



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:32 AM GMT

PDB ID : 3MAV
Title : Crystal structure of Plasmodium vivax putative farnesyl pyrophosphate synthase (Pv092040)
Authors : Dong,A.; Dunford,J.; Lew,J.; Wernimont,A.K.; Ren,H.; Zhao,Y.; Koeieradzki,I.; Opperman,U.; Sundstrom,M.; Weigelt,J.; Edwards,A.M.; Arrow-smith,C.H.; Bochkarev,A.; Hui,R.; Artz,J.D.; Structural Genomics Consortium (SGC)
Deposited on : 2010-03-24
Resolution : 2.10 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
<http://wwpdb.org/validation/2016/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 : 1.7 (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

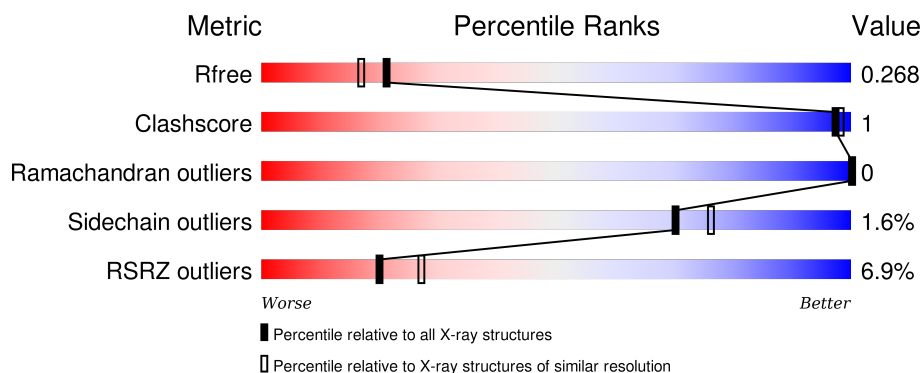
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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. 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	395	<div> <div>4%</div> <div>85%</div> <div>12%</div> </div>
1	B	395	<div> <div>9%</div> <div>83%</div> <div>13%</div> </div>
1	C	395	<div> <div>5%</div> <div>85%</div> <div>11%</div> </div>
1	D	395	<div> <div>7%</div> <div>86%</div> <div>10%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11402 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	348	Total	C	N	O	S	0	3	0
			2787	1808	443	522	14			
1	B	345	Total	C	N	O	S	0	0	0
			2704	1754	431	505	14			
1	C	350	Total	C	N	O	S	0	0	0
			2748	1787	439	508	14			
1	D	356	Total	C	N	O	S	0	0	0
			2748	1780	439	514	15			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	EXPRESSION TAG	UNP A5K4U6
A	2	SER	-	EXPRESSION TAG	UNP A5K4U6
A	3	SER	-	EXPRESSION TAG	UNP A5K4U6
A	4	HIS	-	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	SER	-	EXPRESSION TAG	UNP A5K4U6
A	11	SER	-	EXPRESSION TAG	UNP A5K4U6
A	12	GLY	-	EXPRESSION TAG	UNP A5K4U6
A	13	ARG	-	EXPRESSION TAG	UNP A5K4U6
A	14	GLU	-	EXPRESSION TAG	UNP A5K4U6
A	15	ASN	-	EXPRESSION TAG	UNP A5K4U6
A	16	LEU	-	EXPRESSION TAG	UNP A5K4U6
A	17	TYR	-	EXPRESSION TAG	UNP A5K4U6
A	18	PHE	-	EXPRESSION TAG	UNP A5K4U6
A	19	GLN	-	EXPRESSION TAG	UNP A5K4U6
A	20	GLY	-	EXPRESSION TAG	UNP A5K4U6
A	133	MET	THR	CLONING ARTIFACT	UNP A5K4U6

