



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:26 AM UTC

PDB ID : 6WM8 / pdb_00006wm8
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

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

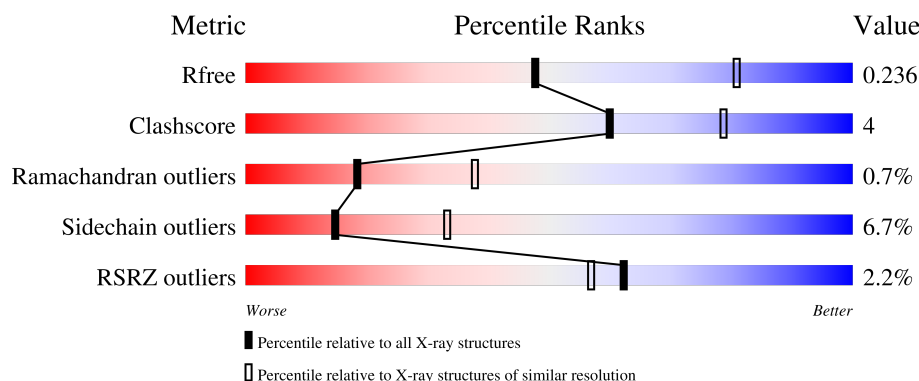
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

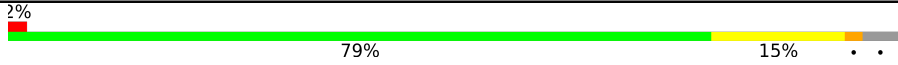
The reported resolution of this entry is 2.60 Å.

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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 ≥ 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
1	A	354	Total	C	N	O	S	0	0	0
			2770	1747	475	531	17			
1	B	353	Total	C	N	O	S	0	0	0
			2761	1742	473	529	17			
1	C	353	Total	C	N	O	S	0	0	0
			2761	1742	473	529	17			

There are 24 discrepancies between the modelled and reference sequences:

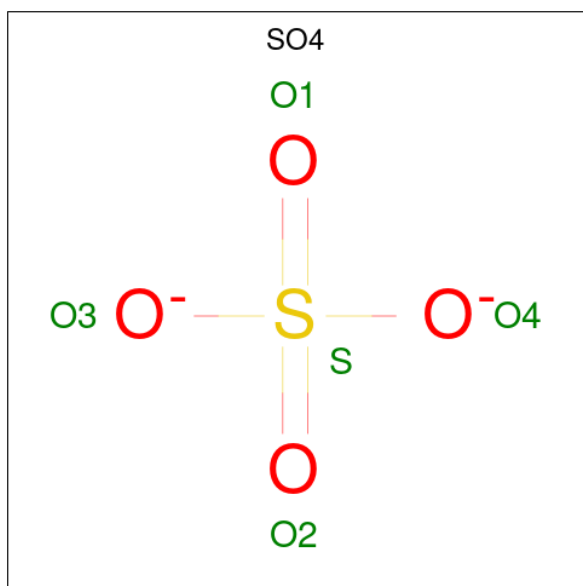
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP Q9UQ80
A	-5	GLY	-	expression tag	UNP Q9UQ80
A	-4	HIS	-	expression tag	UNP Q9UQ80
A	-3	HIS	-	expression tag	UNP Q9UQ80
A	-2	HIS	-	expression tag	UNP Q9UQ80
A	-1	HIS	-	expression tag	UNP Q9UQ80
A	0	HIS	-	expression tag	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 (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	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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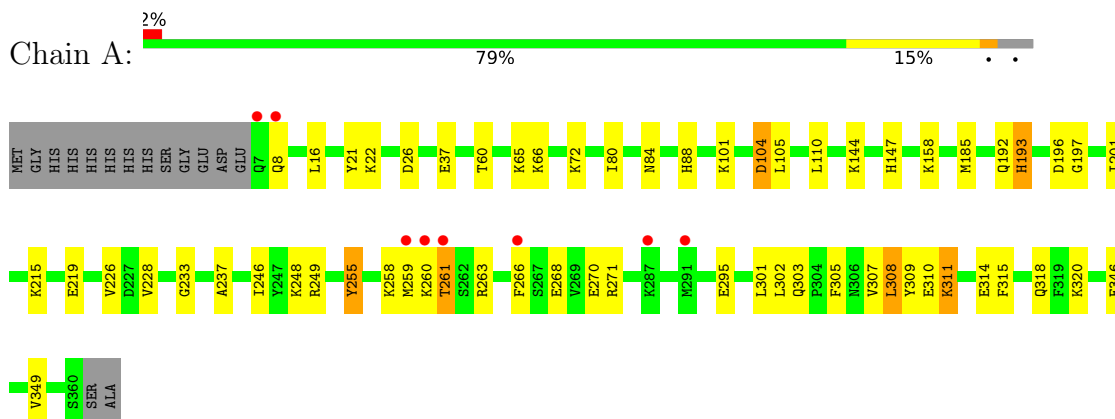
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	32	Total	O	0	0
			32	32		

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.

