



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 25, 2024 – 10:29 PM EDT

PDB ID : 6SS6  
Title : Structure of arginase-2 in complex with the inhibitory human antigen-binding fragment Fab C0020187  
Authors : Burschowsky, D.; Addyman, A.; Fiedler, S.; Groves, M.; Haynes, S.; See-wooruthun, C.; Carr, M.  
Deposited on : 2019-09-06  
Resolution : 3.25 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](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:

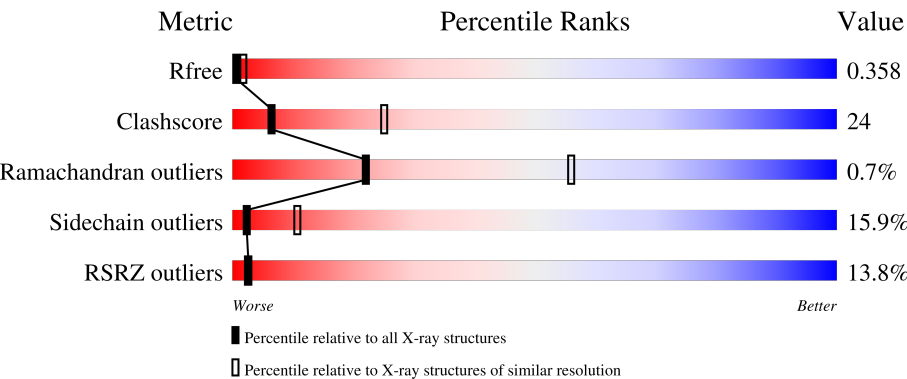
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	AAA	346	<div><div>5%</div><div>52%30%10%8%</div></div>
1	BBB	346	<div><div>4%</div><div>58%24%7%11%</div></div>
1	CCC	346	<div><div>6%</div><div>56%26%8%8%</div></div>
2	HHH	233	<div><div>6%</div><div>68%22%5%5%</div></div>
2	III	233	<div><div>14%</div><div>63%27%5%5%</div></div>

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Mol	Chain	Length	Quality of chain
2	JJJ	233	
3	LLL	220	
3	MMM	220	
3	NNN	220	

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
5	SO4	AAA	405	-	-	-	X
5	SO4	HHH	303	-	-	-	X
5	SO4	HHH	305	-	-	-	X
5	SO4	III	301	-	-	-	X
5	SO4	JJJ	301	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 33558 atoms, of which 16603 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 Arginase-2, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	AAA	318	Total	C	H	N	O	S	121	0	0
			4848	1534	2419	422	464	9			
1	BBB	308	Total	C	H	N	O	S	116	0	0
			4691	1482	2341	411	448	9			
1	CCC	317	Total	C	H	N	O	S	120	0	0
			4837	1531	2414	421	462	9			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	22	MET	-	initiating methionine	UNP P78540
AAA	355	GLY	-	expression tag	UNP P78540
AAA	356	GLY	-	expression tag	UNP P78540
AAA	357	GLY	-	expression tag	UNP P78540
AAA	358	HIS	-	expression tag	UNP P78540
AAA	359	HIS	-	expression tag	UNP P78540
AAA	360	HIS	-	expression tag	UNP P78540
AAA	361	HIS	-	expression tag	UNP P78540
AAA	362	HIS	-	expression tag	UNP P78540
AAA	363	HIS	-	expression tag	UNP P78540
AAA	364	HIS	-	expression tag	UNP P78540
AAA	365	HIS	-	expression tag	UNP P78540
AAA	366	HIS	-	expression tag	UNP P78540
AAA	367	HIS	-	expression tag	UNP P78540
BBB	22	MET	-	initiating methionine	UNP P78540
BBB	355	GLY	-	expression tag	UNP P78540
BBB	356	GLY	-	expression tag	UNP P78540
BBB	357	GLY	-	expression tag	UNP P78540
BBB	358	HIS	-	expression tag	UNP P78540
BBB	359	HIS	-	expression tag	UNP P78540
BBB	360	HIS	-	expression tag	UNP P78540
BBB	361	HIS	-	expression tag	UNP P78540
BBB	362	HIS	-	expression tag	UNP P78540

