



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:20 PM GMT

PDB ID : 1T5F  
Title : arginase I-AOH complex  
Authors : Shin, H.; Cama, E.; Christianson, D.W.  
Deposited on : 2004-05-04  
Resolution : 2.20 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) : **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

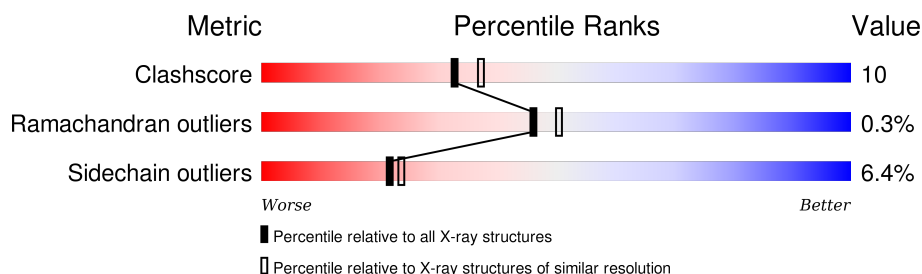
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)

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	314	
1	B	314	
1	C	314	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7442 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 Arginase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	314	Total	C	N	O	S	0	0	0
			2385	1523	402	455	5			
1	B	314	Total	C	N	O	S	0	0	0
			2385	1523	402	455	5			
1	C	314	Total	C	N	O	S	0	0	0
			2385	1523	402	455	5			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	CYS	GLN	ENGINEERED	UNP P07824
A	119	ALA	CYS	ENGINEERED	UNP P07824
A	141	ALA	HIS	ENGINEERED	UNP P07824
A	168	ALA	CYS	ENGINEERED	UNP P07824
A	303	ALA	CYS	ENGINEERED	UNP P07824
B	19	CYS	GLN	ENGINEERED	UNP P07824
B	119	ALA	CYS	ENGINEERED	UNP P07824
B	141	ALA	HIS	ENGINEERED	UNP P07824
B	168	ALA	CYS	ENGINEERED	UNP P07824
B	303	ALA	CYS	ENGINEERED	UNP P07824
C	19	CYS	GLN	ENGINEERED	UNP P07824
C	119	ALA	CYS	ENGINEERED	UNP P07824
C	141	ALA	HIS	ENGINEERED	UNP P07824
C	168	ALA	CYS	ENGINEERED	UNP P07824
C	303	ALA	CYS	ENGINEERED	UNP P07824

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

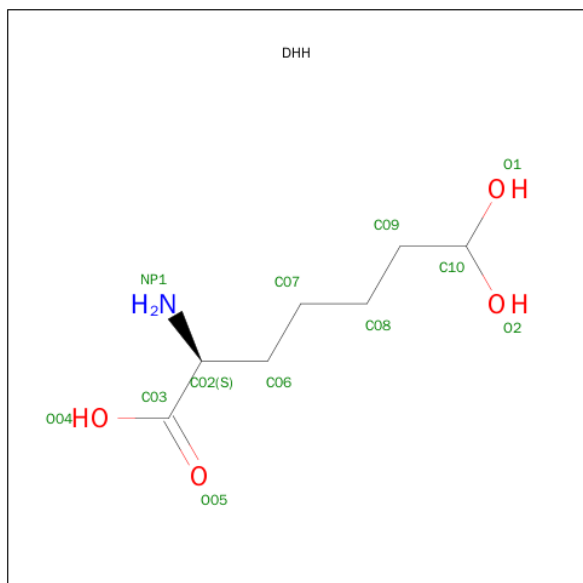
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mn	0	0
			2	2		
2	C	2	Total	Mn	0	0
			2	2		

- Molecule 3 is (S)-2-AMINO-7,7-DIHYDROXYHEPTANOIC ACID (three-letter code: DHH) (formula: C<sub>7</sub>H<sub>15</sub>NO<sub>4</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			12	7	1	4		
3	B	1	Total	C	N	O	0	0
			12	7	1	4		
3	C	1	Total	C	N	O	0	0
			12	7	1	4		

- Molecule 4 is water.

