



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 12:55 pm GMT

PDB ID : 4F7R  
Title : Crystal structure of 14-3-3 protein from Giardia intestinalis  
Authors : Fiorillo, A.; Ilari, A.; Lalle, M.  
Deposited on : 2012-05-16  
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

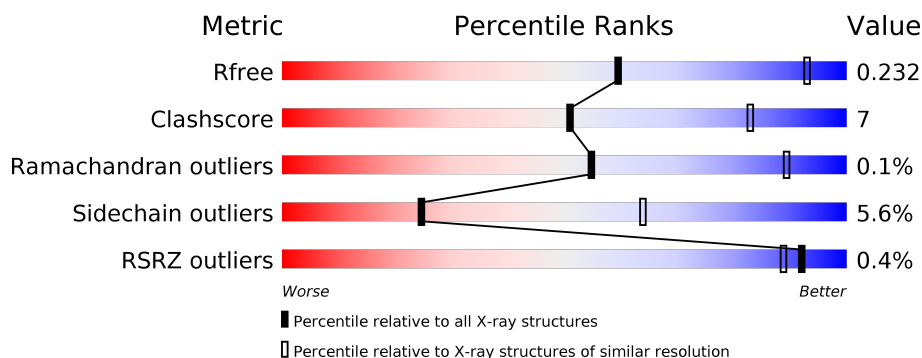
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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))
$R_{free}$	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	253	 79% 12% • 7%
1	B	253	 79% 14% • 6%
1	C	253	 77% 15% • 6%
1	D	253	 75% 17% • 6%

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7801 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 14-3-3 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	0	0	0
			1921	1213	330	370	8			
1	B	237	Total	C	N	O	S	0	0	0
			1929	1217	331	373	8			
1	C	237	Total	C	N	O	S	0	1	0
			1934	1221	331	373	9			
1	D	238	Total	C	N	O	S	0	0	0
			1937	1222	332	374	9			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP Q2QBT8
A	-3	PRO	-	EXPRESSION TAG	UNP Q2QBT8
A	-2	LEU	-	EXPRESSION TAG	UNP Q2QBT8
A	-1	GLY	-	EXPRESSION TAG	UNP Q2QBT8
A	0	SER	-	EXPRESSION TAG	UNP Q2QBT8
B	-4	GLY	-	EXPRESSION TAG	UNP Q2QBT8
B	-3	PRO	-	EXPRESSION TAG	UNP Q2QBT8
B	-2	LEU	-	EXPRESSION TAG	UNP Q2QBT8
B	-1	GLY	-	EXPRESSION TAG	UNP Q2QBT8
B	0	SER	-	EXPRESSION TAG	UNP Q2QBT8
C	-4	GLY	-	EXPRESSION TAG	UNP Q2QBT8
C	-3	PRO	-	EXPRESSION TAG	UNP Q2QBT8
C	-2	LEU	-	EXPRESSION TAG	UNP Q2QBT8
C	-1	GLY	-	EXPRESSION TAG	UNP Q2QBT8
C	0	SER	-	EXPRESSION TAG	UNP Q2QBT8
D	-4	GLY	-	EXPRESSION TAG	UNP Q2QBT8
D	-3	PRO	-	EXPRESSION TAG	UNP Q2QBT8
D	-2	LEU	-	EXPRESSION TAG	UNP Q2QBT8
D	-1	GLY	-	EXPRESSION TAG	UNP Q2QBT8
D	0	SER	-	EXPRESSION TAG	UNP Q2QBT8

- 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		

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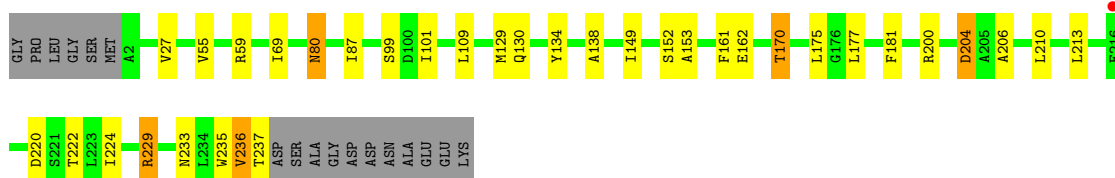
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		

