Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:44 PM GMT

PDB ID	:	1YHM
Title	:	Structure of the complex of Trypanosoma cruzi farnesyl disphosphate synthase with alendronate, Isopentenyl diphosphate and mg+2
Authors	:	Gabelli, S.B.; McLellan, J.S.; Montalvetti, A.; Oldfield, E.; Docampo, R.; Amzel, L.M.
Deposited on	:	2005-01-09
Resolution	:	2.50 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 (i)) were used in the production of this report:

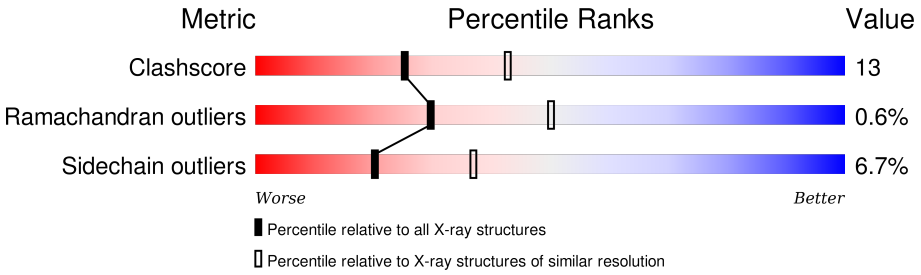
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	362	74% 22%
1	B	362	74% 22%
1	C	362	77% 21%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8891 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	Se	0	0	0
			2891	1857	473	538	8	15			
1	B	362	Total	C	N	O	S	Se	0	0	0
			2891	1857	473	538	8	15			
1	C	362	Total	C	N	O	S	Se	0	0	0
			2891	1857	473	538	8	15			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
A	39	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
A	40	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
A	53	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
A	86	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
A	101	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
A	106	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
A	138	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
A	168	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
A	174	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
A	188	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
A	219	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
A	232	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
A	253	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
B	4	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
B	39	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
B	40	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
B	53	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
B	86	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
B	101	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
B	106	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
B	138	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
B	168	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26

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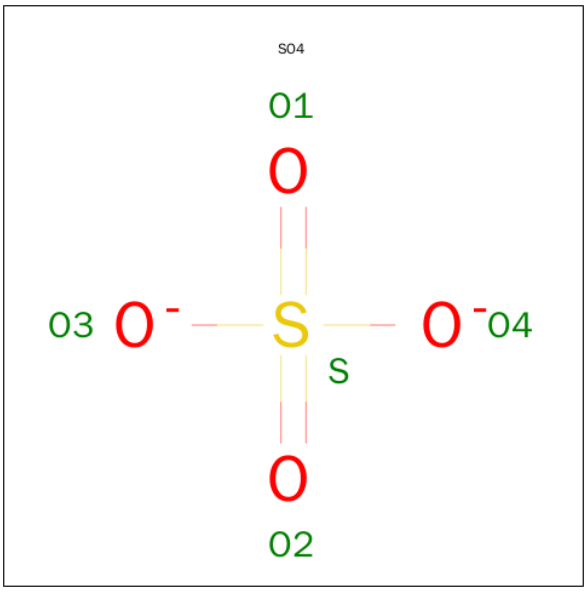
Chain	Residue	Modelled	Actual	Comment	Reference
B	174	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
B	188	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
B	219	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
B	232	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
B	253	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
C	4	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
C	39	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
C	40	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
C	53	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
C	86	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
C	101	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
C	106	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
C	138	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
C	168	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
C	174	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
C	188	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
C	219	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
C	232	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26
C	253	MSE	MET	MODIFIED RESIDUE	UNP Q8WS26

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

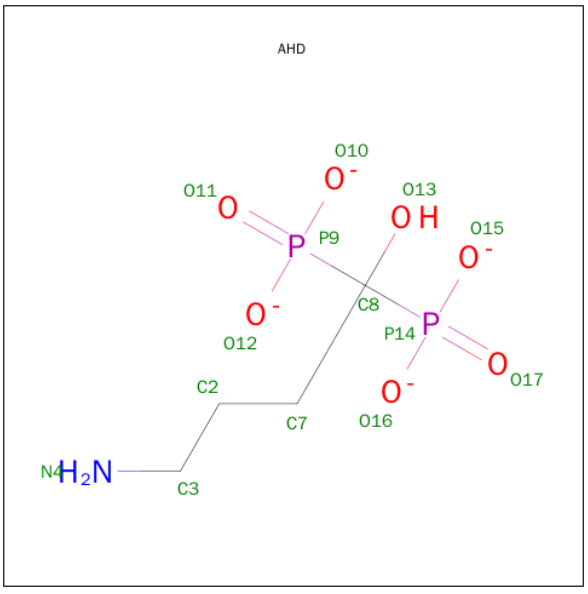
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	3	Total Mg 3 3	0	0
2	A	3	Total Mg 3 3	0	0
2	C	3	Total Mg 3 3	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



