Full wwPDB X-ray Structure Validation Report (i)

Apr 28, 2024 – 03:36 pm BST

PDB ID	:	2VG2
Title	:	Rv2361 with IPP
Authors	:	Naismith, J.H.; Wang, W.; Dong, C.
Deposited on	:	2007-11-07
Resolution	:	1.95 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

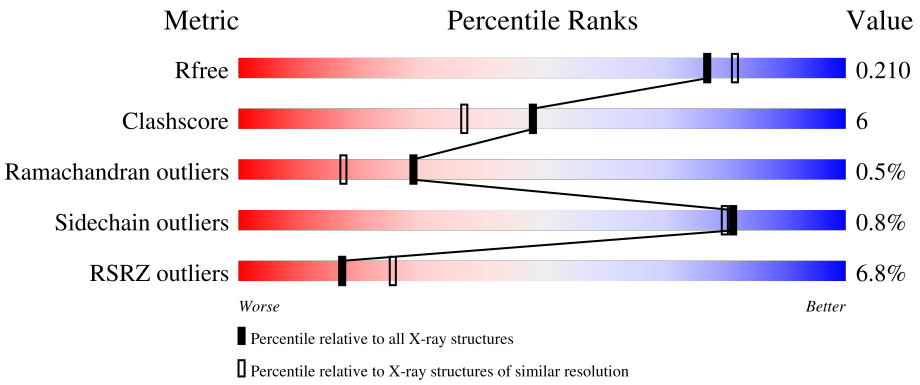
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 1.95 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	284	4% 89% 10% •
1	B	284	6% 88% 10% •
1	C	284	8% 91% 9%
1	D	284	9% 88% 12%

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	DPO	A	1297	-	-	X	-
4	GOL	A	1301	-	-	-	X
4	GOL	A	1302	-	-	X	-
4	GOL	B	1298	-	-	X	-
4	GOL	C	1299	-	-	X	-

2 Entry composition (i)

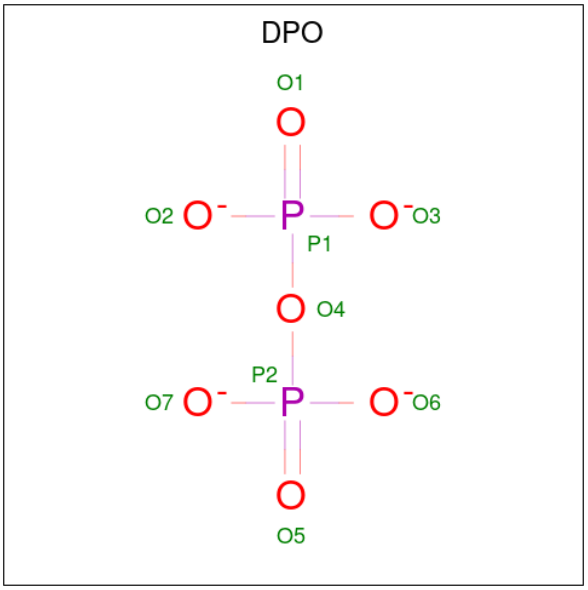
There are 7 unique types of molecules in this entry. The entry contains 10052 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UNDECAPRENYL PYROPHOSPHATE SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	284	2293	1448	422	413	10	0	3	1
1	B	283	2288	1444	421	414	9	0	1	0
1	C	283	2276	1434	421	412	9	0	0	0
1	D	284	2287	1443	422	413	9	0	0	0

- Molecule 2 is DIPHOSPHATE (three-letter code: DPO) (formula: O_7P_2).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	A	1	9	7	2	0	0
2	B	1	9	7	2	0	0

