



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 7, 2026 – 02:00 AM UTC

PDB ID : 6SS2 / pdb\_00006ss2  
Title : Structure of arginase-2 in complex with the inhibitory human antigen-binding fragment Fab C0021158  
Authors : Burschowsky, D.; Addyman, A.; Fiedler, S.; Groves, M.; Haynes, S.; See-wooruthun, C.; Carr, M.  
Deposited on : 2019-09-06  
Resolution : 2.40 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 : 4-5-2 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

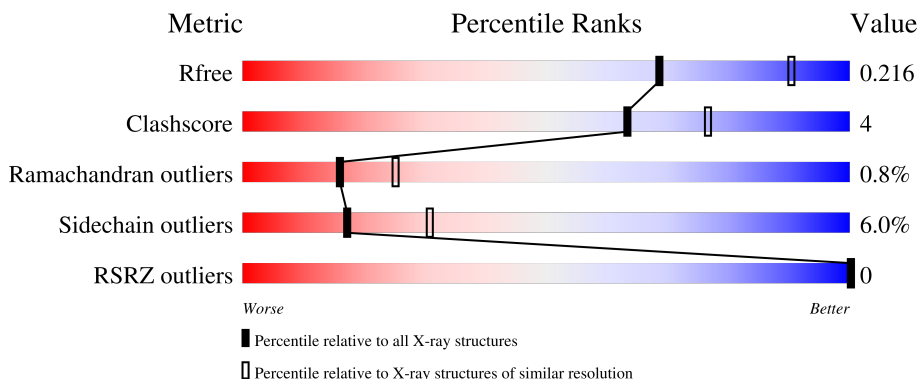
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	339	 81%      12%      • 6%
2	HHH	233	 79%      15%      • 5%
3	LLL	220	 86%      10%      • •

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 11730 atoms, of which 5784 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
			Total	C	H	N	O	S			
1	AAA	320	4884	1544	2439	424	467	10	121	0	0

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	22	MET	-	initiating methionine	UNP P78540
AAA	355	HIS	-	expression tag	UNP P78540
AAA	356	HIS	-	expression tag	UNP P78540
AAA	357	HIS	-	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

- Molecule 2 is a protein called Fab C0021158 heavy chain (IgG1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	HHH	222	3308	1047	1651	284	320	6	87	0	0

- Molecule 3 is a protein called Fab C0021158 light chain (IgG1).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	LLL	213	3112	987	1534	262	325	4	104	0	0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
4	AAA	1	14	3	8	3	2	0
4	AAA	1	14	3	8	3	2	0
4	AAA	1	14	3	8	3	2	0
4	AAA	1	14	3	8	3	2	0
4	AAA	1	14	3	8	3	2	0
4	AAA	1	14	3	8	3	2	0
4	AAA	1	14	3	8	3	2	0
4	AAA	1	14	3	8	3	2	0
4	AAA	1	14	3	8	3	2	0
4	AAA	1	14	3	8	3	2	0
4	AAA	1	14	3	8	3	2	0
4	AAA	1	14	3	8	3	2	0
4	AAA	1	14	3	8	3	2	0
4	AAA	1	14	3	8	3	2	0
4	AAA	1	14	3	8	3	2	0
4	AAA	1	14	3	8	3	2	0
4	HHH	1	14	3	8	3	2	0

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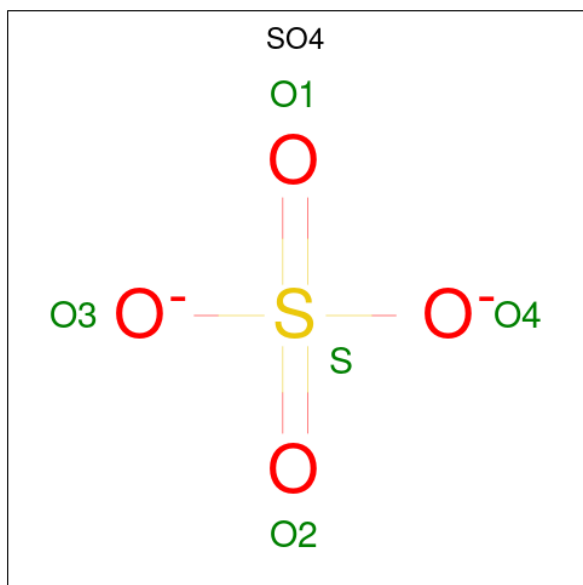
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	HHH	1	Total	C	H	O	2	0
			14	3	8	3		
4	HHH	1	Total	C	H	O	2	0
			14	3	8	3		
4	LLL	1	Total	C	H	O	2	0
			14	3	8	3		
4	LLL	1	Total	C	H	O	2	0
			14	3	8	3		
4	LLL	1	Total	C	H	O	2	0
			14	3	8	3		