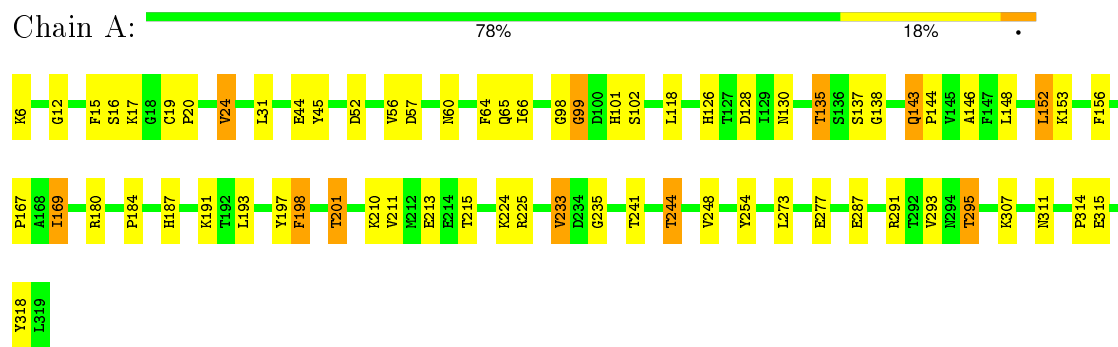
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	71	Total	O	0	0
			71	71		
4	B	94	Total	O	0	0
			94	94		
4	C	80	Total	O	0	0
			80	80		

### 3 Residue-property plots

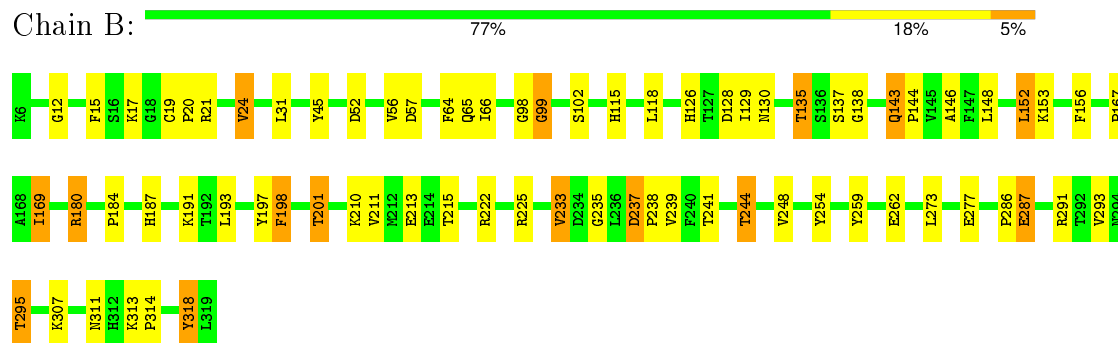
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

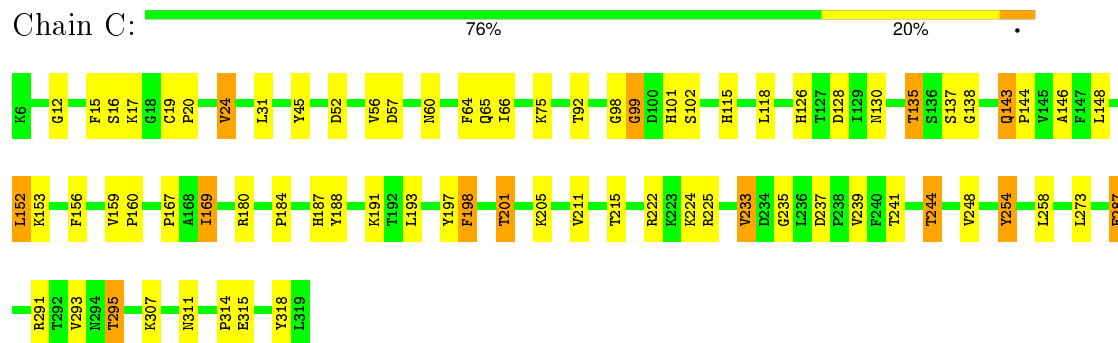
#### • Molecule 1: Arginase 1



#### • Molecule 1: Arginase 1



#### • Molecule 1: Arginase 1



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	87.90 Å 87.90 Å 105.20 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.59 – 2.20	Depositor
% Data completeness (in resolution range)	90.7 (19.59-2.20)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.222 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7442	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

