



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 10:53 pm BST

PDB ID : 3TFO  
Title : Crystal structure of a putative 3-oxoacyl-(acyl-carrier-protein) reductase from *Sinorhizobium meliloti*  
Authors : Agarwal, R.; Chamala, S.; Evans, B.; Foti, R.; Gizzi, A.; Hillerich, B.; Kar, A.; LaFleur, J.; Seidel, R.; Villigas, G.; Zencheck, W.; Almo, S.C.; Swaminathan, S.; New York Structural Genomics Research Consortium (NYSGRG)  
Deposited on : 2011-08-16  
Resolution : 2.08 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](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.

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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 : 2.11  
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) : 2.11

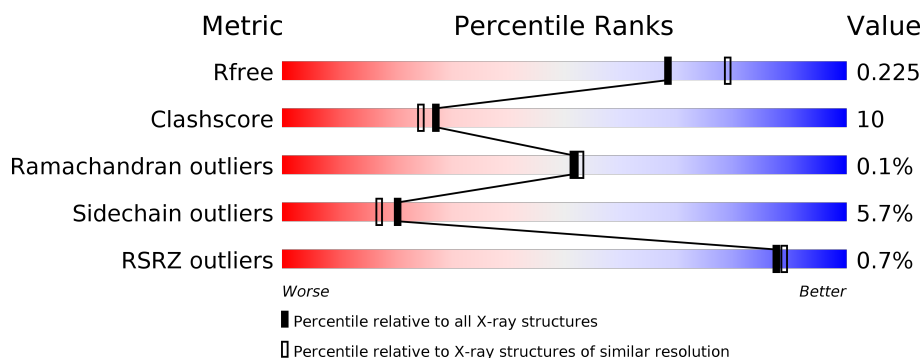
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.08 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	6189 (2.10-2.06)
Clashscore	141614	6738 (2.10-2.06)
Ramachandran outliers	138981	6663 (2.10-2.06)
Sidechain outliers	138945	6664 (2.10-2.06)
RSRZ outliers	127900	6057 (2.10-2.06)

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  $\geq 3$ , 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	A	264	
1	B	264	
1	C	264	
1	D	264	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6839 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 putative 3-oxoacyl-(acyl-carrier-protein) reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	216	Total	C	N	O	S	0	0	0
			1552	975	276	295	6			
1	B	215	Total	C	N	O	S	0	0	0
			1542	969	274	293	6			
1	C	216	Total	C	N	O	S	0	0	0
			1559	977	281	296	5			
1	D	218	Total	C	N	O	S	0	0	0
			1564	982	279	297	6			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q92XI4
A	2	VAL	-	EXPRESSION TAG	UNP Q92XI4
A	243	ALA	-	EXPRESSION TAG	UNP Q92XI4
A	244	GLU	-	EXPRESSION TAG	UNP Q92XI4
A	245	ASN	-	EXPRESSION TAG	UNP Q92XI4
A	246	LEU	-	EXPRESSION TAG	UNP Q92XI4
A	247	TYR	-	EXPRESSION TAG	UNP Q92XI4
A	248	PHE	-	EXPRESSION TAG	UNP Q92XI4
A	249	GLN	-	EXPRESSION TAG	UNP Q92XI4
A	250	SER	-	EXPRESSION TAG	UNP Q92XI4
A	251	HIS	-	EXPRESSION TAG	UNP Q92XI4
A	252	HIS	-	EXPRESSION TAG	UNP Q92XI4
A	253	HIS	-	EXPRESSION TAG	UNP Q92XI4
A	254	HIS	-	EXPRESSION TAG	UNP Q92XI4
A	255	HIS	-	EXPRESSION TAG	UNP Q92XI4
A	256	HIS	-	EXPRESSION TAG	UNP Q92XI4
A	257	TRP	-	EXPRESSION TAG	UNP Q92XI4
A	258	SER	-	EXPRESSION TAG	UNP Q92XI4
A	259	HIS	-	EXPRESSION TAG	UNP Q92XI4
A	260	PRO	-	EXPRESSION TAG	UNP Q92XI4
A	261	GLN	-	EXPRESSION TAG	UNP Q92XI4

