Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2020 – 07:31 AM BST

PDB ID	:	6SS2
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.; Seewooruthun, C.; Carr, M.
Deposited on	:	2019-09-06
Resolution	:	2.40 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 following versions of software and data (see references ⓘ) were used in the production of this report:

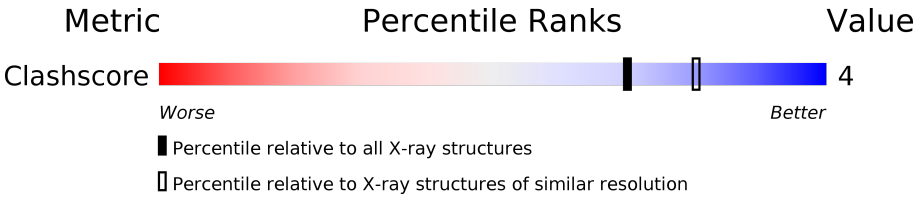
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

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 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))
Clashscore	141614	4398 (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 on 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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	AAA	339	86% 9% 6%
2	HHH	233	88% 8% 5%
3	LLL	220	90% 7% .

2 Entry composition

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
1	AAA	320	Total	C	H	N	O	S	121	0	0
			4884	1544	2439	424	467	10			

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

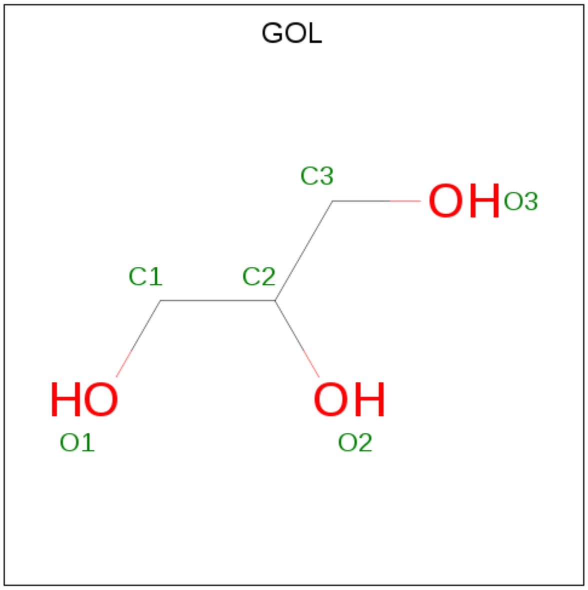
- Molecule 2 is a protein called Fab C0021158 heavy chain (IgG1).

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

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

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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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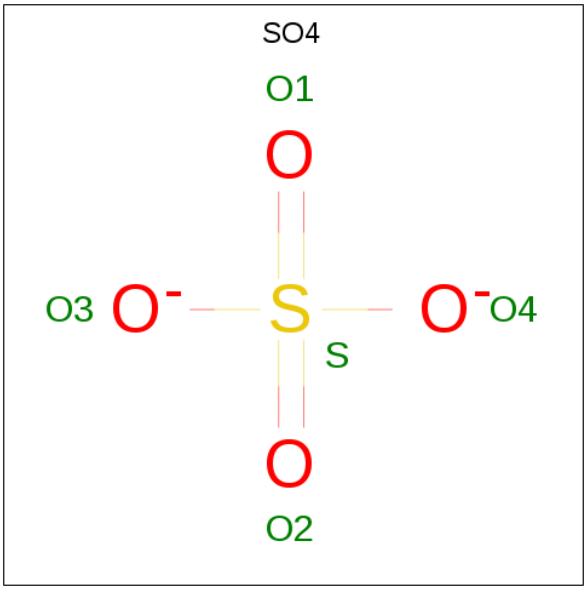
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	HHH	1	Total	C	H	O	2	0
			14	3	8	3		
4	HHH	1	Total	C	H	O	2	0
			14	3	8	3		
4	LLL	1	Total	C	H	O	2	0
			14	3	8	3		
4	LLL	1	Total	C	H	O	2	0
			14	3	8	3		
4	LLL	1	Total	C	H	O	2	0
			14	3	8	3		
4	LLL	1	Total	C	H	O	2	0
			14	3	8	3		

- Molecule 5 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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 5 4 1	0	0
6	AAA	1	Total O S 5 4 1	0	0
6	AAA	1	Total O S 5 4 1	0	0
6	AAA	1	Total O S 5 4 1	0	0
6	AAA	1	Total O S 5 4 1	0	0
6	AAA	1	Total O S 5 4 1	0	0
6	AAA	1	Total O S 5 4 1	0	0
6	HHH	1	Total O S 5 4 1	0	0
6	HHH	1	Total O S 5 4 1	0	0
6	LLL	1	Total O S 5 4 1	0	0
6	LLL	1	Total O S 5 4 1	0	0
6	LLL	1	Total O S 5 4 1	0	0
6	LLL	1	Total O S 5 4 1	0	0
6	LLL	1	Total O S 5 4 1	0	0
6	LLL	1	Total O S 5 4 1	0	0

- Molecule 7 is water.

