Full wwPDB X-ray Structure Validation Report

Feb 1, 2016 – 03:59 PM GMT

PDB ID	:	4DXJ
Title	:	Crystal structure of Trypanosome cruzi farnesyl diphosphate synthase in complex with [2-(n-propylamino)ethane-1,1-diyl]bisphosphonic acid and Mg2+
Authors	:	Aripirala, S.; Amzel, L.M.; Gabelli, S.B.
Deposited on	:	2012-02-27
Resolution	:	2.35 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

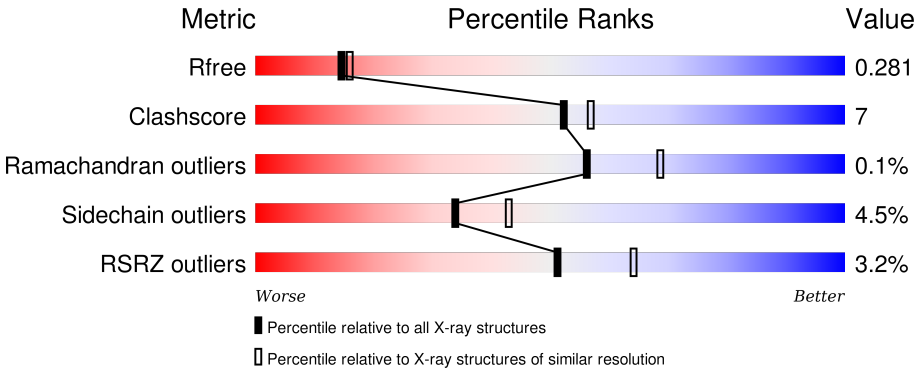
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 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	1352 (2.38-2.34)
Clashscore	102246	1456 (2.38-2.34)
Ramachandran outliers	100387	1435 (2.38-2.34)
Sidechain outliers	100360	1436 (2.38-2.34)
RSRZ outliers	91569	1358 (2.38-2.34)

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 <=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	362	4% 87% 11%
1	B	362	3% 85% 14%
1	C	362	3% 87% 11%

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
4	IPE	B	405	-	-	X	-
5	PEG	A	406	-	-	X	X
5	PEG	B	406	-	-	X	X
5	PEG	C	407	-	-	-	X
5	PEG	C	408	-	-	-	X
7	PGE	B	409	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 9014 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.

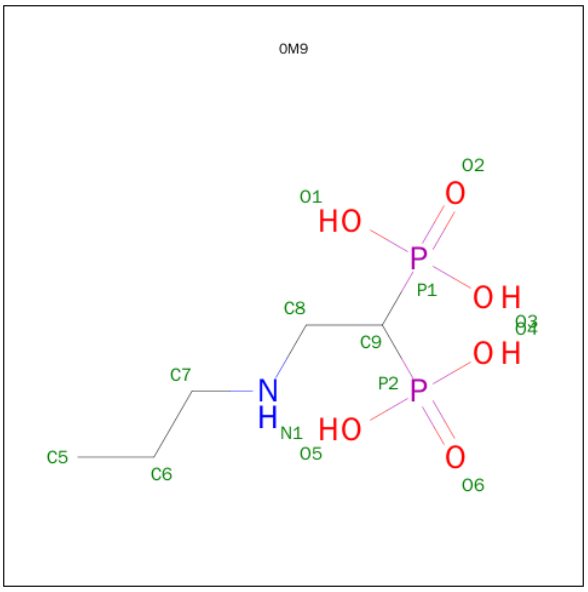
- Molecule 1 is a protein called Farnesyl pyrophosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	2	0
			2907	1866	477	541	23			
1	B	362	Total	C	N	O	S	0	2	0
			2903	1863	475	541	24			
1	C	362	Total	C	N	O	S	0	0	0
			2891	1857	473	538	23			

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

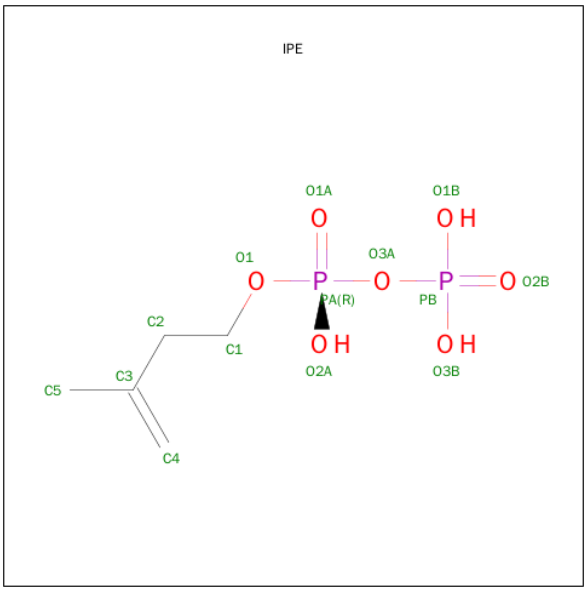
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	3	Total	Mg	0	0
			3	3		
2	A	3	Total	Mg	0	0
			3	3		
2	C	3	Total	Mg	0	0
			3	3		