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	363	HIS	-	expression tag	UNP P78540
BBB	364	HIS	-	expression tag	UNP P78540
BBB	365	HIS	-	expression tag	UNP P78540
BBB	366	HIS	-	expression tag	UNP P78540
BBB	367	HIS	-	expression tag	UNP P78540
CCC	22	MET	-	initiating methionine	UNP P78540
CCC	355	GLY	-	expression tag	UNP P78540
CCC	356	GLY	-	expression tag	UNP P78540
CCC	357	GLY	-	expression tag	UNP P78540
CCC	358	HIS	-	expression tag	UNP P78540
CCC	359	HIS	-	expression tag	UNP P78540
CCC	360	HIS	-	expression tag	UNP P78540
CCC	361	HIS	-	expression tag	UNP P78540
CCC	362	HIS	-	expression tag	UNP P78540
CCC	363	HIS	-	expression tag	UNP P78540
CCC	364	HIS	-	expression tag	UNP P78540
CCC	365	HIS	-	expression tag	UNP P78540
CCC	366	HIS	-	expression tag	UNP P78540
CCC	367	HIS	-	expression tag	UNP P78540

- Molecule 2 is a protein called Fab C0020187 heavy chain (IgG1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	HHH	222	Total	C	H	N	O	S	93	0	0
			3267	1032	1624	280	324	7			
2	III	222	Total	C	H	N	O	S	93	0	0
			3267	1032	1624	280	324	7			
2	JJJ	218	Total	C	H	N	O	S	92	0	0
			3205	1013	1593	275	317	7			

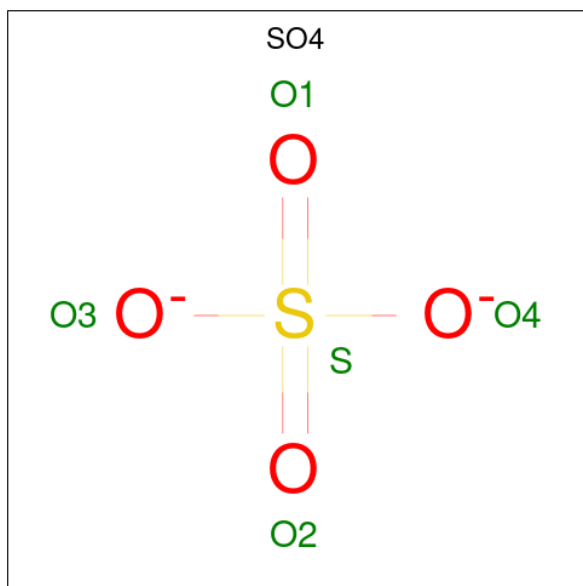
- Molecule 3 is a protein called Fab C0020187 light chain (IgG1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	LLL	214	Total	C	H	N	O	S	103	0	0
			3120	990	1538	262	326	4			
3	MMM	213	Total	C	H	N	O	S	103	0	0
			3105	985	1532	261	323	4			
3	NNN	211	Total	C	H	N	O	S	102	0	0
			3077	976	1518	259	320	4			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	AAA	2	Total	Mn	0	0
			2	2		
4	BBB	2	Total	Mn	0	0
			2	2		
4	CCC	2	Total	Mn	0	0
			2	2		