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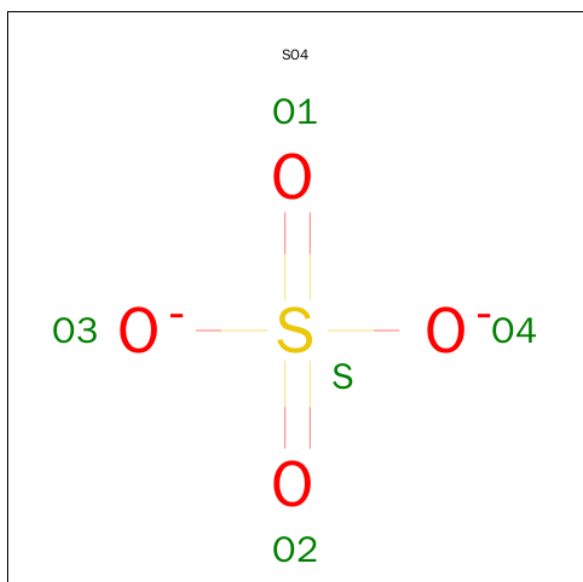
Chain	Residue	Modelled	Actual	Comment	Reference
A	226	ASP	ASN	CLONING ARTIFACT	UNP A5K4U6
B	1	GLY	-	EXPRESSION TAG	UNP A5K4U6
B	2	SER	-	EXPRESSION TAG	UNP A5K4U6
B	3	SER	-	EXPRESSION TAG	UNP A5K4U6
B	4	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	5	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	6	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	7	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	8	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	9	HIS	-	EXPRESSION TAG	UNP A5K4U6
B	10	SER	-	EXPRESSION TAG	UNP A5K4U6
B	11	SER	-	EXPRESSION TAG	UNP A5K4U6
B	12	GLY	-	EXPRESSION TAG	UNP A5K4U6
B	13	ARG	-	EXPRESSION TAG	UNP A5K4U6
B	14	GLU	-	EXPRESSION TAG	UNP A5K4U6
B	15	ASN	-	EXPRESSION TAG	UNP A5K4U6
B	16	LEU	-	EXPRESSION TAG	UNP A5K4U6
B	17	TYR	-	EXPRESSION TAG	UNP A5K4U6
B	18	PHE	-	EXPRESSION TAG	UNP A5K4U6
B	19	GLN	-	EXPRESSION TAG	UNP A5K4U6
B	20	GLY	-	EXPRESSION TAG	UNP A5K4U6
B	133	MET	THR	CLONING ARTIFACT	UNP A5K4U6
B	226	ASP	ASN	CLONING ARTIFACT	UNP A5K4U6
C	1	GLY	-	EXPRESSION TAG	UNP A5K4U6
C	2	SER	-	EXPRESSION TAG	UNP A5K4U6
C	3	SER	-	EXPRESSION TAG	UNP A5K4U6
C	4	HIS	-	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	SER	-	EXPRESSION TAG	UNP A5K4U6
C	11	SER	-	EXPRESSION TAG	UNP A5K4U6
C	12	GLY	-	EXPRESSION TAG	UNP A5K4U6
C	13	ARG	-	EXPRESSION TAG	UNP A5K4U6
C	14	GLU	-	EXPRESSION TAG	UNP A5K4U6
C	15	ASN	-	EXPRESSION TAG	UNP A5K4U6
C	16	LEU	-	EXPRESSION TAG	UNP A5K4U6
C	17	TYR	-	EXPRESSION TAG	UNP A5K4U6
C	18	PHE	-	EXPRESSION TAG	UNP A5K4U6
C	19	GLN	-	EXPRESSION TAG	UNP A5K4U6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	20	GLY	-	EXPRESSION TAG	UNP A5K4U6
C	133	MET	THR	CLONING ARTIFACT	UNP A5K4U6
C	226	ASP	ASN	CLONING ARTIFACT	UNP A5K4U6
D	1	GLY	-	EXPRESSION TAG	UNP A5K4U6
D	2	SER	-	EXPRESSION TAG	UNP A5K4U6
D	3	SER	-	EXPRESSION TAG	UNP A5K4U6
D	4	HIS	-	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	SER	-	EXPRESSION TAG	UNP A5K4U6
D	11	SER	-	EXPRESSION TAG	UNP A5K4U6
D	12	GLY	-	EXPRESSION TAG	UNP A5K4U6
D	13	ARG	-	EXPRESSION TAG	UNP A5K4U6
D	14	GLU	-	EXPRESSION TAG	UNP A5K4U6
D	15	ASN	-	EXPRESSION TAG	UNP A5K4U6
D	16	LEU	-	EXPRESSION TAG	UNP A5K4U6
D	17	TYR	-	EXPRESSION TAG	UNP A5K4U6
D	18	PHE	-	EXPRESSION TAG	UNP A5K4U6
D	19	GLN	-	EXPRESSION TAG	UNP A5K4U6
D	20	GLY	-	EXPRESSION TAG	UNP A5K4U6
D	133	MET	THR	CLONING ARTIFACT	UNP A5K4U6
D	226	ASP	ASN	CLONING ARTIFACT	UNP A5K4U6