- Molecule 3 is [2-(PROPYLAMINO)ETHANE-1,1-DIYL]BIS(PHOSPHONIC ACID) (three-letter code: 0M9) (formula: $C_5H_{15}NO_6P_2$).



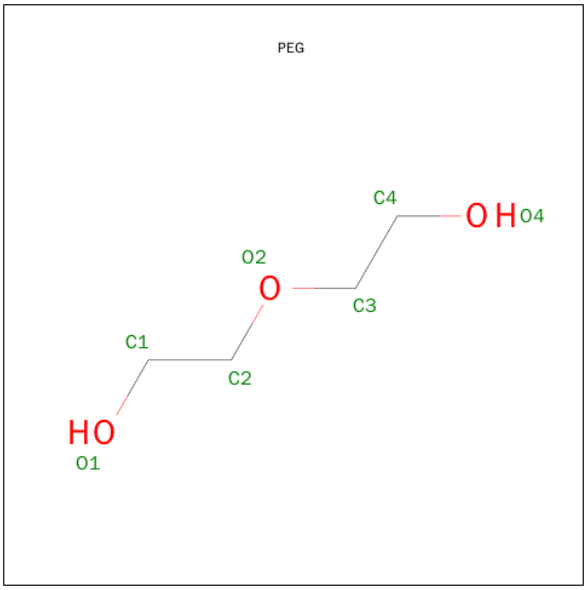
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			14	5	1	6	2		
3	B	1	Total	C	N	O	P	0	0
			14	5	1	6	2		
3	C	1	Total	C	N	O	P	0	0
			14	5	1	6	2		

- Molecule 4 is 3-METHYLBUT-3-ENYL TRIHYDROGEN DIPHOSPHATE (three-letter code: IPE) (formula: $C_5H_{12}O_7P_2$).



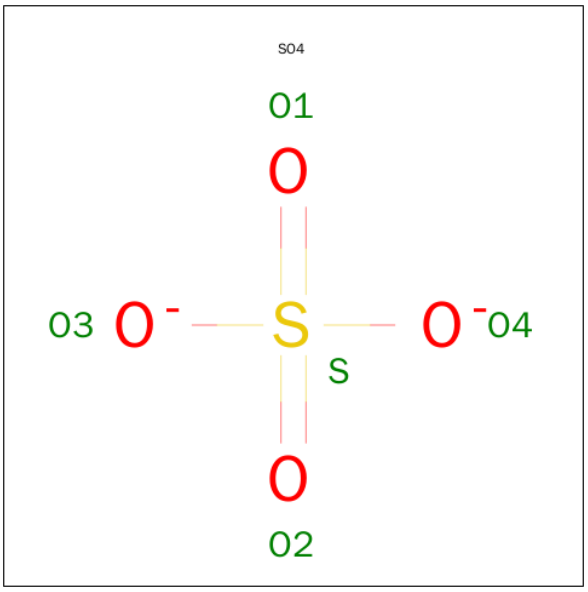
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O P 14 5 7 2	0	0
4	B	1	Total C O P 14 5 7 2	0	0
4	C	1	Total C O P 14 5 7 2	0	0

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



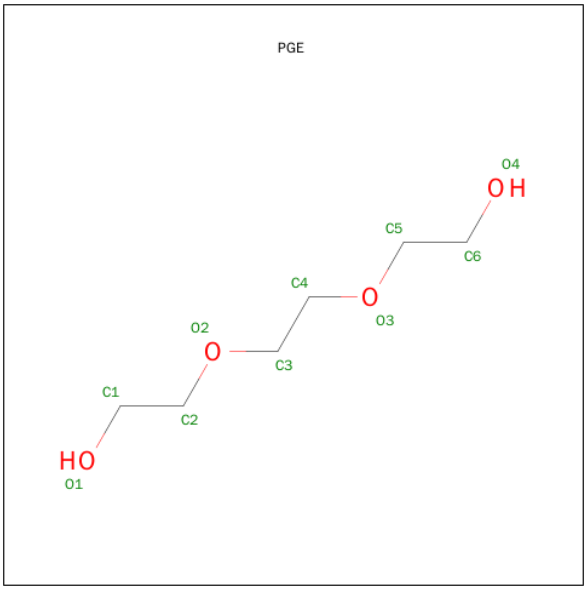
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	B	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0
5	C	1	Total C O 7 4 3	0	0

