



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 9, 2026 – 09:39 PM UTC

PDB ID : 9RVT / pdb\_00009rvt  
Title : ACE2 extracellular domain in complex with the macrocyclic peptide GR1.4  
Authors : Brear, P.; Hyvonen, M.  
Deposited on : 2025-07-08  
Resolution : 2.39 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 : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

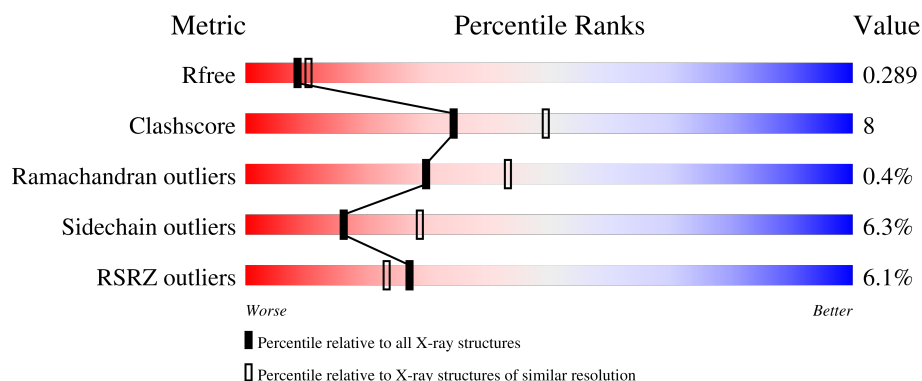
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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))
$R_{free}$	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	609	<div> <div>4%</div> <div>75%</div> <div>21%</div> <div>..</div> </div>
1	B	609	<div> <div>3%</div> <div>76%</div> <div>20%</div> <div>..</div> </div>
1	D	609	<div> <div>9%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
1	G	609	<div> <div>7%</div> <div>74%</div> <div>21%</div> <div>..</div> </div>
2	C	14	<div> <div>21%</div> <div>86%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	14	<div><div></div><div>14%</div><div>86%</div><div>7%</div><div>7%</div></div>
2	F	14	<div><div></div><div>14%</div><div>64%</div><div>21%</div><div>14%</div></div>
2	H	14	<div><div></div><div>14%</div><div>64%</div><div>36%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 20476 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 Processed angiotensin-converting enzyme 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	596	Total	C	N	O	S	0	2	0
			4881	3122	810	920	29			
1	B	596	Total	C	N	O	S	0	0	0
			4862	3111	805	917	29			
1	D	595	Total	C	N	O	S	0	0	0
			4856	3108	804	915	29			
1	G	595	Total	C	N	O	S	0	1	0
			4866	3114	807	916	29			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	GLY	-	expression tag	UNP Q9BYF1
A	616	SER	-	expression tag	UNP Q9BYF1
A	617	SER	-	expression tag	UNP Q9BYF1
A	618	PRO	-	expression tag	UNP Q9BYF1
A	619	HIS	-	expression tag	UNP Q9BYF1
A	620	HIS	-	expression tag	UNP Q9BYF1
A	621	HIS	-	expression tag	UNP Q9BYF1
A	622	HIS	-	expression tag	UNP Q9BYF1
A	623	HIS	-	expression tag	UNP Q9BYF1
A	624	HIS	-	expression tag	UNP Q9BYF1
A	625	HIS	-	expression tag	UNP Q9BYF1
A	626	HIS	-	expression tag	UNP Q9BYF1
B	18	GLY	-	expression tag	UNP Q9BYF1
B	616	SER	-	expression tag	UNP Q9BYF1
B	617	SER	-	expression tag	UNP Q9BYF1
B	618	PRO	-	expression tag	UNP Q9BYF1
B	619	HIS	-	expression tag	UNP Q9BYF1
B	620	HIS	-	expression tag	UNP Q9BYF1
B	621	HIS	-	expression tag	UNP Q9BYF1
B	622	HIS	-	expression tag	UNP Q9BYF1
B	623	HIS	-	expression tag	UNP Q9BYF1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	624	HIS	-	expression tag	UNP Q9BYF1
B	625	HIS	-	expression tag	UNP Q9BYF1
B	626	HIS	-	expression tag	UNP Q9BYF1
D	18	GLY	-	expression tag	UNP Q9BYF1
D	616	SER	-	expression tag	UNP Q9BYF1
D	617	SER	-	expression tag	UNP Q9BYF1
D	618	PRO	-	expression tag	UNP Q9BYF1
D	619	HIS	-	expression tag	UNP Q9BYF1
D	620	HIS	-	expression tag	UNP Q9BYF1
D	621	HIS	-	expression tag	UNP Q9BYF1
D	622	HIS	-	expression tag	UNP Q9BYF1
D	623	HIS	-	expression tag	UNP Q9BYF1
D	624	HIS	-	expression tag	UNP Q9BYF1
D	625	HIS	-	expression tag	UNP Q9BYF1
D	626	HIS	-	expression tag	UNP Q9BYF1
G	18	GLY	-	expression tag	UNP Q9BYF1
G	616	SER	-	expression tag	UNP Q9BYF1
G	617	SER	-	expression tag	UNP Q9BYF1
G	618	PRO	-	expression tag	UNP Q9BYF1
G	619	HIS	-	expression tag	UNP Q9BYF1
G	620	HIS	-	expression tag	UNP Q9BYF1
G	621	HIS	-	expression tag	UNP Q9BYF1
G	622	HIS	-	expression tag	UNP Q9BYF1
G	623	HIS	-	expression tag	UNP Q9BYF1
G	624	HIS	-	expression tag	UNP Q9BYF1
G	625	HIS	-	expression tag	UNP Q9BYF1
G	626	HIS	-	expression tag	UNP Q9BYF1

