



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:18 AM GMT

PDB ID : 3HU1  
Title : Structure of p97 N-D1 R95G mutant in complex with ATPgS  
Authors : Tang, W.-K.  
Deposited on : 2009-06-12  
Resolution : 2.81 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

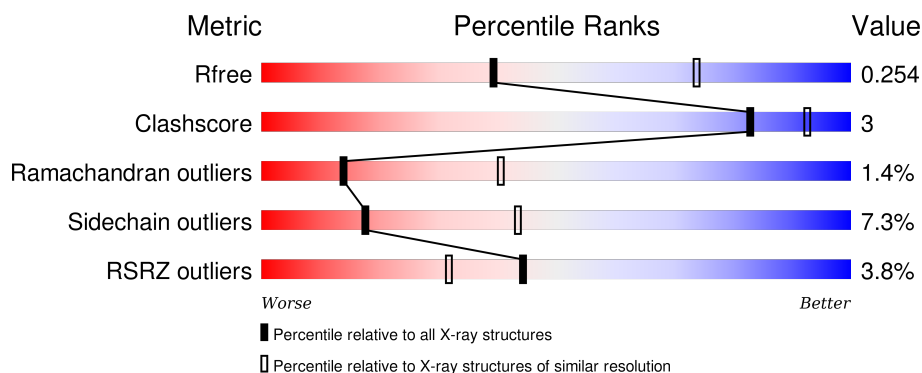
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.81 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	2676 (2.84-2.80)
Clashscore	102246	3124 (2.84-2.80)
Ramachandran outliers	100387	3072 (2.84-2.80)
Sidechain outliers	100360	3074 (2.84-2.80)
RSRZ outliers	91569	2690 (2.84-2.80)

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	489	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>8%</div> </div> </div>
1	B	489	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>8%</div> </div> </div>
1	C	489	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>8%</div> </div> </div>
1	D	489	<div> <div>6%</div> <div> <div></div> <div>80%</div> <div>11%</div> <div>8%</div> </div> </div>
1	E	489	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>8%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	489	<div><div></div><div>2%</div><div>79%</div><div>12%</div><div>8%</div></div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 21445 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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	451	Total	C	N	O	S	0	0	0
			3522	2211	623	670	18			
1	B	451	Total	C	N	O	S	0	0	0
			3522	2211	623	670	18			
1	C	451	Total	C	N	O	S	0	0	0
			3522	2211	623	670	18			
1	D	451	Total	C	N	O	S	0	0	0
			3522	2211	623	670	18			
1	E	451	Total	C	N	O	S	0	0	0
			3522	2211	623	670	18			
1	F	451	Total	C	N	O	S	0	0	0
			3522	2211	623	670	18			

There are 54 discrepancies between the modelled and reference sequences:

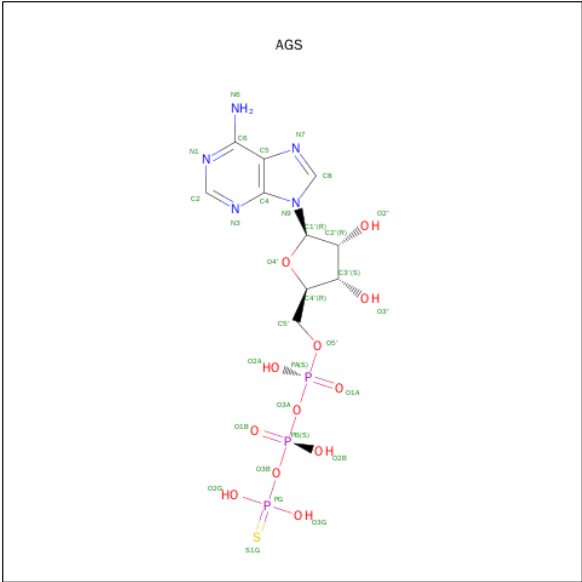
Chain	Residue	Modelled	Actual	Comment	Reference
A	95	GLY	ARG	ENGINEERED MUTATION	UNP P55072
A	482	ARG	-	EXPRESSION TAG	UNP P55072
A	483	SER	-	EXPRESSION TAG	UNP P55072
A	484	HIS	-	EXPRESSION TAG	UNP P55072
A	485	HIS	-	EXPRESSION TAG	UNP P55072
A	486	HIS	-	EXPRESSION TAG	UNP P55072
A	487	HIS	-	EXPRESSION TAG	UNP P55072
A	488	HIS	-	EXPRESSION TAG	UNP P55072
A	489	HIS	-	EXPRESSION TAG	UNP P55072
B	95	GLY	ARG	ENGINEERED MUTATION	UNP P55072
B	482	ARG	-	EXPRESSION TAG	UNP P55072
B	483	SER	-	EXPRESSION TAG	UNP P55072
B	484	HIS	-	EXPRESSION TAG	UNP P55072
B	485	HIS	-	EXPRESSION TAG	UNP P55072
B	486	HIS	-	EXPRESSION TAG	UNP P55072
B	487	HIS	-	EXPRESSION TAG	UNP P55072
B	488	HIS	-	EXPRESSION TAG	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
B	489	HIS	-	EXPRESSION TAG	UNP P55072
C	95	GLY	ARG	ENGINEERED MUTATION	UNP P55072
C	482	ARG	-	EXPRESSION TAG	UNP P55072
C	483	SER	-	EXPRESSION TAG	UNP P55072
C	484	HIS	-	EXPRESSION TAG	UNP P55072
C	485	HIS	-	EXPRESSION TAG	UNP P55072
C	486	HIS	-	EXPRESSION TAG	UNP P55072
C	487	HIS	-	EXPRESSION TAG	UNP P55072
C	488	HIS	-	EXPRESSION TAG	UNP P55072
C	489	HIS	-	EXPRESSION TAG	UNP P55072
D	95	GLY	ARG	ENGINEERED MUTATION	UNP P55072
D	482	ARG	-	EXPRESSION TAG	UNP P55072
D	483	SER	-	EXPRESSION TAG	UNP P55072
D	484	HIS	-	EXPRESSION TAG	UNP P55072
D	485	HIS	-	EXPRESSION TAG	UNP P55072
D	486	HIS	-	EXPRESSION TAG	UNP P55072
D	487	HIS	-	EXPRESSION TAG	UNP P55072
D	488	HIS	-	EXPRESSION TAG	UNP P55072
D	489	HIS	-	EXPRESSION TAG	UNP P55072
E	95	GLY	ARG	ENGINEERED MUTATION	UNP P55072
E	482	ARG	-	EXPRESSION TAG	UNP P55072
E	483	SER	-	EXPRESSION TAG	UNP P55072
E	484	HIS	-	EXPRESSION TAG	UNP P55072
E	485	HIS	-	EXPRESSION TAG	UNP P55072
E	486	HIS	-	EXPRESSION TAG	UNP P55072
E	487	HIS	-	EXPRESSION TAG	UNP P55072
E	488	HIS	-	EXPRESSION TAG	UNP P55072
E	489	HIS	-	EXPRESSION TAG	UNP P55072
F	95	GLY	ARG	ENGINEERED MUTATION	UNP P55072
F	482	ARG	-	EXPRESSION TAG	UNP P55072
F	483	SER	-	EXPRESSION TAG	UNP P55072
F	484	HIS	-	EXPRESSION TAG	UNP P55072
F	485	HIS	-	EXPRESSION TAG	UNP P55072
F	486	HIS	-	EXPRESSION TAG	UNP P55072
F	487	HIS	-	EXPRESSION TAG	UNP P55072
F	488	HIS	-	EXPRESSION TAG	UNP P55072
F	489	HIS	-	EXPRESSION TAG	UNP P55072

