



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 09:52 PM BST

PDB ID : 6V6H  
Title : Crystal structure of histidine ammonia-lyase from Trypanosoma cruzi  
Authors : Miranda, R.R.; Silva, M.; Barison, M.J.; Silber, A.M.; Iulek, J.  
Deposited on : 2019-12-05  
Resolution : 2.55 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

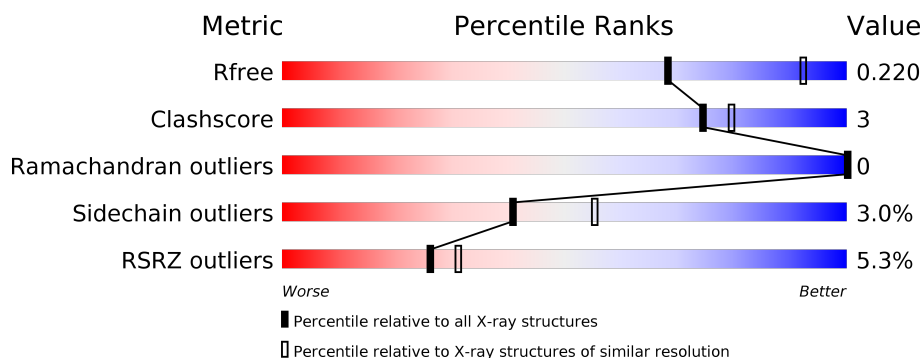
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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))
$R_{free}$	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	538	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>7% • 5%</div> </div> </div>
1	B	538	<div> <div>5%</div> <div> <div></div> <div>87%</div> <div>5% • 6%</div> </div> </div>
1	C	538	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>7% • 5%</div> </div> </div>
1	D	538	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>7% • 6%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15683 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 Histidine ammonia-lyase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	0	1	1
			3782	2398	673	693	18			
1	B	505	Total	C	N	O	S	0	0	1
			3728	2367	663	680	18			
1	C	509	Total	C	N	O	S	0	2	0
			3779	2394	676	691	18			
1	D	505	Total	C	N	O	S	8	2	0
			3742	2385	661	680	16			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	expression tag	UNP Q4E133
A	-4	HIS	-	expression tag	UNP Q4E133
A	-3	HIS	-	expression tag	UNP Q4E133
A	-2	HIS	-	expression tag	UNP Q4E133
A	-1	HIS	-	expression tag	UNP Q4E133
A	0	HIS	-	expression tag	UNP Q4E133
A	124	LEU	VAL	conflict	UNP Q4E133
A	143	MDO	ALA	chromophore	UNP Q4E133
A	143	MDO	SER	chromophore	UNP Q4E133
A	143	MDO	GLY	chromophore	UNP Q4E133
B	-5	HIS	-	expression tag	UNP Q4E133
B	-4	HIS	-	expression tag	UNP Q4E133
B	-3	HIS	-	expression tag	UNP Q4E133
B	-2	HIS	-	expression tag	UNP Q4E133
B	-1	HIS	-	expression tag	UNP Q4E133
B	0	HIS	-	expression tag	UNP Q4E133
B	124	LEU	VAL	conflict	UNP Q4E133
B	143	MDO	ALA	chromophore	UNP Q4E133
B	143	MDO	SER	chromophore	UNP Q4E133
B	143	MDO	GLY	chromophore	UNP Q4E133
C	-5	HIS	-	expression tag	UNP Q4E133

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	HIS	-	expression tag	UNP Q4E133
C	-3	HIS	-	expression tag	UNP Q4E133
C	-2	HIS	-	expression tag	UNP Q4E133
C	-1	HIS	-	expression tag	UNP Q4E133
C	0	HIS	-	expression tag	UNP Q4E133
C	124	LEU	VAL	conflict	UNP Q4E133
C	143	MDO	ALA	chromophore	UNP Q4E133
C	143	MDO	SER	chromophore	UNP Q4E133
C	143	MDO	GLY	chromophore	UNP Q4E133
D	-5	HIS	-	expression tag	UNP Q4E133
D	-4	HIS	-	expression tag	UNP Q4E133
D	-3	HIS	-	expression tag	UNP Q4E133
D	-2	HIS	-	expression tag	UNP Q4E133
D	-1	HIS	-	expression tag	UNP Q4E133
D	0	HIS	-	expression tag	UNP Q4E133
D	124	LEU	VAL	conflict	UNP Q4E133
D	143	MDO	ALA	chromophore	UNP Q4E133
D	143	MDO	SER	chromophore	UNP Q4E133
D	143	MDO	GLY	chromophore	UNP Q4E133

