



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 12, 2023 – 05:26 PM EDT

PDB ID : 6WM8  
Title : Proliferation-Associated protein 2G4 (PA2G4)  
Authors : Gorman, M.A.; Stevenson, B.W.; Parker, M.W.  
Deposited on : 2020-04-20  
Resolution : 2.60 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>.

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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 : 1.8.5 (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

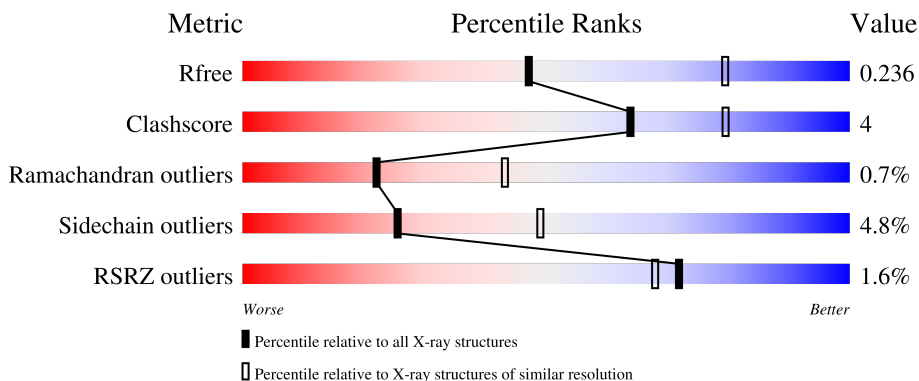
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*




The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	369	
1	B	369	
1	C	369	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 8541 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 Proliferation-associated protein 2G4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	354	2770	1747	475	531	17	0	0	0
1	B	353	2761	1742	473	529	17	0	0	0
1	C	353	2761	1742	473	529	17	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q9UQ80
A	-5	GLY	-	expression tag	UNP Q9UQ80
A	-4	HIS	-	expression tag	UNP Q9UQ80
A	-3	HIS	-	expression tag	UNP Q9UQ80
A	-2	HIS	-	expression tag	UNP Q9UQ80
A	-1	HIS	-	expression tag	UNP Q9UQ80
A	0	HIS	-	expression tag	UNP Q9UQ80
A	1	HIS	-	expression tag	UNP Q9UQ80
B	-6	MET	-	initiating methionine	UNP Q9UQ80
B	-5	GLY	-	expression tag	UNP Q9UQ80
B	-4	HIS	-	expression tag	UNP Q9UQ80
B	-3	HIS	-	expression tag	UNP Q9UQ80
B	-2	HIS	-	expression tag	UNP Q9UQ80
B	-1	HIS	-	expression tag	UNP Q9UQ80
B	0	HIS	-	expression tag	UNP Q9UQ80
B	1	HIS	-	expression tag	UNP Q9UQ80
C	-6	MET	-	initiating methionine	UNP Q9UQ80
C	-5	GLY	-	expression tag	UNP Q9UQ80
C	-4	HIS	-	expression tag	UNP Q9UQ80
C	-3	HIS	-	expression tag	UNP Q9UQ80
C	-2	HIS	-	expression tag	UNP Q9UQ80
C	-1	HIS	-	expression tag	UNP Q9UQ80
C	0	HIS	-	expression tag	UNP Q9UQ80

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1	HIS	-	expression tag	UNP Q9UQ80

- 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	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		

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

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	34	Total	O	0	0
			34	34		
3	B	43	Total	O	0	0
			43	43		

