



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:45 PM GMT

PDB ID : 1GTP  
Title : GTP CYCLOHYDROLASE I  
Authors : Nar, H.; Huber, R.; Meining, W.; Bacher, A.  
Deposited on : 1995-09-16  
Resolution : 3.00 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.

---

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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

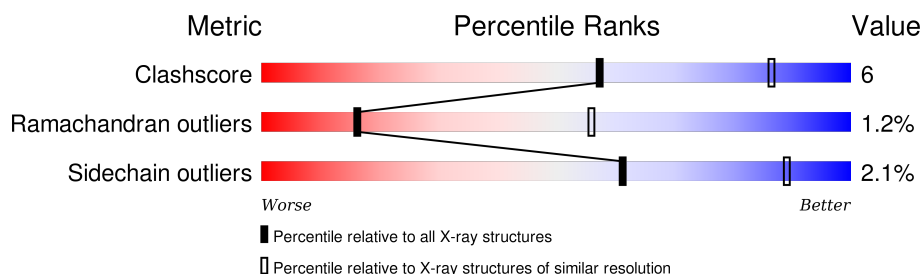
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	221	<div> <div>82%</div> <div>17%</div> </div>
1	B	221	<div> <div>84%</div> <div>15%</div> </div>
1	C	221	<div> <div>82%</div> <div>17%</div> </div>
1	D	221	<div> <div>86%</div> <div>13%</div> </div>
1	E	221	<div> <div>83%</div> <div>15%</div> </div>
1	F	221	<div> <div>81%</div> <div>18%</div> </div>
1	G	221	<div> <div>84%</div> <div>16%</div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	H	221	 81% 18% .
1	I	221	 85% 15%
1	J	221	 85% 14%
1	K	221	 83% 16% .
1	L	221	 80% 19%
1	M	221	 82% 17% .
1	N	221	 81% 18% .
1	O	221	 82% 17% .
1	P	221	 82% 17% .
1	Q	221	 81% 18% .
1	R	221	 83% 17%
1	S	221	 85% 14% .
1	T	221	 81% 19%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 43780 atoms, of which 8720 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 GTP CYCLOHYDROLASE I.

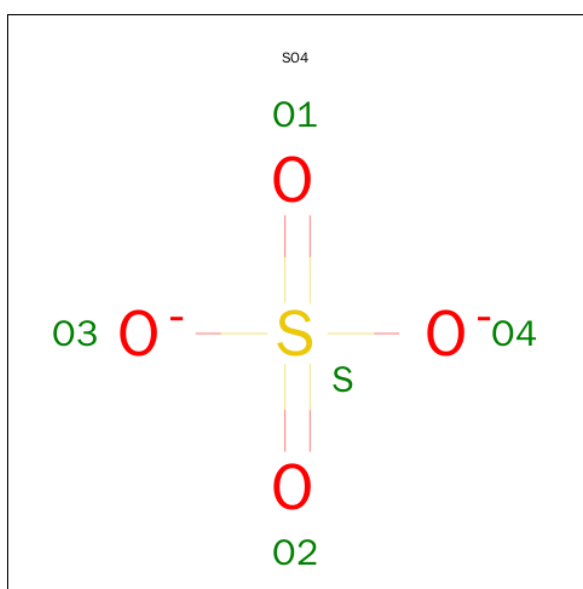
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	B	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	C	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	D	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	E	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	F	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	G	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	H	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	I	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	J	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	K	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	L	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	M	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	N	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	O	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	P	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			

*Continued on next page...*

Continued from previous page...

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	R	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	S	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			
1	T	221	Total	C	H	N	O	S	72	0	0
			2136	1088	404	309	326	9			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	H	1	Total	O	S	0	0
			5	4	1		
2	I	1	Total	O	S	0	0
			5	4	1		
2	J	1	Total	O	S	0	0
			5	4	1		
2	K	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	L	1	Total	O	S	0	0
			5	4	1		
2	N	1	Total	O	S	0	0
			5	4	1		
2	O	1	Total	O	S	0	0
			5	4	1		
2	P	1	Total	O	S	0	0
			5	4	1		
2	Q	1	Total	O	S	0	0
			5	4	1		
2	R	1	Total	O	S	0	0
			5	4	1		
2	S	1	Total	O	S	0	0
			5	4	1		
2	T	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	16	Total	H	O	0	0
			48	32	16		
3	B	14	Total	H	O	0	0
			42	28	14		
3	C	18	Total	H	O	0	0
			54	36	18		
3	D	16	Total	H	O	0	0
			48	32	16		
3	E	16	Total	H	O	0	0
			48	32	16		
3	F	16	Total	H	O	0	0
			48	32	16		

*Continued on next page...*

*Continued from previous page...*

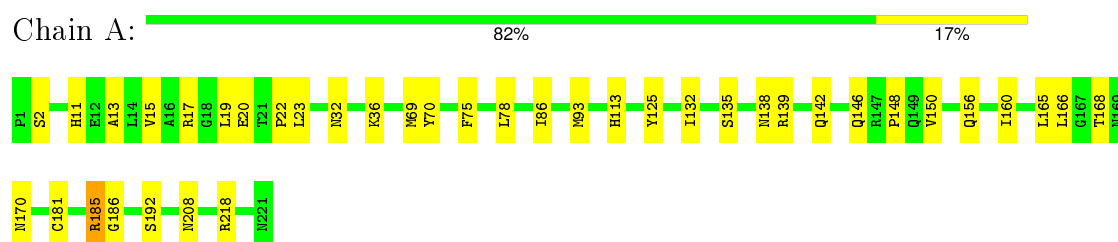
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	G	16	Total 48	H 32	O 16	0	0
3	H	16	Total 48	H 32	O 16	0	0
3	I	16	Total 48	H 32	O 16	0	0
3	J	16	Total 48	H 32	O 16	0	0
3	K	15	Total 45	H 30	O 15	0	0
3	L	17	Total 51	H 34	O 17	0	0
3	M	15	Total 45	H 30	O 15	0	0
3	N	17	Total 51	H 34	O 17	0	0
3	O	16	Total 48	H 32	O 16	0	0
3	P	17	Total 51	H 34	O 17	0	0
3	Q	15	Total 45	H 30	O 15	0	0
3	R	17	Total 51	H 34	O 17	0	0
3	S	16	Total 48	H 32	O 16	0	0
3	T	15	Total 45	H 30	O 15	0	0

### 3 Residue-property plots

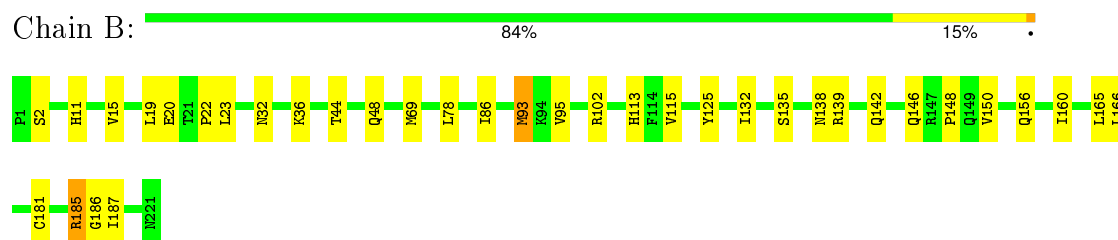
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