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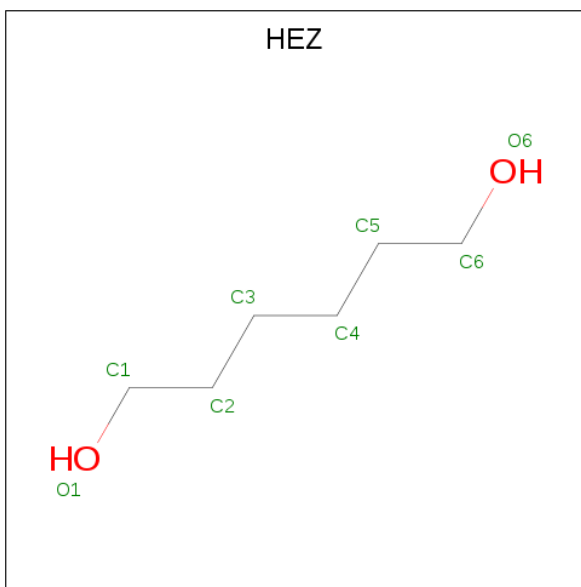
Chain	Residue	Modelled	Actual	Comment	Reference
A	262	PHE	-	EXPRESSION TAG	UNP Q92XI4
A	263	GLU	-	EXPRESSION TAG	UNP Q92XI4
A	264	LYS	-	EXPRESSION TAG	UNP Q92XI4
B	1	MET	-	EXPRESSION TAG	UNP Q92XI4
B	2	VAL	-	EXPRESSION TAG	UNP Q92XI4
B	243	ALA	-	EXPRESSION TAG	UNP Q92XI4
B	244	GLU	-	EXPRESSION TAG	UNP Q92XI4
B	245	ASN	-	EXPRESSION TAG	UNP Q92XI4
B	246	LEU	-	EXPRESSION TAG	UNP Q92XI4
B	247	TYR	-	EXPRESSION TAG	UNP Q92XI4
B	248	PHE	-	EXPRESSION TAG	UNP Q92XI4
B	249	GLN	-	EXPRESSION TAG	UNP Q92XI4
B	250	SER	-	EXPRESSION TAG	UNP Q92XI4
B	251	HIS	-	EXPRESSION TAG	UNP Q92XI4
B	252	HIS	-	EXPRESSION TAG	UNP Q92XI4
B	253	HIS	-	EXPRESSION TAG	UNP Q92XI4
B	254	HIS	-	EXPRESSION TAG	UNP Q92XI4
B	255	HIS	-	EXPRESSION TAG	UNP Q92XI4
B	256	HIS	-	EXPRESSION TAG	UNP Q92XI4
B	257	TRP	-	EXPRESSION TAG	UNP Q92XI4
B	258	SER	-	EXPRESSION TAG	UNP Q92XI4
B	259	HIS	-	EXPRESSION TAG	UNP Q92XI4
B	260	PRO	-	EXPRESSION TAG	UNP Q92XI4
B	261	GLN	-	EXPRESSION TAG	UNP Q92XI4
B	262	PHE	-	EXPRESSION TAG	UNP Q92XI4
B	263	GLU	-	EXPRESSION TAG	UNP Q92XI4
B	264	LYS	-	EXPRESSION TAG	UNP Q92XI4
C	1	MET	-	EXPRESSION TAG	UNP Q92XI4
C	2	VAL	-	EXPRESSION TAG	UNP Q92XI4
C	243	ALA	-	EXPRESSION TAG	UNP Q92XI4
C	244	GLU	-	EXPRESSION TAG	UNP Q92XI4
C	245	ASN	-	EXPRESSION TAG	UNP Q92XI4
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C	249	GLN	-	EXPRESSION TAG	UNP Q92XI4
C	250	SER	-	EXPRESSION TAG	UNP Q92XI4
C	251	HIS	-	EXPRESSION TAG	UNP Q92XI4
C	252	HIS	-	EXPRESSION TAG	UNP Q92XI4
C	253	HIS	-	EXPRESSION TAG	UNP Q92XI4
C	254	HIS	-	EXPRESSION TAG	UNP Q92XI4
C	255	HIS	-	EXPRESSION TAG	UNP Q92XI4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	256	HIS	-	EXPRESSION TAG	UNP Q92XI4
C	257	TRP	-	EXPRESSION TAG	UNP Q92XI4
C	258	SER	-	EXPRESSION TAG	UNP Q92XI4
C	259	HIS	-	EXPRESSION TAG	UNP Q92XI4
C	260	PRO	-	EXPRESSION TAG	UNP Q92XI4
C	261	GLN	-	EXPRESSION TAG	UNP Q92XI4
C	262	PHE	-	EXPRESSION TAG	UNP Q92XI4
C	263	GLU	-	EXPRESSION TAG	UNP Q92XI4
C	264	LYS	-	EXPRESSION TAG	UNP Q92XI4
D	1	MET	-	EXPRESSION TAG	UNP Q92XI4
D	2	VAL	-	EXPRESSION TAG	UNP Q92XI4
D	243	ALA	-	EXPRESSION TAG	UNP Q92XI4
D	244	GLU	-	EXPRESSION TAG	UNP Q92XI4
D	245	ASN	-	EXPRESSION TAG	UNP Q92XI4
D	246	LEU	-	EXPRESSION TAG	UNP Q92XI4
D	247	TYR	-	EXPRESSION TAG	UNP Q92XI4
D	248	PHE	-	EXPRESSION TAG	UNP Q92XI4
D	249	GLN	-	EXPRESSION TAG	UNP Q92XI4
D	250	SER	-	EXPRESSION TAG	UNP Q92XI4
D	251	HIS	-	EXPRESSION TAG	UNP Q92XI4
D	252	HIS	-	EXPRESSION TAG	UNP Q92XI4
D	253	HIS	-	EXPRESSION TAG	UNP Q92XI4
D	254	HIS	-	EXPRESSION TAG	UNP Q92XI4
D	255	HIS	-	EXPRESSION TAG	UNP Q92XI4
D	256	HIS	-	EXPRESSION TAG	UNP Q92XI4
D	257	TRP	-	EXPRESSION TAG	UNP Q92XI4
D	258	SER	-	EXPRESSION TAG	UNP Q92XI4
D	259	HIS	-	EXPRESSION TAG	UNP Q92XI4
D	260	PRO	-	EXPRESSION TAG	UNP Q92XI4
D	261	GLN	-	EXPRESSION TAG	UNP Q92XI4
D	262	PHE	-	EXPRESSION TAG	UNP Q92XI4
D	263	GLU	-	EXPRESSION TAG	UNP Q92XI4
D	264	LYS	-	EXPRESSION TAG	UNP Q92XI4