- Molecule 2 is a protein called macrocyclic peptide GR1.4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	14	Total 103	C 66	N 15	O 20	S 2	0	0	0
2	E	14	Total 103	C 66	N 15	O 20	S 2	0	0	0
2	F	14	Total 103	C 66	N 15	O 20	S 2	0	0	0
2	H	14	Total 103	C 66	N 15	O 20	S 2	0	0	0

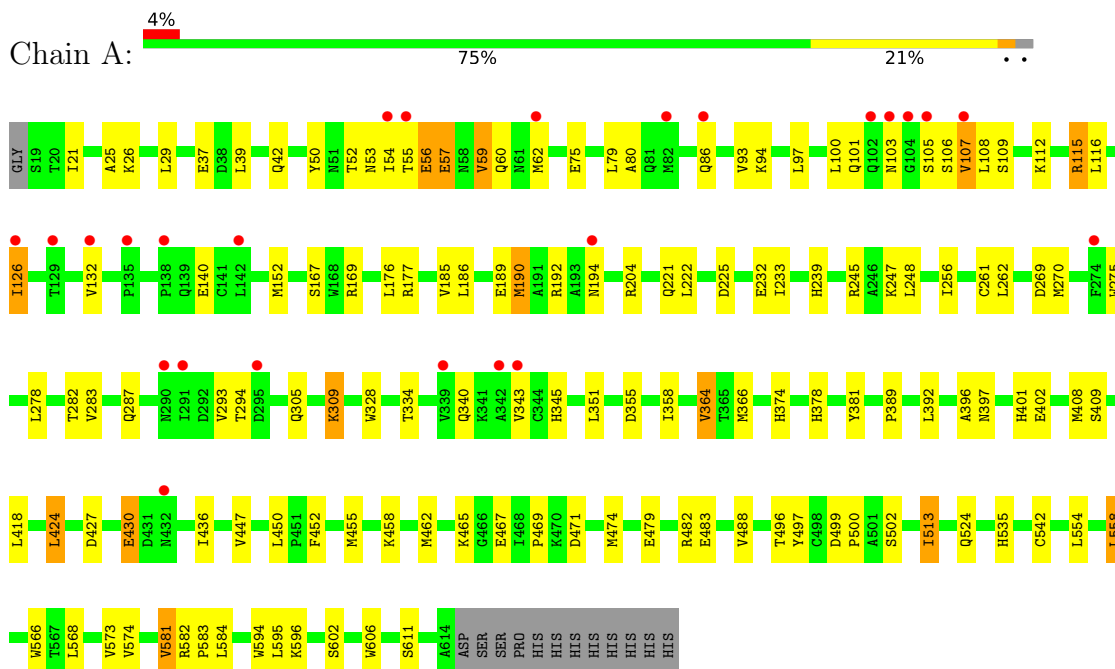
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	180	Total 180	O 180	0	0
3	B	161	Total 161	O 161	0	0
3	C	6	Total 6	O 6	0	0
3	D	102	Total 102	O 102	0	0
3	E	3	Total 3	O 3	0	0
3	F	3	Total 3	O 3	0	0
3	G	142	Total 142	O 142	0	0
3	H	2	Total 2	O 2	0	0