- Molecule 5 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	AAA	2	Total	Mn	0	0
			2	2		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	AAA	1	Total	O	S	0	0
			5	4	1		
6	AAA	1	Total	O	S	0	0
			5	4	1		
6	AAA	1	Total	O	S	0	0
			5	4	1		
6	AAA	1	Total	O	S	0	0
			5	4	1		
6	AAA	1	Total	O	S	0	0
			5	4	1		
6	AAA	1	Total	O	S	0	0
			5	4	1		
6	HHH	1	Total	O	S	0	0
			5	4	1		
6	HHH	1	Total	O	S	0	0
			5	4	1		
6	LLL	1	Total	O	S	0	0
			5	4	1		
6	LLL	1	Total	O	S	0	0
			5	4	1		
6	LLL	1	Total	O	S	0	0
			5	4	1		
6	LLL	1	Total	O	S	0	0
			5	4	1		
6	LLL	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

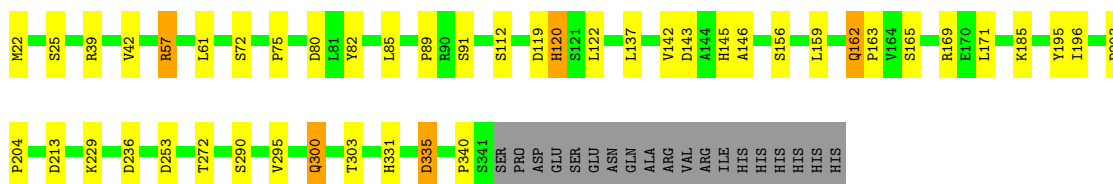
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	AAA	36	Total	O	0	0
			36	36		
7	HHH	11	Total	O	0	0
			11	11		
7	LLL	12	Total	O	0	0
			12	12		

### 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.

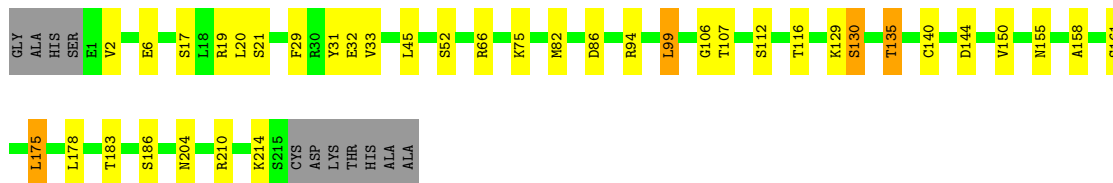
- Molecule 1: Arginase-2, mitochondrial

Chain AAA:  81% 12% • 6%




- Molecule 2: Fab C0021158 heavy chain (IgG1)

Chain HHH:  79% 15% • 5%



- Molecule 3: Fab C0021158 light chain (IgG1)

Chain LLL:  86% 10% • •



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.06Å 149.06Å 123.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.37 – 2.40 45.37 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (45.37-2.40) 89.9 (45.37-2.40)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.93 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, $R_{free}$	0.254 , 0.284 0.184 , 0.216	Depositor DCC
$R_{free}$ test set	1976 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	41.1	Xtriage
Anisotropy	0.174	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 26.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.165 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.801 for H, K, L 0.199 for K, H, -L	Depositor
Outliers	0 of 39902 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11730	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.12% 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: MN, GOL, SO4, CSO