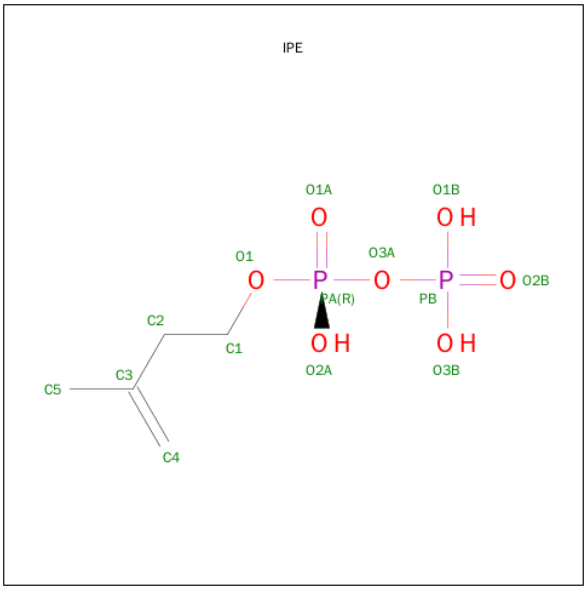
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is 4-AMINO-1-HYDROXYBUTANE-1,1-DIYLDIPHOSPHONATE (three-letter code: AHD) (formula: $C_4H_9NO_7P_2$).



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

- Molecule 5 is 3-METHYLBUT-3-ENYL TRIHYDROGEN DIPHOSPHATE (three-letter code: IPE) (formula: $C_5H_{12}O_7P_2$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	35	Total O 35 35	0	0
6	B	42	Total O 42 42	0	0
6	C	33	Total O 33 33	0	0

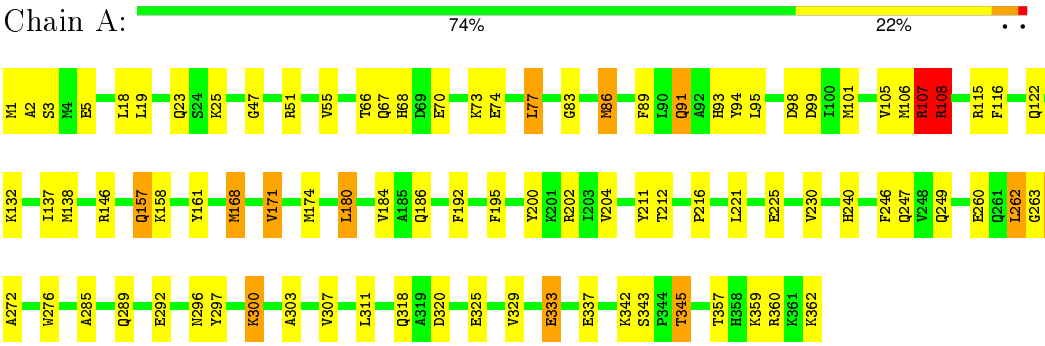
3 Residue-property plots (i)

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.

Note EDS was not executed.

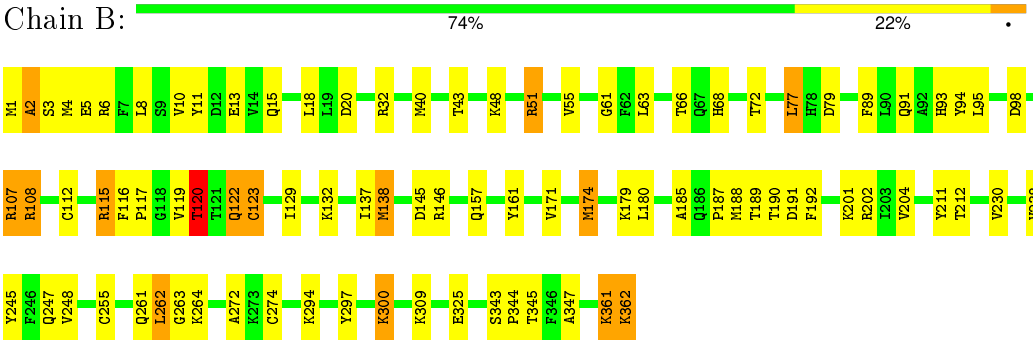
- Molecule 1: farnesyl pyrophosphate synthase

Chain A:



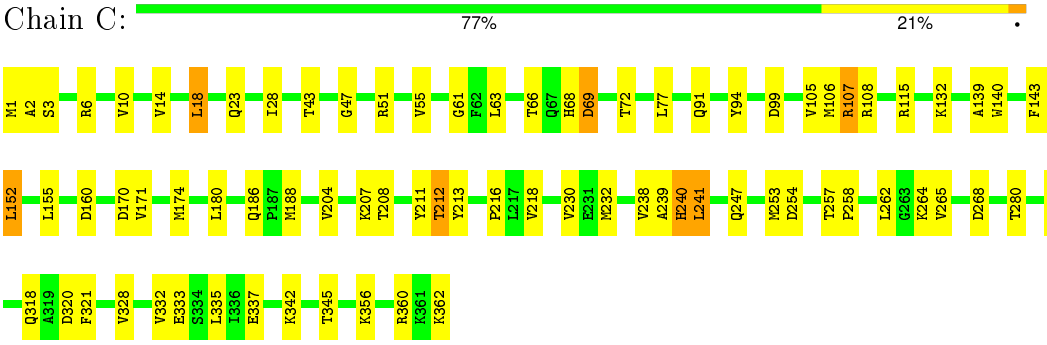
- Molecule 1: farnesyl pyrophosphate synthase