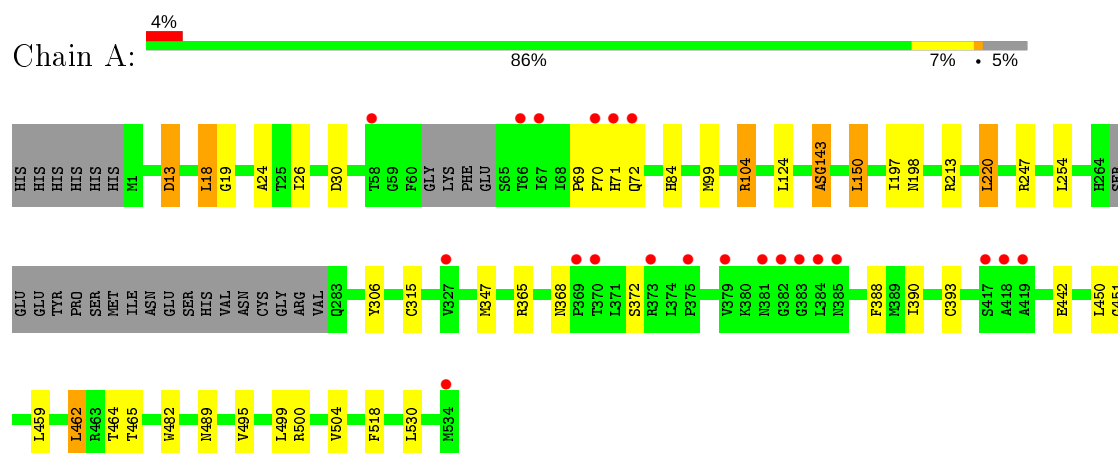
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	180	Total O 180 180	0	0
2	B	148	Total O 148 148	0	0
2	C	178	Total O 178 178	0	0
2	D	146	Total O 146 146	0	0

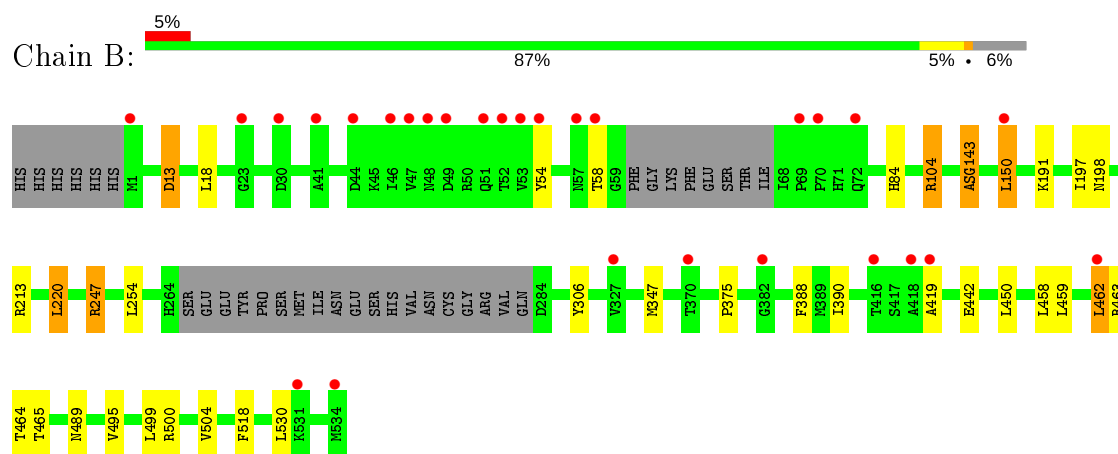
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