- Molecule 2 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	C	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

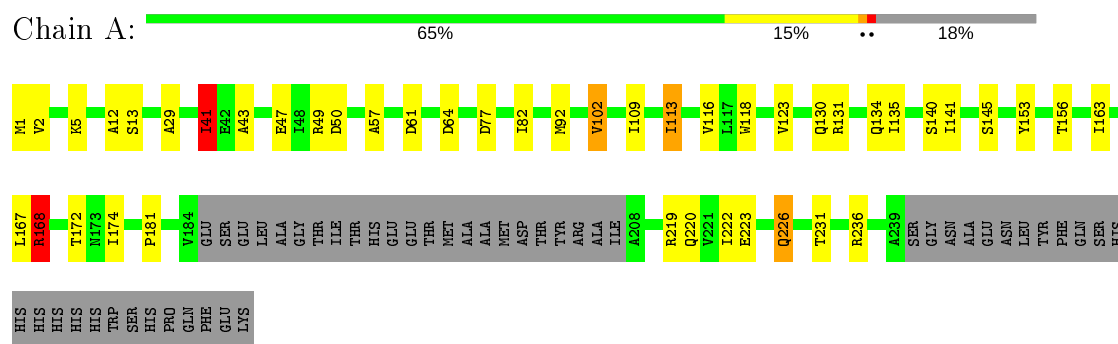
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	142	Total	O	0	0
			142	142		
4	B	137	Total	O	0	0
			137	137		
4	C	152	Total	O	0	0
			152	152		
4	D	120	Total	O	0	0
			120	120		

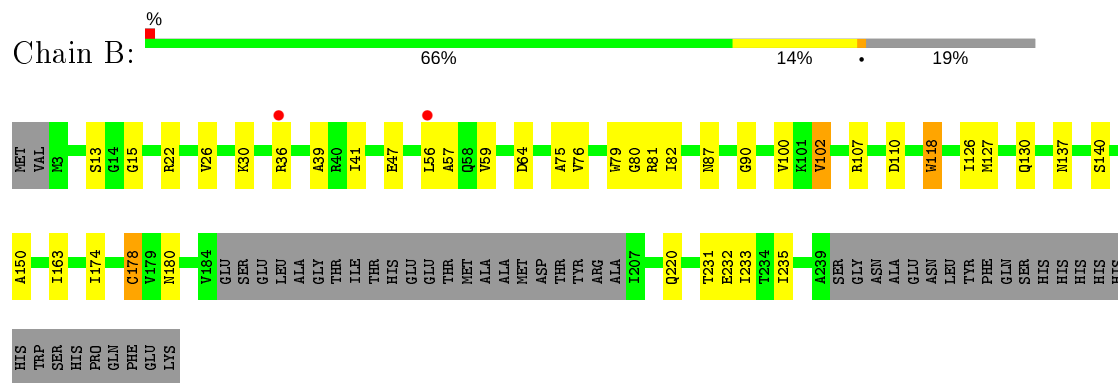
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

