



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:27 PM GMT

PDB ID : 3RBM  
Title : Crystal structure of Plasmodium vivax geranylgeranylpyrophosphate synthase complexed with BPH -703  
Authors : Liu, Y.L.; No, J.H.; Oldfield, E.  
Deposited on : 2011-03-29  
Resolution : 2.61 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

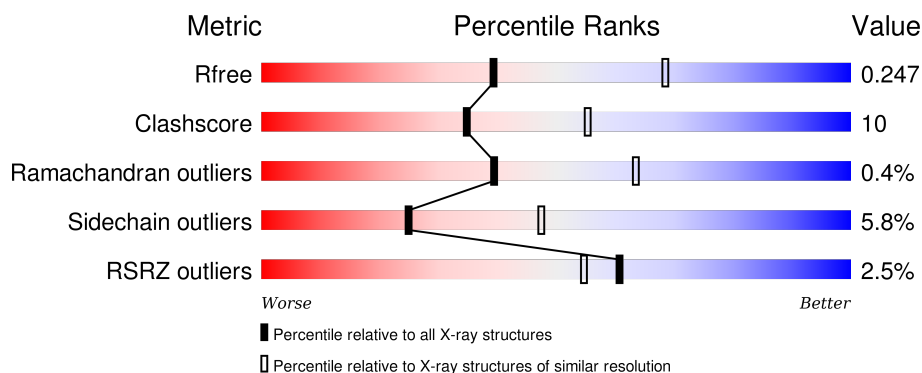
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2700 (2.64-2.60)
Clashscore	102246	3065 (2.64-2.60)
Ramachandran outliers	100387	3015 (2.64-2.60)
Sidechain outliers	100360	3015 (2.64-2.60)
RSRZ outliers	91569	2706 (2.64-2.60)

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. 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	396	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>14%</div> <div>• 10%</div> </div> </div>
1	B	396	<div> <div>%</div> <div> <div></div> <div>74%</div> <div>15%</div> <div>• 9%</div> </div> </div>
1	C	396	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>13%</div> <div>• 10%</div> </div> </div>
1	D	396	<div> <div>4%</div> <div> <div></div> <div>73%</div> <div>16%</div> <div>• 10%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MG	C	1001	-	-	-	X
3	B73	B	2001	-	-	X	-
3	B73	C	2001	-	-	X	-
3	B73	D	2001	-	-	X	-

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12025 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 Farnesyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	355	Total	C	N	O	S	13	0	0
			2888	1882	456	535	15			
1	B	362	Total	C	N	O	S	10	0	0
			2938	1909	467	547	15			
1	C	356	Total	C	N	O	S	13	0	0
			2894	1885	457	537	15			
1	D	357	Total	C	N	O	S	13	1	0
			2899	1888	458	538	15			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP A5K4U6
A	2	GLY	-	EXPRESSION TAG	UNP A5K4U6
A	3	SER	-	EXPRESSION TAG	UNP A5K4U6
A	4	SER	-	EXPRESSION TAG	UNP A5K4U6
A	5	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	6	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	7	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	8	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	9	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	10	HIS	-	EXPRESSION TAG	UNP A5K4U6
A	11	SER	-	EXPRESSION TAG	UNP A5K4U6
A	12	SER	-	EXPRESSION TAG	UNP A5K4U6
A	13	GLY	-	EXPRESSION TAG	UNP A5K4U6
A	14	ARG	-	EXPRESSION TAG	UNP A5K4U6
A	15	GLU	-	EXPRESSION TAG	UNP A5K4U6
A	16	ASN	-	EXPRESSION TAG	UNP A5K4U6
A	17	LEU	-	EXPRESSION TAG	UNP A5K4U6
A	18	TYR	-	EXPRESSION TAG	UNP A5K4U6
A	19	PHE	-	EXPRESSION TAG	UNP A5K4U6
A	20	GLN	-	EXPRESSION TAG	UNP A5K4U6
A	21	GLY	-	EXPRESSION TAG	UNP A5K4U6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	134	MET	THR	SEE REMARK 999	UNP A5K4U6
A	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
B	1	MET	-	EXPRESSION TAG	UNP A5K4U6
B	2	GLY	-	EXPRESSION TAG	UNP A5K4U6
B	3	SER	-	EXPRESSION TAG	UNP A5K4U6
B	4	SER	-	EXPRESSION TAG	UNP A5K4U6
B	5	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	6	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	7	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	8	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	9	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	10	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	11	SER	-	EXPRESSION TAG	UNP A5K4U6
B	12	SER	-	EXPRESSION TAG	UNP A5K4U6
B	13	GLY	-	EXPRESSION TAG	UNP A5K4U6
B	14	ARG	-	EXPRESSION TAG	UNP A5K4U6
B	15	GLU	-	EXPRESSION TAG	UNP A5K4U6
B	16	ASN	-	EXPRESSION TAG	UNP A5K4U6
B	17	LEU	-	EXPRESSION TAG	UNP A5K4U6
B	18	TYR	-	EXPRESSION TAG	UNP A5K4U6
B	19	PHE	-	EXPRESSION TAG	UNP A5K4U6
B	20	GLN	-	EXPRESSION TAG	UNP A5K4U6
B	21	GLY	-	EXPRESSION TAG	UNP A5K4U6
B	134	MET	THR	SEE REMARK 999	UNP A5K4U6
B	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
C	1	MET	-	EXPRESSION TAG	UNP A5K4U6
C	2	GLY	-	EXPRESSION TAG	UNP A5K4U6
C	3	SER	-	EXPRESSION TAG	UNP A5K4U6
C	4	SER	-	EXPRESSION TAG	UNP A5K4U6
C	5	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	6	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	7	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	8	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	9	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	10	HIS	-	EXPRESSION TAG	UNP A5K4U6
C	11	SER	-	EXPRESSION TAG	UNP A5K4U6
C	12	SER	-	EXPRESSION TAG	UNP A5K4U6
C	13	GLY	-	EXPRESSION TAG	UNP A5K4U6
C	14	ARG	-	EXPRESSION TAG	UNP A5K4U6
C	15	GLU	-	EXPRESSION TAG	UNP A5K4U6
C	16	ASN	-	EXPRESSION TAG	UNP A5K4U6
C	17	LEU	-	EXPRESSION TAG	UNP A5K4U6