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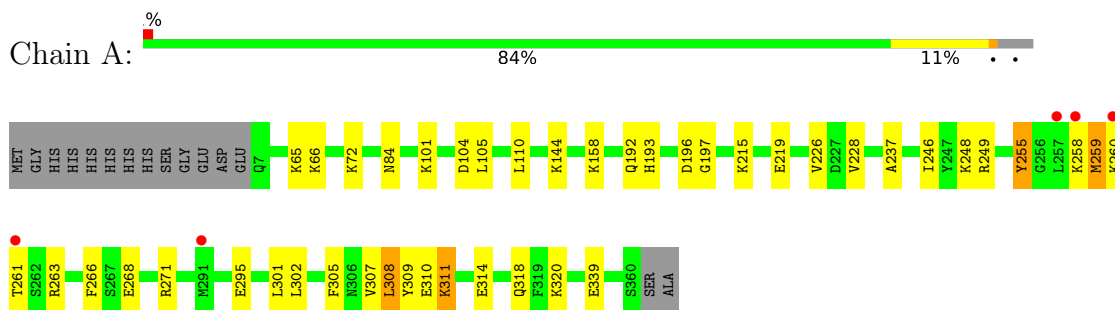
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	C	32	Total	O	0	0
			32	32		

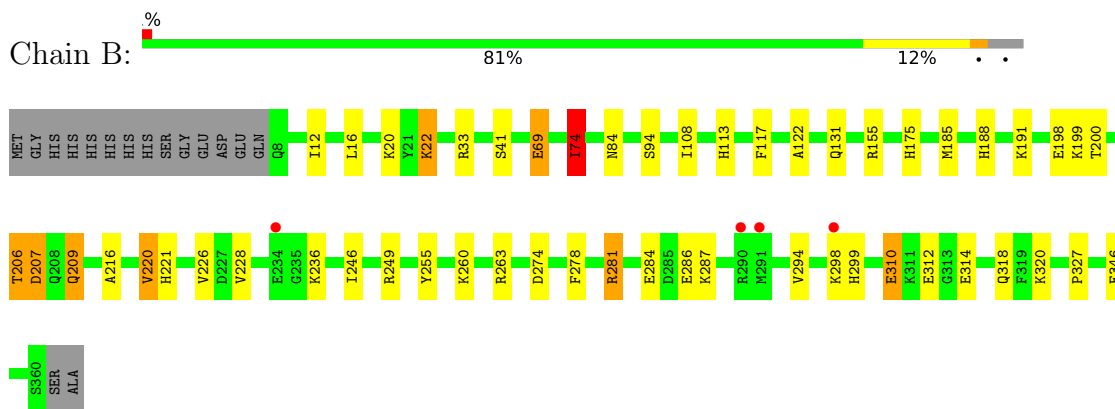
### 3 Residue-property plots [i](#)

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.

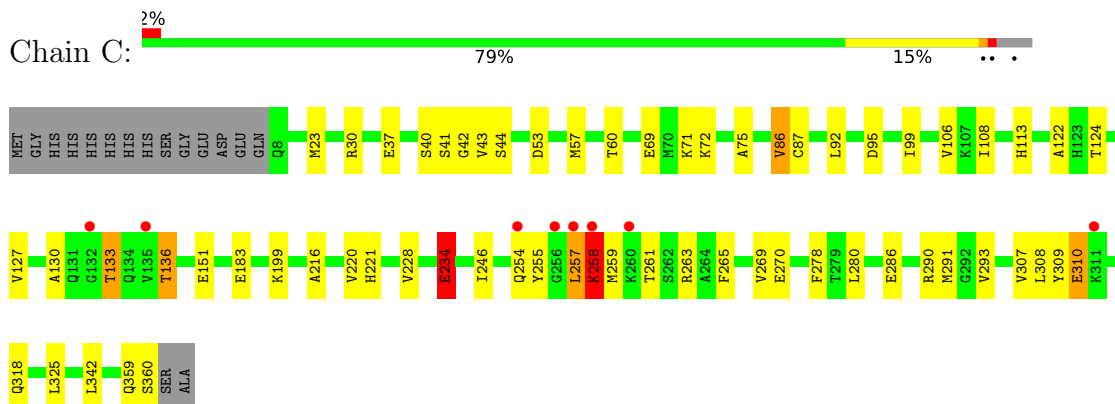
- Molecule 1: Proliferation-associated protein 2G4



