



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:21 AM UTC

PDB ID : 2GHI / pdb_00002ghi
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

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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

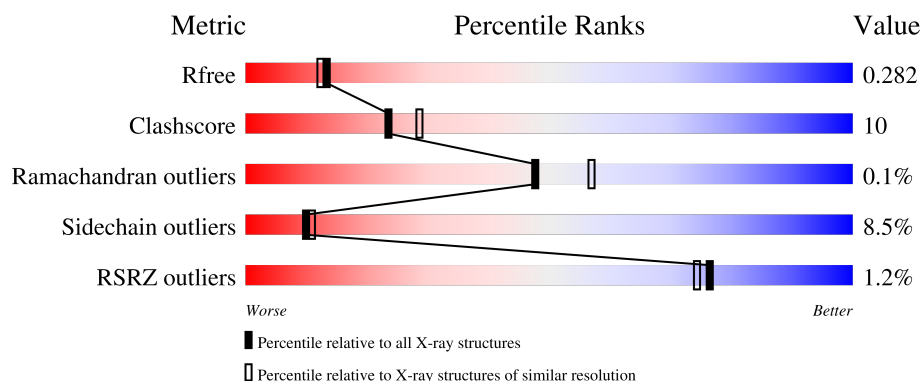
1 Overall quality at a glance

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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 (CCD ID: SO4) (formula: O₄S).



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		

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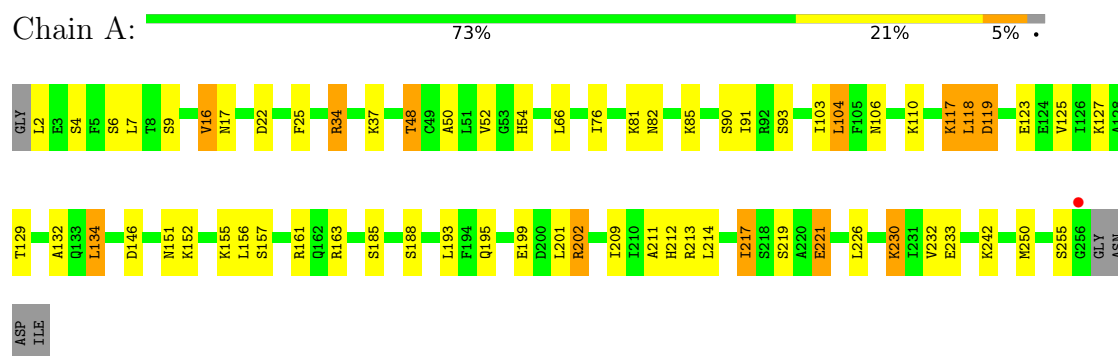
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	93	Total 93	O 93	0	0
3	C	81	Total 81	O 81	0	0
3	D	61	Total 61	O 61	0	0

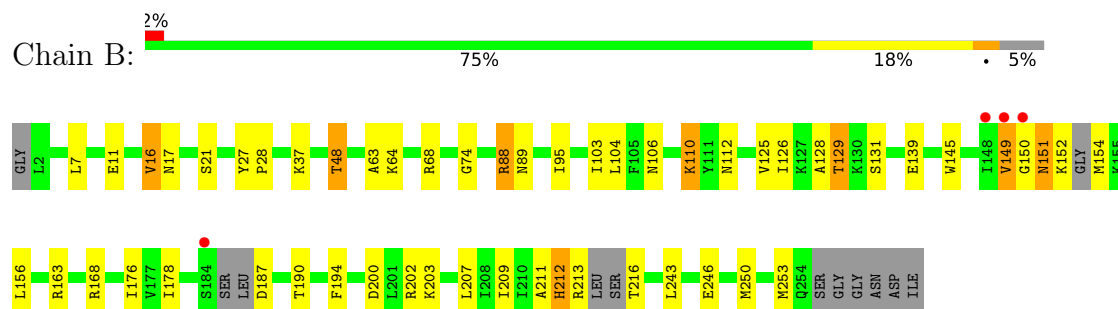
3 Residue-property plots

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.