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

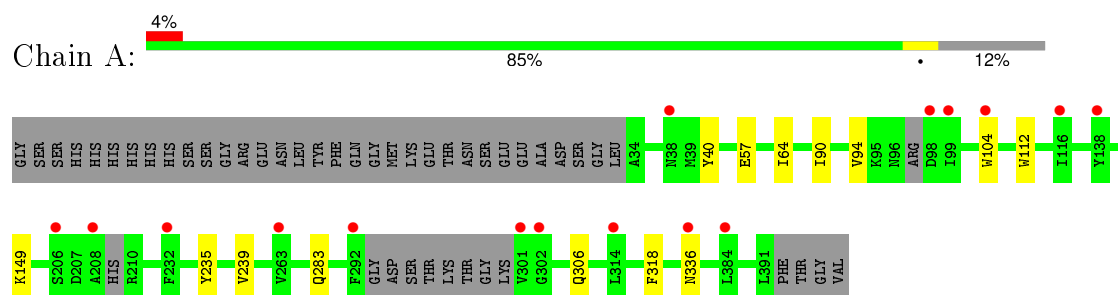
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	105	Total O 105 105	0	0
3	B	97	Total O 97 97	0	0
3	C	91	Total O 91 91	0	0
3	D	77	Total O 77 77	0	0

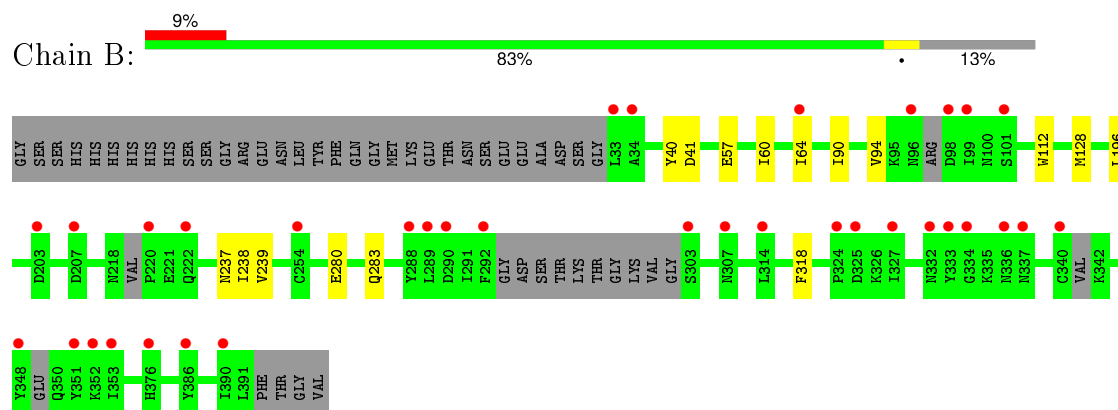
3 Residue-property plots [i](#)

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

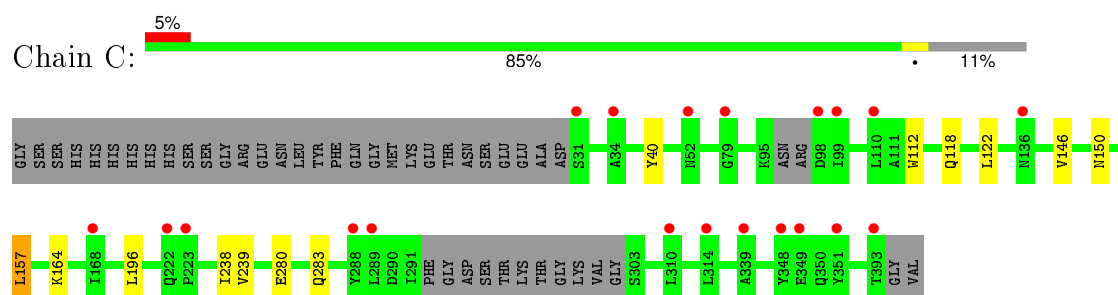
- Molecule 1: Farnesyl pyrophosphate synthase