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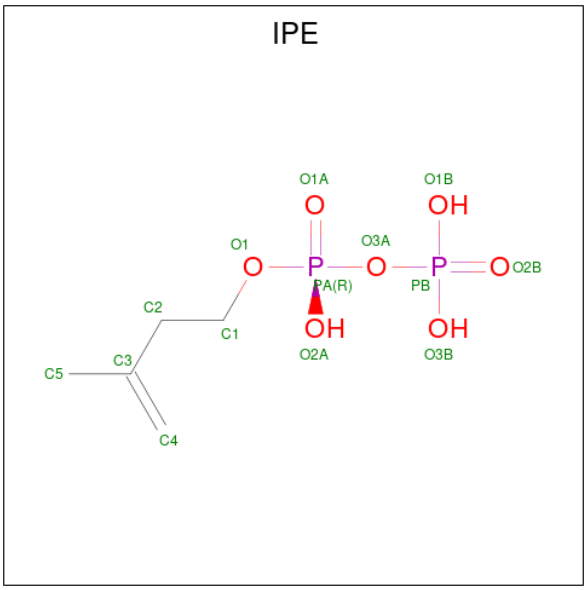
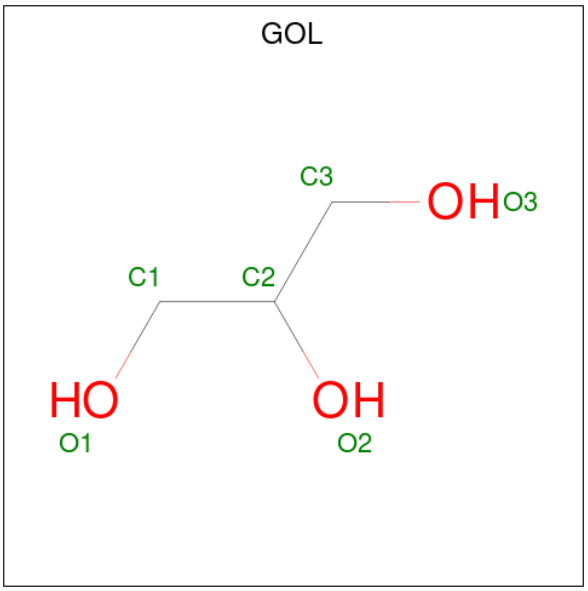
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
2	C	1	9	7	2	0	0

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



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

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

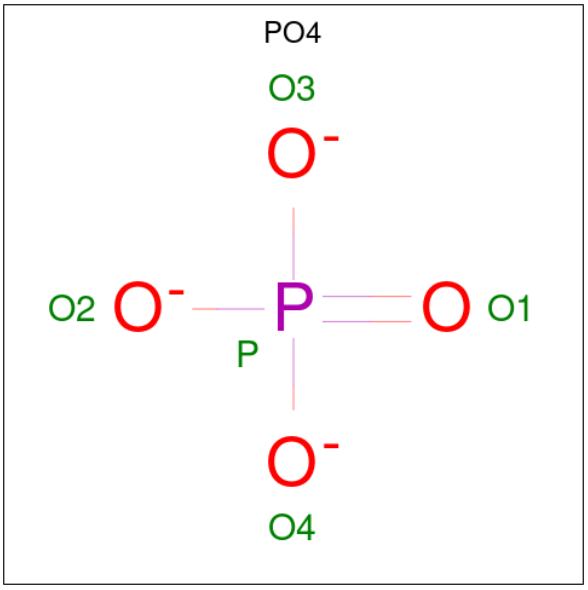


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
4	A	1	6	3	3	0	0
4	A	1	6	3	3	0	0
4	A	1	6	3	3	0	0
4	A	1	6	3	3	0	0
4	A	1	6	3	3	0	0
4	B	1	6	3	3	0	0
4	B	1	6	3	3	0	0
4	B	1	6	3	3	0	0
4	B	1	6	3	3	0	0
4	C	1	6	3	3	0	0
4	C	1	6	3	3	0	0
4	C	1	6	3	3	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	1	1	1	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
6	A	1	5	4	1	0	0
			Total	O	P		
6	C	1	5	4	1	0	0
			Total	O	P		
6	C	1	5	4	1	0	0
			Total	O	P		
6	D	1	5	4	1	0	0
			Total	O	P		
6	D	1	5	4	1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	231	231	231	0	0
			Total	O		
7	B	179	179	179	0	0
			Total	O		
7	C	183	183	183	0	0
			Total	O		
7	D	162	162	162	0	0

3 Residue-property plots (i)

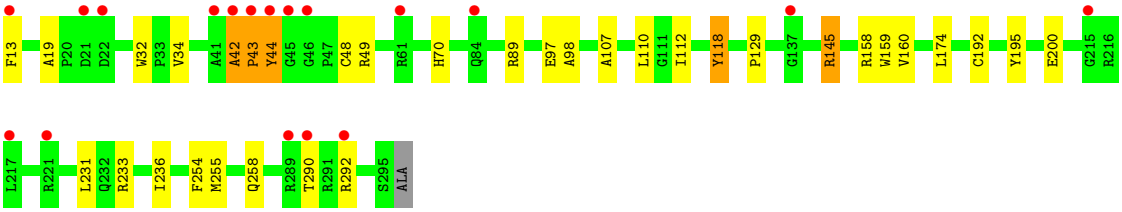
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: UNDECAPRENYL PYROPHOSPHATE SYNTHETASE