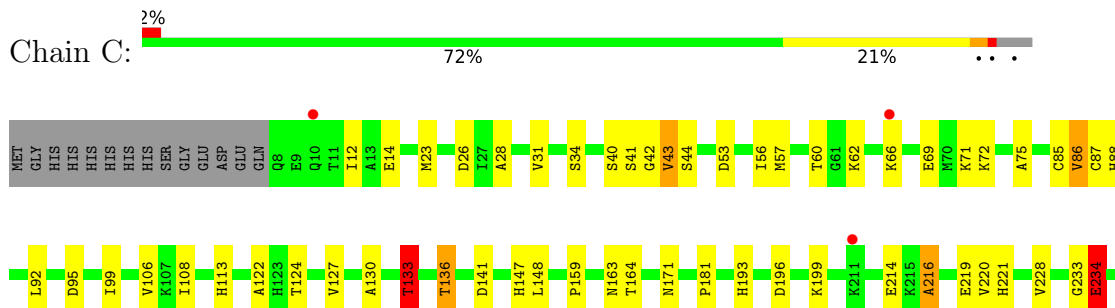
• Molecule 1: Proliferation-associated protein 2G4

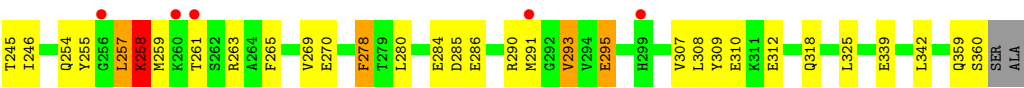


• Molecule 1: Proliferation-associated protein 2G4



• 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	2.22 (at 2.61Å)	Xtriage
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 ²)	58.1	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 37.1	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	0.95	EDS
Total number of atoms	8541	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage'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.*

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	1.25	9/2817 (0.3%)	1.58	13/3791 (0.3%)
1	B	1.26	10/2808 (0.4%)	1.61	25/3779 (0.7%)
1	C	1.25	8/2808 (0.3%)	1.64	28/3779 (0.7%)
All	All	1.25	27/8433 (0.3%)	1.61	66/11349 (0.6%)

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 (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	HIS	CE1-NE2	10.10	1.42	1.32
1	B	193	HIS	CE1-NE2	7.87	1.40	1.32
1	C	193	HIS	CE1-NE2	7.42	1.40	1.32
1	B	307	VAL	C-O	-7.06	1.16	1.24
1	A	37	GLU	C-O	-6.94	1.15	1.24
1	B	223	VAL	C-O	-6.61	1.17	1.24
1	C	88	HIS	CE1-NE2	6.47	1.39	1.32
1	B	147	HIS	CE1-NE2	6.43	1.39	1.32
1	C	147	HIS	CE1-NE2	6.41	1.39	1.32
1	B	265	PHE	C-O	6.32	1.31	1.24
1	B	204	ASN	N-CA	5.71	1.50	1.46
1	B	90	SER	CA-CB	-5.70	1.46	1.53
1	A	16	LEU	C-O	5.64	1.31	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	216	ALA	C-O	-5.59	1.17	1.23
1	A	193	HIS	CE1-NE2	5.45	1.38	1.32
1	A	104	ASP	C-O	5.39	1.30	1.23
1	C	181	PRO	C-O	-5.37	1.17	1.23
1	B	330	PRO	C-O	-5.34	1.17	1.23
1	B	166	VAL	C-O	5.34	1.30	1.24
1	C	28	ALA	C-O	-5.27	1.18	1.24
1	A	88	HIS	CE1-NE2	5.27	1.37	1.32
1	A	26	ASP	C-O	5.20	1.30	1.24
1	C	159	PRO	C-O	-5.17	1.17	1.23
1	B	193	HIS	CG-ND1	5.14	1.44	1.38
1	A	233	GLY	C-O	5.11	1.29	1.24
1	A	349	VAL	C-O	-5.09	1.18	1.24
1	C	56	ILE	C-O	5.03	1.30	1.24