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	1.04	0/2491	1.43	4/3388 (0.1%)
2	HHH	1.06	0/1695	1.32	1/2307 (0.0%)
3	LLL	1.03	0/1616	1.31	2/2210 (0.1%)
All	All	1.04	0/5802	1.37	7/7905 (0.1%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	AAA	253	ASP	CA-CB-CG	7.39	120.00	112.60
2	HHH	106	GLY	CA-C-O	-6.34	117.85	122.23
1	AAA	119	ASP	CA-CB-CG	6.05	118.65	112.60
1	AAA	80	ASP	CA-CB-CG	5.90	118.50	112.60
1	AAA	57	ARG	CG-CD-NE	-5.55	99.78	112.00

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	2445	2439	2423	23	0
2	HHH	1657	1651	1651	16	0
3	LLL	1578	1534	1530	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	AAA	78	104	104	2	0
4	HHH	18	24	24	0	0
4	LLL	24	32	32	1	0
5	AAA	2	0	0	0	0
6	AAA	45	0	0	1	0
6	HHH	10	0	0	1	0
6	LLL	30	0	0	0	0
7	AAA	36	0	0	1	0
7	HHH	11	0	0	0	0
7	LLL	12	0	0	0	0
All	All	5946	5784	5764	46	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.

The worst 5 of 46 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)
2:HHH:45:LEU:O	3:LLL:2:GLN:HG3	1.92	0.69
1:AAA:39:ARG:O	1:AAA:42:VAL:HG12	1.96	0.65
1:AAA:57:ARG:NH1	7:AAA:501:HOH:O	2.31	0.64
1:AAA:335:ASP:OD2	1:AAA:335:ASP:N	2.31	0.63
1:AAA:85:LEU:HD21	2:HHH:33:VAL:HG21	1.83	0.61

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	AAA	317/339 (94%)	308 (97%)	7 (2%)	2 (1%)	21 32
2	HHH	220/233 (94%)	201 (91%)	16 (7%)	3 (1%)	9 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	LLL	211/220 (96%)	199 (94%)	11 (5%)	1 (0%)	24	37
All	All	748/792 (94%)	708 (95%)	34 (4%)	6 (1%)	16	25

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	HHH	2	VAL
3	LLL	3	SER
2	HHH	116	THR
2	HHH	130	SER
1	AAA	162	GLN

### 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	AAA	269/287 (94%)	254 (94%)	15 (6%)	19	33
2	HHH	183/190 (96%)	167 (91%)	16 (9%)	9	16
3	LLL	178/184 (97%)	171 (96%)	7 (4%)	28	48
All	All	630/661 (95%)	592 (94%)	38 (6%)	17	31

5 of 38 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	HHH	204	ASN
3	LLL	167	LYS
2	HHH	210	ARG
3	LLL	18	LYS
3	LLL	205	LYS