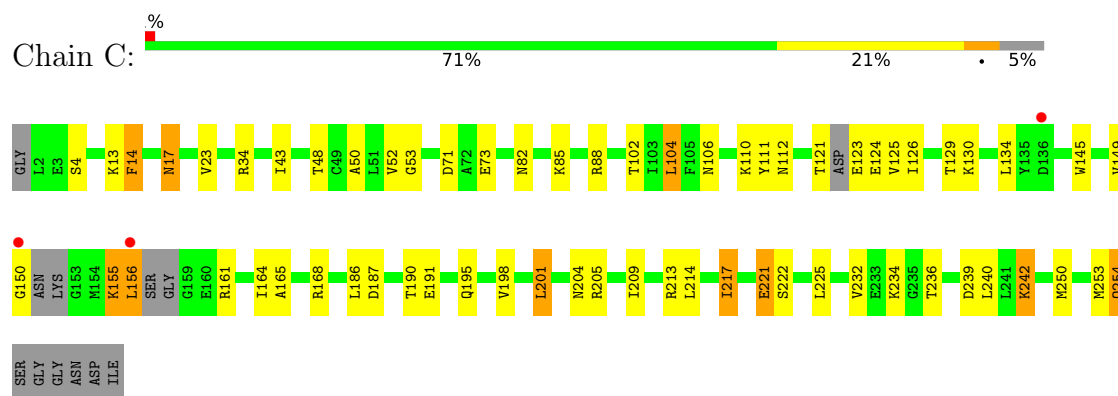
- Molecule 1: transport protein



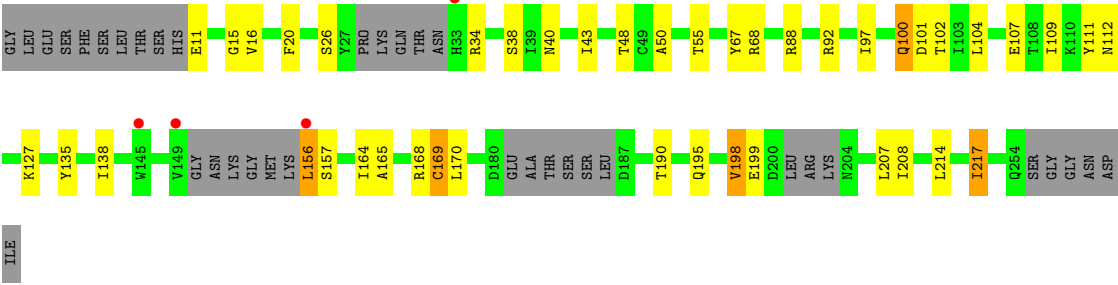
- Molecule 1: transport protein



- Molecule 1: transport protein



- Molecule 1: transport protein



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4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.02Å 70.69Å 74.38Å 69.81° 76.69° 82.29°	Depositor
Resolution (Å)	32.67 – 2.20 32.67 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.1 (32.67-2.20) 99.0 (32.67-2.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.204 , 0.288 0.203 , 0.282	Depositor DCC
R_{free} test set	857 reflections (1.30%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7960	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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	1.22	3/2036 (0.1%)	1.26	8/2741 (0.3%)
1	B	1.10	1/1948 (0.1%)	1.24	15/2630 (0.6%)
1	C	1.14	1/1941 (0.1%)	1.21	4/2616 (0.2%)
1	D	1.01	1/1738 (0.1%)	1.11	5/2343 (0.2%)
All	All	1.12	6/7663 (0.1%)	1.21	32/10330 (0.3%)

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	C	43	ILE	C-O	5.55	1.30	1.24
1	A	66	LEU	N-CA	5.28	1.52	1.46
1	D	198	VAL	CA-CB	5.20	1.61	1.54
1	A	76	ILE	C-O	-5.13	1.18	1.24
1	A	91	ILE	CA-CB	5.13	1.61	1.54
1	B	212	HIS	CA-C	5.09	1.58	1.52