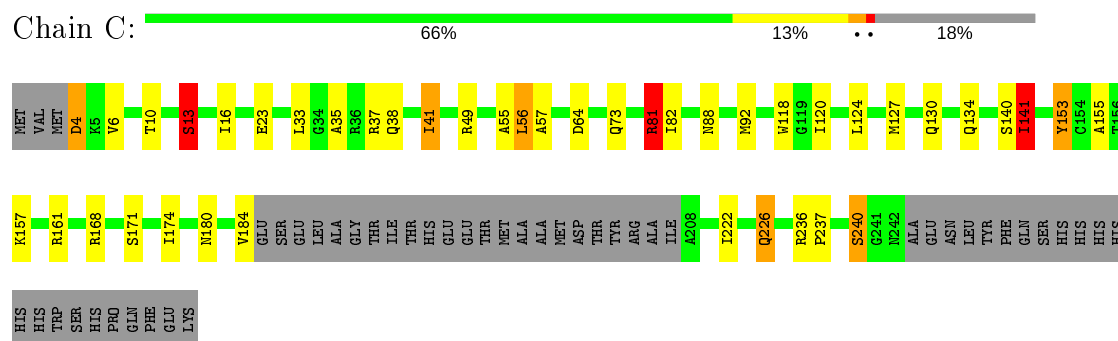
- Molecule 1: putative 3-oxoacyl-(acyl-carrier-protein) reductase



- Molecule 1: putative 3-oxoacyl-(acyl-carrier-protein) reductase

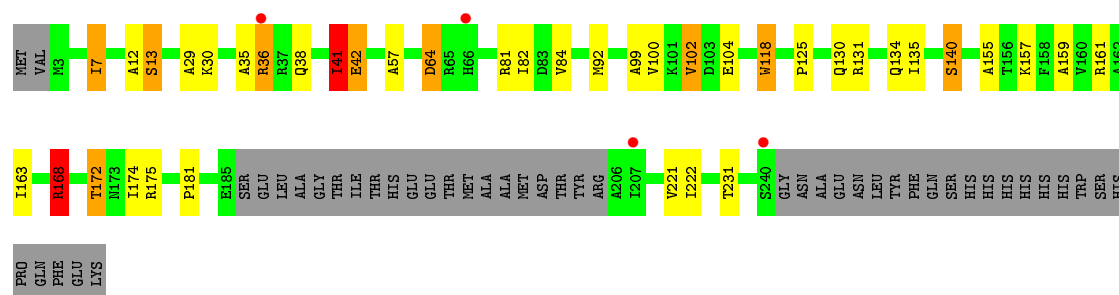


- Molecule 1: putative 3-oxoacyl-(acyl-carrier-protein) reductase





- Chain D:  2% 67% 11% . . 17%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	108.55Å 108.55Å 207.31Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.08 – 2.08 48.08 – 2.08	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.08-2.08) 99.8 (48.08-2.08)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.26 (at 2.08Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.176 , 0.219 0.182 , 0.225	Depositor DCC
$R_{free}$ test set	4270 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.2	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 52.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.016 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	6839	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: SO4, HEZ

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	1.38	3/1568 (0.2%)	1.02	5/2137 (0.2%)
1	B	1.38	6/1558 (0.4%)	1.06	4/2124 (0.2%)
1	C	1.34	5/1575 (0.3%)	1.08	7/2146 (0.3%)
1	D	1.36	4/1580 (0.3%)	1.07	9/2154 (0.4%)
All	All	1.36	18/6281 (0.3%)	1.06	25/8561 (0.3%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	4	ASP	CA-CB	-5.86	1.41	1.53
1	B	13	SER	CB-OG	-5.80	1.34	1.42
1	B	178	CYS	CB-SG	-5.73	1.72	1.81
1	B	26	VAL	CB-CG2	-5.52	1.41	1.52
1	C	6	VAL	CB-CG2	5.50	1.64	1.52
1	B	150	ALA	CA-CB	5.46	1.64	1.52
1	A	102	VAL	CB-CG1	-5.43	1.41	1.52
1	D	221	VAL	CB-CG2	5.42	1.64	1.52
1	C	23	GLU	CG-CD	5.33	1.59	1.51
1	C	153	TYR	CD2-CE2	5.33	1.47	1.39
1	A	123	VAL	CB-CG2	5.27	1.64	1.52
1	B	81	ARG	CB-CG	-5.24	1.38	1.52
1	D	172	THR	CB-CG2	-5.23	1.35	1.52
1	D	99	ALA	CA-CB	5.21	1.63	1.52
1	D	104	GLU	CD-OE1	5.16	1.31	1.25
1	B	75	ALA	CA-CB	5.12	1.63	1.52
1	C	13	SER	CB-OG	-5.08	1.35	1.42
1	A	116	VAL	CB-CG1	-5.04	1.42	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	ILE	CA-CB-CG2	5.98	122.87	110.90
1	A	113	ILE	CA-CB-CG1	5.88	122.18	111.00
1	D	102	VAL	CG1-CB-CG2	5.86	120.27	110.90
1	B	81	ARG	CB-CA-C	-5.77	98.86	110.40
1	A	64	ASP	CB-CG-OD1	5.75	123.47	118.30
1	C	41	ILE	CA-CB-CG2	5.75	122.40	110.90
1	A	61	ASP	CB-CG-OD1	5.67	123.41	118.30
1	B	110	ASP	CB-CG-OD1	5.63	123.37	118.30
1	C	141	ILE	CA-CB-CG2	5.53	121.97	110.90
1	B	81	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	C	41	ILE	N-CA-CB	-5.52	98.11	110.80
1	D	30	LYS	CD-CE-NZ	-5.49	99.08	111.70
1	D	168	ARG	CG-CD-NE	5.41	123.16	111.80
1	C	64	ASP	CB-CG-OD1	5.41	123.17	118.30
1	D	41	ILE	CA-CB-CG2	5.30	121.51	110.90
1	D	172	THR	N-CA-CB	-5.30	100.24	110.30
1	D	161	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	D	172	THR	CA-CB-CG2	5.28	119.79	112.40
1	C	81	ARG	CB-CA-C	-5.25	99.90	110.40
1	D	64	ASP	CB-CG-OD2	5.24	123.01	118.30
1	D	102	VAL	CA-CB-CG1	5.13	118.59	110.90
1	A	168	ARG	CG-CD-NE	5.09	122.48	111.80
1	B	90	GLY	N-CA-C	-5.08	100.39	113.10
1	C	49	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	C	168	ARG	NE-CZ-NH1	-5.04	117.78	120.30