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

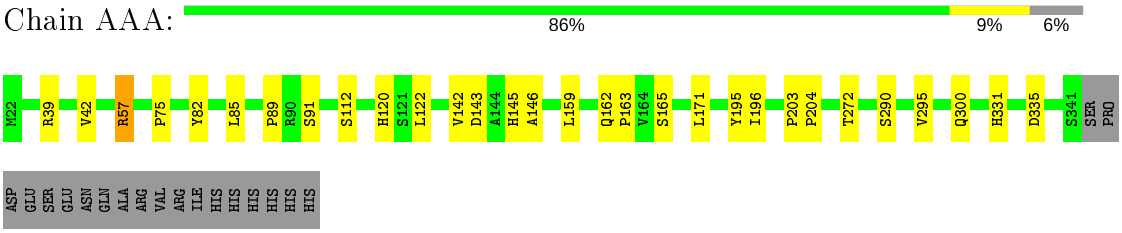
3 Residue-property plots (i)

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. 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. 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.

Note EDS failed to run properly.

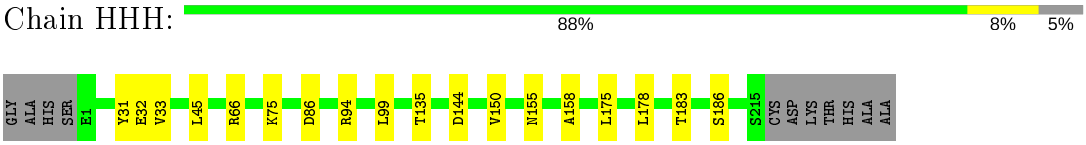
- Molecule 1: Arginase-2, mitochondrial

Chain AAA:



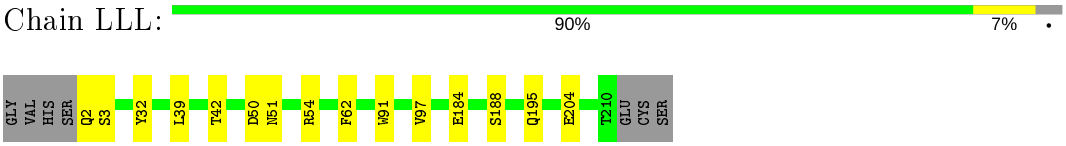
- Molecule 2: Fab C0021158 heavy chain (IgG1)

Chain HHH:



- Molecule 3: Fab C0021158 light chain (IgG1)

Chain LLL:



4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	149.06Å 149.06Å 123.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.37 – 2.40	Depositor
% Data completeness (in resolution range)	99.9 (45.37-2.40)	Depositor
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.93 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.254 , 0.284	Depositor
Wilson B-factor (Å^2)	41.1	Xtriage
Anisotropy	0.174	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	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
Total number of atoms	11730	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, CSO, 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	0.69	0/2491	0.82	1/3388 (0.0%)
2	HHH	0.68	0/1695	0.79	0/2307
3	LLL	0.67	0/1616	0.80	0/2210
All	All	0.68	0/5802	0.80	1/7905 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	AAA	57	ARG	CG-CD-NE	-5.72	99.78	111.80

There are no chirality outliers.

There are no planarity outliers.

