



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 7, 2023 – 04:50 PM EDT

PDB ID : 4Q3V  
Title : Crystal structure of Schistosoma mansoni arginase in complex with inhibitor BEC  
Authors : Hai, Y.; Edwards, J.E.; Van Zandt, M.C.; Hoffmann, K.F.; Christianson, D.W.  
Deposited on : 2014-04-12  
Resolution : 2.70 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)  
Xtriage (Phenix) : 1.13  
EDS : 2.35.1  
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) : 2.35.1

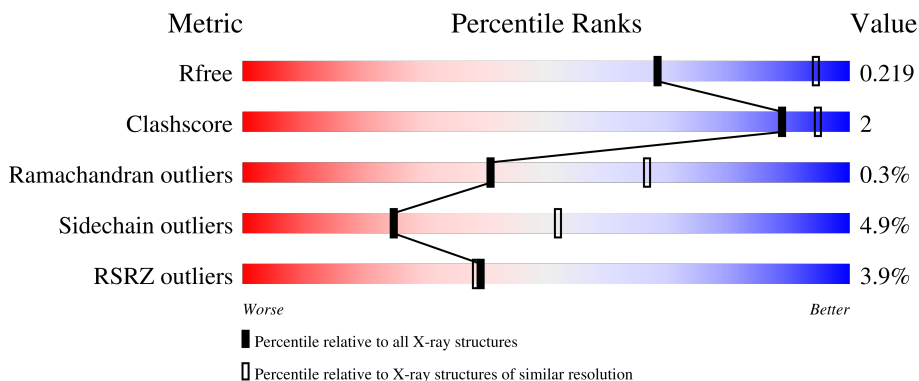
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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  $\leq 5\%$ . 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	385	<div style="display: flex; align-items: center;"> <div style="width: 12%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 6%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">81%      6%      12%</p>
1	B	385	<div style="width: 80%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> <p style="margin-left: 20px;">80%      8%      12%</p>
1	C	385	<div style="display: flex; align-items: center;"> <div style="width: 12%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 81%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 12%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">81%      8%      12%</p>
1	D	385	<div style="display: flex; align-items: center;"> <div style="width: 12%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 15%; height: 10px; background-color: grey;"></div> </div> <p style="margin-left: 20px;">77%      8%      15%</p>

## 2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 10742 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	337	Total 2585	C 1628	N 452	O 490	S 15	0	0	0
1	B	338	Total 2597	C 1636	N 454	O 491	S 16	0	1	0
1	C	339	Total 2603	C 1640	N 456	O 492	S 15	0	0	0
1	D	329	Total 2521	C 1590	N 439	O 477	S 15	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP Q6WVP6
A	-19	GLY	-	expression tag	UNP Q6WVP6
A	-18	SER	-	expression tag	UNP Q6WVP6
A	-17	SER	-	expression tag	UNP Q6WVP6
A	-16	HIS	-	expression tag	UNP Q6WVP6
A	-15	HIS	-	expression tag	UNP Q6WVP6
A	-14	HIS	-	expression tag	UNP Q6WVP6
A	-13	HIS	-	expression tag	UNP Q6WVP6
A	-12	HIS	-	expression tag	UNP Q6WVP6
A	-11	HIS	-	expression tag	UNP Q6WVP6
A	-10	SER	-	expression tag	UNP Q6WVP6
A	-9	SER	-	expression tag	UNP Q6WVP6
A	-8	GLY	-	expression tag	UNP Q6WVP6
A	-7	LEU	-	expression tag	UNP Q6WVP6
A	-6	VAL	-	expression tag	UNP Q6WVP6
A	-5	PRO	-	expression tag	UNP Q6WVP6
A	-4	ARG	-	expression tag	UNP Q6WVP6
A	-3	GLY	-	expression tag	UNP Q6WVP6
A	-2	SER	-	expression tag	UNP Q6WVP6
A	-1	HIS	-	expression tag	UNP Q6WVP6
A	0	MET	-	expression tag	UNP Q6WVP6

