



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:07 PM GMT

PDB ID : 1IV4
Title : Structure of 2C-Methyl-D-erythritol-2,4-cyclodiphosphate Synthase (bound form Substrate)
Authors : Kishida, H.; Wada, T.; Unzai, S.; Kuzuyama, T.; Terada, T.; Sirouzu, M.; Yokoyama, S.; Tame, J.R.H.; Park, S.-Y.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2002-03-11
Resolution : 1.55 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) : **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

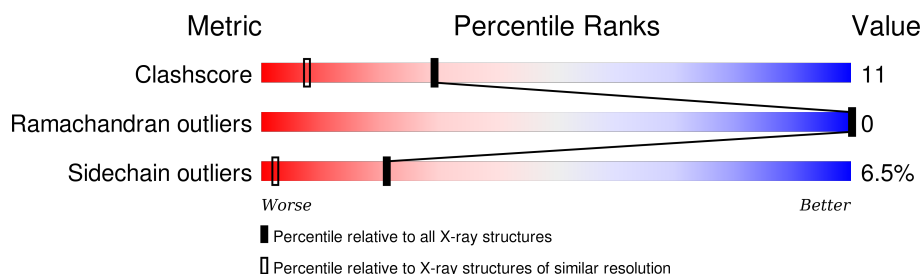
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.55 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	1014 (1.56-1.56)
Ramachandran outliers	100387	1704 (1.58-1.54)
Sidechain outliers	100360	1702 (1.58-1.54)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	152	 78% 18% . .
1	B	152	 77% 18% . .
1	C	152	 66% 25% 7% . .
1	D	152	 78% 16% . .
1	E	152	 74% 18% 6% . .
1	F	152	 71% 20% 7% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7566 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 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	150	Total	C	N	O	S	0	0	0
			1152	726	213	209	4			
1	B	150	Total	C	N	O	S	0	0	0
			1152	726	213	209	4			
1	C	150	Total	C	N	O	S	0	0	0
			1152	726	213	209	4			
1	D	150	Total	C	N	O	S	0	0	0
			1152	726	213	209	4			
1	E	150	Total	C	N	O	S	0	0	0
			1152	726	213	209	4			
1	F	150	Total	C	N	O	S	0	0	0
			1152	726	213	209	4			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	41	MET	LEU	ENGINEERED	UNP Q8RQP5
A	81	MET	LEU	ENGINEERED	UNP Q8RQP5
A	120	MET	LEU	ENGINEERED	UNP Q8RQP5
B	241	MET	LEU	ENGINEERED	UNP Q8RQP5
B	281	MET	LEU	ENGINEERED	UNP Q8RQP5
B	320	MET	LEU	ENGINEERED	UNP Q8RQP5
C	441	MET	LEU	ENGINEERED	UNP Q8RQP5
C	481	MET	LEU	ENGINEERED	UNP Q8RQP5
C	520	MET	LEU	ENGINEERED	UNP Q8RQP5
D	1041	MET	LEU	ENGINEERED	UNP Q8RQP5
D	1081	MET	LEU	ENGINEERED	UNP Q8RQP5
D	1120	MET	LEU	ENGINEERED	UNP Q8RQP5
E	1241	MET	LEU	ENGINEERED	UNP Q8RQP5
E	1281	MET	LEU	ENGINEERED	UNP Q8RQP5
E	1320	MET	LEU	ENGINEERED	UNP Q8RQP5
F	1441	MET	LEU	ENGINEERED	UNP Q8RQP5
F	1481	MET	LEU	ENGINEERED	UNP Q8RQP5

Continued on next page...

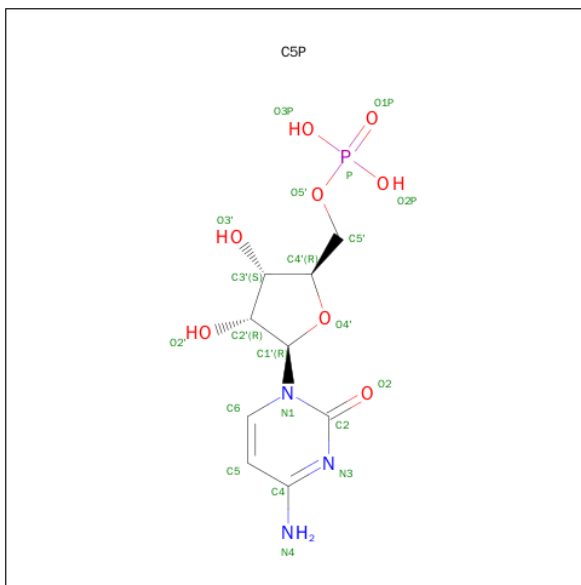
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	1520	MET	LEU	ENGINEERED	UNP Q8RQP5

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	3	Total Mg 3 3	0	0
2	E	1	Total Mg 1 1	0	0
2	B	2	Total Mg 2 2	0	0
2	C	1	Total Mg 1 1	0	0
2	A	3	Total Mg 3 3	0	0
2	F	2	Total Mg 2 2	0	0