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	360	SER	CA-C-O	-15.04	95.22	120.80
1	C	136	THR	CA-CB-OG1	-9.88	94.78	109.60
1	B	207	ASP	CA-CB-CG	8.66	121.26	112.60
1	C	133	THR	CA-CB-OG1	-8.11	97.44	109.60
1	B	74	ILE	CA-CB-CG1	7.48	123.11	110.40
1	B	74	ILE	CB-CA-C	7.15	120.57	110.84
1	A	21	TYR	N-CA-C	-7.03	103.55	111.14
1	A	219	GLU	CB-CG-CD	6.67	123.95	112.60
1	B	339	GLU	CB-CA-C	6.64	118.97	110.34
1	C	147	HIS	CA-CB-CG	-6.35	107.45	113.80
1	C	95	ASP	CB-CA-C	-6.12	98.60	113.15
1	C	214	GLU	CB-CA-C	6.10	120.07	110.19
1	B	350	GLN	CA-C-O	-6.07	112.37	119.05
1	B	117	PHE	CB-CA-C	6.04	120.20	110.29
1	A	147	HIS	CA-CB-CG	-6.00	107.80	113.80
1	B	147	HIS	CA-CB-CG	-5.93	107.86	113.80
1	C	295	GLU	CB-CG-CD	5.92	122.67	112.60
1	B	360	SER	CA-C-O	-5.89	110.79	120.80
1	B	358	LEU	CA-C-O	-5.87	112.39	119.49
1	B	51	LYS	CA-C-N	5.84	126.31	119.94
1	B	51	LYS	C-N-CA	5.84	126.31	119.94
1	B	263	ARG	CG-CD-NE	-5.83	99.17	112.00
1	B	92	LEU	CA-C-O	-5.78	115.17	121.87
1	C	196	ASP	CA-CB-CG	5.76	118.36	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255	TYR	CB-CA-C	5.73	121.83	110.42
1	C	278	PHE	CA-C-O	-5.72	115.15	121.33
1	A	303	GLN	CB-CA-C	5.71	116.72	110.15
1	B	167	THR	CA-C-N	5.67	128.15	120.44
1	B	167	THR	C-N-CA	5.67	128.15	120.44
1	A	60	THR	CA-C-N	5.65	126.38	119.99
1	A	60	THR	C-N-CA	5.65	126.38	119.99
1	B	338	PHE	CA-C-O	-5.64	114.84	121.16
1	A	8	GLN	N-CA-C	-5.64	105.21	111.36
1	C	31	VAL	N-CA-C	-5.63	105.03	110.72
1	C	171	ASN	CA-C-O	-5.62	114.92	120.82
1	C	95	ASP	CA-CB-CG	5.62	118.22	112.60
1	C	85	CYS	CA-C-O	-5.61	114.52	120.92
1	C	285	ASP	CA-CB-CG	5.59	118.19	112.60
1	C	233	GLY	CA-C-N	5.56	132.17	121.54
1	C	233	GLY	C-N-CA	5.56	132.17	121.54
1	B	74	ILE	CB-CG1-CD1	-5.55	102.14	113.80
1	C	339	GLU	CB-CA-C	-5.50	104.72	110.33
1	C	141	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	22	LYS	CB-CA-C	5.35	119.67	110.79
1	B	109	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	261	THR	CA-C-N	5.32	127.35	120.44
1	A	261	THR	C-N-CA	5.32	127.35	120.44
1	C	164	THR	CA-CB-OG1	-5.31	101.63	109.60
1	A	315	PHE	CA-CB-CG	-5.30	108.50	113.80
1	B	270	GLU	N-CA-C	-5.25	105.45	111.07
1	C	34	SER	N-CA-C	-5.22	105.67	111.36
1	C	219	GLU	CB-CG-CD	5.22	121.47	112.60
1	C	310	GLU	CA-C-N	5.21	128.62	120.75
1	C	310	GLU	C-N-CA	5.21	128.62	120.75
1	C	26	ASP	N-CA-C	-5.21	105.61	111.28
1	C	133	THR	CA-CB-CG2	5.17	119.29	110.50
1	C	148	LEU	N-CA-C	-5.15	105.85	111.82
1	B	71	LYS	CB-CA-C	5.10	118.15	109.53
1	B	98	TYR	CA-C-N	5.05	128.69	122.37
1	B	98	TYR	C-N-CA	5.05	128.69	122.37
1	B	159	PRO	CA-C-O	-5.05	115.81	121.32
1	B	48	LEU	N-CA-C	-5.04	105.86	111.36
1	C	245	THR	CB-CA-C	5.03	117.52	109.07
1	C	163	ASN	N-CA-C	-5.02	105.81	111.28
1	A	346	GLU	N-CA-C	-5.00	107.12	113.18
1	B	283	PHE	CA-C-O	-5.00	114.83	120.43

