



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 02:19 pm BST

PDB ID : 2GHI  
Title : Crystal Structure of Plasmodium yoelii Multidrug Resistance Protein 2  
Authors : Dong, A.; Gao, M.; Choe, J.; Zhao, Y.; Lew, J.; Wasney, G.; Alam, Z.; Melone, M.; Kozieradzki, I.; Vedadi, M.; Edwards, A.M.; Arrowsmith, C.H.; Weigelt, J.; Sundstrom, M.; Bochkarev, A.; Hui, R.; Artz, J.D.; Structural Genomics Consortium (SGC)  
Deposited on : 2006-03-27  
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

<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	:	2.11
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)	:	2.11

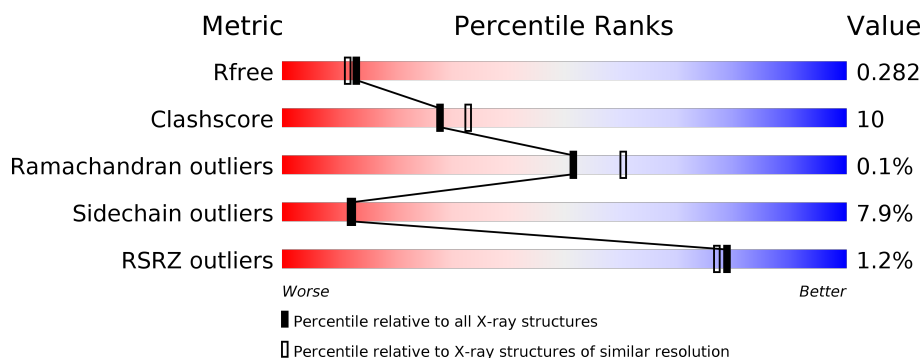
# 1 Overall quality at a glance

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))
$R_{free}$	130704	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (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 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	260	
1	B	260	
1	C	260	
1	D	260	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7960 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 transport protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	0	0	0
			2003	1278	343	377	5			
1	B	248	Total	C	N	O	S	0	0	0
			1919	1222	326	366	5			
1	C	248	Total	C	N	O	S	0	0	0
			1914	1222	328	360	4			
1	D	224	Total	C	N	O	S	0	0	0
			1715	1103	283	325	4			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	CLONING ARTIFACT	UNP Q7RBT4
B	1	GLY	-	CLONING ARTIFACT	UNP Q7RBT4
C	1	GLY	-	CLONING ARTIFACT	UNP Q7RBT4
D	1	GLY	-	CLONING ARTIFACT	UNP Q7RBT4

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



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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	119	Total	O	0	0
			119	119		

*Continued on next page...*

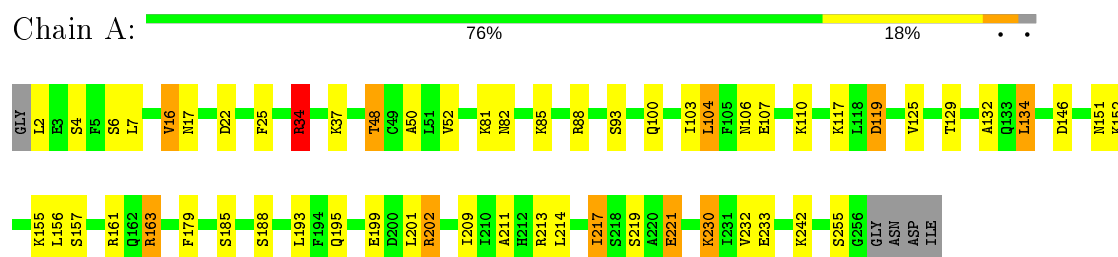
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	93	Total 93	O 93	0	0
3	C	81	Total 81	O 81	0	0
3	D	61	Total 61	O 61	0	0