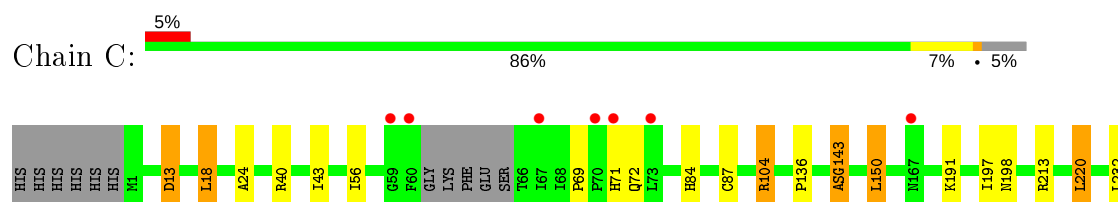
#### • Molecule 1: Histidine ammonia-lyase

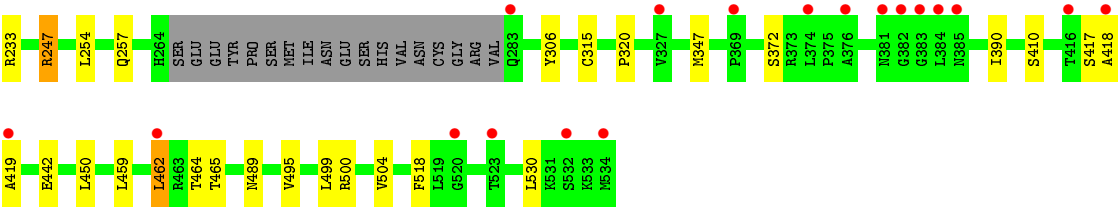


#### • Molecule 1: Histidine ammonia-lyase

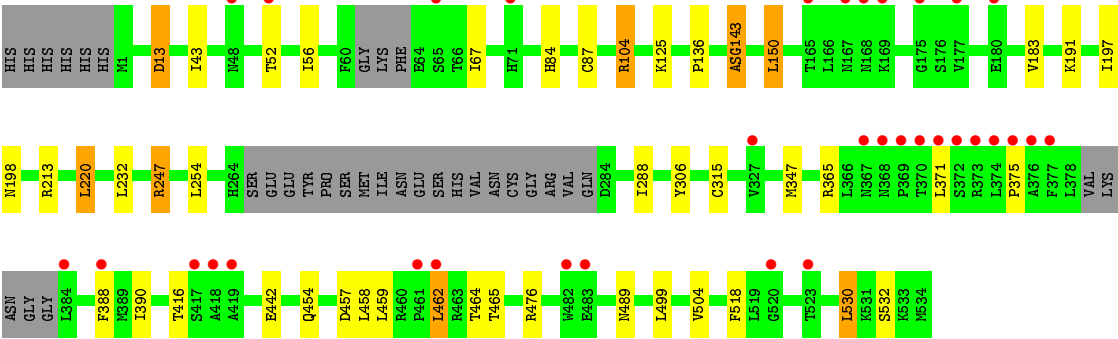
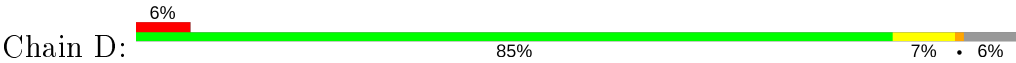


#### • Molecule 1: Histidine ammonia-lyase





● Molecule 1: Histidine ammonia-lyase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.81Å 144.56Å 173.76Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.31 – 2.55 32.31 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.4 (32.31-2.55) 99.4 (32.31-2.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.179 , 0.217 0.183 , 0.220	Depositor DCC
$R_{free}$ test set	2004 reflections (2.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.0	Xtriage
Anisotropy	0.301	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 56.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	15683	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.64% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

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

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

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	0.23	0/3826	0.41	0/5204
1	B	0.23	0/3767	0.41	0/5123
1	C	0.23	0/3826	0.41	0/5204
1	D	0.23	0/3792	0.40	0/5158
All	All	0.23	0/15211	0.41	0/20689