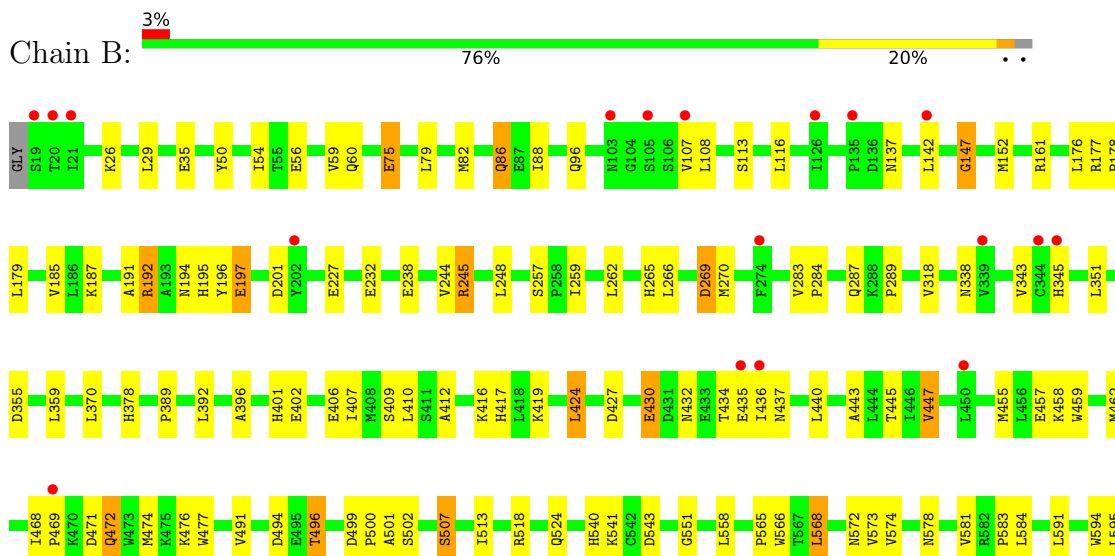
### 3 Residue-property plots [i](#)

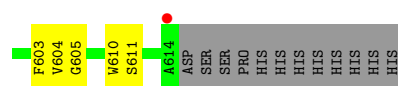
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Processed angiotensin-converting enzyme 2