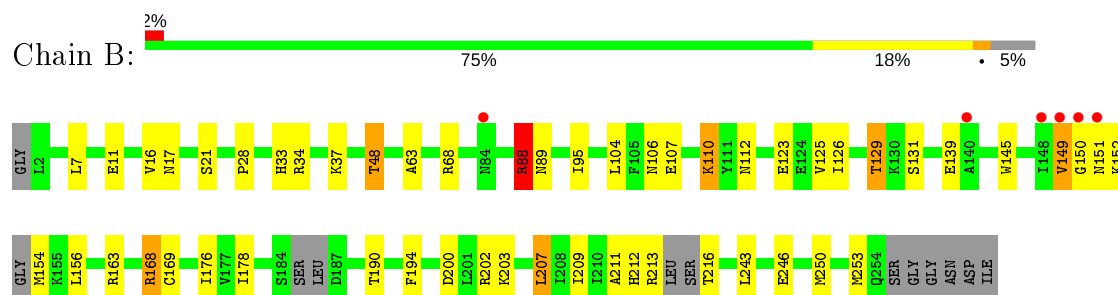
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

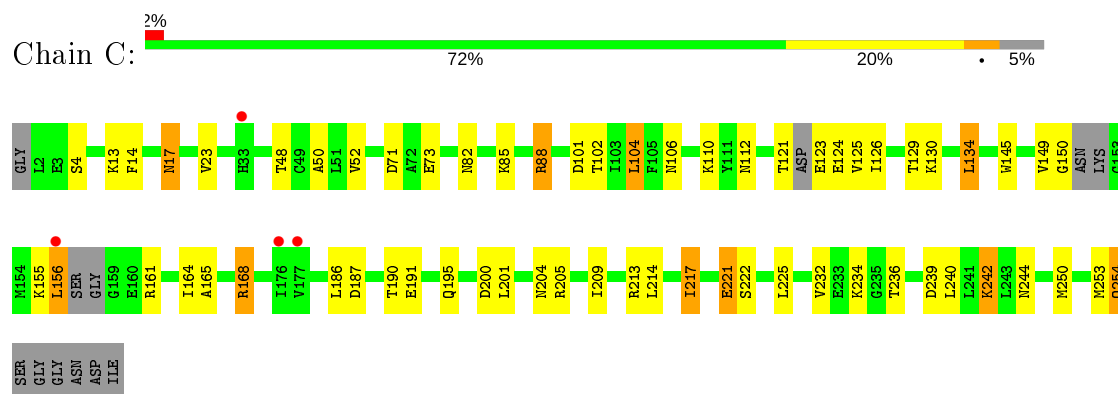
- Molecule 1: transport protein



- Molecule 1: transport protein

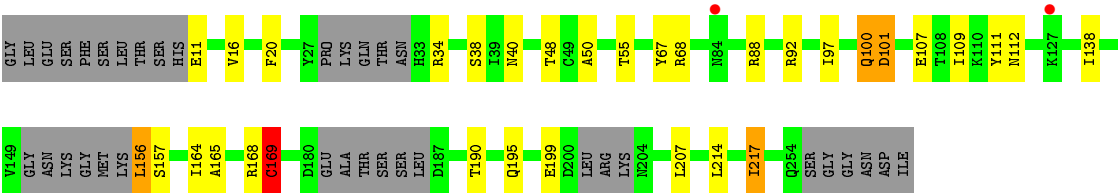


- Molecule 1: transport protein



- Molecule 1: transport protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.02Å 70.69Å 74.38Å 69.81° 76.69° 82.29°	Depositor
Resolution (Å)	32.67 – 2.20 33.11 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (32.67-2.20) 99.1 (33.11-2.20)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.82 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.204 , 0.288 0.204 , 0.282	Depositor DCC
$R_{free}$ test set	857 reflections (1.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.7	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 55.1	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	0.95	EDS
Total number of atoms	7960	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.33% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.98	1/2036 (0.0%)	0.97	5/2741 (0.2%)
1	B	0.86	3/1948 (0.2%)	0.92	5/2630 (0.2%)
1	C	0.90	1/1941 (0.1%)	0.93	4/2616 (0.2%)
1	D	0.79	1/1738 (0.1%)	0.81	0/2343
All	All	0.89	6/7663 (0.1%)	0.91	14/10330 (0.1%)

