



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:18 AM GMT

PDB ID : 2Q5L  
Title : X-ray structure of phenylpyruvate decarboxylase in complex with 2-(1-hydroxyethyl)-3-deaza-ThDP  
Authors : Versees, W.; Spaepen, S.; Wood, M.D.; Leeper, F.J.; Vanderleyden, J.; Steyaert, J.  
Deposited on : 2007-06-01  
Resolution : 1.85 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](mailto: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.

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

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

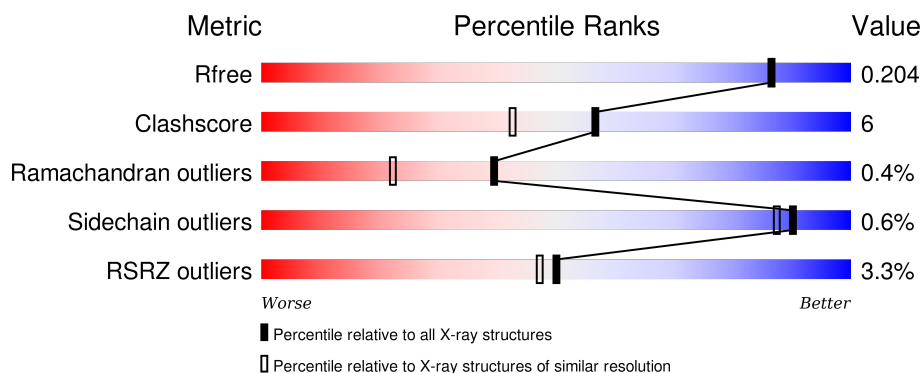
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


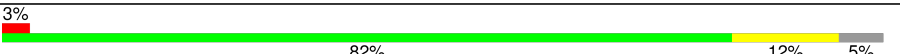
The reported resolution of this entry is 1.85 Å.

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	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	565	
1	B	565	

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
6	GOL	A	4001	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9085 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 PHENYLPYRUVATE DECARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	538	Total	C	N	O	S	0	1	0
			3982	2520	696	743	23			
1	B	535	Total	C	N	O	S	0	1	0
			3961	2510	689	739	23			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P51852
A	-18	GLY	-	EXPRESSION TAG	UNP P51852
A	-17	SER	-	EXPRESSION TAG	UNP P51852
A	-16	SER	-	EXPRESSION TAG	UNP P51852
A	-15	HIS	-	EXPRESSION TAG	UNP P51852
A	-14	HIS	-	EXPRESSION TAG	UNP P51852
A	-13	HIS	-	EXPRESSION TAG	UNP P51852
A	-12	HIS	-	EXPRESSION TAG	UNP P51852
A	-11	HIS	-	EXPRESSION TAG	UNP P51852
A	-10	HIS	-	EXPRESSION TAG	UNP P51852
A	-9	SER	-	EXPRESSION TAG	UNP P51852
A	-8	SER	-	EXPRESSION TAG	UNP P51852
A	-7	GLY	-	EXPRESSION TAG	UNP P51852
A	-6	LEU	-	EXPRESSION TAG	UNP P51852
A	-5	VAL	-	EXPRESSION TAG	UNP P51852
A	-4	PRO	-	EXPRESSION TAG	UNP P51852
A	-3	ARG	-	EXPRESSION TAG	UNP P51852
A	-2	GLY	-	EXPRESSION TAG	UNP P51852
A	-1	SER	-	EXPRESSION TAG	UNP P51852
A	0	HIS	-	EXPRESSION TAG	UNP P51852
A	155	GLN	LEU	EXPRESSION TAG	UNP P51852
A	327	ARG	GLY	SEE REMARK 999	UNP P51852
B	-19	MET	-	EXPRESSION TAG	UNP P51852
B	-18	GLY	-	EXPRESSION TAG	UNP P51852
B	-17	SER	-	EXPRESSION TAG	UNP P51852

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	EXPRESSION TAG	UNP P51852
B	-15	HIS	-	EXPRESSION TAG	UNP P51852
B	-14	HIS	-	EXPRESSION TAG	UNP P51852
B	-13	HIS	-	EXPRESSION TAG	UNP P51852
B	-12	HIS	-	EXPRESSION TAG	UNP P51852
B	-11	HIS	-	EXPRESSION TAG	UNP P51852
B	-10	HIS	-	EXPRESSION TAG	UNP P51852
B	-9	SER	-	EXPRESSION TAG	UNP P51852
B	-8	SER	-	EXPRESSION TAG	UNP P51852
B	-7	GLY	-	EXPRESSION TAG	UNP P51852
B	-6	LEU	-	EXPRESSION TAG	UNP P51852
B	-5	VAL	-	EXPRESSION TAG	UNP P51852
B	-4	PRO	-	EXPRESSION TAG	UNP P51852
B	-3	ARG	-	EXPRESSION TAG	UNP P51852
B	-2	GLY	-	EXPRESSION TAG	UNP P51852
B	-1	SER	-	EXPRESSION TAG	UNP P51852
B	0	HIS	-	EXPRESSION TAG	UNP P51852
B	155	GLN	LEU	EXPRESSION TAG	UNP P51852
B	327	ARG	GLY	SEE REMARK 999	UNP P51852