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	expression tag	UNP Q6WVP6
B	-19	GLY	-	expression tag	UNP Q6WVP6
B	-18	SER	-	expression tag	UNP Q6WVP6
B	-17	SER	-	expression tag	UNP Q6WVP6
B	-16	HIS	-	expression tag	UNP Q6WVP6
B	-15	HIS	-	expression tag	UNP Q6WVP6
B	-14	HIS	-	expression tag	UNP Q6WVP6
B	-13	HIS	-	expression tag	UNP Q6WVP6
B	-12	HIS	-	expression tag	UNP Q6WVP6
B	-11	HIS	-	expression tag	UNP Q6WVP6
B	-10	SER	-	expression tag	UNP Q6WVP6
B	-9	SER	-	expression tag	UNP Q6WVP6
B	-8	GLY	-	expression tag	UNP Q6WVP6
B	-7	LEU	-	expression tag	UNP Q6WVP6
B	-6	VAL	-	expression tag	UNP Q6WVP6
B	-5	PRO	-	expression tag	UNP Q6WVP6
B	-4	ARG	-	expression tag	UNP Q6WVP6
B	-3	GLY	-	expression tag	UNP Q6WVP6
B	-2	SER	-	expression tag	UNP Q6WVP6
B	-1	HIS	-	expression tag	UNP Q6WVP6
B	0	MET	-	expression tag	UNP Q6WVP6
C	-20	MET	-	expression tag	UNP Q6WVP6
C	-19	GLY	-	expression tag	UNP Q6WVP6
C	-18	SER	-	expression tag	UNP Q6WVP6
C	-17	SER	-	expression tag	UNP Q6WVP6
C	-16	HIS	-	expression tag	UNP Q6WVP6
C	-15	HIS	-	expression tag	UNP Q6WVP6
C	-14	HIS	-	expression tag	UNP Q6WVP6
C	-13	HIS	-	expression tag	UNP Q6WVP6
C	-12	HIS	-	expression tag	UNP Q6WVP6
C	-11	HIS	-	expression tag	UNP Q6WVP6
C	-10	SER	-	expression tag	UNP Q6WVP6
C	-9	SER	-	expression tag	UNP Q6WVP6
C	-8	GLY	-	expression tag	UNP Q6WVP6
C	-7	LEU	-	expression tag	UNP Q6WVP6
C	-6	VAL	-	expression tag	UNP Q6WVP6
C	-5	PRO	-	expression tag	UNP Q6WVP6
C	-4	ARG	-	expression tag	UNP Q6WVP6
C	-3	GLY	-	expression tag	UNP Q6WVP6
C	-2	SER	-	expression tag	UNP Q6WVP6
C	-1	HIS	-	expression tag	UNP Q6WVP6
C	0	MET	-	expression tag	UNP Q6WVP6

*Continued on next page...*

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	expression tag	UNP Q6WVP6
D	-19	GLY	-	expression tag	UNP Q6WVP6
D	-18	SER	-	expression tag	UNP Q6WVP6
D	-17	SER	-	expression tag	UNP Q6WVP6
D	-16	HIS	-	expression tag	UNP Q6WVP6
D	-15	HIS	-	expression tag	UNP Q6WVP6
D	-14	HIS	-	expression tag	UNP Q6WVP6
D	-13	HIS	-	expression tag	UNP Q6WVP6
D	-12	HIS	-	expression tag	UNP Q6WVP6
D	-11	HIS	-	expression tag	UNP Q6WVP6
D	-10	SER	-	expression tag	UNP Q6WVP6
D	-9	SER	-	expression tag	UNP Q6WVP6
D	-8	GLY	-	expression tag	UNP Q6WVP6
D	-7	LEU	-	expression tag	UNP Q6WVP6
D	-6	VAL	-	expression tag	UNP Q6WVP6
D	-5	PRO	-	expression tag	UNP Q6WVP6
D	-4	ARG	-	expression tag	UNP Q6WVP6
D	-3	GLY	-	expression tag	UNP Q6WVP6
D	-2	SER	-	expression tag	UNP Q6WVP6
D	-1	HIS	-	expression tag	UNP Q6WVP6
D	0	MET	-	expression tag	UNP Q6WVP6