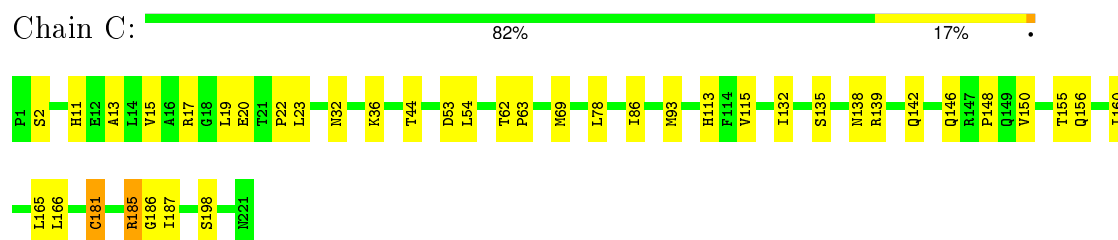
#### • Molecule 1: GTP CYCLOHYDROLASE I



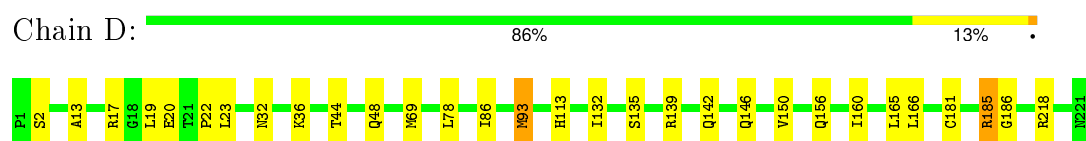
#### • Molecule 1: GTP CYCLOHYDROLASE I



#### • Molecule 1: GTP CYCLOHYDROLASE I

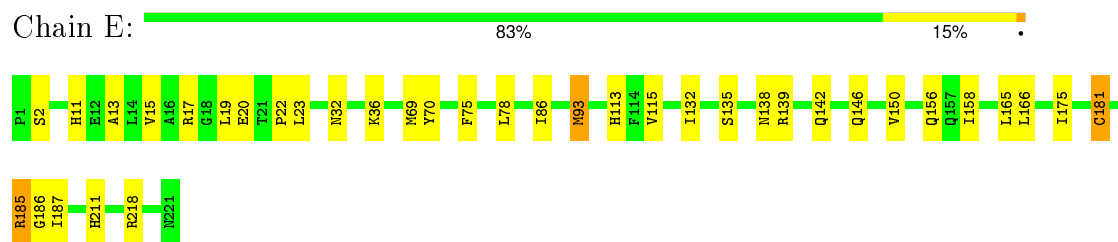


#### • Molecule 1: GTP CYCLOHYDROLASE I

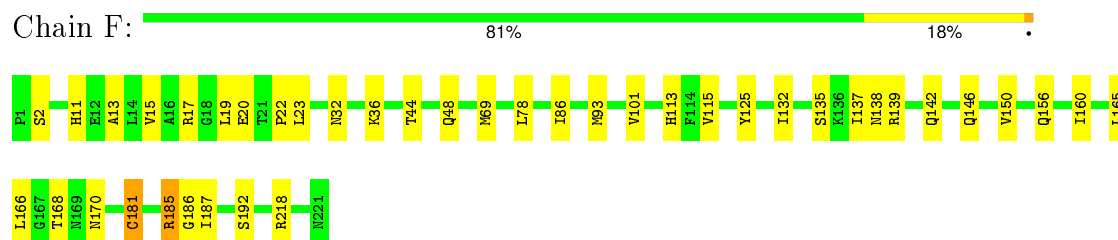


#### • Molecule 1: GTP CYCLOHYDROLASE I

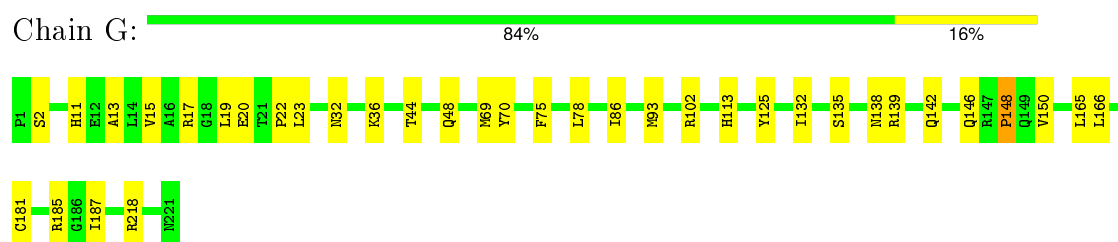




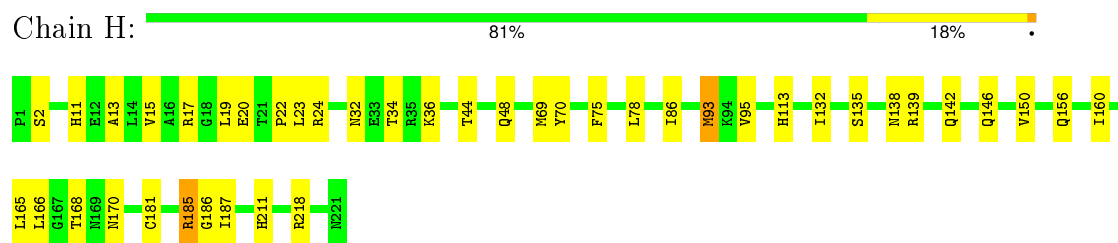
- Molecule 1: GTP CYCLOHYDROLASE I



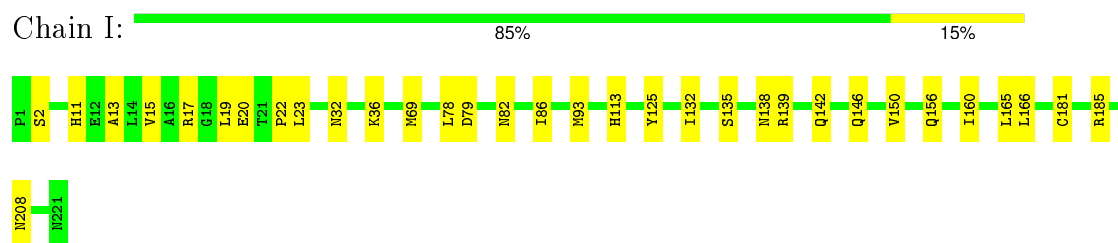
- Molecule 1: GTP CYCLOHYDROLASE I



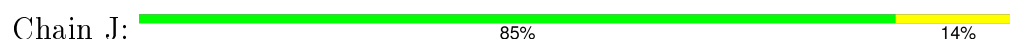
- Molecule 1: GTP CYCLOHYDROLASE I

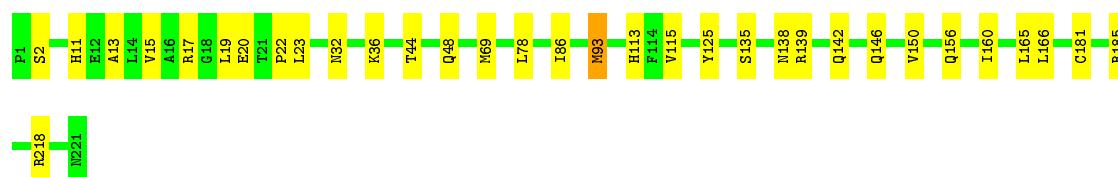


- Molecule 1: GTP CYCLOHYDROLASE I



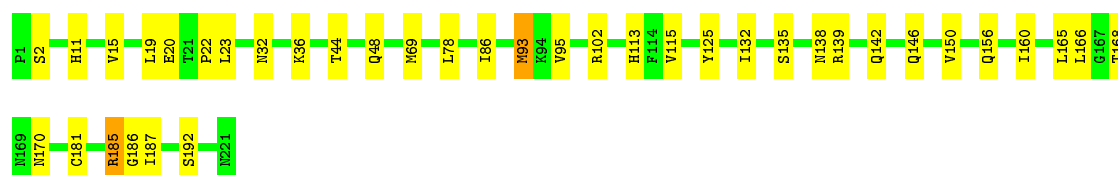
- Molecule 1: GTP CYCLOHYDROLASE I





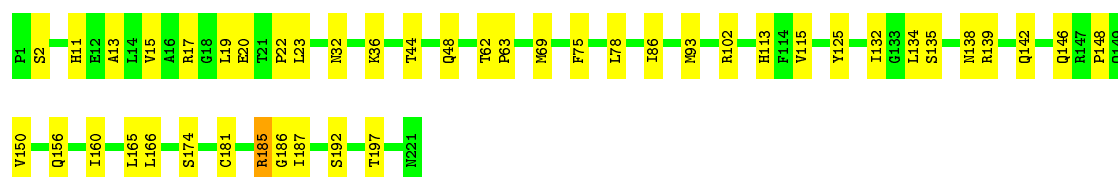
• Molecule 1: GTP CYCLOHYDROLASE I

Chain K: 83% 16%



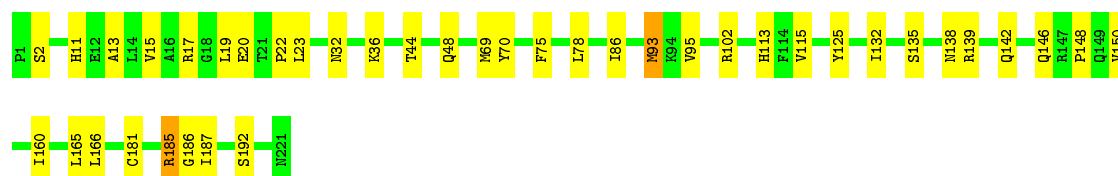
• Molecule 1: GTP CYCLOHYDROLASE I

Chain L: 80% 19%



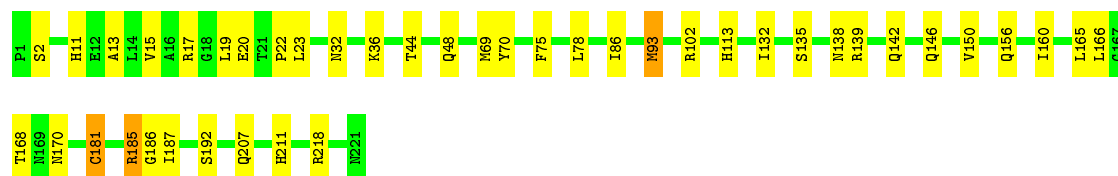
• Molecule 1: GTP CYCLOHYDROLASE I

Chain M: 82% 17%



• Molecule 1: GTP CYCLOHYDROLASE I

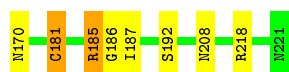
Chain N: 81% 18%



• Molecule 1: GTP CYCLOHYDROLASE I

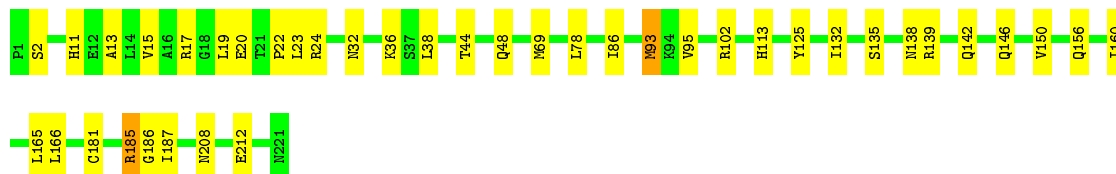
Chain O: 82% 17%





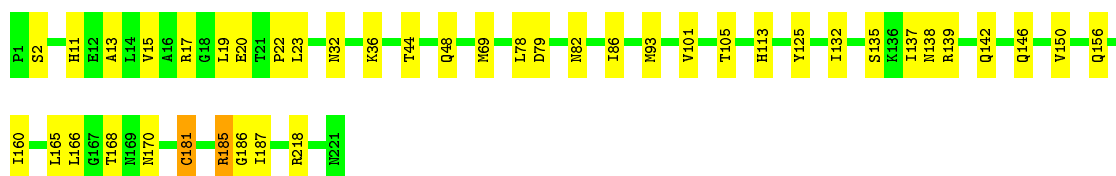
• Molecule 1: GTP CYCLOHYDROLASE I

Chain P: 82% 17%



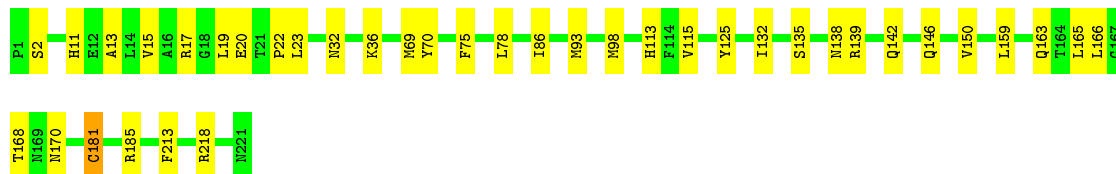
• Molecule 1: GTP CYCLOHYDROLASE I

Chain Q: 81% 18%



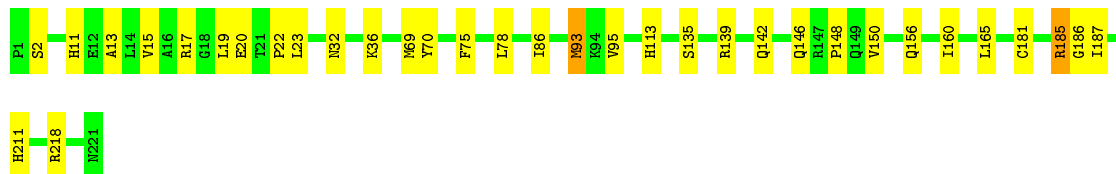
• Molecule 1: GTP CYCLOHYDROLASE I

Chain R: 83% 17%



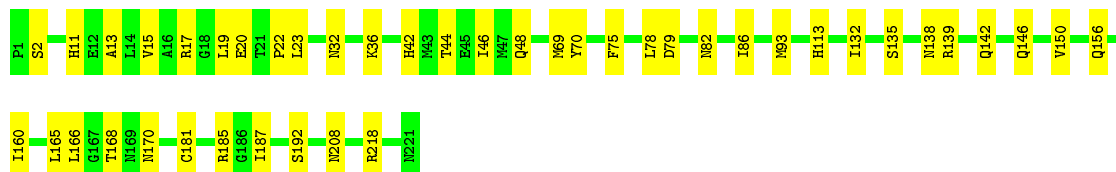
• Molecule 1: GTP CYCLOHYDROLASE I

Chain S: 85% 14%



• Molecule 1: GTP CYCLOHYDROLASE I

Chain T: 81% 19%



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	204.20 Å   210.40 Å   71.80 Å 90.00°   95.80°   90.00°	Depositor
Resolution (Å)	6.00 – 3.00	Depositor
% Data completeness (in resolution range)	92.5 (6.00-3.00)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.189 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	43780	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

## 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: SO4

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	0.40	0/1760	0.73	2/2384 (0.1%)
1	B	0.40	0/1760	0.72	2/2384 (0.1%)
1	C	0.39	0/1760	0.73	2/2384 (0.1%)
1	D	0.40	0/1760	0.73	1/2384 (0.0%)
1	E	0.40	0/1760	0.73	1/2384 (0.0%)
1	F	0.39	0/1760	0.72	1/2384 (0.0%)
1	G	0.41	0/1760	0.73	2/2384 (0.1%)
1	H	0.41	0/1760	0.73	1/2384 (0.0%)
1	I	0.40	0/1760	0.72	1/2384 (0.0%)
1	J	0.41	0/1760	0.73	1/2384 (0.0%)
1	K	0.39	0/1760	0.72	1/2384 (0.0%)
1	L	0.39	0/1760	0.73	1/2384 (0.0%)
1	M	0.39	0/1760	0.73	2/2384 (0.1%)
1	N	0.39	0/1760	0.72	1/2384 (0.0%)
1	O	0.39	0/1760	0.73	2/2384 (0.1%)
1	P	0.40	0/1760	0.73	1/2384 (0.0%)
1	Q	0.38	0/1760	0.71	1/2384 (0.0%)
1	R	0.40	0/1760	0.73	1/2384 (0.0%)
1	S	0.40	0/1760	0.72	2/2384 (0.1%)
1	T	0.40	0/1760	0.71	1/2384 (0.0%)
All	All	0.40	0/35200	0.72	27/47680 (0.1%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	O	150	VAL	N-CA-C	-6.90	92.36	111.00
1	A	150	VAL	N-CA-C	-6.70	92.91	111.00
1	D	150	VAL	N-CA-C	-6.67	92.98	111.00
1	M	150	VAL	N-CA-C	-6.64	93.08	111.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	150	VAL	N-CA-C	-6.61	93.16	111.00
1	R	150	VAL	N-CA-C	-6.58	93.24	111.00
1	C	150	VAL	N-CA-C	-6.50	93.46	111.00
1	I	150	VAL	N-CA-C	-6.49	93.47	111.00
1	T	150	VAL	N-CA-C	-6.46	93.57	111.00
1	L	150	VAL	N-CA-C	-6.45	93.58	111.00
1	G	150	VAL	N-CA-C	-6.45	93.59	111.00
1	K	150	VAL	N-CA-C	-6.40	93.72	111.00
1	B	150	VAL	N-CA-C	-6.38	93.77	111.00
1	F	150	VAL	N-CA-C	-6.38	93.78	111.00
1	N	150	VAL	N-CA-C	-6.38	93.78	111.00
1	J	150	VAL	N-CA-C	-6.20	94.26	111.00
1	E	150	VAL	N-CA-C	-6.17	94.35	111.00
1	P	150	VAL	N-CA-C	-6.15	94.39	111.00
1	H	150	VAL	N-CA-C	-6.13	94.45	111.00
1	S	150	VAL	N-CA-C	-6.01	94.78	111.00
1	M	148	PRO	N-CA-C	-5.20	98.59	112.10
1	B	148	PRO	N-CA-C	-5.18	98.64	112.10
1	C	148	PRO	N-CA-C	-5.13	98.76	112.10
1	A	148	PRO	N-CA-C	-5.09	98.86	112.10
1	S	148	PRO	N-CA-C	-5.07	98.91	112.10
1	O	148	PRO	N-CA-C	-5.06	98.94	112.10
1	G	148	PRO	N-CA-C	-5.05	98.97	112.10

There are no chirality outliers.

There are no planarity outliers.

## 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	1732	404	1766	25	0
1	B	1732	404	1766	23	0
1	C	1732	404	1766	26	0
1	D	1732	404	1766	19	0
1	E	1732	404	1766	22	0
1	F	1732	404	1766	25	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1732	404	1766	20	0
1	H	1732	404	1766	28	0
1	I	1732	404	1766	21	0
1	J	1732	404	1766	18	0
1	K	1732	404	1766	25	0
1	L	1732	404	1766	30	0
1	M	1732	404	1766	28	0
1	N	1732	404	1766	27	0
1	O	1732	404	1766	27	0
1	P	1732	404	1766	29	0
1	Q	1732	404	1766	24	0
1	R	1732	404	1766	24	0
1	S	1732	404	1766	22	0
1	T	1732	404	1766	27	0
2	A	10	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	0	0
2	I	5	0	0	0	0
2	J	5	0	0	0	0
2	K	5	0	0	0	0
2	L	10	0	0	0	0
2	N	5	0	0	0	0
2	O	5	0	0	0	0
2	P	5	0	0	0	0
2	Q	5	0	0	0	0
2	R	5	0	0	0	0
2	S	5	0	0	0	0
2	T	5	0	0	0	0
3	A	16	32	0	0	0
3	B	14	28	0	0	0
3	C	18	36	0	0	0
3	D	16	32	0	0	0
3	E	16	32	0	0	0
3	F	16	32	0	0	0
3	G	16	32	0	0	0
3	H	16	32	0	0	0
3	I	16	32	0	0	0
3	J	16	32	0	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	K	15	30	0	0	0
3	L	17	34	0	1	0
3	M	15	30	0	0	0
3	N	17	34	0	0	0
3	O	16	32	0	0	0
3	P	17	34	0	0	0
3	Q	15	30	0	1	0
3	R	17	34	0	0	0
3	S	16	32	0	0	0
3	T	15	30	0	0	0
All	All	35060	8720	35320	404	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 6.