Chain B:



- Molecule 1: farnesyl pyrophosphate synthase

Chain C:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	103.20Å 103.20Å 385.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	87.71 – 2.50	Depositor
% Data completeness (in resolution range)	99.9 (87.71-2.50)	Depositor
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.208 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8891	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.85	1/2942 (0.0%)	0.90	6/3962 (0.2%)
1	B	0.86	2/2942 (0.1%)	0.87	3/3962 (0.1%)
1	C	0.82	2/2942 (0.1%)	0.83	2/3962 (0.1%)
All	All	0.85	5/8826 (0.1%)	0.87	11/11886 (0.1%)

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	1
1	C	0	1
All	All	0	2

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	240	HIS	C-N	8.65	1.53	1.34
1	B	274	CYS	CB-SG	-6.92	1.70	1.82
1	B	138	MSE	SE-CE	-5.91	1.60	1.95
1	A	94	TYR	CD1-CE1	5.82	1.48	1.39
1	C	241	LEU	N-CA	5.46	1.57	1.46

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	240	HIS	C-N-CA	-12.13	91.38	121.70
1	A	108	ARG	NE-CZ-NH1	9.91	125.26	120.30
1	C	240	HIS	CA-C-N	-8.47	98.56	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	108	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	A	268	ASP	CB-CG-OD1	6.59	124.23	118.30
1	B	107	ARG	CG-CD-NE	-5.85	99.51	111.80
1	A	107	ARG	CG-CD-NE	-5.71	99.80	111.80
1	A	146	ARG	NE-CZ-NH1	5.67	123.13	120.30
1	B	94	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	A	107	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	107	ARG	NE-CZ-NH2	-5.05	117.78	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	361	LYS	Peptide
1	C	240	HIS	Mainchain

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	2891	0	2856	82	0
1	B	2891	0	2856	84	1
1	C	2891	0	2856	56	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	0	0
4	A	14	0	8	5	0
4	B	14	0	8	3	0
4	C	14	0	5	4	0
5	A	14	0	9	3	0
5	B	14	0	9	3	0
5	C	14	0	9	3	0
6	A	35	0	0	7	0
6	B	42	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	33	0	0	3	0
All	All	8891	0	8616	218	1

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 13.