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

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
1	CSO	AAA	134	1	3,6,7	0.84	0	1,6,8	0.36	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
1	CSO	AAA	134	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 39 ligands modelled in this entry, 2 are monoatomic - leaving 37 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
6	SO4	AAA	416	-	4,4,4	0.33	0	6,6,6	0.11	0
4	GOL	AAA	401	-	5,5,5	0.10	0	5,5,5	0.30	0
4	GOL	LLL	304	-	5,5,5	0.09	0	5,5,5	0.26	0
6	SO4	LLL	306	-	4,4,4	0.32	0	6,6,6	0.07	0
6	SO4	LLL	305	-	4,4,4	0.32	0	6,6,6	0.10	0
4	GOL	AAA	411	-	5,5,5	0.11	0	5,5,5	0.25	0
6	SO4	AAA	418	-	4,4,4	0.32	0	6,6,6	0.10	0
4	GOL	HHH	303	-	5,5,5	0.09	0	5,5,5	0.27	0
4	GOL	AAA	405	-	5,5,5	0.08	0	5,5,5	0.28	0
4	GOL	AAA	408	-	5,5,5	0.11	0	5,5,5	0.29	0
4	GOL	AAA	410	-	5,5,5	0.11	0	5,5,5	0.33	0
6	SO4	AAA	419	-	4,4,4	0.35	0	6,6,6	0.08	0
4	GOL	AAA	406	-	5,5,5	0.09	0	5,5,5	0.26	0
4	GOL	AAA	403	-	5,5,5	0.09	0	5,5,5	0.26	0
4	GOL	LLL	303	-	5,5,5	0.13	0	5,5,5	0.37	0
6	SO4	LLL	308	-	4,4,4	0.32	0	6,6,6	0.06	0
4	GOL	AAA	402	-	5,5,5	0.08	0	5,5,5	0.25	0
6	SO4	AAA	422	5	4,4,4	0.29	0	6,6,6	0.08	0
4	GOL	HHH	301	-	5,5,5	0.10	0	5,5,5	0.37	0
6	SO4	AAA	423	-	4,4,4	0.33	0	6,6,6	0.07	0
4	GOL	AAA	412	-	5,5,5	0.12	0	5,5,5	0.39	0
6	SO4	AAA	421	-	4,4,4	0.32	0	6,6,6	0.09	0
4	GOL	AAA	404	-	5,5,5	0.14	0	5,5,5	0.40	0
4	GOL	LLL	301	-	5,5,5	0.09	0	5,5,5	0.29	0
6	SO4	AAA	420	-	4,4,4	0.33	0	6,6,6	0.07	0
6	SO4	HHH	305	-	4,4,4	0.32	0	6,6,6	0.08	0
4	GOL	AAA	407	-	5,5,5	0.09	0	5,5,5	0.25	0
6	SO4	LLL	310	-	4,4,4	0.34	0	6,6,6	0.08	0
4	GOL	LLL	302	-	5,5,5	0.10	0	5,5,5	0.27	0
6	SO4	AAA	417	-	4,4,4	0.32	0	6,6,6	0.07	0
4	GOL	HHH	302	-	5,5,5	0.10	0	5,5,5	0.26	0
6	SO4	LLL	309	-	4,4,4	0.33	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	SO4	HHH	304	-	4,4,4	0.34	0	6,6,6	0.08	0
4	GOL	AAA	409	-	5,5,5	0.10	0	5,5,5	0.32	0
6	SO4	LLL	307	-	4,4,4	0.32	0	6,6,6	0.07	0
4	GOL	AAA	413	-	5,5,5	0.10	0	5,5,5	0.28	0
6	SO4	AAA	424	-	4,4,4	0.32	0	6,6,6	0.07	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
4	GOL	AAA	401	-	-	2/4/4/4	-
4	GOL	LLL	304	-	-	1/4/4/4	-
4	GOL	AAA	411	-	-	2/4/4/4	-
4	GOL	HHH	303	-	-	1/4/4/4	-
4	GOL	AAA	405	-	-	2/4/4/4	-
4	GOL	AAA	408	-	-	0/4/4/4	-
4	GOL	AAA	410	-	-	2/4/4/4	-
4	GOL	AAA	406	-	-	2/4/4/4	-
4	GOL	AAA	403	-	-	2/4/4/4	-
4	GOL	LLL	303	-	-	2/4/4/4	-
4	GOL	AAA	402	-	-	2/4/4/4	-
4	GOL	HHH	301	-	-	4/4/4/4	-
4	GOL	AAA	412	-	-	4/4/4/4	-
4	GOL	AAA	404	-	-	2/4/4/4	-
4	GOL	LLL	301	-	-	0/4/4/4	-
4	GOL	AAA	407	-	-	2/4/4/4	-
4	GOL	LLL	302	-	-	0/4/4/4	-
4	GOL	HHH	302	-	-	2/4/4/4	-
4	GOL	AAA	409	-	-	4/4/4/4	-
4	GOL	AAA	413	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	401	GOL	C1-C2-C3-O3
4	AAA	402	GOL	C1-C2-C3-O3
4	AAA	403	GOL	O1-C1-C2-C3
4	AAA	407	GOL	O1-C1-C2-C3
4	AAA	409	GOL	O1-C1-C2-O2

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	AAA	418	SO4	1	0
4	AAA	402	GOL	1	0
4	AAA	404	GOL	1	0
4	LLL	302	GOL	1	0
6	HHH	304	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	319/339 (94%)	-1.27	0 100 100	30, 41, 62, 102	0
2	HHH	222/233 (95%)	-1.11	0 100 100	40, 60, 94, 112	0
3	LLL	213/220 (96%)	-1.30	0 100 100	36, 50, 62, 72	0
All	All	754/792 (95%)	-1.23	0 100 100	30, 48, 82, 112	0

There are no RSRZ outliers to report.