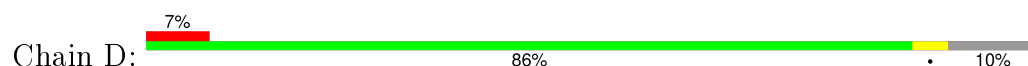
- Molecule 1: Farnesyl pyrophosphate synthase

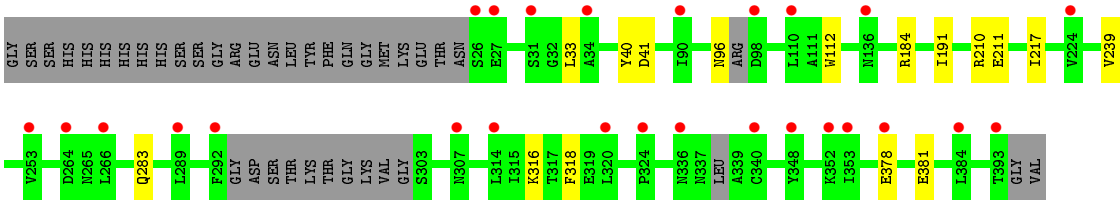


- Molecule 1: Farnesyl pyrophosphate synthase



- Molecule 1: Farnesyl pyrophosphate synthase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.97Å 116.39Å 92.42Å 90.00° 116.01° 90.00°	Depositor
Resolution (Å)	20.99 – 2.10 20.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	2.0 (20.99-2.10) 99.2 (20.99-2.10)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 2.09Å)	Xtriage
Refinement program	COOT 0.5.2, BUSTER 2.8.0	Depositor
R, R_{free}	0.229 , 0.262 0.234 , 0.268	Depositor DCC
R_{free} test set	1850 reflections (2.05%)	DCC
Wilson B-factor (Å ²)	39.6	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 42.5	EDS
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 92136 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11402	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.55	0/2855	0.57	0/3873
1	B	0.55	0/2757	0.56	0/3739
1	C	0.56	0/2806	0.57	0/3817
1	D	0.56	0/2803	0.57	0/3811
All	All	0.56	0/11221	0.56	0/15240

There are no bond length outliers.

There are no bond angle outliers.

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	A	2787	0	2658	7	0
1	B	2704	0	2527	10	0
1	C	2748	0	2586	7	0
1	D	2748	0	2521	5	0
2	A	10	0	0	0	0
2	B	20	0	0	0	0
2	C	5	0	0	0	0
2	D	10	0	0	0	0
3	A	105	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	97	0	0	0	0
3	C	91	0	0	0	0
3	D	77	0	0	0	0
All	All	11402	0	10292	25	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 1.