All (218) 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:1:MSE:CE	1:B:1:MSE:SE	2.14	1.46
1:A:300:LYS:HG2	6:A:936:HOH:O	1.61	0.99
1:A:137:ILE:HG13	1:B:157:GLN:NE2	1.77	0.99
1:B:145:ASP:HB3	6:B:1922:HOH:O	1.60	0.99
1:B:91:GLN:HE21	1:B:95:LEU:HD11	1.27	0.98
1:A:91:GLN:NE2	1:A:95:LEU:HD11	1.82	0.94
1:A:106:MSE:HE3	1:A:263:GLY:C	1.95	0.87
1:A:345:THR:HG22	6:A:925:HOH:O	1.77	0.84
1:B:51:ARG:CZ	1:B:91:GLN:OE1	2.27	0.83
1:C:106:MSE:HE3	1:C:265:VAL:HG23	1.59	0.83
1:B:79:ASP:OD1	1:B:146:ARG:NH1	2.12	0.82
1:B:61:GLY:O	1:B:345:THR:HG21	1.80	0.81
4:A:901:AHD:H72	5:A:900:IPE:H22	1.64	0.80
1:B:106:MSE:HE3	1:B:263:GLY:C	2.03	0.79
1:A:157:GLN:OE1	1:A:158:LYS:HG2	1.82	0.79
1:A:2:ALA:HA	1:A:5:GLU:OE1	1.81	0.79
1:B:89:PHE:CD2	1:B:138:MSE:HE1	2.17	0.78
1:A:360:ARG:NH1	1:A:362:LYS:HG3	1.99	0.78
1:B:2:ALA:O	1:B:3:SER:HB3	1.83	0.78
1:C:51:ARG:NH2	1:C:91:GLN:HE22	1.82	0.76
1:B:300:LYS:H	1:B:300:LYS:HD3	1.50	0.76
1:B:51:ARG:NH1	1:B:212:THR:OG1	2.19	0.75
1:C:208:THR:O	1:C:212:THR:HG23	1.86	0.75
1:A:137:ILE:HG13	1:B:157:GLN:HE22	1.51	0.74
1:B:190:THR:O	1:B:294:LYS:HD3	1.88	0.74
1:B:119:VAL:O	1:B:120:THR:CG2	2.37	0.73
1:C:51:ARG:NH2	1:C:91:GLN:NE2	2.37	0.73
1:A:1:MSE:C	1:A:3:SER:H	1.90	0.72
1:C:69:ASP:HB2	1:C:72:THR:HB	1.71	0.72
1:A:91:GLN:HE21	1:A:95:LEU:HD11	1.55	0.72
1:C:174:MSE:H	1:C:174:MSE:SE	2.23	0.71
1:B:20:ASP:HB3	6:B:1925:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:GLY:O	1:C:345:THR:HG21	1.90	0.71
1:B:119:VAL:O	1:B:120:THR:HG23	1.92	0.70
1:A:168:MSE:HE1	1:B:32:ARG:CD	2.22	0.69
1:A:168:MSE:HE1	1:B:32:ARG:HD3	1.75	0.69
1:C:328:VAL:O	1:C:332:VAL:HG23	1.93	0.68
1:A:91:GLN:HE21	1:A:95:LEU:CD1	2.08	0.66
1:B:300:LYS:N	1:B:300:LYS:HD3	2.10	0.66
1:B:61:GLY:C	1:B:345:THR:HG21	2.16	0.66
1:C:107:ARG:NH2	4:C:2901:AHD:O10	2.26	0.66
1:B:63:LEU:HD11	1:B:77:LEU:HD13	1.78	0.65
1:B:185:ALA:O	1:B:187:PRO:HD3	1.96	0.65
1:B:98:ASP:HA	1:B:101:MSE:CE	2.27	0.64
1:B:264:LYS:NZ	4:B:1901:AHD:O10	2.29	0.64
1:A:91:GLN:HE22	1:A:95:LEU:HD11	1.63	0.63
1:B:261:GLN:NE2	1:B:361:LYS:O	2.30	0.63
1:A:91:GLN:NE2	1:A:95:LEU:CD1	2.61	0.63
1:B:91:GLN:NE2	1:B:95:LEU:HD11	2.07	0.62
1:A:91:GLN:HG3	1:A:211:TYR:HE1	1.64	0.62
1:A:171:VAL:HG22	1:B:122:GLN:HE21	1.63	0.62
1:A:137:ILE:HD11	1:B:161:TYR:CD2	2.35	0.61
1:A:51:ARG:NH2	1:A:91:GLN:OE1	2.34	0.61
1:A:51:ARG:CZ	1:A:91:GLN:OE1	2.49	0.60
1:A:157:GLN:OE1	1:A:158:LYS:CG	2.49	0.60
1:A:161:TYR:CG	1:B:137:ILE:HD11	2.36	0.60
1:B:3:SER:HB2	1:B:6:ARG:NH2	2.17	0.60
1:A:300:LYS:CG	6:A:936:HOH:O	2.33	0.60
1:C:63:LEU:HD11	1:C:77:LEU:HD13	1.82	0.59
1:C:99:ASP:OD2	1:C:107:ARG:HD2	2.03	0.59
1:A:106:MSE:HE3	1:A:263:GLY:CA	2.32	0.58
1:C:204:VAL:HG22	1:C:247:GLN:HG2	1.85	0.58
1:C:239:ALA:C	1:C:241:LEU:N	2.54	0.58
1:C:105:VAL:HA	1:C:115:ARG:HD3	1.85	0.58
1:A:51:ARG:NH1	1:A:211:TYR:CE1	2.71	0.58
1:B:63:LEU:CD1	1:B:77:LEU:HD13	2.32	0.58
1:A:68:HIS:HB2	1:A:73:LYS:HG3	1.86	0.57
1:A:272:ALA:HA	1:A:297:TYR:CE2	2.40	0.56
1:C:51:ARG:HH22	1:C:91:GLN:HE22	1.52	0.56
1:C:69:ASP:HB2	1:C:72:THR:CB	2.34	0.56
1:A:360:ARG:HH11	1:A:362:LYS:HE3	1.71	0.56
1:B:98:ASP:HA	1:B:101:MSE:HE3	1.86	0.56