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C<sub>10</sub>H<sub>16</sub>N<sub>5</sub>O<sub>12</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	D	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

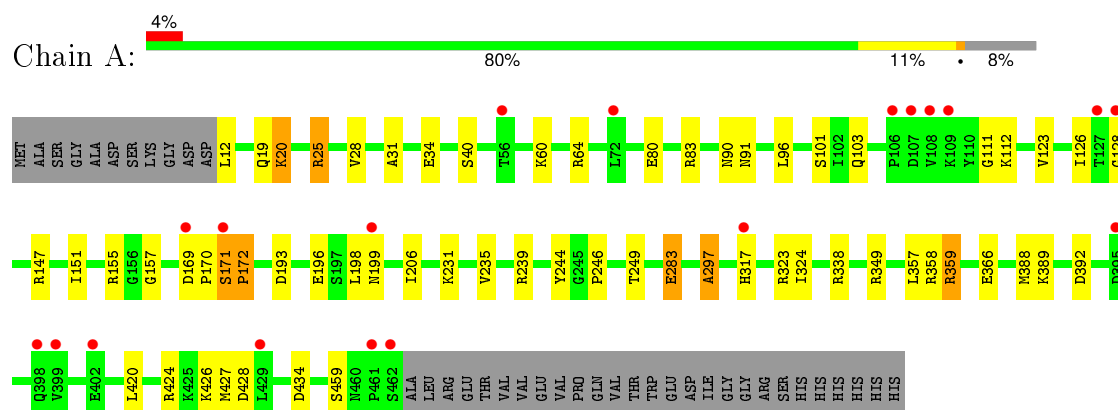
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	27	Total 27	O 27	0	0
4	B	22	Total 22	O 22	0	0
4	C	22	Total 22	O 22	0	0
4	D	16	Total 16	O 16	0	0
4	E	19	Total 19	O 19	0	0
4	F	15	Total 15	O 15	0	0

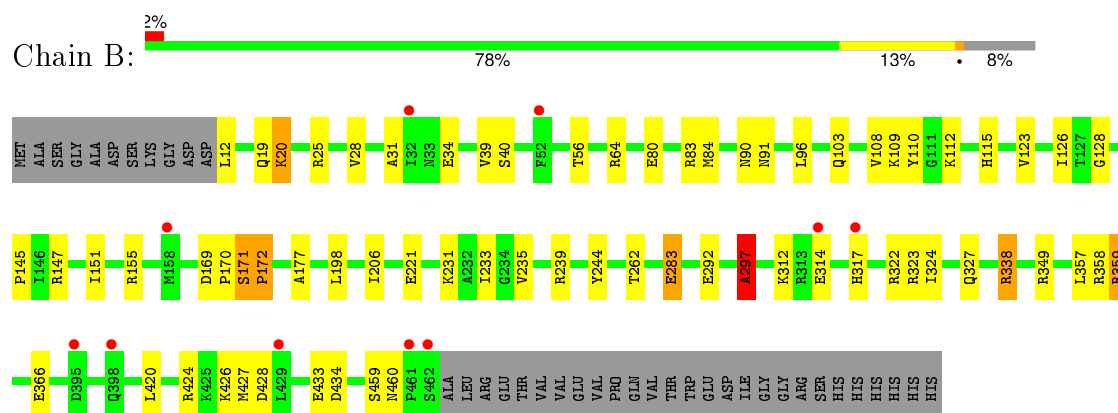
### 3 Residue-property plots

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

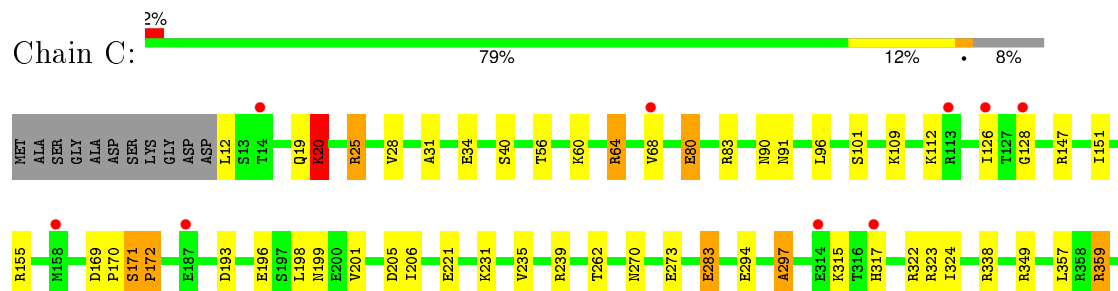
- Molecule 1: Transitional endoplasmic reticulum ATPase