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	AAA	1	Total	O	S	0	0
			5	4	1		
5	AAA	1	Total	O	S	0	0
			5	4	1		
5	AAA	1	Total	O	S	0	0
			5	4	1		
5	BBB	1	Total	O	S	0	0
			5	4	1		
5	BBB	1	Total	O	S	0	0
			5	4	1		
5	BBB	1	Total	O	S	0	0
			5	4	1		
5	CCC	1	Total	O	S	0	0
			5	4	1		
5	CCC	1	Total	O	S	0	0
			5	4	1		
5	CCC	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	CCC	1	Total	O	S	0	0
			5	4	1		
5	CCC	1	Total	O	S	0	0
			5	4	1		
5	CCC	1	Total	O	S	0	0
			5	4	1		
5	HHH	1	Total	O	S	0	0
			5	4	1		
5	HHH	1	Total	O	S	0	0
			5	4	1		
5	HHH	1	Total	O	S	0	0
			5	4	1		
5	HHH	1	Total	O	S	0	0
			5	4	1		
5	HHH	1	Total	O	S	0	0
			5	4	1		
5	III	1	Total	O	S	0	0
			5	4	1		
5	III	1	Total	O	S	0	0
			5	4	1		
5	III	1	Total	O	S	0	0
			5	4	1		
5	III	1	Total	O	S	0	0
			5	4	1		
5	JJJ	1	Total	O	S	0	0
			5	4	1		
5	LLL	1	Total	O	S	0	0
			5	4	1		
5	LLL	1	Total	O	S	0	0
			5	4	1		
5	MMM	1	Total	O	S	0	0
			5	4	1		
5	MMM	1	Total	O	S	0	0
			5	4	1		
5	MMM	1	Total	O	S	0	0
			5	4	1		

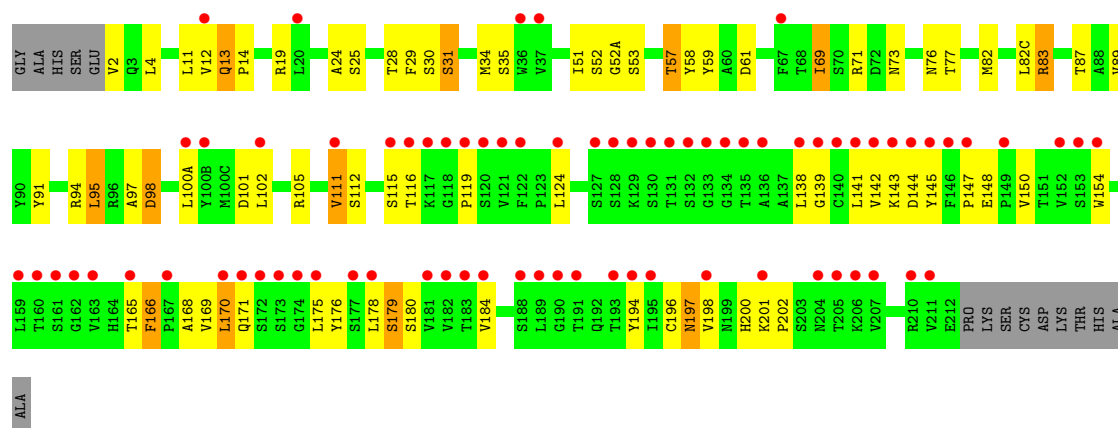


- Molecule 1: Arginase-2, mitochondrial

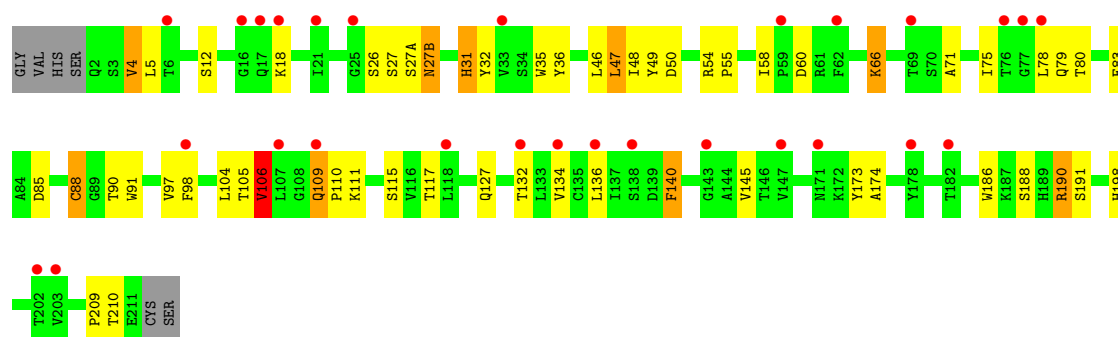
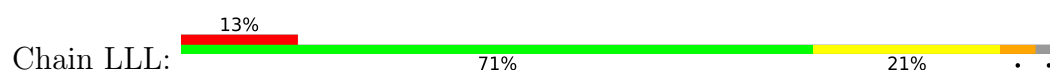