Chain A:

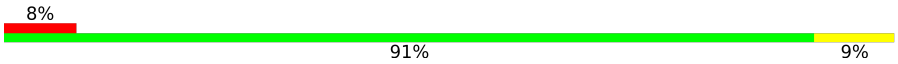
• Molecule 1: UNDECAPRENYL PYROPHOSPHATE SYNTHETASE

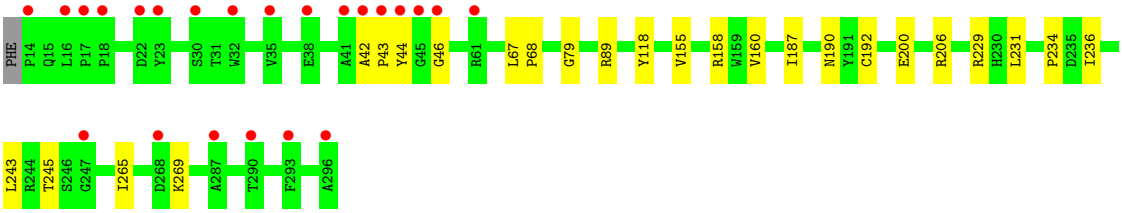
Chain B:



• Molecule 1: UNDECAPRENYL PYROPHOSPHATE SYNTHETASE

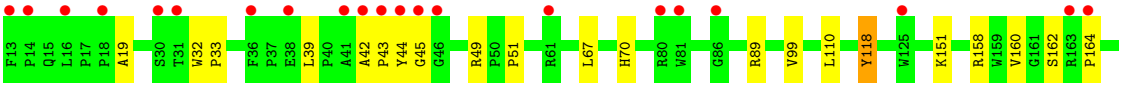
Chain C:

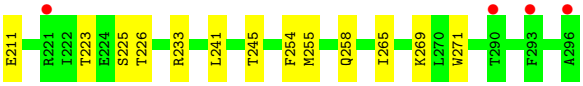




• Molecule 1: UNDECAPRENYL PYROPHOSPHATE SYNTHETASE

Chain D:




E211
R221
I222
T223
E224
S225
T226
R233
L241
T245
F254
M255
Q258
I265
K269
L270
W271
T290
F293
A296

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	87.07Å 87.07Å 183.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	69.84 – 1.95 61.24 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.5 (69.84-1.95) 98.0 (61.24-1.95)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.76 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.185 , 0.211 0.189 , 0.210	Depositor DCC
R_{free} test set	5556 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.006	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.040 for -h,-k,l 0.178 for h,-h-k,-l 0.045 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10052	wwPDB-VP
Average B, all atoms (Å^2)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: IPE, DPO, CL, GOL, PO4

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	0.53	0/2364	0.72	4/3217 (0.1%)
1	B	0.47	0/2353	0.68	3/3201 (0.1%)
1	C	0.43	0/2337	0.59	1/3179 (0.0%)
1	D	0.41	0/2349	0.58	0/3196
All	All	0.46	0/9403	0.65	8/12793 (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	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	145	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	A	145	ARG	NE-CZ-NH2	-9.71	115.44	120.30
1	B	145	ARG	NE-CZ-NH1	9.13	124.87	120.30
1	A	49	ARG	NE-CZ-NH2	-8.79	115.91	120.30
1	A	145	ARG	NE-CZ-NH1	8.55	124.57	120.30
1	A	49	ARG	CG-CD-NE	-5.90	99.40	111.80
1	C	229	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	89	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	13	PHE	Peptide
1	B	13	PHE	Peptide
1	B	42	ALA	Peptide

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	2293	0	2259	33	0
1	B	2288	0	2246	38	0
1	C	2276	0	2237	17	0
1	D	2287	0	2245	21	0
2	A	9	0	0	2	0
2	B	9	0	0	0	0
2	C	9	0	0	0	0
3	A	14	0	9	3	0
3	B	14	0	9	2	0
4	A	30	0	40	11	0
4	B	24	0	32	10	0
4	C	18	0	24	6	0
5	A	1	0	0	0	0
6	A	5	0	0	0	0
6	C	10	0	0	1	0
6	D	10	0	0	0	0
7	A	231	0	0	4	0
7	B	179	0	0	5	0
7	C	183	0	0	1	0
7	D	162	0	0	2	0
All	All	10052	0	9101	110	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 6.