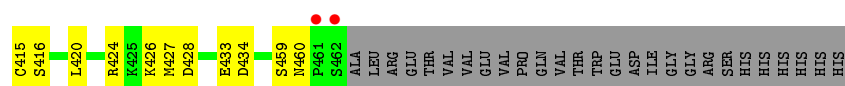
- Molecule 1: Transitional endoplasmic reticulum ATPase



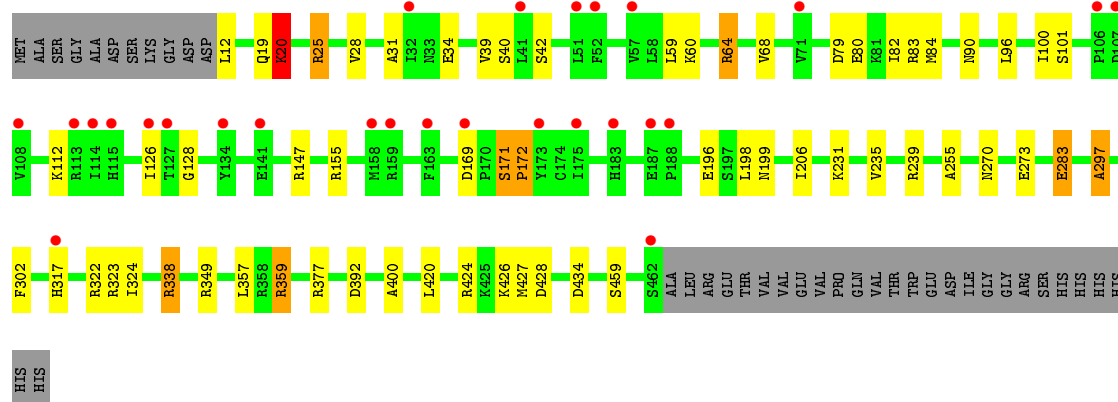
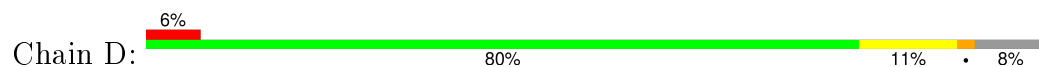
- Molecule 1: Transitional endoplasmic reticulum ATPase



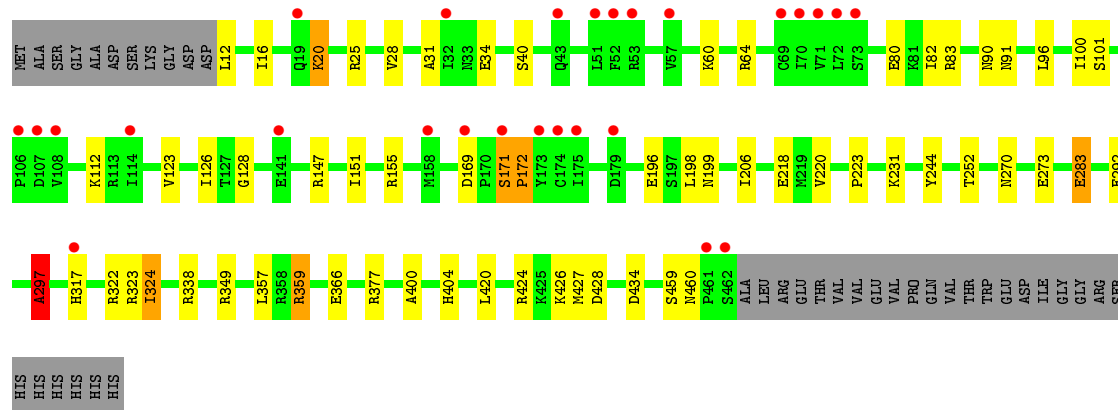
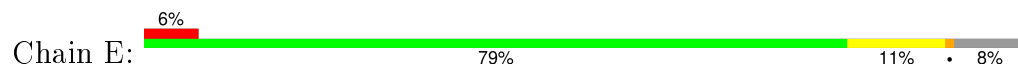




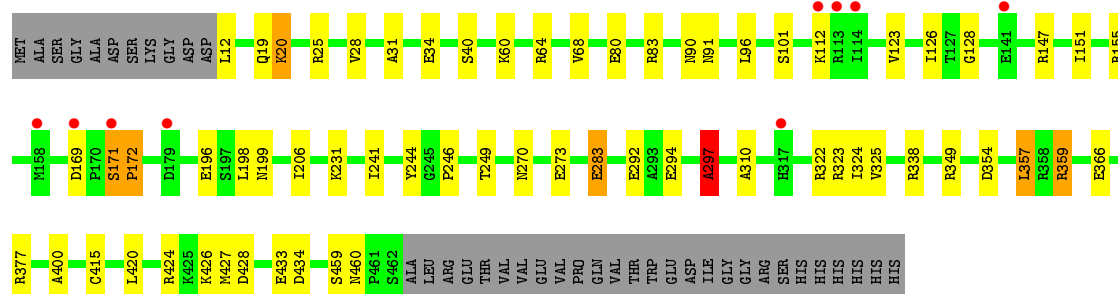
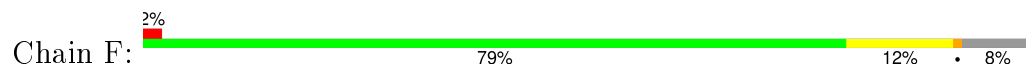
• Molecule 1: Transitional endoplasmic reticulum ATPase



