%)	4	8

5 of 77 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	159	GLU
1	A	302	HIS
1	B	176	ASN
1	B	272	LEU
1	E	80	LEU

### 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	229/316 (72%)	194 (85%)	35 (15%)	3	8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	223/316 (71%)	176 (79%)	47 (21%)	1	3
1	C	230/316 (73%)	182 (79%)	48 (21%)	1	3
1	D	232/316 (73%)	202 (87%)	30 (13%)	5	12
1	E	230/316 (73%)	196 (85%)	34 (15%)	3	9
1	F	232/316 (73%)	198 (85%)	34 (15%)	3	9
1	G	225/316 (71%)	191 (85%)	34 (15%)	3	8
1	H	232/316 (73%)	190 (82%)	42 (18%)	2	5
All	All	1833/2528 (72%)	1529 (83%)	304 (17%)	2	6

5 of 304 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	121	LYS
1	E	146	LYS
1	H	175	ILE
1	D	146	LYS
1	D	258	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 67 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	308	ASN
1	D	250	GLN
1	H	166	ASN
1	D	53	ASN
1	D	179	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 [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 [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	258/349 (73%)	0.99	25 (9%) 8 6	24, 42, 49, 55	0
1	B	252/349 (72%)	1.05	48 (19%) 1 1	27, 42, 48, 52	0
1	C	256/349 (73%)	1.13	55 (21%) 1 1	27, 42, 47, 53	0
1	D	258/349 (73%)	1.00	22 (8%) 11 9	32, 42, 49, 54	0
1	E	258/349 (73%)	1.05	45 (17%) 2 1	26, 42, 48, 51	0
1	F	258/349 (73%)	0.95	42 (16%) 2 1	30, 42, 47, 54	0
1	G	252/349 (72%)	1.16	54 (21%) 1 1	31, 42, 48, 56	0
1	H	258/349 (73%)	0.97	46 (17%) 2 1	34, 42, 48, 53	0
All	All	2050/2792 (73%)	1.04	337 (16%) 2 1	24, 42, 48, 56	0

The worst 5 of 337 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	274	GLY	9.6
1	E	178	THR	8.5
1	G	175	ILE	8.3
1	E	111	LEU	7.9
1	G	146	LYS	7.8

### 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](#)

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	FE	A	350	1/1	0.96	0.26	1.42	47,47,47,47	1
2	FE	E	350	1/1	0.94	0.06	-1.78	63,63,63,63	1
2	FE	G	350	1/1	0.92	0.06	-2.83	58,58,58,58	1
2	FE	F	350	1/1	0.96	0.09	-	54,54,54,54	1
2	FE	B	350	1/1	0.82	0.44	-	65,65,65,65	1
2	FE	C	350	1/1	0.92	0.09	-	61,61,61,61	1
2	FE	D	350	1/1	0.86	0.13	-	49,49,49,49	1
2	FE	H	350	1/1	0.97	0.06	-	53,53,53,53	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.