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

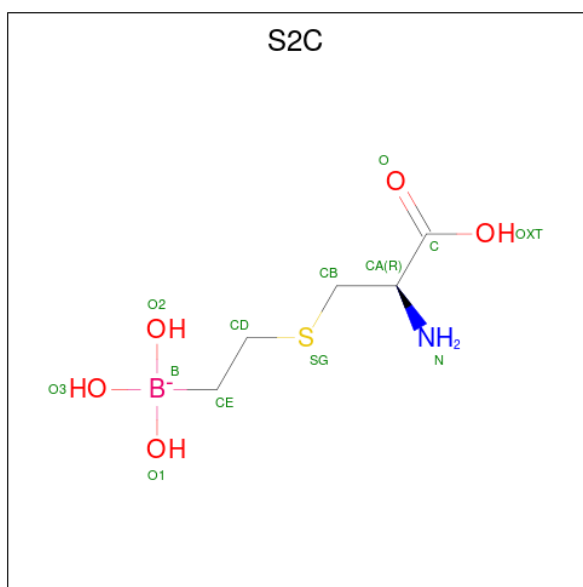
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total Mn 2 2	0	0
2	B	2	Total Mn 2 2	0	0
2	C	2	Total Mn 2 2	0	0
2	D	2	Total Mn 2 2	0	0

- 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
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0
3	C	1	Total C O 6 3 3	0	0

- Molecule 4 is S-2-(BORONOETHYL)-L-CYSTEINE (three-letter code: S2C) (formula:  $C_5H_{13}BNO_5S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	B	C	N	O			S
4	A	1	Total 13	B 1	C 5	N 1	O 5	S 1	0	0
4	B	1	Total 13	B 1	C 5	N 1	O 5	S 1	0	0
4	C	1	Total 13	B 1	C 5	N 1	O 5	S 1	0	0

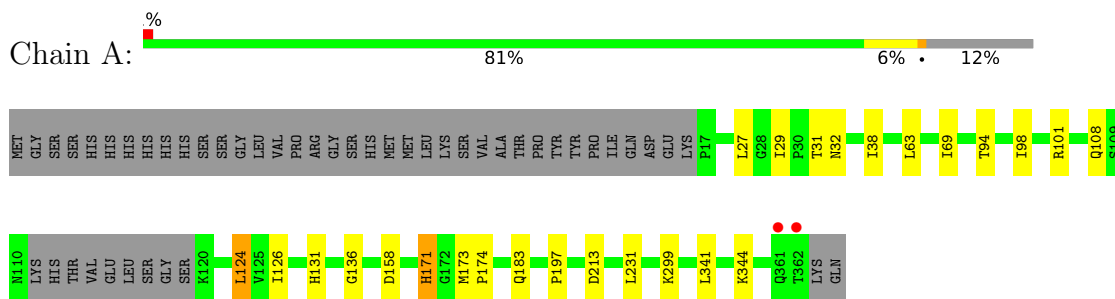
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	135	Total 135	O 135	0	0
5	B	124	Total 124	O 124	0	0
5	C	84	Total 84	O 84	0	0
5	D	10	Total 10	O 10	0	0

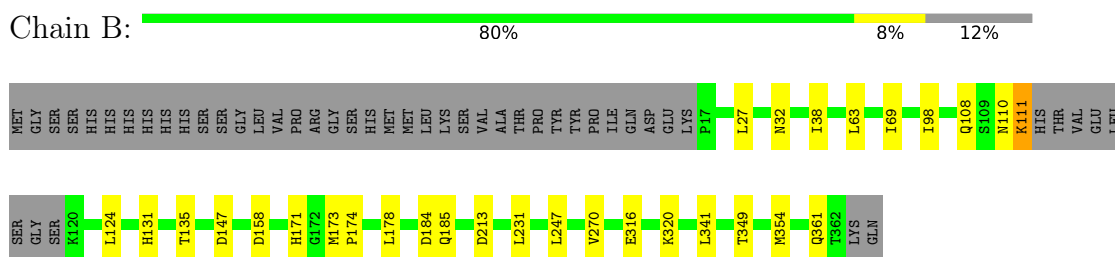
### 3 Residue-property plots [i](#)

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.