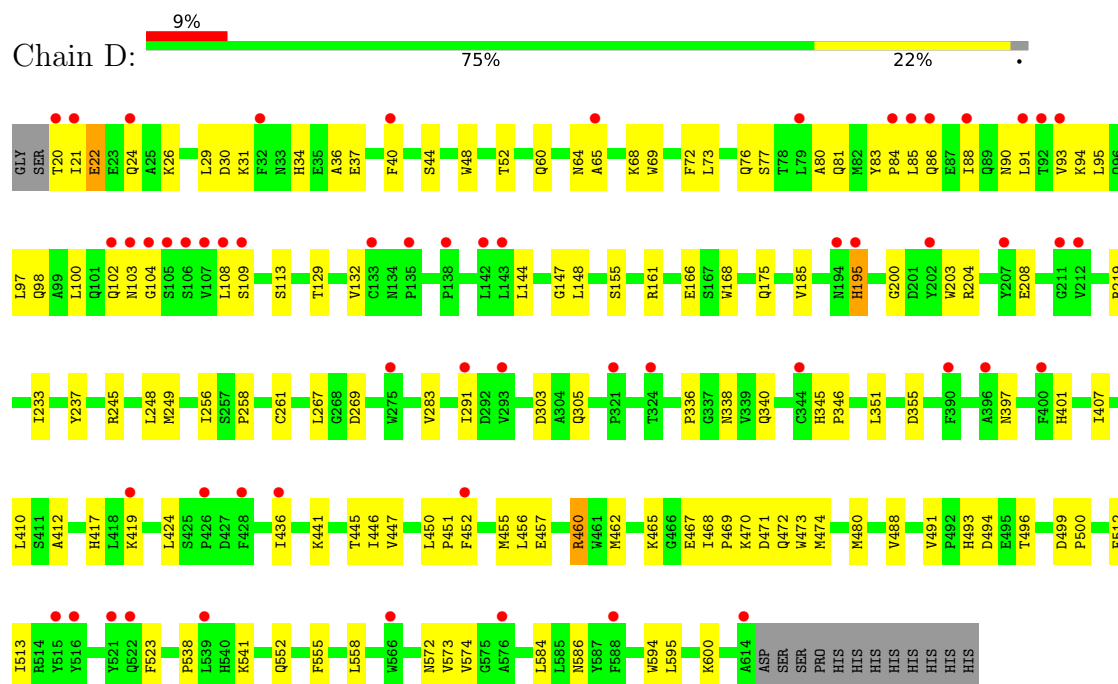


#### • Molecule 1: Processed angiotensin-converting enzyme 2

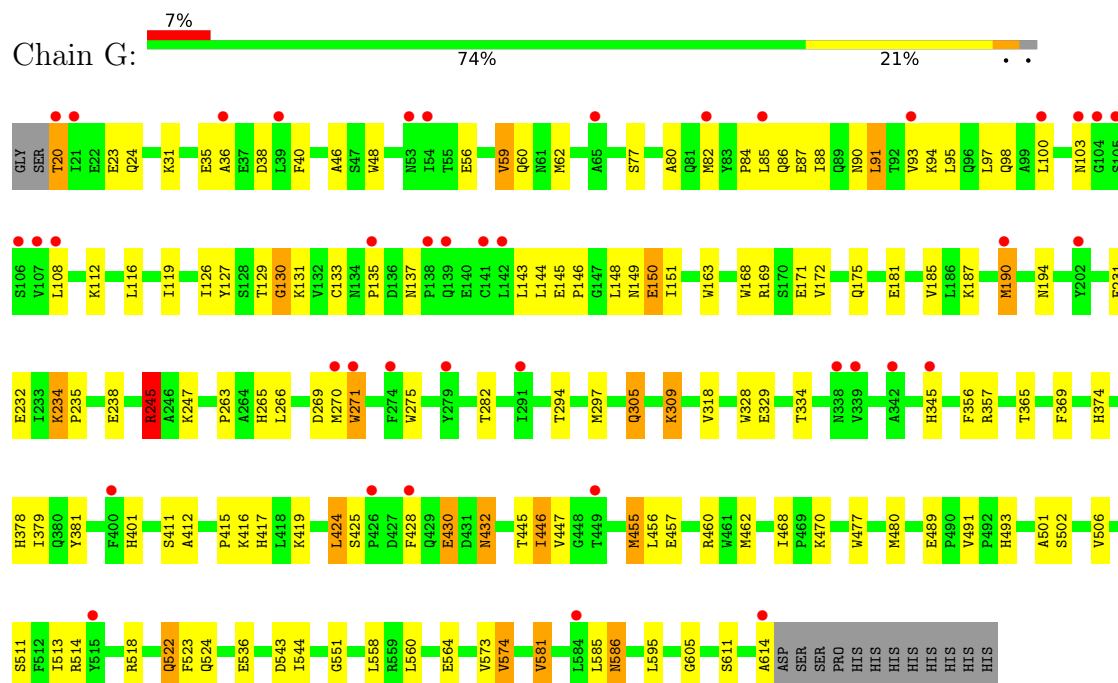




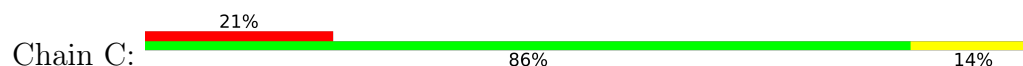
• Molecule 1: Processed angiotensin-converting enzyme 2



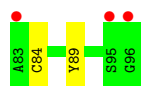
• Molecule 1: Processed angiotensin-converting enzyme 2



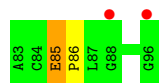
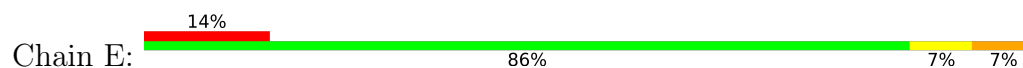
• Molecule 2: macrocyclic peptide GR1.4



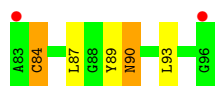




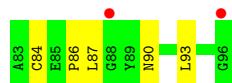
- Molecule 2: macrocyclic peptide GR1.4



- Molecule 2: macrocyclic peptide GR1.4



- Molecule 2: macrocyclic peptide GR1.4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.23Å 77.45Å 153.69Å 90.00° 101.22° 90.00°	Depositor
Resolution (Å)	69.07 – 2.39 69.07 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.4 (69.07-2.39) 99.3 (69.07-2.39)	Depositor EDS
$R_{merge}$	0.40	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.05 (at 2.40Å)	Xtrriage
Refinement program	BUSTER 2.10.4 (10-JUL-2024)	Depositor
R, $R_{free}$	0.249 , 0.298 0.246 , 0.289	Depositor DCC
$R_{free}$ test set	2019 reflections (1.93%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.6	Xtrriage
Anisotropy	0.219	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 49.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	20476	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 34.32 % 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 6.9490e-04. 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