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	2445	2439	2423	23	0
2	HHH	1657	1651	1651	13	0
3	LLL	1578	1534	1530	12	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	42	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 (42) 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
2:HHH:32:GLU:HG2	2:HHH:94:ARG:HD2	1.82	0.60
1:AAA:272:THR:HG21	4:AAA:404:GOL:H31	1.84	0.59
1:AAA:162:GLN:N	1:AAA:163:PRO:CD	2.68	0.56
3:LLL:2:GLN:NE2	3:LLL:97:VAL:HA	2.22	0.55
3:LLL:2:GLN:OE1	3:LLL:3:SER:N	2.38	0.54
3:LLL:54:ARG:NH2	3:LLL:62:PHE:O	2.42	0.53
3:LLL:195:GLN:NE2	3:LLL:204:GLU:OE1	2.41	0.51
2:HHH:135:THR:CG2	2:HHH:183:THR:HG22	2.40	0.50
2:HHH:75:LYS:NZ	6:HHH:304:SO4:O2	2.45	0.49
2:HHH:144:ASP:HB3	2:HHH:175:LEU:HD23	1.94	0.48
1:AAA:331:HIS:HB3	4:AAA:402:GOL:H2	1.95	0.48
1:AAA:165:SER:HA	1:AAA:171:LEU:HD23	1.97	0.47
2:HHH:150:VAL:CG1	2:HHH:178:LEU:HD21	2.45	0.47
1:AAA:122:LEU:HD12	1:AAA:122:LEU:C	2.35	0.47
1:AAA:300:GLN:HB3	2:HHH:31:TYR:HB3	1.97	0.46
1:AAA:75:PRO:HA	1:AAA:91:SER:OG	2.16	0.46
1:AAA:89:PRO:HB3	1:AAA:159:LEU:HD11	2.00	0.44
1:AAA:120:HIS:CG	1:AAA:295:VAL:HG21	2.52	0.44
3:LLL:184:GLU:O	3:LLL:188:SER:HB2	2.18	0.44
1:AAA:162:GLN:H	1:AAA:163:PRO:CD	2.30	0.44
1:AAA:112:SER:HA	1:AAA:290:SER:O	2.18	0.43
1:AAA:162:GLN:N	1:AAA:163:PRO:HD2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:LLL:51:ASN:HD21	4:LLL:302:GOL:H32	1.83	0.43
2:HHH:155:ASN:HB2	2:HHH:158:ALA:HB3	2.01	0.43
2:HHH:66:ARG:NH1	2:HHH:86:ASP:OD1	2.44	0.42
1:AAA:82:TYR:HB2	3:LLL:91:TRP:CE2	2.55	0.42
2:HHH:135:THR:HA	2:HHH:186:SER:OG	2.19	0.42
2:HHH:99:LEU:HB3	3:LLL:32:TYR:CZ	2.55	0.42
3:LLL:39:LEU:O	3:LLL:42:THR:OG1	2.31	0.41
1:AAA:39:ARG:NE	6:AAA:418:SO4:O3	2.53	0.41
1:AAA:143:ASP:HB3	1:AAA:145:HIS:O	2.20	0.41
1:AAA:146:ALA:HA	1:AAA:195:TYR:CE1	2.55	0.41
1:AAA:203:PRO:N	1:AAA:204:PRO:HD2	2.36	0.41
2:HHH:99:LEU:HB3	3:LLL:32:TYR:CE2	2.57	0.40
1:AAA:162:GLN:O	1:AAA:163:PRO:C	2.60	0.40
1:AAA:142:VAL:HA	1:AAA:196:ILE:O	2.21	0.40
3:LLL:32:TYR:HB3	3:LLL:50:ASP:HA	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains (i)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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	0.83	0	0,6,8	0.00	-