All (404) 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:O:86:ILE:HG12	1:O:165:LEU:HD13	1.68	0.76
1:R:19:LEU:HD21	1:S:93:MET:HA	1.67	0.76
1:N:86:ILE:HG12	1:N:165:LEU:HD13	1.67	0.75
1:G:19:LEU:HD21	1:H:93:MET:HA	1.71	0.72
1:A:86:ILE:HG12	1:A:165:LEU:HD13	1.73	0.71
1:P:86:ILE:HG12	1:P:165:LEU:HD13	1.74	0.70
1:E:86:ILE:HG12	1:E:165:LEU:HD13	1.75	0.68
1:C:86:ILE:HG12	1:C:165:LEU:HD13	1.74	0.68
1:S:86:ILE:HG12	1:S:165:LEU:HD13	1.75	0.67
1:K:86:ILE:HG12	1:K:165:LEU:HD13	1.75	0.67
1:L:23:LEU:HD21	1:L:78:LEU:HD22	1.76	0.67
1:N:187:ILE:HD12	1:O:139:ARG:HG2	1.77	0.67
1:I:86:ILE:HG12	1:I:165:LEU:HD13	1.75	0.67
1:L:19:LEU:HD21	1:M:93:MET:HA	1.76	0.67
1:H:187:ILE:HD12	1:I:139:ARG:HG2	1.77	0.67
1:K:23:LEU:HD21	1:K:78:LEU:HD22	1.76	0.66
1:R:19:LEU:CD2	1:S:93:MET:HA	2.25	0.65
1:J:86:ILE:HG12	1:J:165:LEU:HD13	1.78	0.65
1:I:135:SER:O	1:I:139:ARG:HG3	1.98	0.64
1:S:187:ILE:HD12	1:T:139:ARG:HG2	1.78	0.64
1:Q:142:GLN:O	1:Q:146:GLN:HG2	1.97	0.64
1:B:86:ILE:HG12	1:B:165:LEU:HD13	1.79	0.64
1:L:86:ILE:HG12	1:L:165:LEU:HD13	1.81	0.63