### 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	0.74	0/5019	1.16	6/6819 (0.1%)
1	B	0.74	0/4999	1.15	12/6792 (0.2%)
1	D	0.71	0/4993	1.13	11/6784 (0.2%)
1	G	0.74	1/5004 (0.0%)	1.18	19/6799 (0.3%)
2	C	0.81	0/105	1.28	1/140 (0.7%)
2	E	0.72	0/105	1.33	0/140
2	F	0.66	0/105	1.24	1/140 (0.7%)
2	H	0.77	0/105	1.32	1/140 (0.7%)
All	All	0.74	1/20435 (0.0%)	1.16	51/27754 (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	2
1	B	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	194	ASN	C-N	6.69	1.43	1.33

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	269	ASP	CA-CB-CG	9.98	122.58	112.60
1	G	194	ASN	O-C-N	9.33	133.21	122.20
1	A	269	ASP	CA-CB-CG	7.74	120.34	112.60
1	G	585	LEU	CA-C-N	6.88	129.38	120.44
1	G	585	LEU	C-N-CA	6.88	129.38	120.44

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	ARG	Sidechain
1	A	169	ARG	Sidechain
1	B	245	ARG	Sidechain

## 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	4881	0	4652	70	0
1	B	4862	0	4639	62	1
1	D	4856	0	4634	79	1
1	G	4866	0	4640	79	0
2	C	103	0	93	1	0
2	E	103	0	93	2	0
2	F	103	0	93	5	0
2	H	103	0	93	3	0
3	A	180	0	0	3	0
3	B	161	0	0	0	0
3	C	6	0	0	0	0
3	D	102	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	142	0	0	1	0
3	H	2	0	0	0	0
All	All	20476	0	18937	293	1

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 8.