• Molecule 1: Transitional endoplasmic reticulum ATPase



• Molecule 1: Transitional endoplasmic reticulum ATPase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.76 Å 103.28 Å 107.69 Å 97.66° 91.88° 89.75°	Depositor
Resolution (Å)	25.00 – 2.81 43.92 – 2.81	Depositor EDS
% Data completeness (in resolution range)	90.2 (25.00-2.81) 87.1 (43.92-2.81)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.31 (at 2.81 Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.240 , 0.271 0.220 , 0.254	Depositor DCC
$R_{free}$ test set	4322 reflections (5.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.3	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 54.3	EDS
Estimated twinning fraction	0.022 for h,-k,-l 0.016 for -h,-l,-k 0.019 for -h,l,k	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 87228 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	21445	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.95	0/3576	0.73	0/4832
1	B	0.97	1/3576 (0.0%)	0.73	0/4832
1	C	0.97	1/3576 (0.0%)	0.73	0/4832
1	D	0.95	0/3576	0.73	0/4832
1	E	0.99	1/3576 (0.0%)	0.74	0/4832
1	F	0.98	2/3576 (0.1%)	0.73	1/4832 (0.0%)
All	All	0.97	5/21456 (0.0%)	0.73	1/28992 (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	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
All	All	0	5

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	415	CYS	CB-SG	-7.06	1.70	1.82
1	F	415	CYS	CB-SG	-6.36	1.71	1.82
1	E	297	ALA	CA-CB	6.34	1.65	1.52
1	F	297	ALA	CA-CB	6.18	1.65	1.52
1	B	297	ALA	CA-CB	5.94	1.65	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	241	ILE	CG1-CB-CG2	-5.60	99.09	111.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	297	ALA	Peptide
1	C	297	ALA	Peptide
1	D	297	ALA	Peptide
1	E	297	ALA	Peptide
1	F	297	ALA	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	3522	0	3583	24	0
1	B	3522	0	3583	29	0
1	C	3522	0	3583	25	0
1	D	3522	0	3583	26	0
1	E	3522	0	3584	25	0
1	F	3522	0	3583	21	0
2	A	31	0	12	1	0
2	B	31	0	12	1	0
2	C	31	0	12	1	0
2	D	31	0	12	1	0
2	E	31	0	12	1	0
2	F	31	0	12	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	27	0	0	1	0
4	B	22	0	0	3	0
4	C	22	0	0	1	0
4	D	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	19	0	0	1	0
4	F	15	0	0	0	0
All	All	21445	0	21571	132	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 3.