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:ILE:HG12	1:F:165:LEU:HD13	1.81	0.62
1:Q:86:ILE:HG12	1:Q:165:LEU:HD13	1.81	0.62
1:C:19:LEU:HD21	1:D:93:MET:HA	1.81	0.62
1:M:142:GLN:O	1:M:146:GLN:HG2	2.00	0.62
1:D:86:ILE:HG12	1:D:165:LEU:HD13	1.80	0.61
1:G:19:LEU:CD2	1:H:93:MET:HA	2.30	0.61
1:L:19:LEU:CD2	1:M:93:MET:HA	2.31	0.61
1:I:23:LEU:HD21	1:I:78:LEU:HD22	1.83	0.60
1:D:23:LEU:HD21	1:D:78:LEU:HD22	1.82	0.60
1:R:86:ILE:HG12	1:R:165:LEU:HD13	1.82	0.60
1:P:93:MET:HA	1:T:19:LEU:HD21	1.83	0.60
1:P:23:LEU:HD21	1:P:78:LEU:HD22	1.83	0.60
1:E:142:GLN:O	1:E:146:GLN:HG2	2.01	0.60
1:O:23:LEU:HD21	1:O:78:LEU:HD22	1.83	0.60
1:T:86:ILE:HG12	1:T:165:LEU:HD13	1.84	0.60
1:L:142:GLN:O	1:L:146:GLN:HG2	2.02	0.60
1:D:142:GLN:O	1:D:146:GLN:HG2	2.02	0.59
1:C:23:LEU:HD21	1:C:78:LEU:HD22	1.84	0.59
1:H:142:GLN:O	1:H:146:GLN:HG2	2.02	0.59
1:I:142:GLN:O	1:I:146:GLN:HG2	2.02	0.59
1:S:135:SER:O	1:S:139:ARG:HG3	2.02	0.59
1:T:23:LEU:HD21	1:T:78:LEU:HD22	1.85	0.59
1:A:113:HIS:HB3	1:J:69:MET:HE1	1.84	0.59
1:T:135:SER:O	1:T:139:ARG:HG3	2.03	0.58
1:B:142:GLN:O	1:B:146:GLN:HG2	2.02	0.58
1:M:23:LEU:HD21	1:M:78:LEU:HD22	1.83	0.58
1:G:86:ILE:HG12	1:G:165:LEU:HD13	1.84	0.58
1:Q:135:SER:O	1:Q:139:ARG:HG3	2.04	0.58
1:R:23:LEU:HD21	1:R:78:LEU:HD22	1.84	0.58
1:C:19:LEU:CD2	1:D:93:MET:HA	2.33	0.58
1:S:142:GLN:O	1:S:146:GLN:HG2	2.03	0.58
1:F:135:SER:O	1:F:139:ARG:HG3	2.04	0.58
1:C:142:GLN:O	1:C:146:GLN:HG2	2.04	0.58
1:N:142:GLN:O	1:N:146:GLN:HG2	2.04	0.58
1:O:135:SER:O	1:O:139:ARG:HG3	2.03	0.57
1:B:11:HIS:O	1:B:15:VAL:HG23	2.05	0.57
1:B:69:MET:HE1	1:I:113:HIS:HB3	1.85	0.57
1:B:135:SER:O	1:B:139:ARG:HG3	2.04	0.57
1:M:86:ILE:HG12	1:M:165:LEU:HD13	1.86	0.57
1:H:135:SER:O	1:H:139:ARG:HG3	2.04	0.57
1:N:23:LEU:HD21	1:N:78:LEU:HD22	1.86	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:ASN:O	1:C:36:LYS:HG3	2.05	0.57
1:B:23:LEU:HD21	1:B:78:LEU:HD22	1.86	0.56
1:J:23:LEU:HD21	1:J:78:LEU:HD22	1.87	0.56
1:G:23:LEU:HD21	1:G:78:LEU:HD22	1.86	0.56
1:H:23:LEU:HD21	1:H:78:LEU:HD22	1.86	0.56
1:N:69:MET:HE1	1:Q:113:HIS:HB3	1.88	0.56
1:Q:19:LEU:HD12	1:Q:160:ILE:HD11	1.88	0.56
1:C:135:SER:O	1:C:139:ARG:HG3	2.06	0.56
1:F:23:LEU:HD21	1:F:78:LEU:HD22	1.87	0.56
1:K:11:HIS:O	1:K:15:VAL:HG23	2.06	0.56
1:L:135:SER:O	1:L:139:ARG:HG3	2.06	0.56
1:M:135:SER:O	1:M:139:ARG:HG3	2.06	0.56
1:E:23:LEU:HD21	1:E:78:LEU:HD22	1.87	0.56
1:A:142:GLN:O	1:A:146:GLN:HG2	2.05	0.56
1:C:11:HIS:O	1:C:15:VAL:HG23	2.06	0.55
1:K:142:GLN:O	1:K:146:GLN:HG2	2.06	0.55
1:P:93:MET:HA	1:T:19:LEU:CD2	2.36	0.55
1:G:11:HIS:O	1:G:15:VAL:HG23	2.06	0.55
1:K:93:MET:HA	1:O:19:LEU:CD2	2.37	0.55
1:K:187:ILE:HD12	1:L:139:ARG:HG2	1.88	0.55
1:A:135:SER:O	1:A:139:ARG:HG3	2.06	0.55
1:I:19:LEU:HD21	1:J:93:MET:HA	1.88	0.55
1:H:86:ILE:HG12	1:H:165:LEU:HD13	1.88	0.55
1:A:23:LEU:HD21	1:A:78:LEU:HD22	1.87	0.55
1:R:135:SER:O	1:R:139:ARG:HG3	2.08	0.54
1:L:69:MET:HE1	1:S:113:HIS:HB3	1.88	0.54
1:N:113:HIS:HB3	1:Q:69:MET:HE1	1.87	0.54
1:S:23:LEU:HD21	1:S:78:LEU:HD22	1.89	0.54
1:K:69:MET:HE1	1:T:113:HIS:HB3	1.89	0.54
1:J:142:GLN:O	1:J:146:GLN:HG2	2.08	0.54
1:R:142:GLN:O	1:R:146:GLN:HG2	2.07	0.54
1:T:142:GLN:O	1:T:146:GLN:HG2	2.07	0.54
1:O:69:MET:HE1	1:P:113:HIS:HB3	1.90	0.54
1:A:19:LEU:CD2	1:B:93:MET:HA	2.39	0.53
1:E:69:MET:HE1	1:F:113:HIS:HB3	1.91	0.53
1:P:11:HIS:O	1:P:15:VAL:HG23	2.09	0.53
1:J:135:SER:O	1:J:139:ARG:HG3	2.08	0.53
1:K:93:MET:HA	1:O:19:LEU:HD21	1.90	0.53
1:H:34:THR:HG22	1:P:38:LEU:HD23	1.89	0.53
1:J:11:HIS:O	1:J:15:VAL:HG23	2.10	0.52
1:K:135:SER:O	1:K:139:ARG:HG3	2.10	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:11:HIS:O	1:Q:15:VAL:HG23	2.09	0.52
1:L:32:ASN:O	1:L:36:LYS:HG3	2.10	0.51
1:H:32:ASN:O	1:H:36:LYS:HG3	2.09	0.51
1:M:113:HIS:HB3	1:R:69:MET:HE1	1.92	0.51
1:D:135:SER:O	1:D:139:ARG:HG3	2.10	0.51
1:Q:132:ILE:HB	1:Q:166:LEU:HD21	1.91	0.51
1:F:32:ASN:O	1:F:36:LYS:HG3	2.10	0.51
1:F:142:GLN:O	1:F:146:GLN:HG2	2.09	0.51
1:G:70:TYR:O	1:G:75:PHE:HB2	2.10	0.51
1:Q:32:ASN:O	1:Q:36:LYS:HG3	2.11	0.51
1:A:32:ASN:O	1:A:36:LYS:HG3	2.10	0.51
1:P:32:ASN:O	1:P:36:LYS:HG3	2.10	0.51
1:K:113:HIS:HB3	1:T:69:MET:HE1	1.93	0.51
1:F:19:LEU:HD12	1:F:160:ILE:HD11	1.93	0.50
1:J:32:ASN:O	1:J:36:LYS:HG3	2.11	0.50
1:S:11:HIS:O	1:S:15:VAL:HG23	2.10	0.50
1:C:69:MET:HE1	1:H:113:HIS:HB3	1.93	0.50
1:B:187:ILE:HD12	1:C:139:ARG:HG2	1.93	0.50
1:P:13:ALA:O	1:P:17:ARG:HD3	2.12	0.50
1:I:138:ASN:HD22	1:I:138:ASN:H	1.60	0.50
1:I:19:LEU:CD2	1:J:93:MET:HA	2.42	0.50
1:A:139:ARG:HG2	1:E:187:ILE:HD12	1.94	0.50
1:O:142:GLN:O	1:O:146:GLN:HG2	2.11	0.50
1:N:19:LEU:HD13	1:N:156:GLN:HB3	1.93	0.50
1:L:115:VAL:HG21	1:S:69:MET:HE1	1.94	0.50
1:O:32:ASN:O	1:O:36:LYS:HG3	2.11	0.50
1:O:113:HIS:HB3	1:P:69:MET:HE1	1.93	0.50
1:C:113:HIS:HB3	1:H:69:MET:HE1	1.93	0.50
1:A:19:LEU:HD12	1:A:160:ILE:HD11	1.94	0.49
1:S:19:LEU:HD12	1:S:160:ILE:CD1	2.41	0.49
1:S:19:LEU:HD12	1:S:160:ILE:HD11	1.94	0.49
1:E:135:SER:O	1:E:139:ARG:HG3	2.12	0.49
1:A:19:LEU:HD12	1:A:160:ILE:CD1	2.42	0.49
1:Q:23:LEU:HD21	1:Q:78:LEU:HD22	1.93	0.49
1:G:135:SER:O	1:G:139:ARG:HG3	2.12	0.49
1:L:11:HIS:O	1:L:15:VAL:HG23	2.12	0.49
1:D:113:HIS:HB3	1:G:69:MET:HE1	1.95	0.49
1:E:113:HIS:HB3	1:F:69:MET:HE1	1.94	0.49
1:B:138:ASN:H	1:B:138:ASN:HD22	1.60	0.49
1:N:135:SER:O	1:N:139:ARG:HG3	2.13	0.49
1:J:19:LEU:HD12	1:J:160:ILE:HD11	1.93	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:19:LEU:HD12	1:N:160:ILE:HD11	1.94	0.49
1:A:19:LEU:HD21	1:B:93:MET:HA	1.93	0.49
1:R:32:ASN:O	1:R:36:LYS:HG3	2.12	0.49
1:K:125:TYR:CD2	1:K:166:LEU:HD13	2.48	0.49
1:O:11:HIS:O	1:O:15:VAL:HG23	2.13	0.49
1:Q:113:HIS:HB2	1:Q:181:CYS:SG	2.52	0.48
1:Q:187:ILE:HD12	1:R:139:ARG:HG2	1.95	0.48
1:F:19:LEU:HD12	1:F:160:ILE:CD1	2.43	0.48
1:P:44:THR:O	1:P:48:GLN:HG3	2.13	0.48
1:J:19:LEU:HD12	1:J:160:ILE:CD1	2.43	0.48
1:T:11:HIS:O	1:T:15:VAL:HG23	2.13	0.48
1:H:19:LEU:HD12	1:H:160:ILE:CD1	2.42	0.48
1:P:19:LEU:HD12	1:P:160:ILE:HD11	1.95	0.48
1:T:19:LEU:HD12	1:T:160:ILE:CD1	2.44	0.48
1:S:211:HIS:CE1	1:T:208:ASN:OD1	2.66	0.48
1:A:69:MET:HE1	1:J:113:HIS:HB3	1.96	0.48
1:E:70:TYR:O	1:E:75:PHE:HB2	2.14	0.48
1:F:13:ALA:O	1:F:17:ARG:HD3	2.13	0.48
1:N:11:HIS:O	1:N:15:VAL:HG23	2.14	0.48
1:L:132:ILE:HB	1:L:166:LEU:HD21	1.94	0.48
1:B:113:HIS:HB3	1:I:69:MET:HE1	1.96	0.47
1:M:11:HIS:O	1:M:15:VAL:HG23	2.14	0.47
1:H:138:ASN:H	1:H:138:ASN:HD22	1.61	0.47
1:G:142:GLN:O	1:G:146:GLN:HG2	2.14	0.47
1:O:19:LEU:HD12	1:O:160:ILE:CD1	2.44	0.47
1:M:69:MET:HE1	1:R:113:HIS:HB3	1.95	0.47
1:Q:19:LEU:HD13	1:Q:156:GLN:HB3	1.96	0.47
1:B:19:LEU:HD12	1:B:160:ILE:HD11	1.95	0.47
1:E:138:ASN:HD22	1:E:138:ASN:H	1.62	0.47
1:N:70:TYR:O	1:N:75:PHE:HB2	2.15	0.47
1:M:115:VAL:HG21	1:R:69:MET:HE1	1.95	0.47
1:N:19:LEU:HD12	1:N:160:ILE:CD1	2.44	0.47
1:N:32:ASN:O	1:N:36:LYS:HG3	2.15	0.47
1:S:13:ALA:O	1:S:17:ARG:HD3	2.15	0.47
1:T:13:ALA:O	1:T:17:ARG:HD3	2.15	0.47
1:N:132:ILE:HB	1:N:166:LEU:HD21	1.97	0.47
1:M:32:ASN:O	1:M:36:LYS:HG3	2.15	0.47
1:I:32:ASN:O	1:I:36:LYS:HG3	2.15	0.47
1:D:44:THR:O	1:D:48:GLN:HG3	2.14	0.47
1:P:187:ILE:HD12	1:Q:139:ARG:HG2	1.96	0.47
1:C:19:LEU:HD12	1:C:160:ILE:CD1	2.45	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:125:TYR:CD2	1:Q:166:LEU:HD13	2.50	0.47
1:J:44:THR:O	1:J:48:GLN:HG3	2.15	0.47
1:N:168:THR:HG22	1:N:170:ASN:H	1.80	0.46
1:G:32:ASN:O	1:G:36:LYS:HG3	2.15	0.46
1:F:101:VAL:HG21	1:F:137:ILE:HD12	1.97	0.46
1:O:185:ARG:HD2	1:P:69:MET:HE2	1.97	0.46
1:H:11:HIS:O	1:H:15:VAL:HG23	2.15	0.46
1:P:135:SER:O	1:P:139:ARG:HG3	2.15	0.46
1:T:44:THR:O	1:T:48:GLN:HG3	2.15	0.46
1:A:11:HIS:O	1:A:15:VAL:HG23	2.16	0.46
1:F:132:ILE:HB	1:F:166:LEU:HD21	1.97	0.46
1:L:19:LEU:HD12	1:L:160:ILE:HD11	1.98	0.46
1:H:13:ALA:O	1:H:17:ARG:HD3	2.16	0.46
1:C:138:ASN:HD22	1:C:138:ASN:H	1.64	0.46
1:F:138:ASN:H	1:F:138:ASN:HD22	1.63	0.46
1:E:132:ILE:HB	1:E:166:LEU:HD21	1.97	0.46
1:R:168:THR:HG22	1:R:170:ASN:H	1.80	0.46
1:S:19:LEU:HD13	1:S:156:GLN:HB3	1.98	0.46
1:H:132:ILE:HB	1:H:166:LEU:HD21	1.97	0.46
1:F:19:LEU:HD13	1:F:156:GLN:HB3	1.98	0.45
1:B:19:LEU:HD12	1:B:160:ILE:CD1	2.47	0.45
1:B:185:ARG:HG2	1:B:186:GLY:H	1.81	0.45
1:C:187:ILE:HD12	1:D:139:ARG:HA	1.97	0.45
1:H:19:LEU:HD12	1:H:160:ILE:HD11	1.99	0.45
1:M:19:LEU:HD12	1:M:160:ILE:HD11	1.98	0.45
1:K:19:LEU:HD13	1:K:156:GLN:HB3	1.99	0.45
1:A:138:ASN:H	1:A:138:ASN:HD22	1.64	0.45
1:O:168:THR:HG22	1:O:170:ASN:H	1.81	0.45
1:K:168:THR:HG22	1:K:170:ASN:H	1.81	0.45
1:M:13:ALA:O	1:M:17:ARG:HD3	2.17	0.45
1:C:53:ASP:HA	1:H:24:ARG:HG3	1.98	0.45
1:K:19:LEU:HD12	1:K:160:ILE:CD1	2.47	0.45
1:D:32:ASN:O	1:D:36:LYS:HG3	2.16	0.45
1:F:11:HIS:O	1:F:15:VAL:HG23	2.17	0.45
1:T:19:LEU:HD12	1:T:160:ILE:HD11	1.98	0.45
1:C:113:HIS:HB2	1:C:181:CYS:SG	2.57	0.45
1:L:75:PHE:CE1	1:L:148:PRO:HG3	2.52	0.45
1:I:11:HIS:O	1:I:15:VAL:HG23	2.17	0.45
1:E:11:HIS:O	1:E:15:VAL:HG23	2.17	0.45
1:F:113:HIS:HB2	1:F:181:CYS:SG	2.56	0.44