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	A	1552	0	1599	36	0
1	B	1542	0	1585	28	0
1	C	1559	0	1610	35	0
1	D	1564	0	1608	33	0
2	A	8	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	8	0	14	0	0
3	A	15	0	0	1	0
3	B	15	0	0	1	0
3	C	15	0	0	1	0
3	D	10	0	0	1	0
4	A	142	0	0	10	0
4	B	137	0	0	8	0
4	C	152	0	0	5	0
4	D	120	0	0	3	0
All	All	6839	0	6430	128	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 10.

All (128) 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:D:36:ARG:HH11	1:D:36:ARG:HG3	1.03	1.13
4:A:560:HOH:O	1:B:231:THR:HG21	1.50	1.07
1:A:1:MET:O	1:A:5:LYS:HE2	1.61	1.00
1:D:36:ARG:HH11	1:D:36:ARG:CG	1.76	0.98
1:A:41:ILE:HG23	1:A:57:ALA:HB1	1.53	0.91
1:D:36:ARG:HG3	1:D:36:ARG:NH1	1.84	0.88
1:C:92:MET:HE3	1:C:153:TYR:CZ	2.09	0.88
1:A:113:ILE:HD11	1:A:156:THR:HA	1.55	0.87
1:A:2:VAL:HG23	1:A:223:GLU:CG	2.07	0.85
1:C:73:GLN:HG2	4:C:312:HOH:O	1.79	0.81
1:C:41:ILE:HG22	1:C:57:ALA:HB1	1.64	0.80
1:C:92:MET:HE2	1:C:153:TYR:CE2	2.18	0.78
1:C:92:MET:CE	1:C:153:TYR:CE2	2.66	0.78
1:B:178:CYS:HB3	4:B:434:HOH:O	1.82	0.77
1:A:219:ARG:NH2	3:A:266:SO4:O3	2.20	0.75
1:C:4:ASP:CB	4:C:470:HOH:O	2.35	0.75
1:C:41:ILE:CG2	1:C:57:ALA:HB1	2.17	0.74
1:D:100:VAL:HG12	1:D:100:VAL:O	1.88	0.73
1:D:131:ARG:HD2	4:D:682:HOH:O	1.88	0.73
1:C:82:ILE:H	1:C:130:GLN:HE22	1.37	0.73
1:B:82:ILE:H	1:B:130:GLN:HE22	1.39	0.70
1:A:2:VAL:HG23	1:A:223:GLU:HG3	1.73	0.69
1:C:81:ARG:HG2	1:C:81:ARG:NH1	2.08	0.69
1:D:41:ILE:CG2	1:D:57:ALA:HB1	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:SER:HB3	4:A:302:HOH:O	1.94	0.67
1:A:2:VAL:HG23	1:A:223:GLU:HG2	1.75	0.67
1:A:113:ILE:HD11	1:A:156:THR:CA	2.23	0.67
1:B:102:VAL:HG22	1:D:118:TRP:CZ3	2.30	0.67
1:C:134:GLN:HE22	1:C:222:ILE:HA	1.59	0.66
1:A:77:ASP:HB3	4:A:349:HOH:O	1.96	0.66
1:C:35:ALA:HB3	1:C:41:ILE:HG13	1.77	0.66
1:B:100:VAL:HG12	4:B:268:HOH:O	1.95	0.65
1:C:81:ARG:HG2	1:C:81:ARG:HH11	1.61	0.64
1:A:226:GLN:HG2	4:A:319:HOH:O	1.97	0.64
1:B:178:CYS:CB	4:B:434:HOH:O	2.41	0.64
1:A:82:ILE:H	1:A:130:GLN:HE22	1.45	0.64
1:A:220:GLN:NE2	2:A:265:HEZ:H21	2.12	0.63
1:A:77:ASP:CB	4:A:349:HOH:O	2.47	0.63