- Molecule 3 is CYTIDINE-5'-MONOPHOSPHATE (three-letter code: C5P) (formula: C₉H₁₄N₃O₈P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total C N O P 21 9 3 8 1	0	0
3	A	1	Total C N O P 21 9 3 8 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			21	9	3	8	1		
3	F	1	Total	C	N	O	P	0	0
			21	9	3	8	1		
3	D	1	Total	C	N	O	P	0	0
			21	9	3	8	1		
3	F	1	Total	C	N	O	P	0	0
			21	9	3	8	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	98	Total	O	0	0
			98	98		
4	B	91	Total	O	0	0
			91	91		
4	C	86	Total	O	0	0
			86	86		
4	D	88	Total	O	0	0
			88	88		
4	E	73	Total	O	0	0
			73	73		
4	F	80	Total	O	0	0
			80	80		

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.

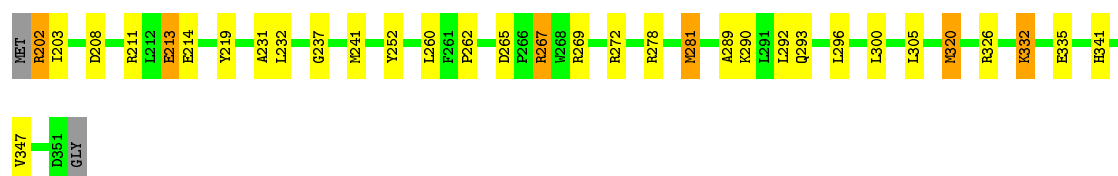
- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

Chain A: 



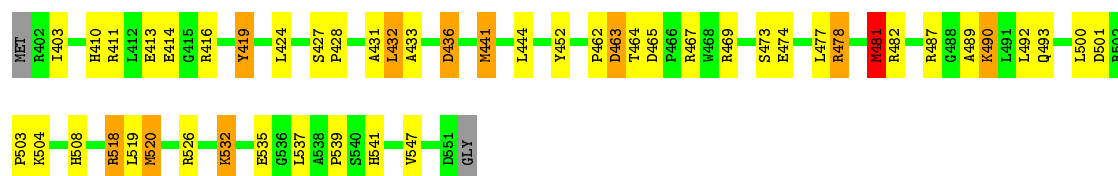
- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

Chain B: 




- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

Chain C: 



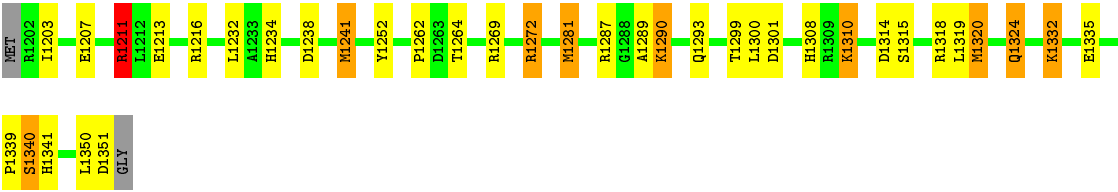
- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

Chain D: 

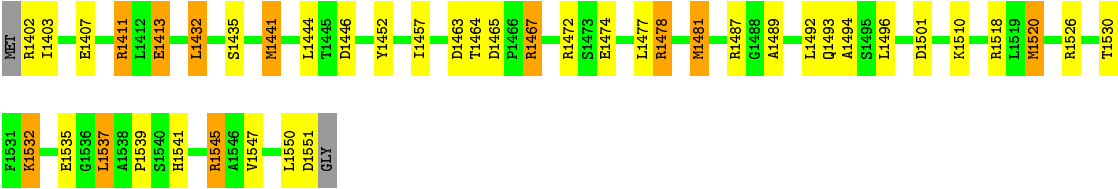


- Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase

Chain E: 



• Molecule 1: 2-C-methyl-D-erythritol 2,4-cyclodiphosphate synthase



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	106.36 Å 106.36 Å 149.19 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.55	Depositor
% Data completeness (in resolution range)	90.5 (20.00-1.55)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.206 , 0.257	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7566	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

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: MG, C5P

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	0.51	2/1173 (0.2%)	1.14	8/1587 (0.5%)
1	B	0.47	0/1173	1.18	11/1587 (0.7%)
1	C	0.53	2/1173 (0.2%)	1.24	12/1587 (0.8%)
1	D	0.45	0/1173	1.21	16/1587 (1.0%)
1	E	0.50	1/1173 (0.1%)	1.24	13/1587 (0.8%)
1	F	0.46	1/1173 (0.1%)	1.19	13/1587 (0.8%)
All	All	0.49	6/7038 (0.1%)	1.20	73/9522 (0.8%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	81	MET	C-O	6.81	1.36	1.23
1	E	1320	MET	CA-C	6.31	1.69	1.52
1	F	1481	MET	CA-C	6.08	1.68	1.52
1	C	520	MET	CA-C	5.90	1.68	1.52
1	C	520	MET	C-O	-5.49	1.12	1.23
1	A	41	MET	C-O	5.25	1.33	1.23