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



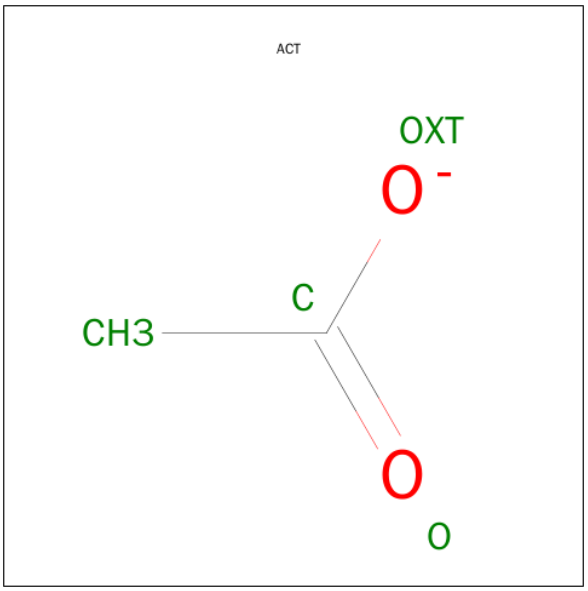
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0

- Molecule 7 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	1	Total C O 10 6 4	0	0

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	1	Total C O 4 2 2	0	0

- Molecule 9 is water.

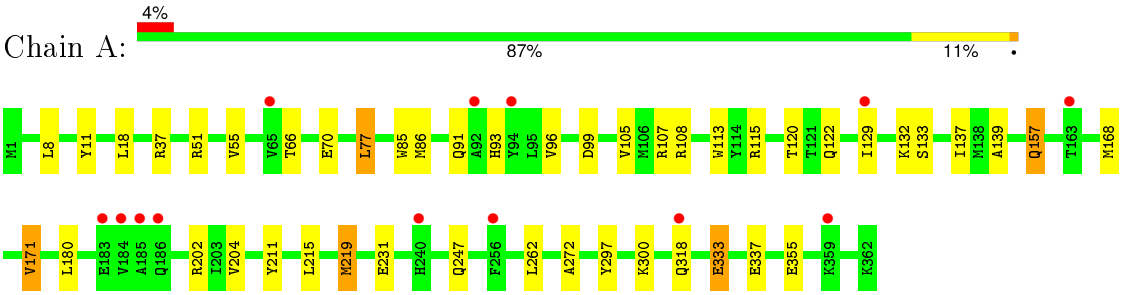
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	55	Total O 55 55	0	0
9	B	62	Total O 62 62	0	0
9	C	44	Total O 44 44	0	0

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.

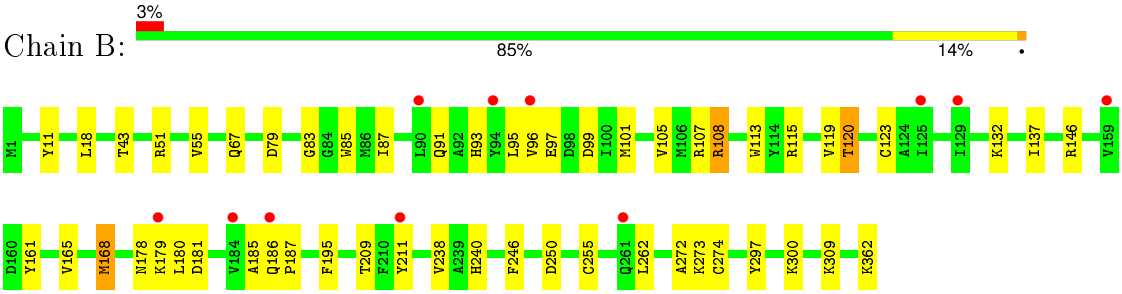
- Molecule 1: Farnesyl pyrophosphate synthase

Chain A:



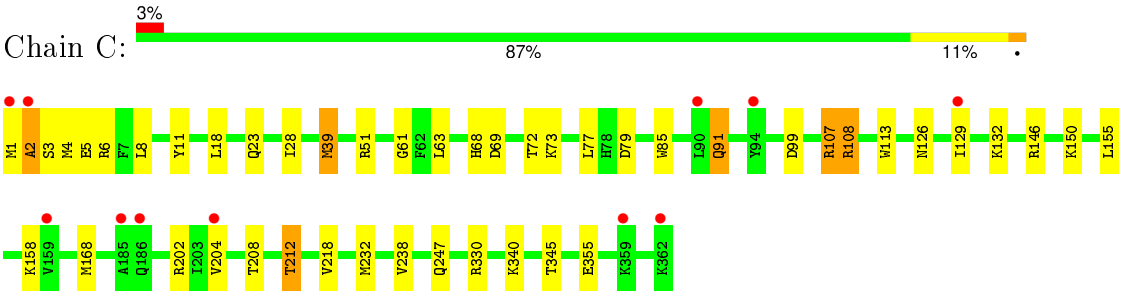
- Molecule 1: Farnesyl pyrophosphate synthase

Chain B:



- Molecule 1: Farnesyl pyrophosphate synthase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	103.22Å 103.22Å 386.66Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	38.72 – 2.35 38.72 – 2.35	Depositor EDS
% Data completeness (in resolution range)	95.2 (38.72-2.35) 95.3 (38.72-2.35)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.220 , 0.285 0.216 , 0.281	Depositor DCC
R_{free} test set	2537 reflections (5.42%)	DCC
Wilson B-factor (Å^2)	40.3	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 33.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	2 of 49555 reflections (0.004%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9014	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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, 0.375 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, PGE, IPE, 0M9, SO4, ACT, PEG

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	0.47	0/2973	0.56	0/4028
1	B	0.49	0/2968	0.58	0/4021
1	C	0.45	0/2956	0.55	0/4004
All	All	0.47	0/8897	0.57	0/12053

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	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	2	ALA	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	2907	0	2867	33	0
1	B	2903	0	2865	53	0
1	C	2891	0	2856	33	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
3	A	14	0	13	3	0
3	B	14	0	13	1	0
3	C	14	0	13	0	0
4	A	14	0	9	5	0
4	B	14	0	9	7	0
4	C	14	0	9	3	0
5	A	7	0	10	7	0
5	B	14	0	20	8	0
5	C	14	0	20	2	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	B	10	0	14	10	0
8	C	4	0	3	0	0
9	A	55	0	0	0	0
9	B	62	0	0	0	0
9	C	44	0	0	2	0
All	All	9014	0	8721	117	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 7.