All (110) 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:34:VAL:HG13	4:B:1298:GOL:H32	1.29	1.07
1:B:34:VAL:HG13	4:B:1298:GOL:C3	1.91	1.00
1:B:34:VAL:CG1	4:B:1298:GOL:H32	1.90	1.00
1:C:231:LEU:HD12	4:C:1299:GOL:H32	1.52	0.92
1:A:98:ALA:HB2	4:A:1302:GOL:H2	1.60	0.84
1:B:48:CYS:SG	7:B:2023:HOH:O	2.41	0.78
1:A:34[B]:VAL:HG23	4:A:1302:GOL:H32	1.71	0.73
4:A:1301:GOL:H11	7:A:2062:HOH:O	1.88	0.72
1:A:255:MET:HE3	1:A:258:GLN:HB2	1.71	0.71
1:B:98:ALA:HB2	4:B:1298:GOL:H2	1.75	0.68
1:A:32:TRP:CD1	4:A:1302:GOL:H12	2.29	0.67
1:B:32:TRP:CD1	4:B:1298:GOL:H12	2.30	0.67
1:B:97:GLU:OE2	1:B:145:ARG:HD2	1.95	0.67
1:A:34[A]:VAL:HG13	4:A:1302:GOL:H32	1.76	0.66
1:A:70:HIS:CE1	1:A:255:MET:HE2	2.30	0.66
1:A:118:TYR:O	3:A:1298:IPE:H41	1.96	0.66
1:A:34[B]:VAL:HG23	4:A:1302:GOL:C3	2.28	0.64
1:B:255:MET:HE3	1:B:258:GLN:HB2	1.79	0.64
1:C:236:ILE:HB	4:C:1299:GOL:C1	2.27	0.64
1:B:42:ALA:HB1	1:B:43:PRO:CD	2.27	0.64
1:B:70:HIS:CE1	1:B:255:MET:HE2	2.32	0.64
2:A:1297:DPO:O3	2:A:1297:DPO:O6	2.12	0.64
3:B:1297:IPE:H42	7:B:2176:HOH:O	1.97	0.64
1:A:34[A]:VAL:HG13	4:A:1302:GOL:C3	2.28	0.63
1:B:292:ARG:HH21	1:D:89:ARG:HH22	1.49	0.60
1:C:231:LEU:HD12	4:C:1299:GOL:C3	2.27	0.60
1:C:234:PRO:HA	4:C:1299:GOL:H31	1.84	0.60
1:B:34:VAL:HG11	4:B:1298:GOL:H32	1.83	0.60
1:A:255:MET:HE3	1:A:258:GLN:CB	2.32	0.59
1:A:70:HIS:HE1	1:A:255:MET:HE2	1.66	0.59
1:D:255:MET:HE3	1:D:258:GLN:HB2	1.84	0.59
3:B:1297:IPE:C4	7:B:2176:HOH:O	2.49	0.58
1:C:236:ILE:HB	4:C:1299:GOL:H11	1.84	0.58
1:A:98:ALA:HB2	4:A:1302:GOL:C2	2.34	0.57
1:B:42:ALA:HB1	1:B:43:PRO:HD3	1.86	0.57
1:B:34:VAL:HG13	4:B:1298:GOL:H31	1.85	0.56
1:A:75:MET:N	3:A:1298:IPE:H42	2.20	0.56
1:C:200:GLU:HG2	1:C:231:LEU:HD22	1.88	0.55
1:D:223:THR:HG23	1:D:225:SER:N	2.22	0.55
1:D:241:LEU:HD11	1:D:265:ILE:HD12	1.89	0.55
1:A:75:MET:H	3:A:1298:IPE:H42	1.73	0.53
1:A:118:TYR:OH	1:A:121:SER:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:HIS:HE1	1:B:255:MET:HE2	1.74	0.53
1:B:98:ALA:HB2	4:B:1298:GOL:C2	2.39	0.52
1:D:160:VAL:HG22	1:D:233:ARG:HG3	1.92	0.52
1:C:236:ILE:HB	4:C:1299:GOL:H12	1.91	0.52
1:B:255:MET:HE3	1:B:258:GLN:CB	2.39	0.51
1:D:42:ALA:O	1:D:45:GLY:N	2.33	0.51
1:B:42:ALA:CB	1:B:43:PRO:CD	2.89	0.51
6:C:1298:PO4:O4	7:C:2178:HOH:O	2.17	0.51
1:C:42:ALA:HB1	1:C:43:PRO:HD2	1.92	0.51
1:A:168:ARG:HH21	1:B:290:THR:HG22	1.77	0.50
1:A:263:GLU:OE2	1:A:289:ARG:NH1	2.45	0.50
1:C:245:THR:HB	1:C:269:LYS:O	2.11	0.50
1:B:159:TRP:HB2	1:B:174:LEU:HD13	1.94	0.48
1:A:79:GLY:N	2:A:1297:DPO:O6	2.37	0.48
1:D:70:HIS:CE1	1:D:255:MET:HE2	2.48	0.47