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	272	ARG	NE-CZ-NH2	-11.50	114.55	120.30
1	D	1072	ARG	NE-CZ-NH2	-9.99	115.30	120.30
1	F	1472	ARG	NE-CZ-NH2	-9.91	115.35	120.30
1	D	1121	ARG	NE-CZ-NH1	9.58	125.09	120.30
1	C	487	ARG	CD-NE-CZ	9.18	136.45	123.60
1	E	1211	ARG	CD-NE-CZ	9.04	136.26	123.60
1	E	1269	ARG	NE-CZ-NH1	-8.93	115.84	120.30
1	B	326	ARG	NE-CZ-NH2	-8.80	115.90	120.30
1	E	1287	ARG	NE-CZ-NH1	8.67	124.64	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	1287	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	F	1545	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	B	219	TYR	CB-CG-CD1	-8.05	116.17	121.00
1	F	1487	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	C	487	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	E	1272	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	F	1526	ARG	NE-CZ-NH1	7.40	124.00	120.30
1	F	1478	ARG	NE-CZ-NH1	-7.12	116.74	120.30
1	F	1550	LEU	C-N-CA	7.11	139.46	121.70
1	D	1102	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	C	478	ARG	NE-CZ-NH1	6.93	123.76	120.30
1	C	482	ARG	NE-CZ-NH1	-6.80	116.90	120.30
1	D	1087	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	E	1272	ARG	CD-NE-CZ	6.60	132.84	123.60
1	A	72	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	D	1121	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	D	1126	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	A	87	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	C	487	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	B	278	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	82	ARG	NE-CZ-NH1	-6.13	117.23	120.30
1	D	1065	ASP	CB-CG-OD1	6.11	123.80	118.30
1	F	1526	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	D	1121	ARG	CD-NE-CZ	5.99	131.98	123.60
1	D	1145	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	F	1472	ARG	NH1-CZ-NH2	5.92	125.91	119.40
1	B	202	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	D	1120	MET	CG-SD-CE	5.77	109.43	100.20
1	F	1481	MET	CG-SD-CE	5.76	109.42	100.20
1	A	67	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	B	281	MET	CG-SD-CE	5.75	109.40	100.20
1	A	120	MET	CG-SD-CE	5.75	109.40	100.20
1	A	41	MET	CG-SD-CE	5.75	109.39	100.20
1	B	241	MET	CG-SD-CE	5.73	109.37	100.20
1	F	1520	MET	CG-SD-CE	5.72	109.35	100.20
1	B	320	MET	CG-SD-CE	5.72	109.35	100.20
1	E	1281	MET	CG-SD-CE	5.71	109.34	100.20
1	A	81	MET	CG-SD-CE	5.71	109.33	100.20
1	C	441	MET	CG-SD-CE	5.70	109.33	100.20
1	D	1041	MET	CG-SD-CE	5.70	109.32	100.20
1	D	1081	MET	CG-SD-CE	5.69	109.30	100.20
1	E	1320	MET	CG-SD-CE	5.69	109.30	100.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	1441	MET	CG-SD-CE	5.68	109.29	100.20
1	C	481	MET	CG-SD-CE	5.68	109.28	100.20
1	C	520	MET	CG-SD-CE	5.67	109.27	100.20
1	E	1241	MET	CG-SD-CE	5.67	109.27	100.20
1	D	1087	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	B	272	ARG	NH1-CZ-NH2	5.59	125.55	119.40
1	B	267	ARG	CD-NE-CZ	5.59	131.43	123.60
1	E	1320	MET	CB-CA-C	-5.55	99.29	110.40
1	C	526	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	E	1238	ASP	CB-CG-OD1	5.45	123.20	118.30
1	F	1411	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	D	1072	ARG	NH1-CZ-NH2	5.38	125.31	119.40
1	C	436	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	267	ARG	NE-CZ-NH1	5.35	122.98	120.30
1	C	419	TYR	CB-CG-CD1	-5.25	117.85	121.00
1	E	1320	MET	CA-C-N	-5.25	105.65	117.20
1	C	478	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	D	1082	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	A	102	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	F	1518	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	E	1287	ARG	CD-NE-CZ	5.07	130.70	123.60
1	D	1011	ARG	NE-CZ-NH1	-5.01	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1152	0	1182	25	0
1	B	1152	0	1182	22	0
1	C	1152	0	1182	49	0
1	D	1152	0	1182	26	0
1	E	1152	0	1182	36	0
1	F	1152	0	1182	33	0
2	A	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	3	0	0	0	0
2	E	1	0	0	0	0
2	F	2	0	0	0	0
3	A	21	0	11	0	0
3	B	21	0	11	0	0
3	C	21	0	11	0	0
3	D	21	0	11	1	0
3	F	42	0	22	0	0
4	A	98	0	0	1	0
4	B	91	0	0	3	0
4	C	86	0	0	8	0
4	D	88	0	0	6	0
4	E	73	0	0	1	0
4	F	80	0	0	5	0
All	All	7566	0	7158	161	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 11.