### 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.

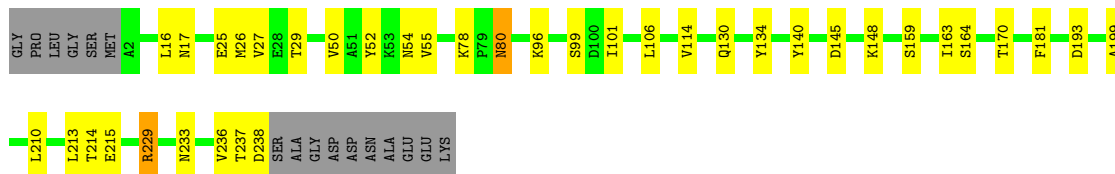
- Molecule 1: 14-3-3 protein

Chain A: 



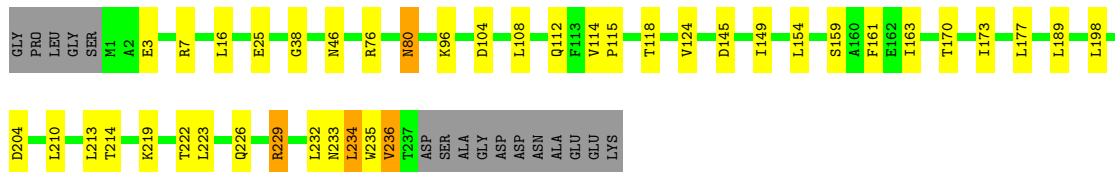
- Molecule 1: 14-3-3 protein

Chain B: 




- Molecule 1: 14-3-3 protein

Chain C: 



- Molecule 1: 14-3-3 protein

Chain D: 



F161	E162	I163	T170	L177	A178	L179	N180	F181	S182	V183	R194	R200	L213	T214	E215	D220	S221	T222	R229	D230	N233	L234	D238	SER	ALA	GLY	ASP	ASP	ASN	ALA	GLU	GLU	LYS
------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.88Å 100.88Å 140.56Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 3.20 47.48 – 3.20	Depositor EDS
% Data completeness (in resolution range)	100.0 (50.00-3.20) 100.0 (47.48-3.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.66 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.185 , 0.232 0.192 , 0.232	Depositor DCC
$R_{free}$ test set	1338 reflections (5.34%)	DCC
Wilson B-factor (Å <sup>2</sup> )	70.8	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 35.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.011 for -h,-k,l 0.049 for h,-h-k,-l 0.029 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7801	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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: 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	0.36	0/1954	0.50	0/2632
1	B	0.37	0/1962	0.48	0/2643
1	C	0.35	0/1970	0.49	0/2653
1	D	0.36	1/1970 (0.1%)	0.47	0/2653
All	All	0.36	1/7856 (0.0%)	0.49	0/10581

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	63	TRP	CD2-CE2	5.05	1.47	1.41

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	1921	0	1908	25	0
1	B	1929	0	1912	23	0
1	C	1934	0	1924	30	0
1	D	1937	0	1924	27	0
2	A	25	0	0	0	0
2	B	20	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	25	0	0	0	0
2	D	10	0	0	0	0
All	All	7801	0	7668	101	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 7.