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	2
All	All	0	8

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	143	MDO	Mainchain,Peptide
1	B	143	MDO	Mainchain,Peptide
1	C	143	MDO	Mainchain,Peptide
1	D	143	MDO	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	3782	0	3777	25	0
1	B	3728	0	3733	23	0
1	C	3779	0	3777	31	0
1	D	3742	0	3728	31	0
2	A	180	0	0	1	1
2	B	148	0	0	2	0
2	C	178	0	0	2	1
2	D	146	0	0	1	0
All	All	15683	0	15015	96	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (96) 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:A:365:ARG:NH1	1:B:419:ALA:O	2.21	0.73
1:C:347:MET:HG2	1:D:347:MET:HG2	1.72	0.71
1:C:233[A]:ARG:NH1	1:C:372:SER:O	2.25	0.69
1:A:500:ARG:NH2	2:A:601:HOH:O	2.26	0.67
1:B:104:ARG:NH2	1:B:198:ASN:O	2.29	0.66
1:C:104:ARG:NH2	1:C:198:ASN:O	2.29	0.66
1:D:104:ARG:NH2	1:D:198:ASN:O	2.29	0.65
1:A:104:ARG:NH2	1:A:198:ASN:O	2.29	0.65
1:A:347:MET:HG2	1:B:347:MET:HG2	1.79	0.65
1:B:500:ARG:NH2	2:B:601:HOH:O	2.31	0.64
1:D:13:ASP:OD2	1:D:306:TYR:OH	2.17	0.63
1:A:13:ASP:OD2	1:A:306:TYR:OH	2.17	0.63
1:A:150:LEU:HB3	1:A:197:ILE:HA	1.81	0.62
1:B:150:LEU:HB3	1:B:197:ILE:HA	1.81	0.62
1:D:150:LEU:HB3	1:D:197:ILE:HA	1.82	0.61
1:A:26:ILE:HG13	1:A:124:LEU:HD12	1.83	0.61
1:C:13:ASP:OD2	1:C:306:TYR:OH	2.17	0.61
1:B:13:ASP:OD2	1:B:306:TYR:OH	2.17	0.61
1:C:150:LEU:HB3	1:C:197:ILE:HA	1.81	0.61