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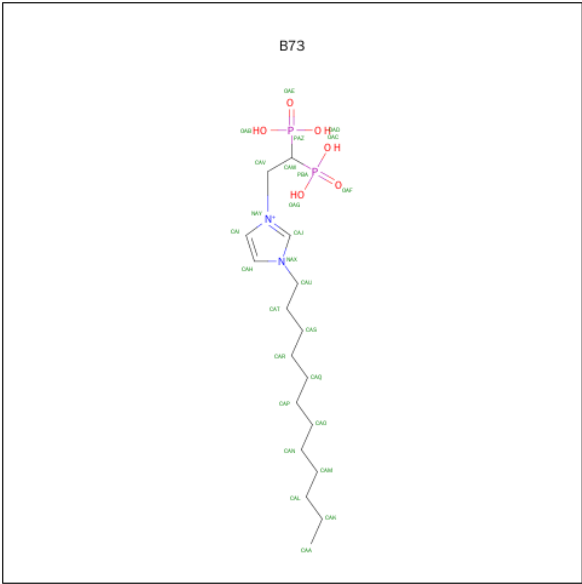
Chain	Residue	Modelled	Actual	Comment	Reference
C	18	TYR	-	EXPRESSION TAG	UNP A5K4U6
C	19	PHE	-	EXPRESSION TAG	UNP A5K4U6
C	20	GLN	-	EXPRESSION TAG	UNP A5K4U6
C	21	GLY	-	EXPRESSION TAG	UNP A5K4U6
C	134	MET	THR	SEE REMARK 999	UNP A5K4U6
C	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6
D	1	MET	-	EXPRESSION TAG	UNP A5K4U6
D	2	GLY	-	EXPRESSION TAG	UNP A5K4U6
D	3	SER	-	EXPRESSION TAG	UNP A5K4U6
D	4	SER	-	EXPRESSION TAG	UNP A5K4U6
D	5	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	6	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	7	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	8	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	9	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	10	HIS	-	EXPRESSION TAG	UNP A5K4U6
D	11	SER	-	EXPRESSION TAG	UNP A5K4U6
D	12	SER	-	EXPRESSION TAG	UNP A5K4U6
D	13	GLY	-	EXPRESSION TAG	UNP A5K4U6
D	14	ARG	-	EXPRESSION TAG	UNP A5K4U6
D	15	GLU	-	EXPRESSION TAG	UNP A5K4U6
D	16	ASN	-	EXPRESSION TAG	UNP A5K4U6
D	17	LEU	-	EXPRESSION TAG	UNP A5K4U6
D	18	TYR	-	EXPRESSION TAG	UNP A5K4U6
D	19	PHE	-	EXPRESSION TAG	UNP A5K4U6
D	20	GLN	-	EXPRESSION TAG	UNP A5K4U6
D	21	GLY	-	EXPRESSION TAG	UNP A5K4U6
D	134	MET	THR	SEE REMARK 999	UNP A5K4U6
D	227	ASP	ASN	SEE REMARK 999	UNP A5K4U6

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Mg 3 3	0	0
2	A	3	Total Mg 3 3	0	0
2	D	3	Total Mg 3 3	0	0
2	C	3	Total Mg 3 3	0	0

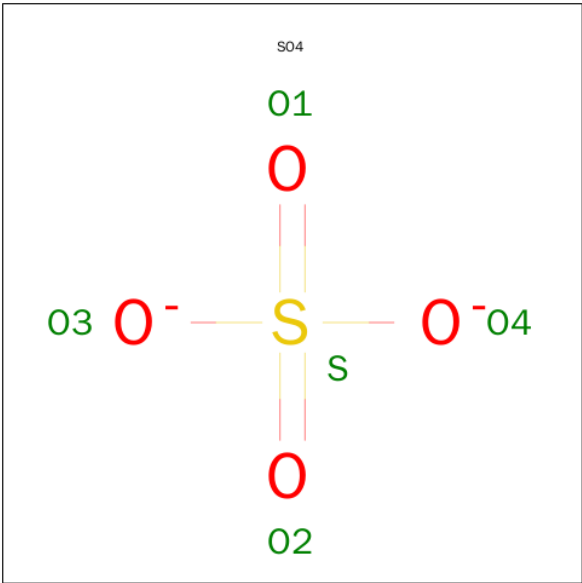
- Molecule 3 is 3-(2,2-DIPHOSPHONOETHYL)-1-DODECYL-1H-IMIDAZOL-3-IUM

(three-letter code: B73) (formula: C<sub>17</sub>H<sub>35</sub>N<sub>2</sub>O<sub>6</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	17	2	6	2		
3	B	1	Total	C	N	O	P	0	0
			27	17	2	6	2		
3	C	1	Total	C	N	O	P	0	0
			27	17	2	6	2		
3	D	1	Total	C	N	O	P	0	0
			27	17	2	6	2		

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



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

- Molecule 5 is water.

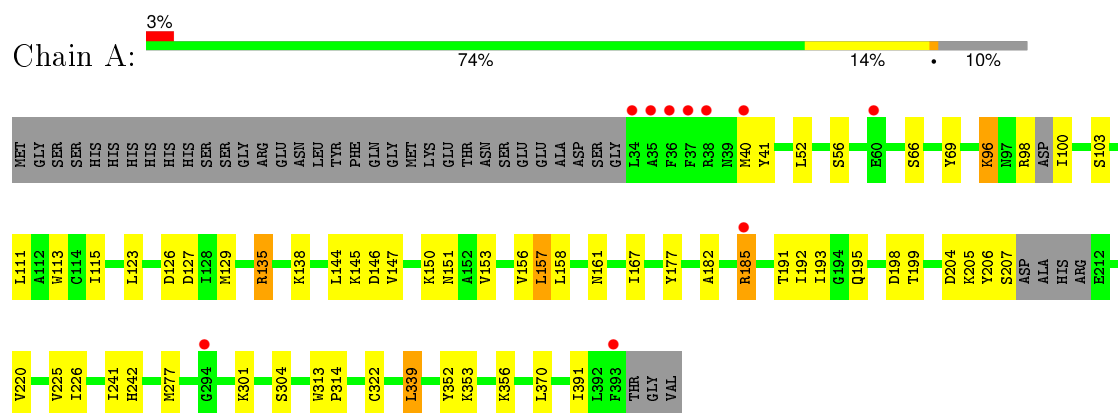
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	72	Total O 72 72	0	0
5	B	81	Total O 81 81	0	0
5	C	56	Total O 56 56	0	0
5	D	57	Total O 57 57	0	0



