



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2023 – 08:40 PM EDT

PDB ID : 1P8N  
Title : Structural and Functional Importance of First-Shell Metal Ligands in the Binuclear Manganese Cluster of Arginase I.  
Authors : Cama, E.; Emig, F.A.; Ash, D.E.; Christianson, D.W.  
Deposited on : 2003-05-07  
Resolution : 2.90 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

---

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)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.35

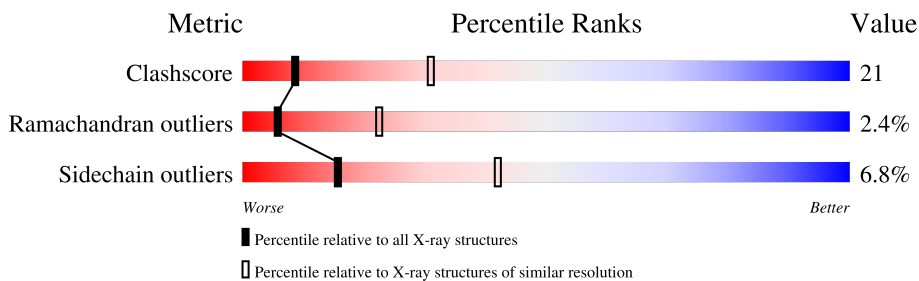
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)

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 of 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  $\leq 5\%$ .

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 7240 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
			Total	C	N	O	S			
1	A	314	2393	1527	405	454	7	0	0	0
1	B	314	2393	1527	405	454	7	3	0	0
1	C	314	2393	1527	405	454	7	3	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	ALA	ASP	engineered mutation	UNP P07824
B	232	ALA	ASP	engineered mutation	UNP P07824
C	232	ALA	ASP	engineered mutation	UNP P07824

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 6 3 3	0	0

- Molecule 4 is water.

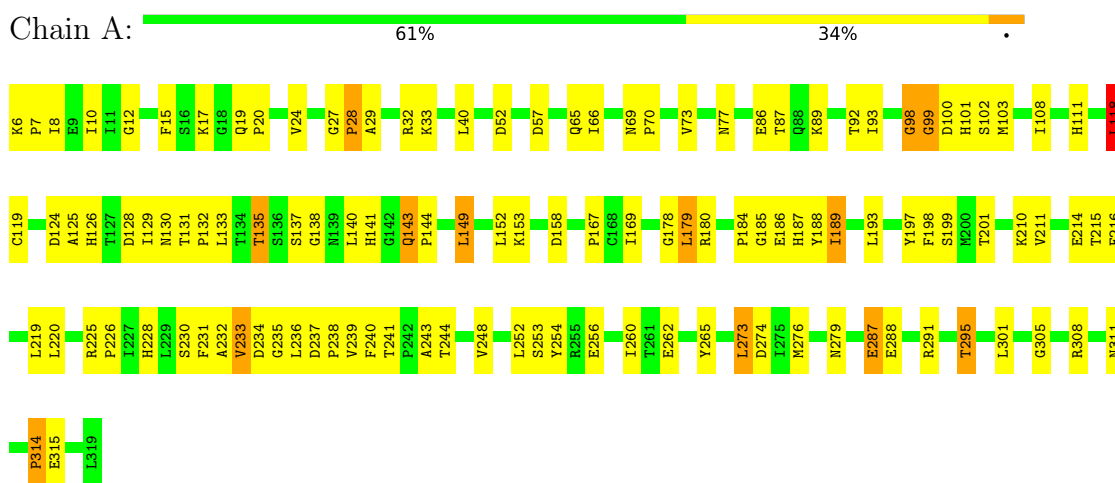
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	18	Total O 18 18	0	0
4	B	19	Total O 19 19	0	0
4	C	15	Total O 15 15	0	0

### 3 Residue-property plots

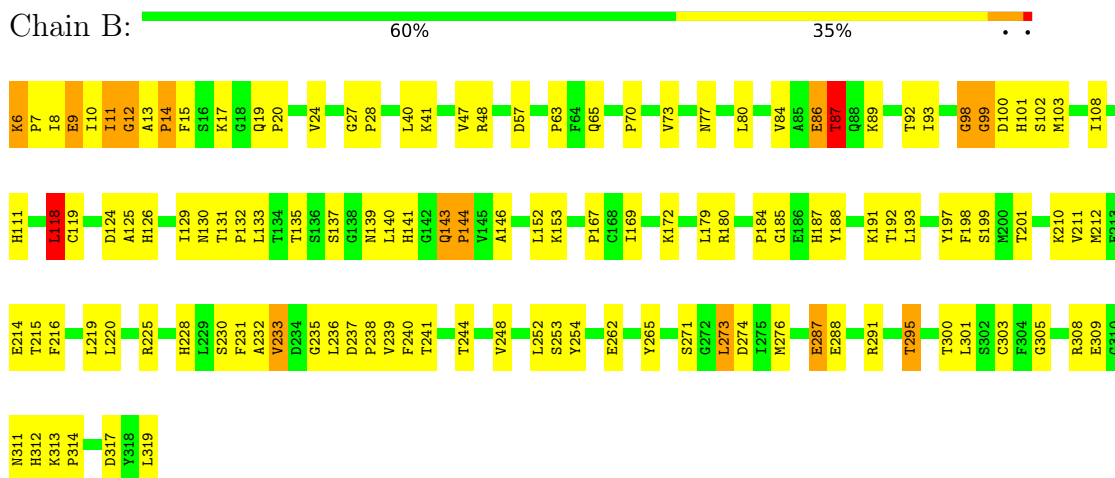
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