All (161) 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:E:1216:ARG:NH2	1:E:1232:LEU:CD1	1.84	1.37
1:E:1216:ARG:NH2	1:E:1232:LEU:HD12	1.54	1.15
1:E:1216:ARG:NH2	1:E:1232:LEU:HD13	1.61	1.15
1:E:1281:MET:HE2	1:E:1320:MET:HA	1.24	1.09
1:E:1216:ARG:CZ	1:E:1232:LEU:HD12	1.86	1.04
1:E:1216:ARG:HH21	1:E:1232:LEU:HD13	1.20	0.99
1:E:1281:MET:CE	1:E:1320:MET:HA	1.99	0.91
1:C:478:ARG:HA	1:C:481:MET:HG3	1.58	0.85
1:C:477:LEU:O	1:C:481:MET:HG2	1.75	0.84
1:E:1216:ARG:HH22	1:E:1232:LEU:CD1	1.95	0.79
1:C:532:LYS:HD2	4:C:1614:HOH:O	1.84	0.77
1:E:1281:MET:HE2	1:E:1320:MET:CA	2.10	0.76
1:C:463:ASP:O	1:C:469:ARG:HD3	1.86	0.76
1:D:1132:LYS:HD2	4:D:76:HOH:O	1.87	0.75
1:E:1211:ARG:HH11	1:E:1211:ARG:HG3	1.51	0.75
1:A:77:LEU:O	1:A:81:MET:HG3	1.88	0.73
1:F:1413:GLU:OE1	1:F:1432:LEU:HD22	1.87	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1465:ASP:OD1	1:F:1467:ARG:HG3	1.88	0.73
1:B:213:GLU:OE1	1:B:232:LEU:HD22	1.89	0.73
1:E:1216:ARG:CZ	1:E:1232:LEU:CD1	2.58	0.72
1:B:332:LYS:HD2	4:B:1619:HOH:O	1.91	0.71
1:E:1332:LYS:HD2	4:F:142:HOH:O	1.90	0.70
1:A:132:LYS:HD2	4:A:1640:HOH:O	1.90	0.70
1:C:444:LEU:HD22	1:C:520:MET:HE1	1.72	0.69
1:F:1532:LYS:HD2	4:F:117:HOH:O	1.94	0.68
1:E:1213:GLU:OE2	1:E:1232:LEU:HD13	1.94	0.68
1:A:13:GLU:OE1	1:A:32:LEU:HB2	1.94	0.67
1:C:431:ALA:HB1	4:C:1684:HOH:O	1.94	0.67
1:C:478:ARG:NH2	1:C:518:ARG:HH12	1.92	0.67
1:D:1013:GLU:OE1	1:D:1032:LEU:HB3	1.95	0.65
1:F:1474:GLU:O	1:F:1478:ARG:HG2	1.97	0.65
1:F:1501:ASP:OD2	1:F:1539:PRO:HA	1.97	0.65
1:B:332:LYS:HE2	4:B:1640:HOH:O	1.98	0.64
1:D:1067:ARG:HG3	4:D:297:HOH:O	1.98	0.63
1:C:441:MET:CE	1:C:474:GLU:HA	2.29	0.63
1:C:478:ARG:HA	1:C:481:MET:CG	2.29	0.63
1:C:441:MET:CE	1:C:477:LEU:HD22	2.29	0.62
1:A:8:ASP:HA	1:C:532:LYS:HE2	1.81	0.62
1:C:441:MET:HE2	1:C:474:GLU:HA	1.80	0.62
1:E:1211:ARG:NH1	1:E:1340:SER:HB2	2.16	0.61
1:D:1003:ILE:HD13	1:F:1547:VAL:HG11	1.82	0.60
1:F:1481:MET:HE2	1:F:1520:MET:HA	1.82	0.60
1:F:1432:LEU:HG	1:F:1432:LEU:O	2.03	0.58
1:C:532:LYS:HE3	4:C:1623:HOH:O	2.03	0.58
1:B:347:VAL:HG11	1:C:403:ILE:HD13	1.85	0.58
1:A:93:GLN:NE2	1:B:203:ILE:H	2.01	0.57
1:A:141:HIS:CD2	1:C:537:LEU:HD13	2.39	0.57
1:C:504:LYS:HG2	4:C:1674:HOH:O	2.04	0.57
1:D:1135:GLU:O	1:E:1341:HIS:HE1	1.88	0.57
1:C:462:PRO:HB2	1:C:464:THR:OG1	2.05	0.57
1:E:1332:LYS:HD3	1:F:1407:GLU:O	2.06	0.56
1:A:3:ILE:H	1:C:493:GLN:NE2	2.03	0.56
1:E:1252:TYR:OH	1:E:1289:ALA:HB2	2.03	0.56
1:A:19:TYR:CE1	1:A:24:LEU:HD23	2.40	0.56
1:A:141:HIS:HE1	1:C:535:GLU:O	1.89	0.56
1:A:135:GLU:O	1:B:341:HIS:HE1	1.89	0.56
1:B:211:ARG:HD3	4:B:1694:HOH:O	2.06	0.56
1:C:508:HIS:HD2	4:C:1611:HOH:O	1.89	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:419:TYR:CZ	1:C:424:LEU:HD12	2.41	0.56