1:A:160:VAL:HG22	1:A:233:ARG:HG3	1.97	0.47
1:A:32:TRP:NE1	4:A:1302:GOL:H12	2.30	0.47
1:B:200:GLU:HG2	1:B:231:LEU:HD22	1.96	0.47
1:B:292:ARG:NH2	1:D:89:ARG:HH22	2.10	0.47
1:B:42:ALA:C	1:B:44:TYR:N	2.69	0.46
1:B:42:ALA:HB3	7:B:2006:HOH:O	2.16	0.46
1:A:70:HIS:HE1	1:A:255:MET:CE	2.29	0.46
1:D:67:LEU:HD11	1:D:110:LEU:HG	1.98	0.46
1:C:160:VAL:O	1:C:192:CYS:HA	2.16	0.46
1:A:222:ILE:HB	1:C:206:ARG:HG3	1.98	0.45
1:D:211:GLU:HG2	7:D:2104:HOH:O	2.17	0.45
1:D:151:LYS:NZ	7:D:2071:HOH:O	2.49	0.45
1:D:19:ALA:HB2	1:D:49:ARG:CZ	2.47	0.45
1:D:223:THR:HG23	1:D:225:SER:H	1.80	0.45
1:B:70:HIS:HE1	1:B:255:MET:CE	2.29	0.45
1:B:110:LEU:HD23	1:B:112:ILE:HD11	1.97	0.45
1:D:39:LEU:HD11	1:D:51:PRO:HD3	1.97	0.45
1:C:243:LEU:HD23	1:C:265:ILE:HB	1.98	0.44
1:B:160:VAL:HG22	1:B:233:ARG:HG3	1.98	0.44
1:B:129:PRO:HD3	4:B:1300:GOL:H2	1.98	0.44
1:B:160:VAL:O	1:B:192:CYS:HA	2.18	0.44
1:B:290:THR:HG23	7:B:2175:HOH:O	2.18	0.44
1:C:79:GLY:HA3	1:C:89:ARG:NH1	2.33	0.44
1:C:67:LEU:HD12	1:C:68:PRO:HD2	2.00	0.43
1:A:245:THR:HB	1:A:269:LYS:O	2.19	0.43
1:A:34[A]:VAL:HG13	4:A:1302:GOL:C2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:LEU:CD2	1:C:265:ILE:HB	2.48	0.43
1:B:118:TYR:CE1	1:B:254:PHE:HB2	2.54	0.43
1:B:107:ALA:HA	1:B:112:ILE:HD12	2.01	0.43
1:A:97:GLU:OE2	1:A:145:ARG:HD2	2.19	0.42
1:A:159:TRP:HB2	1:A:174:LEU:HD13	2.00	0.42
1:D:245:THR:HB	1:D:269:LYS:O	2.19	0.42
1:A:168:ARG:HH21	1:B:290:THR:CG2	2.32	0.42
1:A:295:SER:OG	1:A:296:ALA:N	2.52	0.42
1:D:162:SER:OG	1:D:164:PRO:HD2	2.19	0.42
1:B:236:ILE:HG21	1:B:255:MET:HE1	2.01	0.42
1:C:160:VAL:HG21	1:C:190:ASN:HB3	2.02	0.42
1:B:42:ALA:O	1:B:44:TYR:N	2.53	0.42
1:D:19:ALA:HB2	1:D:49:ARG:NH1	2.34	0.42
1:D:223:THR:HG23	1:D:226:THR:H	1.84	0.42
1:B:19:ALA:HB2	1:B:49:ARG:CZ	2.50	0.42
1:A:118:TYR:CE1	1:A:254:PHE:HB2	2.55	0.41
1:B:195:TYR:CD1	1:B:195:TYR:C	2.94	0.41
1:D:99:VAL:HG12	1:D:271:TRP:CZ2	2.55	0.41
1:A:200:GLU:HG2	1:A:231:LEU:HD22	2.03	0.41
1:D:118:TYR:CE1	1:D:254:PHE:HB2	2.55	0.41
1:A:160:VAL:O	1:A:192:CYS:HA	2.20	0.41
1:C:155:VAL:HG22	1:C:187:ILE:CG2	2.50	0.41
1:A:152:LYS:NZ	7:A:2118:HOH:O	2.54	0.41
1:B:32:TRP:NE1	4:B:1298:GOL:H12	2.36	0.41
1:D:32:TRP:HA	1:D:33:PRO:C	2.41	0.41
1:A:13:PHE:HA	7:A:2057:HOH:O	2.21	0.40
4:A:1302:GOL:H32	7:A:2231:HOH:O	2.22	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	285/284 (100%)	280 (98%)	5 (2%)	0	100	100
1	B	282/284 (99%)	271 (96%)	9 (3%)	2 (1%)	22	11
1	C	281/284 (99%)	272 (97%)	7 (2%)	2 (1%)	22	11
1	D	282/284 (99%)	274 (97%)	6 (2%)	2 (1%)	22	11
All	All	1130/1136 (100%)	1097 (97%)	27 (2%)	6 (0%)	29	17