1:O:185:ARG:HG2	1:O:186:GLY:N	2.32	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:19:LEU:HD12	1:P:160:ILE:CD1	2.48	0.44
1:A:185:ARG:HG2	1:A:186:GLY:N	2.32	0.44
1:R:70:TYR:O	1:R:75:PHE:HB2	2.17	0.44
1:B:132:ILE:HB	1:B:166:LEU:HD21	1.99	0.44
1:Q:101:VAL:HG21	1:Q:137:ILE:HD12	1.98	0.44
1:T:42:HIS:O	1:T:46:ILE:HG13	2.17	0.44
1:J:13:ALA:O	1:J:17:ARG:HD3	2.17	0.44
1:D:69:MET:HE1	1:G:113:HIS:HB3	2.00	0.44
1:A:19:LEU:HD23	1:A:19:LEU:HA	1.86	0.44
1:I:19:LEU:HD12	1:I:160:ILE:CD1	2.48	0.44
1:Q:44:THR:O	1:Q:48:GLN:HG3	2.17	0.44
1:L:138:ASN:HD22	1:L:138:ASN:H	1.66	0.44
1:K:93:MET:HB2	1:K:95:VAL:HG23	1.99	0.44
1:N:192:SER:HA	1:O:102:ARG:O	2.17	0.44
1:M:70:TYR:O	1:M:75:PHE:HB2	2.17	0.44
1:A:70:TYR:O	1:A:75:PHE:HB2	2.17	0.44
1:T:19:LEU:HA	1:T:19:LEU:HD23	1.81	0.44
1:O:19:LEU:HD12	1:O:160:ILE:HD11	2.00	0.44
1:L:113:HIS:HB3	1:S:69:MET:HE1	2.00	0.44
1:G:13:ALA:O	1:G:17:ARG:HD3	2.17	0.44
1:G:125:TYR:CD2	1:G:166:LEU:HD13	2.53	0.44
1:H:19:LEU:HD13	1:H:156:GLN:HB3	2.00	0.44
1:P:19:LEU:HD13	1:P:156:GLN:HB3	2.00	0.44
1:B:19:LEU:HD13	1:B:156:GLN:HB3	1.99	0.44
1:F:192:SER:HA	1:G:102:ARG:O	2.17	0.44
1:P:93:MET:HB2	1:P:95:VAL:HG23	1.99	0.44
1:I:19:LEU:HD13	1:I:156:GLN:HB3	1.99	0.44
1:C:13:ALA:O	1:C:17:ARG:HD3	2.17	0.44
1:L:13:ALA:O	1:L:17:ARG:HD3	2.17	0.44
1:B:185:ARG:HG2	1:B:186:GLY:N	2.33	0.44
1:N:13:ALA:O	1:N:17:ARG:HD3	2.18	0.44
1:K:138:ASN:H	1:K:138:ASN:HD22	1.66	0.44
1:T:19:LEU:HD13	1:T:156:GLN:HB3	1.99	0.43
1:N:207:GLN:HG3	1:O:208:ASN:OD1	2.17	0.43
1:T:132:ILE:HB	1:T:166:LEU:HD21	2.00	0.43
1:Q:105:THR:HG23	3:Q:228:HOH:O	2.18	0.43
1:P:138:ASN:H	1:P:138:ASN:HD22	1.66	0.43
1:C:132:ILE:HB	1:C:166:LEU:HD21	1.99	0.43
1:H:211:HIS:CE1	1:I:208:ASN:OD1	2.70	0.43
1:L:187:ILE:HD13	1:M:138:ASN:HB3	2.01	0.43
1:M:44:THR:O	1:M:48:GLN:HG3	2.18	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:102:ARG:O	1:O:192:SER:HA	2.18	0.43
1:T:79:ASP:HB3	1:T:82:ASN:ND2	2.34	0.43
1:P:187:ILE:HD13	1:Q:138:ASN:HB3	2.00	0.43
1:M:19:LEU:HD21	1:N:93:MET:HA	1.99	0.43
1:R:11:HIS:O	1:R:15:VAL:HG23	2.19	0.43
1:N:211:HIS:CE1	1:O:208:ASN:OD1	2.72	0.43
1:O:13:ALA:O	1:O:17:ARG:HD3	2.18	0.43
1:R:13:ALA:O	1:R:17:ARG:HD3	2.18	0.43
1:E:185:ARG:HG2	1:E:186:GLY:H	1.84	0.43
1:E:115:VAL:HG21	1:F:69:MET:HE1	2.01	0.43
1:D:132:ILE:HB	1:D:166:LEU:HD21	2.00	0.43
1:O:113:HIS:HB2	1:O:181:CYS:SG	2.58	0.43
1:L:125:TYR:CD2	1:L:166:LEU:HD13	2.54	0.43
1:J:138:ASN:H	1:J:138:ASN:HD22	1.67	0.43
1:Q:19:LEU:HD12	1:Q:160:ILE:CD1	2.48	0.43
1:F:187:ILE:HD12	1:G:139:ARG:HG2	2.01	0.43
1:H:44:THR:O	1:H:48:GLN:HG3	2.18	0.43
1:G:138:ASN:HD22	1:G:138:ASN:H	1.66	0.43
1:K:115:VAL:HG21	1:T:69:MET:HE1	2.00	0.43
1:F:19:LEU:HD23	1:F:19:LEU:HA	1.84	0.43
1:I:125:TYR:CD2	1:I:166:LEU:HD13	2.52	0.43
1:P:142:GLN:O	1:P:146:GLN:HG2	2.19	0.43
1:E:13:ALA:O	1:E:17:ARG:HD3	2.19	0.43
1:D:185:ARG:HG2	1:D:186:GLY:N	2.33	0.43
1:K:192:SER:HA	1:L:102:ARG:O	2.18	0.43
1:K:138:ASN:HB3	1:O:187:ILE:HD13	2.01	0.43
1:S:32:ASN:O	1:S:36:LYS:HG3	2.18	0.43
1:T:32:ASN:O	1:T:36:LYS:HG3	2.19	0.43
1:A:69:MET:HE1	1:J:115:VAL:HG21	2.01	0.42
1:D:19:LEU:HD12	1:D:160:ILE:CD1	2.48	0.42
1:M:19:LEU:CD2	1:N:93:MET:HA	2.49	0.42
1:P:132:ILE:HB	1:P:166:LEU:HD21	1.99	0.42
1:L:19:LEU:HD13	1:L:156:GLN:HB3	2.01	0.42
1:L:19:LEU:HD12	1:L:160:ILE:CD1	2.50	0.42
1:G:187:ILE:HD12	1:H:139:ARG:HA	2.01	0.42
1:L:185:ARG:HG2	1:L:186:GLY:N	2.34	0.42
1:L:44:THR:O	1:L:48:GLN:HG3	2.19	0.42
1:T:168:THR:HG22	1:T:170:ASN:H	1.83	0.42
1:N:44:THR:O	1:N:48:GLN:HG3	2.18	0.42
1:G:75:PHE:CE1	1:G:148:PRO:HG3	2.55	0.42
1:P:125:TYR:CD2	1:P:166:LEU:HD13	2.55	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:192:SER:HA	1:M:102:ARG:O	2.18	0.42
1:I:13:ALA:O	1:I:17:ARG:HD3	2.19	0.42
1:P:102:ARG:O	1:T:192:SER:HA	2.19	0.42
1:R:132:ILE:HB	1:R:166:LEU:HD21	2.00	0.42
1:K:132:ILE:HB	1:K:166:LEU:HD21	2.01	0.42
1:A:168:THR:HG22	1:A:170:ASN:H	1.83	0.42
1:E:32:ASN:O	1:E:36:LYS:HG3	2.19	0.42
1:M:185:ARG:HG2	1:M:186:GLY:N	2.34	0.42
1:A:132:ILE:HB	1:A:166:LEU:HD21	2.00	0.42
1:L:174:SER:CB	1:L:197:THR:HG22	2.50	0.42
1:B:32:ASN:O	1:B:36:LYS:HG3	2.19	0.42
1:O:185:ARG:HG2	1:O:186:GLY:H	1.84	0.42
1:R:125:TYR:CD2	1:R:166:LEU:HD13	2.55	0.42
1:K:185:ARG:HG2	1:K:186:GLY:H	1.84	0.42
1:B:93:MET:HB2	1:B:95:VAL:HG23	2.02	0.42
1:M:69:MET:HE1	1:R:115:VAL:HG21	2.01	0.42
1:B:125:TYR:CD2	1:B:166:LEU:HD13	2.55	0.42
1:G:44:THR:O	1:G:48:GLN:HG3	2.19	0.42
1:N:138:ASN:HD22	1:N:138:ASN:H	1.67	0.42
1:R:138:ASN:H	1:R:138:ASN:HD22	1.68	0.42
1:M:125:TYR:CD2	1:M:166:LEU:HD13	2.55	0.42
1:L:185:ARG:HG2	1:L:186:GLY:H	1.85	0.42
1:C:155:THR:HG22	1:C:198:SER:OG	2.19	0.42
1:C:19:LEU:HA	1:C:19:LEU:HD23	1.86	0.41
1:F:125:TYR:CD2	1:F:166:LEU:HD13	2.55	0.41
1:P:185:ARG:HG2	1:P:186:GLY:N	2.35	0.41
1:K:44:THR:O	1:K:48:GLN:HG3	2.20	0.41
1:M:93:MET:HB2	1:M:95:VAL:HG23	2.02	0.41
1:B:115:VAL:HG21	1:I:69:MET:HE1	2.02	0.41
1:D:19:LEU:CD2	1:E:93:MET:HA	2.50	0.41
1:A:125:TYR:CD2	1:A:166:LEU:HD13	2.55	0.41
1:O:132:ILE:HB	1:O:166:LEU:HD21	2.01	0.41
1:N:113:HIS:HB2	1:N:181:CYS:SG	2.61	0.41
1:C:185:ARG:HG2	1:C:186:GLY:N	2.35	0.41
1:G:132:ILE:HB	1:G:166:LEU:HD21	2.01	0.41
1:D:13:ALA:O	1:D:17:ARG:HD3	2.20	0.41
1:R:98:MET:HE1	1:R:213:PHE:HA	2.01	0.41
1:O:53:ASP:HA	1:P:24:ARG:HG3	2.00	0.41
1:I:19:LEU:HA	1:I:19:LEU:HD23	1.83	0.41
1:J:19:LEU:HD13	1:J:156:GLN:HB3	2.03	0.41
1:S:185:ARG:HG2	1:S:186:GLY:H	1.85	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:168:THR:HG22	1:F:170:ASN:H	1.85	0.41
1:R:19:LEU:HD21	1:S:93:MET:CA	2.42	0.41
1:E:69:MET:HE1	1:F:115:VAL:HG21	2.02	0.41
1:N:185:ARG:HG2	1:N:186:GLY:H	1.86	0.41
1:K:187:ILE:HD13	1:L:138:ASN:HB3	2.02	0.41
1:I:132:ILE:HB	1:I:166:LEU:HD21	2.02	0.41
1:H:168:THR:HG22	1:H:170:ASN:H	1.86	0.41
1:O:19:LEU:HD13	1:O:156:GLN:HB3	2.03	0.41
1:M:185:ARG:HD2	1:R:69:MET:HE2	2.02	0.41
1:D:19:LEU:HD21	1:E:93:MET:HA	2.03	0.41
1:Q:79:ASP:HB3	1:Q:82:ASN:ND2	2.36	0.41
1:A:208:ASN:OD1	1:E:211:HIS:CE1	2.73	0.41
1:E:113:HIS:HB2	1:E:181:CYS:SG	2.61	0.41
1:E:19:LEU:HD13	1:E:156:GLN:HB3	2.03	0.41
1:C:115:VAL:HG21	1:H:69:MET:HE1	2.02	0.41
1:M:19:LEU:HD12	1:M:160:ILE:CD1	2.51	0.41
1:D:185:ARG:HG2	1:D:186:GLY:H	1.85	0.41
1:A:13:ALA:O	1:A:17:ARG:HD3	2.20	0.41
1:Q:13:ALA:O	1:Q:17:ARG:HD3	2.21	0.41
1:L:134:LEU:HB3	3:L:232:HOH:O	2.21	0.41
1:S:93:MET:HB2	1:S:95:VAL:HG23	2.03	0.41
1:T:70:TYR:O	1:T:75:PHE:HB2	2.21	0.41
1:Q:185:ARG:HG2	1:Q:186:GLY:H	1.86	0.41
1:M:187:ILE:HD12	1:N:139:ARG:HG2	2.04	0.40
1:R:113:HIS:HB2	1:R:181:CYS:SG	2.62	0.40
1:M:132:ILE:HB	1:M:166:LEU:HD21	2.02	0.40
1:P:185:ARG:HG2	1:P:186:GLY:H	1.85	0.40
1:S:185:ARG:HG2	1:S:186:GLY:N	2.36	0.40
1:Q:168:THR:HG22	1:Q:170:ASN:H	1.85	0.40
1:J:125:TYR:CD2	1:J:166:LEU:HD13	2.56	0.40
1:M:192:SER:HA	1:N:102:ARG:O	2.21	0.40
1:A:192:SER:HA	1:B:102:ARG:O	2.21	0.40
1:C:185:ARG:HD2	1:H:69:MET:CE	2.51	0.40
1:C:44:THR:HG23	1:C:54:LEU:HD13	2.03	0.40
1:H:185:ARG:HG2	1:H:186:GLY:N	2.36	0.40
1:T:138:ASN:HD22	1:T:138:ASN:H	1.69	0.40
1:I:79:ASP:HB3	1:I:82:ASN:ND2	2.36	0.40
1:P:138:ASN:HB3	1:T:187:ILE:HD13	2.03	0.40
1:D:19:LEU:HD13	1:D:156:GLN:HB3	2.03	0.40
1:P:208:ASN:O	1:P:212:GLU:HG3	2.21	0.40
1:F:44:THR:O	1:F:48:GLN:HG3	2.21	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:THR:O	1:B:48:GLN:HG3	2.21	0.40
1:H:70:TYR:O	1:H:75:PHE:HB2	2.22	0.40
1:E:158:ILE:HD12	1:E:175:ILE:HD11	2.02	0.40
1:C:62:THR:HB	1:C:63:PRO:HD3	2.04	0.40
1:H:93:MET:HB2	1:H:95:VAL:HG23	2.04	0.40
1:C:19:LEU:HD13	1:C:156:GLN:HB3	2.02	0.40
1:A:19:LEU:HD13	1:A:156:GLN:HB3	2.03	0.40
1:F:185:ARG:HG2	1:F:186:GLY:N	2.37	0.40
1:L:62:THR:HB	1:L:63:PRO:HD3	2.03	0.40
1:S:70:TYR:O	1:S:75:PHE:HB2	2.21	0.40
1:R:159:LEU:O	1:R:163:GLN:HG3	2.22	0.40
1:K:32:ASN:O	1:K:36:LYS:HG3	2.21	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	219/221 (99%)	203 (93%)	13 (6%)	3 (1%)	14	51
1	B	219/221 (99%)	202 (92%)	15 (7%)	2 (1%)	21	64
1	C	219/221 (99%)	204 (93%)	13 (6%)	2 (1%)	21	64
1	D	219/221 (99%)	203 (93%)	13 (6%)	3 (1%)	14	51
1	E	219/221 (99%)	205 (94%)	11 (5%)	3 (1%)	14	51
1	F	219/221 (99%)	206 (94%)	10 (5%)	3 (1%)	14	51
1	G	219/221 (99%)	204 (93%)	12 (6%)	3 (1%)	14	51
1	H	219/221 (99%)	202 (92%)	14 (6%)	3 (1%)	14	51
1	I	219/221 (99%)	203 (93%)	14 (6%)	2 (1%)	21	64
1	J	219/221 (99%)	204 (93%)	12 (6%)	3 (1%)	14	51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	219/221 (99%)	204 (93%)	13 (6%)	2 (1%)	21	64
1	L	219/221 (99%)	203 (93%)	14 (6%)	2 (1%)	21	64
1	M	219/221 (99%)	207 (94%)	10 (5%)	2 (1%)	21	64
1	N	219/221 (99%)	204 (93%)	12 (6%)	3 (1%)	14	51
1	O	219/221 (99%)	203 (93%)	13 (6%)	3 (1%)	14	51
1	P	219/221 (99%)	203 (93%)	14 (6%)	2 (1%)	21	64
1	Q	219/221 (99%)	204 (93%)	12 (6%)	3 (1%)	14	51
1	R	219/221 (99%)	205 (94%)	11 (5%)	3 (1%)	14	51
1	S	219/221 (99%)	203 (93%)	13 (6%)	3 (1%)	14	51
1	T	219/221 (99%)	206 (94%)	10 (5%)	3 (1%)	14	51
All	All	4380/4420 (99%)	4078 (93%)	249 (6%)	53 (1%)	16	56