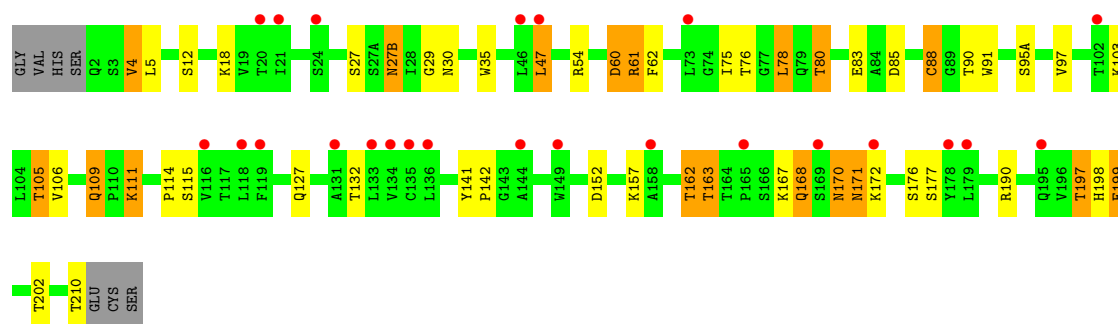
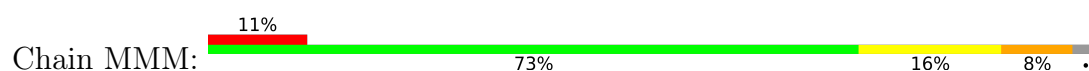




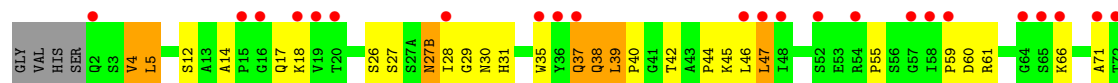
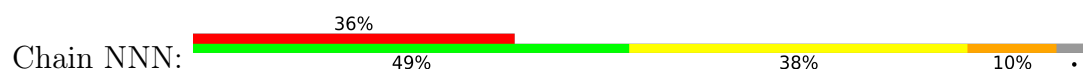
• Molecule 3: Fab C0020187 light chain (IgG1)

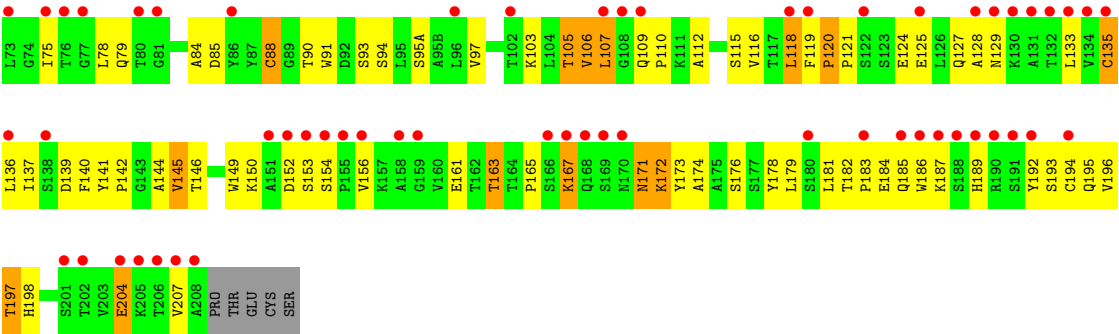


• Molecule 3: Fab C0020187 light chain (IgG1)



• Molecule 3: Fab C0020187 light chain (IgG1)