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	43	PRO
1	B	44	TYR
1	D	43	PRO
1	D	44	TYR
1	C	44	TYR
1	C	46	GLY

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	242/239 (101%)	240 (99%)	2 (1%)	81	80
1	B	240/239 (100%)	238 (99%)	2 (1%)	81	80
1	C	238/239 (100%)	236 (99%)	2 (1%)	81	80
1	D	239/239 (100%)	237 (99%)	2 (1%)	81	80
All	All	959/956 (100%)	951 (99%)	8 (1%)	81	80

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	TYR
1	A	158	ARG
1	B	118	TYR
1	B	158	ARG
1	C	118	TYR

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Mol	Chain	Res	Type
1	C	158	ARG
1	D	118	TYR
1	D	158	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 23 ligands modelled in this entry, 1 is monoatomic - leaving 22 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	$\#\|Z\| > 2$
4	GOL	A	1300	-	5,5,5	0.35	0	5,5,5	0.15	0
6	PO4	D	1297	-	4,4,4	0.93	0	6,6,6	0.54	0
3	IPE	B	1297	-	11,13,13	2.50	2 (18%)	15,19,19	1.41	3 (20%)
6	PO4	C	1298	-	4,4,4	0.96	0	6,6,6	0.45	0
2	DPO	A	1297	-	6,8,8	1.07	0	13,13,13	1.52	2 (15%)
4	GOL	A	1299	-	5,5,5	0.38	0	5,5,5	0.26	0
2	DPO	B	1296	-	6,8,8	0.87	0	13,13,13	1.34	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	B	1301	-	5,5,5	0.37	0	5,5,5	0.29	0
4	GOL	C	1301	-	5,5,5	0.38	0	5,5,5	0.26	0
6	PO4	C	1302	-	4,4,4	1.37	0	6,6,6	0.64	0
4	GOL	A	1302	-	5,5,5	0.81	0	5,5,5	0.86	0
4	GOL	A	1301	-	5,5,5	0.38	0	5,5,5	0.45	0
3	IPE	A	1298	-	11,13,13	2.62	2 (18%)	15,19,19	1.06	0
2	DPO	C	1297	-	6,8,8	0.81	0	13,13,13	1.50	1 (7%)
4	GOL	B	1299	-	5,5,5	0.41	0	5,5,5	0.07	0
4	GOL	A	1305	-	5,5,5	0.34	0	5,5,5	0.25	0
6	PO4	A	1304	-	4,4,4	0.70	0	6,6,6	0.53	0
4	GOL	C	1299	-	5,5,5	0.82	0	5,5,5	1.03	0
4	GOL	B	1300	-	5,5,5	0.40	0	5,5,5	0.20	0
4	GOL	C	1300	-	5,5,5	0.45	0	5,5,5	0.45	0
6	PO4	D	1298	-	4,4,4	0.63	0	6,6,6	0.95	0
4	GOL	B	1298	-	5,5,5	0.78	0	5,5,5	0.90	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
4	GOL	A	1300	-	-	4/4/4/4	-
4	GOL	A	1305	-	-	0/4/4/4	-
2	DPO	B	1296	-	-	1/6/6/6	-
4	GOL	B	1301	-	-	2/4/4/4	-
4	GOL	C	1299	-	-	2/4/4/4	-
4	GOL	C	1301	-	-	4/4/4/4	-
3	IPE	B	1297	-	-	4/13/13/13	-
3	IPE	A	1298	-	-	4/13/13/13	-
2	DPO	C	1297	-	-	2/6/6/6	-
4	GOL	A	1302	-	-	2/4/4/4	-
4	GOL	A	1301	-	-	2/4/4/4	-
4	GOL	B	1299	-	-	2/4/4/4	-
4	GOL	B	1300	-	-	2/4/4/4	-
4	GOL	B	1298	-	-	4/4/4/4	-
2	DPO	A	1297	-	-	3/6/6/6	-
4	GOL	C	1300	-	-	2/4/4/4	-
4	GOL	A	1299	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1298	IPE	C4-C3	7.71	1.54	1.33
3	B	1297	IPE	C4-C3	7.30	1.53	1.33
3	A	1298	IPE	C5-C3	-2.25	1.39	1.48
3	B	1297	IPE	C5-C3	-2.09	1.40	1.48