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	1.16	23/2437 (0.9%)	0.91	20/3310 (0.6%)
1	B	0.84	22/2437 (0.9%)	0.84	5/3310 (0.2%)
1	C	0.99	25/2437 (1.0%)	0.90	14/3310 (0.4%)
All	All	1.01	70/7311 (1.0%)	0.88	39/9930 (0.4%)

All (70) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	318	TYR	CE2-CZ	-15.44	1.18	1.38
1	C	254	TYR	CE2-CZ	-14.45	1.19	1.38
1	C	254	TYR	CE1-CZ	-14.07	1.20	1.38
1	A	318	TYR	CE1-CZ	-14.07	1.20	1.38
1	A	197	TYR	CE2-CZ	-13.20	1.21	1.38
1	A	45	TYR	CE1-CZ	-12.75	1.22	1.38
1	A	197	TYR	CE1-CZ	-12.63	1.22	1.38
1	A	45	TYR	CE2-CZ	-12.63	1.22	1.38
1	A	45	TYR	CG-CD1	-12.55	1.22	1.39
1	A	197	TYR	CG-CD1	-12.39	1.23	1.39
1	A	198	PHE	CE1-CZ	-12.32	1.14	1.37
1	C	156	PHE	CE1-CZ	-12.21	1.14	1.37
1	A	197	TYR	CG-CD2	-12.09	1.23	1.39
1	A	45	TYR	CG-CD2	-12.06	1.23	1.39
1	C	156	PHE	CG-CD2	-11.86	1.21	1.38
1	A	318	TYR	CG-CD1	-11.78	1.23	1.39
1	C	254	TYR	CG-CD2	-11.03	1.24	1.39
1	C	156	PHE	CE2-CZ	-10.97	1.16	1.37
1	A	318	TYR	CG-CD2	-10.91	1.25	1.39
1	C	254	TYR	CG-CD1	-10.80	1.25	1.39
1	A	198	PHE	CE2-CZ	-10.62	1.17	1.37
1	A	198	PHE	CG-CD2	-10.48	1.23	1.38
1	A	198	PHE	CG-CD1	-10.09	1.23	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	156	PHE	CG-CD1	-9.92	1.23	1.38
1	B	156	PHE	CE1-CZ	-9.21	1.19	1.37
1	B	45	TYR	CE2-CZ	-8.55	1.27	1.38
1	B	197	TYR	CE1-CZ	-8.35	1.27	1.38
1	C	318	TYR	CE2-CZ	-8.32	1.27	1.38
1	B	45	TYR	CE1-CZ	-8.31	1.27	1.38
1	B	197	TYR	CE2-CZ	-8.13	1.27	1.38
1	B	318	TYR	CG-CD1	-7.85	1.28	1.39
1	A	254	TYR	CE2-CZ	-7.85	1.28	1.38
1	A	254	TYR	CE1-CZ	-7.56	1.28	1.38
1	C	318	TYR	CE1-CZ	-7.45	1.28	1.38
1	B	254	TYR	CG-CD1	-7.16	1.29	1.39
1	C	197	TYR	CE1-CZ	-7.11	1.29	1.38
1	B	318	TYR	CE2-CZ	-7.11	1.29	1.38
1	B	198	PHE	CE2-CZ	-7.01	1.24	1.37
1	B	318	TYR	CG-CD2	-6.98	1.30	1.39
1	B	254	TYR	CE1-CZ	-6.96	1.29	1.38
1	A	156	PHE	CE1-CZ	-6.76	1.24	1.37
1	B	254	TYR	CG-CD2	-6.71	1.30	1.39
1	B	318	TYR	CE1-CZ	-6.68	1.29	1.38
1	C	45	TYR	CE2-CZ	-6.65	1.29	1.38
1	B	156	PHE	CG-CD2	-6.64	1.28	1.38
1	C	45	TYR	CG-CD2	-6.54	1.30	1.39
1	C	197	TYR	CE2-CZ	-6.52	1.30	1.38
1	C	45	TYR	CG-CD1	-6.41	1.30	1.39
1	C	318	TYR	CG-CD2	-6.38	1.30	1.39
1	C	197	TYR	CG-CD2	-6.34	1.30	1.39
1	B	198	PHE	CG-CD2	-6.19	1.29	1.38
1	C	318	TYR	CG-CD1	-6.12	1.31	1.39
1	C	197	TYR	CG-CD1	-6.07	1.31	1.39
1	C	45	TYR	CE1-CZ	-6.05	1.30	1.38
1	A	254	TYR	CG-CD2	-6.05	1.31	1.39
1	A	254	TYR	CG-CD1	-6.04	1.31	1.39
1	C	198	PHE	CE1-CZ	-6.03	1.25	1.37
1	B	198	PHE	CE1-CZ	-6.02	1.25	1.37
1	B	254	TYR	CE2-CZ	-6.01	1.30	1.38
1	A	156	PHE	CG-CD2	-5.64	1.30	1.38
1	B	197	TYR	CG-CD2	-5.64	1.31	1.39
1	B	156	PHE	CE2-CZ	-5.53	1.26	1.37
1	B	45	TYR	CG-CD2	-5.49	1.32	1.39
1	A	156	PHE	CE2-CZ	-5.49	1.26	1.37
1	C	198	PHE	CG-CD2	-5.45	1.30	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	45	TYR	CG-CD1	-5.34	1.32	1.39
1	C	237	ASP	CG-OD1	-5.28	1.13	1.25
1	C	198	PHE	CG-CD1	-5.21	1.30	1.38
1	B	197	TYR	CG-CD1	-5.13	1.32	1.39
1	C	237	ASP	CG-OD2	-5.03	1.13	1.25

