



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 12:48 PM GMT

PDB ID : 3S24
Title : Crystal structure of human mRNA guanylyltransferase
Authors : Das, K.; Chu, C.; Thyminski, J.R.; Bauman, J.D.; Guan, R.; Qiu, W.; Montelione, G.T.; Arnold, E.; Shatkin, A.J.
Deposited on : 2011-05-16
Resolution : 3.01 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at 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.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

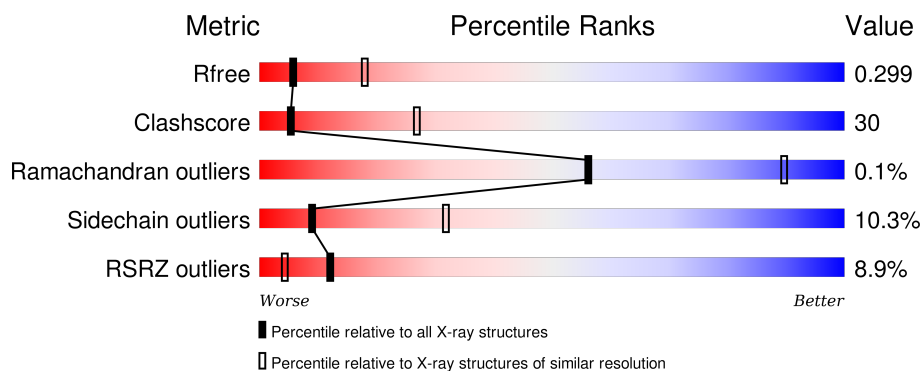
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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}	91344	1773 (3.04-3.00)
Clashscore	102246	2117 (3.04-3.00)
Ramachandran outliers	100387	2050 (3.04-3.00)
Sidechain outliers	100360	2053 (3.04-3.00)
RSRZ outliers	91569	1788 (3.04-3.00)

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 ≥ 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	347	<div> <div>5%</div> <div>49%</div> <div>38%</div> <div>8%</div> <div>5%</div> </div>
1	B	347	<div> <div>13%</div> <div>39%</div> <div>45%</div> <div>7%</div> <div>9%</div> </div>
1	C	347	<div> <div>9%</div> <div>44%</div> <div>41%</div> <div>5%</div> <div>10%</div> </div>
1	D	347	<div> <div>6%</div> <div>51%</div> <div>39%</div> <div>5%</div> <div>5%</div> </div>
1	E	347	<div> <div>11%</div> <div>47%</div> <div>44%</div> <div>•</div> <div>5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	347	
1	G	347	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	5	-	-	X	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18387 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 mRNA-capping enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	328	Total	C	N	O	S	0	0	0
			2646	1688	457	481	20			
1	B	316	Total	C	N	O	S	0	0	0
			2561	1637	440	465	19			
1	C	314	Total	C	N	O	S	0	0	0
			2547	1628	438	462	19			
1	D	328	Total	C	N	O	S	0	0	0
			2646	1688	457	481	20			
1	E	329	Total	C	N	O	S	0	0	0
			2649	1689	456	483	21			
1	G	329	Total	C	N	O	S	0	0	0
			2651	1691	458	482	20			
1	F	333	Total	C	N	O	S	0	0	0
			2662	1698	460	484	20			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	568	LEU	-	EXPRESSION TAG	UNP O60942
A	569	GLU	-	EXPRESSION TAG	UNP O60942
A	570	HIS	-	EXPRESSION TAG	UNP O60942
A	571	HIS	-	EXPRESSION TAG	UNP O60942
A	572	HIS	-	EXPRESSION TAG	UNP O60942
A	573	HIS	-	EXPRESSION TAG	UNP O60942
A	574	HIS	-	EXPRESSION TAG	UNP O60942
A	575	HIS	-	EXPRESSION TAG	UNP O60942
B	568	LEU	-	EXPRESSION TAG	UNP O60942
B	569	GLU	-	EXPRESSION TAG	UNP O60942
B	570	HIS	-	EXPRESSION TAG	UNP O60942
B	571	HIS	-	EXPRESSION TAG	UNP O60942
B	572	HIS	-	EXPRESSION TAG	UNP O60942
B	573	HIS	-	EXPRESSION TAG	UNP O60942
B	574	HIS	-	EXPRESSION TAG	UNP O60942