All (101) 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:C:234:LEU:HD12	1:C:234:LEU:O	1.37	1.20
1:C:235:TRP:O	1:C:236:VAL:HG23	1.52	1.08
1:C:234:LEU:HD12	1:C:234:LEU:C	1.76	1.00
1:A:220:ASP:O	1:A:224:ILE:HD12	1.77	0.84
1:A:235:TRP:O	1:A:236:VAL:HB	1.76	0.82
1:C:235:TRP:O	1:C:236:VAL:CG2	2.30	0.80
1:A:235:TRP:O	1:A:236:VAL:CB	2.31	0.78
1:D:214:THR:OG1	1:D:222:THR:HG21	1.85	0.77
1:C:104:ASP:O	1:C:108:LEU:HD12	1.84	0.76
1:C:235:TRP:C	1:C:236:VAL:CG2	2.54	0.76
1:C:234:LEU:C	1:C:234:LEU:CD1	2.52	0.75
1:C:234:LEU:O	1:C:234:LEU:CD1	2.30	0.71
1:B:170:THR:HB	1:B:213:LEU:HD21	1.72	0.71
1:D:214:THR:CG2	1:D:222:THR:HG21	2.20	0.71
1:D:55:VAL:HG12	1:D:101:ILE:HD13	1.74	0.69
1:D:214:THR:HG21	1:D:222:THR:HG21	1.75	0.67
1:B:159:SER:O	1:B:163:ILE:HD12	1.94	0.67
1:C:235:TRP:C	1:C:236:VAL:HG23	2.18	0.63
1:C:232:LEU:O	1:C:236:VAL:CG2	2.48	0.62
1:D:145:ASP:O	1:D:149:ILE:HD12	2.00	0.62
1:B:99:SER:HG	1:B:140:TYR:HH	1.45	0.59
1:B:199:ALA:HB3	1:C:232:LEU:HD21	1.86	0.57
1:C:145:ASP:O	1:C:149:ILE:HD12	2.05	0.57
1:A:236:VAL:HG12	1:A:236:VAL:O	2.05	0.57
1:C:170:THR:HB	1:C:213:LEU:HD21	1.87	0.56
1:D:214:THR:HG21	1:D:222:THR:CG2	2.35	0.56
1:A:235:TRP:O	1:A:236:VAL:HG23	2.08	0.54
1:A:235:TRP:O	1:A:236:VAL:CG2	2.54	0.54
1:D:17:ASN:HD22	1:D:26:MET:HA	1.73	0.54
1:A:55:VAL:HG12	1:A:101:ILE:HD13	1.90	0.54
1:C:159:SER:O	1:C:163:ILE:HD13	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:LEU:O	1:C:236:VAL:HG23	2.09	0.53
1:B:214:THR:HG22	1:B:215:GLU:O	2.09	0.53
1:B:55:VAL:HG12	1:B:101:ILE:HD13	1.92	0.52
1:A:229:ARG:HD3	1:A:233:ASN:ND2	2.24	0.52
1:A:27:VAL:HG21	1:A:55:VAL:HG21	1.91	0.51
1:C:235:TRP:C	1:C:236:VAL:HG22	2.31	0.51
1:B:99:SER:OG	1:B:140:TYR:OH	2.21	0.51
1:D:179:LEU:O	1:D:183:VAL:HG23	2.11	0.51
1:B:229:ARG:HD3	1:B:233:ASN:ND2	2.26	0.51
1:A:87:ILE:HG12	1:B:16:LEU:HD11	1.93	0.50
1:C:159:SER:O	1:C:163:ILE:CD1	2.59	0.50
1:B:55:VAL:HG12	1:B:101:ILE:CD1	2.42	0.50
1:B:17:ASN:HD22	1:B:26:MET:HA	1.76	0.50
1:D:32:LYS:O	1:D:36:MET:HG2	2.12	0.50
1:D:161:PHE:HA	1:D:177:LEU:HD21	1.94	0.49
1:D:214:THR:CB	1:D:222:THR:HG21	2.41	0.49
1:D:170:THR:HB	1:D:213:LEU:HD21	1.94	0.49
1:A:80:ASN:C	1:A:80:ASN:HD22	2.16	0.49
1:A:170:THR:HB	1:A:213:LEU:HD21	1.94	0.49
1:D:230:ASP:O	1:D:234:LEU:HD13	2.14	0.48
1:B:237:THR:O	1:B:238:ASP:CB	2.61	0.48
1:C:229:ARG:HD3	1:C:233:ASN:ND2	2.29	0.48