1:A:132:LYS:HZ2	1:B:129:ILE:HG23	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:901:AHD:H32	5:A:900:IPE:H53	1.87	0.54
1:A:161:TYR:CD2	1:B:137:ILE:HD11	2.42	0.54
1:B:68:HIS:HB3	1:B:72:THR:HB	1.88	0.54
1:A:360:ARG:HH11	1:A:362:LYS:HG3	1.72	0.54
4:A:901:AHD:O16	6:A:905:HOH:O	2.18	0.54
1:B:204:VAL:HG22	1:B:247:GLN:HG2	1.89	0.54
1:C:106:MSE:HE3	1:C:265:VAL:CG2	2.33	0.54
4:B:1901:AHD:H72	5:B:1900:IPE:H22	1.89	0.54
1:A:137:ILE:HD11	1:B:161:TYR:CG	2.43	0.54
1:B:106:MSE:HE3	1:B:264:LYS:N	2.22	0.54
1:B:51:ARG:NH1	1:B:211:TYR:CE1	2.76	0.53
1:B:112:CYS:HB2	1:B:115:ARG:HG3	1.89	0.53
1:A:66:THR:HB	1:A:68:HIS:NE2	2.24	0.53
1:A:262:LEU:HD13	1:A:264:LYS:HG3	1.89	0.53
1:A:174:MSE:H	1:A:174:MSE:SE	2.41	0.53
1:B:2:ALA:O	1:B:3:SER:CB	2.48	0.53
1:A:212:THR:O	1:A:216:PRO:HG2	2.09	0.53
1:A:204:VAL:HG22	1:A:247:GLN:HG2	1.90	0.53
1:C:10:VAL:O	1:C:14:VAL:HG23	2.09	0.53
1:B:174:MSE:SE	1:B:174:MSE:H	2.41	0.52
1:C:239:ALA:C	1:C:241:LEU:H	2.12	0.52
1:B:98:ASP:HA	1:B:101:MSE:HE2	1.91	0.52
1:C:1:MSE:CG	1:C:2:ALA:N	2.73	0.52
1:B:255:CYS:SG	1:B:309:LYS:HG2	2.49	0.52
1:B:51:ARG:NH2	1:B:91:GLN:OE1	2.43	0.52
1:A:105:VAL:HA	1:A:115:ARG:HD3	1.91	0.52
1:A:132:LYS:NZ	1:B:129:ILE:HG23	2.24	0.52
1:A:122:GLN:HB3	6:A:928:HOH:O	2.09	0.51
1:B:240:HIS:HB3	6:B:1936:HOH:O	2.11	0.51
1:A:89:PHE:CD2	1:A:138:MSE:HE1	2.46	0.51
1:A:83:GLY:HA2	1:A:86:MSE:HG3	1.92	0.51
1:A:157:GLN:OE1	1:A:158:LYS:N	2.44	0.51
1:C:254:ASP:OD2	1:C:268:ASP:HB2	2.11	0.50
1:C:132:LYS:HE2	1:C:160:ASP:OD1	2.12	0.50
1:A:51:ARG:NH1	1:A:212:THR:OG1	2.44	0.50
1:A:362:LYS:NZ	5:A:900:IPE:O1B	2.45	0.50
1:A:1:MSE:C	1:A:3:SER:N	2.64	0.50
1:B:106:MSE:HG2	1:B:263:GLY:O	2.11	0.49
1:B:48:LYS:HG2	6:B:1943:HOH:O	2.11	0.49
1:C:1:MSE:HG2	1:C:2:ALA:N	2.27	0.49
1:B:89:PHE:CE2	1:B:138:MSE:HE1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:TYR:OH	1:C:160:ASP:OD1	2.19	0.49
1:C:47:GLY:HA2	1:C:108:ARG:HD2	1.93	0.49
1:C:1:MSE:CG	1:C:2:ALA:H	2.25	0.49
1:B:108:ARG:NH1	5:B:1900:IPE:O1B	2.45	0.49
1:B:66:THR:HG22	1:B:68:HIS:CE1	2.48	0.48
4:C:2901:AHD:H72	5:C:2900:IPE:H22	1.94	0.48
1:B:120:THR:HG23	1:B:123:CYS:SG	2.53	0.48
1:A:25:LYS:NZ	6:A:917:HOH:O	2.46	0.48
1:A:93:HIS:NE2	1:A:132:LYS:HE3	2.28	0.48
1:B:116:PHE:O	1:B:117:PRO:C	2.52	0.48
1:B:48:LYS:HB2	6:B:1924:HOH:O	2.13	0.48
1:A:325:GLU:O	1:A:329:VAL:HG23	2.13	0.48
1:A:246:PHE:HD2	1:A:357:THR:CG2	2.27	0.48
1:C:51:ARG:HD3	1:C:212:THR:HA	1.96	0.48
1:A:360:ARG:HH11	1:A:362:LYS:CG	2.26	0.47
1:B:262:LEU:HD13	1:B:264:LYS:CG	2.44	0.47
1:A:184:VAL:O	1:A:186:GLN:HG3	2.14	0.47
1:C:155:LEU:HD22	1:C:218:VAL:HG11	1.95	0.47
1:C:51:ARG:NH1	1:C:212:THR:HB	2.30	0.47
1:A:106:MSE:HE3	1:A:264:LYS:N	2.28	0.47
1:B:362:LYS:NZ	5:B:1900:IPE:O1A	2.46	0.47
1:B:272:ALA:HA	1:B:297:TYR:CE2	2.50	0.47
5:C:2900:IPE:H41	5:C:2900:IPE:H12	1.55	0.47
1:A:128:GLY:HA2	1:A:131:LEU:HD12	1.97	0.47
1:C:23:GLN:HA	1:C:28:ILE:HG22	1.97	0.47
1:C:152:LEU:HD23	1:C:152:LEU:O	2.14	0.46
1:C:333:GLU:O	1:C:337:GLU:HG2	2.15	0.46
1:A:51:ARG:NE	1:A:91:GLN:OE1	2.49	0.46
1:C:321:PHE:C	1:C:321:PHE:CD2	2.89	0.46
1:B:15:GLN:HE21	1:B:40:MSE:SE	2.49	0.46
1:B:10:VAL:O	1:B:13:GLU:HB2	2.15	0.46
1:A:1:MSE:O	1:A:2:ALA:HB3	2.16	0.46
1:B:230:VAL:HG12	1:B:343:SER:OG	2.15	0.46