- Molecule 1: Proliferation-associated protein 2G4



- Molecule 1: Proliferation-associated protein 2G4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.37Å 138.37Å 220.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.92 – 2.60 48.92 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.92-2.60) 100.0 (48.92-2.60)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 2.61Å)	Xtrriage
Refinement program	REFMAC 5.8.0258	Depositor
R, $R_{free}$	0.194 , 0.238 0.198 , 0.236	Depositor DCC
$R_{free}$ test set	3295 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.1	Xtrriage
Anisotropy	0.149	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 33.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8541	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	65.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.20% 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	0.89	2/2817 (0.1%)	1.05	1/3791 (0.0%)
1	B	0.89	1/2808 (0.0%)	1.07	5/3779 (0.1%)
1	C	0.88	4/2808 (0.1%)	1.09	5/3779 (0.1%)
All	All	0.89	7/8433 (0.1%)	1.07	11/11349 (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
1	C	0	1
All	All	0	3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	339	GLU	CD-OE1	6.33	1.32	1.25
1	C	151	GLU	CD-OE2	6.30	1.32	1.25
1	C	37	GLU	CD-OE2	6.07	1.32	1.25
1	A	219	GLU	CD-OE1	5.80	1.32	1.25
1	B	69	GLU	CD-OE2	5.67	1.31	1.25
1	C	183	GLU	CD-OE1	-5.67	1.19	1.25
1	C	310	GLU	CD-OE1	5.57	1.31	1.25

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	360	SER	CA-C-O	-11.85	95.22	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	136	THR	CA-CB-OG1	-6.77	94.78	109.00
1	B	74	ILE	CA-CB-CG1	6.38	123.11	111.00
1	C	30	ARG	NE-CZ-NH2	-6.25	117.18	120.30
1	B	263	ARG	CG-CD-NE	-6.01	99.17	111.80
1	C	95	ASP	CB-CA-C	-5.90	98.60	110.40
1	A	255	TYR	CB-CA-C	5.71	121.83	110.40
1	B	281	ARG	NE-CZ-NH2	-5.53	117.53	120.30
1	B	33	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	B	263	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	C	133	THR	CA-CB-OG1	-5.50	97.44	109.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	188	HIS	Peptide
1	B	206	THR	Peptide
1	C	359	GLN	Peptide

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

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2770	0	2781	21	0
1	B	2761	0	2773	24	0
1	C	2761	0	2773	27	0
2	A	45	0	0	1	0
2	B	45	0	0	1	0
2	C	50	0	0	0	0
3	A	34	0	0	0	0
3	B	43	0	0	4	0
3	C	32	0	0	0	0
All	All	8541	0	8327	71	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 4.