1:A:109:LEU:HD11	1:A:129:MET:HG2	1.96	0.47
1:A:237:THR:O	1:A:237:THR:CG2	2.62	0.47
1:B:50:VAL:O	1:B:54:ASN:ND2	2.47	0.47
1:A:235:TRP:N	1:A:235:TRP:CD1	2.81	0.47
1:A:235:TRP:C	1:A:236:VAL:HG23	2.35	0.47
1:D:13:MET:HE2	1:D:13:MET:HA	1.96	0.47
1:A:69:ILE:HG22	1:A:87:ILE:HD13	1.96	0.47
1:D:229:ARG:HD3	1:D:233:ASN:ND2	2.30	0.47
1:D:7:ARG:NH1	1:D:44:GLU:OE1	2.48	0.46
1:A:210:LEU:HG	1:A:222:THR:HG23	1.98	0.46
1:B:114:VAL:HG21	1:B:130:GLN:HE21	1.80	0.46
1:C:154:LEU:HD13	1:C:189:LEU:HD11	1.97	0.46
1:B:170:THR:CB	1:B:213:LEU:HD21	2.43	0.46
1:A:204:ASP:OD1	1:A:229:ARG:NE	2.47	0.45
1:D:138:ALA:HB2	1:D:149:ILE:CG2	2.46	0.45
1:C:214:THR:HG21	1:C:222:THR:OG1	2.17	0.45
1:B:233:ASN:O	1:B:236:VAL:HG12	2.17	0.45
1:C:7:ARG:NH1	1:C:38:GLY:O	2.49	0.45
1:D:214:THR:HG22	1:D:215:GLU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:40:LEU:CD2	1:D:40:LEU:N	2.79	0.44
1:B:114:VAL:HG21	1:B:130:GLN:NE2	2.33	0.44
1:C:161:PHE:HA	1:C:177:LEU:HD21	1.99	0.44
1:B:106:LEU:HD22	1:B:134:TYR:CE2	2.52	0.44
1:D:134:TYR:HB3	1:D:153:ALA:HB2	1.99	0.44
1:A:134:TYR:HB3	1:A:153:ALA:HB2	1.99	0.43
1:A:233:ASN:O	1:A:235:TRP:O	2.37	0.43
1:D:55:VAL:HG12	1:D:101:ILE:CD1	2.46	0.43
1:B:25:GLU:O	1:B:29:THR:HG23	2.18	0.43
1:B:210:LEU:HD11	1:C:210:LEU:HD11	2.00	0.43
1:D:138:ALA:HB2	1:D:149:ILE:HG22	2.00	0.42
1:B:237:THR:O	1:B:238:ASP:HB2	2.19	0.42
1:D:124:VAL:HG22	1:D:163:ILE:HB	2.01	0.42
1:C:114:VAL:HB	1:C:115:PRO:HD3	2.02	0.42
1:A:161:PHE:HA	1:A:177:LEU:HD21	2.02	0.42
1:A:170:THR:HG22	1:A:213:LEU:HD11	2.01	0.42
1:C:124:VAL:HG12	1:C:173:ILE:HG22	2.01	0.42
1:A:175:LEU:HD21	1:A:206:ALA:HB2	2.01	0.41
1:C:80:ASN:C	1:C:80:ASN:HD22	2.24	0.41
1:D:26:MET:HG2	1:D:51:ALA:HB2	2.02	0.41
1:D:31:ARG:NH2	1:D:104:ASP:OD1	2.54	0.41
1:B:27:VAL:HG13	1:B:52:TYR:CZ	2.56	0.41
1:C:25:GLU:OE1	1:D:93:LYS:NZ	2.49	0.41
1:D:52:TYR:CE2	1:D:105:ILE:HD13	2.56	0.41
1:C:223:LEU:HD12	1:C:226:GLN:HE21	1.86	0.40
1:B:80:ASN:C	1:B:80:ASN:HD22	2.23	0.40
1:C:198:LEU:O	1:C:198:LEU:HD12	2.21	0.40
1:A:138:ALA:HB2	1:A:149:ILE:HG22	2.02	0.40
1:C:124:VAL:CG1	1:C:173:ILE:HG22	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	234/253 (92%)	230 (98%)	3 (1%)	1 (0%)	38	77
1	B	235/253 (93%)	233 (99%)	2 (1%)	0	100	100
1	C	236/253 (93%)	232 (98%)	4 (2%)	0	100	100
1	D	236/253 (93%)	232 (98%)	4 (2%)	0	100	100
All	All	941/1012 (93%)	927 (98%)	13 (1%)	1 (0%)	55	89