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
4	GOL	AAA	413	-	5,5,5	0.10	0	5,5,5	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	SO4	LLL	305	-	4,4,4	0.37	0	6,6,6	0.07	0
4	GOL	AAA	408	-	5,5,5	0.12	0	5,5,5	0.29	0
4	GOL	AAA	401	-	5,5,5	0.10	0	5,5,5	0.31	0
6	SO4	AAA	421	-	4,4,4	0.37	0	6,6,6	0.06	0
6	SO4	LLL	306	-	4,4,4	0.36	0	6,6,6	0.06	0
6	SO4	AAA	418	-	4,4,4	0.36	0	6,6,6	0.08	0
4	GOL	HHH	302	-	5,5,5	0.10	0	5,5,5	0.27	0
6	SO4	HHH	304	-	4,4,4	0.39	0	6,6,6	0.06	0
4	GOL	AAA	404	-	5,5,5	0.14	0	5,5,5	0.40	0
4	GOL	AAA	403	-	5,5,5	0.09	0	5,5,5	0.27	0
6	SO4	AAA	419	-	4,4,4	0.38	0	6,6,6	0.05	0
4	GOL	AAA	406	-	5,5,5	0.09	0	5,5,5	0.27	0
4	GOL	AAA	402	-	5,5,5	0.09	0	5,5,5	0.26	0
4	GOL	HHH	301	-	5,5,5	0.10	0	5,5,5	0.37	0
6	SO4	LLL	310	-	4,4,4	0.39	0	6,6,6	0.06	0
4	GOL	LLL	301	-	5,5,5	0.09	0	5,5,5	0.30	0
6	SO4	AAA	416	-	4,4,4	0.37	0	6,6,6	0.07	0
4	GOL	AAA	409	-	5,5,5	0.11	0	5,5,5	0.33	0
4	GOL	AAA	405	-	5,5,5	0.08	0	5,5,5	0.29	0
4	GOL	LLL	303	-	5,5,5	0.13	0	5,5,5	0.37	0
4	GOL	AAA	412	-	5,5,5	0.13	0	5,5,5	0.39	0
6	SO4	AAA	417	-	4,4,4	0.37	0	6,6,6	0.06	0
6	SO4	AAA	422	5	4,4,4	0.33	0	6,6,6	0.08	0
4	GOL	AAA	407	-	5,5,5	0.10	0	5,5,5	0.27	0
4	GOL	AAA	410	-	5,5,5	0.12	0	5,5,5	0.33	0
4	GOL	LLL	302	-	5,5,5	0.10	0	5,5,5	0.28	0
6	SO4	LLL	307	-	4,4,4	0.36	0	6,6,6	0.05	0
6	SO4	AAA	423	-	4,4,4	0.37	0	6,6,6	0.05	0
4	GOL	HHH	303	-	5,5,5	0.10	0	5,5,5	0.28	0
6	SO4	AAA	424	-	4,4,4	0.36	0	6,6,6	0.05	0
6	SO4	LLL	308	-	4,4,4	0.37	0	6,6,6	0.06	0
6	SO4	HHH	305	-	4,4,4	0.36	0	6,6,6	0.06	0
6	SO4	AAA	420	-	4,4,4	0.37	0	6,6,6	0.04	0
4	GOL	LLL	304	-	5,5,5	0.10	0	5,5,5	0.27	0
4	GOL	AAA	411	-	5,5,5	0.11	0	5,5,5	0.26	0
6	SO4	LLL	309	-	4,4,4	0.37	0	6,6,6	0.05	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	LLL	302	-	-	0/4/4/4	-
4	GOL	AAA	413	-	-	2/4/4/4	-
4	GOL	HHH	303	-	-	1/4/4/4	-
4	GOL	AAA	405	-	-	1/4/4/4	-
4	GOL	AAA	408	-	-	0/4/4/4	-
4	GOL	LLL	303	-	-	2/4/4/4	-
4	GOL	AAA	401	-	-	2/4/4/4	-
4	GOL	AAA	412	-	-	4/4/4/4	-
4	GOL	AAA	406	-	-	2/4/4/4	-
4	GOL	LLL	304	-	-	1/4/4/4	-
4	GOL	AAA	402	-	-	2/4/4/4	-
4	GOL	HHH	301	-	-	4/4/4/4	-
4	GOL	AAA	403	-	-	2/4/4/4	-
4	GOL	LLL	301	-	-	0/4/4/4	-
4	GOL	AAA	404	-	-	2/4/4/4	-
4	GOL	AAA	407	-	-	2/4/4/4	-
4	GOL	HHH	302	-	-	2/4/4/4	-
4	GOL	AAA	411	-	-	2/4/4/4	-
4	GOL	AAA	409	-	-	4/4/4/4	-
4	GOL	AAA	410	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	AAA	413	GOL	C1-C2-C3-O3
4	AAA	401	GOL	C1-C2-C3-O3
4	AAA	403	GOL	O1-C1-C2-C3
4	AAA	402	GOL	C1-C2-C3-O3
4	HHH	301	GOL	C1-C2-C3-O3
4	HHH	301	GOL	O2-C2-C3-O3
4	AAA	409	GOL	O1-C1-C2-O2
4	AAA	409	GOL	O1-C1-C2-C3
4	LLL	303	GOL	C1-C2-C3-O3
4	AAA	407	GOL	O1-C1-C2-C3
4	AAA	411	GOL	C1-C2-C3-O3
4	LLL	303	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	HHH	302	GOL	O1-C1-C2-C3
4	AAA	404	GOL	O1-C1-C2-C3
4	AAA	406	GOL	O1-C1-C2-C3
4	HHH	301	GOL	O1-C1-C2-C3
4	AAA	409	GOL	C1-C2-C3-O3
4	AAA	412	GOL	C1-C2-C3-O3
4	AAA	410	GOL	C1-C2-C3-O3
4	LLL	304	GOL	O1-C1-C2-C3
4	AAA	401	GOL	O2-C2-C3-O3
4	AAA	404	GOL	O1-C1-C2-O2
4	AAA	403	GOL	O1-C1-C2-O2
4	AAA	402	GOL	O2-C2-C3-O3
4	AAA	411	GOL	O2-C2-C3-O3
4	AAA	413	GOL	O2-C2-C3-O3
4	HHH	302	GOL	O1-C1-C2-O2
4	AAA	406	GOL	O1-C1-C2-O2
4	HHH	301	GOL	O1-C1-C2-O2
4	AAA	409	GOL	O2-C2-C3-O3
4	AAA	412	GOL	O1-C1-C2-O2
4	AAA	407	GOL	O1-C1-C2-O2
4	AAA	410	GOL	O2-C2-C3-O3
4	AAA	405	GOL	O1-C1-C2-C3
4	AAA	412	GOL	O1-C1-C2-C3
4	AAA	412	GOL	O2-C2-C3-O3
4	HHH	303	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
6	HHH	304	SO4	1	0
4	AAA	404	GOL	1	0
4	AAA	402	GOL	1	0
4	LLL	302	GOL	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.