### 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSO	AAA	134	7/8	1.00	0.02	20,43,44,44	1

### 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, 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( $\text{\AA}^2$ )	Q<0.9
4	GOL	AAA	411	6/6	0.91	0.09	30,78,79,80	2
4	GOL	AAA	406	6/6	0.92	0.11	30,83,86,86	2
4	GOL	AAA	410	6/6	0.95	0.09	30,61,65,66	2
4	GOL	AAA	407	6/6	0.95	0.07	30,76,79,79	2
4	GOL	AAA	409	6/6	0.96	0.19	30,60,61,62	2
4	GOL	LLL	304	6/6	0.96	0.05	30,74,77,77	2
6	SO4	HHH	305	5/5	0.96	0.05	83,87,92,94	0
4	GOL	AAA	408	6/6	0.97	0.06	30,73,74,74	2
4	GOL	AAA	412	6/6	0.97	0.08	30,61,62,62	2
4	GOL	HHH	301	6/6	0.97	0.07	30,57,58,59	2
4	GOL	HHH	302	6/6	0.97	0.05	30,83,84,84	2
4	GOL	HHH	303	6/6	0.97	0.06	30,64,66,66	2
4	GOL	LLL	301	6/6	0.97	0.08	30,89,90,91	2
4	GOL	LLL	303	6/6	0.97	0.09	30,52,53,53	2
4	GOL	AAA	401	6/6	0.97	0.08	30,59,60,60	2
6	SO4	AAA	419	5/5	0.97	0.05	82,85,86,86	0
6	SO4	AAA	424	5/5	0.97	0.05	84,88,89,89	0
4	GOL	AAA	403	6/6	0.97	0.05	30,72,73,75	2
4	GOL	AAA	402	6/6	0.98	0.06	30,64,66,70	2
6	SO4	AAA	416	5/5	0.98	0.08	54,56,59,60	0
6	SO4	AAA	418	5/5	0.98	0.08	68,69,75,78	0
4	GOL	AAA	404	6/6	0.98	0.10	30,42,45,45	2
4	GOL	LLL	302	6/6	0.98	0.06	30,63,65,66	2
4	GOL	AAA	405	6/6	0.98	0.08	30,78,79,80	2
6	SO4	LLL	306	5/5	0.98	0.04	78,83,84,85	0
6	SO4	LLL	307	5/5	0.98	0.04	74,77,81,82	0
6	SO4	LLL	308	5/5	0.98	0.07	75,76,82,82	0
6	SO4	LLL	309	5/5	0.98	0.04	81,81,84,84	0
6	SO4	LLL	310	5/5	0.98	0.04	93,99,101,102	0
6	SO4	AAA	417	5/5	0.99	0.04	56,57,61,62	0
6	SO4	LLL	305	5/5	0.99	0.04	65,66,67,67	0
6	SO4	AAA	420	5/5	0.99	0.02	80,81,87,88	0
6	SO4	AAA	421	5/5	0.99	0.03	76,79,83,86	0
6	SO4	AAA	423	5/5	0.99	0.04	88,89,90,91	0
4	GOL	AAA	413	6/6	0.99	0.05	30,69,71,71	2
6	SO4	HHH	304	5/5	0.99	0.03	60,66,66,68	0
5	MN	AAA	415	1/1	1.00	0.02	44,44,44,44	0
6	SO4	AAA	422	5/5	1.00	0.03	62,72,80,82	0
5	MN	AAA	414	1/1	1.00	0.01	47,47,47,47	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.