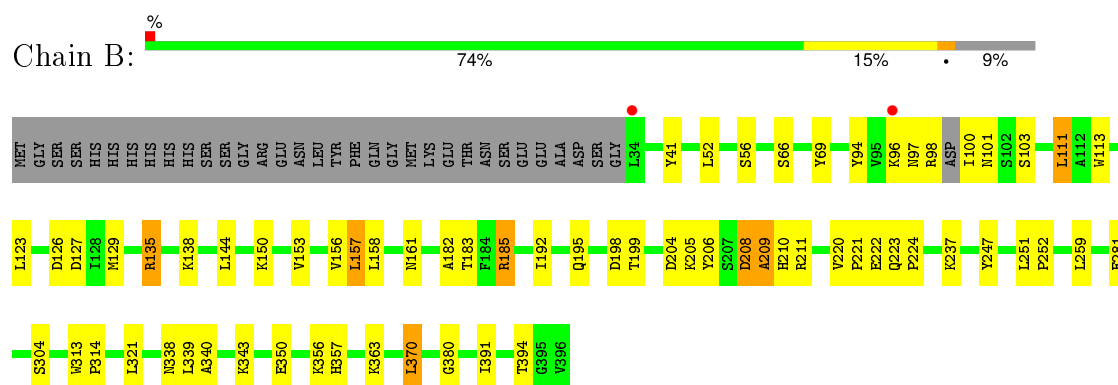
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

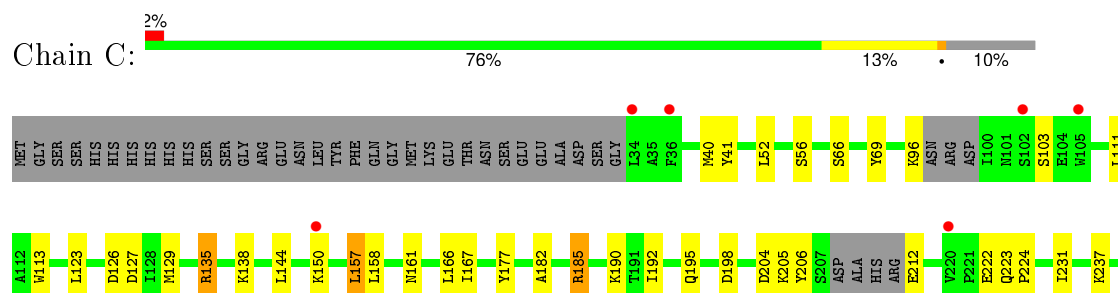
#### • Molecule 1: Farnesyl pyrophosphate synthase



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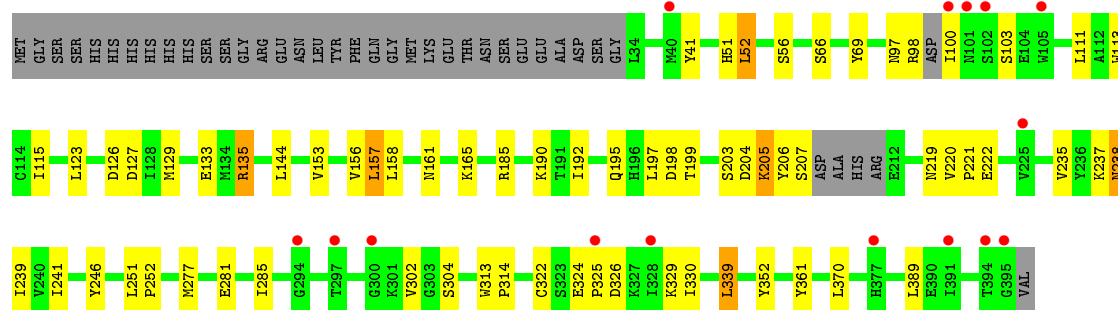