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.13Å 138.13Å 551.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.76 – 3.25 48.78 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.76-3.25) 100.0 (48.78-3.25)	Depositor EDS
$R_{merge}$	0.78	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.54 (at 3.25Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.300 , 0.361 0.298 , 0.358	Depositor DCC
$R_{free}$ test set	2549 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	87.5	Xtriage
Anisotropy	0.564	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 66.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.36$ , $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.88	EDS
Total number of atoms	33558	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.82% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, 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	AAA	0.66	0/2483	0.81	0/3380
1	BBB	0.67	0/2401	0.85	3/3265 (0.1%)
1	CCC	0.67	0/2477	0.86	1/3372 (0.0%)
2	HHH	0.68	0/1679	0.81	0/2283
2	III	0.68	0/1679	0.85	1/2283 (0.0%)
2	JJJ	0.69	0/1647	0.81	0/2240
3	LLL	0.67	0/1621	0.81	0/2216
3	MMM	0.66	0/1612	0.78	0/2204
3	NNN	0.68	0/1597	0.86	0/2182
All	All	0.67	0/17196	0.83	5/23425 (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	CCC	0	2

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	BBB	82	TYR	CB-CA-C	9.43	129.25	110.40
1	CCC	77	PRO	N-CA-CB	-8.01	93.69	103.30
2	III	213	PRO	CA-N-CD	-5.89	103.25	111.50
1	BBB	82	TYR	CA-CB-CG	5.63	124.09	113.40
1	BBB	88	ASN	CB-CA-C	5.00	120.41	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	CCC	157	GLY	Peptide
1	CCC	158	ASN	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	AAA	2429	2419	2406	148	4
1	BBB	2350	2341	2328	127	4
1	CCC	2423	2414	2399	135	0
2	HHH	1643	1624	1624	60	1
2	III	1643	1624	1624	74	1
2	JJJ	1612	1593	1590	84	0
3	LLL	1582	1538	1534	50	3
3	MMM	1573	1532	1528	35	0
3	NNN	1559	1518	1514	137	7
4	AAA	2	0	0	0	0
4	BBB	2	0	0	0	0
4	CCC	2	0	0	0	0
5	AAA	15	0	0	1	0
5	BBB	15	0	0	0	0
5	CCC	30	0	0	1	0
5	HHH	25	0	0	0	0
5	III	20	0	0	0	0
5	JJJ	5	0	0	0	0
5	LLL	10	0	0	0	0
5	MMM	15	0	0	0	0
All	All	16955	16603	16547	799	12

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 24.

The worst 5 of 799 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)
3:NNN:149:TRP:CZ3	3:NNN:194:CYS:CB	2.11	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:149:ASN:HB3	1:BBB:154:THR:CG2	1.58	1.32
1:BBB:149:ASN:CB	1:BBB:154:THR:HG21	1.62	1.30
1:CCC:88:ASN:OD1	1:CCC:89:PRO:HD3	1.41	1.19
1:AAA:150:THR:HG23	1:AAA:153:THR:HG21	1.25	1.18

The worst 5 of 12 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:76:VAL:HG12	3:NNN:95(A):SER:HG[8_555]	0.79	0.81
1:AAA:300:GLN:OE1	1:AAA:300:GLN:OE1[8_555]	1.48	0.72
1:AAA:40:LYS:HZ3	1:AAA:40:LYS:HZ3[8_555]	1.17	0.43
1:AAA:40:LYS:HZ2	1:AAA:40:LYS:HZ2[8_555]	1.20	0.40
3:LLL:188:SER:HG	3:NNN:26:SER:OG[8_545]	1.35	0.25

## 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	AAA	316/346 (91%)	287 (91%)	27 (8%)	2 (1%)	25	59
1	BBB	306/346 (88%)	278 (91%)	25 (8%)	3 (1%)	15	47
1	CCC	315/346 (91%)	282 (90%)	28 (9%)	5 (2%)	9	37
2	HHH	220/233 (94%)	206 (94%)	13 (6%)	1 (0%)	29	62
2	III	220/233 (94%)	205 (93%)	13 (6%)	2 (1%)	17	50
2	JJJ	216/233 (93%)	206 (95%)	9 (4%)	1 (0%)	29	62
3	LLL	212/220 (96%)	198 (93%)	13 (6%)	1 (0%)	29	62
3	MMM	211/220 (96%)	195 (92%)	16 (8%)	0	100	100
3	NNN	209/220 (95%)	189 (90%)	19 (9%)	1 (0%)	29	62
All	All	2225/2397 (93%)	2046 (92%)	163 (7%)	16 (1%)	22	56