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	236	VAL

### 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	205/217 (94%)	194 (95%)	11 (5%)	26	65
1	B	206/217 (95%)	197 (96%)	9 (4%)	33	70
1	C	207/217 (95%)	194 (94%)	13 (6%)	21	59
1	D	207/217 (95%)	194 (94%)	13 (6%)	21	59
All	All	825/868 (95%)	779 (94%)	46 (6%)	25	64

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ARG
1	A	80	ASN
1	A	99	SER
1	A	130	GLN
1	A	152	SER
1	A	162	GLU
1	A	170	THR
1	A	181	PHE
1	A	200	ARG
1	A	204	ASP

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Mol	Chain	Res	Type
1	A	229	ARG
1	B	78	LYS
1	B	80	ASN
1	B	96	LYS
1	B	145	ASP
1	B	148	LYS
1	B	164	SER
1	B	181	PHE
1	B	193	ASP
1	B	229	ARG
1	C	3	GLU
1	C	16	LEU
1	C	46	ASN
1	C	76	ARG
1	C	80	ASN
1	C	96	LYS
1	C	112	GLN
1	C	118	THR
1	C	204	ASP
1	C	219	LYS
1	C	229	ARG
1	C	234	LEU
1	C	236	VAL
1	D	13	MET
1	D	16	LEU
1	D	40	LEU
1	D	72	LYS
1	D	116	ARG
1	D	123	LYS
1	D	144	GLU
1	D	181	PHE
1	D	194	ARG
1	D	200	ARG
1	D	220	ASP
1	D	229	ARG
1	D	238	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	ASN
1	A	19	ASN

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Mol	Chain	Res	Type
1	A	80	ASN
1	B	17	ASN
1	B	80	ASN
1	B	110	GLN
1	B	130	GLN
1	C	17	ASN
1	C	80	ASN
1	C	92	GLN
1	C	112	GLN
1	C	226	GLN
1	C	233	ASN
1	D	17	ASN
1	D	54	ASN
1	D	110	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

