



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:48 PM GMT

PDB ID : 1HCJ  
Title : Photoproduct of the wild-type Aequorea victoria Green Fluorescent Protein  
Authors : Van Thor, J.J.; Gensch, T.; Hellingwerf, K.J.; Johnson, L.  
Deposited on : 2001-05-04  
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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

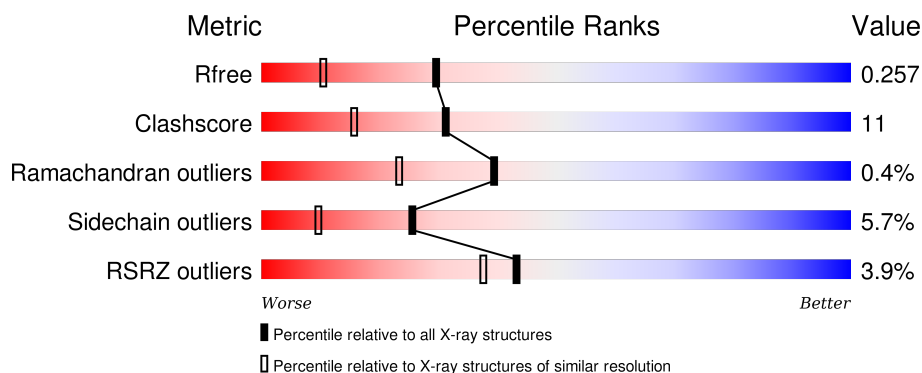
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	236	<div> <div>2%</div> <div>67% 22% 6% . .</div> </div>
1	B	236	<div> <div>3%</div> <div>69% 24% . .</div> </div>
1	C	236	<div> <div>6%</div> <div>67% 22% 6% . .</div> </div>
1	D	236	<div> <div>4%</div> <div>70% 22% . .</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7879 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 GREEN FLUORESCENT PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1817	1158	310	343	6			
1	B	227	Total	C	N	O	S	0	0	0
			1813	1157	308	342	6			
1	C	228	Total	C	N	O	S	0	0	0
			1818	1158	307	347	6			
1	D	227	Total	C	N	O	S	0	0	0
			1798	1149	305	338	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	GLY	CONFLICT	UNP P42212
B	2	SER	GLY	CONFLICT	UNP P42212
C	2	SER	GLY	CONFLICT	UNP P42212
D	2	SER	GLY	CONFLICT	UNP P42212
A	66	GYS	SER	CHROMOPHORE	UNP P42212
A	66	GYS	TYR	CHROMOPHORE	UNP P42212
A	66	GYS	GLY	CHROMOPHORE	UNP P42212
B	66	GYS	SER	CHROMOPHORE	UNP P42212
B	66	GYS	TYR	CHROMOPHORE	UNP P42212
B	66	GYS	GLY	CHROMOPHORE	UNP P42212
C	66	GYS	SER	CHROMOPHORE	UNP P42212
C	66	GYS	TYR	CHROMOPHORE	UNP P42212
C	66	GYS	GLY	CHROMOPHORE	UNP P42212
D	66	GYS	SER	CHROMOPHORE	UNP P42212
D	66	GYS	TYR	CHROMOPHORE	UNP P42212
D	66	GYS	GLY	CHROMOPHORE	UNP P42212

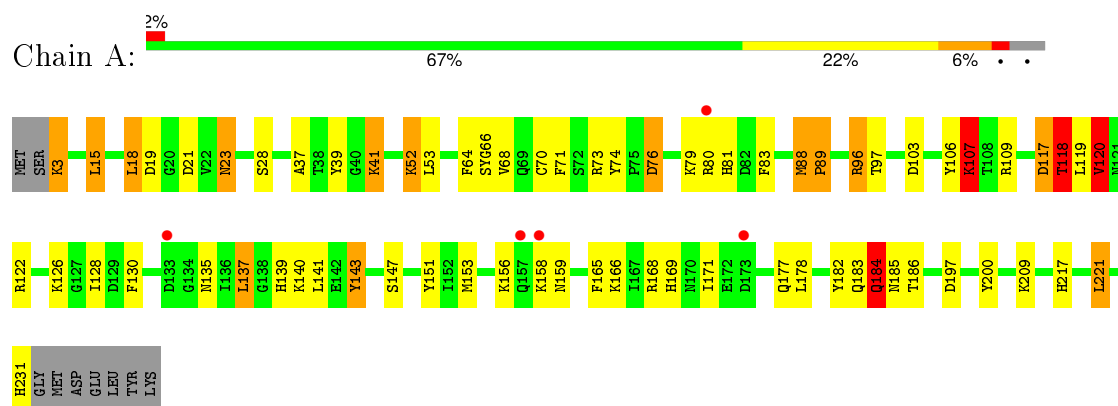
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	202	Total 202	O 202	0	0
2	B	153	Total 153	O 153	0	0
2	C	147	Total 147	O 147	0	0
2	D	131	Total 131	O 131	0	0

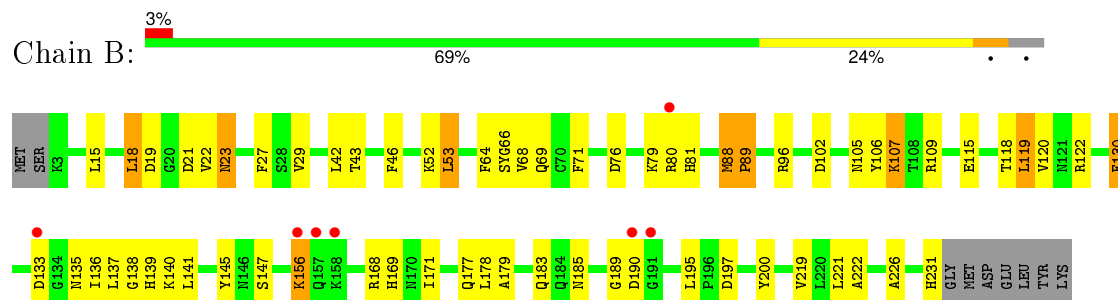
### 3 Residue-property plots [i](#)

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.