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:530:LEU:HB3	1:D:532:SER:O	2.08	0.53
1:D:125:LYS:HG2	1:D:183:VAL:HG22	1.91	0.53
1:B:191:LYS:HD3	1:B:191:LYS:O	2.10	0.52
1:A:459:LEU:O	1:A:462:LEU:HB2	2.09	0.52
1:B:388:PHE:HE2	1:B:450:LEU:HG	1.74	0.52
1:D:52:THR:OG1	1:D:67:ILE:HG13	2.10	0.52
1:D:459:LEU:O	1:D:462:LEU:HB2	2.10	0.51
1:B:84:HIS:CG	1:D:390:ILE:HG13	2.46	0.51
1:C:459:LEU:O	1:C:462:LEU:HB2	2.10	0.51
1:A:69:PRO:HB2	1:A:71:HIS:CE1	2.45	0.51
1:B:459:LEU:O	1:B:462:LEU:HB2	2.10	0.51
1:A:450:LEU:HD13	1:A:495:VAL:HG21	1.93	0.50
1:A:84:HIS:CG	1:C:390:ILE:HG13	2.47	0.50
1:D:191:LYS:HD3	1:D:191:LYS:O	2.11	0.50
1:C:69:PRO:HB2	1:C:71:HIS:CE1	2.47	0.49
1:D:388[A]:PHE:CE1	1:D:454:GLN:HG2	2.48	0.49
1:C:257:GLN:NE2	1:D:532:SER:O	2.44	0.49
1:A:388[B]:PHE:HE1	1:A:482:TRP:CE3	2.30	0.49
1:A:18:LEU:HD12	1:A:24:ALA:HB1	1.94	0.48
1:C:464:THR:OG1	1:C:465:THR:N	2.46	0.48
1:B:54:TYR:HA	1:B:58:THR:HG21	1.95	0.48
1:D:191:LYS:NZ	2:D:608:HOH:O	2.45	0.48
1:C:410:SER:O	2:C:601:HOH:O	2.20	0.48
1:A:388[B]:PHE:CE2	1:A:451:GLY:HA2	2.49	0.47
1:C:43:ILE:HD12	1:C:56:ILE:HD12	1.96	0.47
1:C:191:LYS:O	1:C:191:LYS:HD3	2.14	0.47
1:D:375:PRO:HD2	1:D:458:LEU:HD13	1.97	0.47
1:C:499:LEU:HD23	1:C:504:VAL:HG21	1.97	0.47
1:D:499:LEU:HD23	1:D:504:VAL:HG21	1.97	0.47
1:C:71:HIS:CD2	1:C:72:GLN:HG3	2.50	0.47
1:D:464:THR:OG1	1:D:465:THR:N	2.46	0.47
1:A:368:ASN:HD21	1:C:418:ALA:HB3	1.78	0.47
1:B:375:PRO:HD2	1:B:458:LEU:HD13	1.96	0.47
1:D:388[A]:PHE:HE1	1:D:454:GLN:HG2	1.78	0.47
1:B:450:LEU:HD13	1:B:495:VAL:HG21	1.97	0.46
1:B:499:LEU:HD23	1:B:504:VAL:HG21	1.97	0.46
1:C:417:SER:C	1:C:419:ALA:H	2.19	0.46
1:A:464:THR:OG1	1:A:465:THR:N	2.46	0.46
1:B:463:ARG:NH2	2:B:607:HOH:O	2.45	0.46
1:C:232:LEU:HA	1:C:233[A]:ARG:HH11	1.80	0.46
1:A:499:LEU:HD23	1:A:504:VAL:HG21	1.97	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:418:ALA:O	1:D:371:LEU:HD21	2.16	0.45
1:C:500:ARG:NH2	2:C:602:HOH:O	2.50	0.45
1:A:71:HIS:CD2	1:A:72:GLN:HG3	2.52	0.45
1:D:457:ASP:OD2	1:D:476:ARG:NH2	2.38	0.45
1:D:232:LEU:HD12	1:D:288:ILE:HD11	1.99	0.45
1:C:220:LEU:HG	1:C:499:LEU:HD22	2.00	0.44
1:B:464:THR:OG1	1:B:465:THR:N	2.46	0.44
1:C:247:ARG:HG2	1:D:315:CYS:HB3	2.00	0.44
1:D:43:ILE:HD12	1:D:56:ILE:HD12	2.00	0.44
1:D:220:LEU:HG	1:D:499:LEU:HD22	2.00	0.44
1:A:220:LEU:HG	1:A:499:LEU:HD22	2.00	0.44
1:B:220:LEU:HG	1:B:499:LEU:HD22	2.00	0.44
1:C:18:LEU:HD12	1:C:24:ALA:HB1	2.00	0.44
1:A:213:ARG:HD2	1:A:442:GLU:OE2	2.18	0.44
1:B:213:ARG:HD2	1:B:442:GLU:OE2	2.18	0.44
1:C:213:ARG:HD2	1:C:442:GLU:OE2	2.18	0.43
1:B:84:HIS:HA	1:D:390:ILE:HG13	2.00	0.43
1:D:213:ARG:HD2	1:D:442:GLU:OE2	2.18	0.43
1:B:390:ILE:HG13	1:D:84:HIS:CG	2.54	0.42
1:C:315:CYS:HB3	1:D:247:ARG:HG2	2.02	0.42
1:C:40:ARG:HD2	1:C:40:ARG:HA	1.92	0.41
1:B:220:LEU:HD12	1:B:220:LEU:HA	1.94	0.41
1:C:450:LEU:HD13	1:C:495:VAL:HG21	2.02	0.41
1:C:18:LEU:HA	1:C:18:LEU:HD12	1.86	0.41
1:D:365:ARG:NH2	1:D:371:LEU:HD22	2.35	0.41
1:A:69:PRO:HA	1:A:70:PRO:HD3	1.96	0.41
1:D:150:LEU:HA	1:D:150:LEU:HD12	1.92	0.41
1:A:365:ARG:O	1:A:372:SER:HB3	2.21	0.41
1:A:19:GLY:HA3	1:A:99:MET:HG3	2.03	0.41
1:A:315:CYS:HB3	1:B:247:ARG:HG2	2.02	0.40
1:A:390:ILE:HG13	1:C:84:HIS:CG	2.55	0.40
1:B:462:LEU:HA	1:B:462:LEU:HD12	1.90	0.40
1:D:462:LEU:HD12	1:D:462:LEU:HA	1.89	0.40
1:C:191:LYS:HE2	1:C:320:PRO:HD2	2.03	0.40
1:C:87:CYS:HB3	1:C:136:PRO:HB2	2.04	0.40
1:D:87:CYS:HB3	1:D:136:PRO:HB2	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:765:HOH:O	2:C:627:HOH:O[4_566]	2.19	0.01