All (117) 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:B:113:TRP:H	5:B:406:PEG:H22	1.10	1.14
3:A:404:0M9:H7	4:A:405:IPE:H22	1.27	1.11
1:A:132:LYS:HB3	7:B:409:PGE:H6	1.35	1.06
1:B:132:LYS:HD2	7:B:409:PGE:H12	1.43	0.97
1:C:51:ARG:HH11	1:C:212:THR:HB	1.37	0.87
1:B:96:VAL:HA	5:B:406:PEG:H11	1.56	0.86
1:A:96:VAL:HA	5:A:406:PEG:H22	1.59	0.84
3:A:404:0M9:H7	4:A:405:IPE:C2	2.09	0.83
1:B:51:ARG:HH22	4:B:405:IPE:H11	1.49	0.78
1:B:113:TRP:N	5:B:406:PEG:H22	1.96	0.76
1:C:208:THR:O	1:C:212:THR:HG23	1.84	0.76
1:A:91:GLN:HG3	1:A:211:TYR:HE1	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:VAL:HA	5:A:406:PEG:C2	2.19	0.72
1:A:99:ASP:HB2	5:A:406:PEG:H11	1.70	0.72
1:B:79:ASP:OD1	1:B:146:ARG:NH1	2.23	0.72
1:B:51:ARG:HH22	4:B:405:IPE:C1	2.04	0.70
3:A:404:0M9:C8	4:A:405:IPE:H22	2.15	0.69
1:B:132:LYS:HB3	7:B:409:PGE:H12	1.75	0.68
1:B:119:VAL:O	1:B:120:THR:HG22	1.96	0.66
1:A:91:GLN:HG3	1:A:211:TYR:CE1	2.30	0.65
1:C:51:ARG:HD3	1:C:212:THR:HB	1.78	0.64
1:A:113:TRP:N	5:A:406:PEG:H12	2.14	0.63
1:B:99:ASP:HB2	5:B:406:PEG:H12	1.78	0.63
1:A:211:TYR:OH	4:A:405:IPE:H41	1.99	0.62
1:C:99:ASP:OD2	1:C:107:ARG:HD2	1.99	0.62
1:A:132:LYS:CB	7:B:409:PGE:H6	2.23	0.62
1:C:1:MET:HG3	1:C:2:ALA:H	1.65	0.62
1:C:51:ARG:NH2	1:C:91:GLN:OE1	2.32	0.61
1:A:113:TRP:H	5:A:406:PEG:H12	1.66	0.61
4:C:405:IPE:H21	4:C:405:IPE:O2A	1.99	0.61
1:A:157:GLN:HE21	1:B:137:ILE:HD13	1.66	0.60
1:C:51:ARG:NH1	1:C:212:THR:HB	2.12	0.60
1:B:250:ASP:OD1	4:B:405:IPE:H42	2.02	0.60
1:A:105:VAL:HA	1:A:115:ARG:HD3	1.83	0.59
1:B:120:THR:HG22	1:B:123[A]:CYS:SG	2.43	0.59
1:C:1:MET:HG3	1:C:2:ALA:N	2.18	0.58
1:B:181:ASP:H	1:B:186:GLN:HE22	1.51	0.58
1:A:107:ARG:HG3	1:A:108:ARG:HG3	1.85	0.58
1:C:51:ARG:HH22	4:C:405:IPE:PA	2.26	0.57
1:A:333:GLU:O	1:A:337:GLU:HG2	2.04	0.57
1:C:2:ALA:O	1:C:4:MET:N	2.38	0.56
1:C:204:VAL:HG22	1:C:247:GLN:HG2	1.85	0.56
1:B:181:ASP:H	1:B:186:GLN:NE2	2.03	0.56
1:A:96:VAL:HG22	5:A:406:PEG:H21	1.88	0.56
1:B:99:ASP:CB	5:B:406:PEG:H12	2.37	0.55
1:B:96:VAL:HA	5:B:406:PEG:C1	2.31	0.54
1:A:51:ARG:NH2	4:A:405:IPE:O1A	2.41	0.53
1:B:51:ARG:NH2	4:B:405:IPE:C1	2.70	0.53
1:A:8:LEU:HD13	1:C:5:GLU:HG3	1.89	0.53
1:A:99:ASP:CB	5:A:406:PEG:H11	2.39	0.53
1:B:97:GLU:O	1:B:101:MET:HG3	2.09	0.52
1:B:132:LYS:CD	7:B:409:PGE:H12	2.28	0.52
1:B:93:HIS:NE2	1:B:132:LYS:HE3	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ASN:ND2	1:B:179:LYS:HD2	2.25	0.51
1:B:99:ASP:HB2	5:B:406:PEG:C1	2.41	0.50
1:B:93:HIS:CD2	1:B:132:LYS:HE3	2.46	0.50
1:B:51:ARG:NH2	4:B:405:IPE:H12	2.26	0.50
1:A:204:VAL:HG22	1:A:247:GLN:HG2	1.94	0.50
1:C:69:ASP:HB3	1:C:72:THR:H	1.77	0.49
1:C:63:LEU:HD22	1:C:73:LYS:HG2	1.94	0.48
1:A:132:LYS:HD3	7:B:409:PGE:H32	1.95	0.48