#### • Molecule 1: Farnesyl pyrophosphate synthase





- Molecule 1: Farnesyl pyrophosphate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.68Å 107.95Å 140.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.58 – 2.61 45.58 – 2.61	Depositor EDS
% Data completeness (in resolution range)	99.2 (45.58-2.61) 99.2 (45.58-2.61)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	7.08 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.208 , 0.253 0.205 , 0.247	Depositor DCC
$R_{free}$ test set	2550 reflections (5.35%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.6	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 40.9	EDS
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 50270 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	12025	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, B73, SO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.50	0/2948	0.55	1/3985 (0.0%)
1	B	0.49	0/3000	0.54	1/4058 (0.0%)
1	C	0.48	0/2954	0.53	2/3993 (0.1%)
1	D	0.52	0/2959	0.54	0/4000
All	All	0.50	0/11861	0.54	4/16036 (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	B	0	2
1	D	0	1
All	All	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	356	LYS	CB-CG-CD	-5.95	96.13	111.60
1	B	209	ALA	CB-CA-C	-5.70	101.55	110.10
1	A	356	LYS	CB-CG-CD	-5.54	97.20	111.60
1	C	356	LYS	CG-CD-CE	-5.16	96.42	111.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	97	ASN	Mainchain,Peptide
1	D	97	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	A	2888	0	2840	63	0
1	B	2938	0	2875	59	0
1	C	2894	0	2848	47	0
1	D	2899	0	2850	73	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
3	A	27	0	31	18	0
3	B	27	0	31	23	0
3	C	27	0	31	28	0
3	D	27	0	31	21	0
4	A	5	0	0	1	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	72	0	0	3	0
5	B	81	0	0	0	0
5	C	56	0	0	3	0
5	D	57	0	0	1	0
All	All	12025	0	11537	230	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 (230) 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:C:2001:B73:HAAA	1:D:157:LEU:CB	1.72	1.19
1:A:98:ARG:O	1:A:100:ILE:N	1.77	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:LEU:HB2	3:B:2001:B73:HALA	1.16	1.14
3:C:2001:B73:CAL	1:D:157:LEU:HB2	1.77	1.14
1:C:192:ILE:HD11	1:D:157:LEU:HD13	1.27	1.12
3:C:2001:B73:CAA	1:D:157:LEU:HG	1.86	1.05
3:C:2001:B73:HAL	1:D:157:LEU:CB	1.87	1.05
1:A:185:ARG:HH21	1:A:185:ARG:HB3	1.21	1.05
3:C:2001:B73:HAL	1:D:157:LEU:HB2	1.38	1.05
1:A:157:LEU:HD13	1:B:192:ILE:HD11	1.39	1.03
3:A:2001:B73:HAAB	1:B:157:LEU:HG	1.40	1.02
3:C:2001:B73:HAA	3:D:2001:B73:CAA	1.89	1.00
3:C:2001:B73:CAK	1:D:157:LEU:HB2	1.90	1.00
3:C:2001:B73:HAAA	1:D:157:LEU:CG	1.90	1.00
1:A:192:ILE:HD11	1:B:157:LEU:HD13	1.44	1.00
3:A:2001:B73:HALA	1:B:153:VAL:CG1	1.95	0.97
1:D:156:VAL:HG12	3:D:2001:B73:CAA	1.94	0.96
3:C:2001:B73:HAA	3:D:2001:B73:HAAA	1.47	0.94
3:A:2001:B73:HALA	1:B:153:VAL:HG12	1.50	0.94
1:A:182:ALA:HA	1:A:185:ARG:HH22	1.32	0.93
3:C:2001:B73:HAAB	1:D:157:LEU:HG	1.53	0.91
1:B:98:ARG:CB	1:B:100:ILE:N	2.35	0.90
1:A:182:ALA:HA	1:A:185:ARG:NH2	1.87	0.89
3:C:2001:B73:CAA	1:D:157:LEU:CB	2.50	0.89
1:D:156:VAL:HG12	3:D:2001:B73:HAAB	1.54	0.88
1:B:156:VAL:HG11	3:B:2001:B73:HAM	1.57	0.87
3:C:2001:B73:CAA	1:D:157:LEU:CG	2.49	0.86
1:D:156:VAL:CG1	3:D:2001:B73:CAA	2.53	0.86
3:C:2001:B73:HAAA	1:D:157:LEU:CA	2.06	0.85
1:A:157:LEU:HB2	3:B:2001:B73:CAL	2.04	0.85
3:C:2001:B73:HAL	1:D:157:LEU:CG	2.08	0.82
1:D:156:VAL:CG1	3:D:2001:B73:HAAB	2.10	0.81
3:C:2001:B73:HAA	3:D:2001:B73:HAA	1.63	0.81
3:C:2001:B73:CAA	1:D:157:LEU:HB2	2.09	0.79
1:C:185:ARG:CZ	5:C:443:HOH:O	2.30	0.78
1:B:208:ASP:O	1:B:210:HIS:N	2.16	0.77
1:B:204:ASP:OD2	1:B:222:GLU:HG3	1.83	0.77
1:A:199:THR:HG23	1:B:150:LYS:HE2	1.67	0.77
1:A:157:LEU:CB	3:B:2001:B73:HALA	2.08	0.75
1:A:69:TYR:CE1	1:A:158:LEU:HD22	2.22	0.74
1:C:182:ALA:HA	1:C:185:ARG:HH22	1.52	0.74
1:A:241:ILE:HG23	1:A:277:MET:SD	2.27	0.74
1:A:153:VAL:HG13	3:B:2001:B73:HAA	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:185:ARG:HB3	1:C:185:ARG:HH21	1.54	0.72
1:A:129:MET:HE1	1:A:195:GLN:HG3	1.72	0.71
1:D:156:VAL:HG12	3:D:2001:B73:HAA	1.71	0.71
3:A:2001:B73:HALA	1:B:153:VAL:HG13	1.72	0.69
1:C:182:ALA:HA	1:C:185:ARG:NH2	2.06	0.69