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	B	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	169	CYS	CB-SG	-5.78	1.72	1.81
1	B	123	GLU	CG-CD	5.70	1.60	1.51
1	B	123	GLU	CB-CG	5.30	1.62	1.52
1	A	88	ARG	CZ-NH2	5.27	1.39	1.33
1	C	101	ASP	CB-CG	5.21	1.62	1.51
1	B	169	CYS	CB-SG	-5.05	1.73	1.81

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	ARG	NE-CZ-NH1	8.44	124.52	120.30
1	A	119	ASP	CB-CG-OD2	-7.09	111.92	118.30
1	B	168	ARG	NE-CZ-NH2	-7.04	116.78	120.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	ARG	NE-CZ-NH1	-6.55	117.03	120.30
1	B	207	LEU	CA-CB-CG	6.53	130.31	115.30
1	A	163	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	34	ARG	CG-CD-NE	-6.10	98.99	111.80
1	C	168	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	C	88	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	B	88	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	C	88	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	A	119	ASP	CB-CG-OD1	5.46	123.21	118.30
1	C	134	LEU	CB-CG-CD1	-5.31	101.98	111.00
1	B	34	ARG	NE-CZ-NH2	5.02	122.81	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	149	VAL	Peptide
1	B	150	GLY	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	2003	0	2044	39	0
1	B	1919	0	1892	42	0
1	C	1914	0	1920	52	0
1	D	1715	0	1695	19	0
2	A	20	0	0	0	0
2	B	15	0	0	0	0
2	C	15	0	0	0	0
2	D	5	0	0	0	0
3	A	119	0	0	4	0
3	B	93	0	0	3	0
3	C	81	0	0	0	0
3	D	61	0	0	2	0
All	All	7960	0	7551	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:B:151:ASN:H	1:B:152:LYS:C	1.56	1.07
1:B:106:ASN:HD21	1:B:151:ASN:CB	1.71	1.01
1:C:155:LYS:HA	1:C:156:LEU:HB2	1.42	0.99
1:B:106:ASN:HD21	1:B:151:ASN:HB2	1.39	0.88
1:C:253:MET:O	1:C:254:GLN:HB2	1.70	0.87
1:B:106:ASN:HD21	1:B:151:ASN:HB3	1.43	0.82
1:B:212:HIS:H	1:B:213:ARG:CB	1.92	0.82
1:A:50:ALA:HB2	1:A:217:ILE:HG13	1.61	0.81
1:C:17:ASN:H	1:C:17:ASN:HD22	1.28	0.81
1:A:82:ASN:HB3	1:A:85:LYS:HE2	1.62	0.79
1:A:185:SER:HB3	1:A:213:ARG:NH1	1.99	0.78
1:D:112:ASN:O	1:D:168:ARG:HD3	1.83	0.78
1:C:106:ASN:HA	1:C:150:GLY:HA3	1.64	0.78
1:C:155:LYS:HA	1:C:156:LEU:CB	2.14	0.77
1:A:185:SER:HB3	1:A:213:ARG:HH11	1.48	0.77
1:B:7:LEU:CD2	1:B:16:VAL:HG11	2.13	0.77
1:B:151:ASN:N	1:B:152:LYS:C	2.37	0.76
1:B:104:LEU:HD21	1:B:156:LEU:HD12	1.69	0.75
1:A:132:ALA:O	1:A:163:ARG:HG2	1.87	0.74
1:B:194:PHE:HD1	3:B:2018:HOH:O	1.69	0.74
1:A:2:LEU:N	3:A:2067:HOH:O	2.20	0.73
1:B:126:ILE:O	1:B:129:THR:HG22	1.90	0.71
1:A:219:SER:HB3	3:A:2116:HOH:O	1.89	0.71
1:B:212:HIS:N	1:B:213:ARG:CB	2.54	0.71
1:B:63:ALA:HB1	1:B:178:ILE:HG21	1.74	0.70
1:B:7:LEU:CD2	1:B:16:VAL:CG1	2.69	0.70
1:A:125:VAL:O	1:A:129:THR:HG23	1.92	0.69
1:C:155:LYS:CA	1:C:156:LEU:HB2	2.20	0.69
1:C:17:ASN:ND2	1:C:17:ASN:H	1.91	0.69
1:B:7:LEU:HD21	1:B:16:VAL:HG11	1.72	0.69
1:B:48:THR:HB	1:B:207:LEU:HB3	1.76	0.68
1:D:68:ARG:HB3	1:D:88:ARG:HG2	1.75	0.68
1:A:134:LEU:HG	1:A:163:ARG:HB3	1.76	0.67
1:A:157:SER:O	1:A:161:ARG:HG3	1.95	0.66
1:C:50:ALA:HB1	1:C:217:ILE:HG12	1.77	0.66
1:D:48:THR:HG22	1:D:207:LEU:HB2	1.76	0.66
1:A:50:ALA:CB	1:A:217:ILE:HG13	2.25	0.66