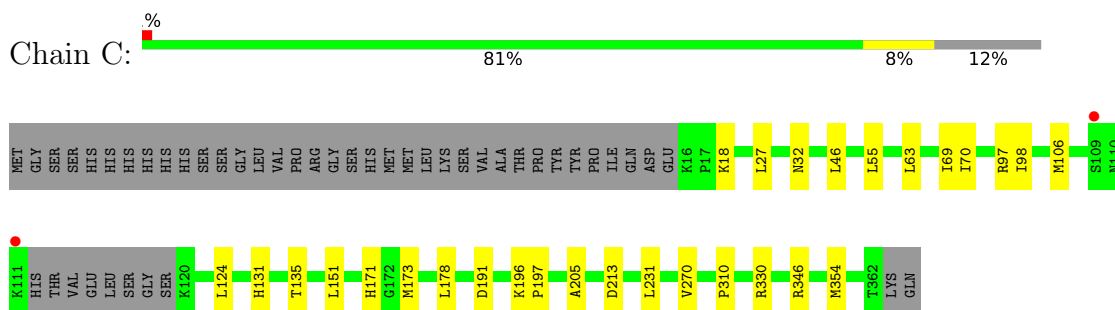
- Molecule 1: Arginase



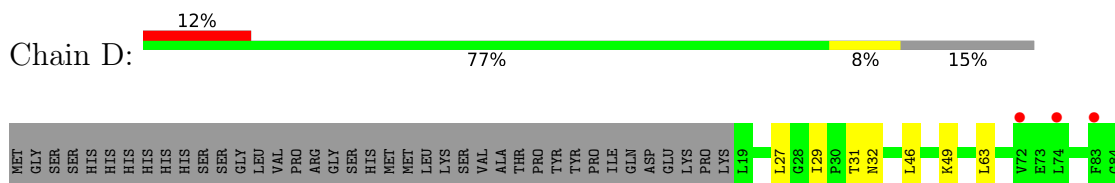
- Molecule 1: Arginase



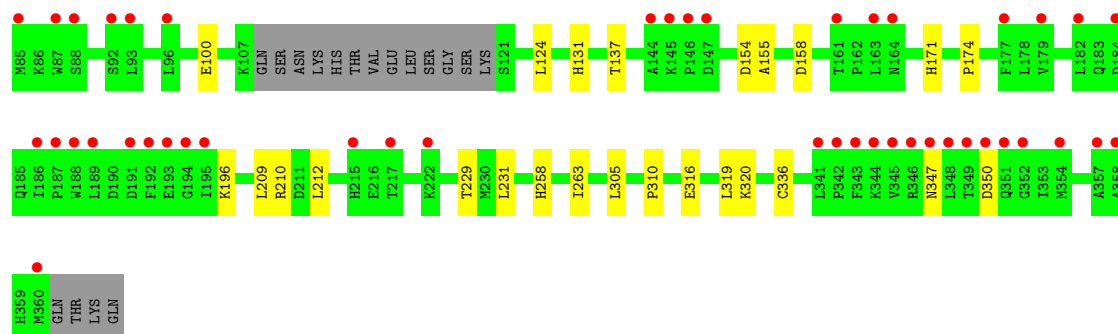
- Molecule 1: Arginase



- Molecule 1: Arginase







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	178.39Å 178.39Å 178.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.48 – 2.70 49.48 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.48-2.70) 98.5 (49.48-2.70)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	0.16	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 2.69Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8.3_1479)	Depositor
R, $R_{free}$	0.167 , 0.217 0.172 , 0.219	Depositor DCC
$R_{free}$ test set	2637 reflections (5.12%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.4	Xtrriage
Anisotropy	0.000	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.025 for l,-k,h	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10742	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.92% 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: MN, S2C, 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	0.24	0/2633	0.43	0/3568
1	B	0.22	0/2648	0.42	0/3587
1	C	0.22	0/2651	0.42	0/3591
1	D	0.21	0/2568	0.40	0/3482
All	All	0.22	0/10500	0.42	0/14228

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	2585	0	2600	11	0
1	B	2597	0	2618	6	0
1	C	2603	0	2625	9	0
1	D	2521	0	2532	12	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	12	0	16	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	16	0	0
3	C	12	0	16	0	0
4	A	13	0	10	2	0
4	B	13	0	11	3	0
4	C	13	0	11	1	0
5	A	135	0	0	0	0
5	B	124	0	0	0	0
5	C	84	0	0	0	0
5	D	10	0	0	0	0
All	All	10742	0	10455	40	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 2.