3:A:2001:B73:HAK	3:B:2001:B73:HAAA	1.76	0.68
1:A:153:VAL:HG12	3:B:2001:B73:HAKA	1.75	0.68
3:C:2001:B73:HAOA	1:D:157:LEU:HD12	1.74	0.68
1:A:153:VAL:HG13	3:B:2001:B73:CAK	2.24	0.67
1:A:127:ASP:OD2	1:A:135:ARG:HD2	1.95	0.67
1:A:153:VAL:CG1	3:B:2001:B73:HAKA	2.25	0.66
1:A:185:ARG:HB3	1:A:185:ARG:NH2	2.04	0.66
1:C:241:ILE:HG23	1:C:277:MET:SD	2.36	0.65
1:A:41:TYR:HB2	1:A:113:TRP:CZ2	2.31	0.65
1:C:129:MET:HE1	1:C:195:GLN:HG3	1.79	0.65
1:A:157:LEU:HD12	3:B:2001:B73:HAOA	1.79	0.64
1:C:157:LEU:HD22	1:C:161:ASN:ND2	2.12	0.64
1:A:156:VAL:HG11	3:A:2001:B73:HAKA	1.78	0.64
1:B:135:ARG:NH2	3:B:2001:B73:OAD	2.29	0.64
1:B:204:ASP:N	1:B:222:GLU:OE2	2.22	0.64
1:C:205:LYS:HB3	1:C:206:TYR:HD2	1.63	0.64
1:C:185:ARG:NH2	5:C:443:HOH:O	2.29	0.63
1:B:127:ASP:OD2	1:B:135:ARG:HD2	1.99	0.63
4:A:3001:SO4:O3	5:A:427:HOH:O	2.16	0.62
1:D:129:MET:HE1	1:D:195:GLN:HG3	1.81	0.62
1:A:153:VAL:HG13	3:B:2001:B73:CAA	2.30	0.61
3:C:2001:B73:HAAA	1:D:157:LEU:HA	1.82	0.61
1:C:313:TRP:HB3	1:C:314:PRO:HD3	1.83	0.61
1:D:69:TYR:CE1	1:D:158:LEU:HD22	2.36	0.61
1:A:313:TRP:HB3	1:A:314:PRO:HD3	1.83	0.61
3:C:2001:B73:HAL	1:D:157:LEU:HG	1.82	0.60
1:C:245:ALA:HB2	1:C:280:GLY:HA3	1.82	0.60
1:B:69:TYR:CE1	1:B:158:LEU:HD22	2.35	0.60
1:A:153:VAL:CG1	3:B:2001:B73:CAK	2.80	0.59
1:C:353:LYS:O	1:C:357:HIS:HD2	1.86	0.59
1:A:157:LEU:HG	3:B:2001:B73:HAMA	1.84	0.58
1:A:185:ARG:HH21	1:A:185:ARG:CB	2.08	0.58
1:C:192:ILE:CD1	1:D:157:LEU:HD13	2.19	0.58
1:B:208:ASP:C	1:B:210:HIS:H	2.08	0.57
1:A:339:LEU:HD23	1:C:339:LEU:CD2	2.35	0.57
1:A:339:LEU:HD23	1:C:339:LEU:HD21	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:GLU:N	5:C:408:HOH:O	2.37	0.57
1:C:167:ILE:HG22	1:C:177:TYR:HE1	1.70	0.57
1:A:156:VAL:CG1	3:A:2001:B73:HAKA	2.35	0.56
3:A:2001:B73:HAAB	1:B:157:LEU:CG	2.26	0.56
1:D:156:VAL:HG11	3:D:2001:B73:HAKA	1.87	0.56
3:A:2001:B73:CAK	3:B:2001:B73:HAAA	2.35	0.56
1:C:204:ASP:N	1:C:222:GLU:OE2	2.34	0.56
1:B:338:ASN:HD21	1:D:133:GLU:CD	2.08	0.56
1:A:145:LYS:HE3	1:B:221:PRO:HG3	1.88	0.56
1:A:98:ARG:HA	1:A:100:ILE:HG13	1.89	0.55
1:D:126:ASP:OD2	3:D:2001:B73:HAW	2.07	0.55
1:B:340:ALA:HB2	1:D:302:VAL:CG1	2.37	0.55
1:D:313:TRP:HB3	1:D:314:PRO:HD3	1.88	0.55
3:A:2001:B73:HAK	3:B:2001:B73:CAA	2.37	0.55
1:B:251:LEU:N	1:B:252:PRO:HD2	2.21	0.54
1:C:41:TYR:HB2	1:C:113:TRP:CZ2	2.43	0.54
3:A:2001:B73:HAN	1:B:157:LEU:HD12	1.88	0.54
3:A:2001:B73:HAA	3:B:2001:B73:HAL	1.89	0.54
1:B:157:LEU:HD22	1:B:161:ASN:ND2	2.23	0.54
3:C:2001:B73:CAA	3:D:2001:B73:HAA	2.35	0.53
3:A:2001:B73:CAA	3:B:2001:B73:HAL	2.38	0.53
1:D:156:VAL:HG11	3:D:2001:B73:CAK	2.38	0.53
1:D:156:VAL:CG1	3:D:2001:B73:HAKA	2.39	0.53
1:B:237:LYS:HD3	1:B:281:GLU:OE2	2.09	0.53
1:A:182:ALA:CA	1:A:185:ARG:HH22	2.14	0.53
1:C:69:TYR:CE1	1:C:158:LEU:HD22	2.43	0.53
1:B:111:LEU:HD22	1:B:259:LEU:HD22	1.90	0.52
1:C:40:MET:HA	1:C:40:MET:CE	2.39	0.52
1:D:157:LEU:HD22	1:D:161:ASN:ND2	2.25	0.52
1:C:192:ILE:HD11	1:D:157:LEU:CD1	2.20	0.52
1:C:157:LEU:HD13	1:D:192:ILE:HD11	1.91	0.52
1:B:340:ALA:HB2	1:D:302:VAL:HG11	1.91	0.52
1:C:185:ARG:NH2	1:C:185:ARG:HB3	2.21	0.51
1:D:98:ARG:O	1:D:100:ILE:N	2.42	0.51
1:C:127:ASP:OD2	1:C:135:ARG:HD2	2.11	0.51
1:A:158:LEU:HB2	1:B:192:ILE:HG21	1.92	0.51
1:D:190:LYS:HD3	1:D:246:TYR:CE1	2.44	0.51
1:B:313:TRP:HB3	1:B:314:PRO:HD3	1.92	0.51
1:A:241:ILE:CG2	1:A:277:MET:SD	2.97	0.50
1:D:156:VAL:CG1	3:D:2001:B73:CAK	2.89	0.50
1:A:157:LEU:HG	3:B:2001:B73:CAL	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:127:ASP:OD2	1:D:135:ARG:HD2	2.12	0.50
1:D:197:LEU:HB3	1:D:239:ILE:HG12	1.93	0.50
3:C:2001:B73:HAK	1:D:153:VAL:O	2.10	0.50
1:B:41:TYR:HB2	1:B:113:TRP:CZ2	2.47	0.49
1:D:324:GLU:N	1:D:325:PRO:CD	2.75	0.49
3:C:2001:B73:HAAA	1:D:157:LEU:CD2	2.41	0.49
1:D:135:ARG:NH2	3:D:2001:B73:OAD	2.39	0.49
1:A:157:LEU:HD22	1:A:161:ASN:ND2	2.26	0.49
1:A:153:VAL:O	3:B:2001:B73:HAK	2.13	0.49
1:A:225:VAL:HG13	5:A:411:HOH:O	2.11	0.49
1:A:69:TYR:CD1	1:A:158:LEU:HD22	2.47	0.49
1:C:126:ASP:OD2	3:C:2001:B73:HAW	2.12	0.49
1:C:231:ILE:O	1:C:231:ILE:HG22	2.12	0.49
1:A:145:LYS:HE3	1:B:221:PRO:CG	2.42	0.49
1:D:241:ILE:HG23	1:D:277:MET:SD	2.53	0.49
1:C:157:LEU:HD12	3:D:2001:B73:HAO	1.94	0.48
1:B:183:THR:HG22	1:B:251:LEU:CD1	2.43	0.48