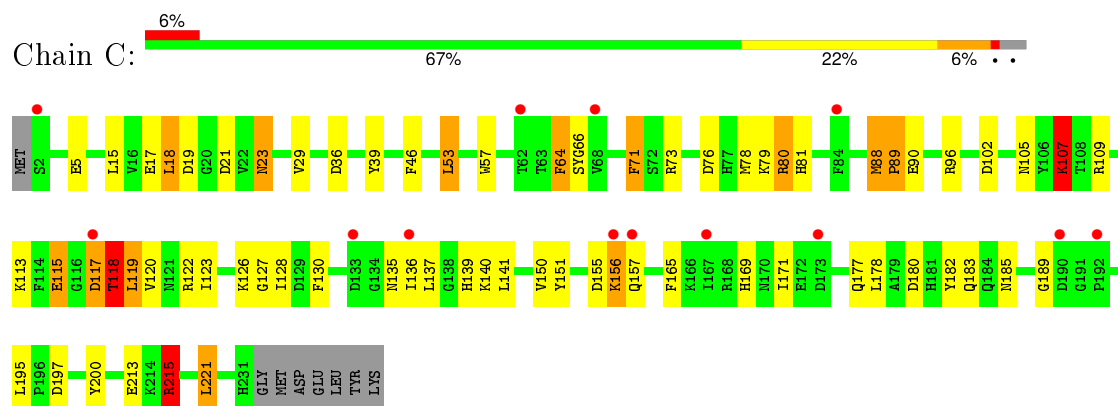
#### • Molecule 1: GREEN FLUORESCENT PROTEIN



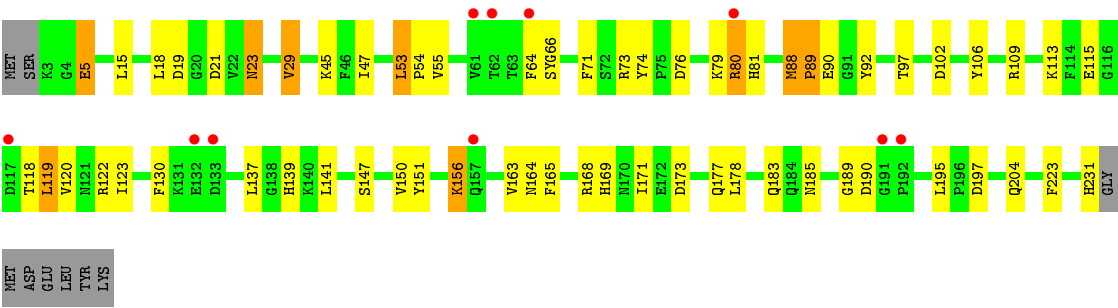
#### • Molecule 1: GREEN FLUORESCENT PROTEIN



#### • Molecule 1: GREEN FLUORESCENT PROTEIN



#### • Molecule 1: GREEN FLUORESCENT PROTEIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.77Å 65.67Å 110.50Å 90.00° 103.88° 90.00°	Depositor
Resolution (Å)	33.15 – 1.80 28.05 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (33.15-1.80) 96.3 (28.05-1.80)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.09 (at 1.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.209 , 0.267 0.206 , 0.257	Depositor DCC
$R_{free}$ test set	4506 reflections (5.32%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.6	Xtriage
Anisotropy	0.478	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 58.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 89190 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7879	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.56% 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, 0.375 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: ABA, GYS

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	0.92	0/1831	1.78	44/2472 (1.8%)
1	B	0.88	0/1827	1.81	43/2467 (1.7%)
1	C	0.84	0/1832	1.85	41/2476 (1.7%)
1	D	0.75	0/1812	1.54	27/2450 (1.1%)
All	All	0.85	0/7302	1.75	155/9865 (1.6%)

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	2
1	C	0	2
1	D	0	3
All	All	0	9

There are no bond length outliers.