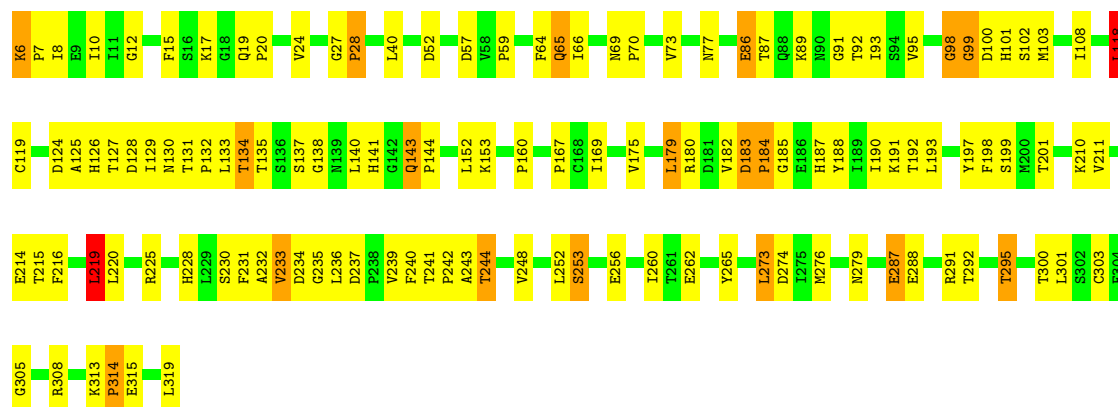


- Molecule 1: Arginase 1



- Molecule 1: Arginase 1





## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.34Å 90.34Å 104.98Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.57 – 2.90	Depositor
% Data completeness (in resolution range)	91.6 (29.57-2.90)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.286 , 0.305	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7240	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	80.0	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: MN, GOL

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	0.58	3/2446 (0.1%)	0.77	5/3321 (0.2%)
1	B	0.59	2/2446 (0.1%)	0.78	7/3321 (0.2%)
1	C	0.59	4/2446 (0.2%)	0.80	6/3321 (0.2%)
All	All	0.58	9/7338 (0.1%)	0.78	18/9963 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	11	ILE	C-O	-10.29	1.03	1.23
1	B	87	THR	CB-CG2	-9.80	1.20	1.52
1	A	149	LEU	CG-CD2	-8.72	1.19	1.51
1	A	149	LEU	CG-CD1	-8.57	1.20	1.51
1	C	219	LEU	CG-CD2	-7.41	1.24	1.51
1	C	201	THR	CB-CG2	-7.37	1.28	1.52
1	C	134	THR	CB-CG2	-6.48	1.30	1.52
1	A	87	THR	CB-CG2	-5.32	1.34	1.52
1	C	87	THR	CB-CG2	-5.10	1.35	1.52

All (18) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	99	GLY	N-CA-C	8.98	135.55	113.10
1	C	99	GLY	N-CA-C	8.83	135.18	113.10
1	B	99	GLY	N-CA-C	8.52	134.39	113.10
1	C	219	LEU	CB-CG-CD2	-8.32	96.85	111.00
1	B	11	ILE	CA-C-N	8.29	132.79	116.20
1	C	6	LYS	C-N-CD	-8.21	102.53	120.60
1	A	149	LEU	CD1-CG-CD2	-7.97	86.58	110.50
1	B	12	GLY	N-CA-C	-7.93	93.26	113.10
1	A	118	LEU	CA-CB-CG	6.60	130.49	115.30
1	C	219	LEU	CB-CG-CD1	6.53	122.09	111.00
1	B	11	ILE	O-C-N	-6.51	112.14	123.20
1	A	6	LYS	C-N-CD	-6.27	106.80	120.60
1	B	87	THR	OG1-CB-CG2	-5.77	96.72	110.00
1	C	201	THR	OG1-CB-CG2	-5.60	97.12	110.00
1	B	118	LEU	CA-CB-CG	5.55	128.06	115.30
1	A	149	LEU	CB-CG-CD1	5.54	120.42	111.00
1	C	118	LEU	CA-CB-CG	5.43	127.79	115.30
1	B	6	LYS	C-N-CD	-5.21	109.13	120.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	GLY	Peptide
1	B	98	GLY	Peptide
1	C	98	GLY	Peptide

## 5.2 Too-close contacts [i](#)

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	2393	0	2421	92	0
1	B	2393	0	2421	113	0
1	C	2393	0	2421	107	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	6	0	8	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	18	0	0	4	0
4	B	19	0	0	6	0
4	C	15	0	0	1	0
All	All	7240	0	7271	298	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 21.