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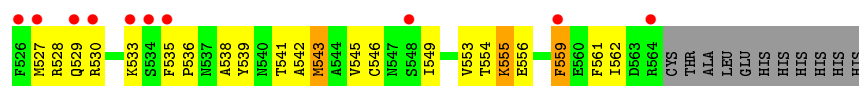
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Chain	Residue	Modelled	Actual	Comment	Reference
B	575	HIS	-	EXPRESSION TAG	UNP O60942
C	568	LEU	-	EXPRESSION TAG	UNP O60942
C	569	GLU	-	EXPRESSION TAG	UNP O60942
C	570	HIS	-	EXPRESSION TAG	UNP O60942
C	571	HIS	-	EXPRESSION TAG	UNP O60942
C	572	HIS	-	EXPRESSION TAG	UNP O60942
C	573	HIS	-	EXPRESSION TAG	UNP O60942
C	574	HIS	-	EXPRESSION TAG	UNP O60942
C	575	HIS	-	EXPRESSION TAG	UNP O60942
D	568	LEU	-	EXPRESSION TAG	UNP O60942
D	569	GLU	-	EXPRESSION TAG	UNP O60942
D	570	HIS	-	EXPRESSION TAG	UNP O60942
D	571	HIS	-	EXPRESSION TAG	UNP O60942
D	572	HIS	-	EXPRESSION TAG	UNP O60942
D	573	HIS	-	EXPRESSION TAG	UNP O60942
D	574	HIS	-	EXPRESSION TAG	UNP O60942
D	575	HIS	-	EXPRESSION TAG	UNP O60942
E	568	LEU	-	EXPRESSION TAG	UNP O60942
E	569	GLU	-	EXPRESSION TAG	UNP O60942
E	570	HIS	-	EXPRESSION TAG	UNP O60942
E	571	HIS	-	EXPRESSION TAG	UNP O60942
E	572	HIS	-	EXPRESSION TAG	UNP O60942
E	573	HIS	-	EXPRESSION TAG	UNP O60942
E	574	HIS	-	EXPRESSION TAG	UNP O60942
E	575	HIS	-	EXPRESSION TAG	UNP O60942
G	568	LEU	-	EXPRESSION TAG	UNP O60942
G	569	GLU	-	EXPRESSION TAG	UNP O60942
G	570	HIS	-	EXPRESSION TAG	UNP O60942
G	571	HIS	-	EXPRESSION TAG	UNP O60942
G	572	HIS	-	EXPRESSION TAG	UNP O60942
G	573	HIS	-	EXPRESSION TAG	UNP O60942
G	574	HIS	-	EXPRESSION TAG	UNP O60942
G	575	HIS	-	EXPRESSION TAG	UNP O60942
F	568	LEU	-	EXPRESSION TAG	UNP O60942
F	569	GLU	-	EXPRESSION TAG	UNP O60942
F	570	HIS	-	EXPRESSION TAG	UNP O60942
F	571	HIS	-	EXPRESSION TAG	UNP O60942
F	572	HIS	-	EXPRESSION TAG	UNP O60942
F	573	HIS	-	EXPRESSION TAG	UNP O60942
F	574	HIS	-	EXPRESSION TAG	UNP O60942
F	575	HIS	-	EXPRESSION TAG	UNP O60942