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:VAL:O	1:C:150:GLY:C	2.35	0.66
1:D:195:GLN:O	1:D:199:GLU:HG2	1.96	0.66
1:A:48:THR:HG21	3:A:2123:HOH:O	1.95	0.66
1:C:48:THR:HG22	1:C:221:GLU:OE1	1.97	0.65
1:B:149:VAL:HG11	1:B:156:LEU:CD1	2.26	0.65
1:C:125:VAL:O	1:C:129:THR:HG23	1.96	0.65
1:B:68:ARG:HB3	1:B:88:ARG:HD2	1.79	0.64
1:C:50:ALA:CB	1:C:217:ILE:HG12	2.27	0.64
1:B:7:LEU:HD22	1:B:16:VAL:CG1	2.28	0.63
1:D:50:ALA:HB2	1:D:217:ILE:HG13	1.81	0.63
1:C:104:LEU:HD22	1:C:161:ARG:HG2	1.81	0.63
1:C:225:LEU:HD11	1:C:250:MET:CE	2.30	0.61
1:A:50:ALA:HB1	1:A:217:ILE:HG12	1.82	0.60
1:A:232:VAL:HG23	1:A:233:GLU:HG3	1.84	0.59
1:A:50:ALA:CB	1:A:217:ILE:CG1	2.80	0.59
1:C:104:LEU:CD2	1:C:161:ARG:HG2	2.33	0.59
1:C:13:LYS:HE3	1:C:14:PHE:CE2	2.38	0.59
1:C:71:ASP:OD1	1:C:88:ARG:NH2	2.31	0.59
1:C:209:ILE:HG21	1:C:217:ILE:HD11	1.85	0.58
1:D:50:ALA:CB	1:D:217:ILE:HG13	2.33	0.58
1:B:209:ILE:HG22	1:B:211:ALA:HB2	1.85	0.58
1:D:101:ASP:HA	3:D:2070:HOH:O	2.03	0.58
1:A:209:ILE:HG21	1:A:217:ILE:HD11	1.85	0.58
1:A:199:GLU:HA	1:A:202:ARG:HD2	1.86	0.58
1:C:225:LEU:HD11	1:C:250:MET:HE1	1.87	0.57
1:B:125:VAL:O	1:B:129:THR:HB	2.05	0.56
1:C:186:LEU:HB3	1:C:190:THR:HG23	1.86	0.56
1:C:106:ASN:HA	1:C:150:GLY:CA	2.34	0.56
1:D:20:PHE:O	1:D:40:ASN:HA	2.06	0.56
1:C:112:ASN:O	1:C:168:ARG:HD3	2.06	0.56
1:B:151:ASN:H	1:B:152:LYS:CA	2.19	0.55
1:C:209:ILE:CG2	1:C:217:ILE:HD11	2.37	0.55
1:B:106:ASN:ND2	1:B:151:ASN:HB3	2.17	0.55
1:D:48:THR:HG23	3:D:2025:HOH:O	2.05	0.55
1:B:212:HIS:CA	1:B:213:ARG:CB	2.85	0.54
1:A:25:PHE:O	1:A:34:ARG:HB2	2.08	0.54
1:C:191:GLU:O	1:C:195:GLN:HG3	2.08	0.54
1:B:112:ASN:O	1:B:168:ARG:HD3	2.08	0.54
1:C:52:VAL:HG23	1:C:225:LEU:HD13	1.90	0.53
1:B:203:LYS:HB3	3:B:2062:HOH:O	2.07	0.53
1:A:209:ILE:CG2	1:A:217:ILE:HD11	2.39	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:ASN:ND2	1:B:151:ASN:HB2	2.17	0.53
1:D:165:ALA:O	1:D:169:CYS:HB3	2.08	0.53
1:A:50:ALA:HB2	1:A:217:ILE:CG1	2.37	0.52
1:A:82:ASN:CB	1:A:85:LYS:HE2	2.35	0.52
1:D:88:ARG:O	1:D:92:ARG:HG3	2.10	0.52
1:A:104:LEU:HD22	1:A:161:ARG:HD2	1.93	0.51
1:C:225:LEU:CD1	1:C:250:MET:HE1	2.40	0.51
1:C:104:LEU:HD12	1:C:112:ASN:CG	2.30	0.51
1:A:103:ILE:H	1:A:103:ILE:HD12	1.76	0.51
1:A:152:LYS:HA	1:C:232:VAL:HG12	1.93	0.51
1:A:34:ARG:HG3	1:A:37:LYS:HG2	1.92	0.50
1:C:239:ASP:HA	1:C:242:LYS:HE3	1.93	0.50
1:C:164:ILE:O	1:C:168:ARG:HG3	2.12	0.50
1:D:164:ILE:O	1:D:168:ARG:HG3	2.12	0.49
1:B:48:THR:HG21	1:B:207:LEU:HD23	1.95	0.49
1:C:155:LYS:CA	1:C:156:LEU:CB	2.88	0.49
1:A:48:THR:HG23	1:A:221:GLU:OE1	2.13	0.49
1:C:201:LEU:O	1:C:205:ARG:HD2	2.12	0.49