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	237	ASP	CB-CG-OD2	10.68	127.92	118.30
1	B	99	GLY	N-CA-C	-10.64	86.49	113.10
1	C	99	GLY	N-CA-C	-10.46	86.96	113.10
1	A	99	GLY	N-CA-C	-10.45	86.97	113.10
1	C	237	ASP	OD1-CG-OD2	-8.71	106.76	123.30
1	C	237	ASP	CB-CG-OD1	7.78	125.30	118.30
1	C	156	PHE	CB-CG-CD1	7.63	126.14	120.80
1	A	318	TYR	CB-CG-CD2	7.39	125.44	121.00
1	A	198	PHE	CB-CG-CD2	7.12	125.79	120.80
1	A	318	TYR	CD1-CG-CD2	-6.69	110.55	117.90
1	C	156	PHE	CD1-CG-CD2	-6.42	109.95	118.30
1	A	45	TYR	CD1-CE1-CZ	6.20	125.38	119.80
1	C	254	TYR	CB-CG-CD1	6.19	124.71	121.00
1	A	318	TYR	CD1-CE1-CZ	6.18	125.36	119.80
1	C	254	TYR	CD1-CG-CD2	-6.13	111.16	117.90
1	A	197	TYR	CD1-CE1-CZ	6.12	125.31	119.80
1	A	198	PHE	CD1-CG-CD2	-6.09	110.38	118.30
1	A	45	TYR	CZ-CE2-CD2	6.09	125.28	119.80
1	B	180	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	B	237	ASP	CB-CG-OD1	5.92	123.63	118.30
1	C	254	TYR	CD1-CE1-CZ	5.81	125.03	119.80
1	A	197	TYR	CZ-CE2-CD2	5.81	125.03	119.80
1	C	156	PHE	CZ-CE2-CD2	5.67	126.91	120.10
1	A	318	TYR	CZ-CE2-CD2	5.64	124.88	119.80
1	A	45	TYR	CE1-CZ-CE2	-5.62	110.81	119.80
1	B	98	GLY	CA-C-N	-5.55	105.11	116.20
1	C	254	TYR	CZ-CE2-CD2	5.46	124.71	119.80
1	A	197	TYR	CE1-CZ-CE2	-5.38	111.19	119.80
1	B	98	GLY	N-CA-C	5.29	126.33	113.10
1	C	254	TYR	CB-CG-CD2	5.15	124.09	121.00
1	A	45	TYR	CB-CG-CD1	5.14	124.08	121.00
1	C	98	GLY	N-CA-C	5.14	125.96	113.10
1	A	98	GLY	N-CA-C	5.14	125.95	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	197	TYR	CD1-CG-CD2	-5.09	112.31	117.90
1	A	98	GLY	CA-C-N	-5.07	106.07	116.20
1	A	45	TYR	CD1-CG-CD2	-5.06	112.33	117.90
1	A	197	TYR	CB-CG-CD1	5.04	124.02	121.00
1	A	318	TYR	CB-CG-CD1	5.03	124.02	121.00
1	C	98	GLY	CA-C-N	-5.00	106.20	116.20