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

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	25	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	72	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 (72) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:LEU:C	1:A:105:LEU:HD23	2.26	0.59
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: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:A:268:GLU:CD	1:A:271:ARG:HH21	2.19	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: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:O	1:B:281:ARG:HG2	2.13	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:110:LEU:HD12	1:A:110:LEU:C	2.41	0.46
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:C:220:VAL:O	1:C:221:HIS:HB2	2.16	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:110:LEU:C	1:B:110:LEU:HD12	2.45	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: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%)	36	58
1	B	351/369 (95%)	330 (94%)	19 (5%)	2 (1%)	21	42
1	C	351/369 (95%)	333 (95%)	14 (4%)	4 (1%)	11	25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1054/1107 (95%)	994 (94%)	53 (5%)	7 (1%)	18	38

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 ⓘ

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%)	290 (95%)	14 (5%)	24	49
1	B	303/316 (96%)	281 (93%)	22 (7%)	13	29
1	C	303/316 (96%)	278 (92%)	25 (8%)	10	23
All	All	910/948 (96%)	849 (93%)	61 (7%)	15	33

All (61) 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
1	A	80	ILE
1	A	185	MET
1	A	201	ILE
1	A	215	LYS
1	A	255	TYR
1	A	260	LYS

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Mol	Chain	Res	Type
1	A	261	THR
1	A	270	GLU
1	A	295	GLU
1	A	308	LEU
1	A	311	LYS
1	B	14	GLU
1	B	69	GLU
1	B	74	ILE
1	B	131	GLN
1	B	155	ARG
1	B	172	LYS
1	B	185	MET
1	B	191	LYS
1	B	207	ASP
1	B	209	GLN
1	B	220	VAL
1	B	236	LYS
1	B	238	LYS
1	B	249	ARG
1	B	271	ARG
1	B	284	GLU
1	B	287	LYS
1	B	294	VAL
1	B	298	LYS
1	B	310	GLU
1	B	312	GLU
1	B	346	GLU
1	C	12	ILE
1	C	14	GLU
1	C	41	SER
1	C	43	VAL
1	C	44	SER
1	C	62	LYS
1	C	66	LYS
1	C	69	GLU
1	C	71	LYS
1	C	86	VAL
1	C	133	THR
1	C	136	THR
1	C	234	GLU
1	C	254	GLN
1	C	258	LYS