1:B:243:LEU:HG	1:B:243:LEU:O	2.13	0.48
1:C:50:ALA:HB2	1:C:217:ILE:CG1	2.43	0.48
1:B:194:PHE:C	1:B:194:PHE:CD2	2.87	0.48
1:B:246:GLU:O	1:B:250:MET:HG3	2.14	0.48
1:C:102:THR:OG1	1:C:165:ALA:HB2	2.13	0.48
1:C:23:VAL:HA	1:C:73:GLU:O	2.14	0.48
1:C:134:LEU:HD11	1:C:164:ILE:HG13	1.96	0.47
1:C:214:LEU:HD12	1:C:214:LEU:H	1.79	0.47
1:B:110:LYS:HG3	1:B:145:TRP:HB3	1.95	0.47
1:C:121:THR:OG1	1:C:124:GLU:HG3	2.14	0.47
1:B:149:VAL:HG13	1:B:154:MET:O	2.14	0.47
1:B:28:PRO:HA	1:C:234:LYS:O	2.15	0.47
1:A:50:ALA:HB1	1:A:217:ILE:CG1	2.43	0.46
1:A:7:LEU:HD22	1:A:16:VAL:HG13	1.97	0.46
1:D:11:GLU:HG3	1:D:16:VAL:HG12	1.98	0.46
1:A:7:LEU:CD2	1:A:16:VAL:HG11	2.46	0.46
1:B:131:SER:HB3	1:B:200:ASP:OD1	2.16	0.46
1:D:67:TYR:CD1	1:D:97:ILE:HD11	2.50	0.46
1:A:242:LYS:HB2	1:A:242:LYS:NZ	2.31	0.46
1:D:214:LEU:O	1:D:217:ILE:HG22	2.15	0.46
1:A:185:SER:CB	1:A:213:ARG:NH1	2.76	0.45
1:C:236:THR:O	1:C:240:LEU:HG	2.17	0.45
1:B:149:VAL:HG11	1:B:156:LEU:HD11	1.95	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:ASN:HD21	1:A:152:LYS:H	1.65	0.44
1:B:163:ARG:HD3	3:B:2013:HOH:O	2.17	0.44
1:C:82:ASN:H	1:C:85:LYS:NZ	2.16	0.43
1:A:106:ASN:HD21	1:A:151:ASN:N	2.15	0.43
1:C:13:LYS:O	1:C:204:ASN:HB3	2.19	0.43
1:A:7:LEU:HD22	1:A:16:VAL:CG1	2.49	0.43
1:B:212:HIS:CG	1:B:213:ARG:CB	3.02	0.43
1:C:110:LYS:HB2	1:C:145:TRP:HB3	2.01	0.43
1:C:225:LEU:HD11	1:C:250:MET:HE3	1.99	0.43
1:A:52:VAL:HG12	1:A:211:ALA:HB3	2.01	0.42
1:A:217:ILE:HA	1:A:217:ILE:HD12	1.67	0.42
1:B:7:LEU:HD22	1:B:11:GLU:HB3	2.00	0.42
1:C:50:ALA:HB2	1:C:217:ILE:HG13	2.01	0.42
1:C:104:LEU:CD2	1:C:161:ARG:CG	2.96	0.42
1:B:95:ILE:HA	1:B:176:ILE:O	2.20	0.42
1:D:109:ILE:HD13	1:D:138:ILE:HG12	2.02	0.42
1:B:202:ARG:CB	1:B:207:LEU:HD22	2.50	0.42
1:C:121:THR:O	1:C:123:GLU:N	2.53	0.41
1:C:187:ASP:H	1:C:190:THR:CG2	2.33	0.41
1:B:202:ARG:HB3	1:B:207:LEU:HD22	2.03	0.41
1:C:52:VAL:HG23	1:C:225:LEU:CD1	2.50	0.41
1:A:193:LEU:HA	1:A:193:LEU:HD23	1.90	0.41
1:A:37:LYS:HB2	1:A:230:LYS:HG3	2.03	0.41
1:D:100:GLN:HE21	1:D:100:GLN:HB2	1.64	0.41
1:D:156:LEU:N	1:D:156:LEU:HD23	2.36	0.41
1:B:149:VAL:HG11	1:B:156:LEU:HD12	2.00	0.41
1:C:104:LEU:HD11	1:C:164:ILE:HD13	2.02	0.41
1:D:107:GLU:HG3	1:D:111:TYR:CZ	2.56	0.41
1:C:126:ILE:O	1:C:130:LYS:HG3	2.21	0.40
1:A:155:LYS:CB	3:A:2088:HOH:O	2.68	0.40
1:C:13:LYS:CE	1:C:14:PHE:CE2	3.03	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	253/260 (97%)	241 (95%)	11 (4%)	1 (0%)	34	37
1	B	240/260 (92%)	232 (97%)	8 (3%)	0	100	100
1	C	240/260 (92%)	230 (96%)	10 (4%)	0	100	100
1	D	214/260 (82%)	203 (95%)	11 (5%)	0	100	100
All	All	947/1040 (91%)	906 (96%)	40 (4%)	1 (0%)	51	60