1:A:249:GLN:HB2	1:A:360:ARG:HH21	1.80	0.45
1:B:362:LYS:HG3	6:B:1943:HOH:O	2.15	0.45
1:A:221:LEU:HD13	1:A:230:VAL:HG21	1.98	0.45
1:A:99:ASP:OD2	1:A:107:ARG:HG2	2.16	0.45
1:C:254:ASP:HB2	6:C:2909:HOH:O	2.16	0.45
1:A:77:LEU:HA	1:A:77:LEU:HD12	1.86	0.45
1:B:2:ALA:O	1:B:4:MSE:N	2.50	0.45
1:C:253:MSE:HE1	1:C:360:ARG:NH1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ARG:NE	1:B:91:GLN:OE1	2.48	0.45
1:C:43:THR:O	1:C:108:ARG:NH2	2.50	0.45
1:A:246:PHE:HD2	1:A:357:THR:HG23	1.80	0.45
1:A:106:MSE:CE	1:A:264:LYS:N	2.80	0.45
1:C:6:ARG:CZ	1:C:77:LEU:HD23	2.46	0.44
1:C:170:ASP:OD1	1:C:207:LYS:NZ	2.40	0.44
1:C:51:ARG:NH2	5:C:2900:IPE:O2A	2.51	0.44
1:C:47:GLY:CA	1:C:108:ARG:HD2	2.48	0.44
1:B:262:LEU:HD13	1:B:264:LYS:HG2	1.99	0.44
1:A:70:GLU:OE2	1:A:74:GLU:HG3	2.17	0.44
1:C:180:LEU:HA	1:C:186:GLN:NE2	2.33	0.44
1:B:43:THR:O	1:B:108:ARG:NH2	2.51	0.44
1:C:264:LYS:NZ	4:C:2901:AHD:O10	2.46	0.44
1:A:174:MSE:HB3	1:A:272:ALA:O	2.16	0.44
1:A:292:GLU:HB3	1:A:311:LEU:HD11	2.00	0.44
1:B:1:MSE:C	1:B:2:ALA:O	2.54	0.44
1:B:79:ASP:CG	1:B:146:ARG:NH1	2.69	0.44
1:C:51:ARG:NH1	1:C:212:THR:CG2	2.81	0.44
1:B:105:VAL:HA	1:B:115:ARG:HD3	2.00	0.43
1:A:132:LYS:HB3	6:B:1914:HOH:O	2.17	0.43
1:C:18:LEU:HA	1:C:18:LEU:HD12	1.87	0.43
1:C:318:GLN:HG2	6:C:2919:HOH:O	2.17	0.43
1:A:98:ASP:HA	1:A:101:MSE:HE3	2.00	0.43
1:A:180:LEU:HD23	1:A:186:GLN:OE1	2.18	0.43
1:A:333:GLU:O	1:A:337:GLU:HG2	2.18	0.43
1:C:139:ALA:O	1:C:143:PHE:HB2	2.19	0.42
1:C:264:LYS:HZ2	4:C:2901:AHD:P9	2.42	0.42
1:B:245:TYR:OH	1:B:325:GLU:OE2	2.29	0.42
1:C:140:TRP:O	1:C:144:ALA:HB2	2.18	0.42
1:A:285:ALA:HB1	1:A:289:GLN:HB2	2.00	0.42
1:B:61:GLY:CA	1:B:345:THR:HG21	2.49	0.42
1:A:19:LEU:HD23	1:A:19:LEU:HA	1.92	0.42
1:A:221:LEU:CD1	1:A:230:VAL:HG21	2.50	0.42
1:A:303:ALA:O	1:A:307:VAL:HG23	2.18	0.42
1:C:238:VAL:HA	1:C:335:LEU:HD13	2.02	0.42
1:A:296:ASN:ND2	1:A:307:VAL:HG11	2.34	0.42
4:A:901:AHD:H31	4:A:901:AHD:O15	2.20	0.42
1:C:51:ARG:NH1	1:C:211:TYR:CE1	2.87	0.42
1:B:66:THR:CG2	1:B:68:HIS:CE1	3.02	0.42
1:B:93:HIS:CD2	1:B:132:LYS:HE3	2.55	0.42
1:A:240:HIS:HB2	6:A:921:HOH:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:LEU:O	1:B:11:TYR:HB3	2.20	0.41
1:C:257:THR:HA	1:C:258:PRO:HD3	1.92	0.41
1:B:79:ASP:CG	1:B:146:ARG:HH11	2.23	0.41
1:A:106:MSE:HG2	1:A:263:GLY:O	2.20	0.41
1:B:244:GLU:O	1:B:248:VAL:HG23	2.19	0.41
1:C:68:HIS:HB2	6:C:2931:HOH:O	2.19	0.41
1:A:47:GLY:HA2	1:A:108:ARG:HD2	2.02	0.41
1:A:264:LYS:NZ	4:A:901:AHD:O11	2.46	0.41
1:A:200:TYR:CZ	1:A:276:TRP:HB2	2.55	0.41
1:B:262:LEU:HD22	1:B:362:LYS:HD3	2.03	0.41
1:C:63:LEU:HD11	1:C:77:LEU:CD1	2.50	0.41
1:B:201:LYS:HG2	1:B:244:GLU:OE2	2.20	0.41
1:A:51:ARG:NH1	1:A:212:THR:HG23	2.36	0.41
1:B:119:VAL:O	1:B:120:THR:HG22	2.18	0.41
1:C:301:ASP:HB3	1:C:304:LYS:HG3	2.03	0.41
1:A:192:PHE:O	1:A:195:PHE:HB2	2.21	0.41
1:C:51:ARG:HH22	1:C:91:GLN:NE2	2.13	0.40
1:B:344:PRO:O	1:B:347:ALA:HB3	2.20	0.40
1:C:213:TYR:C	1:C:216:PRO:HD2	2.41	0.40
1:B:188:MSE:CG	1:B:189:THR:N	2.84	0.40
1:B:191:ASP:O	1:B:192:PHE:HB2	2.21	0.40
1:B:264:LYS:NZ	4:B:1901:AHD:P9	2.94	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:GLU:OE1	1:B:5:GLU:OE1[8_676]	2.09	0.11