All (298) 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:308:ARG:HE	1:B:201:THR:HG22	1.19	1.08
1:B:8:ILE:HG22	1:B:10:ILE:HD11	1.37	1.04
1:C:119:CYS:CB	1:C:219:LEU:HD21	1.89	1.02
1:C:119:CYS:HB2	1:C:219:LEU:HD21	1.03	1.00
1:C:119:CYS:HB2	1:C:219:LEU:CD2	1.93	0.98
1:B:8:ILE:HG22	1:B:10:ILE:CD1	1.94	0.98
1:B:311:ASN:O	1:C:184:PRO:HA	1.68	0.94
1:C:210:LYS:HE3	1:C:214:GLU:OE2	1.69	0.91
1:A:201:THR:HG22	1:C:308:ARG:HE	1.34	0.90
1:A:308:ARG:NE	1:B:201:THR:HG22	1.85	0.89
1:B:9:GLU:C	1:B:10:ILE:HD12	1.95	0.86
1:C:12:GLY:HA3	1:C:52:ASP:OD1	1.75	0.86
1:A:143:GLN:H	1:A:144:PRO:HD3	1.42	0.85
1:B:7:PRO:CB	1:B:92:THR:HG22	2.07	0.85
1:A:28:PRO:HD3	1:A:98:GLY:O	1.78	0.83
1:A:12:GLY:HA3	1:A:52:ASP:OD1	1.82	0.80
1:B:87:THR:HG23	1:B:92:THR:OG1	1.82	0.79
1:C:143:GLN:H	1:C:144:PRO:HD3	1.47	0.79
1:B:143:GLN:H	1:B:144:PRO:HD3	1.47	0.79
1:B:8:ILE:CG2	1:B:10:ILE:HD11	2.11	0.78
1:A:7:PRO:CB	1:A:92:THR:HG22	2.13	0.78
1:A:143:GLN:H	1:A:144:PRO:CD	1.97	0.78
1:B:143:GLN:H	1:B:144:PRO:CD	1.96	0.77
1:C:130:ASN:OD1	1:C:134:THR:HG23	1.85	0.77
1:C:7:PRO:CB	1:C:92:THR:HG22	2.15	0.76
1:C:143:GLN:H	1:C:144:PRO:CD	2.01	0.74
1:C:216:PHE:O	1:C:220:LEU:HB2	1.89	0.73
1:B:10:ILE:HD12	1:B:10:ILE:N	2.03	0.73
1:B:230:SER:HA	1:B:274:ASP:HB2	1.72	0.72
1:C:230:SER:HA	1:C:274:ASP:HB2	1.72	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:GLU:OE2	1:B:308:ARG:HG3	1.92	0.70
1:A:143:GLN:N	1:A:144:PRO:CD	2.53	0.70
1:B:28:PRO:HD3	1:B:98:GLY:O	1.92	0.69
1:A:262:GLU:OE2	1:A:308:ARG:HG3	1.92	0.69
1:B:135:THR:HB	1:B:137:SER:O	1.92	0.69
1:A:233:VAL:HG13	1:A:241:THR:HB	1.75	0.68
1:C:126:HIS:HB3	4:C:802:HOH:O	1.92	0.68
1:B:143:GLN:N	1:B:144:PRO:CD	2.56	0.68
1:C:119:CYS:CB	1:C:219:LEU:CD2	2.64	0.68
1:C:125:ALA:HB1	1:C:180:ARG:HG2	1.76	0.68
1:C:19:GLN:HB2	1:C:20:PRO:HD2	1.75	0.68
1:A:125:ALA:HB1	1:A:180:ARG:HG2	1.75	0.67
1:A:135:THR:HB	1:A:137:SER:O	1.93	0.67
1:B:130:ASN:HB3	1:B:135:THR:HG23	1.77	0.67
1:A:119:CYS:HB2	1:A:219:LEU:HD22	1.77	0.67
1:C:102:SER:HA	1:C:144:PRO:HG3	1.75	0.66
1:A:130:ASN:HB3	1:A:135:THR:HG23	1.78	0.66
1:A:198:PHE:CE1	1:A:215:THR:HG22	2.31	0.66
1:B:119:CYS:HB2	1:B:219:LEU:HD22	1.77	0.66
1:A:291:ARG:O	1:A:295:THR:HG23	1.96	0.65
1:B:102:SER:HA	1:B:144:PRO:HG3	1.77	0.65
1:A:211:VAL:O	1:A:215:THR:HG23	1.95	0.65
1:C:130:ASN:HB3	1:C:135:THR:HG23	1.79	0.65
1:C:291:ARG:O	1:C:295:THR:HG23	1.96	0.65
1:B:125:ALA:HB1	1:B:180:ARG:HG2	1.79	0.65
1:B:9:GLU:OE1	1:B:48:ARG:HD3	1.95	0.65
1:C:143:GLN:N	1:C:144:PRO:CD	2.59	0.64
1:C:180:ARG:NH2	1:C:235:GLY:O	2.31	0.64
1:C:210:LYS:O	1:C:214:GLU:HG3	1.98	0.63
1:A:216:PHE:O	1:A:220:LEU:HB2	1.98	0.63