All (40) 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:D:209:LEU:HD13	1:D:212:LEU:HD21	1.75	0.68
1:A:213:ASP:OD1	4:A:405:S2C:N	2.31	0.63
1:C:213:ASP:OD2	4:C:405:S2C:N	2.31	0.63
1:D:158:ASP:HB3	1:D:174:PRO:HD2	1.83	0.60
1:D:137:THR:HG22	1:D:258:HIS:HE1	1.69	0.58
1:A:69:ILE:HG21	1:A:98:ILE:HD13	1.86	0.57
1:D:46:LEU:HD22	1:D:310:PRO:HG3	1.87	0.56
1:B:213:ASP:OD1	4:B:405:S2C:N	2.41	0.53
1:A:69:ILE:HD11	1:A:101:ARG:HB3	1.91	0.53
1:A:94:THR:O	1:A:98:ILE:HG12	2.08	0.53
1:C:70:ILE:O	1:C:97:ARG:NH1	2.36	0.52
4:B:405:S2C:CD	4:B:405:S2C:O3	2.57	0.52
1:D:29:ILE:HG22	1:D:31:THR:HG23	1.92	0.51
1:A:29:ILE:HD13	1:A:98:ILE:HD12	1.93	0.50
1:B:158:ASP:HB3	1:B:174:PRO:HD2	1.92	0.50
1:A:124:LEU:HD13	1:A:126:ILE:HD11	1.95	0.49
1:D:209:LEU:HB2	1:D:229:THR:HG22	1.96	0.47
1:C:55:LEU:HB3	1:C:330:ARG:NE	2.30	0.47
1:A:29:ILE:HG22	1:A:31:THR:HG23	1.97	0.47
1:C:135:THR:HA	1:C:178:LEU:HD11	1.97	0.47
4:B:405:S2C:O3	4:B:405:S2C:HD2	2.14	0.46
1:D:347:ASN:HB3	1:D:350:ASP:HB2	1.96	0.46
1:C:46:LEU:HD22	1:C:310:PRO:HG3	1.97	0.46
1:D:154:ASP:OD1	1:D:155:ALA:N	2.48	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:191:ASP:OD2	1:C:191:ASP:N	2.41	0.46
1:A:158:ASP:HB3	1:A:174:PRO:HD2	1.97	0.46
1:C:69:ILE:HD13	1:C:98:ILE:HA	1.98	0.46
1:A:171:HIS:CE1	4:A:405:S2C:HE1	2.50	0.45
1:A:183:GLN:HG3	1:A:197:PRO:HG3	1.97	0.45
1:D:137:THR:HG22	1:D:258:HIS:CE1	2.51	0.44
1:B:69:ILE:HD13	1:B:98:ILE:HA	1.99	0.44
1:B:110:ASN:O	1:B:111:LYS:NZ	2.46	0.44
1:B:316:GLU:HG2	1:B:320:LYS:HE3	2.00	0.44
1:B:135:THR:HA	1:B:178:LEU:HD11	1.99	0.43
1:C:196:LYS:HA	1:C:197:PRO:HD3	1.80	0.43
1:D:316:GLU:HG2	1:D:320:LYS:HE3	2.00	0.42
1:C:151:LEU:HD23	1:C:205:ALA:HB3	2.03	0.41
1:D:316:GLU:O	1:D:320:LYS:HG3	2.21	0.41
1:A:98:ILE:HB	1:A:136:GLY:HA3	2.03	0.40
1:D:263:ILE:HD13	1:D:305:LEU:HD11	2.04	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	333/385 (86%)	326 (98%)	6 (2%)	1 (0%)	41	66
1	B	335/385 (87%)	325 (97%)	9 (3%)	1 (0%)	41	66
1	C	335/385 (87%)	328 (98%)	6 (2%)	1 (0%)	41	66
1	D	325/385 (84%)	315 (97%)	9 (3%)	1 (0%)	41	66
All	All	1328/1540 (86%)	1294 (97%)	30 (2%)	4 (0%)	41	66

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	210	ARG
1	B	173	MET
1	C	173	MET
1	A	173	MET