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	117	LYS

### 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	219/226 (97%)	192 (88%)	27 (12%)	4	4
1	B	202/226 (89%)	188 (93%)	14 (7%)	15	16
1	C	202/226 (89%)	190 (94%)	12 (6%)	19	23
1	D	177/226 (78%)	167 (94%)	10 (6%)	21	25
All	All	800/904 (88%)	737 (92%)	63 (8%)	12	12

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	6	SER
1	A	16	VAL
1	A	17	ASN
1	A	22	ASP
1	A	34	ARG
1	A	48	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	81	LYS
1	A	93	SER
1	A	100	GLN
1	A	104	LEU
1	A	107	GLU
1	A	110	LYS
1	A	119	ASP
1	A	134	LEU
1	A	146	ASP
1	A	156	LEU
1	A	179	PHE
1	A	188	SER
1	A	195	GLN
1	A	201	LEU
1	A	202	ARG
1	A	214	LEU
1	A	217	ILE
1	A	221	GLU
1	A	230	LYS
1	A	255	SER
1	B	17	ASN
1	B	21	SER
1	B	33	HIS
1	B	37	LYS
1	B	48	THR
1	B	88	ARG
1	B	89	ASN
1	B	107	GLU
1	B	110	LYS
1	B	129	THR
1	B	139	GLU
1	B	190	THR
1	B	216	THR
1	B	253	MET
1	C	4	SER
1	C	17	ASN
1	C	104	LEU
1	C	156	LEU
1	C	200	ASP
1	C	213	ARG
1	C	217	ILE
1	C	221	GLU