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	151	ASN	N-CA-C	-9.16	102.01	113.55
1	B	212	HIS	N-CA-C	8.26	123.67	112.68
1	A	118	LEU	CA-C-N	7.48	131.05	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	118	LEU	C-N-CA	7.48	131.05	120.28
1	A	119	ASP	N-CA-C	7.36	120.17	111.71
1	A	90	SER	N-CA-C	-6.87	104.72	113.23
1	D	135	TYR	N-CA-C	6.62	118.15	111.07
1	B	64	LYS	N-CA-C	6.49	119.18	111.33
1	D	43	ILE	CA-C-N	-6.45	113.14	119.78
1	D	43	ILE	C-N-CA	-6.45	113.14	119.78
1	A	34	ARG	CG-CD-NE	-5.91	98.99	112.00
1	A	212	HIS	N-CA-C	-5.65	106.93	113.88
1	D	170	LEU	N-CA-C	5.54	118.08	111.71
1	D	15	GLY	CA-C-O	-5.52	118.48	122.45
1	B	151	ASN	CA-C-N	5.44	131.49	121.70
1	B	151	ASN	C-N-CA	5.44	131.49	121.70
1	C	201	LEU	N-CA-C	-5.37	105.87	112.90
1	B	27	TYR	CA-C-N	5.33	125.40	119.32
1	B	27	TYR	C-N-CA	5.33	125.40	119.32
1	B	74	GLY	N-CA-C	-5.24	104.32	112.45
1	B	128	ALA	CA-C-N	5.23	127.28	120.28
1	B	128	ALA	C-N-CA	5.23	127.28	120.28
1	A	117	LYS	CA-C-N	5.19	127.96	120.38
1	A	117	LYS	C-N-CA	5.19	127.96	120.38
1	B	212	HIS	CA-C-N	5.18	131.03	121.70
1	B	212	HIS	C-N-CA	5.18	131.03	121.70
1	B	27	TYR	N-CA-C	-5.11	102.84	110.20
1	B	16	VAL	CA-C-N	-5.10	111.81	122.07
1	B	16	VAL	C-N-CA	-5.10	111.81	122.07
1	C	155	LYS	CA-C-N	5.08	130.83	121.70
1	C	155	LYS	C-N-CA	5.08	130.83	121.70
1	C	14	PHE	N-CA-C	5.00	120.77	114.31

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	40	0
1	B	1919	0	1892	43	0
1	C	1914	0	1920	55	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	155	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 (155) 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	1.11
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:C:225:LEU:HD11	1:C:250:MET:HE3	1.60	0.82
1:A:50:ALA:HB2	1:A:217:ILE:HG13	1.61	0.81
1:C:17:ASN:HD22	1:C:17:ASN:H	1.28	0.81
1:B:151:ASN:N	1:B:152:LYS:C	2.37	0.80
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:A:54:HIS:CE1	1:A:250:MET:HE2	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:53:GLY:HA2	1:C:250:MET:HE1	1.68	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:C:149:VAL:O	1:C:150:GLY:C	2.35	0.70
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:H	1:C:17:ASN:ND2	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
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:A:50:ALA:HB1	1:A:217:ILE:HG12	1.82	0.60
1:C:225:LEU:HD11	1:C:250:MET:CE	2.30	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:104:LEU:HD12	1:C:112:ASN:CG	2.30	0.56
1:C:112:ASN:O	1:C:168:ARG:HD3	2.06	0.56
1:C:225:LEU:CD1	1:C:250:MET:HE3	2.32	0.56
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
1:B:194:PHE:C	1:B:194:PHE:CD2	2.87	0.53
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:B:151:ASN:H	1:B:152:LYS:CA	2.19	0.51
1:A:103:ILE:HD12	1:A:103:ILE:H	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:C:50:ALA:HB2	1:C:217:ILE:CG1	2.43	0.48
1:B:246:GLU:O	1:B:250:MET:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:VAL:HA	1:C:73:GLU:O	2.14	0.48
1:C:102:THR:OG1	1:C:165:ALA:HB2	2.13	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:B:243:LEU:HG	1:B:243:LEU:O	2.13	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:53:GLY:CA	1:C:250:MET:HE1	2.44	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
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:A:52:VAL:HG12	1:A:211:ALA:HB3	2.01	0.42
1:A:217:ILE:HD12	1:A:217:ILE:HA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:TYR:CD2	1:C:111:TYR:C	2.99	0.41
1:C:187:ASP:CG	1:C:190:THR:HG22	2.46	0.41
1:A:37:LYS:HB2	1:A:230:LYS:HG3	2.03	0.41
1:A:193:LEU:HD23	1:A:193:LEU:HA	1.90	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:100:GLN:HE21	1:D:100:GLN:HB2	1.64	0.41
1:D:156:LEU:HD23	1:D:156:LEU:N	2.36	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:B:187:ASP:OD2	1:B:187:ASP:C	2.65	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%)	30	34
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%)	48	57

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%)	191 (87%)	28 (13%)	4	4
1	B	202/226 (89%)	189 (94%)	13 (6%)	16	19
1	C	202/226 (89%)	190 (94%)	12 (6%)	18	22
1	D	177/226 (78%)	162 (92%)	15 (8%)	10	11
All	All	800/904 (88%)	732 (92%)	68 (8%)	10	11

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	6	SER
1	A	9	SER
1	A	16	VAL
1	A	17	ASN
1	A	22	ASP
1	A	48	THR
1	A	81	LYS
1	A	93	SER
1	A	104	LEU
1	A	110	LYS
1	A	118	LEU
1	A	119	ASP
1	A	123	GLU
1	A	127	LYS
1	A	134	LEU
1	A	146	ASP
1	A	156	LEU
1	A	188	SER
1	A	195	GLN
1	A	201	LEU
1	A	202	ARG
1	A	214	LEU
1	A	217	ILE