## 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	503/538 (94%)	493 (98%)	10 (2%)	0	100	100
1	B	497/538 (92%)	482 (97%)	15 (3%)	0	100	100
1	C	503/538 (94%)	489 (97%)	14 (3%)	0	100	100
1	D	497/538 (92%)	485 (98%)	12 (2%)	0	100	100
All	All	2000/2152 (93%)	1949 (98%)	51 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	382/445 (86%)	370 (97%)	12 (3%)	40	54
1	B	374/445 (84%)	363 (97%)	11 (3%)	42	57
1	C	381/445 (86%)	370 (97%)	11 (3%)	42	57
1	D	373/445 (84%)	362 (97%)	11 (3%)	42	57
All	All	1510/1780 (85%)	1465 (97%)	45 (3%)	41	55

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	A	18	LEU
1	A	30	ASP
1	A	104	ARG
1	A	150	LEU
1	A	220	LEU
1	A	247	ARG
1	A	254	LEU
1	A	462	LEU
1	A	489	ASN
1	A	518	PHE
1	A	530	LEU
1	B	13	ASP
1	B	18	LEU
1	B	104	ARG
1	B	150	LEU
1	B	220	LEU
1	B	247	ARG
1	B	254	LEU
1	B	462	LEU
1	B	489	ASN
1	B	518	PHE
1	B	530	LEU
1	C	13	ASP
1	C	18	LEU
1	C	104	ARG
1	C	150	LEU
1	C	220	LEU
1	C	247	ARG
1	C	254	LEU
1	C	462	LEU
1	C	489	ASN
1	C	518	PHE
1	C	530	LEU
1	D	13	ASP
1	D	104	ARG
1	D	150	LEU
1	D	220	LEU
1	D	247	ARG
1	D	254	LEU
1	D	416	THR
1	D	462	LEU
1	D	489	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	518	PHE
1	D	530	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	GLN
1	A	198	ASN
1	A	494	ASN
1	B	121	GLN
1	B	198	ASN
1	B	229	HIS
1	B	494	ASN
1	C	198	ASN
1	C	229	HIS
1	C	494	ASN
1	D	198	ASN
1	D	494	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	MDO	B	143	1	12,13,14	3.84	3 (25%)	15,18,20	6.74	7 (46%)
1	CSS	D	393	1	4,6,7	1.20	0	1,6,8	0.72	0
1	CSS	A	393	1	4,6,7	1.22	1 (25%)	1,6,8	0.69	0
1	CSS	C	393	1	4,6,7	1.12	0	1,6,8	1.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	CSS	B	393	1	4,6,7	1.10	0	1,6,8	0.92	0
1	MDO	C	143	1	12,13,14	3.83	4 (33%)	15,18,20	6.48	7 (46%)
1	MDO	A	143	1	12,13,14	3.85	4 (33%)	15,18,20	6.41	7 (46%)
1	MDO	D	143	1	12,13,14	3.81	3 (25%)	15,18,20	6.61	6 (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	MDO	B	143	1	-	2/4/23/24	0/1/1/1
1	CSS	D	393	1	-	1/1/5/7	-
1	CSS	A	393	1	-	1/1/5/7	-
1	CSS	C	393	1	-	1/1/5/7	-
1	CSS	B	393	1	-	1/1/5/7	-
1	MDO	C	143	1	-	2/4/23/24	0/1/1/1
1	MDO	A	143	1	-	2/4/23/24	0/1/1/1
1	MDO	D	143	1	-	2/4/23/24	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	143	MDO	O2-C2	11.93	1.48	1.23
1	B	143	MDO	O2-C2	11.91	1.48	1.23
1	C	143	MDO	O2-C2	11.89	1.48	1.23
1	D	143	MDO	O2-C2	11.71	1.47	1.23
1	D	143	MDO	C1-N2	3.94	1.38	1.32
1	A	143	MDO	C1-N2	3.85	1.37	1.32
1	B	143	MDO	C1-N2	3.55	1.37	1.32
1	C	143	MDO	C1-N2	3.50	1.37	1.32
1	D	143	MDO	C2-N3	-3.17	1.32	1.39
1	A	143	MDO	C2-N3	-3.12	1.32	1.39
1	B	143	MDO	C2-N3	-3.08	1.32	1.39
1	C	143	MDO	C2-N3	-3.07	1.32	1.39
1	A	143	MDO	CA2-C2	2.20	1.47	1.43
1	C	143	MDO	CA2-C2	2.11	1.47	1.43
1	A	393	CSS	CB-SG	-2.02	1.75	1.81