3:C:2001:B73:CAL	1:D:157:LEU:HG	2.43	0.48
1:C:205:LYS:HB3	1:C:206:TYR:CD2	2.47	0.48
1:C:223:GLN:HA	1:C:224:PRO:HD3	1.74	0.48
1:C:237:LYS:HD3	1:C:281:GLU:OE2	2.12	0.48
1:A:146:ASP:O	1:B:205:LYS:NZ	2.37	0.48
1:D:41:TYR:HB2	1:D:113:TRP:CZ2	2.48	0.48
1:D:156:VAL:HG11	3:D:2001:B73:HAAB	1.93	0.48
1:D:322:CYS:HA	1:D:352:TYR:CE2	2.49	0.48
1:A:205:LYS:HB3	1:A:206:TYR:HD2	1.79	0.48
1:B:185:ARG:HB3	1:B:185:ARG:NH2	2.29	0.47
3:C:2001:B73:HANA	1:D:157:LEU:CD1	2.44	0.47
1:C:129:MET:HE1	1:C:195:GLN:CG	2.43	0.47
1:D:205:LYS:HB3	1:D:206:TYR:HD2	1.79	0.47
1:A:158:LEU:O	1:A:158:LEU:HG	2.13	0.47
1:B:223:GLN:HA	1:B:224:PRO:HD3	1.71	0.47
1:D:251:LEU:N	1:D:252:PRO:HD2	2.30	0.47
3:C:2001:B73:CAO	1:D:157:LEU:HD12	2.41	0.47
1:D:156:VAL:HG11	3:D:2001:B73:CAA	2.39	0.47
1:D:51:HIS:CE1	1:D:165:LYS:HE3	2.49	0.47
3:C:2001:B73:OAG	3:C:2001:B73:NAY	2.48	0.47
1:B:204:ASP:OD2	1:B:222:GLU:CG	2.60	0.47
1:C:129:MET:CE	1:C:195:GLN:HG3	2.45	0.47
1:B:321:LEU:HD11	1:B:357:HIS:CE1	2.49	0.46
1:C:391:ILE:O	1:C:391:ILE:HD12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:183:THR:HG22	1:B:251:LEU:HD12	1.98	0.46
1:A:96:LYS:HA	1:A:96:LYS:HE2	1.97	0.46
1:B:182:ALA:HA	1:B:185:ARG:NH2	2.31	0.46
1:C:135:ARG:NH2	3:C:2001:B73:OAD	2.45	0.45
1:A:41:TYR:HB2	1:A:113:TRP:CE2	2.52	0.45
1:C:204:ASP:O	1:C:205:LYS:C	2.54	0.45
1:B:185:ARG:HB3	1:B:185:ARG:HH21	1.80	0.45
1:C:158:LEU:O	1:C:158:LEU:HG	2.16	0.45
1:B:340:ALA:CB	1:D:302:VAL:HG11	2.47	0.45
1:B:391:ILE:HA	1:B:394:THR:HG22	1.99	0.45
1:A:157:LEU:HG	3:B:2001:B73:CAM	2.47	0.44
1:C:69:TYR:CD1	1:C:158:LEU:HD22	2.52	0.44
1:D:156:VAL:HB	3:D:2001:B73:HAKA	1.99	0.44
1:A:322:CYS:HA	1:A:352:TYR:CE2	2.52	0.44
1:B:339:LEU:HD21	1:D:339:LEU:HA	1.99	0.44
3:D:2001:B73:HAMA	3:D:2001:B73:HAAB	1.65	0.44
1:C:157:LEU:HD22	1:C:161:ASN:HD22	1.81	0.44
3:A:2001:B73:HAOA	1:B:157:LEU:HD12	1.98	0.44
1:C:251:LEU:HB3	1:C:252:PRO:CD	2.47	0.44
1:D:203:SER:OG	1:D:205:LYS:HB2	2.18	0.43
1:A:147:VAL:O	1:A:151:ASN:HB2	2.18	0.43
1:D:326:ASP:O	1:D:330:ILE:HG13	2.18	0.43
1:D:389:LEU:HD12	1:D:389:LEU:HA	1.85	0.43
1:B:251:LEU:HB3	1:B:252:PRO:CD	2.48	0.43
1:C:370:LEU:HD13	1:C:389:LEU:HD23	2.01	0.43
1:A:167:ILE:HG22	1:A:177:TYR:HE1	1.83	0.43
1:A:129:MET:CE	1:A:195:GLN:HG3	2.45	0.43
1:D:219:ASN:HB2	5:D:402:HOH:O	2.19	0.42
1:A:220:VAL:HG22	1:D:220:VAL:HG22	2.00	0.42
3:A:2001:B73:CAN	1:B:157:LEU:HD12	2.48	0.42
1:D:313:TRP:N	1:D:314:PRO:CD	2.82	0.42
1:A:191:THR:HA	1:A:242:HIS:O	2.18	0.42
1:A:40:MET:CE	1:A:40:MET:HA	2.49	0.42
1:D:156:VAL:CB	3:D:2001:B73:HAKA	2.49	0.42
1:B:205:LYS:HB3	1:B:206:TYR:HD2	1.85	0.42
1:B:129:MET:HE1	1:B:195:GLN:HG3	2.02	0.42
1:A:126:ASP:OD2	3:A:2001:B73:HAW	2.19	0.42
3:A:2001:B73:HAAB	1:B:157:LEU:HB2	2.00	0.42
1:B:158:LEU:HG	1:B:158:LEU:O	2.17	0.42
1:A:145:LYS:CE	1:B:221:PRO:HG3	2.49	0.42
1:D:237:LYS:HD3	1:D:281:GLU:OE2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:370:LEU:HD12	1:B:370:LEU:HA	1.94	0.42
1:B:126:ASP:OD2	3:B:2001:B73:HAW	2.20	0.42
1:C:167:ILE:HG22	1:C:177:TYR:CE1	2.54	0.41
1:D:204:ASP:N	1:D:222:GLU:OE2	2.37	0.41
1:B:101:ASN:C	1:B:101:ASN:OD1	2.58	0.41
1:A:204:ASP:O	1:A:205:LYS:C	2.58	0.41
1:A:352:TYR:O	1:A:353:LYS:HB2	2.20	0.41
1:D:235:VAL:O	1:D:238:ASN:HB2	2.21	0.41
1:C:182:ALA:CA	1:C:185:ARG:HH22	2.29	0.41
1:D:52:LEU:HD12	1:D:52:LEU:HA	1.90	0.41
3:A:2001:B73:HAAB	1:B:157:LEU:CB	2.50	0.41
1:D:285:ILE:HD12	1:D:361:TYR:CZ	2.56	0.41
1:A:145:LYS:HG3	1:B:220:VAL:O	2.21	0.41
1:A:391:ILE:HD12	1:A:391:ILE:O	2.21	0.41
1:B:343:LYS:HG2	1:D:339:LEU:HD21	2.03	0.41
1:C:150:LYS:HE3	1:D:199:THR:HG23	2.02	0.41
1:A:150:LYS:HE3	1:B:199:THR:HG23	2.04	0.40
1:B:156:VAL:CG1	3:B:2001:B73:HAM	2.40	0.40
1:B:94:TYR:O	1:B:380:GLY:HA3	2.22	0.40
1:C:166:LEU:HD23	1:C:166:LEU:HA	1.95	0.40
1:A:207:SER:O	5:A:399:HOH:O	2.22	0.40
1:A:225:VAL:HG12	1:A:226:ILE:N	2.37	0.40
1:C:190:LYS:HD3	1:C:246:TYR:CE1	2.56	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	349/396 (88%)	337 (97%)	11 (3%)	1 (0%)	46 70
1	B	358/396 (90%)	341 (95%)	15 (4%)	2 (1%)	30 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	350/396 (88%)	334 (95%)	15 (4%)	1 (0%)	46	70
1	D	351/396 (89%)	336 (96%)	14 (4%)	1 (0%)	46	70
All	All	1408/1584 (89%)	1348 (96%)	55 (4%)	5 (0%)	39	63