### 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	284/327 (87%)	272 (96%)	12 (4%)	30	58
1	B	286/327 (88%)	267 (93%)	19 (7%)	16	38
1	C	286/327 (88%)	274 (96%)	12 (4%)	30	58
1	D	276/327 (84%)	264 (96%)	12 (4%)	29	57
All	All	1132/1308 (86%)	1077 (95%)	55 (5%)	25	52

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	32	ASN
1	A	38	ILE
1	A	63	LEU
1	A	108	GLN
1	A	124	LEU
1	A	131	HIS
1	A	171	HIS
1	A	231	LEU
1	A	299	LYS
1	A	341	LEU
1	A	344	LYS
1	B	27	LEU
1	B	32	ASN
1	B	38	ILE
1	B	63	LEU
1	B	108	GLN
1	B	111	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	124	LEU
1	B	131	HIS
1	B	147	ASP
1	B	171	HIS
1	B	184	ASP
1	B	185	GLN
1	B	231	LEU
1	B	247	LEU
1	B	270	VAL
1	B	341	LEU
1	B	349	THR
1	B	354	MET
1	B	361	GLN
1	C	18	LYS
1	C	27	LEU
1	C	32	ASN
1	C	63	LEU
1	C	106	MET
1	C	124	LEU
1	C	131	HIS
1	C	171	HIS
1	C	231	LEU
1	C	270	VAL
1	C	346	ARG
1	C	354	MET
1	D	27	LEU
1	D	32	ASN
1	D	49	LYS
1	D	63	LEU
1	D	100	GLU
1	D	124	LEU
1	D	131	HIS
1	D	171	HIS
1	D	196	LYS
1	D	231	LEU
1	D	319	LEU
1	D	336	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	171	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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 17 ligands modelled in this entry, 8 are monoatomic - leaving 9 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	404	-	5,5,5	0.38	0	5,5,5	0.29	0
3	GOL	C	403	-	5,5,5	0.36	0	5,5,5	0.32	0
4	S2C	A	405	2	8,12,12	1.31	1 (12%)	11,16,16	1.63	3 (27%)
4	S2C	C	405	2	8,12,12	1.11	0	11,16,16	1.70	4 (36%)
3	GOL	C	404	-	5,5,5	0.37	0	5,5,5	0.27	0
3	GOL	A	403	-	5,5,5	0.34	0	5,5,5	0.40	0
3	GOL	B	403	-	5,5,5	0.37	0	5,5,5	0.33	0
3	GOL	B	404	-	5,5,5	0.36	0	5,5,5	0.32	0
4	S2C	B	405	2	8,12,12	1.09	0	11,16,16	1.61	3 (27%)

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	404	-	-	2/4/4/4	-
3	GOL	C	403	-	-	3/4/4/4	-
4	S2C	A	405	2	-	1/8/12/12	-
4	S2C	C	405	2	-	4/8/12/12	-
3	GOL	C	404	-	-	2/4/4/4	-
3	GOL	A	403	-	-	2/4/4/4	-
3	GOL	B	403	-	-	0/4/4/4	-
3	GOL	B	404	-	-	2/4/4/4	-
4	S2C	B	405	2	-	0/8/12/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	405	S2C	CE-CD	-2.48	1.52	1.54

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	405	S2C	O3-B-O2	-2.58	99.90	109.18
4	C	405	S2C	O3-B-O2	-2.58	99.92	109.18
4	B	405	S2C	O3-B-O2	-2.56	99.97	109.18
4	C	405	S2C	O3-B-O1	-2.50	100.19	109.18
4	B	405	S2C	CB-SG-CD	2.37	109.38	102.27
4	A	405	S2C	O3-B-O1	-2.37	100.68	109.18
4	A	405	S2C	O1-B-O2	2.31	117.47	109.18
4	B	405	S2C	O3-B-O1	-2.31	100.89	109.18
4	C	405	S2C	O1-B-O2	2.16	116.95	109.18
4	C	405	S2C	CB-SG-CD	2.15	108.70	102.27