All (155) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	80	ARG	NE-CZ-NH1	21.06	130.83	120.30
1	B	109	ARG	NE-CZ-NH2	-18.84	110.88	120.30
1	C	80	ARG	NE-CZ-NH2	-17.45	111.57	120.30
1	B	168	ARG	CD-NE-CZ	16.99	147.38	123.60
1	C	215	ARG	NE-CZ-NH1	16.82	128.71	120.30
1	C	73	ARG	NE-CZ-NH2	-15.35	112.63	120.30
1	B	122	ARG	NE-CZ-NH2	-13.04	113.78	120.30
1	C	215	ARG	NE-CZ-NH2	-12.89	113.86	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	109	ARG	NE-CZ-NH1	-10.91	114.84	120.30
1	C	215	ARG	CD-NE-CZ	10.57	138.41	123.60
1	A	21	ASP	CB-CG-OD1	10.14	127.43	118.30
1	B	130	PHE	CB-CG-CD1	-9.92	113.86	120.80
1	A	117	ASP	CB-CG-OD1	9.73	127.06	118.30
1	C	96	ARG	NE-CZ-NH2	-9.57	115.51	120.30
1	A	106	TYR	CB-CG-CD1	9.19	126.51	121.00
1	A	200	TYR	CB-CG-CD1	-9.14	115.51	121.00
1	A	109	ARG	NE-CZ-NH1	-8.82	115.89	120.30
1	D	5	GLU	CA-CB-CG	8.66	132.46	113.40
1	D	88	MET	CA-C-O	-8.65	101.93	120.10
1	A	74	TYR	CB-CG-CD2	-8.59	115.85	121.00
1	A	18	LEU	CA-CB-CG	8.48	134.81	115.30
1	B	200	TYR	CB-CG-CD1	-8.43	115.94	121.00
1	B	231	HIS	CA-C-O	-8.20	102.89	120.10
1	A	122	ARG	NE-CZ-NH2	-8.08	116.26	120.30
1	A	118	THR	CA-CB-OG1	8.04	125.89	109.00
1	C	29	VAL	CA-CB-CG1	7.91	122.76	110.90
1	D	21	ASP	CB-CG-OD1	7.90	125.41	118.30
1	B	18	LEU	CB-CG-CD1	7.81	124.28	111.00
1	B	102	ASP	CB-CG-OD2	7.73	125.26	118.30
1	C	89	PRO	N-CA-CB	7.72	112.56	103.30
1	B	88	MET	CA-C-O	-7.70	103.93	120.10
1	A	120	VAL	CA-CB-CG2	7.52	122.19	110.90
1	B	80	ARG	CD-NE-CZ	7.51	134.12	123.60
1	C	64	PHE	CB-CG-CD2	7.50	126.05	120.80
1	B	18	LEU	CA-CB-CG	7.50	132.54	115.30
1	D	89	PRO	N-CA-CB	7.43	112.22	103.30
1	A	184	GLN	CA-CB-CG	7.42	129.73	113.40
1	D	109	ARG	NE-CZ-NH1	-7.40	116.60	120.30
1	B	109	ARG	CG-CD-NE	-7.36	96.34	111.80
1	A	74	TYR	CB-CG-CD1	7.32	125.39	121.00
1	A	231	HIS	CA-C-O	-7.31	104.75	120.10
1	C	64	PHE	CB-CG-CD1	-7.29	115.70	120.80
1	B	64	PHE	CA-C-O	7.24	135.31	120.10
1	B	89	PRO	CA-N-CD	-7.12	101.53	111.50
1	C	122	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	C	102	ASP	CB-CG-OD1	7.04	124.64	118.30
1	C	119	LEU	CA-CB-CG	-7.04	99.11	115.30
1	B	89	PRO	N-CA-CB	7.00	111.70	103.30
1	A	151	TYR	CB-CG-CD1	6.96	125.18	121.00
1	D	173	ASP	CB-CG-OD1	6.94	124.55	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	71	PHE	CB-CG-CD2	-6.93	115.95	120.80
1	D	151	TYR	CB-CG-CD2	6.86	125.12	121.00
1	C	200	TYR	CB-CG-CD1	-6.79	116.93	121.00
1	D	151	TYR	CB-CG-CD1	-6.78	116.93	121.00
1	A	64	PHE	CB-CA-C	-6.77	96.86	110.40
1	D	106	TYR	CB-CG-CD1	6.75	125.05	121.00
1	A	89	PRO	CA-N-CD	-6.74	102.07	111.50
1	C	117	ASP	CB-CG-OD1	6.71	124.34	118.30
1	B	21	ASP	CB-CG-OD1	6.68	124.31	118.30
1	B	106	TYR	CB-CG-CD1	6.67	125.00	121.00
1	D	122	ARG	NE-CZ-NH1	6.63	123.62	120.30
1	B	130	PHE	CB-CG-CD2	6.56	125.39	120.80
1	D	173	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	C	115	GLU	OE1-CD-OE2	-6.54	115.45	123.30
1	A	88	MET	CA-C-O	-6.48	106.49	120.10
1	B	68	VAL	CB-CA-C	6.45	123.66	111.40
1	C	73	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	B	119	LEU	CA-CB-CG	-6.43	100.52	115.30
1	A	89	PRO	N-CA-CB	6.42	111.01	103.30
1	C	96	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	D	74	TYR	CZ-CE2-CD2	-6.38	114.06	119.80
1	B	46	PHE	CB-CG-CD2	-6.38	116.34	120.80
1	A	168	ARG	NE-CZ-NH1	-6.33	117.14	120.30
1	C	36	ASP	CB-CG-OD1	6.33	124.00	118.30
1	D	102	ASP	CB-CG-OD1	6.31	123.98	118.30
1	D	74	TYR	CG-CD2-CE2	6.31	126.34	121.30
1	B	19	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	C	151	TYR	CB-CG-CD2	6.28	124.77	121.00
1	C	107	LYS	CA-CB-CG	-6.26	99.63	113.40
1	C	89	PRO	CA-N-CD	-6.25	102.75	111.50
1	D	231	HIS	CA-C-O	-6.20	107.07	120.10
1	B	109	ARG	NH1-CZ-NH2	6.20	126.22	119.40
1	A	73	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	C	109	ARG	NH1-CZ-NH2	6.07	126.07	119.40
1	D	92	TYR	CB-CG-CD2	-6.04	117.37	121.00
1	B	189	GLY	C-N-CA	6.04	136.79	121.70
1	A	73	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	B	43	THR	CA-CB-CG2	-6.01	103.98	112.40
1	B	168	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	D	89	PRO	CA-N-CD	-6.00	103.09	111.50
1	D	223	PHE	CB-CG-CD2	-5.98	116.62	120.80
1	C	78	MET	CG-SD-CE	5.97	109.76	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	21	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	D	19	ASP	CB-CG-OD1	5.92	123.63	118.30
1	D	119	LEU	CA-CB-CG	-5.83	101.88	115.30
1	A	217	HIS	O-C-N	5.80	131.98	122.70
1	C	17	GLU	OE1-CD-OE2	-5.79	116.35	123.30
1	B	64	PHE	CB-CA-C	-5.76	98.87	110.40
1	A	76	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	A	221	LEU	CB-CG-CD1	5.70	120.70	111.00
1	C	39	TYR	CB-CG-CD2	-5.67	117.60	121.00
1	C	89	PRO	N-CD-CG	5.66	111.69	103.20
1	B	29	VAL	CA-CB-CG1	5.65	119.37	110.90
1	C	180	ASP	CB-CG-OD1	5.63	123.36	118.30
1	C	182	TYR	CB-CG-CD1	-5.60	117.64	121.00
1	C	151	TYR	CB-CG-CD1	-5.58	117.65	121.00
1	C	80	ARG	CB-CA-C	-5.55	99.31	110.40
1	A	80	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	102	ASP	CB-CG-OD1	-5.54	113.32	118.30
1	A	73	ARG	NH1-CZ-NH2	5.51	125.46	119.40
1	B	219	VAL	O-C-N	5.49	131.49	122.70
1	B	168	ARG	CG-CD-NE	-5.48	100.29	111.80
1	C	88	MET	CA-C-O	-5.43	108.69	120.10
1	D	73	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	A	68	VAL	CB-CA-C	5.41	121.68	111.40
1	A	122	ARG	CD-NE-CZ	-5.41	116.03	123.60
1	B	119	LEU	CD1-CG-CD2	5.40	126.69	110.50
1	D	29	VAL	CA-CB-CG1	5.39	118.99	110.90
1	A	19	ASP	CA-CB-CG	-5.35	101.64	113.40
1	A	107	LYS	CD-CE-NZ	5.33	123.96	111.70
1	A	137	LEU	CB-CG-CD2	-5.33	101.94	111.00
1	C	21	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	A	83	PHE	CB-CG-CD1	5.32	124.52	120.80
1	A	97	THR	N-CA-CB	5.32	120.41	110.30
1	C	221	LEU	CA-CB-CG	5.31	127.52	115.30
1	B	42	LEU	CB-CG-CD1	5.28	119.97	111.00
1	A	37	ALA	N-CA-CB	5.26	117.46	110.10
1	D	97	THR	N-CA-CB	5.25	120.28	110.30
1	B	29	VAL	N-CA-CB	5.23	123.00	111.50
1	C	118	THR	CA-CB-OG1	5.22	119.96	109.00
1	A	53	LEU	CA-CB-CG	5.20	127.25	115.30
1	A	143	TYR	CG-CD2-CE2	5.20	125.46	121.30
1	A	182	TYR	CB-CG-CD2	-5.19	117.89	121.00
1	D	168	ARG	NE-CZ-NH1	-5.19	117.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	SER	N-CA-CB	5.17	118.26	110.50
1	A	165	PHE	CB-CG-CD1	-5.16	117.19	120.80
1	D	21	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	B	89	PRO	N-CD-CG	5.15	110.92	103.20
1	A	83	PHE	CB-CG-CD2	-5.15	117.20	120.80
1	B	80	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	C	39	TYR	CB-CG-CD1	5.13	124.08	121.00
1	D	80	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	B	109	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	122	ARG	NH1-CZ-NH2	5.11	125.02	119.40
1	C	57	TRP	CH2-CZ2-CE2	5.11	122.51	117.40
1	B	53	LEU	CB-CG-CD2	5.11	119.68	111.00
1	B	179	ALA	N-CA-CB	5.11	117.25	110.10
1	D	164	ASN	CB-CG-OD1	5.08	131.76	121.60
1	B	145	TYR	CB-CG-CD2	-5.06	117.96	121.00
1	A	103	ASP	CB-CG-OD1	5.06	122.85	118.30
1	C	53	LEU	CA-CB-CG	5.04	126.90	115.30
1	A	96	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	B	69	GLN	O-C-N	-5.03	114.66	122.70
1	B	226	ALA	CB-CA-C	-5.03	102.56	110.10
1	A	39	TYR	CB-CG-CD1	-5.02	117.99	121.00