1:A:11:TYR:HB2	1:A:85:TRP:CZ2	2.49	0.48
1:C:8:LEU:O	1:C:11:TYR:HB3	2.14	0.48
1:C:79:ASP:OD1	1:C:146:ARG:NH1	2.47	0.48
1:C:51:ARG:HH11	1:C:212:THR:CB	2.18	0.48
1:C:11:TYR:HB2	1:C:85:TRP:CZ2	2.48	0.48
1:A:93:HIS:NE2	1:A:132:LYS:HE3	2.29	0.47
1:B:79:ASP:CG	1:B:146:ARG:NH1	2.67	0.47
1:B:11:TYR:HB2	1:B:85:TRP:CZ2	2.49	0.47
1:B:91:GLN:NE2	4:B:405:IPE:H12	2.30	0.47
1:A:272:ALA:HA	1:A:297:TYR:CE2	2.50	0.47
1:A:157:GLN:NE2	1:B:137:ILE:HD13	2.30	0.47
1:B:272:ALA:HA	1:B:297:TYR:CE2	2.50	0.47
1:B:246:PHE:HE1	4:B:405:IPE:H52	1.81	0.46
1:B:107:ARG:HH12	3:B:404:0M9:H1	1.63	0.46
1:A:171:VAL:CG1	1:B:123[A]:CYS:HB3	2.46	0.46
1:B:11:TYR:HB2	1:B:85:TRP:CE2	2.49	0.46
1:B:132:LYS:HB3	7:B:409:PGE:C1	2.42	0.46
1:B:165:VAL:O	1:B:168:MET:HG3	2.16	0.46
1:B:105:VAL:HA	1:B:115:ARG:HD3	1.97	0.46
1:B:119:VAL:O	1:B:123[A]:CYS:SG	2.74	0.46
1:A:37:ARG:HH11	1:A:37:ARG:HG3	1.80	0.45
1:B:209:THR:OG1	1:B:240:HIS:HD2	2.00	0.45
1:A:215:LEU:O	1:A:219:MET:HB3	2.16	0.45
1:C:1:MET:CG	1:C:2:ALA:H	2.25	0.45
1:C:61:GLY:O	1:C:345:THR:HG21	2.18	0.44
1:B:255:CYS:SG	1:B:309:LYS:HG2	2.57	0.44
1:B:107:ARG:HG3	1:B:108:ARG:HG3	1.98	0.44
1:C:126:ASN:HA	1:C:129:ILE:HD12	1.99	0.44
1:A:77:LEU:HA	1:A:77:LEU:HD12	1.90	0.44
1:A:157:GLN:HE21	1:B:137:ILE:HA	1.81	0.44
1:A:120:THR:HB	1:A:122:GLN:NE2	2.32	0.44
1:C:73:LYS:HE2	9:C:530:HOH:O	2.18	0.43
1:B:83:GLY:O	1:B:87:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:LYS:NZ	9:C:513:HOH:O	2.40	0.43
1:B:180:LEU:HA	1:B:186:GLN:HE22	1.83	0.43
1:C:39:MET:HB2	1:C:113:TRP:CZ2	2.53	0.43
1:C:6:ARG:CZ	1:C:77:LEU:HD23	2.48	0.43
1:A:137:ILE:HD11	1:B:161:TYR:CG	2.54	0.43
1:C:23:GLN:HA	1:C:28:ILE:HG22	2.01	0.42
1:C:155:LEU:HD13	5:C:407:PEG:H42	2.00	0.42
1:B:132:LYS:HD2	7:B:409:PGE:C1	2.30	0.42
1:A:129:ILE:HG23	7:B:409:PGE:HO4	1.84	0.42
1:A:86:MET:HE1	1:A:139:ALA:HB2	2.01	0.42
1:B:43:THR:HG22	5:B:406:PEG:H32	2.00	0.42
1:B:91:GLN:HG3	1:B:211:TYR:HE1	1.84	0.42
1:B:91:GLN:NE2	1:B:95:LEU:HD11	2.35	0.42
1:B:132:LYS:NZ	7:B:409:PGE:O4	2.48	0.42
1:C:155:LEU:HD22	1:C:218:VAL:HG11	2.01	0.42
1:C:108:ARG:HD3	4:C:405:IPE:O1B	2.20	0.41
1:C:39:MET:CB	1:C:113:TRP:CZ2	3.02	0.41
1:B:273:LYS:HD3	1:B:273:LYS:HA	1.95	0.41
1:C:232:MET:CG	5:C:407:PEG:H32	2.51	0.41
1:C:208:THR:O	1:C:212:THR:CG2	2.63	0.40
1:B:195:PHE:CE2	1:B:274:CYS:HA	2.56	0.40
1:C:68:HIS:CD2	1:C:72:THR:HG21	2.57	0.40
1:B:185:ALA:O	1:B:187:PRO:HD3	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	362/362 (100%)	356 (98%)	6 (2%)	0	100	100
1	B	362/362 (100%)	356 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	360/362 (99%)	352 (98%)	7 (2%)	1 (0%)	46 55
All	All	1084/1086 (100%)	1064 (98%)	19 (2%)	1 (0%)	56 69