All (132) 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:F:424:ARG:HA	1:F:427:MET:HG2	1.69	0.74
1:E:424:ARG:HA	1:E:427:MET:HG2	1.73	0.71
2:B:800:AGS:S1G	1:C:359:ARG:HG2	2.31	0.71
1:D:424:ARG:HA	1:D:427:MET:HG2	1.71	0.70
2:C:800:AGS:S1G	1:D:359:ARG:HG2	2.31	0.69
1:A:193:ASP:HA	1:B:338:ARG:HH12	1.57	0.68
2:E:800:AGS:S1G	1:F:359:ARG:HG2	2.33	0.68
1:C:424:ARG:HA	1:C:427:MET:HG2	1.75	0.68
1:B:424:ARG:HA	1:B:427:MET:HG2	1.76	0.67
1:A:193:ASP:HA	1:B:338:ARG:NH1	2.10	0.66
1:D:428:ASP:HA	1:E:20:LYS:HD3	1.78	0.66
1:E:428:ASP:HA	1:F:20:LYS:HD3	1.78	0.65
1:F:40:SER:HB2	1:F:83:ARG:HB2	1.80	0.64
1:B:40:SER:HB2	1:B:83:ARG:HB2	1.79	0.64
1:A:359:ARG:HG2	2:F:800:AGS:S1G	2.37	0.64
1:A:40:SER:HB2	1:A:83:ARG:HB2	1.80	0.63
1:E:40:SER:HB2	1:E:83:ARG:HB2	1.79	0.63
1:D:40:SER:HB2	1:D:83:ARG:HB2	1.80	0.63
1:C:40:SER:HB2	1:C:83:ARG:HB2	1.81	0.62
1:A:424:ARG:HA	1:A:427:MET:HG2	1.80	0.62
1:A:239:ARG:HD3	4:A:500:HOH:O	2.00	0.61
1:B:115:HIS:HB2	4:B:508:HOH:O	2.00	0.60
1:B:31:ALA:HA	1:B:83:ARG:HB3	1.84	0.59
1:C:317:HIS:HB2	1:D:322:ARG:HH12	1.68	0.59
1:F:377:ARG:NH1	1:F:400:ALA:O	2.36	0.59
1:E:252:THR:OG1	4:E:804:HOH:O	2.17	0.58
1:D:317:HIS:HB2	1:E:322:ARG:HH12	1.68	0.58
1:C:428:ASP:HA	1:D:20:LYS:HD2	1.86	0.57
1:A:317:HIS:HB2	1:B:322:ARG:HH12	1.71	0.56
1:B:317:HIS:HB2	1:C:322:ARG:HH12	1.72	0.55
1:E:60:LYS:HB2	1:E:101:SER:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:193:ASP:HA	1:D:338:ARG:HH12	1.74	0.53
1:F:28:VAL:HG23	1:F:96:LEU:HA	1.91	0.53
1:B:110:TYR:HD2	1:B:177:ALA:HB2	1.75	0.52
2:D:800:AGS:S1G	1:E:359:ARG:HG2	2.48	0.52
1:E:91:ASN:HD21	1:E:151:ILE:H	1.57	0.52
1:B:283:GLU:HB3	1:B:327:GLN:HE21	1.75	0.52
1:A:428:ASP:HA	1:B:20:LYS:HD3	1.93	0.51
1:C:112:LYS:HB3	1:C:169:ASP:HB3	1.92	0.51
1:A:31:ALA:HA	1:A:83:ARG:HB3	1.91	0.51
1:E:28:VAL:HG23	1:E:96:LEU:HA	1.93	0.51
1:C:109:LYS:HD2	1:C:170:PRO:HB3	1.92	0.50
1:B:171:SER:CB	1:B:172:PRO:HD3	2.41	0.50
1:F:60:LYS:HB2	1:F:101:SER:HB2	1.94	0.50
1:E:270:ASN:HB2	1:E:273:GLU:HB2	1.94	0.50
1:C:221:GLU:OE2	1:C:262:THR:HG22	2.12	0.50
1:D:283:GLU:OE2	1:D:323:ARG:HD2	2.11	0.50
1:B:28:VAL:HG23	1:B:96:LEU:HA	1.93	0.49
1:A:283:GLU:OE2	1:A:323:ARG:HD2	2.12	0.49
1:B:428:ASP:HA	1:C:20:LYS:HD2	1.94	0.49
1:D:31:ALA:HA	1:D:83:ARG:HB3	1.94	0.48
1:F:91:ASN:HD21	1:F:151:ILE:H	1.62	0.48
1:C:201:VAL:HG13	1:C:205:ASP:HB2	1.95	0.48
1:F:270:ASN:HB2	1:F:273:GLU:HB2	1.96	0.48
1:C:91:ASN:HD21	1:C:151:ILE:H	1.61	0.48
1:A:91:ASN:HD21	1:A:151:ILE:H	1.62	0.47
1:B:109:LYS:HD2	1:B:170:PRO:HB3	1.95	0.47
1:E:31:ALA:HA	1:E:83:ARG:HB3	1.97	0.47
1:C:433:GLU:HG3	1:D:25:ARG:HH21	1.80	0.47
1:F:31:ALA:HA	1:F:83:ARG:HB3	1.97	0.47
1:F:244:TYR:HE2	1:F:366:GLU:HB3	1.81	0.46
1:D:60:LYS:HB2	1:D:101:SER:HB2	1.97	0.46
1:E:283:GLU:OE2	1:E:323:ARG:HD2	2.16	0.46
2:A:800:AGS:S1G	1:B:359:ARG:HG2	2.55	0.46
1:C:28:VAL:HG23	1:C:96:LEU:HA	1.97	0.46
1:D:171:SER:HB2	1:D:172:PRO:HD3	1.98	0.46
1:C:31:ALA:HA	1:C:83:ARG:HB3	1.97	0.45
1:E:196:GLU:HA	1:E:199:ASN:HB2	1.98	0.45
1:D:28:VAL:HG23	1:D:96:LEU:HA	1.97	0.45
1:A:112:LYS:HB3	1:A:169:ASP:HB3	1.99	0.45
1:F:91:ASN:ND2	1:F:151:ILE:H	2.15	0.45
1:D:82:ILE:HG21	1:D:100:ILE:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:GLU:OE2	1:B:323:ARG:HD2	2.17	0.44
1:C:283:GLU:OE2	1:C:323:ARG:HD2	2.17	0.44
1:C:60:LYS:HB2	1:C:101:SER:HB2	1.99	0.44
1:E:244:TYR:HE2	1:E:366:GLU:HB3	1.83	0.44
1:A:171:SER:CB	1:A:172:PRO:HD3	2.46	0.44
1:A:389:LYS:HE3	4:B:496:HOH:O	2.16	0.44
1:A:60:LYS:HB2	1:A:101:SER:HB2	1.99	0.44
1:A:244:TYR:HE2	1:A:366:GLU:HB3	1.83	0.44
1:E:16:ILE:HG21	1:E:218:GLU:HG3	1.99	0.44
1:A:25:ARG:HH21	1:F:433:GLU:HG3	1.82	0.44
1:D:42:SER:OG	1:D:79:ASP:HA	2.18	0.43
1:B:91:ASN:HD21	1:B:151:ILE:H	1.65	0.43
1:B:56:THR:HG22	1:B:145:PRO:HG3	2.00	0.43
1:B:221:GLU:OE2	1:B:262:THR:HG22	2.18	0.43
1:D:196:GLU:HA	1:D:199:ASN:HB2	2.00	0.43
1:E:283:GLU:HG3	1:E:324:ILE:HG13	2.00	0.43
1:B:39:VAL:HG12	1:B:84:MET:HB3	2.01	0.43
1:C:171:SER:HB2	1:C:172:PRO:HD3	2.01	0.43
1:C:171:SER:CB	1:C:172:PRO:HD3	2.48	0.43
1:D:255:ALA:HB2	1:D:302:PHE:CZ	2.54	0.43
1:A:246:PRO:HD2	1:A:249:THR:HG21	2.00	0.43
1:D:270:ASN:HB2	1:D:273:GLU:HB2	2.01	0.43
1:F:354:ASP:HB3	1:F:357:LEU:HD12	2.01	0.42
1:E:220:VAL:O	1:E:223:PRO:HD2	2.18	0.42
1:A:91:ASN:ND2	1:A:151:ILE:H	2.17	0.42
1:B:171:SER:HB2	1:B:172:PRO:HD3	2.00	0.42
1:F:310:ALA:HA	1:F:325:VAL:HG22	2.01	0.42
1:F:283:GLU:OE2	1:F:323:ARG:HD2	2.19	0.42
1:A:196:GLU:HA	1:A:199:ASN:HB2	2.00	0.42
1:E:171:SER:CB	1:E:172:PRO:HD3	2.50	0.42
1:C:80:GLU:HB3	4:C:498:HOH:O	2.19	0.42
1:B:110:TYR:CD2	1:B:177:ALA:HB2	2.54	0.42
1:B:433:GLU:HG3	1:C:25:ARG:HH21	1.84	0.42
1:A:28:VAL:HG23	1:A:96:LEU:HA	2.02	0.42
1:D:171:SER:CB	1:D:172:PRO:HD3	2.50	0.42
1:F:112:LYS:HB3	1:F:169:ASP:HB3	2.02	0.42
1:A:388:MET:HA	1:B:233:ILE:O	2.20	0.41
1:D:64:ARG:HG3	1:D:64:ARG:O	2.20	0.41
1:F:196:GLU:HA	1:F:199:ASN:HB2	2.01	0.41
1:E:317:HIS:HB2	1:F:322:ARG:HH12	1.85	0.41
1:B:312:LYS:HB3	1:B:314:GLU:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:377:ARG:NH1	1:E:400:ALA:O	2.48	0.41
1:D:317:HIS:HB2	1:E:322:ARG:NH1	2.34	0.41
1:A:171:SER:HB2	1:A:172:PRO:HD3	2.02	0.41
1:B:297:ALA:O	4:B:500:HOH:O	2.22	0.41
1:D:112:LYS:HB3	1:D:169:ASP:HB3	2.01	0.41
1:E:82:ILE:HG21	1:E:100:ILE:HD11	2.02	0.41
1:D:39:VAL:HG11	1:D:59:LEU:HD11	2.02	0.41
1:B:112:LYS:HB3	1:B:169:ASP:HB3	2.02	0.41
1:F:246:PRO:HD2	1:F:249:THR:HG21	2.02	0.41
1:A:111:GLY:HA2	1:A:170:PRO:HG2	2.03	0.41
1:E:112:LYS:HB3	1:E:169:ASP:HB3	2.02	0.41
1:C:64:ARG:HG3	1:C:64:ARG:O	2.21	0.41
1:B:244:TYR:HE2	1:B:366:GLU:HB3	1.84	0.41
1:D:377:ARG:NH1	1:D:400:ALA:O	2.47	0.40
1:E:91:ASN:ND2	1:E:151:ILE:H	2.18	0.40
1:D:39:VAL:HG12	1:D:84:MET:HB3	2.02	0.40
1:F:171:SER:HB2	1:F:172:PRO:HD3	2.04	0.40
1:C:270:ASN:HB2	1:C:273:GLU:HB2	2.04	0.40
1:C:196:GLU:HA	1:C:199:ASN:HB2	2.03	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	449/489 (92%)	419 (93%)	23 (5%)	7 (2%)	12	36
1	B	449/489 (92%)	422 (94%)	21 (5%)	6 (1%)	15	42
1	C	449/489 (92%)	421 (94%)	22 (5%)	6 (1%)	15	42
1	D	449/489 (92%)	420 (94%)	23 (5%)	6 (1%)	15	42
1	E	449/489 (92%)	420 (94%)	23 (5%)	6 (1%)	15	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	449/489 (92%)	419 (93%)	24 (5%)	6 (1%)	15	42
All	All	2694/2934 (92%)	2521 (94%)	136 (5%)	37 (1%)	14	40