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	143	MDO	CA2-C2-N3	18.49	112.11	103.37
1	D	143	MDO	CA2-C2-N3	18.48	112.11	103.37
1	C	143	MDO	CA2-C2-N3	18.11	111.93	103.37
1	A	143	MDO	CA2-C2-N3	18.04	111.90	103.37
1	B	143	MDO	O2-C2-CA2	-12.59	123.89	130.96
1	D	143	MDO	O2-C2-CA2	-12.29	124.06	130.96
1	A	143	MDO	O2-C2-CA2	-11.08	124.74	130.96
1	C	143	MDO	O2-C2-CA2	-10.69	124.96	130.96
1	B	143	MDO	C2-CA2-N2	-10.57	101.53	108.93
1	C	143	MDO	C2-CA2-N2	-10.55	101.54	108.93
1	A	143	MDO	C2-CA2-N2	-10.22	101.78	108.93
1	D	143	MDO	C2-CA2-N2	-10.14	101.83	108.93
1	C	143	MDO	CA2-N2-C1	5.42	110.31	105.40
1	B	143	MDO	CA2-N2-C1	5.17	110.08	105.40
1	A	143	MDO	CA2-N2-C1	5.06	109.98	105.40
1	B	143	MDO	C2-N3-C1	-4.86	105.50	107.97
1	D	143	MDO	CA2-N2-C1	4.83	109.77	105.40
1	C	143	MDO	C2-N3-C1	-4.72	105.58	107.97
1	D	143	MDO	C2-N3-C1	-4.59	105.64	107.97
1	A	143	MDO	C2-N3-C1	-4.22	105.83	107.97
1	C	143	MDO	CB2-CA2-C2	3.74	129.62	122.76
1	A	143	MDO	CB2-CA2-C2	3.15	128.52	122.76
1	B	143	MDO	CB2-CA2-C2	3.14	128.52	122.76
1	D	143	MDO	CB2-CA2-C2	2.75	127.80	122.76
1	C	143	MDO	O-C-CA3	-2.28	119.51	126.39
1	A	143	MDO	O-C-CA3	-2.28	119.52	126.39
1	B	143	MDO	O-C-CA3	-2.16	119.88	126.39

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	393	CSS	N-CA-CB-SG
1	A	393	CSS	N-CA-CB-SG
1	C	393	CSS	N-CA-CB-SG
1	B	393	CSS	N-CA-CB-SG
1	B	143	MDO	N2-C1-CA-CB
1	C	143	MDO	N2-C1-CA-CB
1	A	143	MDO	N2-C1-CA-CB
1	D	143	MDO	N2-C1-CA-CB
1	B	143	MDO	N3-C1-CA-CB
1	C	143	MDO	N3-C1-CA-CB
1	A	143	MDO	N3-C1-CA-CB