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	360/362 (99%)	345 (96%)	15 (4%)	0	100	100
1	B	360/362 (99%)	346 (96%)	11 (3%)	3 (1%)	24	41
1	C	360/362 (99%)	335 (93%)	22 (6%)	3 (1%)	24	41
All	All	1080/1086 (99%)	1026 (95%)	48 (4%)	6 (1%)	30	50

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	69	ASP
1	B	2	ALA
1	C	3	SER
1	C	188	MSE
1	B	120	THR
1	B	180	LEU

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	309/294 (105%)	282 (91%)	27 (9%)	13	24
1	B	309/294 (105%)	291 (94%)	18 (6%)	25	45
1	C	309/294 (105%)	292 (94%)	17 (6%)	27	48
All	All	927/882 (105%)	865 (93%)	62 (7%)	20	37

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	LEU
1	A	23	GLN
1	A	55	VAL
1	A	67	GLN
1	A	77	LEU
1	A	86	MSE
1	A	91	GLN

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Mol	Chain	Res	Type
1	A	107	ARG
1	A	108	ARG
1	A	116	PHE
1	A	157	GLN
1	A	168	MSE
1	A	171	VAL
1	A	180	LEU
1	A	202	ARG
1	A	225	GLU
1	A	260	GLU
1	A	262	LEU
1	A	264	LYS
1	A	300	LYS
1	A	318	GLN
1	A	320	ASP
1	A	333	GLU
1	A	342	LYS
1	A	343	SER
1	A	345	THR
1	A	359	LYS
1	B	18	LEU
1	B	51	ARG
1	B	55	VAL
1	B	77	LEU
1	B	107	ARG
1	B	108	ARG
1	B	115	ARG
1	B	120	THR
1	B	122	GLN
1	B	123	CYS
1	B	171	VAL
1	B	174	MSE
1	B	179	LYS
1	B	202	ARG
1	B	238	VAL
1	B	262	LEU
1	B	300	LYS
1	B	362	LYS
1	C	18	LEU
1	C	55	VAL
1	C	66	THR
1	C	107	ARG

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Mol	Chain	Res	Type
1	C	150	LYS
1	C	152	LEU
1	C	171	VAL
1	C	212	THR
1	C	230	VAL
1	C	232	MSE
1	C	262	LEU
1	C	280	THR
1	C	300	LYS
1	C	320	ASP
1	C	342	LYS
1	C	356	LYS
1	C	362	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	15	GLN
1	B	68	HIS
1	B	122	GLN
1	B	157	GLN
1	C	91	GLN
1	C	186	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 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 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	SO4	A	370	-	4,4,4	0.32	0	6,6,6	0.28	0
5	IPE	A	900	-	10,13,13	0.53	0	14,19,19	1.33	3 (21%)
4	AHD	A	901	2	13,13,13	4.42	6 (46%)	18,21,21	3.51	11 (61%)
3	SO4	B	1370	-	4,4,4	0.30	0	6,6,6	0.13	0
5	IPE	B	1900	-	10,13,13	0.68	0	14,19,19	1.25	2 (14%)
4	AHD	B	1901	2	13,13,13	7.21	9 (69%)	18,21,21	3.01	10 (55%)
3	SO4	C	2370	-	4,4,4	0.15	0	6,6,6	0.25	0
5	IPE	C	2900	-	10,13,13	0.59	0	14,19,19	1.22	2 (14%)
4	AHD	C	2901	2	13,13,13	7.68	10 (76%)	18,21,21	5.94	7 (38%)

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	SO4	A	370	-	-	0/0/0/0	0/0/0/0
5	IPE	A	900	-	-	0/13/13/13	0/0/0/0
4	AHD	A	901	2	-	0/23/23/23	0/0/0/0
3	SO4	B	1370	-	-	0/0/0/0	0/0/0/0
5	IPE	B	1900	-	-	0/13/13/13	0/0/0/0
4	AHD	B	1901	2	-	0/23/23/23	0/0/0/0
3	SO4	C	2370	-	-	0/0/0/0	0/0/0/0
5	IPE	C	2900	-	-	0/13/13/13	0/0/0/0
4	AHD	C	2901	2	-	1/23/23/23	0/0/0/0