1:C:95:VAL:HG13	1:C:273:LEU:HD13	1.80	0.63
1:B:198:PHE:CE1	1:B:215:THR:HG22	2.34	0.63
1:B:198:PHE:CD2	1:B:211:VAL:HG13	2.33	0.63
1:B:152:LEU:CD1	1:B:193:LEU:HD21	2.28	0.63
1:C:28:PRO:HD3	1:C:98:GLY:O	1.99	0.63
1:B:180:ARG:NH2	1:B:235:GLY:O	2.32	0.63
1:B:237:ASP:OD1	1:B:239:VAL:HG23	1.99	0.62
1:C:135:THR:HB	1:C:137:SER:O	1.99	0.62
1:C:198:PHE:CE1	1:C:215:THR:HG22	2.35	0.62
1:B:7:PRO:HB3	1:B:92:THR:HG22	1.82	0.62
1:C:314:PRO:O	1:C:315:GLU:HB2	1.99	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLN:HB2	1:A:20:PRO:HD2	1.81	0.62
1:A:152:LEU:CD1	1:A:193:LEU:HD21	2.30	0.62
1:B:291:ARG:O	1:B:295:THR:HG23	2.01	0.61
1:C:262:GLU:OE2	1:C:308:ARG:HG3	2.00	0.61
1:C:236:LEU:HD23	1:C:252:LEU:HB2	1.82	0.61
1:A:102:SER:HA	1:A:144:PRO:HG3	1.83	0.61
1:B:216:PHE:O	1:B:220:LEU:HB2	2.01	0.61
1:B:87:THR:CG2	1:B:92:THR:OG1	2.49	0.61
1:A:180:ARG:HD2	1:A:248:VAL:HB	1.83	0.60
1:B:19:GLN:HB2	1:B:20:PRO:HD2	1.82	0.60
1:B:10:ILE:CD1	1:B:10:ILE:N	2.64	0.60
1:C:211:VAL:O	1:C:215:THR:HG23	2.01	0.60
1:B:180:ARG:HD2	1:B:248:VAL:HB	1.83	0.60
1:B:153:LYS:HD2	1:B:167:PRO:HG2	1.83	0.59
1:A:33:LYS:HB3	4:A:805:HOH:O	2.01	0.59
1:A:308:ARG:HE	1:B:201:THR:CG2	2.05	0.59
1:B:8:ILE:HD13	1:B:93:ILE:HB	1.85	0.59
1:A:180:ARG:HG3	1:A:248:VAL:HG11	1.83	0.59
1:A:230:SER:HA	1:A:274:ASP:HB2	1.85	0.59
1:B:11:ILE:CD1	1:B:84:VAL:HG22	2.33	0.58
1:C:175:VAL:HG23	1:C:219:LEU:HD12	1.85	0.58
1:A:236:LEU:HD23	1:A:252:LEU:HB2	1.86	0.58
1:B:15:PHE:CZ	1:B:17:LYS:HB2	2.38	0.58
1:B:140:LEU:O	1:B:144:PRO:HD3	2.04	0.58
1:B:8:ILE:HG22	1:B:10:ILE:HD12	1.83	0.58
1:C:140:LEU:O	1:C:144:PRO:HD3	2.04	0.58
1:C:287:GLU:HG3	1:C:288:GLU:N	2.18	0.57
1:B:7:PRO:HB2	1:B:92:THR:HA	1.85	0.57
1:C:152:LEU:CD1	1:C:193:LEU:HD21	2.33	0.57
1:A:29:ALA:O	1:A:33:LYS:HB2	2.05	0.57
1:A:7:PRO:HB2	1:A:92:THR:HG22	1.87	0.57
1:C:180:ARG:HD2	1:C:248:VAL:HB	1.85	0.57
1:A:8:ILE:HD13	1:A:93:ILE:HB	1.87	0.56
1:B:7:PRO:HB2	1:B:92:THR:HG22	1.84	0.56
1:C:15:PHE:CZ	1:C:17:LYS:HB2	2.41	0.56
1:C:180:ARG:HG3	1:C:248:VAL:HG11	1.87	0.56
1:A:287:GLU:HG3	1:A:288:GLU:N	2.21	0.56
1:B:180:ARG:HG3	1:B:248:VAL:HG11	1.87	0.55
1:C:10:ILE:HD12	1:C:10:ILE:N	2.21	0.55
1:B:233:VAL:HG13	1:B:241:THR:HB	1.87	0.55
1:C:153:LYS:HD2	1:C:167:PRO:HG2	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:VAL:HG12	1:B:239:VAL:O	2.06	0.55
1:A:201:THR:HG22	1:C:262:GLU:OE1	2.06	0.54
1:A:15:PHE:CZ	1:A:17:LYS:HB2	2.41	0.54
1:B:13:ALA:N	1:B:14:PRO:CD	2.70	0.54
1:B:265:TYR:CE2	1:B:305:GLY:HA2	2.43	0.54
1:A:10:ILE:HD12	1:A:10:ILE:N	2.22	0.54
1:A:231:PHE:CD1	1:A:232:ALA:O	2.61	0.54