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	88	MET	Mainchain,Peptide
1	B	88	MET	Mainchain,Peptide
1	C	88	MET	Mainchain,Peptide
1	D	64	PHE	Mainchain
1	D	88	MET	Mainchain,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	1817	0	1764	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1813	0	1756	33	0
1	C	1818	0	1743	45	0
1	D	1798	0	1724	29	0
2	A	202	0	0	13	0
2	B	153	0	0	6	0
2	C	147	0	0	8	0
2	D	131	0	0	1	0
All	All	7879	0	6987	154	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 11.

All (154) 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:171:ILE:HD11	1:C:177:GLN:HB2	1.45	0.99
1:C:183:GLN:HE21	1:C:185:ASN:HD21	1.16	0.93
1:B:183:GLN:HE21	1:B:185:ASN:HD21	1.18	0.89
1:A:70:CYS:SG	1:A:119:LEU:HD11	2.15	0.86
1:A:183:GLN:HE21	1:A:185:ASN:HD21	1.24	0.83
1:D:156:LYS:HG3	1:D:195:LEU:HD13	1.60	0.81
1:B:23:ASN:HD21	1:B:130:PHE:H	1.28	0.80
1:D:81:HIS:HD2	1:D:197:ASP:H	1.32	0.77
1:A:130:PHE:HB3	1:A:137:LEU:CD2	2.15	0.77
1:A:118:THR:HG21	2:A:2113:HOH:O	1.83	0.76
1:D:76:ASP:HA	1:D:79:LYS:HD2	1.66	0.76
1:C:115:GLU:OE2	1:C:120:VAL:HG21	1.85	0.75
1:C:81:HIS:HD2	1:C:197:ASP:H	1.34	0.75
1:A:130:PHE:HB3	1:A:137:LEU:HD21	1.67	0.75
1:A:130:PHE:CB	1:A:137:LEU:HD21	2.18	0.74
1:B:81:HIS:HD2	1:B:197:ASP:H	1.37	0.73
1:C:71:PHE:HE2	1:C:119:LEU:HD22	1.52	0.73
1:D:171:ILE:HD11	1:D:177:GLN:HB2	1.69	0.72
1:B:130:PHE:HB3	1:B:137:LEU:HD23	1.69	0.72
1:C:171:ILE:HD11	1:C:177:GLN:CB	2.20	0.72
1:D:183:GLN:HE21	1:D:185:ASN:HD21	1.38	0.71
1:B:107:LYS:HE3	2:B:2076:HOH:O	1.91	0.70
1:C:120:VAL:HG23	2:C:2088:HOH:O	1.93	0.68
1:B:141:LEU:HD13	1:B:169:HIS:HB3	1.75	0.68
1:B:81:HIS:CD2	1:B:197:ASP:H	2.13	0.67
1:C:105:ASN:HD21	1:C:128:ILE:HD11	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ASN:HD22	1:B:140:LYS:HD2	1.60	0.66
1:A:23:ASN:HD21	1:A:130:PHE:H	1.42	0.65
1:C:81:HIS:CD2	1:C:197:ASP:H	2.15	0.65
1:C:23:ASN:HD21	1:C:130:PHE:H	1.45	0.65
1:A:137:LEU:HD22	1:A:137:LEU:H	1.62	0.64
1:C:130:PHE:HB3	1:C:137:LEU:HD23	1.79	0.64
1:A:41:LYS:HD2	1:A:221:LEU:HD11	1.80	0.64
1:B:76:ASP:HA	1:B:79:LYS:HD2	1.80	0.63
1:B:115:GLU:OE2	1:B:120:VAL:HG21	1.98	0.62
1:A:117:ASP:OD1	1:A:118:THR:HG22	1.99	0.61
1:A:107:LYS:HE2	1:A:107:LYS:N	2.15	0.61
1:D:81:HIS:CD2	1:D:197:ASP:H	2.15	0.61
1:A:81:HIS:CD2	1:A:197:ASP:H	2.18	0.61
1:A:81:HIS:HD2	1:A:197:ASP:H	1.49	0.61
1:A:183:GLN:HE21	1:A:185:ASN:ND2	1.95	0.61
1:C:71:PHE:CE2	1:C:119:LEU:HD22	2.35	0.61
1:D:130:PHE:HB3	1:D:137:LEU:HD23	1.81	0.60
1:D:171:ILE:HD11	1:D:177:GLN:CB	2.32	0.60
1:B:120:VAL:HG23	2:B:2082:HOH:O	2.01	0.60
1:A:139:HIS:HD2	2:A:2025:HOH:O	1.84	0.60
1:D:23:ASN:HD21	1:D:130:PHE:H	1.50	0.59
1:A:186:THR:HG23	2:A:2097:HOH:O	2.02	0.59
1:B:133:ASP:HB3	1:D:80:ARG:HH12	1.68	0.58
1:D:115:GLU:OE2	1:D:120:VAL:HG21	2.03	0.58
1:C:107:LYS:NZ	1:C:128:ILE:HG13	2.18	0.57
1:A:153:MET:HE3	2:A:2168:HOH:O	2.05	0.56
1:C:183:GLN:HE21	1:C:185:ASN:ND2	1.94	0.56
1:A:141:LEU:HD22	1:A:171:ILE:CD1	2.36	0.56
1:A:66:GYS:HD1	1:A:66:GYS:N2	2.21	0.56
1:D:66:GYS:HD1	1:D:66:GYS:N2	2.21	0.55
1:C:81:HIS:HE1	2:C:2062:HOH:O	1.89	0.55
1:A:171:ILE:HD11	1:A:177:GLN:CB	2.37	0.55
1:B:81:HIS:HE1	2:B:2151:HOH:O	1.90	0.55
1:B:139:HIS:HD2	2:B:2014:HOH:O	1.90	0.54
1:D:141:LEU:HD13	1:D:169:HIS:HB3	1.90	0.54
1:A:197:ASP:HB3	2:A:2169:HOH:O	2.07	0.54
1:C:66:GYS:HD1	1:C:66:GYS:N2	2.24	0.53
1:C:118:THR:HG21	2:C:2092:HOH:O	2.08	0.53
1:C:107:LYS:HE2	1:C:126:LYS:O	2.08	0.53
1:D:130:PHE:HB3	1:D:137:LEU:CD2	2.39	0.52
1:C:105:ASN:O	1:C:127:GLY:HA2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:LEU:HD22	1:C:19:ASP:N	2.25	0.52
1:B:183:GLN:HE21	1:B:185:ASN:ND2	1.98	0.52
1:A:96:ARG:HG2	1:A:183:GLN:HB2	1.90	0.51