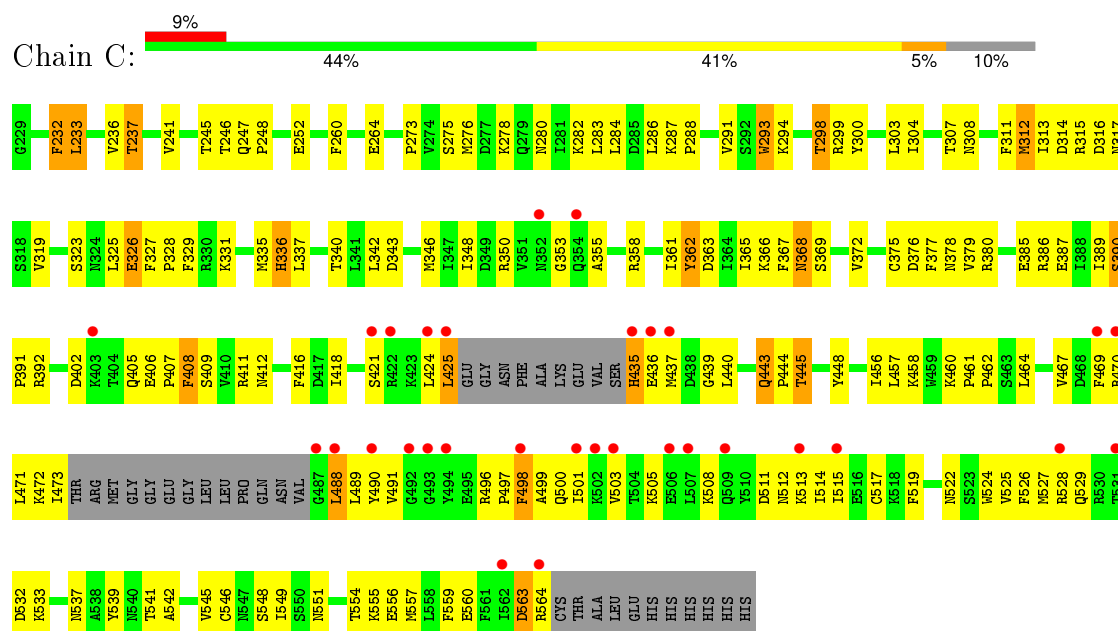
- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



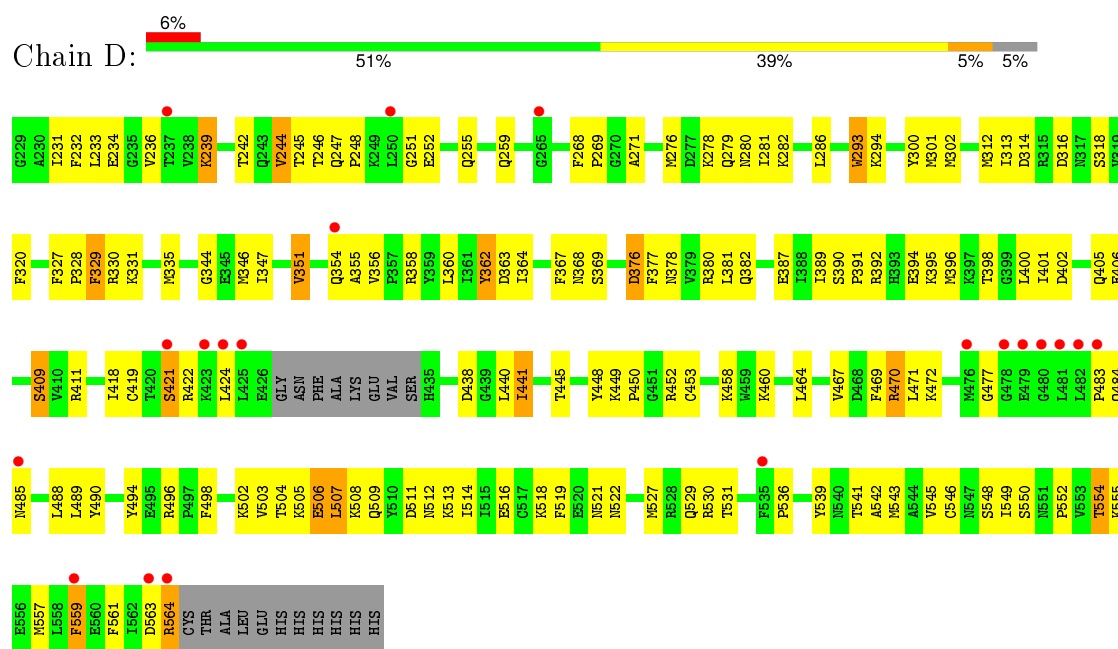
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		