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	77	PRO
1	CCC	77	PRO
1	CCC	162	GLN
2	III	56	SER
2	III	213	PRO

### 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	AAA	268/292 (92%)	219 (82%)	49 (18%)	1	7
1	BBB	258/292 (88%)	221 (86%)	37 (14%)	3	14
1	CCC	267/292 (91%)	219 (82%)	48 (18%)	1	7
2	HHH	183/190 (96%)	157 (86%)	26 (14%)	3	15
2	III	183/190 (96%)	156 (85%)	27 (15%)	3	13
2	JJJ	179/190 (94%)	158 (88%)	21 (12%)	5	21
3	LLL	179/184 (97%)	155 (87%)	24 (13%)	4	16
3	MMM	178/184 (97%)	149 (84%)	29 (16%)	2	10
3	NNN	176/184 (96%)	140 (80%)	36 (20%)	1	4
All	All	1871/1998 (94%)	1574 (84%)	297 (16%)	2	11

5 of 297 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	LLL	210	THR
3	NNN	154	SER
3	MMM	61	ARG
3	MMM	210	THR
1	CCC	81	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.



### 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 monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 33 ligands modelled in this entry, 6 are monoatomic - leaving 27 for Mogul analysis.

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	$\# Z  > 2$
5	SO4	JJJ	301	-	4,4,4	0.38	0	6,6,6	0.07	0
5	SO4	CCC	407	-	4,4,4	0.38	0	6,6,6	0.04	0
5	SO4	CCC	403	-	4,4,4	0.38	0	6,6,6	0.05	0
5	SO4	CCC	405	-	4,4,4	0.38	0	6,6,6	0.05	0
5	SO4	LLL	302	-	4,4,4	0.39	0	6,6,6	0.05	0
5	SO4	HHH	303	-	4,4,4	0.39	0	6,6,6	0.05	0
5	SO4	AAA	405	-	4,4,4	0.38	0	6,6,6	0.05	0
5	SO4	III	304	-	4,4,4	0.38	0	6,6,6	0.06	0
5	SO4	MMM	303	-	4,4,4	0.37	0	6,6,6	0.05	0
5	SO4	MMM	301	-	4,4,4	0.37	0	6,6,6	0.05	0
5	SO4	CCC	404	-	4,4,4	0.38	0	6,6,6	0.04	0
5	SO4	AAA	404	-	4,4,4	0.37	0	6,6,6	0.08	0
5	SO4	III	301	-	4,4,4	0.38	0	6,6,6	0.04	0
5	SO4	CCC	406	-	4,4,4	0.39	0	6,6,6	0.05	0
5	SO4	BBB	404	-	4,4,4	0.38	0	6,6,6	0.05	0
5	SO4	III	302	-	4,4,4	0.38	0	6,6,6	0.05	0
5	SO4	HHH	305	-	4,4,4	0.38	0	6,6,6	0.04	0
5	SO4	AAA	403	-	4,4,4	0.36	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
5	SO4	HHH	301	-	4,4,4	0.38	0	6,6,6	0.06	0
5	SO4	BBB	405	-	4,4,4	0.38	0	6,6,6	0.06	0
5	SO4	LLL	301	-	4,4,4	0.38	0	6,6,6	0.05	0
5	SO4	MMM	302	-	4,4,4	0.38	0	6,6,6	0.06	0
5	SO4	CCC	408	-	4,4,4	0.39	0	6,6,6	0.05	0
5	SO4	III	303	-	4,4,4	0.40	0	6,6,6	0.06	0
5	SO4	HHH	304	-	4,4,4	0.37	0	6,6,6	0.05	0
5	SO4	HHH	302	-	4,4,4	0.37	0	6,6,6	0.05	0
5	SO4	BBB	403	-	4,4,4	0.38	0	6,6,6	0.04	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
5	CCC	407	SO4	1	0
5	AAA	404	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	AAA	318/346 (91%)	0.43	19 (5%) 21 21	44, 91, 128, 203	0
1	BBB	308/346 (89%)	0.48	13 (4%) 36 33	50, 95, 129, 150	0
1	CCC	317/346 (91%)	0.57	22 (6%) 16 16	59, 96, 133, 215	0
2	HHH	222/233 (95%)	0.52	15 (6%) 17 16	55, 91, 154, 190	0
2	III	222/233 (95%)	0.76	33 (14%) 2 2	50, 101, 175, 204	0
2	JJJ	218/233 (93%)	1.92	76 (34%) 0 0	74, 117, 213, 245	0
3	LLL	214/220 (97%)	0.76	28 (13%) 3 3	71, 105, 128, 159	0
3	MMM	213/220 (96%)	0.60	24 (11%) 5 5	35, 111, 147, 165	0
3	NNN	211/220 (95%)	1.65	80 (37%) 0 0	87, 140, 185, 224	0
All	All	2243/2397 (93%)	0.81	310 (13%) 2 2	35, 102, 176, 245	0