1:B:236:LEU:HD23	1:B:252:LEU:HB2	1.90	0.54
1:C:7:PRO:HB3	1:C:92:THR:HG22	1.88	0.54
1:C:8:ILE:HD13	1:C:93:ILE:HB	1.89	0.54
1:C:231:PHE:CD1	1:C:232:ALA:O	2.61	0.54
1:A:311:ASN:O	1:B:184:PRO:HA	2.09	0.53
1:C:7:PRO:HB2	1:C:92:THR:HA	1.90	0.53
1:C:7:PRO:HB2	1:C:92:THR:HG22	1.91	0.53
1:A:7:PRO:HB3	1:A:92:THR:HG22	1.90	0.53
1:C:73:VAL:HG21	1:C:140:LEU:HD12	1.91	0.53
1:A:140:LEU:O	1:A:144:PRO:HD3	2.08	0.52
1:A:180:ARG:NH2	1:A:235:GLY:O	2.42	0.52
1:B:231:PHE:CD1	1:B:232:ALA:O	2.62	0.52
1:B:312:HIS:HB3	1:C:184:PRO:O	2.09	0.52
1:B:11:ILE:HG21	1:B:80:LEU:CD1	2.39	0.52
1:B:11:ILE:HG21	1:B:80:LEU:HD11	1.91	0.52
1:B:108:ILE:HG12	1:B:228:HIS:CD2	2.45	0.52
1:B:77:ASN:OD1	1:B:103:MET:HA	2.10	0.51
1:A:73:VAL:HG21	1:A:140:LEU:HD12	1.91	0.51
1:B:86:GLU:O	1:B:89:LYS:HB3	2.10	0.51
1:B:103:MET:HB2	1:B:276:MET:CE	2.41	0.51
1:B:287:GLU:HG3	1:B:288:GLU:N	2.26	0.51
1:B:70:PRO:HD2	4:B:826:HOH:O	2.11	0.51
1:A:314:PRO:O	1:A:315:GLU:HB2	2.11	0.51
1:B:101:HIS:O	1:B:144:PRO:HG2	2.11	0.50
1:B:73:VAL:HG21	1:B:140:LEU:HD12	1.92	0.50
1:B:131:THR:O	1:B:133:LEU:N	2.44	0.50
1:C:233:VAL:O	1:C:235:GLY:N	2.44	0.50
1:A:198:PHE:CD2	1:A:211:VAL:HG13	2.47	0.50
1:B:13:ALA:N	1:B:14:PRO:HD3	2.27	0.50
1:C:240:PHE:CE2	1:C:253:SER:HA	2.46	0.50
1:A:108:ILE:HG12	1:A:228:HIS:CD2	2.47	0.50
1:C:6:LYS:HE2	1:C:91:GLY:O	2.12	0.50
1:C:101:HIS:O	1:C:144:PRO:HG2	2.11	0.50
1:A:7:PRO:HB2	1:A:92:THR:HA	1.93	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:ASP:HA	4:A:817:HOH:O	2.12	0.49
1:C:86:GLU:O	1:C:89:LYS:N	2.41	0.49
1:B:309:GLU:O	1:C:182:VAL:HB	2.12	0.49
1:C:131:THR:O	1:C:133:LEU:N	2.45	0.49
1:B:9:GLU:CA	1:B:10:ILE:HD12	2.43	0.49
1:A:73:VAL:HG11	1:A:140:LEU:HD13	1.94	0.49
1:A:187:HIS:O	1:A:188:TYR:C	2.50	0.49
1:C:27:GLY:O	1:C:28:PRO:C	2.51	0.49
1:A:128:ASP:HA	4:A:849:HOH:O	2.11	0.49
1:A:186:GLU:O	1:A:187:HIS:C	2.51	0.49
1:B:152:LEU:HD13	1:B:193:LEU:HD21	1.94	0.48
1:C:57:ASP:O	1:C:59:PRO:HD3	2.13	0.48
1:C:108:ILE:HG12	1:C:228:HIS:CD2	2.49	0.48
1:C:239:VAL:HG12	1:C:239:VAL:O	2.12	0.48
1:A:124:ASP:OD2	1:A:126:HIS:N	2.39	0.48
1:B:73:VAL:HG11	1:B:140:LEU:HD13	1.95	0.48
1:C:86:GLU:O	1:C:89:LYS:HB3	2.13	0.48
1:A:189:ILE:HD11	1:C:319:LEU:HD21	1.95	0.48
1:B:179:LEU:HB2	1:B:199:SER:HA	1.95	0.48
1:B:212:MET:HA	4:B:842:HOH:O	2.13	0.48
1:A:201:THR:CG2	1:C:262:GLU:OE1	2.62	0.47
1:C:179:LEU:HB2	1:C:199:SER:HA	1.97	0.47
1:A:152:LEU:HD13	1:A:193:LEU:HD21	1.95	0.47
1:C:131:THR:C	1:C:133:LEU:H	2.17	0.47
1:A:131:THR:O	1:A:133:LEU:N	2.47	0.47
1:A:240:PHE:CE2	1:A:253:SER:HA	2.49	0.47
1:B:300:THR:O	1:B:303:CYS:HB2	2.14	0.47
1:C:73:VAL:HG11	1:C:140:LEU:HD13	1.96	0.47