1:B:66:GYS:HD1	1:B:66:GYS:N2	2.25	0.51
1:A:171:ILE:HD11	1:A:177:GLN:HB3	1.92	0.51
1:C:113:LYS:O	1:C:120:VAL:HG22	2.11	0.50
1:A:52:LYS:HB2	1:A:52:LYS:HZ2	1.75	0.50
1:A:135:ASN:HD22	1:A:140:LYS:HD2	1.75	0.50
1:C:107:LYS:HE3	2:C:2084:HOH:O	2.11	0.50
1:A:81:HIS:HE1	2:A:2202:HOH:O	1.94	0.50
1:A:137:LEU:HD22	1:A:137:LEU:N	2.25	0.50
1:A:126:LYS:HE3	1:A:128:ILE:CG2	2.42	0.50
1:B:171:ILE:HD11	1:B:177:GLN:HB2	1.93	0.49
1:C:115:GLU:CD	1:C:120:VAL:HG21	2.30	0.49
1:B:96:ARG:HG2	1:B:183:GLN:HB2	1.94	0.49
1:A:71:PHE:CE2	1:A:119:LEU:HD13	2.47	0.49
1:C:5:GLU:OE1	1:C:79:LYS:HD3	2.11	0.49
1:D:45:LYS:HE2	1:D:47:ILE:HD11	1.94	0.49
1:C:117:ASP:OD1	1:C:118:THR:HG22	2.13	0.48
1:A:130:PHE:HB2	1:A:137:LEU:HD21	1.96	0.48
1:B:141:LEU:HB3	2:B:2092:HOH:O	2.12	0.48
1:D:139:HIS:HD2	2:D:2017:HOH:O	1.97	0.48
1:C:155:ASP:OD1	1:C:157:GLN:NE2	2.47	0.48
1:D:53:LEU:HD13	1:D:55:VAL:O	2.14	0.47
1:C:90:GLU:OE1	1:C:189:GLY:HA3	2.14	0.47
1:C:76:ASP:OD1	1:C:79:LYS:HE2	2.13	0.47
1:D:183:GLN:HE21	1:D:185:ASN:ND2	2.09	0.47
1:A:169:HIS:HD2	2:A:2134:HOH:O	1.98	0.46
1:C:107:LYS:HZ1	1:C:128:ILE:HG13	1.80	0.46
1:A:52:LYS:HB2	1:A:52:LYS:NZ	2.29	0.46
1:A:76:ASP:OD1	1:A:79:LYS:HE2	2.15	0.46
1:A:183:GLN:NE2	1:A:185:ASN:HD21	2.03	0.46
1:C:139:HIS:HD2	2:C:2018:HOH:O	1.98	0.46
1:A:143:TYR:CZ	1:A:209:LYS:HE2	2.52	0.45
1:B:138:GLY:HA3	1:B:140:LYS:NZ	2.31	0.45
1:A:126:LYS:HE3	1:A:128:ILE:HG22	1.99	0.45
1:B:105:ASN:OD1	1:B:107:LYS:CD	2.64	0.45
1:D:90:GLU:OE2	1:D:189:GLY:HA3	2.16	0.45
1:B:130:PHE:CB	1:B:137:LEU:HD23	2.44	0.45
1:B:169:HIS:HD2	2:B:2096:HOH:O	1.99	0.45
1:D:18:LEU:HD23	1:D:123:ILE:CG2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:221:LEU:C	1:B:221:LEU:HD23	2.37	0.45
1:D:71:PHE:CE2	1:D:119:LEU:HD22	2.52	0.45
1:A:158:LYS:HD2	1:A:184:GLN:HE21	1.81	0.44
1:C:169:HIS:HD2	2:C:2103:HOH:O	2.00	0.44
1:D:53:LEU:HD22	1:D:54:PRO:HD2	2.00	0.44
1:C:105:ASN:HD21	1:C:128:ILE:CD1	2.28	0.44
1:C:135:ASN:HD22	1:C:140:LYS:HD2	1.82	0.44
1:D:147:SER:HB3	1:D:204:GLN:HG2	1.98	0.44
1:A:158:LYS:HD2	1:A:184:GLN:NE2	2.33	0.44
1:A:159:ASN:ND2	2:A:2146:HOH:O	2.50	0.44
1:A:107:LYS:HE2	1:A:107:LYS:H	1.82	0.44
1:D:141:LEU:HD22	1:D:171:ILE:CD1	2.48	0.44
1:C:18:LEU:HD23	1:C:123:ILE:HB	1.99	0.43
1:C:80:ARG:NE	2:C:2063:HOH:O	2.52	0.43
1:D:163:VAL:HB	1:D:183:GLN:HB3	2.01	0.43
1:D:150:VAL:HA	1:D:165:PHE:HB3	2.01	0.43
1:B:136:ILE:N	1:B:136:ILE:HD12	2.34	0.43
1:A:169:HIS:HE1	2:A:2057:HOH:O	2.02	0.43
1:B:141:LEU:HD22	1:B:171:ILE:CD1	2.48	0.42
1:C:213:GLU:OE2	1:C:215:ARG:HB2	2.18	0.42
1:C:156:LYS:HD2	1:C:195:LEU:HD13	2.01	0.42
1:A:107:LYS:NZ	1:A:128:ILE:HG12	2.34	0.42
1:B:133:ASP:CB	1:D:80:ARG:HH12	2.31	0.42
1:B:221:LEU:HD23	1:B:222:ABA:N	2.34	0.42
1:A:166:LYS:HD2	2:A:2158:HOH:O	2.18	0.42
1:C:136:ILE:HG22	1:C:137:LEU:HD22	2.01	0.42
1:B:22:VAL:HG23	1:B:27:PHE:HE1	1.84	0.42
1:B:120:VAL:O	1:B:120:VAL:HG23	2.19	0.42
1:C:90:GLU:HG3	2:C:2073:HOH:O	2.19	0.42
1:B:156:LYS:HD3	1:B:195:LEU:HD13	2.02	0.42
1:A:15:LEU:HD23	2:A:2017:HOH:O	2.20	0.42
1:C:120:VAL:HG23	1:C:120:VAL:O	2.19	0.42
1:B:71:PHE:HE2	1:B:119:LEU:HD22	1.85	0.41
1:B:107:LYS:HE2	1:B:107:LYS:HB2	1.60	0.41
1:C:18:LEU:HD23	1:C:123:ILE:CG2	2.51	0.41
1:C:141:LEU:CD2	1:C:171:ILE:HD13	2.51	0.41
1:D:137:LEU:HD22	1:D:137:LEU:N	2.35	0.41
1:A:15:LEU:O	1:A:120:VAL:HA	2.21	0.41
1:C:107:LYS:HE2	1:C:107:LYS:N	2.35	0.41
1:D:141:LEU:HD22	1:D:171:ILE:HD13	2.02	0.41
1:A:171:ILE:HD11	1:A:177:GLN:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:PHE:CZ	1:C:64:PHE:HB3	2.56	0.41
1:A:15:LEU:HD13	2:A:2029:HOH:O	2.21	0.41
1:C:150:VAL:HA	1:C:165:PHE:HB3	2.03	0.40
1:A:141:LEU:HD13	1:A:169:HIS:HB3	2.02	0.40
1:A:3:LYS:HB3	2:A:2090:HOH:O	2.20	0.40