All (53) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	2	SER
1	A	2	SER
1	B	2	SER
1	C	2	SER
1	D	2	SER
1	F	2	SER
1	G	2	SER
1	H	2	SER
1	I	2	SER
1	J	2	SER
1	K	2	SER
1	L	2	SER
1	M	2	SER
1	N	2	SER
1	O	2	SER
1	P	2	SER
1	Q	2	SER
1	R	2	SER
1	S	2	SER
1	T	2	SER
1	S	218	ARG
1	T	218	ARG
1	C	22	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	218	ARG
1	E	218	ARG
1	G	218	ARG
1	H	22	PRO
1	J	218	ARG
1	N	22	PRO
1	P	22	PRO
1	Q	218	ARG
1	R	218	ARG
1	S	22	PRO
1	T	22	PRO
1	A	22	PRO
1	A	218	ARG
1	B	22	PRO
1	D	22	PRO
1	E	22	PRO
1	F	218	ARG
1	H	218	ARG
1	I	22	PRO
1	J	22	PRO
1	K	22	PRO
1	N	218	ARG
1	O	218	ARG
1	Q	22	PRO
1	R	22	PRO
1	F	22	PRO
1	G	22	PRO
1	L	22	PRO
1	M	22	PRO
1	O	22	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	194/194 (100%)	190 (98%)	4 (2%)	61 89