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1297	DPO	P2-O4-P1	-4.53	117.28	132.83
2	C	1297	DPO	P2-O4-P1	-3.73	120.02	132.83
3	B	1297	IPE	PA-O3A-PB	-3.57	120.58	132.83
2	B	1296	DPO	P2-O4-P1	-3.45	120.97	132.83
3	B	1297	IPE	C5-C3-C2	2.16	122.01	115.24
3	B	1297	IPE	O1B-PB-O3A	2.11	111.73	104.64
2	A	1297	DPO	O7-P2-O4	2.10	111.66	104.64

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1297	DPO	P1-O4-P2-O6
2	B	1296	DPO	P1-O4-P2-O6
2	C	1297	DPO	P2-O4-P1-O3
3	A	1298	IPE	O1-C1-C2-C3
3	A	1298	IPE	C1-O1-PA-O1A
3	A	1298	IPE	C1-O1-PA-O2A
3	B	1297	IPE	C1-C2-C3-C4
3	B	1297	IPE	C1-C2-C3-C5
3	B	1297	IPE	PA-O3A-PB-O1B
4	A	1299	GOL	C1-C2-C3-O3
4	A	1301	GOL	C1-C2-C3-O3
4	A	1301	GOL	O2-C2-C3-O3
4	A	1302	GOL	O1-C1-C2-C3
4	B	1298	GOL	C1-C2-C3-O3
4	B	1299	GOL	O1-C1-C2-C3
4	B	1300	GOL	C1-C2-C3-O3
4	B	1301	GOL	O1-C1-C2-C3
4	C	1299	GOL	C1-C2-C3-O3
4	C	1300	GOL	C1-C2-C3-O3
4	C	1301	GOL	O1-C1-C2-C3
4	C	1301	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	B	1299	GOL	O1-C1-C2-O2
4	C	1299	GOL	O2-C2-C3-O3
4	A	1300	GOL	C1-C2-C3-O3
4	B	1298	GOL	O1-C1-C2-C3
4	A	1299	GOL	O2-C2-C3-O3
4	A	1300	GOL	O2-C2-C3-O3
4	A	1302	GOL	O1-C1-C2-O2
4	B	1298	GOL	O1-C1-C2-O2
4	B	1298	GOL	O2-C2-C3-O3
4	B	1300	GOL	O2-C2-C3-O3
4	C	1300	GOL	O2-C2-C3-O3
4	C	1301	GOL	O1-C1-C2-O2
4	C	1301	GOL	O2-C2-C3-O3
4	B	1301	GOL	O1-C1-C2-O2
2	A	1297	DPO	P2-O4-P1-O1
3	A	1298	IPE	C1-O1-PA-O3A
3	B	1297	IPE	PA-O3A-PB-O2B
4	A	1300	GOL	O1-C1-C2-C3
2	A	1297	DPO	P1-O4-P2-O7
2	C	1297	DPO	P2-O4-P1-O2
4	A	1300	GOL	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1297	IPE	2	0
6	C	1298	PO4	1	0
2	A	1297	DPO	2	0
4	A	1302	GOL	10	0
4	A	1301	GOL	1	0
3	A	1298	IPE	3	0
4	C	1299	GOL	6	0
4	B	1300	GOL	1	0
4	B	1298	GOL	9	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	284/284 (100%)	0.50	11 (3%)	39	49	31, 39, 48, 61	0
1	B	283/284 (99%)	0.60	18 (6%)	19	28	36, 39, 50, 60	0
1	C	283/284 (99%)	0.65	23 (8%)	12	18	31, 39, 48, 55	0
1	D	284/284 (100%)	0.78	25 (8%)	10	16	29, 40, 49, 56	0
All	All	1134/1136 (99%)	0.63	77 (6%)	17	25	29, 39, 49, 61	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	44	TYR	13.7
1	D	44	TYR	12.7
1	C	44	TYR	9.6
1	D	43	PRO	8.3
1	B	45	GLY	8.1
1	B	43	PRO	8.1
1	C	43	PRO	7.8
1	C	45	GLY	7.5
1	D	13	PHE	6.8
1	C	42	ALA	6.5
1	C	296	ALA	6.5