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Mol	Chain	Res	Type
1	A	221	GLU
1	A	226	LEU
1	A	230	LYS
1	A	255	SER
1	B	17	ASN
1	B	21	SER
1	B	37	LYS
1	B	48	THR
1	B	88	ARG
1	B	89	ASN
1	B	103	ILE
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	34	ARG
1	C	104	LEU
1	C	156	LEU
1	C	198	VAL
1	C	213	ARG
1	C	217	ILE
1	C	221	GLU
1	C	222	SER
1	C	242	LYS
1	C	254	GLN
1	D	26	SER
1	D	34	ARG
1	D	38	SER
1	D	55	THR
1	D	100	GLN
1	D	102	THR
1	D	104	LEU
1	D	127	LYS
1	D	156	LEU
1	D	157	SER
1	D	169	CYS
1	D	190	THR
1	D	198	VAL

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Mol	Chain	Res	Type
1	D	208	ILE
1	D	217	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	HIS
1	A	54	HIS
1	A	106	ASN
1	A	244	ASN
1	B	17	ASN
1	B	33	HIS
1	B	54	HIS
1	B	106	ASN
1	B	133	GLN
1	B	151	ASN
1	B	227	ASN
1	B	254	GLN
1	C	10	HIS
1	C	17	ASN
1	C	54	HIS
1	C	87	ASN
1	C	162	GLN
1	C	227	ASN
1	C	244	ASN
1	C	254	GLN
1	D	100	GLN
1	D	244	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	2011	-	4,4,4	0.25	0	6,6,6	0.35	0
2	SO4	B	2007	-	4,4,4	0.31	0	6,6,6	0.32	0
2	SO4	A	2001	-	4,4,4	0.38	0	6,6,6	0.51	0
2	SO4	C	2002	-	4,4,4	0.29	0	6,6,6	0.84	0
2	SO4	A	2004	-	4,4,4	0.37	0	6,6,6	0.56	0
2	SO4	A	2009	-	4,4,4	0.16	0	6,6,6	0.54	0
2	SO4	D	2010	-	4,4,4	0.23	0	6,6,6	0.55	0
2	SO4	B	2005	-	4,4,4	0.23	0	6,6,6	0.82	0
2	SO4	C	2006	-	4,4,4	0.25	0	6,6,6	0.61	0
2	SO4	A	2003	-	4,4,4	0.21	0	6,6,6	0.69	0
2	SO4	C	2008	-	4,4,4	0.16	0	6,6,6	0.54	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 [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](#)

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, 95th 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 ²)	Q<0.9
1	A	255/260 (98%)	-0.19	1 (0%) 88 87	26, 39, 51, 59	0
1	B	248/260 (95%)	0.05	4 (1%) 70 67	31, 45, 69, 78	0
1	C	248/260 (95%)	-0.03	3 (1%) 76 74	32, 44, 57, 68	0
1	D	224/260 (86%)	0.19	4 (1%) 67 64	31, 51, 64, 71	0
All	All	975/1040 (93%)	-0.00	12 (1%) 76 74	26, 45, 62, 78	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	145	TRP	4.6
1	D	156	LEU	3.3
1	D	149	VAL	3.0
1	C	156	LEU	2.7
1	B	150	GLY	2.4
1	B	184	SER	2.4
1	B	149	VAL	2.4
1	C	136	ASP	2.2
1	B	148	ILE	2.1
1	A	256	GLY	2.1
1	D	33	HIS	2.1
1	C	150	GLY	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 oligosaccharides 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, 95th 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	0.84	0.10	91,91,92,94	0
2	SO4	A	2003	5/5	0.91	0.08	58,58,60,63	0
2	SO4	A	2009	5/5	0.95	0.07	54,57,60,60	0
2	SO4	B	2005	5/5	0.96	0.08	53,53,55,57	0
2	SO4	C	2006	5/5	0.96	0.05	58,58,60,61	0
2	SO4	C	2008	5/5	0.97	0.05	48,49,49,51	0
2	SO4	D	2010	5/5	0.97	0.05	55,58,60,61	0
2	SO4	A	2004	5/5	0.98	0.05	46,47,49,50	0
2	SO4	B	2007	5/5	0.98	0.04	36,37,39,41	0
2	SO4	A	2001	5/5	0.98	0.05	43,47,49,50	0
2	SO4	C	2002	5/5	0.99	0.04	36,38,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.