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2901	AHD	P14-C8	-21.70	1.69	1.85
4	B	1901	AHD	P9-C8	-17.22	1.73	1.85
4	B	1901	AHD	O13-C8	-15.12	1.24	1.44
4	A	901	AHD	O13-C8	-12.86	1.27	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	2901	AHD	P9-C8	-11.65	1.77	1.85
4	B	1901	AHD	C7-C8	-10.35	1.42	1.54
4	C	2901	AHD	C2-C3	-7.73	1.13	1.51
4	A	901	AHD	C7-C8	-5.58	1.48	1.54
4	C	2901	AHD	C7-C8	-3.93	1.49	1.54
4	C	2901	AHD	O13-C8	-3.69	1.39	1.44
4	B	1901	AHD	P14-O17	-3.10	1.45	1.50
4	C	2901	AHD	P9-O12	-3.06	1.48	1.54
4	A	901	AHD	P14-O16	-2.97	1.49	1.54
4	A	901	AHD	P9-O12	-2.58	1.49	1.54
4	B	1901	AHD	P14-C8	-2.46	1.83	1.85
4	B	1901	AHD	P14-O16	-2.38	1.50	1.54
4	C	2901	AHD	P14-O15	-2.32	1.50	1.54
4	B	1901	AHD	P14-O15	-2.18	1.50	1.54
4	B	1901	AHD	P9-O12	-2.10	1.50	1.54
4	C	2901	AHD	P14-O17	2.69	1.54	1.50
4	B	1901	AHD	P9-O10	3.02	1.60	1.54
4	A	901	AHD	P14-O15	3.39	1.61	1.54
4	C	2901	AHD	P9-O10	3.62	1.61	1.54
4	A	901	AHD	P9-O11	4.49	1.57	1.50
4	C	2901	AHD	P14-O16	5.78	1.65	1.54

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	901	AHD	O17-P14-C8	-5.95	93.94	109.95
4	A	901	AHD	O15-P14-O17	-5.32	100.42	113.04
4	B	1901	AHD	O16-P14-O15	-4.28	96.14	108.24
4	B	1901	AHD	O15-P14-C8	-4.09	96.79	105.90
4	B	1901	AHD	O10-P9-O12	-3.87	97.31	108.24
4	C	2901	AHD	O15-P14-C8	-3.56	97.95	105.90
4	A	901	AHD	O12-P9-O11	-3.52	104.69	113.04
4	B	1901	AHD	P14-C8-P9	-3.47	107.54	112.84
4	C	2901	AHD	O16-P14-O15	-3.36	98.73	108.24
4	A	901	AHD	P14-C8-P9	-3.32	107.77	112.84
4	B	1901	AHD	O12-P9-O11	-2.61	106.86	113.04
5	C	2900	IPE	O1B-PB-O3A	-2.58	93.38	105.09
4	C	2901	AHD	O10-P9-O11	-2.39	107.36	113.04
4	A	901	AHD	O15-P14-C8	-2.37	100.62	105.90
4	A	901	AHD	O10-P9-O11	-2.32	107.53	113.04
5	A	900	IPE	O1-C1-C2	-2.26	97.77	108.63
5	B	1900	IPE	O3A-PA-O1	-2.20	97.09	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	900	IPE	O2A-PA-O1A	2.07	123.72	112.53
5	C	2900	IPE	O1B-PB-O2B	2.26	117.87	110.58
4	A	901	AHD	O16-P14-C8	2.36	111.17	105.90
5	B	1900	IPE	O3B-PB-O2B	2.42	118.37	110.58
4	B	1901	AHD	O16-P14-O17	2.57	119.12	113.04
4	C	2901	AHD	O12-P9-C8	2.70	111.93	105.90
4	B	1901	AHD	O16-P14-C8	2.77	112.07	105.90
4	B	1901	AHD	C7-C2-C3	2.81	118.30	112.72
5	A	900	IPE	O1B-PB-O2B	2.84	119.73	110.58
4	C	2901	AHD	O16-P14-O17	3.37	121.02	113.04
4	C	2901	AHD	C2-C7-C8	3.46	123.81	116.60
4	A	901	AHD	C7-C2-C3	3.49	119.65	112.72
4	A	901	AHD	O12-P9-C8	3.93	114.66	105.90
4	B	1901	AHD	C2-C7-C8	4.39	125.75	116.60
4	A	901	AHD	C2-C7-C8	5.64	128.34	116.60
4	B	1901	AHD	O12-P9-C8	6.41	120.19	105.90
4	A	901	AHD	O16-P14-O15	7.18	128.52	108.24
4	C	2901	AHD	C7-C2-C3	23.68	159.76	112.72

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	2901	AHD	C8-C7-C2-C3

There are no ring outliers.

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	900	IPE	3	0
4	A	901	AHD	5	0
5	B	1900	IPE	3	0
4	B	1901	AHD	3	0
5	C	2900	IPE	3	0
4	C	2901	AHD	4	0

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.