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	2385	0	2415	46	0
1	B	2385	0	2415	57	0
1	C	2385	0	2415	54	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	12	0	13	3	0
3	B	12	0	13	3	0
3	C	12	0	13	3	0
4	A	71	0	0	5	0
4	B	94	0	0	6	0
4	C	80	0	0	5	0
All	All	7442	0	7284	150	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 10.

All (150) 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:6:LYS:HB2	4:A:842:HOH:O	1.49	1.11
1:B:135:THR:HB	1:B:137:SER:O	1.81	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:211:VAL:O	1:C:215:THR:HG23	1.80	0.80
1:B:128:ASP:OD1	3:B:1001:DHH:H092	1.83	0.79
1:A:135:THR:HB	1:A:137:SER:O	1.82	0.78
1:C:128:ASP:OD1	3:C:1002:DHH:H092	1.85	0.77
1:A:128:ASP:OD1	3:A:1000:DHH:H092	1.86	0.75
1:B:211:VAL:O	1:B:215:THR:HG23	1.86	0.75
1:C:135:THR:HB	1:C:137:SER:O	1.86	0.74
1:A:211:VAL:O	1:A:215:THR:HG23	1.87	0.74
1:C:143:GLN:N	1:C:144:PRO:HD3	2.05	0.71
1:B:128:ASP:HB3	1:B:144:PRO:HD2	1.74	0.69
4:A:609:HOH:O	1:B:201:THR:HG21	1.92	0.69
1:C:153:LYS:HD3	1:C:167:PRO:HG2	1.75	0.69
1:B:198:PHE:CE2	1:B:215:THR:HG22	2.30	0.67
1:B:143:GLN:N	1:B:144:PRO:HD3	2.09	0.67
1:A:153:LYS:HD3	1:A:167:PRO:HG2	1.76	0.67
1:A:143:GLN:N	1:A:144:PRO:HD3	2.10	0.67
1:A:128:ASP:HB3	1:A:144:PRO:HD2	1.76	0.67
1:C:143:GLN:H	1:C:144:PRO:HD3	1.59	0.66
1:C:128:ASP:HB3	1:C:144:PRO:HD2	1.78	0.66
1:C:198:PHE:CE2	1:C:215:THR:HG22	2.31	0.66
1:B:153:LYS:HD3	1:B:167:PRO:HG2	1.78	0.65
1:A:184:PRO:HA	1:C:311:ASN:O	1.95	0.65
1:C:307:LYS:H	1:C:311:ASN:HD21	1.47	0.63
1:B:311:ASN:O	1:C:184:PRO:HA	1.98	0.63
1:B:143:GLN:H	1:B:144:PRO:HD3	1.65	0.62
1:C:143:GLN:N	1:C:144:PRO:CD	2.63	0.61
1:A:180:ARG:NH2	1:A:235:GLY:O	2.34	0.61
1:C:180:ARG:NH2	1:C:235:GLY:O	2.33	0.61
1:B:130:ASN:ND2	3:B:1001:DHH:O05	2.34	0.60
1:B:233:VAL:HG22	1:B:241:THR:HG21	1.83	0.60
1:A:143:GLN:H	1:A:144:PRO:HD3	1.68	0.59
1:B:291:ARG:O	1:B:295:THR:CG2	2.51	0.58
1:B:180:ARG:NH2	1:B:235:GLY:O	2.34	0.58
1:A:126:HIS:HB3	4:A:647:HOH:O	2.03	0.58
1:A:307:LYS:H	1:A:311:ASN:HD21	1.49	0.58
1:C:115:HIS:HE1	4:C:751:HOH:O	1.87	0.58
1:B:143:GLN:N	1:B:144:PRO:CD	2.66	0.57
1:A:130:ASN:ND2	3:A:1000:DHH:O05	2.36	0.57
1:C:135:THR:CG2	4:C:839:HOH:O	2.51	0.57
1:B:128:ASP:OD1	3:B:1001:DHH:C09	2.52	0.57
1:C:130:ASN:ND2	3:C:1002:DHH:O05	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:LYS:H	1:B:311:ASN:HD21	1.53	0.57
1:A:233:VAL:HG22	1:A:241:THR:HG21	1.87	0.56
1:B:15:PHE:CZ	1:B:17:LYS:HB2	2.40	0.56