16 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	301	-	4,4,4	0.38	0	6,6,6	0.20	0
2	SO4	A	302	-	4,4,4	0.42	0	6,6,6	0.10	0
2	SO4	A	303	-	4,4,4	0.41	0	6,6,6	0.11	0
2	SO4	A	304	-	4,4,4	0.42	0	6,6,6	0.10	0
2	SO4	A	305	-	4,4,4	0.48	0	6,6,6	0.21	0
2	SO4	B	301	-	4,4,4	0.42	0	6,6,6	0.16	0
2	SO4	B	302	-	4,4,4	0.37	0	6,6,6	0.13	0
2	SO4	B	303	-	4,4,4	0.43	0	6,6,6	0.11	0
2	SO4	B	304	-	4,4,4	0.44	0	6,6,6	0.10	0
2	SO4	C	301	-	4,4,4	0.42	0	6,6,6	0.14	0
2	SO4	C	302	-	4,4,4	0.41	0	6,6,6	0.09	0
2	SO4	C	303	-	4,4,4	0.41	0	6,6,6	0.17	0
2	SO4	C	304	-	4,4,4	0.41	0	6,6,6	0.15	0
2	SO4	C	305	-	4,4,4	0.44	0	6,6,6	0.08	0
2	SO4	D	301	-	4,4,4	0.36	0	6,6,6	0.22	0
2	SO4	D	302	-	4,4,4	0.41	0	6,6,6	0.08	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
2	SO4	A	301	-	-	0/0/0/0	0/0/0/0
2	SO4	A	302	-	-	0/0/0/0	0/0/0/0
2	SO4	A	303	-	-	0/0/0/0	0/0/0/0
2	SO4	A	304	-	-	0/0/0/0	0/0/0/0
2	SO4	A	305	-	-	0/0/0/0	0/0/0/0
2	SO4	B	301	-	-	0/0/0/0	0/0/0/0
2	SO4	B	302	-	-	0/0/0/0	0/0/0/0
2	SO4	B	303	-	-	0/0/0/0	0/0/0/0
2	SO4	B	304	-	-	0/0/0/0	0/0/0/0
2	SO4	C	301	-	-	0/0/0/0	0/0/0/0
2	SO4	C	302	-	-	0/0/0/0	0/0/0/0
2	SO4	C	303	-	-	0/0/0/0	0/0/0/0
2	SO4	C	304	-	-	0/0/0/0	0/0/0/0
2	SO4	C	305	-	-	0/0/0/0	0/0/0/0
2	SO4	D	301	-	-	0/0/0/0	0/0/0/0
2	SO4	D	302	-	-	0/0/0/0	0/0/0/0

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	236/253 (93%)	0.06	1 (0%) 92 89	36, 56, 80, 98	0
1	B	237/253 (93%)	0.13	0 100 100	41, 61, 86, 103	0
1	C	237/253 (93%)	0.11	0 100 100	41, 57, 78, 97	0
1	D	238/253 (94%)	0.26	3 (1%) 77 65	46, 70, 97, 113	0
All	All	948/1012 (93%)	0.14	4 (0%) 92 89	36, 60, 89, 113	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	78	LYS	2.6
1	D	79	PRO	2.2
1	A	216	GLU	2.2
1	D	117	SER	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SO4	A	305	5/5	0.74	0.29	1.18	90,95,98,99	0
2	SO4	C	305	5/5	0.85	0.24	-0.06	95,98,99,100	0
2	SO4	B	304	5/5	0.86	0.17	-1.66	99,102,103,105	0
2	SO4	C	301	5/5	0.97	0.17	-1.93	54,55,56,57	0
2	SO4	C	303	5/5	0.87	0.16	-3.17	73,75,76,77	0
2	SO4	B	302	5/5	0.92	0.16	-	75,79,79,81	0
2	SO4	D	301	5/5	0.94	0.17	-	71,72,72,75	0
2	SO4	B	303	5/5	0.90	0.18	-	96,98,100,102	0
2	SO4	A	304	5/5	0.91	0.18	-	103,103,104,105	0
2	SO4	D	302	5/5	0.94	0.17	-	78,79,80,81	0
2	SO4	B	301	5/5	0.97	0.15	-	50,51,53,53	0
2	SO4	A	301	5/5	0.97	0.16	-	57,57,58,59	0
2	SO4	C	302	5/5	0.90	0.18	-	92,96,97,97	0
2	SO4	C	304	5/5	0.92	0.21	-	83,85,87,88	0
2	SO4	A	302	5/5	0.91	0.21	-	82,83,85,85	0
2	SO4	A	303	5/5	0.94	0.14	-	83,86,87,88	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.