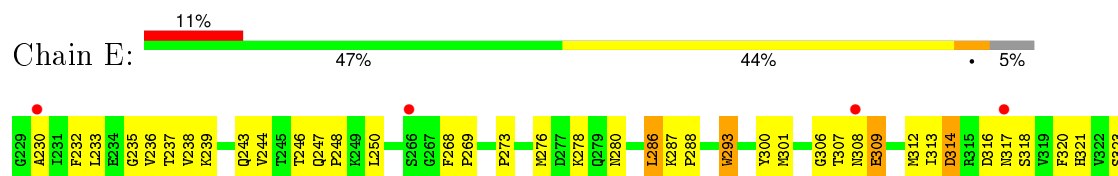
• Molecule 1: mRNA-capping enzyme

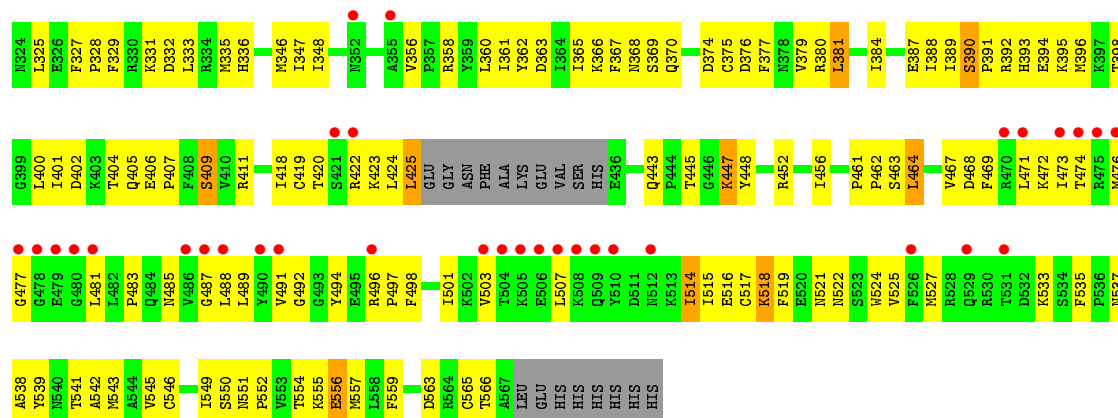


• Molecule 1: mRNA-capping enzyme

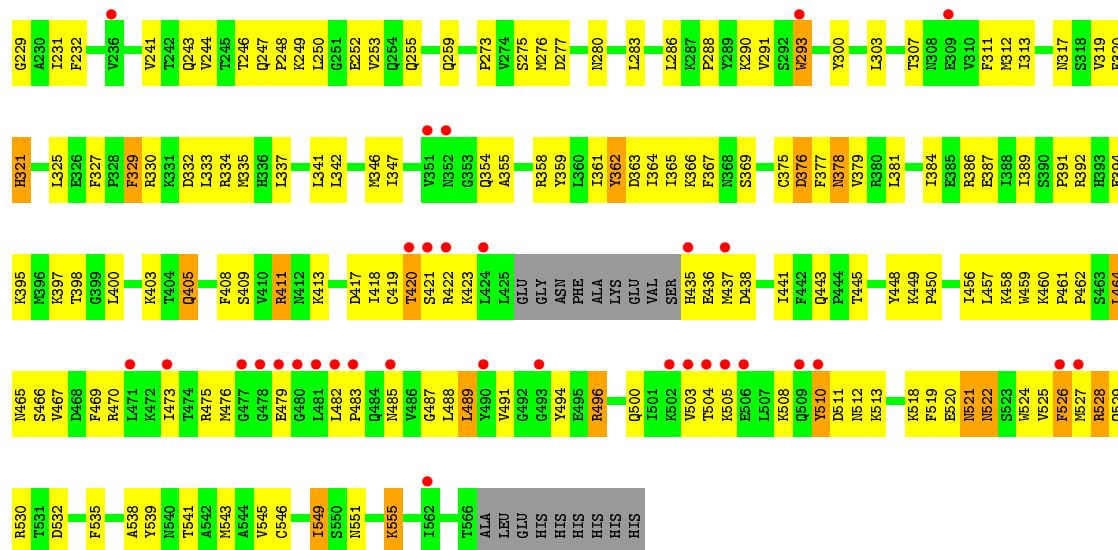


• Molecule 1: mRNA-capping enzyme

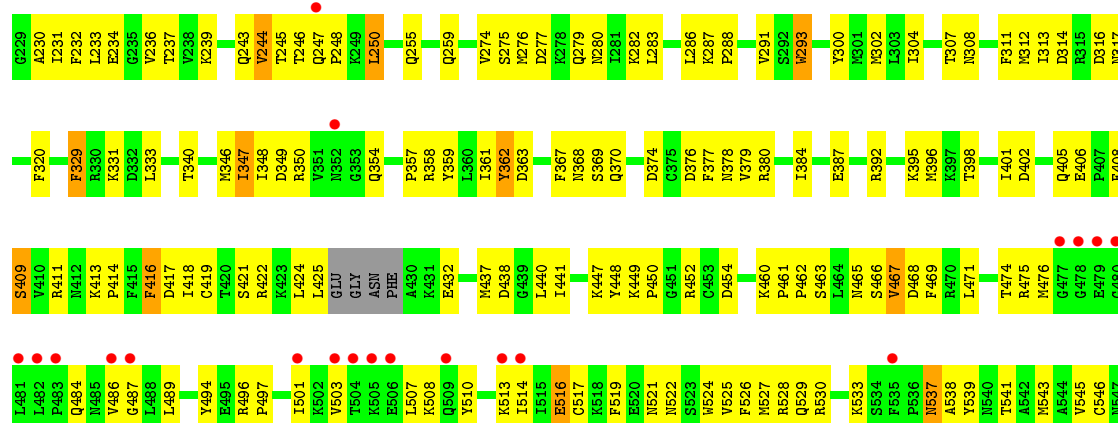




• Molecule 1: mRNA-capping enzyme



• Molecule 1: mRNA-capping enzyme



S548	S549	S550	S551	P552	V553	T554	K555	E556	M557	E560	F561	L562	D563	R564	C565	THR	ALA	LEU	GLU	HIS	HIS	HIS	HIS	HIS	HIS
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.12Å 104.66Å 149.57Å 90.00° 94.95° 90.00°	Depositor
Resolution (Å)	35.43 – 3.01 35.43 – 3.01	Depositor EDS
% Data completeness (in resolution range)	95.1 (35.43-3.01) 95.0 (35.43-3.01)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 3.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.258 , 0.296 0.254 , 0.299	Depositor DCC
R_{free} test set	2724 reflections (5.38%)	DCC
Wilson B-factor (Å ²)	94.6	Xtriage
Anisotropy	0.139	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 38.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 53399 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	18387	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z > 5	RMSZ	# Z > 5