1:C:66:ILE:HG22	1:C:138:GLY:CA	2.35	0.56
1:C:180:ARG:HG3	1:C:248:VAL:HG11	1.87	0.56
1:B:180:ARG:HG3	1:B:248:VAL:HG11	1.88	0.56
1:A:143:GLN:N	1:A:144:PRO:CD	2.69	0.56
1:B:115:HIS:HE1	4:B:612:HOH:O	1.88	0.55
1:A:66:ILE:HG22	1:A:138:GLY:CA	2.36	0.55
1:A:130:ASN:HB3	1:A:135:THR:HG23	1.88	0.54
1:C:15:PHE:CZ	1:C:17:LYS:HB2	2.41	0.54
1:A:291:ARG:O	1:A:295:THR:CG2	2.55	0.54
1:B:66:ILE:HG22	1:B:138:GLY:CA	2.38	0.54
1:B:148:LEU:O	1:B:169:ILE:HD13	2.07	0.54
1:C:233:VAL:HG22	1:C:241:THR:HG21	1.90	0.53
1:C:128:ASP:OD1	3:C:1002:DHH:C09	2.56	0.53
1:A:118:LEU:O	1:A:118:LEU:HD12	2.08	0.52
1:A:148:LEU:O	1:A:169:ILE:HD13	2.10	0.52
1:B:146:ALA:HA	1:B:152:LEU:HD23	1.92	0.52
1:C:291:ARG:O	1:C:295:THR:CG2	2.57	0.52
1:A:146:ALA:HA	1:A:152:LEU:HD23	1.90	0.52
1:B:130:ASN:HB3	1:B:135:THR:HG23	1.90	0.52
1:A:180:ARG:HG3	1:A:248:VAL:HG11	1.92	0.51
1:C:130:ASN:HB3	1:C:135:THR:HG23	1.92	0.51
4:B:654:HOH:O	1:C:201:THR:HG21	2.11	0.51
1:A:15:PHE:CZ	1:A:17:LYS:HB2	2.46	0.51
1:A:128:ASP:OD1	3:A:1000:DHH:C09	2.55	0.51
1:A:201:THR:HG21	4:C:700:HOH:O	2.10	0.51
1:B:291:ARG:O	1:B:295:THR:HG23	2.11	0.50
1:C:118:LEU:O	1:C:118:LEU:HD12	2.11	0.50
1:C:146:ALA:HA	1:C:152:LEU:HD23	1.92	0.50
1:B:118:LEU:HD12	1:B:118:LEU:O	2.11	0.50
1:A:44:GLU:HG2	4:A:721:HOH:O	2.12	0.50
1:A:24:VAL:O	1:A:99:GLY:HA2	2.12	0.50
1:A:102:SER:HA	1:A:144:PRO:HG3	1.94	0.49
1:A:118:LEU:HD12	1:A:118:LEU:C	2.33	0.49
1:C:148:LEU:O	1:C:169:ILE:HD13	2.12	0.49
1:B:262:GLU:OE1	1:C:201:THR:HB	2.12	0.49
1:C:31:LEU:HD23	1:C:293:VAL:HG13	1.95	0.49
1:A:135:THR:CG2	4:A:837:HOH:O	2.61	0.49
1:C:118:LEU:HD12	1:C:118:LEU:C	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:LEU:HD13	1:A:193:LEU:HD21	1.95	0.48
1:B:118:LEU:HD12	1:B:118:LEU:C	2.33	0.48
1:C:102:SER:HA	1:C:144:PRO:HG3	1.95	0.48
1:B:19:CYS:HB2	1:B:20:PRO:HD2	1.96	0.48
1:B:24:VAL:O	1:B:99:GLY:HA2	2.13	0.48
1:B:102:SER:HA	1:B:144:PRO:HG3	1.96	0.47
1:C:291:ARG:O	1:C:295:THR:HG23	2.14	0.47
1:C:24:VAL:O	1:C:99:GLY:HA2	2.13	0.47
1:B:233:VAL:HG12	1:B:244:THR:HG23	1.97	0.47
1:B:244:THR:CG2	1:B:277:GLU:O	2.64	0.46
1:B:210:LYS:HD2	1:B:213:GLU:OE2	2.15	0.46
1:B:259:TYR:CE1	1:C:205:LYS:HB2	2.50	0.46
1:B:244:THR:HG23	1:B:277:GLU:O	2.17	0.45
1:C:152:LEU:HD13	1:C:193:LEU:HD21	1.97	0.45
1:B:291:ARG:O	1:B:295:THR:HG22	2.17	0.45
1:A:291:ARG:O	1:A:295:THR:HG23	2.16	0.45
1:C:233:VAL:HG12	1:C:244:THR:HG23	1.98	0.45
1:B:12:GLY:HA3	1:B:52:ASP:OD1	2.17	0.45