The worst 5 of 310 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	JJJ	152	VAL	11.5
2	JJJ	134	GLY	10.0
2	III	137	ALA	9.4
2	JJJ	173	SER	8.6
2	JJJ	128	SER	8.1

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

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
5	SO4	AAA	405	5/5	0.40	0.42	186,188,190,191	0
5	SO4	HHH	305	5/5	0.47	0.60	178,183,184,185	0
5	SO4	CCC	405	5/5	0.48	0.38	161,163,168,170	0
5	SO4	BBB	405	5/5	0.56	0.35	175,175,179,180	0
5	SO4	CCC	407	5/5	0.57	0.31	138,141,146,155	0
5	SO4	III	304	5/5	0.58	0.28	175,175,182,186	0
5	SO4	JJJ	301	5/5	0.59	0.57	171,176,180,185	0
5	SO4	MMM	302	5/5	0.61	0.33	145,147,149,150	0
5	SO4	HHH	304	5/5	0.62	0.39	152,160,162,162	0
5	SO4	LLL	301	5/5	0.64	0.24	157,157,159,161	0
5	SO4	CCC	406	5/5	0.65	0.29	170,174,176,180	0
5	SO4	III	301	5/5	0.68	0.45	181,182,187,189	0
5	SO4	CCC	408	5/5	0.69	0.30	162,164,169,169	0
5	SO4	AAA	404	5/5	0.70	0.28	111,115,116,121	0
5	SO4	HHH	303	5/5	0.75	0.52	177,184,188,189	0
4	MN	CCC	402	1/1	0.78	0.14	121,121,121,121	0
5	SO4	III	302	5/5	0.78	0.39	129,130,132,135	0
5	SO4	HHH	302	5/5	0.79	0.27	102,103,106,107	0
5	SO4	BBB	404	5/5	0.79	0.29	152,155,156,156	0
5	SO4	MMM	303	5/5	0.79	0.30	132,133,137,138	0
5	SO4	BBB	403	5/5	0.81	0.27	155,161,163,166	0
5	SO4	III	303	5/5	0.83	0.28	140,142,146,148	0
4	MN	AAA	402	1/1	0.84	0.14	100,100,100,100	0
5	SO4	LLL	302	5/5	0.84	0.18	135,136,138,140	0
5	SO4	AAA	403	5/5	0.85	0.14	117,119,122,124	0
5	SO4	MMM	301	5/5	0.86	0.25	129,133,136,136	0
5	SO4	CCC	404	5/5	0.88	0.17	141,145,148,156	0
5	SO4	HHH	301	5/5	0.92	0.15	103,104,107,108	0
5	SO4	CCC	403	5/5	0.93	0.15	111,111,113,117	0
4	MN	BBB	401	1/1	0.95	0.18	87,87,87,87	0
4	MN	BBB	402	1/1	0.95	0.16	98,98,98,98	0
4	MN	AAA	401	1/1	0.97	0.16	75,75,75,75	0
4	MN	CCC	401	1/1	0.97	0.13	86,86,86,86	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.