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	3	SER

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	311/309 (101%)	293 (94%)	18 (6%)	25 29
1	B	311/309 (101%)	301 (97%)	10 (3%)	46 59
1	C	309/309 (100%)	295 (96%)	14 (4%)	34 43
All	All	931/927 (100%)	889 (96%)	42 (4%)	34 43

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	55	VAL
1	A	66	THR
1	A	70	GLU
1	A	77	LEU
1	A	133	SER
1	A	157	GLN
1	A	168	MET
1	A	171	VAL
1	A	180	LEU
1	A	202	ARG
1	A	219	MET
1	A	231	GLU
1	A	262	LEU

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Mol	Chain	Res	Type
1	A	300	LYS
1	A	318	GLN
1	A	333	GLU
1	A	355	GLU
1	B	18	LEU
1	B	55	VAL
1	B	67	GLN
1	B	108	ARG
1	B	120	THR
1	B	168	MET
1	B	238	VAL
1	B	262	LEU
1	B	300	LYS
1	B	362	LYS
1	C	18	LEU
1	C	39	MET
1	C	91	GLN
1	C	107	ARG
1	C	108	ARG
1	C	150	LYS
1	C	158	LYS
1	C	168	MET
1	C	202	ARG
1	C	212	THR
1	C	238	VAL
1	C	330	ARG
1	C	340	LYS
1	C	355	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	GLN
1	A	122	GLN
1	A	157	GLN
1	A	318	GLN
1	B	67	GLN
1	B	78	HIS
1	B	91	GLN
1	B	178	ASN
1	B	186	GLN
1	B	240	HIS

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Mol	Chain	Res	Type
1	C	91	GLN
1	C	338	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

Of 24 ligands modelled in this entry, 9 are monoatomic - leaving 15 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	0M9	A	404	2	12,13,13	1.31	1 (8%)	13,19,19	1.45	3 (23%)
4	IPE	A	405	-	10,13,13	0.51	0	14,19,19	1.06	1 (7%)
5	PEG	A	406	-	6,6,6	0.66	0	5,5,5	0.41	0
6	SO4	A	407	-	4,4,4	0.23	0	6,6,6	0.19	0
3	0M9	B	404	2	12,13,13	1.57	4 (33%)	13,19,19	1.71	4 (30%)
4	IPE	B	405	-	10,13,13	0.56	0	14,19,19	1.20	0
5	PEG	B	406	-	6,6,6	0.59	0	5,5,5	0.50	0
5	PEG	B	407	-	6,6,6	0.54	0	5,5,5	0.22	0
6	SO4	B	408	-	4,4,4	0.21	0	6,6,6	0.19	0
7	PGE	B	409	-	9,9,9	0.57	0	8,8,8	0.32	0
3	0M9	C	404	2	12,13,13	1.33	0	13,19,19	2.08	4 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	IPE	C	405	-	10,13,13	0.64	0	14,19,19	1.09	0
8	ACT	C	406	-	1,3,3	1.14	0	0,3,3	0.00	-
5	PEG	C	407	-	6,6,6	0.48	0	5,5,5	0.36	0
5	PEG	C	408	-	6,6,6	0.49	0	5,5,5	0.32	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	0M9	A	404	2	-	0/15/17/17	0/0/0/0
4	IPE	A	405	-	-	0/13/13/13	0/0/0/0
5	PEG	A	406	-	-	0/4/4/4	0/0/0/0
6	SO4	A	407	-	-	0/0/0/0	0/0/0/0
3	0M9	B	404	2	-	0/15/17/17	0/0/0/0
4	IPE	B	405	-	-	0/13/13/13	0/0/0/0
5	PEG	B	406	-	-	0/4/4/4	0/0/0/0
5	PEG	B	407	-	-	0/4/4/4	0/0/0/0
6	SO4	B	408	-	-	0/0/0/0	0/0/0/0
7	PGE	B	409	-	-	0/7/7/7	0/0/0/0
3	0M9	C	404	2	-	0/15/17/17	0/0/0/0
4	IPE	C	405	-	-	0/13/13/13	0/0/0/0
8	ACT	C	406	-	-	0/0/0/0	0/0/0/0
5	PEG	C	407	-	-	0/4/4/4	0/0/0/0
5	PEG	C	408	-	-	0/4/4/4	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	404	0M9	P2-O5	-2.41	1.50	1.54
3	B	404	0M9	P2-O4	-2.41	1.50	1.54
3	B	404	0M9	P1-O1	-2.37	1.50	1.54
3	B	404	0M9	P1-O3	-2.28	1.51	1.54
3	A	404	0M9	P1-O1	-2.28	1.51	1.54