1:B:198:PHE:HE2	1:B:215:THR:HG22	1.77	0.45
1:B:152:LEU:HD13	1:B:193:LEU:HD21	1.99	0.44
1:C:64:PHE:O	1:C:65:GLN:HB2	2.17	0.44
1:A:187:HIS:O	1:A:191:LYS:HG2	2.17	0.44
1:C:75:LYS:HD2	1:C:75:LYS:HA	1.85	0.44
1:C:287:GLU:OE2	1:C:291:ARG:NE	2.48	0.44
1:A:291:ARG:O	1:A:295:THR:HG22	2.17	0.44
1:C:314:PRO:O	1:C:315:GLU:HB2	2.17	0.44
1:B:126:HIS:HB3	4:B:608:HOH:O	2.17	0.44
1:B:187:HIS:O	1:B:191:LYS:HG2	2.18	0.44
1:A:64:PHE:O	1:A:65:GLN:HB2	2.18	0.44
1:A:198:PHE:CE1	1:A:215:THR:HG22	2.53	0.44
1:C:19:CYS:HB2	1:C:20:PRO:HD2	1.99	0.44
1:B:318:TYR:HB2	1:C:188:TYR:CD2	2.53	0.44
1:B:135:THR:CG2	4:B:658:HOH:O	2.67	0.43
1:C:92:THR:HG21	4:C:706:HOH:O	2.18	0.43
1:A:19:CYS:HB2	1:A:20:PRO:HD2	2.00	0.43
1:C:16:SER:CB	1:C:24:VAL:HG23	2.48	0.43
1:B:237:ASP:HA	1:B:238:PRO:HD3	1.91	0.43
1:B:64:PHE:O	1:B:65:GLN:HB2	2.18	0.43
1:B:169:ILE:HD13	1:B:169:ILE:H	1.84	0.43
1:A:210:LYS:HD2	1:A:213:GLU:OE2	2.18	0.43
1:A:233:VAL:HG12	1:A:244:THR:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LEU:HD23	1:B:293:VAL:HG13	2.01	0.43
1:B:233:VAL:HG12	1:B:244:THR:CG2	2.48	0.42
1:B:129:ILE:O	1:B:129:ILE:HG12	2.20	0.42
1:A:311:ASN:O	1:B:184:PRO:HA	2.19	0.42
1:A:12:GLY:HA3	1:A:52:ASP:OD1	2.19	0.42
1:A:16:SER:CB	1:A:24:VAL:HG23	2.49	0.42
1:A:314:PRO:O	1:A:315:GLU:HB2	2.18	0.42
1:B:287:GLU:OE2	1:B:291:ARG:NE	2.49	0.42
1:B:21:ARG:NH1	4:B:736:HOH:O	2.53	0.42
1:C:254:TYR:CE1	1:C:258:LEU:HD11	2.55	0.42
1:A:244:THR:CG2	1:A:277:GLU:O	2.68	0.41
1:C:233:VAL:HG12	1:C:244:THR:CG2	2.50	0.41
1:C:159:VAL:HA	1:C:160:PRO:HD3	1.97	0.41
1:C:233:VAL:CG1	1:C:244:THR:HG23	2.51	0.41
1:B:313:LYS:HA	1:B:314:PRO:HD3	1.91	0.41
1:C:169:ILE:HD13	1:C:169:ILE:H	1.86	0.41
1:B:318:TYR:HD1	1:C:188:TYR:CG	2.39	0.41
1:C:187:HIS:O	1:C:191:LYS:HG2	2.21	0.41
1:B:233:VAL:CG1	1:B:244:THR:HG23	2.51	0.41
1:A:31:LEU:HD23	1:A:293:VAL:HG13	2.03	0.41
1:B:135:THR:HG22	4:B:658:HOH:O	2.20	0.41
1:C:198:PHE:HE2	1:C:215:THR:HG22	1.83	0.40
1:A:169:ILE:HD13	1:A:169:ILE:H	1.85	0.40
1:C:12:GLY:HA3	1:C:52:ASP:OD1	2.22	0.40
1:C:126:HIS:HB3	4:C:624:HOH:O	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	312/314 (99%)	303 (97%)	8 (3%)	1 (0%)	46 50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	312/314 (99%)	305 (98%)	6 (2%)	1 (0%)	46	50
1	C	312/314 (99%)	304 (97%)	7 (2%)	1 (0%)	46	50
All	All	936/942 (99%)	912 (97%)	21 (2%)	3 (0%)	46	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	143	GLN
1	A	143	GLN
1	B	143	GLN