All (71) 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:GLU:HA	1:C:234:GLU:OE1	1.87	0.73
1:B:94:SER:HB3	1:B:286:GLU:OE2	1.92	0.70
1:C:257:LEU:HD23	1:C:263:ARG:HA	1.77	0.66
1:C:286:GLU:O	1:C:290:ARG:HG3	1.95	0.66
1:B:175:HIS:HB3	3:B:542:HOH:O	1.97	0.65
1:B:294:VAL:O	1:B:298:LYS:HB3	1.99	0.63
1:C:130:ALA:O	1:C:133:THR:HB	1.99	0.62
1:B:255:TYR:CE2	1:B:299:HIS:CD2	2.87	0.61
1:A:259:MET:O	1:A:263:ARG:HD3	2.00	0.60
1:C:258:LYS:HG2	1:C:259:MET:N	2.20	0.56
1:A:84:ASN:HB3	1:A:314:GLU:O	2.06	0.56
1:C:307:VAL:HG12	1:C:309:TYR:CE1	2.40	0.56
1:B:84:ASN:HB3	1:B:314:GLU:O	2.05	0.56
1:A:196:ASP:OD2	1:A:248:LYS:HE2	2.07	0.55
1:B:22:LYS:HE2	3:B:506:HOH:O	2.06	0.55
1:A:144:LYS:HE3	2:A:509:SO4:O2	2.06	0.55
1:A:105:LEU:C	1:A:105:LEU:HD23	2.26	0.54
1:A:237:ALA:HB1	1:A:308:LEU:HB3	1.90	0.54
1:B:198:GLU:O	1:B:200:THR:HG23	2.08	0.54
1:C:228:VAL:O	1:C:318:GLN:HA	2.08	0.53
1:A:310:GLU:HG3	1:A:311:LYS:H	1.73	0.53
1:B:327:PRO:HD2	3:B:529:HOH:O	2.10	0.52
1:C:265:PHE:CZ	1:C:293:VAL:HG23	2.45	0.51
1:A:249:ARG:HA	1:A:302:LEU:HD23	1.92	0.51
1:C:86:VAL:HG23	1:C:87:CYS:SG	2.50	0.51
1:A:158:LYS:HE3	1:C:23:MET:SD	2.50	0.51
1:B:16:LEU:O	1:B:20:LYS:HG3	2.12	0.50
1:A:259:MET:O	1:A:263:ARG:CD	2.60	0.50
1:B:113:HIS:HA	1:B:117:PHE:O	2.11	0.50
1:C:92:LEU:HD21	1:C:280:LEU:HB2	1.93	0.50
1:B:220:VAL:O	1:B:221:HIS:HB2	2.12	0.49
1:C:234:GLU:OE1	1:C:234:GLU:CA	2.57	0.49
1:C:325:LEU:HD23	1:C:325:LEU:N	2.26	0.49
1:C:199:LYS:HE3	1:C:216:ALA:HB1	1.95	0.49
1:B:281:ARG:O	1:B:281:ARG:HG2	2.13	0.48
1:A:226:VAL:O	1:A:320:LYS:HA	2.12	0.48
1:B:228:VAL:O	1:B:318:GLN:HA	2.14	0.48
1:B:281:ARG:HD3	3:B:514:HOH:O	2.14	0.47
1:B:255:TYR:CD2	1:B:299:HIS:CD2	3.03	0.46
1:A:268:GLU:CD	1:A:271:ARG:HH21	2.19	0.46
1:C:220:VAL:O	1:C:221:HIS:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:265:PHE:CE2	1:C:293:VAL:HG23	2.51	0.45
1:B:199:LYS:HE3	1:B:216:ALA:HB1	1.97	0.45
1:B:74:ILE:HD13	1:B:74:ILE:HG21	1.29	0.45
1:C:60:THR:O	1:C:72:LYS:HE3	2.16	0.45
1:A:258:LYS:HG3	1:A:258:LYS:O	2.17	0.44
1:A:310:GLU:HG3	1:A:311:LYS:N	2.32	0.44
1:A:192:GLN:HG2	1:A:193:HIS:ND1	2.33	0.44
1:B:41:SER:OG	2:B:408:SO4:O4	2.24	0.44
1:A:266:PHE:CE1	1:A:301:LEU:HB3	2.53	0.44
1:B:236:LYS:O	1:B:310:GLU:HG2	2.17	0.44
1:C:258:LYS:HG2	1:C:259:MET:H	1.82	0.43
1:C:42:GLY:HA2	1:C:99:ILE:CG2	2.48	0.43
1:B:226:VAL:O	1:B:320:LYS:HA	2.19	0.42
1:C:246:ILE:HA	1:C:278:PHE:O	2.19	0.42
1:A:307:VAL:HG12	1:A:309:TYR:CE1	2.54	0.42
1:C:86:VAL:CG2	1:C:87:CYS:SG	3.07	0.42
1:A:101:LYS:O	1:A:104:ASP:HB2	2.20	0.42
1:B:108:ILE:O	1:B:122:ALA:HA	2.19	0.41
1:C:53:ASP:O	1:C:57:MET:HG2	2.20	0.41
1:C:106:VAL:O	1:C:124:THR:HA	2.20	0.41
1:A:110:LEU:HD12	1:A:110:LEU:C	2.41	0.41
1:C:40:SER:HA	1:C:127:VAL:HG13	2.02	0.41
1:B:12:ILE:CG1	1:B:221:HIS:HA	2.51	0.41
1:C:75:ALA:HB2	1:C:113:HIS:HB3	2.03	0.41
1:B:246:ILE:HA	1:B:278:PHE:O	2.21	0.41
1:C:40:SER:O	1:C:43:VAL:HG13	2.21	0.41
1:A:228:VAL:O	1:A:318:GLN:HA	2.20	0.40
1:A:246:ILE:HG22	1:A:305:PHE:HB2	2.03	0.40
1:B:206:THR:OG1	1:B:209:GLN:HB2	2.22	0.40
1:C:108:ILE:O	1:C:122:ALA:HA	2.22	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	352/369 (95%)	331 (94%)	20 (6%)	1 (0%)	41	64
1	B	351/369 (95%)	330 (94%)	19 (5%)	2 (1%)	25	47
1	C	351/369 (95%)	333 (95%)	14 (4%)	4 (1%)	14	30
All	All	1054/1107 (95%)	994 (94%)	53 (5%)	7 (1%)	22	43