1	B	42	ALA	6.0
1	D	41	ALA	5.6
1	D	42	ALA	5.6
1	A	296	ALA	5.5
1	A	44	TYR	5.2
1	D	45	GLY	4.9
1	B	41	ALA	4.6
1	B	13	PHE	4.5
1	A	292	ARG	4.5
1	A	13	PHE	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	293	PHE	4.1
1	C	46	GLY	4.0
1	C	61	ARG	3.9
1	D	46	GLY	3.8
1	C	38	GLU	3.8
1	D	14	PRO	3.6
1	D	221	ARG	3.5
1	C	41	ALA	3.4
1	A	45	GLY	3.3
1	B	221	ARG	3.3
1	A	46	GLY	3.3
1	C	14	PRO	3.2
1	D	293	PHE	3.2
1	D	80	ARG	3.1
1	D	290	THR	3.1
1	D	18	PRO	3.0
1	D	31	THR	2.7
1	D	61	ARG	2.7
1	C	17	PRO	2.7
1	D	36	PHE	2.7
1	C	22	ASP	2.6
1	A	86	GLY	2.6
1	D	86	GLY	2.5
1	A	289	ARG	2.5
1	B	292	ARG	2.5
1	C	16	LEU	2.5
1	D	30	SER	2.5
1	B	21	ASP	2.4
1	A	61	ARG	2.4
1	C	30	SER	2.3
1	A	87	LEU	2.3
1	B	46	GLY	2.3
1	B	22	ASP	2.3
1	B	217	LEU	2.3
1	C	287	ALA	2.3
1	B	215	GLY	2.3
1	B	289	ARG	2.3
1	C	23	TYR	2.2
1	D	163	ARG	2.3
1	B	84	GLN	2.2
1	D	125	TRP	2.2
1	D	38	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	18	PRO	2.2
1	A	295	SER	2.2
1	C	32	TRP	2.2
1	D	16	LEU	2.2
1	C	290	THR	2.2
1	D	296	ALA	2.2
1	B	290	THR	2.1
1	D	164	PRO	2.1
1	B	61	ARG	2.1
1	C	35	VAL	2.1
1	D	81	TRP	2.1
1	B	137	GLY	2.0
1	C	247	GLY	2.0
1	C	268	ASP	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors(Å^2)	Q<0.9
4	GOL	A	1305	6/6	0.57	0.40	77,79,79,80	0
4	GOL	B	1299	6/6	0.71	0.39	62,63,63,64	0
4	GOL	A	1301	6/6	0.74	0.47	59,60,60,61	0
4	GOL	C	1301	6/6	0.75	0.36	59,59,60,60	0
3	IPE	A	1298	14/14	0.76	0.31	42,49,56,56	0
4	GOL	B	1301	6/6	0.78	0.40	58,59,59,59	0
2	DPO	C	1297	9/9	0.80	0.26	60,62,68,69	0
6	PO4	C	1298	5/5	0.81	0.35	93,93,94,94	0
4	GOL	C	1300	6/6	0.82	0.34	52,54,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	PO4	D	1298	5/5	0.83	0.26	49,50,51,55	0
4	GOL	B	1300	6/6	0.84	0.25	55,56,56,57	0
4	GOL	A	1300	6/6	0.84	0.24	58,58,59,59	0
3	IPE	B	1297	14/14	0.84	0.28	49,59,60,60	0
2	DPO	B	1296	9/9	0.86	0.28	49,51,55,56	0
2	DPO	A	1297	9/9	0.86	0.22	56,58,64,64	0
4	GOL	A	1299	6/6	0.87	0.18	56,56,56,56	0
6	PO4	A	1304	5/5	0.90	0.22	56,57,59,60	0
4	GOL	C	1299	6/6	0.92	0.40	33,37,39,39	0
4	GOL	A	1302	6/6	0.93	0.35	30,33,35,36	0
4	GOL	B	1298	6/6	0.94	0.39	29,33,34,36	0
6	PO4	D	1297	5/5	0.95	0.17	62,62,62,63	0
5	CL	A	1303	1/1	0.98	0.20	37,37,37,37	0
6	PO4	C	1302	5/5	0.98	0.14	35,36,38,39	0

6.5 Other polymers (i)

There are no such residues in this entry.