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	GOL	O1-C1-C2-C3
3	A	404	GOL	O1-C1-C2-C3
3	C	404	GOL	O1-C1-C2-C3
3	B	404	GOL	O1-C1-C2-C3
3	C	403	GOL	O1-C1-C2-C3
3	A	403	GOL	O1-C1-C2-O2
3	A	404	GOL	O1-C1-C2-O2
3	C	403	GOL	O1-C1-C2-O2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	C	404	GOL	O1-C1-C2-O2
3	C	403	GOL	C1-C2-C3-O3
4	C	405	S2C	OXT-C-CA-N
4	C	405	S2C	O-C-CA-N
4	C	405	S2C	CE-CD-SG-CB
3	B	404	GOL	O1-C1-C2-O2
4	A	405	S2C	CE-CD-SG-CB
4	C	405	S2C	N-CA-CB-SG

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	405	S2C	2	0
4	C	405	S2C	1	0
4	B	405	S2C	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

### 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	337/385 (87%)	-0.43	2 (0%) 89 91	8, 17, 44, 67	8 (2%)
1	B	338/385 (87%)	-0.61	0 100 100	8, 16, 44, 66	5 (1%)
1	C	339/385 (88%)	-0.46	2 (0%) 89 91	15, 25, 47, 65	6 (1%)
1	D	329/385 (85%)	0.68	48 (14%) 2 1	37, 56, 68, 86	51 (15%)
All	All	1343/1540 (87%)	-0.21	52 (3%) 39 38	8, 24, 63, 86	70 (5%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	350	ASP	5.0
1	D	351	GLN	4.9
1	D	360	MET	4.5
1	D	187	PRO	4.3
1	D	357	ALA	4.3
1	D	144	ALA	4.2
1	D	343	PHE	4.0
1	D	344	LYS	3.9
1	D	184	ASP	3.8
1	D	349	THR	3.8
1	D	195	ILE	3.7
1	D	192	PHE	3.7
1	D	193	GLU	3.6
1	D	146	PRO	3.6
1	D	96	LEU	3.3
1	D	74	LEU	3.2
1	D	345	VAL	3.2
1	D	346	ARG	3.1
1	D	348	LEU	3.1
1	D	354	MET	2.9
1	D	347	ASN	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	177	PHE	2.9
1	D	92	SER	2.9
1	D	215	HIS	2.8
1	D	179	VAL	2.7
1	D	72	VAL	2.6
1	D	188	TRP	2.6
1	A	361	GLN	2.6
1	D	85	MET	2.6
1	A	362	THR	2.4
1	D	182	LEU	2.4
1	D	161	THR	2.4
1	D	189	LEU	2.4
1	D	145	LYS	2.4
1	D	341	LEU	2.4
1	D	186	ILE	2.4
1	D	93	LEU	2.4
1	C	109	SER	2.3
1	D	147	ASP	2.3
1	D	88	SER	2.3
1	C	111	LYS	2.3
1	D	342	PRO	2.2
1	D	164	ASN	2.2
1	D	191	ASP	2.2
1	D	352	GLY	2.2
1	D	222	LYS	2.2
1	D	163	LEU	2.2
1	D	194	GLY	2.2
1	D	358	ALA	2.2
1	D	87	TRP	2.1
1	D	217	THR	2.1
1	D	83	PHE	2.1

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
3	GOL	A	404	6/6	0.93	0.22	21,33,42,52	0
3	GOL	C	404	6/6	0.94	0.21	36,39,41,52	0
3	GOL	B	404	6/6	0.95	0.11	23,26,28,37	0
3	GOL	B	403	6/6	0.95	0.15	16,20,27,36	1
2	MN	D	400	1/1	0.96	0.08	55,55,55,55	0
3	GOL	A	403	6/6	0.96	0.13	18,26,28,29	1
4	S2C	A	405	13/13	0.96	0.15	17,34,40,41	0
4	S2C	C	405	13/13	0.96	0.18	22,30,49,55	0
3	GOL	C	403	6/6	0.97	0.15	30,34,37,42	1
4	S2C	B	405	13/13	0.97	0.14	15,27,36,44	0
2	MN	D	401	1/1	0.97	0.07	56,56,56,56	0
2	MN	C	402	1/1	0.99	0.13	19,19,19,19	0
2	MN	A	402	1/1	0.99	0.15	10,10,10,10	0
2	MN	B	401	1/1	0.99	0.12	12,12,12,12	0
2	MN	B	402	1/1	0.99	0.11	10,10,10,10	0
2	MN	A	401	1/1	1.00	0.15	12,12,12,12	0
2	MN	C	401	1/1	1.00	0.14	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.