1:E:1335:GLU:O	1:F:1541:HIS:HE1	1.89	0.56
1:E:1315:SER:O	1:E:1319:LEU:HD23	2.05	0.56
1:D:1141:HIS:HE1	1:F:1535:GLU:O	1.88	0.55
1:B:335:GLU:O	1:C:541:HIS:HE1	1.90	0.55
1:E:1211:ARG:HH12	1:E:1340:SER:HB2	1.72	0.55
1:F:1535:GLU:HA	4:F:497:HOH:O	2.07	0.55
1:E:1308:HIS:HE1	4:E:224:HOH:O	1.89	0.54
1:D:1145:ARG:HD2	1:E:1207:GLU:OE2	2.07	0.54
1:E:1332:LYS:HE2	4:F:193:HOH:O	2.06	0.54
1:D:1150:LEU:O	1:D:1151:ASP:HB2	2.06	0.54
1:E:1310:LYS:HD3	1:E:1314:ASP:OD2	2.08	0.53
1:C:452:TYR:OH	1:C:489:ALA:HB2	2.09	0.53
1:C:492:LEU:HD12	4:C:1620:HOH:O	2.08	0.53
1:E:1350:LEU:O	1:E:1351:ASP:HB2	2.10	0.52
1:A:3:ILE:HD13	1:C:547:VAL:HG11	1.91	0.52
1:E:1301:ASP:OD2	1:E:1339:PRO:HA	2.10	0.52
1:F:1481:MET:CE	1:F:1520:MET:HA	2.40	0.52
1:F:1441:MET:CE	1:F:1477:LEU:HD22	2.41	0.51
1:E:1252:TYR:CE1	1:E:1289:ALA:HB2	2.46	0.51
1:D:1093:GLN:NE2	1:E:1203:ILE:H	2.09	0.51
1:A:150:LEU:O	1:A:151:ASP:HB2	2.10	0.50
1:B:281:MET:HE3	1:B:320:MET:HA	1.94	0.50
1:B:267:ARG:HG2	1:D:1087:ARG:HH21	1.76	0.49
1:C:477:LEU:O	1:C:481:MET:CG	2.55	0.49
1:B:293:GLN:NE2	1:C:403:ILE:H	2.10	0.49
1:A:19:TYR:CZ	1:A:24:LEU:HD23	2.48	0.49
1:A:137:LEU:HD13	1:B:341:HIS:CD2	2.47	0.49
1:C:419:TYR:CE1	1:C:424:LEU:HD12	2.48	0.48
1:D:1056:ASP:HB3	1:F:1530:THR:HG22	1.95	0.48
1:C:489:ALA:C	1:C:490:LYS:HD3	2.34	0.48
1:C:532:LYS:HB3	1:C:532:LYS:HE3	1.67	0.47
1:D:1003:ILE:CD1	1:F:1547:VAL:HG11	2.44	0.47
1:C:441:MET:HE3	1:C:477:LEU:HD22	1.95	0.47
1:D:1141:HIS:HD2	4:D:136:HOH:O	1.97	0.47
1:C:478:ARG:CA	1:C:481:MET:HG3	2.39	0.47
1:F:1452:TYR:CE1	1:F:1489:ALA:HB2	2.50	0.47
1:E:1299:THR:O	1:E:1300:LEU:HB3	2.15	0.47
1:F:1532:LYS:HE3	1:F:1532:LYS:HB3	1.61	0.47
1:B:267:ARG:HG2	1:D:1087:ARG:NH2	2.30	0.47
1:D:1141:HIS:CD2	1:F:1537:LEU:HD13	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:7:GLU:O	1:C:532:LYS:HD3	2.14	0.47
1:D:1007:GLU:HG2	1:D:1145:ARG:HG2	1.96	0.47
1:C:433:ALA:HB2	4:C:1684:HOH:O	2.13	0.46
1:A:59:LEU:HG	1:A:60:LEU:HD23	1.97	0.46
1:E:1252:TYR:CZ	1:E:1289:ALA:HB2	2.50	0.46
1:E:1281:MET:CE	1:E:1320:MET:HG2	2.46	0.46
1:A:32:LEU:HG	1:A:32:LEU:O	2.15	0.46
1:F:1411:ARG:HG2	1:F:1413:GLU:OE2	2.16	0.46
1:F:1492:LEU:HD12	4:F:213:HOH:O	2.16	0.46
1:E:1314:ASP:OD1	1:E:1324:GLN:NE2	2.48	0.46
1:C:501:ASP:OD2	1:C:539:PRO:HA	2.16	0.45
1:A:132:LYS:HE3	1:A:132:LYS:HB3	1.47	0.45
1:D:1014:GLU:OE1	1:D:1102:ARG:NH2	2.49	0.45
1:C:452:TYR:CZ	1:C:489:ALA:HB2	2.50	0.45
1:C:413:GLU:OE1	1:C:432:LEU:HD13	2.16	0.45
1:B:252:TYR:CZ	1:B:289:ALA:HB2	2.52	0.45
1:C:410:HIS:HB3	4:C:1684:HOH:O	2.15	0.45
1:D:1063:ASP:O	1:D:1069:ARG:HB2	2.17	0.45
1:C:500:LEU:HD23	1:C:500:LEU:N	2.32	0.45