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	207	ASP
1	A	197	GLY
1	B	274	ASP
1	C	257	LEU
1	C	258	LYS
1	C	234	GLU
1	C	255	TYR

### 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	304/316 (96%)	293 (96%)	11 (4%)	35	61
1	B	303/316 (96%)	286 (94%)	17 (6%)	21	42
1	C	303/316 (96%)	287 (95%)	16 (5%)	22	45
All	All	910/948 (96%)	866 (95%)	44 (5%)	25	49

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LYS
1	A	66	LYS
1	A	72	LYS

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Mol	Chain	Res	Type
1	A	215	LYS
1	A	255	TYR
1	A	259	MET
1	A	260	LYS
1	A	261	THR
1	A	295	GLU
1	A	308	LEU
1	A	311	LYS
1	B	22	LYS
1	B	69	GLU
1	B	74	ILE
1	B	131	GLN
1	B	155	ARG
1	B	185	MET
1	B	191	LYS
1	B	207	ASP
1	B	209	GLN
1	B	220	VAL
1	B	249	ARG
1	B	260	LYS
1	B	284	GLU
1	B	287	LYS
1	B	310	GLU
1	B	312	GLU
1	B	346	GLU
1	C	41	SER
1	C	44	SER
1	C	69	GLU
1	C	71	LYS
1	C	86	VAL
1	C	136	THR
1	C	234	GLU
1	C	254	GLN
1	C	258	LYS
1	C	261	THR
1	C	269	VAL
1	C	270	GLU
1	C	291	MET
1	C	308	LEU
1	C	310	GLU
1	C	342	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	306	ASN
1	C	178	ASN