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	SER
1	B	171	SER
1	C	171	SER
1	D	171	SER
1	E	171	SER
1	F	171	SER
1	A	126	ILE
1	A	128	GLY
1	A	297	ALA
1	B	20	LYS
1	B	126	ILE
1	B	128	GLY
1	C	126	ILE
1	D	126	ILE
1	E	20	LYS
1	E	126	ILE
1	E	128	GLY
1	F	20	LYS
1	F	126	ILE
1	F	128	GLY
1	A	20	LYS
1	A	172	PRO
1	B	172	PRO
1	B	297	ALA
1	C	20	LYS
1	C	172	PRO
1	C	297	ALA
1	D	20	LYS
1	D	128	GLY
1	D	172	PRO
1	D	297	ALA
1	E	172	PRO
1	E	297	ALA
1	F	172	PRO
1	F	297	ALA
1	C	128	GLY

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Mol	Chain	Res	Type
1	A	157	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	386/417 (93%)	358 (93%)	28 (7%)	17	43
1	B	386/417 (93%)	356 (92%)	30 (8%)	16	40
1	C	386/417 (93%)	355 (92%)	31 (8%)	15	39
1	D	386/417 (93%)	359 (93%)	27 (7%)	19	46
1	E	386/417 (93%)	361 (94%)	25 (6%)	21	50
1	F	386/417 (93%)	358 (93%)	28 (7%)	17	43
All	All	2316/2502 (93%)	2147 (93%)	169 (7%)	17	43

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	LEU
1	A	19	GLN
1	A	20	LYS
1	A	25	ARG
1	A	34	GLU
1	A	64	ARG
1	A	80	GLU
1	A	90	ASN
1	A	103	GLN
1	A	123	VAL
1	A	147	ARG
1	A	155	ARG
1	A	198	LEU
1	A	206	ILE
1	A	231	LYS
1	A	235	VAL
1	A	283	GLU

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Mol	Chain	Res	Type
1	A	324	ILE
1	A	338	ARG
1	A	349	ARG
1	A	357	LEU
1	A	358	ARG
1	A	359	ARG
1	A	392	ASP
1	A	420	LEU
1	A	426	LYS
1	A	434	ASP
1	A	459	SER
1	B	12	LEU
1	B	19	GLN
1	B	25	ARG
1	B	34	GLU
1	B	64	ARG
1	B	80	GLU
1	B	90	ASN
1	B	103	GLN
1	B	108	VAL
1	B	123	VAL
1	B	147	ARG
1	B	155	ARG
1	B	198	LEU
1	B	206	ILE
1	B	231	LYS
1	B	235	VAL
1	B	239	ARG
1	B	283	GLU
1	B	292	GLU
1	B	324	ILE
1	B	338	ARG
1	B	349	ARG
1	B	357	LEU
1	B	358	ARG
1	B	359	ARG
1	B	420	LEU
1	B	426	LYS
1	B	434	ASP
1	B	459	SER
1	B	460	ASN
1	C	12	LEU

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Mol	Chain	Res	Type
1	C	19	GLN
1	C	20	LYS
1	C	25	ARG
1	C	34	GLU
1	C	56	THR
1	C	64	ARG
1	C	68	VAL
1	C	80	GLU
1	C	90	ASN
1	C	147	ARG
1	C	155	ARG
1	C	198	LEU
1	C	206	ILE
1	C	231	LYS
1	C	235	VAL
1	C	239	ARG
1	C	283	GLU
1	C	294	GLU
1	C	315	LYS
1	C	324	ILE
1	C	338	ARG
1	C	349	ARG
1	C	357	LEU
1	C	359	ARG
1	C	416	SER
1	C	420	LEU
1	C	426	LYS
1	C	434	ASP
1	C	459	SER
1	C	460	ASN
1	D	12	LEU
1	D	19	GLN
1	D	20	LYS
1	D	25	ARG
1	D	34	GLU
1	D	64	ARG
1	D	68	VAL
1	D	80	GLU
1	D	90	ASN
1	D	147	ARG
1	D	155	ARG
1	D	198	LEU