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
1	D	143	MDO	N3-C1-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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	508/538 (94%)	-0.13	21 (4%)	37	44	16, 27, 71, 119	0
1	B	503/538 (93%)	0.00	28 (5%)	24	29	20, 33, 62, 135	0
1	C	507/538 (94%)	-0.15	25 (4%)	29	35	17, 28, 61, 109	0
1	D	503/538 (93%)	0.06	34 (6%)	17	20	18, 32, 68, 119	0
All	All	2021/2152 (93%)	-0.05	108 (5%)	26	31	16, 30, 65, 135	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	382	GLY	6.6
1	A	418	ALA	5.7
1	C	416	THR	4.9
1	A	381	ASN	4.6
1	D	374	LEU	4.6
1	B	52	THR	4.6
1	D	461	PRO	4.6
1	B	418	ALA	4.5
1	B	382	GLY	4.5
1	C	60	PHE	4.4
1	D	370	THR	4.3
1	D	418	ALA	4.3
1	A	419	ALA	4.3
1	D	371	LEU	4.2
1	D	48	ASN	4.1
1	C	418	ALA	4.1
1	D	375	PRO	4.0
1	B	53	VAL	4.0
1	A	327	VAL	4.0
1	B	51	GLN	3.9
1	A	369	PRO	3.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	419	ALA	3.8
1	B	534	MET	3.8
1	D	167	ASN	3.6
1	D	369	PRO	3.6
1	C	419	ALA	3.6
1	B	54	TYR	3.6
1	B	70	PRO	3.6
1	A	66	THR	3.5
1	D	523	THR	3.5
1	A	67	ILE	3.4
1	A	370	THR	3.4
1	A	373	ARG	3.4
1	B	416	THR	3.4
1	C	67	ILE	3.3
1	D	377	PHE	3.3
1	B	58	THR	3.3
1	A	383	GLY	3.3
1	C	374	LEU	3.2
1	B	48	ASN	3.2
1	D	376	ALA	3.2
1	D	65	SER	3.1
1	C	167	ASN	3.1
1	D	417	SER	3.1
1	C	384	LEU	3.1
1	C	327	VAL	3.1
1	D	462	LEU	3.0
1	B	72	GLN	3.0
1	D	372	SER	2.9
1	D	384	LEU	2.9
1	D	373	ARG	2.9
1	A	534	MET	2.8
1	B	23	GLY	2.8
1	D	520	GLY	2.8
1	A	70	PRO	2.8
1	D	71[A]	HIS	2.7
1	A	385	ASN	2.7
1	D	327	VAL	2.7
1	D	368	ASN	2.7
1	A	375	PRO	2.7
1	B	327	VAL	2.6
1	B	57	ASN	2.6
1	D	419	ALA	2.5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	388[A]	PHE	2.5
1	B	46	ILE	2.5
1	C	383	GLY	2.5
1	B	531	LYS	2.5
1	B	370	THR	2.5
1	B	1	MET	2.5
1	C	70	PRO	2.5
1	B	49	ASP	2.5
1	D	168	ASN	2.4
1	C	369	PRO	2.4
1	C	283	GLN	2.4
1	D	482	TRP	2.4
1	D	52	THR	2.4
1	B	41	ALA	2.3
1	B	44	ASP	2.3
1	D	169	LYS	2.3
1	D	175	GLY	2.3
1	D	367	ASN	2.3
1	A	384	LEU	2.3
1	C	382	GLY	2.2
1	C	376	ALA	2.2
1	B	30	ASP	2.2
1	B	47	VAL	2.2
1	C	534	MET	2.2
1	D	177	VAL	2.2
1	B	462	LEU	2.2
1	A	71	HIS	2.2
1	D	180	GLU	2.2
1	A	379	VAL	2.2
1	C	462	LEU	2.2
1	C	520	GLY	2.1
1	C	523	THR	2.1
1	A	72	GLN	2.1
1	B	69	PRO	2.1
1	A	417	SER	2.1
1	C	385	ASN	2.1
1	D	483	GLU	2.1
1	C	381	ASN	2.1
1	C	71	HIS	2.1
1	B	150	LEU	2.1
1	C	59	GLY	2.1
1	A	58	THR	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	532	SER	2.0
1	D	165	THR	2.0
1	C	73	LEU	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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	CSS	D	393	7/8	0.88	0.18	36,40,59,95	0
1	CSS	B	393	7/8	0.89	0.16	24,26,41,79	0
1	CSS	A	393	7/8	0.91	0.16	27,29,59,62	0
1	MDO	D	143	13/14	0.93	0.19	22,26,32,33	0
1	CSS	C	393	7/8	0.94	0.17	26,28,53,64	0
1	MDO	C	143	13/14	0.95	0.20	22,31,36,37	0
1	MDO	B	143	13/14	0.95	0.17	30,31,37,46	0
1	MDO	A	143	13/14	0.96	0.22	15,24,33,34	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.