All (25) 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:A:57:GLU:H	1:B:237:ASN:HD21	1.36	0.71
1:B:239:VAL:HG22	1:B:283:GLN:HG2	1.83	0.59
1:B:239:VAL:HG11	1:B:280:GLU:HA	1.84	0.58
1:D:239:VAL:HG22	1:D:283:GLN:HG2	1.92	0.52
1:C:118:GLN:O	1:C:122:LEU:HG	2.12	0.50
1:D:378:GLU:HA	1:D:381:GLU:HB2	1.93	0.50
1:B:239:VAL:CG1	1:B:280:GLU:HA	2.42	0.50
1:C:239:VAL:HG22	1:C:283:GLN:HG2	1.95	0.49
1:C:40:TYR:HB2	1:C:112:TRP:CZ2	2.49	0.48
1:B:57:GLU:HB2	1:B:60:ILE:HD12	1.96	0.47
1:A:57:GLU:H	1:B:237:ASN:ND2	2.11	0.45
1:C:146:VAL:O	1:C:150:ASN:HB2	2.17	0.45
1:A:149:LYS:HA	1:B:128:MET:HG2	1.99	0.44
1:C:157:LEU:HB2	1:D:191:ILE:HG21	2.00	0.44
1:C:239:VAL:HG11	1:C:280:GLU:HA	2.00	0.43
1:B:196:LEU:HB3	1:B:238:ILE:HG12	2.00	0.43
1:A:239:VAL:HG22	1:A:283:GLN:HG2	1.99	0.43
1:A:40:TYR:HB2	1:A:112:TRP:CZ2	2.53	0.42
1:A:235:TYR:CZ	1:A:239:VAL:HG21	2.54	0.42
1:A:90:ILE:O	1:A:94:VAL:HG23	2.20	0.41
1:B:40:TYR:HB2	1:B:112:TRP:CZ2	2.55	0.41
1:C:196:LEU:HB3	1:C:238:ILE:HG12	2.01	0.40
1:D:40:TYR:HB2	1:D:112:TRP:CZ2	2.57	0.40
1:D:210:ARG:HG2	1:D:211:GLU:HG2	2.02	0.40
1:B:90:ILE:O	1:B:94:VAL:HG23	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	344/395 (87%)	335 (97%)	9 (3%)	0	100	100
1	B	333/395 (84%)	324 (97%)	9 (3%)	0	100	100
1	C	344/395 (87%)	335 (97%)	9 (3%)	0	100	100
1	D	348/395 (88%)	340 (98%)	8 (2%)	0	100	100
All	All	1369/1580 (87%)	1334 (97%)	35 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	A	286/356 (80%)	281 (98%)	5 (2%)	68	74
1	B	268/356 (75%)	265 (99%)	3 (1%)	80	85
1	C	272/356 (76%)	270 (99%)	2 (1%)	88	92
1	D	264/356 (74%)	257 (97%)	7 (3%)	52	56
All	All	1090/1424 (76%)	1073 (98%)	17 (2%)	70	76

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ILE
1	A	104	TRP

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Mol	Chain	Res	Type
1	A	306	GLN
1	A	318	PHE
1	A	336	ASN
1	B	41	ASP
1	B	64	ILE
1	B	318	PHE
1	C	157	LEU
1	C	164	LYS
1	D	33	LEU
1	D	41	ASP
1	D	96	ASN
1	D	184	ARG
1	D	217	ILE
1	D	316	LYS
1	D	318	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	B	63	HIS
1	B	194	GLN
1	B	237	ASN
1	C	100	ASN
1	C	153	ASN
1	D	194	GLN

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 ⓘ

9 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
2	SO4	A	2003	-	4,4,4	0.34	0	6,6,6	0.14	0
2	SO4	A	2005	-	4,4,4	0.10	0	6,6,6	0.06	0
2	SO4	B	2002	-	4,4,4	0.38	0	6,6,6	0.12	0
2	SO4	B	2008	-	4,4,4	0.05	0	6,6,6	0.08	0
2	SO4	B	2009	-	4,4,4	0.21	0	6,6,6	0.09	0
2	SO4	B	2010	-	4,4,4	0.16	0	6,6,6	0.13	0
2	SO4	C	2011	-	4,4,4	0.10	0	6,6,6	0.10	0
2	SO4	D	2001	-	4,4,4	0.34	0	6,6,6	0.11	0
2	SO4	D	2004	-	4,4,4	0.43	0	6,6,6	0.06	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	SO4	A	2003	-	-	0/0/0/0	0/0/0/0
2	SO4	A	2005	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2002	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2008	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2009	-	-	0/0/0/0	0/0/0/0
2	SO4	B	2010	-	-	0/0/0/0	0/0/0/0
2	SO4	C	2011	-	-	0/0/0/0	0/0/0/0
2	SO4	D	2001	-	-	0/0/0/0	0/0/0/0
2	SO4	D	2004	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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 ⓘ