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	194/194 (100%)	190 (98%)	4 (2%)	61	89
1	C	194/194 (100%)	190 (98%)	4 (2%)	61	89
1	D	194/194 (100%)	190 (98%)	4 (2%)	61	89
1	E	194/194 (100%)	190 (98%)	4 (2%)	61	89
1	F	194/194 (100%)	190 (98%)	4 (2%)	61	89
1	G	194/194 (100%)	190 (98%)	4 (2%)	61	89
1	H	194/194 (100%)	190 (98%)	4 (2%)	61	89
1	I	194/194 (100%)	190 (98%)	4 (2%)	61	89
1	J	194/194 (100%)	190 (98%)	4 (2%)	61	89
1	K	194/194 (100%)	190 (98%)	4 (2%)	61	89
1	L	194/194 (100%)	190 (98%)	4 (2%)	61	89
1	M	194/194 (100%)	190 (98%)	4 (2%)	61	89
1	N	194/194 (100%)	190 (98%)	4 (2%)	61	89
1	O	194/194 (100%)	189 (97%)	5 (3%)	54	85
1	P	194/194 (100%)	190 (98%)	4 (2%)	61	89
1	Q	194/194 (100%)	190 (98%)	4 (2%)	61	89
1	R	194/194 (100%)	190 (98%)	4 (2%)	61	89
1	S	194/194 (100%)	190 (98%)	4 (2%)	61	89
1	T	194/194 (100%)	190 (98%)	4 (2%)	61	89
All	All	3880/3880 (100%)	3799 (98%)	81 (2%)	61	89