1:D:1085:GLU:OE2	1:D:1121:ARG:NH2	2.50	0.45
1:C:413:GLU:CD	1:C:432:LEU:HD13	2.36	0.44
1:E:1293:GLN:NE2	1:F:1403:ILE:H	2.16	0.44
1:D:1002:ARG:N	4:D:310:HOH:O	2.50	0.44
1:F:1441:MET:HE1	1:F:1477:LEU:HD22	1.99	0.44
1:C:478:ARG:HH21	1:C:518:ARG:HH12	1.66	0.44
1:F:1494:ALA:CB	1:F:1520:MET:HE1	2.48	0.44
1:B:252:TYR:CE1	1:B:289:ALA:HB2	2.53	0.44
1:C:427:SER:HB2	1:C:503:PRO:HG3	1.99	0.44
1:F:1444:LEU:HD22	1:F:1520:MET:HE1	2.00	0.44
1:C:441:MET:CE	1:C:477:LEU:CD2	2.96	0.43
1:F:1478:ARG:HD2	1:F:1478:ARG:HH11	1.55	0.43
1:D:1003:ILE:H	1:F:1493:GLN:NE2	2.15	0.43
1:F:1535:GLU:HA	1:F:1535:GLU:OE1	2.19	0.43
1:C:413:GLU:OE1	1:C:416:ARG:NH2	2.49	0.43
1:D:1132:LYS:HE3	1:D:1132:LYS:HB3	1.69	0.43
1:F:1474:GLU:OE2	1:F:1478:ARG:NH2	2.49	0.43
1:C:414:GLU:HA	1:C:428:PRO:O	2.18	0.43
1:A:96:LEU:HD23	1:A:96:LEU:N	2.34	0.43
1:C:436:ASP:OD2	1:C:473:SER:OG	2.30	0.42
1:C:481:MET:HG2	1:C:481:MET:H	1.40	0.42
1:E:1289:ALA:C	1:E:1290:LYS:HD2	2.39	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:1496:LEU:HD23	1:F:1496:LEU:N	2.34	0.42
1:B:300:LEU:HD21	1:B:305:LEU:CD1	2.50	0.42
3:D:1605:C5P:H5'2	4:D:459:HOH:O	2.19	0.42
1:B:262:PRO:HG2	1:B:265:ASP:HB2	2.01	0.42
1:A:100:LEU:HD23	1:A:100:LEU:N	2.35	0.42
1:D:1032:LEU:O	1:D:1032:LEU:HG	2.20	0.42
1:C:465:ASP:OD1	1:C:467:ARG:HG3	2.20	0.42
1:A:132:LYS:HE2	1:B:208:ASP:HA	2.00	0.42
1:B:231:ALA:CB	1:B:237:GLY:HA3	2.50	0.42
1:C:410:HIS:HD1	1:C:433:ALA:HB2	1.86	0.41
1:D:1132:LYS:HE3	4:D:161:HOH:O	2.19	0.41
1:A:93:GLN:HE22	1:B:202:ARG:HA	1.86	0.41
1:F:1446:ASP:OD1	1:F:1457:ILE:HG23	2.21	0.41
1:B:296:LEU:N	1:B:296:LEU:HD23	2.35	0.41
1:E:1293:GLN:HE22	1:F:1402:ARG:HA	1.86	0.41
1:D:1027:SER:OG	1:D:1103:PRO:HD3	2.21	0.41
1:A:104:LYS:HE2	1:A:104:LYS:HB3	1.84	0.40
1:A:93:GLN:HE22	1:B:203:ILE:H	1.69	0.40
1:A:74:GLU:OE2	1:A:78:ARG:NE	2.49	0.40
1:E:1262:PRO:HB2	1:E:1264:THR:OG1	2.21	0.40
1:D:1007:GLU:OE2	1:F:1545:ARG:HD2	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	148/152 (97%)	147 (99%)	1 (1%)	0	100	100
1	B	148/152 (97%)	147 (99%)	1 (1%)	0	100	100
1	C	148/152 (97%)	145 (98%)	3 (2%)	0	100	100
1	D	148/152 (97%)	146 (99%)	2 (1%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	148/152 (97%)	147 (99%)	1 (1%)	0	100	100
1	F	148/152 (97%)	147 (99%)	1 (1%)	0	100	100
All	All	888/912 (97%)	879 (99%)	9 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	121/122 (99%)	114 (94%)	7 (6%)	25	3
1	B	121/122 (99%)	114 (94%)	7 (6%)	25	3
1	C	121/122 (99%)	113 (93%)	8 (7%)	21	2
1	D	121/122 (99%)	116 (96%)	5 (4%)	37	7
1	E	121/122 (99%)	111 (92%)	10 (8%)	14	1
1	F	121/122 (99%)	111 (92%)	10 (8%)	14	1
All	All	726/732 (99%)	679 (94%)	47 (6%)	21	2