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	209	ALA
1	C	304	SER
1	B	304	SER
1	A	304	SER
1	D	304	SER

### 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	309/357 (87%)	291 (94%)	18 (6%)	25	47
1	B	313/357 (88%)	293 (94%)	20 (6%)	22	42
1	C	310/357 (87%)	295 (95%)	15 (5%)	31	57
1	D	310/357 (87%)	291 (94%)	19 (6%)	23	44
All	All	1242/1428 (87%)	1170 (94%)	72 (6%)	25	47

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	LEU
1	A	56	SER
1	A	66	SER
1	A	96	LYS
1	A	103	SER
1	A	111	LEU
1	A	115	ILE

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Mol	Chain	Res	Type
1	A	123	LEU
1	A	135	ARG
1	A	138	LYS
1	A	144	LEU
1	A	157	LEU
1	A	185	ARG
1	A	193	ILE
1	A	198	ASP
1	A	301	LYS
1	A	339	LEU
1	A	370	LEU
1	B	52	LEU
1	B	56	SER
1	B	66	SER
1	B	96	LYS
1	B	103	SER
1	B	111	LEU
1	B	123	LEU
1	B	135	ARG
1	B	138	LYS
1	B	144	LEU
1	B	157	LEU
1	B	185	ARG
1	B	198	ASP
1	B	208	ASP
1	B	211	ARG
1	B	247	TYR
1	B	350	GLU
1	B	356	LYS
1	B	363	LYS
1	B	370	LEU
1	C	52	LEU
1	C	56	SER
1	C	66	SER
1	C	96	LYS
1	C	103	SER
1	C	111	LEU
1	C	123	LEU
1	C	135	ARG
1	C	138	LYS
1	C	144	LEU
1	C	157	LEU

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Mol	Chain	Res	Type
1	C	185	ARG
1	C	198	ASP
1	C	353	LYS
1	C	370	LEU
1	D	52	LEU
1	D	56	SER
1	D	66	SER
1	D	103	SER
1	D	111	LEU
1	D	115	ILE
1	D	123	LEU
1	D	135	ARG
1	D	144	LEU
1	D	157	LEU
1	D	185	ARG
1	D	198	ASP
1	D	205	LYS
1	D	207	SER
1	D	221	PRO
1	D	238	ASN
1	D	329	LYS
1	D	339	LEU
1	D	370	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	337	ASN
1	A	357	HIS
1	B	82	ASN
1	B	210	HIS
1	B	286	HIS
1	B	307	GLN
1	B	338	ASN
1	C	161	ASN
1	C	357	HIS
1	D	51	HIS
1	D	82	ASN
1	D	195	GLN
1	D	337	ASN
1	D	357	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 12 are monoatomic - leaving 8 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$
3	B73	A	2001	2	26,27,27	3.03	6 (23%)	30,36,36	2.28	9 (30%)
4	SO4	A	3001	-	4,4,4	1.19	0	6,6,6	0.27	0
3	B73	B	2001	2	26,27,27	3.21	7 (26%)	30,36,36	2.21	6 (20%)
4	SO4	B	3001	-	4,4,4	1.08	0	6,6,6	0.25	0
3	B73	C	2001	2	26,27,27	3.88	8 (30%)	30,36,36	1.84	7 (23%)
4	SO4	C	3001	-	4,4,4	0.96	0	6,6,6	0.17	0
3	B73	D	2001	2	26,27,27	2.99	6 (23%)	30,36,36	2.29	9 (30%)
4	SO4	D	3001	-	4,4,4	1.01	0	6,6,6	0.50	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
3	B73	A	2001	2	-	0/24/28/28	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	A	3001	-	-	0/0/0/0	0/0/0/0
3	B73	B	2001	2	-	0/24/28/28	0/1/1/1
4	SO4	B	3001	-	-	0/0/0/0	0/0/0/0
3	B73	C	2001	2	-	0/24/28/28	0/1/1/1
4	SO4	C	3001	-	-	0/0/0/0	0/0/0/0
3	B73	D	2001	2	-	0/24/28/28	0/1/1/1
4	SO4	D	3001	-	-	0/0/0/0	0/0/0/0

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2001	B73	PBA-OAC	-3.74	1.48	1.54
3	B	2001	B73	PBA-OAC	-3.49	1.49	1.54
3	A	2001	B73	PAZ-OAB	-3.38	1.49	1.54
3	D	2001	B73	PBA-OAC	-3.20	1.49	1.54
3	D	2001	B73	PAZ-OAB	-3.19	1.49	1.54
3	C	2001	B73	PBA-OAC	-3.14	1.49	1.54
3	B	2001	B73	PAZ-OAB	-2.58	1.50	1.54
3	C	2001	B73	PAZ-OAB	-2.43	1.50	1.54
3	C	2001	B73	PBA-CAW	-2.31	1.78	1.81
3	B	2001	B73	PBA-CAW	-2.04	1.78	1.81
3	C	2001	B73	CAV-NAY	2.20	1.50	1.48
3	B	2001	B73	PAZ-OAD	4.71	1.62	1.54
3	C	2001	B73	PAZ-OAE	5.47	1.59	1.49
3	A	2001	B73	PAZ-OAD	5.48	1.63	1.54
3	D	2001	B73	PAZ-OAD	5.62	1.64	1.54
3	B	2001	B73	PBA-OAG	6.70	1.65	1.54
3	D	2001	B73	PAZ-OAE	6.97	1.62	1.49
3	D	2001	B73	PBA-OAF	7.03	1.62	1.49
3	A	2001	B73	PBA-OAG	7.13	1.66	1.54
3	B	2001	B73	PAZ-OAE	7.13	1.62	1.49
3	C	2001	B73	PAZ-OAD	7.28	1.66	1.54
3	C	2001	B73	PBA-OAG	7.31	1.66	1.54
3	A	2001	B73	PBA-OAF	7.60	1.63	1.49
3	A	2001	B73	PAZ-OAE	7.86	1.64	1.49
3	D	2001	B73	PBA-OAG	8.17	1.68	1.54
3	B	2001	B73	PBA-OAF	10.70	1.69	1.49
3	C	2001	B73	PBA-OAF	14.75	1.76	1.49