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, 95th 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 ²)	Q<0.9
1	A	348/395 (88%)	0.22	16 (4%) 36 45	27, 41, 63, 98	0
1	B	345/395 (87%)	0.45	35 (10%) 9 12	28, 43, 75, 97	0
1	C	350/395 (88%)	0.31	20 (5%) 27 35	26, 43, 65, 92	0
1	D	356/395 (90%)	0.46	26 (7%) 18 24	25, 49, 71, 95	0
All	All	1399/1580 (88%)	0.36	97 (6%) 20 27	25, 44, 70, 98	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301	VAL	9.4
1	B	289	LEU	5.8
1	A	104	TRP	5.7
1	D	289	LEU	5.3
1	A	302	GLY	5.0
1	C	34	ALA	4.9
1	D	348	TYR	4.5
1	B	101	SER	4.3
1	D	353	ILE	4.2
1	C	339	ALA	4.1
1	B	314	LEU	4.0
1	B	336	ASN	4.0
1	D	324	PRO	4.0
1	C	136	ASN	3.9
1	B	220	PRO	3.9
1	C	393	THR	3.9
1	B	307	ASN	3.8
1	C	31	SER	3.7
1	B	351	TYR	3.6
1	D	292	PHE	3.6
1	B	303	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	98	ASP	3.5
1	D	34	ALA	3.5
1	B	222	GLN	3.3
1	B	324	PRO	3.2
1	B	288	TYR	3.2
1	C	168	ILE	3.1
1	A	336	ASN	3.1
1	A	232	PHE	3.1
1	D	266	LEU	3.1
1	B	353	ILE	3.0
1	B	348	TYR	3.0
1	D	314	LEU	3.0
1	C	98	ASP	3.0
1	A	208	ALA	3.0
1	C	351	TYR	2.9
1	B	337	ASN	2.9
1	B	390	ILE	2.9
1	D	320	LEU	2.9
1	B	96	ASN	2.9
1	C	314	LEU	2.8
1	B	290	ASP	2.8
1	B	332	ASN	2.8
1	A	206	SER	2.8
1	D	90	ILE	2.8
1	C	52	ASN	2.8
1	D	136	ASN	2.8
1	C	99	ILE	2.7
1	D	336	ASN	2.7
1	B	292	PHE	2.7
1	A	99	ILE	2.7
1	B	340	CYS	2.7
1	B	325	ASP	2.6
1	D	378	GLU	2.6
1	B	386	TYR	2.6
1	C	79	GLY	2.6
1	A	314	LEU	2.6
1	B	98	ASP	2.6
1	C	288	TYR	2.5
1	B	34	ALA	2.5
1	D	27	GLU	2.5
1	B	99	ILE	2.5
1	B	327	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	223	PRO	2.4
1	C	110	LEU	2.4
1	C	310	LEU	2.4
1	C	349	GLU	2.4
1	D	98	ASP	2.4
1	B	334	GLY	2.3
1	A	384	LEU	2.3
1	C	222	GLN	2.3
1	B	352	LYS	2.3
1	B	33	LEU	2.3
1	D	31	SER	2.2
1	A	292	PHE	2.2
1	D	264	ASP	2.2
1	B	376	HIS	2.2
1	D	26	SER	2.2
1	D	352	LYS	2.2
1	C	348	TYR	2.2
1	D	253	VAL	2.2
1	C	289	LEU	2.2
1	B	203	ASP	2.2
1	B	333	TYR	2.2
1	B	254	CYS	2.1
1	D	224	VAL	2.1
1	B	64	ILE	2.1
1	B	207	ASP	2.1
1	D	393	THR	2.1
1	D	110	LEU	2.1
1	D	307	ASN	2.1
1	D	340	CYS	2.1
1	A	38	ASN	2.0
1	D	384	LEU	2.0
1	A	138	TYR	2.0
1	A	263	VAL	2.0
1	A	116	ILE	2.0

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

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, 95th 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(\AA^2)	Q<0.9
2	SO4	B	2010	5/5	0.91	0.12	-0.17	98,102,103,103	0
2	SO4	A	2003	5/5	0.98	0.09	-1.25	46,50,51,51	0
2	SO4	D	2001	5/5	0.99	0.07	-1.28	43,47,48,49	0
2	SO4	B	2002	5/5	0.99	0.06	-2.30	49,53,54,55	0
2	SO4	A	2005	5/5	0.85	0.20	-	106,110,111,112	0
2	SO4	C	2011	5/5	0.79	0.22	-	108,113,113,114	0
2	SO4	B	2008	5/5	0.69	0.28	-	143,147,148,148	0
2	SO4	D	2004	5/5	0.94	0.16	-	71,75,76,77	0
2	SO4	B	2009	5/5	0.87	0.28	-	120,124,125,125	0

6.5 Other polymers [i](#)

There are no such residues in this entry.