1:B:36:ARG:O	1:B:59:VAL:HG23	1.99	0.63
1:A:1:MET:O	1:A:5:LYS:CE	2.43	0.60
1:A:50:ASP:HB2	4:A:391:HOH:O	2.02	0.60
1:D:134:GLN:HE22	1:D:222:ILE:HA	1.67	0.59
1:D:41:ILE:HG23	1:D:57:ALA:HB1	1.84	0.59
1:A:43:ALA:O	1:A:47:GLU:HG3	2.02	0.58
1:D:36:ARG:CG	1:D:36:ARG:NH1	2.47	0.58
1:C:37:ARG:CB	4:C:382:HOH:O	2.51	0.58
1:C:33:LEU:HB3	1:C:41:ILE:HD12	1.85	0.57
1:B:100:VAL:O	1:B:100:VAL:HG12	2.05	0.57
4:B:384:HOH:O	1:D:125:PRO:HG3	2.04	0.57
1:B:22:ARG:NH2	1:B:47:GLU:OE1	2.29	0.56
1:D:82:ILE:H	1:D:130:GLN:HE22	1.52	0.56
1:A:49:ARG:NH2	4:A:446:HOH:O	2.39	0.55
1:A:77:ASP:CG	4:A:349:HOH:O	2.46	0.54
1:C:35:ALA:CB	1:C:41:ILE:HG13	2.38	0.53
1:C:13:SER:HB2	3:C:266:SO4:O4	2.08	0.53
1:D:41:ILE:HG22	1:D:57:ALA:HB1	1.89	0.53
1:C:92:MET:HE3	1:C:153:TYR:CE2	2.34	0.53
1:B:87:ASN:HB2	1:B:137:ASN:HD22	1.73	0.53
1:A:134:GLN:HE22	1:A:222:ILE:HA	1.73	0.52
1:D:131:ARG:CD	4:D:682:HOH:O	2.54	0.52
1:A:168:ARG:HD3	1:A:231:THR:HG21	1.93	0.51
1:B:107:ARG:HD3	4:B:278:HOH:O	2.10	0.51
1:A:226:GLN:CG	4:A:319:HOH:O	2.55	0.51
1:B:56:LEU:HD23	4:B:335:HOH:O	2.12	0.50
1:B:30:LYS:HD3	1:B:79:TRP:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:GLN:HG2	4:C:332:HOH:O	2.11	0.49
1:C:55:ALA:O	1:C:56:LEU:HD23	2.13	0.49
1:B:127:MET:HB3	1:B:174:ILE:HD12	1.93	0.49
1:D:13:SER:HB2	3:D:265:SO4:O3	2.12	0.49
1:A:130:GLN:O	1:A:131:ARG:HB2	2.13	0.48
1:B:178:CYS:SG	4:B:434:HOH:O	2.59	0.48
1:B:127:MET:HB3	1:B:174:ILE:CD1	2.44	0.48
1:A:92:MET:HG3	1:A:153:TYR:CD1	2.48	0.47
1:A:2:VAL:HG12	1:A:29:ALA:HB2	1.95	0.47
1:C:127:MET:HB3	1:C:174:ILE:CD1	2.45	0.47
1:C:127:MET:HB3	1:C:174:ILE:HD12	1.97	0.47
1:C:81:ARG:CG	1:C:81:ARG:HH11	2.27	0.47
1:D:100:VAL:O	1:D:100:VAL:CG1	2.61	0.46
1:C:10:THR:O	1:C:88:ASN:HB3	2.15	0.46
1:D:35:ALA:HB3	1:D:41:ILE:HG12	1.97	0.46
1:D:38:GLN:HE21	1:D:42:GLU:HG3	1.81	0.46
1:D:140:SER:HA	1:D:181:PRO:HD2	1.97	0.46
1:D:157:LYS:HA	1:D:157:LYS:HD2	1.60	0.46
1:C:120:ILE:O	1:C:124:LEU:HB2	2.16	0.45
1:D:12:ALA:C	1:D:41:ILE:HD11	2.36	0.45
1:D:168:ARG:HD2	1:D:168:ARG:HH11	1.66	0.45
1:B:102:VAL:HG22	1:D:118:TRP:HZ3	1.81	0.45
1:A:50:ASP:CB	4:A:391:HOH:O	2.63	0.45