All (31) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2001	B73	NAY-CAJ-NAX	-7.32	104.07	108.75
3	D	2001	B73	NAY-CAJ-NAX	-6.58	104.54	108.75
3	B	2001	B73	NAY-CAJ-NAX	-6.40	104.65	108.75
3	D	2001	B73	OAG-PBA-OAF	-5.43	99.05	113.49
3	C	2001	B73	NAY-CAJ-NAX	-5.31	105.36	108.75
3	B	2001	B73	OAD-PAZ-OAE	-5.17	99.76	113.49
3	D	2001	B73	OAD-PAZ-OAE	-4.59	101.28	113.49
3	A	2001	B73	OAG-PBA-OAF	-4.47	101.61	113.49
3	B	2001	B73	OAG-PBA-OAF	-3.93	103.04	113.49
3	C	2001	B73	CAV-NAY-CAI	-3.65	117.84	125.97
3	C	2001	B73	OAG-PBA-OAF	-3.38	104.51	113.49
3	C	2001	B73	OAD-PAZ-OAE	-3.31	104.69	113.49
3	D	2001	B73	CAV-NAY-CAI	-2.95	119.40	125.97
3	B	2001	B73	CAV-NAY-CAI	-2.88	119.56	125.97
3	A	2001	B73	CAV-NAY-CAI	-2.80	119.72	125.97
3	A	2001	B73	OAD-PAZ-OAE	-2.77	106.12	113.49
3	A	2001	B73	CAI-CAH-NAX	-2.07	105.14	107.15
3	D	2001	B73	OAC-PBA-CAW	2.02	113.51	106.44
3	C	2001	B73	OAB-PAZ-CAW	2.05	113.63	106.44
3	D	2001	B73	OAG-PBA-OAC	2.16	114.06	107.57
3	A	2001	B73	OAG-PBA-OAC	2.27	114.39	107.57
3	D	2001	B73	OAB-PAZ-OAE	2.32	119.65	113.49
3	C	2001	B73	OAD-PAZ-OAB	2.69	115.65	107.57
3	D	2001	B73	CAI-NAY-CAJ	2.76	110.81	108.21
3	C	2001	B73	OAC-PBA-CAW	3.01	117.00	106.44
3	A	2001	B73	CAH-NAX-CAJ	3.07	111.10	108.21
3	B	2001	B73	OAC-PBA-CAW	3.12	117.39	106.44
3	A	2001	B73	OAC-PBA-CAW	3.50	118.70	106.44
3	D	2001	B73	OAB-PAZ-CAW	3.54	118.85	106.44
3	B	2001	B73	OAB-PAZ-CAW	3.91	120.15	106.44
3	A	2001	B73	OAB-PAZ-CAW	4.08	120.76	106.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 82 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2001	B73	18	0
4	A	3001	SO4	1	0
3	B	2001	B73	23	0
3	C	2001	B73	28	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2001	B73	21	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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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	355/396 (89%)	-0.02	10 (2%) 56 50	24, 28, 53, 217	21 (5%)
1	B	362/396 (91%)	-0.10	2 (0%) 90 88	25, 28, 54, 137	20 (5%)
1	C	356/396 (89%)	-0.05	9 (2%) 61 55	25, 29, 59, 181	21 (5%)
1	D	357/396 (90%)	-0.07	15 (4%) 40 33	24, 29, 58, 174	21 (5%)
All	All	1430/1584 (90%)	-0.06	36 (2%) 61 55	24, 28, 57, 217	83 (5%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	34	LEU	8.4
1	A	35	ALA	7.2
1	D	101	ASN	3.6
1	A	37	PHE	3.5
1	D	328	ILE	3.4
1	B	96	LYS	3.4
1	D	100	ILE	3.3
1	C	34	LEU	3.1
1	A	185	ARG	3.0
1	C	347	SER	3.0
1	D	297	THR	2.9
1	D	325	PRO	2.9
1	B	34	LEU	2.8
1	D	394	THR	2.8
1	D	225	VAL	2.7
1	C	220	VAL	2.6
1	A	393	PHE	2.6
1	D	300	GLY	2.6
1	A	40	MET	2.4
1	C	105	TRP	2.4
1	D	105	TRP	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	150	LYS	2.3
1	D	40	MET	2.3
1	A	36	PHE	2.3
1	D	377	HIS	2.3
1	A	294	GLY	2.2
1	C	36	PHE	2.1
1	C	348	LEU	2.1
1	C	323	SER	2.1
1	D	102	SER	2.1
1	C	102	SER	2.1
1	D	294	GLY	2.1
1	D	391	ILE	2.1
1	D	395	GLY	2.1
1	A	38	ARG	2.0
1	A	60	GLU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	MG	C	1001	1/1	0.94	0.24	8.80	20,20,20,20	0
3	B73	C	2001	27/27	0.97	0.13	-1.05	2,8,30,34	0
3	B73	B	2001	27/27	0.97	0.13	-1.11	2,11,49,60	0
3	B73	A	2001	27/27	0.96	0.13	-1.30	2,8,41,52	0
4	SO4	A	3001	5/5	0.97	0.11	-1.32	9,10,16,23	0
2	MG	B	1002	1/1	0.95	0.11	-1.45	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	B73	D	2001	27/27	0.98	0.10	-1.61	5,10,47,57	0
4	SO4	C	3001	5/5	0.99	0.09	-1.73	16,17,24,26	0
2	MG	B	1001	1/1	0.97	0.08	-1.93	9,9,9,9	0
4	SO4	B	3001	5/5	0.98	0.10	-2.34	8,9,15,19	0
4	SO4	D	3001	5/5	0.99	0.09	-2.82	14,15,22,24	0
2	MG	A	1001	1/1	0.98	0.02	-3.09	12,12,12,12	0
2	MG	D	1001	1/1	0.96	0.08	-3.23	18,18,18,18	0
2	MG	C	1002	1/1	0.98	0.07	-3.38	13,13,13,13	0
2	MG	A	1002	1/1	0.89	0.09	-3.44	16,16,16,16	0
2	MG	D	1002	1/1	0.93	0.05	-3.79	19,19,19,19	0
2	MG	A	1003	1/1	0.95	0.07	-	4,4,4,4	0
2	MG	B	1003	1/1	0.90	0.09	-	6,6,6,6	0
2	MG	D	1003	1/1	0.89	0.06	-	8,8,8,8	0
2	MG	C	1003	1/1	0.87	0.08	-	3,3,3,3	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.