1	A	0.56	0/2704	0.70	1/3643 (0.0%)
1	B	0.48	0/2617	0.65	2/3525 (0.1%)
1	C	0.54	0/2603	0.69	1/3505 (0.0%)
1	D	0.53	0/2704	0.68	1/3643 (0.0%)
1	E	0.55	0/2706	0.73	0/3646
1	F	0.56	0/2719	0.71	2/3665 (0.1%)
1	G	0.49	0/2709	0.66	1/3650 (0.0%)
All	All	0.53	0/18762	0.69	8/25277 (0.0%)

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	A	0	2

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	362	TYR	CB-CA-C	6.10	122.60	110.40
1	A	362	TYR	CB-CA-C	6.01	122.41	110.40
1	C	362	TYR	CB-CA-C	5.63	121.67	110.40
1	B	362	TYR	CA-CB-CG	5.53	123.90	113.40
1	F	362	TYR	CA-CB-CG	5.30	123.48	113.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	351	VAL	Peptide
1	A	480	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	2646	0	2650	157	0
1	B	2561	0	2567	169	0
1	C	2547	0	2551	150	0
1	D	2646	0	2650	156	0
1	E	2649	0	2658	178	0
1	F	2662	0	2654	161	0
1	G	2651	0	2652	164	0
2	A	20	0	0	2	0
2	B	5	0	0	0	0
All	All	18387	0	18382	1106	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 30.