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	222	SER
1	C	242	LYS
1	C	244	ASN
1	C	254	GLN
1	D	34	ARG
1	D	38	SER
1	D	55	THR
1	D	100	GLN
1	D	101	ASP
1	D	156	LEU
1	D	157	SER
1	D	169	CYS
1	D	190	THR
1	D	217	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	106	ASN
1	B	17	ASN
1	B	89	ASN
1	B	106	ASN
1	B	151	ASN
1	B	254	GLN
1	C	17	ASN
1	C	244	ASN
1	C	254	GLN
1	D	100	GLN

### 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 ⓘ

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	SO4	A	2001	-	4,4,4	0.36	0	6,6,6	0.54	0
2	SO4	C	2002	-	4,4,4	0.29	0	6,6,6	0.86	0
2	SO4	A	2004	-	4,4,4	0.33	0	6,6,6	0.72	0
2	SO4	A	2009	-	4,4,4	0.16	0	6,6,6	0.59	0
2	SO4	A	2003	-	4,4,4	0.11	0	6,6,6	0.77	0
2	SO4	C	2008	-	4,4,4	0.14	0	6,6,6	0.53	0
2	SO4	B	2011	-	4,4,4	0.14	0	6,6,6	0.36	0
2	SO4	B	2005	-	4,4,4	0.23	0	6,6,6	0.89	0
2	SO4	C	2006	-	4,4,4	0.20	0	6,6,6	0.62	0
2	SO4	D	2010	-	4,4,4	0.13	0	6,6,6	0.52	0
2	SO4	B	2007	-	4,4,4	0.28	0	6,6,6	0.35	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

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

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

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	255/260 (98%)	-0.28	0 100 100	26, 39, 51, 59	0
1	B	248/260 (95%)	0.05	6 (2%) 59 56	31, 45, 69, 78	0
1	C	248/260 (95%)	-0.04	4 (1%) 72 70	32, 44, 57, 68	0
1	D	224/260 (86%)	0.06	2 (0%) 84 83	31, 51, 65, 71	0
All	All	975/1040 (93%)	-0.06	12 (1%) 79 77	26, 45, 62, 78	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	140	ALA	3.1
1	C	176	ILE	3.0
1	B	148	ILE	3.0
1	B	84	ASN	2.7
1	B	150	GLY	2.5
1	C	156	LEU	2.3
1	D	127	LYS	2.1
1	B	151	ASN	2.1
1	D	84	ASN	2.1
1	B	149	VAL	2.0
1	C	33	HIS	2.0
1	C	177	VAL	2.0

### 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 carbohydrates 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( $\text{\AA}^2$ )	Q<0.9
2	SO4	B	2011	5/5	0.91	0.11	91,91,92,94	0
2	SO4	A	2003	5/5	0.98	0.07	58,58,60,63	0
2	SO4	A	2009	5/5	0.98	0.09	54,57,60,60	0
2	SO4	C	2006	5/5	0.98	0.09	58,58,60,61	0
2	SO4	D	2010	5/5	0.98	0.08	55,58,60,61	0
2	SO4	C	2008	5/5	0.99	0.09	48,49,49,51	0
2	SO4	A	2004	5/5	0.99	0.09	46,47,49,50	0
2	SO4	B	2005	5/5	0.99	0.10	53,53,55,57	0
2	SO4	A	2001	5/5	0.99	0.11	43,47,49,50	0
2	SO4	C	2002	5/5	0.99	0.09	36,38,41,41	0
2	SO4	B	2007	5/5	0.99	0.07	36,37,39,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.