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	32	LEU
1	A	60	LEU
1	A	81	MET
1	A	90	LYS
1	A	104	LYS
1	A	132	LYS
1	B	213	GLU
1	B	214	GLU
1	B	260	LEU
1	B	269	ARG
1	B	290	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	292	LEU
1	B	332	LYS
1	C	411	ARG
1	C	432	LEU
1	C	463	ASP
1	C	481	MET
1	C	490	LYS
1	C	518	ARG
1	C	519	LEU
1	C	532	LYS
1	D	1014	GLU
1	D	1032	LEU
1	D	1060	LEU
1	D	1102	ARG
1	D	1132	LYS
1	E	1211	ARG
1	E	1234	HIS
1	E	1241	MET
1	E	1272	ARG
1	E	1290	LYS
1	E	1310	LYS
1	E	1318	ARG
1	E	1324	GLN
1	E	1332	LYS
1	E	1340	SER
1	F	1413	GLU
1	F	1432	LEU
1	F	1435	SER
1	F	1463	ASP
1	F	1464	THR
1	F	1467	ARG
1	F	1510	LYS
1	F	1532	LYS
1	F	1537	LEU
1	F	1551	ASP

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

Mol	Chain	Res	Type
1	A	93	GLN
1	A	141	HIS
1	B	293	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	341	HIS
1	C	493	GLN
1	C	508	HIS
1	C	541	HIS
1	D	1093	GLN
1	D	1141	HIS
1	E	1293	GLN
1	E	1308	HIS
1	E	1341	HIS
1	F	1493	GLN
1	F	1541	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 12 are monoatomic - leaving 6 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	C5P	A	1602	2	17,22,22	2.04	2 (11%)	22,33,33	2.86	10 (45%)
3	C5P	B	1603	2	17,22,22	1.93	2 (11%)	22,33,33	3.06	12 (54%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	C5P	C	1601	2	17,22,22	1.96	2 (11%)	22,33,33	2.94	13 (59%)
3	C5P	D	1605	2	17,22,22	1.91	3 (17%)	22,33,33	2.88	10 (45%)
3	C5P	F	1604	2	17,22,22	2.00	2 (11%)	22,33,33	2.97	10 (45%)
3	C5P	F	1606	2	17,22,22	2.05	3 (17%)	22,33,33	3.20	10 (45%)

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	C5P	A	1602	2	-	0/6/26/26	0/2/2/2
3	C5P	B	1603	2	-	0/6/26/26	0/2/2/2
3	C5P	C	1601	2	-	0/6/26/26	0/2/2/2
3	C5P	D	1605	2	-	0/6/26/26	0/2/2/2
3	C5P	F	1604	2	-	0/6/26/26	0/2/2/2
3	C5P	F	1606	2	-	0/6/26/26	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1605	C5P	C5'-C4'	-2.01	1.45	1.51
3	F	1606	C5P	P-O1P	-2.00	1.44	1.51
3	F	1604	C5P	C4-N3	3.67	1.42	1.35
3	D	1605	C5P	C4-N3	3.85	1.42	1.35
3	B	1603	C5P	C4-N3	3.96	1.42	1.35
3	F	1606	C5P	C4-N3	3.98	1.42	1.35
3	A	1602	C5P	C4-N3	4.04	1.43	1.35
3	C	1601	C5P	C4-N3	4.08	1.43	1.35
3	D	1605	C5P	C6-N1	5.54	1.43	1.35
3	C	1601	C5P	C6-N1	5.63	1.43	1.35
3	B	1603	C5P	C6-N1	5.78	1.43	1.35
3	F	1604	C5P	C6-N1	6.20	1.44	1.35
3	A	1602	C5P	C6-N1	6.24	1.44	1.35
3	F	1606	C5P	C6-N1	6.42	1.44	1.35