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	404	0M9	C9-C8-N1	-4.26	103.28	112.13
3	B	404	0M9	C9-C8-N1	-3.17	105.55	112.13
3	A	404	0M9	C9-C8-N1	-3.03	105.83	112.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	404	0M9	O3-P1-C9	-2.72	96.90	106.44
3	B	404	0M9	O5-P2-C9	-2.71	96.92	106.44
3	C	404	0M9	O5-P2-C9	-2.32	98.30	106.44
3	B	404	0M9	O3-P1-C9	-2.10	99.07	106.44
3	A	404	0M9	O5-P2-O4	2.08	113.82	107.57
4	A	405	IPE	O3B-PB-O1B	2.36	116.37	107.38
3	A	404	0M9	C8-N1-C7	2.77	119.96	113.53
3	B	404	0M9	C8-N1-C7	3.17	120.89	113.53
3	C	404	0M9	C8-N1-C7	4.21	123.32	113.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 43 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	0M9	3	0
4	A	405	IPE	5	0
5	A	406	PEG	7	0
3	B	404	0M9	1	0
4	B	405	IPE	7	0
5	B	406	PEG	8	0
7	B	409	PGE	10	0
4	C	405	IPE	3	0
5	C	407	PEG	2	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^{th} 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	362/362 (100%)	0.21	13 (3%)	46	60	26, 41, 59, 74	0
1	B	362/362 (100%)	0.14	11 (3%)	54	66	25, 36, 50, 60	0
1	C	362/362 (100%)	0.22	11 (3%)	54	66	25, 41, 57, 66	0
All	All	1086/1086 (100%)	0.19	35 (3%)	51	64	25, 39, 57, 74	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	186	GLN	4.8
1	A	65	VAL	4.3
1	B	129	ILE	3.8
1	A	129	ILE	3.7
1	B	94	TYR	3.7
1	C	129	ILE	3.3
1	A	184	VAL	3.3
1	C	94	TYR	3.3
1	A	185	ALA	3.0
1	A	94	TYR	2.9
1	C	185	ALA	2.8
1	A	318	GLN	2.7
1	C	159	VAL	2.7
1	C	2	ALA	2.6
1	A	183	GLU	2.6
1	B	179	LYS	2.6
1	B	90	LEU	2.5
1	A	163	THR	2.4
1	C	359	LYS	2.4
1	C	362	LYS	2.4
1	B	184	VAL	2.4
1	C	204	VAL	2.4
1	A	256	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	261	GLN	2.2
1	B	211	TYR	2.2
1	C	90	LEU	2.2
1	A	186	GLN	2.2
1	A	92	ALA	2.2
1	A	359	LYS	2.2
1	C	186	GLN	2.2
1	B	159	VAL	2.1
1	B	125	ILE	2.1
1	B	96	VAL	2.1
1	C	1	MET	2.1
1	A	240[A]	HIS	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^{th} 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^2)	Q<0.9
5	PEG	A	406	7/7	0.86	0.31	4.16	40,44,47,47	0
5	PEG	C	408	7/7	0.74	0.20	3.72	62,63,64,65	0
5	PEG	B	406	7/7	0.83	0.33	2.87	45,46,48,48	0
5	PEG	C	407	7/7	0.76	0.27	2.79	64,64,65,65	0
7	PGE	B	409	10/10	0.80	0.28	0.86	33,44,46,47	0
2	MG	B	401	1/1	0.81	0.18	0.63	33,33,33,33	0
4	IPE	C	405	14/14	0.92	0.18	0.28	48,56,58,58	0
3	0M9	C	404	14/14	0.96	0.16	-0.22	29,33,34,34	0
3	0M9	B	404	14/14	0.98	0.14	-0.39	30,33,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	0M9	A	404	14/14	0.95	0.12	-0.58	31,34,36,36	0
2	MG	A	401	1/1	0.81	0.13	-0.85	35,35,35,35	0
4	IPE	A	405	14/14	0.96	0.12	-0.95	44,48,50,50	0
4	IPE	B	405	14/14	0.97	0.10	-0.99	39,45,48,48	0
2	MG	C	403	1/1	0.97	0.09	-1.42	35,35,35,35	0
2	MG	C	401	1/1	0.97	0.12	-1.46	35,35,35,35	0
2	MG	B	403	1/1	0.98	0.08	-1.51	28,28,28,28	0
2	MG	A	403	1/1	0.97	0.08	-1.88	34,34,34,34	0
5	PEG	B	407	7/7	0.62	0.43	-	58,60,61,61	0
6	SO4	A	407	5/5	0.94	0.17	-	66,66,66,67	0
8	ACT	C	406	4/4	0.91	0.10	-	61,61,61,61	0
2	MG	B	402	1/1	0.87	0.13	-	30,30,30,30	0
2	MG	C	402	1/1	0.90	0.13	-	32,32,32,32	0
2	MG	A	402	1/1	0.86	0.16	-	35,35,35,35	0
6	SO4	B	408	5/5	0.92	0.16	-	68,69,69,69	0

6.5 Other polymers (i)

There are no such residues in this entry.