### 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](#)

28 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	406	-	4,4,4	0.29	0	6,6,6	0.24	0
2	SO4	C	410	-	4,4,4	0.33	0	6,6,6	0.09	0
2	SO4	A	501	-	4,4,4	0.36	0	6,6,6	0.22	0
2	SO4	A	505	-	4,4,4	0.28	0	6,6,6	0.06	0
2	SO4	B	402	-	4,4,4	0.32	0	6,6,6	0.06	0
2	SO4	B	407	-	4,4,4	0.29	0	6,6,6	0.09	0
2	SO4	A	503	-	4,4,4	0.21	0	6,6,6	0.14	0
2	SO4	B	409	-	4,4,4	0.29	0	6,6,6	0.08	0
2	SO4	B	403	-	4,4,4	0.45	0	6,6,6	0.26	0
2	SO4	A	502	-	4,4,4	0.31	0	6,6,6	0.26	0
2	SO4	C	407	-	4,4,4	0.32	0	6,6,6	0.06	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	A	504	-	4,4,4	0.37	0	6,6,6	0.20	0
2	SO4	B	404	-	4,4,4	0.33	0	6,6,6	0.07	0
2	SO4	A	507	-	4,4,4	0.32	0	6,6,6	0.11	0
2	SO4	C	409	-	4,4,4	0.31	0	6,6,6	0.05	0
2	SO4	B	405	-	4,4,4	0.33	0	6,6,6	0.07	0
2	SO4	A	509	-	4,4,4	0.23	0	6,6,6	0.12	0
2	SO4	A	506	-	4,4,4	0.30	0	6,6,6	0.16	0
2	SO4	C	406	-	4,4,4	0.29	0	6,6,6	0.16	0
2	SO4	A	508	-	4,4,4	0.30	0	6,6,6	0.07	0
2	SO4	B	401	-	4,4,4	0.31	0	6,6,6	0.41	0
2	SO4	C	403	-	4,4,4	0.21	0	6,6,6	0.25	0
2	SO4	C	408	-	4,4,4	0.31	0	6,6,6	0.08	0
2	SO4	C	402	-	4,4,4	0.38	0	6,6,6	0.30	0
2	SO4	C	405	-	4,4,4	0.34	0	6,6,6	0.09	0
2	SO4	C	404	-	4,4,4	0.28	0	6,6,6	0.13	0
2	SO4	B	408	-	4,4,4	0.21	0	6,6,6	0.27	0
2	SO4	C	401	-	4,4,4	0.36	0	6,6,6	0.11	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	509	SO4	1	0
2	B	408	SO4	1	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 [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	354/369 (95%)	-0.15	5 (1%) 75 71	40, 57, 107, 155	0
1	B	353/369 (95%)	-0.10	4 (1%) 80 78	41, 57, 95, 116	0
1	C	353/369 (95%)	-0.05	8 (2%) 60 54	39, 61, 102, 143	0
All	All	1060/1107 (95%)	-0.10	17 (1%) 72 68	39, 59, 104, 155	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	291	MET	3.7
1	B	298	LYS	3.5
1	A	261	THR	3.1
1	C	254	GLN	3.1
1	A	260	LYS	3.1
1	B	290	ARG	3.0
1	A	258	LYS	2.8
1	A	257	LEU	2.7
1	C	256	GLY	2.6
1	C	135	VAL	2.5
1	C	258	LYS	2.3
1	B	234	GLU	2.2
1	B	291	MET	2.2
1	C	311	LYS	2.2
1	C	257	LEU	2.1
1	C	260	LYS	2.1
1	C	132	GLY	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 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
2	SO4	B	406	5/5	0.81	0.21	90,104,120,121	0
2	SO4	C	405	5/5	0.83	0.39	106,112,132,142	0
2	SO4	C	404	5/5	0.85	0.19	88,102,119,121	0
2	SO4	A	506	5/5	0.86	0.17	90,103,114,118	0
2	SO4	B	409	5/5	0.87	0.35	105,110,127,129	0
2	SO4	A	509	5/5	0.87	0.40	75,112,123,128	0
2	SO4	A	505	5/5	0.87	0.26	104,117,124,138	0
2	SO4	A	508	5/5	0.88	0.39	87,117,135,135	0
2	SO4	C	408	5/5	0.89	0.21	91,113,124,129	0
2	SO4	C	409	5/5	0.90	0.25	83,109,116,123	0
2	SO4	C	406	5/5	0.91	0.36	94,104,117,130	0
2	SO4	B	404	5/5	0.92	0.13	95,107,120,127	0
2	SO4	B	407	5/5	0.92	0.21	91,115,124,126	0
2	SO4	B	402	5/5	0.93	0.17	87,91,100,115	0
2	SO4	C	407	5/5	0.93	0.14	92,98,130,135	0
2	SO4	A	507	5/5	0.94	0.35	86,91,105,113	0
2	SO4	A	503	5/5	0.94	0.13	79,85,105,106	0
2	SO4	C	410	5/5	0.94	0.18	91,94,102,116	0
2	SO4	C	403	5/5	0.96	0.16	68,70,82,106	0
2	SO4	B	405	5/5	0.96	0.31	100,111,119,132	0
2	SO4	B	408	5/5	0.96	0.10	67,70,73,81	0
2	SO4	B	401	5/5	0.96	0.14	50,51,63,64	0
2	SO4	A	504	5/5	0.97	0.14	73,74,81,82	0
2	SO4	C	402	5/5	0.97	0.11	51,62,64,75	0
2	SO4	A	501	5/5	0.98	0.11	63,64,73,75	0
2	SO4	B	403	5/5	0.98	0.13	55,58,67,71	0
2	SO4	C	401	5/5	0.98	0.13	62,65,68,79	0
2	SO4	A	502	5/5	0.98	0.10	59,64,67,79	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.