The worst 5 of 293 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:D:24:GLN:HG2	1:D:83:TYR:CE1	2.02	0.94
1:D:21:ILE:HG21	1:D:84:PRO:HD2	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:GLN:HG2	1:D:83:TYR:HE1	1.40	0.83
1:A:105:SER:HA	1:A:194:ASN:HD21	1.46	0.79
1:A:56:GLU:HB3	3:A:866:HOH:O	1.85	0.76

All (1) 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:B:195:HIS:O	1:D:195:HIS:O[2_445]	1.64	0.56

## 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	596/609 (98%)	577 (97%)	17 (3%)	2 (0%)	36	50
1	B	594/609 (98%)	570 (96%)	22 (4%)	2 (0%)	36	50
1	D	593/609 (97%)	573 (97%)	17 (3%)	3 (0%)	24	37
1	G	594/609 (98%)	569 (96%)	23 (4%)	2 (0%)	36	50
2	C	12/14 (86%)	11 (92%)	1 (8%)	0	100	100
2	E	12/14 (86%)	11 (92%)	1 (8%)	0	100	100
2	F	12/14 (86%)	7 (58%)	4 (33%)	1 (8%)	0	0
2	H	12/14 (86%)	9 (75%)	3 (25%)	0	100	100
All	All	2425/2492 (97%)	2327 (96%)	88 (4%)	10 (0%)	30	43

5 of 10 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	137	ASN
1	A	107	VAL

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Mol	Chain	Res	Type
2	F	84	CYS
1	G	130	GLY
1	D	147	GLY

### 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	528/538 (98%)	491 (93%)	37 (7%)	14	24
1	B	526/538 (98%)	490 (93%)	36 (7%)	14	25
1	D	525/538 (98%)	503 (96%)	22 (4%)	26	45
1	G	526/538 (98%)	487 (93%)	39 (7%)	13	22
2	C	11/11 (100%)	11 (100%)	0	100	100
2	E	11/11 (100%)	10 (91%)	1 (9%)	9	14
2	F	11/11 (100%)	11 (100%)	0	100	100
2	H	11/11 (100%)	11 (100%)	0	100	100
All	All	2149/2196 (98%)	2014 (94%)	135 (6%)	16	29

5 of 135 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	305	GLN
1	G	401	HIS
1	G	573	VAL
1	B	192	ARG
1	B	185	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	556	ASN
1	G	442	GLN

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Mol	Chain	Res	Type
1	D	96	GLN
1	G	417	HIS
1	G	586	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	596/609 (97%)	0.54	25 (4%)	40	36	24, 51, 80, 96	2 (0%)
1	B	596/609 (97%)	0.54	19 (3%)	50	46	36, 52, 79, 101	0
1	D	595/609 (97%)	1.00	56 (9%)	14	11	41, 62, 102, 124	0
1	G	595/609 (97%)	0.77	40 (6%)	24	20	25, 56, 83, 100	1 (0%)
2	C	14/14 (100%)	0.99	3 (21%)	2	2	44, 53, 58, 65	0
2	E	14/14 (100%)	0.98	2 (14%)	6	5	45, 54, 58, 64	0
2	F	14/14 (100%)	0.62	2 (14%)	6	5	53, 57, 63, 68	0
2	H	14/14 (100%)	1.03	2 (14%)	6	5	51, 53, 61, 66	0
All	All	2438/2492 (97%)	0.72	149 (6%)	27	23	24, 54, 86, 124	3 (0%)

The worst 5 of 149 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	195	HIS	6.8
1	D	105	SER	6.6
1	D	107	VAL	6.1
1	A	105	SER	5.3
1	D	108	LEU	4.8

### 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 oligosaccharides 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.