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Mol	Chain	Res	Type
1	D	206	ILE
1	D	231	LYS
1	D	235	VAL
1	D	239	ARG
1	D	283	GLU
1	D	324	ILE
1	D	338	ARG
1	D	349	ARG
1	D	357	LEU
1	D	359	ARG
1	D	392	ASP
1	D	420	LEU
1	D	426	LYS
1	D	434	ASP
1	D	459	SER
1	E	12	LEU
1	E	25	ARG
1	E	34	GLU
1	E	64	ARG
1	E	80	GLU
1	E	90	ASN
1	E	123	VAL
1	E	147	ARG
1	E	155	ARG
1	E	198	LEU
1	E	206	ILE
1	E	231	LYS
1	E	283	GLU
1	E	292	GLU
1	E	324	ILE
1	E	338	ARG
1	E	349	ARG
1	E	357	LEU
1	E	359	ARG
1	E	404	HIS
1	E	420	LEU
1	E	426	LYS
1	E	434	ASP
1	E	459	SER
1	E	460	ASN
1	F	12	LEU
1	F	19	GLN

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Mol	Chain	Res	Type
1	F	25	ARG
1	F	34	GLU
1	F	64	ARG
1	F	68	VAL
1	F	80	GLU
1	F	90	ASN
1	F	123	VAL
1	F	147	ARG
1	F	155	ARG
1	F	198	LEU
1	F	206	ILE
1	F	231	LYS
1	F	283	GLU
1	F	292	GLU
1	F	294	GLU
1	F	324	ILE
1	F	338	ARG
1	F	349	ARG
1	F	357	LEU
1	F	359	ARG
1	F	420	LEU
1	F	426	LYS
1	F	428	ASP
1	F	434	ASP
1	F	459	SER
1	F	460	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	260	ASN
1	A	285	ASN
1	A	327	GLN
1	B	91	ASN
1	B	260	ASN
1	B	285	ASN
1	B	327	GLN
1	C	91	ASN
1	C	260	ASN
1	C	327	GLN
1	D	91	ASN

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Mol	Chain	Res	Type
1	D	260	ASN
1	D	285	ASN
1	D	327	GLN
1	E	91	ASN
1	E	260	ASN
1	E	285	ASN
1	E	327	GLN
1	F	91	ASN
1	F	260	ASN
1	F	285	ASN
1	F	327	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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	$\# Z  > 2$
2	AGS	A	800	3	24,33,33	1.50	2 (8%)	28,52,52	2.06	5 (17%)
2	AGS	B	800	3	24,33,33	1.64	3 (12%)	28,52,52	2.02	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	AGS	C	800	3	24,33,33	1.61	4 (16%)	28,52,52	1.98	5 (17%)
2	AGS	D	800	3	24,33,33	1.53	2 (8%)	28,52,52	2.00	4 (14%)
2	AGS	E	800	3	24,33,33	1.43	3 (12%)	28,52,52	1.91	4 (14%)
2	AGS	F	800	3	24,33,33	1.62	2 (8%)	28,52,52	1.90	5 (17%)

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
2	AGS	A	800	3	-	0/15/38/38	0/3/3/3
2	AGS	B	800	3	-	0/15/38/38	0/3/3/3
2	AGS	C	800	3	-	0/15/38/38	0/3/3/3
2	AGS	D	800	3	-	0/15/38/38	0/3/3/3
2	AGS	E	800	3	-	0/15/38/38	0/3/3/3
2	AGS	F	800	3	-	0/15/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	800	AGS	C5-N7	-2.24	1.31	1.39
2	B	800	AGS	C5-N7	-2.15	1.32	1.39
2	C	800	AGS	C5-N7	-2.07	1.32	1.39
2	C	800	AGS	C5-C4	2.01	1.45	1.40
2	B	800	AGS	C5-C4	2.14	1.45	1.40
2	E	800	AGS	C5-C4	2.19	1.45	1.40
2	A	800	AGS	C5-C4	2.57	1.46	1.40
2	C	800	AGS	C2-N3	2.60	1.36	1.32
2	F	800	AGS	C5-C4	2.62	1.46	1.40
2	D	800	AGS	C5-C4	2.77	1.46	1.40
2	E	800	AGS	PG-S1G	4.59	1.99	1.90
2	D	800	AGS	PG-S1G	5.22	2.00	1.90
2	A	800	AGS	PG-S1G	5.31	2.00	1.90
2	B	800	AGS	PG-S1G	5.74	2.01	1.90
2	F	800	AGS	PG-S1G	5.74	2.01	1.90
2	C	800	AGS	PG-S1G	5.77	2.01	1.90

All (27) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	AGS	N3-C2-N1	-8.57	122.33	128.89
2	D	800	AGS	N3-C2-N1	-8.30	122.54	128.89
2	B	800	AGS	N3-C2-N1	-8.22	122.60	128.89
2	F	800	AGS	N3-C2-N1	-7.91	122.84	128.89
2	E	800	AGS	N3-C2-N1	-7.66	123.03	128.89
2	C	800	AGS	N3-C2-N1	-7.59	123.08	128.89
2	B	800	AGS	C2'-C1'-N9	-3.41	109.08	114.29
2	C	800	AGS	C2'-C1'-N9	-3.38	109.12	114.29
2	E	800	AGS	C2'-C1'-N9	-3.33	109.20	114.29
2	C	800	AGS	C4-C5-N7	-3.21	106.53	109.48
2	B	800	AGS	PA-O3A-PB	-3.04	124.19	132.73
2	A	800	AGS	PA-O3A-PB	-2.96	124.42	132.73
2	D	800	AGS	C2'-C1'-N9	-2.83	109.96	114.29
2	A	800	AGS	C4-C5-N7	-2.78	106.92	109.48
2	C	800	AGS	PA-O3A-PB	-2.77	124.95	132.73
2	F	800	AGS	C2'-C1'-N9	-2.64	110.27	114.29
2	B	800	AGS	C4-C5-N7	-2.64	107.06	109.48
2	F	800	AGS	C4-C5-N7	-2.57	107.11	109.48
2	E	800	AGS	PA-O3A-PB	-2.55	125.56	132.73
2	D	800	AGS	PA-O3A-PB	-2.53	125.62	132.73
2	E	800	AGS	PB-O3B-PG	-2.52	124.22	132.67
2	A	800	AGS	PB-O3B-PG	-2.49	124.32	132.67
2	A	800	AGS	C2'-C1'-N9	-2.37	110.67	114.29
2	C	800	AGS	PB-O3B-PG	-2.37	124.73	132.67
2	F	800	AGS	PA-O3A-PB	-2.29	126.28	132.73
2	F	800	AGS	PB-O3B-PG	-2.08	125.70	132.67
2	D	800	AGS	C2-N1-C6	2.08	122.48	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	AGS	1	0
2	B	800	AGS	1	0
2	C	800	AGS	1	0
2	D	800	AGS	1	0
2	E	800	AGS	1	0
2	F	800	AGS	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	451/489 (92%)	0.28	19 (4%)	40	28	62, 65, 67, 72	0
1	B	451/489 (92%)	0.19	10 (2%)	65	54	62, 65, 67, 71	0
1	C	451/489 (92%)	0.21	11 (2%)	62	50	62, 65, 67, 70	0
1	D	451/489 (92%)	0.38	27 (5%)	25	15	62, 65, 67, 71	0
1	E	451/489 (92%)	0.31	27 (5%)	25	15	62, 65, 67, 77	0
1	F	451/489 (92%)	0.23	9 (1%)	68	58	62, 65, 67, 70	0
All	All	2706/2934 (92%)	0.27	103 (3%)	44	32	62, 65, 67, 77	0