1:D:64:ASP:C	1:D:64:ASP:OD1	2.55	0.45
1:B:64:ASP:OD1	1:B:64:ASP:C	2.54	0.45
1:B:39:ALA:N	3:B:266:SO4:O3	2.46	0.44
1:B:232:GLU:HG3	4:B:325:HOH:O	2.17	0.44
1:C:140:SER:HB3	1:C:157:LYS:HG3	1.99	0.44
1:C:41:ILE:HG23	1:C:57:ALA:HB1	1.97	0.44
1:D:118:TRP:HA	1:D:118:TRP:CE3	2.53	0.43
1:A:13:SER:HA	1:A:41:ILE:CD1	2.48	0.43
1:C:141:ILE:HG12	1:C:236:ARG:NH1	2.33	0.43
2:A:265:HEZ:H51	1:B:220:GLN:NE2	2.33	0.43
1:B:233:ILE:HG22	1:B:235:ILE:HG13	2.01	0.43
1:B:180:ASN:ND2	1:B:232:GLU:OE2	2.50	0.43
1:D:118:TRP:HA	1:D:118:TRP:HE3	1.83	0.43
1:B:41:ILE:HD12	1:B:57:ALA:HB1	2.01	0.43
1:C:161:ARG:HD3	1:C:161:ARG:HH11	1.71	0.42
1:A:2:VAL:CG2	1:A:223:GLU:HG3	2.45	0.42
1:A:13:SER:HA	1:A:41:ILE:HD12	2.02	0.42
1:B:118:TRP:CE3	1:B:118:TRP:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ILE:HD12	1:A:236:ARG:CZ	2.50	0.41
1:B:118:TRP:HA	1:B:118:TRP:HE3	1.84	0.41
1:B:76:VAL:O	1:B:80:GLY:HA2	2.20	0.41
1:C:140:SER:H	1:C:180:ASN:HD22	1.69	0.41
1:D:36:ARG:HH11	1:D:36:ARG:CB	2.31	0.41
1:D:159:ALA:O	1:D:163:ILE:HG12	2.21	0.41
1:D:7:ILE:HG13	1:D:29:ALA:HB1	2.01	0.41
1:C:237:PRO:O	1:C:240:SER:HB2	2.21	0.41
1:A:12:ALA:C	1:A:41:ILE:HD11	2.41	0.41
1:D:100:VAL:HG12	4:D:321:HOH:O	2.20	0.41
1:A:135:ILE:HD12	1:A:167:LEU:HD21	2.03	0.41
1:A:2:VAL:O	1:A:2:VAL:HG12	2.21	0.40
1:A:163:ILE:HG13	1:C:155:ALA:HB2	2.02	0.40
1:B:163:ILE:HG13	1:D:155:ALA:HB2	2.02	0.40
1:A:141:ILE:HG23	1:A:141:ILE:HD12	1.80	0.40
1:C:16:ILE:HD11	1:C:184:VAL:HG21	2.03	0.40
1:C:41:ILE:HA	1:C:41:ILE:HD13	1.77	0.40
1:C:4:ASP:N	4:C:661:HOH:O	2.54	0.40
1:D:7:ILE:HD13	1:D:84:VAL:HB	2.03	0.40
1:A:140:SER:HA	1:A:181:PRO:HD2	2.03	0.40
1:C:236:ARG:HD3	1:C:236:ARG:HH11	1.74	0.40
1:D:134:GLN:HA	1:D:175:ARG:O	2.21	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	212/264 (80%)	207 (98%)	5 (2%)	0	100	100
1	B	211/264 (80%)	207 (98%)	3 (1%)	1 (0%)	29	25
1	C	212/264 (80%)	208 (98%)	4 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	214/264 (81%)	209 (98%)	5 (2%)	0	100	100
All	All	849/1056 (80%)	831 (98%)	17 (2%)	1 (0%)	51	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	15	GLY