1:C:152:LEU:HD13	1:C:193:LEU:HD21	1.97	0.47
1:C:233:VAL:C	1:C:235:GLY:H	2.19	0.47
1:B:187:HIS:O	1:B:191:LYS:HG2	2.16	0.46
1:A:237:ASP:OD1	1:A:239:VAL:HG23	2.15	0.46
1:B:131:THR:C	1:B:133:LEU:H	2.19	0.46
1:A:153:LYS:HD2	1:A:167:PRO:HG2	1.96	0.46
1:B:124:ASP:OD2	1:B:126:HIS:N	2.40	0.46
1:B:210:LYS:HE3	1:B:214:GLU:OE2	2.16	0.46
1:A:40:LEU:HD23	1:A:301:LEU:HD23	1.97	0.46
1:B:20:PRO:HD3	1:B:139:ASN:OD1	2.16	0.46
1:A:32:ARG:HG3	1:A:32:ARG:HH11	1.81	0.46
1:A:308:ARG:CZ	1:B:201:THR:HG22	2.44	0.46
1:B:40:LEU:HD23	1:B:301:LEU:HD23	1.96	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:ASN:N	1:A:70:PRO:CD	2.79	0.46
1:B:11:ILE:HG22	1:B:12:GLY:O	2.16	0.46
1:B:198:PHE:CE1	1:B:215:THR:CG2	2.99	0.46
1:B:9:GLU:OE2	1:B:48:ARG:NH1	2.49	0.46
1:B:13:ALA:O	1:B:15:PHE:N	2.46	0.46
1:B:180:ARG:HH22	1:B:235:GLY:C	2.19	0.46
1:C:66:ILE:O	1:C:138:GLY:HA3	2.16	0.46
1:C:131:THR:H	1:C:134:THR:HG22	1.79	0.45
1:C:233:VAL:HG12	1:C:244:THR:CG2	2.46	0.45
1:A:273:LEU:HD22	1:A:274:ASP:N	2.32	0.45
1:C:103:MET:HB2	1:C:276:MET:HE1	1.97	0.45
1:C:103:MET:HB2	1:C:276:MET:CE	2.46	0.45
1:A:265:TYR:CE2	1:A:305:GLY:HA2	2.52	0.45
1:A:273:LEU:CD2	1:A:274:ASP:N	2.80	0.45
1:B:240:PHE:CE2	1:B:253:SER:HA	2.51	0.45
1:C:237:ASP:OD1	1:C:239:VAL:HG23	2.16	0.45
1:C:313:LYS:HB2	1:C:313:LYS:HE3	1.73	0.45
1:C:129:ILE:HG12	1:C:129:ILE:O	2.17	0.45
1:C:187:HIS:O	1:C:191:LYS:HG2	2.17	0.45
1:A:131:THR:C	1:A:133:LEU:H	2.20	0.45
1:C:124:ASP:OD2	1:C:126:HIS:N	2.40	0.45
1:C:183:ASP:HB3	1:C:184:PRO:HD2	1.98	0.45
1:C:243:ALA:HB1	1:C:279:ASN:O	2.17	0.45
1:A:77:ASN:OD1	1:A:103:MET:HA	2.17	0.44
1:B:313:LYS:HB2	1:B:313:LYS:HE3	1.74	0.44
1:A:185:GLY:O	1:A:188:TYR:HB3	2.18	0.44
1:B:27:GLY:O	1:B:28:PRO:C	2.55	0.44
1:C:119:CYS:SG	1:C:219:LEU:CD2	3.05	0.44
1:C:197:TYR:CD1	1:C:197:TYR:C	2.91	0.44
1:A:129:ILE:HG12	1:A:129:ILE:O	2.18	0.44
1:C:242:PRO:HD2	1:C:292:THR:OG1	2.17	0.44
1:C:198:PHE:CD2	1:C:211:VAL:HG13	2.53	0.44
1:A:265:TYR:HB3	4:A:841:HOH:O	2.18	0.43
1:A:86:GLU:O	1:A:89:LYS:HB3	2.19	0.43
1:B:143:GLN:O	1:B:144:PRO:C	2.57	0.43
1:B:185:GLY:O	1:B:188:TYR:HB3	2.19	0.43
1:C:233:VAL:HG22	1:C:241:THR:HG21	2.00	0.43
1:A:201:THR:HG22	1:C:308:ARG:NE	2.16	0.43
1:B:146:ALA:HA	1:B:152:LEU:HD23	2.01	0.43
1:A:103:MET:HB2	1:A:276:MET:CE	2.48	0.43
1:A:111:HIS:ND1	1:A:228:HIS:ND1	2.63	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:MET:HB2	1:B:276:MET:HE3	2.01	0.43
1:B:131:THR:C	1:B:133:LEU:N	2.72	0.43
1:B:233:VAL:C	1:B:235:GLY:H	2.22	0.43
1:C:40:LEU:HD23	1:C:301:LEU:HD23	2.01	0.43
1:C:6:LYS:HA	1:C:7:PRO:HD2	1.75	0.43
1:C:66:ILE:HG22	1:C:138:GLY:HA2	2.01	0.43