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	93	MET
1	A	181	CYS
1	A	185	ARG
1	B	20	GLU
1	B	93	MET
1	B	181	CYS
1	B	185	ARG
1	C	20	GLU
1	C	93	MET
1	C	181	CYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	185	ARG
1	D	20	GLU
1	D	93	MET
1	D	181	CYS
1	D	185	ARG
1	E	20	GLU
1	E	93	MET
1	E	181	CYS
1	E	185	ARG
1	F	20	GLU
1	F	93	MET
1	F	181	CYS
1	F	185	ARG
1	G	20	GLU
1	G	93	MET
1	G	181	CYS
1	G	185	ARG
1	H	20	GLU
1	H	93	MET
1	H	181	CYS
1	H	185	ARG
1	I	20	GLU
1	I	93	MET
1	I	181	CYS
1	I	185	ARG
1	J	20	GLU
1	J	93	MET
1	J	181	CYS
1	J	185	ARG
1	K	20	GLU
1	K	93	MET
1	K	181	CYS
1	K	185	ARG
1	L	20	GLU
1	L	93	MET
1	L	181	CYS
1	L	185	ARG
1	M	20	GLU
1	M	93	MET
1	M	181	CYS
1	M	185	ARG
1	N	20	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	N	93	MET
1	N	181	CYS
1	N	185	ARG
1	O	20	GLU
1	O	63	PRO
1	O	93	MET
1	O	181	CYS
1	O	185	ARG
1	P	20	GLU
1	P	93	MET
1	P	181	CYS
1	P	185	ARG
1	Q	20	GLU
1	Q	93	MET
1	Q	181	CYS
1	Q	185	ARG
1	R	20	GLU
1	R	93	MET
1	R	181	CYS
1	R	185	ARG
1	S	20	GLU
1	S	93	MET
1	S	181	CYS
1	S	185	ARG
1	T	20	GLU
1	T	93	MET
1	T	181	CYS
1	T	185	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	138	ASN
1	B	138	ASN
1	B	163	GLN
1	C	138	ASN
1	C	163	GLN
1	C	207	GLN
1	C	211	HIS
1	D	138	ASN
1	D	163	GLN
1	D	211	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	E	138	ASN
1	E	163	GLN
1	E	207	GLN
1	F	138	ASN
1	F	163	GLN
1	F	211	HIS
1	G	138	ASN
1	G	163	GLN
1	G	207	GLN
1	G	211	HIS
1	H	138	ASN
1	H	163	GLN
1	H	207	GLN
1	I	138	ASN
1	I	163	GLN
1	I	207	GLN
1	I	211	HIS
1	J	138	ASN
1	J	163	GLN
1	K	42	HIS
1	K	138	ASN
1	K	163	GLN
1	K	207	GLN
1	L	138	ASN
1	L	163	GLN
1	L	207	GLN
1	L	211	HIS
1	M	138	ASN
1	M	163	GLN
1	M	207	GLN
1	M	211	HIS
1	N	138	ASN
1	N	163	GLN
1	N	207	GLN
1	N	211	HIS
1	O	138	ASN
1	O	163	GLN
1	P	138	ASN
1	P	163	GLN
1	Q	138	ASN
1	Q	163	GLN
1	Q	207	GLN

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	Q	211	HIS
1	R	138	ASN
1	R	163	GLN
1	R	207	GLN
1	R	211	HIS
1	S	138	ASN
1	S	163	GLN
1	S	207	GLN
1	T	82	ASN
1	T	138	ASN
1	T	163	GLN
1	T	207	GLN
1	T	211	HIS

### 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](#)

20 ligands 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	$\# Z  > 2$
2	SO4	A	222	-	4,4,4	1.43	0	6,6,6	0.33	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	223	-	4,4,4	1.30	0	6,6,6	0.64	0
2	SO4	C	222	-	4,4,4	1.20	0	6,6,6	0.26	0
2	SO4	D	222	-	4,4,4	1.36	1 (25%)	6,6,6	0.65	0
2	SO4	E	222	-	4,4,4	1.20	0	6,6,6	0.41	0
2	SO4	F	222	-	4,4,4	1.19	0	6,6,6	0.45	0
2	SO4	G	222	-	4,4,4	1.26	0	6,6,6	0.48	0
2	SO4	H	222	-	4,4,4	1.50	1 (25%)	6,6,6	0.72	0
2	SO4	I	222	-	4,4,4	1.12	0	6,6,6	0.27	0
2	SO4	J	222	-	4,4,4	1.30	0	6,6,6	0.64	0
2	SO4	K	222	-	4,4,4	1.32	0	6,6,6	0.59	0
2	SO4	L	222	-	4,4,4	1.20	0	6,6,6	0.27	0
2	SO4	L	223	-	4,4,4	1.41	0	6,6,6	0.66	0
2	SO4	N	222	-	4,4,4	1.26	0	6,6,6	0.50	0
2	SO4	O	222	-	4,4,4	1.19	0	6,6,6	0.42	0
2	SO4	P	222	-	4,4,4	1.17	0	6,6,6	0.66	0
2	SO4	Q	222	-	4,4,4	1.16	0	6,6,6	0.40	0
2	SO4	R	222	-	4,4,4	1.31	0	6,6,6	0.53	0
2	SO4	S	222	-	4,4,4	1.41	1 (25%)	6,6,6	0.77	0
2	SO4	T	222	-	4,4,4	1.14	0	6,6,6	0.28	0

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	SO4	A	222	-	-	0/0/0/0	0/0/0/0
2	SO4	A	223	-	-	0/0/0/0	0/0/0/0
2	SO4	C	222	-	-	0/0/0/0	0/0/0/0
2	SO4	D	222	-	-	0/0/0/0	0/0/0/0
2	SO4	E	222	-	-	0/0/0/0	0/0/0/0
2	SO4	F	222	-	-	0/0/0/0	0/0/0/0
2	SO4	G	222	-	-	0/0/0/0	0/0/0/0
2	SO4	H	222	-	-	0/0/0/0	0/0/0/0
2	SO4	I	222	-	-	0/0/0/0	0/0/0/0
2	SO4	J	222	-	-	0/0/0/0	0/0/0/0
2	SO4	K	222	-	-	0/0/0/0	0/0/0/0
2	SO4	L	222	-	-	0/0/0/0	0/0/0/0
2	SO4	L	223	-	-	0/0/0/0	0/0/0/0
2	SO4	N	222	-	-	0/0/0/0	0/0/0/0
2	SO4	O	222	-	-	0/0/0/0	0/0/0/0
2	SO4	P	222	-	-	0/0/0/0	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SO4	Q	222	-	-	0/0/0/0	0/0/0/0
2	SO4	R	222	-	-	0/0/0/0	0/0/0/0
2	SO4	S	222	-	-	0/0/0/0	0/0/0/0
2	SO4	T	222	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	S	222	SO4	O1-S	-2.07	1.40	1.47
2	H	222	SO4	O1-S	-2.04	1.40	1.47
2	D	222	SO4	O1-S	-2.01	1.40	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.