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1605	C5P	O4'-C1'-N1	-8.39	90.39	108.08
3	B	1603	C5P	O4'-C1'-N1	-8.11	90.98	108.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1602	C5P	O4'-C1'-N1	-7.67	91.90	108.08
3	F	1606	C5P	O4'-C1'-N1	-7.56	92.14	108.08
3	F	1604	C5P	O4'-C1'-N1	-6.99	93.35	108.08
3	C	1601	C5P	O4'-C1'-N1	-6.79	93.76	108.08
3	F	1606	C5P	O2'-C2'-C3'	-5.35	94.44	111.83
3	B	1603	C5P	O2'-C2'-C3'	-5.28	94.64	111.83
3	F	1606	C5P	C6-N1-C2	-5.11	113.00	121.28
3	F	1604	C5P	O2'-C2'-C3'	-4.88	95.96	111.83
3	F	1604	C5P	C6-N1-C2	-4.82	113.47	121.28
3	B	1603	C5P	C6-N1-C2	-4.71	113.64	121.28
3	A	1602	C5P	C6-N1-C2	-4.69	113.68	121.28
3	D	1605	C5P	O2'-C2'-C3'	-4.47	97.27	111.83
3	C	1601	C5P	C6-N1-C2	-4.30	114.32	121.28
3	C	1601	C5P	O2P-P-O5'	-4.20	94.48	106.56
3	D	1605	C5P	C6-N1-C2	-4.14	114.58	121.28
3	F	1604	C5P	O2P-P-O5'	-3.99	95.09	106.56
3	C	1601	C5P	O2'-C2'-C3'	-3.95	98.99	111.83
3	A	1602	C5P	O2'-C2'-C3'	-3.79	99.51	111.83
3	F	1606	C5P	O2P-P-O5'	-3.64	96.10	106.56
3	A	1602	C5P	O2P-P-O5'	-3.06	97.74	106.56
3	B	1603	C5P	O2P-P-O5'	-2.93	98.11	106.56
3	D	1605	C5P	O2P-P-O5'	-2.64	98.95	106.56
3	C	1601	C5P	C5-C4-N4	-2.09	118.10	121.31
3	D	1605	C5P	O2P-P-O1P	2.03	117.11	110.58
3	A	1602	C5P	C5-C6-N1	2.05	125.62	120.58
3	D	1605	C5P	O2P-P-O3P	2.07	115.25	107.38
3	B	1603	C5P	C5-C6-N1	2.11	125.76	120.58
3	B	1603	C5P	O2P-P-O3P	2.23	115.86	107.38
3	B	1603	C5P	N4-C4-N3	2.33	120.75	116.50
3	C	1601	C5P	O2P-P-O3P	2.33	116.26	107.38
3	A	1602	C5P	N4-C4-N3	2.34	120.76	116.50
3	D	1605	C5P	C2-N3-C4	2.36	118.94	115.61
3	C	1601	C5P	N4-C4-N3	2.39	120.86	116.50
3	F	1604	C5P	C5-C6-N1	2.45	126.58	120.58
3	C	1601	C5P	C5-C6-N1	2.47	126.63	120.58
3	A	1602	C5P	O3'-C3'-C2'	2.67	120.52	111.83
3	C	1601	C5P	O3'-C3'-C4'	2.72	119.22	111.05
3	B	1603	C5P	O2P-P-O1P	2.74	119.40	110.58
3	F	1606	C5P	C5-C6-N1	2.83	127.52	120.58
3	F	1606	C5P	O2P-P-O1P	2.88	119.84	110.58
3	C	1601	C5P	O2P-P-O1P	2.93	120.03	110.58
3	F	1604	C5P	O2P-P-O1P	3.02	120.29	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1603	C5P	O3'-C3'-C2'	3.16	122.09	111.83
3	D	1605	C5P	O3'-C3'-C4'	3.23	120.73	111.05
3	D	1605	C5P	O3'-C3'-C2'	3.41	122.93	111.83
3	F	1604	C5P	O3'-C3'-C4'	3.52	121.61	111.05
3	B	1603	C5P	O3'-C3'-C4'	3.62	121.91	111.05
3	A	1602	C5P	C2-N3-C4	3.62	120.72	115.61
3	F	1604	C5P	O3'-C3'-C2'	3.64	123.65	111.83
3	A	1602	C5P	O4'-C4'-C5'	3.64	122.34	109.32
3	B	1603	C5P	C2-N3-C4	3.66	120.77	115.61
3	F	1604	C5P	O4'-C4'-C5'	3.71	122.59	109.32
3	B	1603	C5P	O4'-C4'-C5'	3.91	123.29	109.32
3	C	1601	C5P	O3'-C3'-C2'	3.92	124.59	111.83
3	C	1601	C5P	C2-N3-C4	3.95	121.18	115.61
3	F	1606	C5P	O3'-C3'-C4'	3.95	122.90	111.05
3	F	1606	C5P	O3'-C3'-C2'	4.21	125.53	111.83
3	F	1606	C5P	O4'-C4'-C5'	4.37	124.95	109.32
3	F	1606	C5P	C2-N3-C4	4.39	121.80	115.61
3	C	1601	C5P	O4'-C4'-C5'	4.41	125.09	109.32
3	A	1602	C5P	O3'-C3'-C4'	4.49	124.52	111.05
3	F	1604	C5P	C2-N3-C4	4.50	121.96	115.61
3	D	1605	C5P	O4'-C4'-C5'	4.52	125.50	109.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1605	C5P	1	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.