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	223/236 (94%)	218 (98%)	4 (2%)	1 (0%)	39	23
1	B	223/236 (94%)	216 (97%)	6 (3%)	1 (0%)	39	23
1	C	224/236 (95%)	220 (98%)	3 (1%)	1 (0%)	39	23
1	D	223/236 (94%)	219 (98%)	3 (1%)	1 (0%)	39	23
All	All	893/944 (95%)	873 (98%)	16 (2%)	4 (0%)	39	23

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	89	PRO
1	B	89	PRO
1	D	89	PRO
1	C	89	PRO

### 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	196/205 (96%)	183 (93%)	13 (7%)	21	7
1	B	194/205 (95%)	183 (94%)	11 (6%)	25	10
1	C	194/205 (95%)	184 (95%)	10 (5%)	29	12
1	D	189/205 (92%)	179 (95%)	10 (5%)	28	11
All	All	773/820 (94%)	729 (94%)	44 (6%)	25	10

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	15	LEU
1	A	18	LEU
1	A	23	ASN
1	A	41	LYS
1	A	52	LYS
1	A	107	LYS
1	A	118	THR
1	A	120	VAL
1	A	147	SER
1	A	156	LYS
1	A	178	LEU
1	A	184	GLN
1	B	15	LEU
1	B	18	LEU
1	B	23	ASN
1	B	52	LYS
1	B	53	LEU
1	B	107	LYS
1	B	118	THR
1	B	147	SER
1	B	156	LYS
1	B	178	LEU
1	B	190	ASP
1	C	15	LEU
1	C	18	LEU
1	C	23	ASN
1	C	53	LEU
1	C	107	LYS
1	C	118	THR