The worst 5 of 1106 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:246:THR:HG22	1:B:248:PRO:HD2	1.22	1.13
1:D:239:LYS:HD3	1:D:239:LYS:H	1.17	1.08
1:C:462:PRO:HD2	1:C:555:LYS:HE3	1.37	1.06
1:A:230:ALA:HA	1:A:243:GLN:HE22	1.21	1.05
1:F:537:ASN:ND2	1:F:537:ASN:H	1.53	1.03

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	324/347 (93%)	313 (97%)	11 (3%)	0	100	100
1	B	310/347 (89%)	291 (94%)	18 (6%)	1 (0%)	46	82
1	C	308/347 (89%)	296 (96%)	11 (4%)	1 (0%)	46	82
1	D	324/347 (93%)	313 (97%)	11 (3%)	0	100	100
1	E	325/347 (94%)	308 (95%)	17 (5%)	0	100	100
1	F	329/347 (95%)	312 (95%)	17 (5%)	0	100	100
1	G	325/347 (94%)	307 (94%)	18 (6%)	0	100	100
All	All	2245/2429 (92%)	2140 (95%)	103 (5%)	2 (0%)	56	90

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	236	VAL
1	C	232	PHE

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	296/313 (95%)	255 (86%)	41 (14%)	4	19
1	B	288/313 (92%)	250 (87%)	38 (13%)	5	21
1	C	286/313 (91%)	258 (90%)	28 (10%)	10	35
1	D	296/313 (95%)	267 (90%)	29 (10%)	10	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	297/313 (95%)	276 (93%)	21 (7%)	18	53
1	F	294/313 (94%)	273 (93%)	21 (7%)	18	53
1	G	296/313 (95%)	262 (88%)	34 (12%)	7	27
All	All	2053/2191 (94%)	1841 (90%)	212 (10%)	9	32

5 of 212 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	435	HIS
1	D	381	LEU
1	F	293	TRP
1	C	457	LEU
1	D	239	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	412	ASN
1	D	280	ASN
1	G	435	HIS
1	C	280	ASN
1	G	529	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

5 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	1	-	4,4,4	0.14	0	6,6,6	0.37	0
2	SO4	A	2	-	4,4,4	0.11	0	6,6,6	0.14	0
2	SO4	A	3	-	4,4,4	0.36	0	6,6,6	0.29	0
2	SO4	A	5	-	4,4,4	0.12	0	6,6,6	0.18	0
2	SO4	B	4	-	4,4,4	0.17	0	6,6,6	0.44	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	1	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2	-	-	0/0/0/0	0/0/0/0
2	SO4	A	3	-	-	0/0/0/0	0/0/0/0
2	SO4	A	5	-	-	0/0/0/0	0/0/0/0
2	SO4	B	4	-	-	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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	5	SO4	2	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, 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	328/347 (94%)	0.32	17 (5%) 31 12	28, 51, 102, 136	0
1	B	316/347 (91%)	0.65	45 (14%) 4 1	29, 67, 127, 137	0
1	C	314/347 (90%)	0.46	31 (9%) 9 3	26, 59, 121, 135	0
1	D	328/347 (94%)	0.31	20 (6%) 25 9	28, 55, 112, 143	0
1	E	329/347 (94%)	0.59	37 (11%) 7 2	22, 59, 128, 144	0
1	F	333/347 (95%)	0.32	20 (6%) 25 9	23, 52, 119, 148	0
1	G	329/347 (94%)	0.42	33 (10%) 9 3	30, 61, 127, 149	0
All	All	2277/2429 (93%)	0.44	203 (8%) 12 4	22, 57, 123, 149	0

The worst 5 of 203 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	526	PHE	8.3
1	B	504	THR	7.6
1	E	512	ASN	7.4
1	A	564	ARG	7.3
1	G	483	PRO	7.0

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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	SO4	A	3	5/5	0.98	0.28	0.97	41,46,53,55	0
2	SO4	A	5	5/5	0.91	0.22	-0.70	72,75,93,93	0
2	SO4	A	2	5/5	0.96	0.12	-5.12	47,58,60,63	0
2	SO4	A	1	5/5	0.84	0.27	-	68,72,86,94	0
2	SO4	B	4	5/5	0.90	0.18	-	75,79,82,89	0

6.5 Other polymers [i](#)

There are no such residues in this entry.