1:B:86:GLU:O	1:B:89:LYS:N	2.45	0.42
1:B:211:VAL:HG12	4:B:842:HOH:O	2.17	0.42
1:B:254:TYR:CE1	1:B:295:THR:HB	2.54	0.42
1:A:66:ILE:O	1:A:138:GLY:HA3	2.19	0.42
1:A:180:ARG:HG3	1:A:248:VAL:CG1	2.49	0.42
1:C:131:THR:N	1:C:134:THR:HG22	2.34	0.42
1:C:180:ARG:HH22	1:C:235:GLY:C	2.21	0.42
1:C:190:ILE:HD12	1:C:197:TYR:CD2	2.53	0.42
1:A:197:TYR:CD1	1:A:197:TYR:C	2.92	0.42
1:A:231:PHE:HD1	1:A:232:ALA:O	2.03	0.42
1:A:178:GLY:O	1:A:179:LEU:C	2.57	0.42
1:C:77:ASN:OD1	1:C:103:MET:HA	2.18	0.42
1:A:239:VAL:HG12	1:A:239:VAL:O	2.18	0.42
1:B:41:LYS:HG2	1:B:47:VAL:HB	2.00	0.42
1:B:124:ASP:OD2	1:B:125:ALA:N	2.53	0.42
1:B:317:ASP:OD2	1:B:319:LEU:OXT	2.37	0.42
1:C:185:GLY:O	1:C:188:TYR:HB3	2.20	0.42
1:A:103:MET:HB2	1:A:276:MET:HE1	2.01	0.42
1:C:192:THR:HG22	1:C:193:LEU:HD12	2.02	0.42
1:A:256:GLU:O	1:A:260:ILE:HG13	2.19	0.42
1:B:7:PRO:CB	1:B:92:THR:CG2	2.90	0.42
1:B:15:PHE:CE2	1:B:73:VAL:HG22	2.55	0.42
1:C:69:ASN:N	1:C:70:PRO:CD	2.83	0.42
1:C:265:TYR:CE2	1:C:305:GLY:HA2	2.54	0.42
1:C:256:GLU:O	1:C:260:ILE:HG13	2.20	0.42
1:A:101:HIS:O	1:A:144:PRO:HG2	2.20	0.42
1:A:237:ASP:OD1	1:A:238:PRO:HD2	2.20	0.42
1:B:9:GLU:HG3	1:B:10:ILE:N	2.35	0.42
1:B:63:PRO:HA	4:B:826:HOH:O	2.20	0.42
1:B:146:ALA:HA	1:B:152:LEU:CD2	2.50	0.42
1:B:197:TYR:CD1	1:B:197:TYR:C	2.93	0.42
1:B:273:LEU:HD22	1:B:274:ASP:N	2.35	0.42
1:C:64:PHE:O	1:C:65:GLN:HB2	2.20	0.41
1:C:131:THR:C	1:C:133:LEU:N	2.73	0.41
1:C:231:PHE:CE1	1:C:232:ALA:O	2.73	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:THR:HG23	1:C:308:ARG:HB2	2.03	0.41
1:C:300:THR:O	1:C:303:CYS:HB2	2.20	0.41
1:C:6:LYS:CE	1:C:91:GLY:O	2.68	0.41
1:A:254:TYR:CE1	1:A:295:THR:HB	2.56	0.41
1:B:6:LYS:N	4:B:840:HOH:O	2.54	0.41
1:B:273:LEU:CD2	1:B:274:ASP:N	2.84	0.41
1:C:127:THR:O	1:C:128:ASP:C	2.57	0.41
1:A:179:LEU:HB2	1:A:199:SER:HA	2.02	0.41
1:A:243:ALA:HB1	1:A:279:ASN:O	2.21	0.41
1:B:129:ILE:HG12	1:B:129:ILE:O	2.20	0.41
1:A:210:LYS:HE3	1:A:214:GLU:OE2	2.20	0.41
1:A:273:LEU:HD23	1:A:274:ASP:H	1.85	0.41
1:B:111:HIS:CE1	1:B:271:SER:HB3	2.55	0.41
1:A:27:GLY:O	1:A:28:PRO:C	2.58	0.41
1:A:128:ASP:HB3	1:A:144:PRO:HD2	2.02	0.41
1:B:15:PHE:HE2	1:B:73:VAL:HG22	1.86	0.41
1:B:172:LYS:HA	1:B:172:LYS:HD2	1.90	0.41
1:C:233:VAL:HG13	1:C:241:THR:HB	2.03	0.41
1:B:126:HIS:HB3	4:B:801:HOH:O	2.21	0.40
1:B:192:THR:HG22	1:B:193:LEU:HD12	2.02	0.40
1:C:210:LYS:O	1:C:210:LYS:HG3	2.20	0.40
1:C:233:VAL:HG22	1:C:241:THR:CG2	2.52	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	312/314 (99%)	284 (91%)	21 (7%)	7 (2%)	6	24
1	B	312/314 (99%)	274 (88%)	31 (10%)	7 (2%)	6	24
1	C	312/314 (99%)	277 (89%)	27 (9%)	8 (3%)	5	20