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Mol	Chain	Res	Type
1	C	156	LYS
1	C	178	LEU
1	C	215	ARG
1	C	221	LEU
1	D	5	GLU
1	D	15	LEU
1	D	23	ASN
1	D	29	VAL
1	D	53	LEU
1	D	113	LYS
1	D	118	THR
1	D	156	LYS
1	D	178	LEU
1	D	190	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	81	HIS
1	A	121	ASN
1	A	135	ASN
1	A	139	HIS
1	A	149	ASN
1	A	157	GLN
1	A	159	ASN
1	A	169	HIS
1	A	177	GLN
1	A	184	GLN
1	A	185	ASN
1	A	212	ASN
1	B	23	ASN
1	B	81	HIS
1	B	121	ASN
1	B	135	ASN
1	B	139	HIS
1	B	149	ASN
1	B	164	ASN
1	B	169	HIS
1	B	177	GLN
1	B	185	ASN
1	C	23	ASN

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Mol	Chain	Res	Type
1	C	81	HIS
1	C	121	ASN
1	C	135	ASN
1	C	139	HIS
1	C	149	ASN
1	C	169	HIS
1	C	177	GLN
1	C	185	ASN
1	D	23	ASN
1	D	81	HIS
1	D	121	ASN
1	D	135	ASN
1	D	139	HIS
1	D	149	ASN
1	D	157	GLN
1	D	169	HIS
1	D	177	GLN
1	D	185	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	ABA	A	222	1	4,5,6	0.41	0	3,5,7	0.79	0
1	GYS	A	66	1	22,22,23	3.29	11 (50%)	27,30,32	3.89	9 (33%)
1	ABA	B	222	1	4,5,6	0.79	0	3,5,7	1.62	1 (33%)
1	GYS	B	66	1	22,22,23	3.78	13 (59%)	27,30,32	4.12	7 (25%)
1	ABA	C	222	1	4,5,6	1.43	0	3,5,7	1.98	2 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	GYS	C	66	1	22,22,23	3.78	14 (63%)	27,30,32	3.97	8 (29%)
1	ABA	D	222	1	4,5,6	0.80	0	3,5,7	1.31	1 (33%)
1	GYS	D	66	1	22,22,23	3.69	12 (54%)	27,30,32	3.96	11 (40%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	ABA	A	222	1	-	0/2/4/6	0/0/0/0
1	GYS	A	66	1	-	0/8/29/30	0/2/2/2
1	ABA	B	222	1	-	0/2/4/6	0/0/0/0
1	GYS	B	66	1	-	0/8/29/30	0/2/2/2
1	ABA	C	222	1	-	0/2/4/6	0/0/0/0
1	GYS	C	66	1	-	0/8/29/30	0/2/2/2
1	ABA	D	222	1	-	0/2/4/6	0/0/0/0
1	GYS	D	66	1	-	0/8/29/30	0/2/2/2

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	66	GYS	CA2-C2	-11.40	1.36	1.48
1	B	66	GYS	CA2-C2	-10.49	1.37	1.48
1	A	66	GYS	CA2-C2	-10.37	1.37	1.48
1	D	66	GYS	CA2-C2	-9.61	1.38	1.48
1	B	66	GYS	CB2-CA2	-7.99	1.27	1.35
1	D	66	GYS	CA3-N3	-7.68	1.34	1.47
1	C	66	GYS	CA3-N3	-7.01	1.35	1.47
1	D	66	GYS	CG2-CB2	-5.13	1.36	1.46
1	A	66	GYS	C1-N3	-4.23	1.29	1.37
1	B	66	GYS	C1-N3	-3.97	1.30	1.37
1	C	66	GYS	C1-N3	-3.71	1.30	1.37
1	B	66	GYS	C2-N3	-3.47	1.32	1.39
1	D	66	GYS	CB2-CA2	-3.38	1.32	1.35
1	A	66	GYS	CA3-N3	-3.30	1.41	1.47
1	B	66	GYS	CA3-N3	-3.17	1.42	1.47
1	B	66	GYS	C1-N2	-3.02	1.27	1.32
1	D	66	GYS	C1-N2	-2.89	1.27	1.32
1	D	66	GYS	C2-N3	-2.88	1.33	1.39
1	C	66	GYS	CG2-CB2	-2.82	1.41	1.46
1	B	66	GYS	CG2-CB2	-2.81	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	66	GYS	CG2-CB2	-2.79	1.41	1.46
1	A	66	GYS	CA1-C1	-2.75	1.47	1.51
1	A	66	GYS	CB2-CA2	-2.58	1.32	1.35
1	C	66	GYS	CA1-C1	-2.56	1.47	1.51
1	D	66	GYS	C1-N3	-2.54	1.32	1.37
1	A	66	GYS	C2-N3	-2.45	1.34	1.39
1	C	66	GYS	C2-N3	-2.41	1.34	1.39
1	C	66	GYS	C1-N2	-2.31	1.28	1.32
1	B	66	GYS	CA1-C1	-2.21	1.47	1.51
1	B	66	GYS	CB1-CA1	2.04	1.57	1.52
1	B	66	GYS	CE1-CZ	2.08	1.43	1.38
1	C	66	GYS	CE1-CZ	2.12	1.43	1.38
1	A	66	GYS	CE1-CZ	2.12	1.43	1.38
1	D	66	GYS	CE1-CZ	2.14	1.43	1.38
1	C	66	GYS	CB2-CA2	2.15	1.37	1.35
1	C	66	GYS	CB1-CA1	2.38	1.58	1.52
1	D	66	GYS	CA2-N2	2.49	1.43	1.38
1	C	66	GYS	CE1-CD1	2.93	1.44	1.38
1	A	66	GYS	CE1-CD1	2.95	1.44	1.38
1	B	66	GYS	CE1-CD1	2.96	1.44	1.38
1	D	66	GYS	CE1-CD1	3.00	1.44	1.38
1	A	66	GYS	O-C	3.32	1.41	1.19
1	C	66	GYS	O-C	3.42	1.41	1.19
1	C	66	GYS	CA2-N2	3.52	1.46	1.38
1	B	66	GYS	O-C	3.59	1.43	1.19
1	D	66	GYS	O-C	4.13	1.46	1.19
1	C	66	GYS	OH-CZ	6.23	1.52	1.37
1	D	66	GYS	OH-CZ	6.24	1.52	1.37
1	A	66	GYS	OH-CZ	6.25	1.52	1.37
1	B	66	GYS	OH-CZ	6.27	1.52	1.37