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Mol	Chain	Res	Type
1	C	261	THR
1	C	269	VAL
1	C	270	GLU
1	C	284	GLU
1	C	291	MET
1	C	293	VAL
1	C	295	GLU
1	C	308	LEU
1	C	312	GLU
1	C	342	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	GLN
1	A	162	GLN
1	A	306	ASN
1	B	209	GLN
1	B	299	HIS
1	B	318	GLN
1	B	328	ASN
1	C	208	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 oligosaccharides 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	A	506	-	4,4,4	0.24	0	6,6,6	0.17	0
2	SO4	C	403	-	4,4,4	0.17	0	6,6,6	0.24	0
2	SO4	B	406	-	4,4,4	0.31	0	6,6,6	0.24	0
2	SO4	A	507	-	4,4,4	0.29	0	6,6,6	0.10	0
2	SO4	C	404	-	4,4,4	0.28	0	6,6,6	0.14	0
2	SO4	A	505	-	4,4,4	0.29	0	6,6,6	0.09	0
2	SO4	C	402	-	4,4,4	0.39	0	6,6,6	0.33	0
2	SO4	C	405	-	4,4,4	0.29	0	6,6,6	0.10	0
2	SO4	C	407	-	4,4,4	0.32	0	6,6,6	0.10	0
2	SO4	A	508	-	4,4,4	0.28	0	6,6,6	0.09	0
2	SO4	A	509	-	4,4,4	0.21	0	6,6,6	0.13	0
2	SO4	C	401	-	4,4,4	0.32	0	6,6,6	0.14	0
2	SO4	B	403	-	4,4,4	0.49	0	6,6,6	0.25	0
2	SO4	A	504	-	4,4,4	0.31	0	6,6,6	0.18	0
2	SO4	B	404	-	4,4,4	0.29	0	6,6,6	0.07	0
2	SO4	B	409	-	4,4,4	0.28	0	6,6,6	0.08	0
2	SO4	C	408	-	4,4,4	0.30	0	6,6,6	0.10	0
2	SO4	A	503	-	4,4,4	0.21	0	6,6,6	0.15	0
2	SO4	C	409	-	4,4,4	0.30	0	6,6,6	0.08	0
2	SO4	C	406	-	4,4,4	0.26	0	6,6,6	0.18	0
2	SO4	B	407	-	4,4,4	0.28	0	6,6,6	0.11	0
2	SO4	B	401	-	4,4,4	0.33	0	6,6,6	0.42	0
2	SO4	B	408	-	4,4,4	0.28	0	6,6,6	0.27	0
2	SO4	B	405	-	4,4,4	0.30	0	6,6,6	0.09	0
2	SO4	B	402	-	4,4,4	0.32	0	6,6,6	0.04	0
2	SO4	C	410	-	4,4,4	0.32	0	6,6,6	0.12	0
2	SO4	A	501	-	4,4,4	0.34	0	6,6,6	0.25	0
2	SO4	A	502	-	4,4,4	0.30	0	6,6,6	0.27	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	354/369 (95%)	-0.20	8 (2%) 61 55	40, 57, 107, 155	0
1	B	353/369 (95%)	-0.26	7 (1%) 65 60	41, 57, 95, 116	0
1	C	353/369 (95%)	-0.15	8 (2%) 61 55	39, 61, 102, 143	0
All	All	1060/1107 (95%)	-0.21	23 (2%) 62 57	39, 59, 104, 155	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	260	LYS	3.9
1	A	8	GLN	3.3
1	A	7	GLN	3.2
1	C	66	LYS	3.0
1	B	255	TYR	3.0
1	C	261	THR	2.7
1	C	299	HIS	2.6
1	C	256	GLY	2.6
1	B	298	LYS	2.6
1	A	291	MET	2.6
1	B	299	HIS	2.5
1	A	259	MET	2.4
1	C	291	MET	2.4
1	B	297	ALA	2.3
1	C	211	LYS	2.3
1	B	234	GLU	2.2
1	A	266	PHE	2.2
1	B	207	ASP	2.2
1	A	287	LYS	2.2
1	C	260	LYS	2.2
1	C	10	GLN	2.1
1	B	287	LYS	2.1
1	A	261	THR	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 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	A	505	5/5	0.64	0.11	104,117,124,138	0
2	SO4	A	506	5/5	0.64	0.12	90,103,114,118	0
2	SO4	B	406	5/5	0.65	0.17	90,104,120,121	0
2	SO4	B	407	5/5	0.66	0.12	91,115,124,126	0
2	SO4	B	409	5/5	0.67	0.12	105,110,127,129	0
2	SO4	C	406	5/5	0.69	0.13	94,104,117,130	0
2	SO4	A	508	5/5	0.71	0.11	87,117,135,135	0
2	SO4	C	404	5/5	0.72	0.14	88,102,119,121	0
2	SO4	C	407	5/5	0.72	0.11	92,98,130,135	0
2	SO4	C	405	5/5	0.76	0.09	106,112,132,142	0
2	SO4	A	509	5/5	0.79	0.13	75,112,123,128	0
2	SO4	C	408	5/5	0.80	0.11	91,113,124,129	0
2	SO4	B	404	5/5	0.82	0.13	95,107,120,127	0
2	SO4	C	409	5/5	0.83	0.10	83,109,116,123	0
2	SO4	B	405	5/5	0.84	0.07	100,111,119,132	0
2	SO4	A	503	5/5	0.86	0.16	79,85,105,106	0
2	SO4	A	507	5/5	0.88	0.10	86,91,105,113	0
2	SO4	C	410	5/5	0.88	0.10	91,94,102,116	0
2	SO4	A	504	5/5	0.90	0.19	73,74,81,82	0
2	SO4	B	402	5/5	0.90	0.09	87,91,100,115	0
2	SO4	C	403	5/5	0.92	0.18	68,70,82,106	0
2	SO4	B	408	5/5	0.92	0.19	67,70,73,81	0
2	SO4	C	402	5/5	0.95	0.12	51,62,64,75	0
2	SO4	A	501	5/5	0.95	0.08	63,64,73,75	0
2	SO4	B	403	5/5	0.95	0.12	55,58,67,71	0
2	SO4	B	401	5/5	0.96	0.12	50,51,63,64	0
2	SO4	A	502	5/5	0.96	0.14	59,64,67,79	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	C	401	5/5	0.97	0.11	62,65,68,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.