### 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	260/260 (100%)	244 (94%)	16 (6%)	23	25
1	B	260/260 (100%)	244 (94%)	16 (6%)	23	25
1	C	260/260 (100%)	242 (93%)	18 (7%)	19	20
All	All	780/780 (100%)	730 (94%)	50 (6%)	22	24

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	56	VAL
1	A	57	ASP
1	A	60	ASN
1	A	101	HIS
1	A	135	THR
1	A	152	LEU
1	A	169	ILE
1	A	201	THR
1	A	224	LYS
1	A	225	ARG

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Mol	Chain	Res	Type
1	A	233	VAL
1	A	244	THR
1	A	273	LEU
1	A	287	GLU
1	A	295	THR
1	B	24	VAL
1	B	56	VAL
1	B	57	ASP
1	B	135	THR
1	B	152	LEU
1	B	169	ILE
1	B	201	THR
1	B	222	ARG
1	B	225	ARG
1	B	233	VAL
1	B	239	VAL
1	B	244	THR
1	B	273	LEU
1	B	286	PRO
1	B	287	GLU
1	B	295	THR
1	C	24	VAL
1	C	56	VAL
1	C	57	ASP
1	C	60	ASN
1	C	101	HIS
1	C	135	THR
1	C	152	LEU
1	C	169	ILE
1	C	201	THR
1	C	222	ARG
1	C	224	LYS
1	C	225	ARG
1	C	233	VAL
1	C	239	VAL
1	C	244	THR
1	C	273	LEU
1	C	287	GLU
1	C	295	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:



Mol	Chain	Res	Type
1	A	79	GLN
1	A	311	ASN
1	B	115	HIS
1	B	311	ASN
1	C	79	GLN
1	C	115	HIS
1	C	311	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 6 are monoatomic - leaving 3 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	$\# Z  > 2$
3	DHH	A	1000	2	5,11,11	0.91	0	4,13,13	1.35	1 (25%)
3	DHH	B	1001	2	5,11,11	0.91	0	4,13,13	1.35	1 (25%)
3	DHH	C	1002	2	5,11,11	0.91	0	4,13,13	1.35	1 (25%)

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
3	DHH	A	1000	2	-	0/5/11/11	0/0/0/0
3	DHH	B	1001	2	-	0/5/11/11	0/0/0/0
3	DHH	C	1002	2	-	0/5/11/11	0/0/0/0

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1000	DHH	C08-C07-C06	-2.03	106.43	113.66
3	C	1002	DHH	C08-C07-C06	-2.03	106.45	113.66
3	B	1001	DHH	C08-C07-C06	-2.03	106.45	113.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1000	DHH	3	0
3	B	1001	DHH	3	0
3	C	1002	DHH	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

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

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

### 6.3 Carbohydrates [i](#)

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

### 6.4 Ligands [i](#)

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

### 6.5 Other polymers [i](#)

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