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	936/942 (99%)	835 (89%)	79 (8%)	22 (2%)	6	22

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	GLY
1	B	99	GLY
1	C	99	GLY
1	A	143	GLN
1	B	143	GLN
1	C	86	GLU
1	C	143	GLN
1	C	234	ASP
1	A	118	LEU
1	A	179	LEU
1	B	65	GLN
1	B	86	GLU
1	B	118	LEU
1	C	65	GLN
1	C	118	LEU
1	C	132	PRO
1	A	65	GLN
1	A	132	PRO
1	B	132	PRO
1	A	234	ASP
1	B	14	PRO
1	C	179	LEU

### 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	263/263 (100%)	244 (93%)	19 (7%)	14	39
1	B	263/263 (100%)	246 (94%)	17 (6%)	17	45
1	C	263/263 (100%)	245 (93%)	18 (7%)	16	42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	789/789 (100%)	735 (93%)	54 (7%)	16	42

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	VAL
1	A	28	PRO
1	A	57	ASP
1	A	100	ASP
1	A	118	LEU
1	A	135	THR
1	A	141	HIS
1	A	149	LEU
1	A	169	ILE
1	A	184	PRO
1	A	189	ILE
1	A	225	ARG
1	A	226	PRO
1	A	233	VAL
1	A	244	THR
1	A	273	LEU
1	A	287	GLU
1	A	295	THR
1	A	314	PRO
1	B	9	GLU
1	B	24	VAL
1	B	57	ASP
1	B	87	THR
1	B	100	ASP
1	B	118	LEU
1	B	141	HIS
1	B	144	PRO
1	B	169	ILE
1	B	225	ARG
1	B	233	VAL
1	B	238	PRO
1	B	244	THR
1	B	273	LEU
1	B	287	GLU
1	B	295	THR
1	B	314	PRO
1	C	24	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	28	PRO
1	C	100	ASP
1	C	118	LEU
1	C	141	HIS
1	C	160	PRO
1	C	169	ILE
1	C	183	ASP
1	C	184	PRO
1	C	219	LEU
1	C	225	ARG
1	C	233	VAL
1	C	244	THR
1	C	253	SER
1	C	273	LEU
1	C	287	GLU
1	C	295	THR
1	C	314	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	GOL	A	1000	-	5,5,5	0.91	0	5,5,5	0.31	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
3	GOL	A	1000	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1000	GOL	C1-C2-C3-O3

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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.