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	66	GYS	O2-C2-CA2	-14.27	123.24	130.95
1	A	66	GYS	O2-C2-CA2	-12.42	124.24	130.95
1	C	66	GYS	CA3-N3-C2	-9.33	108.80	123.99
1	D	66	GYS	CA3-N3-C2	-7.80	111.29	123.99
1	B	66	GYS	C2-CA2-N2	-7.44	102.97	108.91
1	D	66	GYS	C2-CA2-N2	-6.87	103.42	108.91
1	B	66	GYS	OG1-CB1-CA1	-6.30	97.72	111.16
1	C	66	GYS	OG1-CB1-CA1	-5.70	99.00	111.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	GYS	C2-CA2-N2	-5.61	104.43	108.91
1	A	66	GYS	OG1-CB1-CA1	-5.47	99.50	111.16
1	A	66	GYS	CA3-N3-C2	-5.17	115.58	123.99
1	D	66	GYS	OG1-CB1-CA1	-4.27	102.06	111.16
1	A	66	GYS	C2-CA2-N2	-4.12	105.62	108.91
1	D	66	GYS	O2-C2-CA2	-3.93	128.82	130.95
1	D	66	GYS	CG2-CB2-CA2	-3.52	125.64	130.22
1	B	222	ABA	O-C-CA	-2.69	118.48	125.49
1	C	222	ABA	O-C-CA	-2.40	119.23	125.49
1	C	222	ABA	CG-CB-CA	-2.38	107.29	113.44
1	C	66	GYS	O2-C2-N3	-2.16	119.85	124.50
1	D	222	ABA	O-C-CA	-2.14	119.92	125.49
1	B	66	GYS	CB1-CA1-C1	2.15	116.28	110.43
1	D	66	GYS	CB2-CA2-N2	2.40	132.97	128.67
1	D	66	GYS	CB1-CA1-C1	2.54	117.36	110.43
1	B	66	GYS	CA2-N2-C1	2.56	108.03	105.71
1	D	66	GYS	CA2-N2-C1	2.68	108.14	105.71
1	A	66	GYS	N3-C1-N2	2.75	113.68	111.56
1	A	66	GYS	CB2-CA2-C2	2.92	126.63	122.36
1	C	66	GYS	CB2-CA2-C2	2.93	126.65	122.36
1	B	66	GYS	CB2-CA2-C2	3.05	126.83	122.36
1	C	66	GYS	CB1-CA1-C1	3.48	119.92	110.43
1	D	66	GYS	C-CA3-N3	3.53	120.72	113.00
1	A	66	GYS	CB1-CA1-C1	4.79	123.47	110.43
1	A	66	GYS	CA3-N3-C1	6.72	135.16	127.36
1	A	66	GYS	CA2-C2-N3	8.96	107.89	103.40
1	C	66	GYS	CA2-C2-N3	9.57	108.19	103.40
1	D	66	GYS	CA2-C2-N3	10.61	108.72	103.40
1	D	66	GYS	CA3-N3-C1	10.72	139.81	127.36
1	B	66	GYS	CA2-C2-N3	11.29	109.06	103.40
1	C	66	GYS	CA3-N3-C1	11.83	141.10	127.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	66	GYS	1	0
1	B	222	ABA	1	0
1	B	66	GYS	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	66	GYS	1	0
1	D	66	GYS	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates 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 ⓘ

### 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	225/236 (95%)	0.19	5 (2%) 65 60	20, 28, 41, 58	0
1	B	225/236 (95%)	0.20	7 (3%) 52 47	21, 29, 44, 57	0
1	C	226/236 (95%)	0.37	13 (5%) 26 21	23, 31, 49, 60	0
1	D	225/236 (95%)	0.44	10 (4%) 38 32	25, 35, 52, 62	0
All	All	901/944 (95%)	0.30	35 (3%) 43 37	20, 31, 49, 62	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	157	GLN	4.9
1	C	2	SER	4.2
1	A	157	GLN	4.1
1	B	157	GLN	4.0
1	D	191	GLY	3.9
1	B	190	ASP	3.6
1	C	190	ASP	3.5
1	C	157	GLN	3.1
1	A	158	LYS	3.0
1	C	133	ASP	3.0
1	D	192	PRO	3.0
1	C	173	ASP	3.0
1	C	156	LYS	2.7
1	B	80	ARG	2.7
1	D	117	ASP	2.6
1	A	80	ARG	2.6
1	B	133	ASP	2.6
1	A	133	ASP	2.5
1	D	132	GLU	2.5
1	D	62	THR	2.5
1	C	62	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	156	LYS	2.4
1	D	61	VAL	2.4
1	A	173	ASP	2.4
1	C	68	VAL	2.4
1	D	80	ARG	2.4
1	C	117	ASP	2.4
1	C	192	PRO	2.2
1	D	133	ASP	2.2
1	C	84	PHE	2.1
1	C	136	ILE	2.1
1	C	167	ILE	2.1
1	B	191	GLY	2.1
1	D	64	PHE	2.0
1	B	158	LYS	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	GYS	D	66	21/22	0.90	0.17	-	24,27,30,31	0
1	GYS	C	66	21/22	0.93	0.16	-	22,24,28,29	0
1	ABA	D	222	6/7	0.94	0.14	-	23,24,25,26	0
1	GYS	A	66	21/22	0.93	0.16	-	20,22,24,25	0
1	ABA	B	222	6/7	0.96	0.10	-	22,22,23,24	0
1	ABA	C	222	6/7	0.93	0.14	-	23,24,24,25	0
1	ABA	A	222	6/7	0.92	0.18	-	20,22,23,24	0
1	GYS	B	66	21/22	0.93	0.16	-	20,23,25,26	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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.