### 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	158/204 (78%)	150 (95%)	8 (5%)	24	21
1	B	156/204 (76%)	152 (97%)	4 (3%)	46	49
1	C	159/204 (78%)	150 (94%)	9 (6%)	20	17
1	D	158/204 (78%)	143 (90%)	15 (10%)	8	5
All	All	631/816 (77%)	595 (94%)	36 (6%)	20	17

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	ILE
1	A	102	VAL
1	A	109	ILE
1	A	118	TRP
1	A	168	ARG
1	A	172	THR
1	A	174	ILE
1	A	226	GLN
1	B	102	VAL
1	B	118	TRP
1	B	126	ILE
1	B	140	SER
1	C	13	SER

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Mol	Chain	Res	Type
1	C	38	GLN
1	C	56	LEU
1	C	81	ARG
1	C	118	TRP
1	C	141	ILE
1	C	171	SER
1	C	226	GLN
1	C	240	SER
1	D	7	ILE
1	D	13	SER
1	D	36	ARG
1	D	41	ILE
1	D	42	GLU
1	D	81	ARG
1	D	92	MET
1	D	102	VAL
1	D	118	TRP
1	D	135	ILE
1	D	140	SER
1	D	168	ARG
1	D	172	THR
1	D	174	ILE
1	D	231	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	A	87	ASN
1	A	130	GLN
1	A	134	GLN
1	A	220	GLN
1	B	87	ASN
1	B	130	GLN
1	B	137	ASN
1	B	169	GLN
1	B	173	ASN
1	B	220	GLN
1	C	87	ASN
1	C	130	GLN
1	C	134	GLN
1	C	180	ASN

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Mol	Chain	Res	Type
1	D	38	GLN
1	D	87	ASN
1	D	130	GLN
1	D	134	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

13 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	$\# Z  > 2$
3	SO4	C	267	-	4,4,4	0.40	0	6,6,6	0.31	0
2	HEZ	A	265	-	7,7,7	1.08	1 (14%)	6,6,6	0.97	0
2	HEZ	C	265	-	7,7,7	0.52	0	6,6,6	1.09	1 (16%)
3	SO4	B	265	-	4,4,4	0.50	0	6,6,6	1.00	0
3	SO4	D	265	-	4,4,4	0.30	0	6,6,6	0.77	0
3	SO4	C	268	-	4,4,4	0.68	0	6,6,6	0.83	0
3	SO4	B	266	-	4,4,4	0.38	0	6,6,6	0.32	0
3	SO4	A	268	-	4,4,4	0.36	0	6,6,6	0.72	0
3	SO4	A	266	-	4,4,4	1.21	0	6,6,6	1.90	1 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	C	266	-	4,4,4	0.24	0	6,6,6	1.18	1 (16%)
3	SO4	B	267	-	4,4,4	0.76	0	6,6,6	1.49	1 (16%)
3	SO4	A	267	-	4,4,4	0.16	0	6,6,6	0.45	0
3	SO4	D	266	-	4,4,4	0.19	0	6,6,6	0.61	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	HEZ	A	265	-	-	3/5/5/5	-
2	HEZ	C	265	-	-	1/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	265	HEZ	O1-C1	2.13	1.53	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	266	SO4	O4-S-O3	-4.21	91.11	109.06
3	B	267	SO4	O4-S-O3	-2.60	97.98	109.06
2	C	265	HEZ	C5-C4-C3	-2.24	103.03	114.42
3	C	266	SO4	O4-S-O3	2.11	118.07	109.06

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	265	HEZ	C2-C3-C4-C5
2	A	265	HEZ	O1-C1-C2-C3
2	C	265	HEZ	O1-C1-C2-C3
2	A	265	HEZ	C3-C4-C5-C6

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	265	HEZ	2	0
3	D	265	SO4	1	0
3	B	266	SO4	1	0
3	A	266	SO4	1	0
3	C	266	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	A	216/264 (81%)	-0.48	0 <a href="#">100</a> <a href="#">100</a>	20, 30, 45, 56	0
1	B	215/264 (81%)	-0.53	2 (0%) <a href="#">84</a> <a href="#">86</a>	23, 31, 43, 55	0
1	C	216/264 (81%)	-0.59	0 <a href="#">100</a> <a href="#">100</a>	20, 29, 42, 57	0
1	D	218/264 (82%)	-0.41	4 (1%) <a href="#">68</a> <a href="#">71</a>	22, 31, 46, 58	0
All	All	865/1056 (81%)	-0.50	6 (0%) <a href="#">87</a> <a href="#">89</a>	20, 30, 44, 58	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	66	HIS	2.9
1	D	207	ILE	2.8
1	B	36	ARG	2.7
1	D	240	SER	2.7
1	B	56	LEU	2.1
1	D	36	ARG	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 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. 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
3	SO4	B	267	5/5	0.71	0.26	69,69,77,78	0
3	SO4	D	265	5/5	0.85	0.15	39,40,45,45	5
3	SO4	B	266	5/5	0.89	0.26	83,85,86,86	0
3	SO4	D	266	5/5	0.91	0.15	50,52,54,55	5
3	SO4	C	267	5/5	0.92	0.13	41,44,47,48	5
2	HEZ	A	265	8/8	0.92	0.21	40,42,47,49	0
2	HEZ	C	265	8/8	0.94	0.20	35,42,52,53	0
3	SO4	C	266	5/5	0.94	0.18	32,35,37,39	5
3	SO4	A	268	5/5	0.96	0.25	33,35,37,39	5
3	SO4	A	266	5/5	0.97	0.14	29,38,43,45	1
3	SO4	B	265	5/5	0.98	0.35	30,35,36,36	5
3	SO4	A	267	5/5	0.99	0.07	42,45,48,51	0
3	SO4	C	268	5/5	0.99	0.11	47,48,52,57	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.