All (103) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	158	MET	4.5
1	E	106	PRO	4.3
1	D	169	ASP	4.1
1	E	158	MET	3.9
1	D	114	ILE	3.8
1	C	462	SER	3.7
1	E	173	TYR	3.7
1	F	114	ILE	3.6
1	E	169	ASP	3.5
1	E	52	PHE	3.5
1	A	128	GLY	3.5
1	E	114	ILE	3.4
1	E	462	SER	3.4
1	D	32	ILE	3.3
1	E	171	SER	3.3
1	A	109	LYS	3.3
1	B	462	SER	3.3
1	D	187	GLU	3.2
1	D	57	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	106	PRO	3.2
1	A	171	SER	3.2
1	F	113	ARG	3.1
1	D	183	HIS	3.1
1	A	72	LEU	3.1
1	A	317	HIS	3.1
1	C	461	PRO	3.1
1	A	169	ASP	3.1
1	D	173	TYR	3.1
1	D	52	PHE	3.0
1	D	141	GLU	2.9
1	A	395	ASP	2.9
1	C	317	HIS	2.9
1	F	158	MET	2.9
1	E	179	ASP	2.8
1	E	107	ASP	2.8
1	C	158	MET	2.8
1	E	19	GLN	2.8
1	E	175	ILE	2.8
1	A	402	GLU	2.8
1	D	113	ARG	2.7
1	E	317	HIS	2.7
1	D	159	ARG	2.7
1	A	107	ASP	2.7
1	D	107	ASP	2.6
1	E	72	LEU	2.6
1	B	395	ASP	2.6
1	E	57	VAL	2.6
1	E	69	CYS	2.6
1	A	127	THR	2.6
1	D	41	LEU	2.6
1	C	126	ILE	2.6
1	F	112	LYS	2.5
1	C	128	GLY	2.5
1	C	187	GLU	2.5
1	F	169	ASP	2.5
1	A	461	PRO	2.5
1	D	175	ILE	2.5
1	B	158	MET	2.5
1	D	462	SER	2.4
1	D	188	PRO	2.4
1	E	51	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	171	SER	2.4
1	F	141	GLU	2.4
1	D	51	LEU	2.4
1	E	32	ILE	2.4
1	E	108	VAL	2.4
1	F	179	ASP	2.4
1	B	461	PRO	2.4
1	D	126	ILE	2.4
1	D	108	VAL	2.4
1	C	14	THR	2.4
1	E	70	ILE	2.3
1	B	317	HIS	2.3
1	D	317	HIS	2.3
1	A	398	GLN	2.3
1	B	429	LEU	2.2
1	A	108	VAL	2.2
1	F	317	HIS	2.2
1	C	68	VAL	2.2
1	D	134	TYR	2.2
1	A	399	VAL	2.2
1	D	163	PHE	2.2
1	E	174	CYS	2.2
1	B	32	ILE	2.2
1	D	71	VAL	2.2
1	C	314	GLU	2.2
1	E	71	VAL	2.1
1	A	56	THR	2.1
1	E	73	SER	2.1
1	A	106	PRO	2.1
1	B	398	GLN	2.1
1	B	314	GLU	2.1
1	A	429	LEU	2.1
1	E	141	GLU	2.1
1	C	113	ARG	2.1
1	D	115	HIS	2.1
1	E	53	ARG	2.1
1	D	127	THR	2.0
1	A	199	ASN	2.0
1	E	43	GLN	2.0
1	B	52	PHE	2.0
1	E	461	PRO	2.0
1	A	462	SER	2.0

## 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	AGS	A	800	31/31	0.97	0.17	-0.99	53,60,62,64	0
2	AGS	B	800	31/31	0.98	0.14	-1.47	51,60,63,65	0
2	AGS	F	800	31/31	0.98	0.13	-1.64	51,60,62,64	0
2	AGS	D	800	31/31	0.98	0.12	-1.66	53,60,62,65	0
2	AGS	C	800	31/31	0.98	0.14	-1.88	53,61,62,65	0
2	AGS	E	800	31/31	0.99	0.15	-1.88	51,60,62,64	0
3	MG	D	801	1/1	0.96	0.12	-	55,55,55,55	0
3	MG	B	801	1/1	0.97	0.10	-	55,55,55,55	0
3	MG	E	801	1/1	0.99	0.14	-	54,54,54,54	0
3	MG	F	801	1/1	0.97	0.09	-	55,55,55,55	0
3	MG	C	801	1/1	0.98	0.12	-	54,54,54,54	0
3	MG	A	801	1/1	0.96	0.18	-	55,55,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.