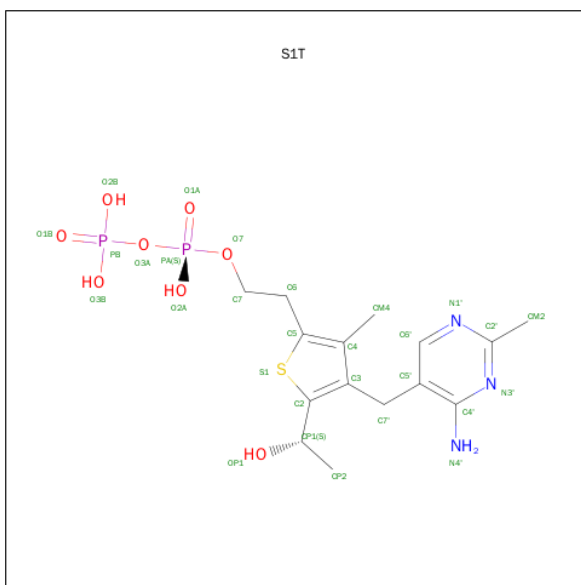
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

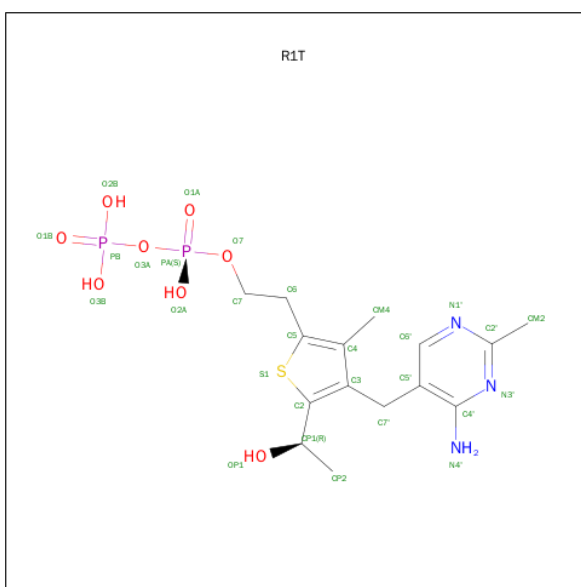
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0

- Molecule 4 is 2-{4-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-5-[(1S)-1-HYDROXYETHYL]-3-METHYL-2-THIENYL}ETHYL TRIHYDROGEN DIPHOSPHATE (three-letter code: S1T) (formula: C<sub>15</sub>H<sub>23</sub>N<sub>3</sub>O<sub>8</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	B	1	Total 29	C 15	N 3	O 8	P 2	S 1	0	1
4	A	1	Total 29	C 15	N 3	O 8	P 2	S 1	0	1

- Molecule 5 is 2-{4-[(4-AMINO-2-METHYLPYRIMIDIN-5-YL)METHYL]-5-[(1R)-1-HYDROXYETHYL]-3-METHYL-2-THIENYL}ETHYL TRIHYDROGEN DIPHOSPHATE (three-letter code: R1T) (formula: C<sub>15</sub>H<sub>23</sub>N<sub>3</sub>O<sub>8</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	S	0	1
			29	15	3	8	2	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	1
			29	15	3	8	2	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

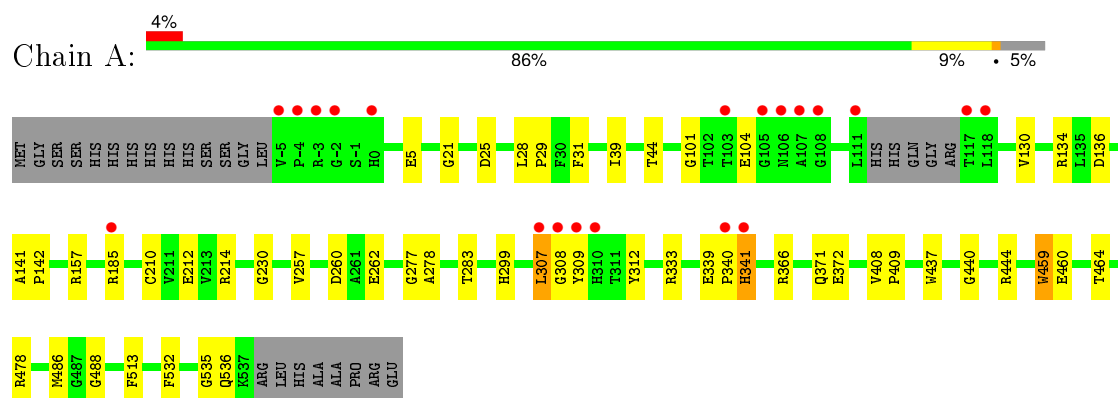
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	534	Total	O	0	0
			534	534		
7	B	476	Total	O	0	0
			476	476		

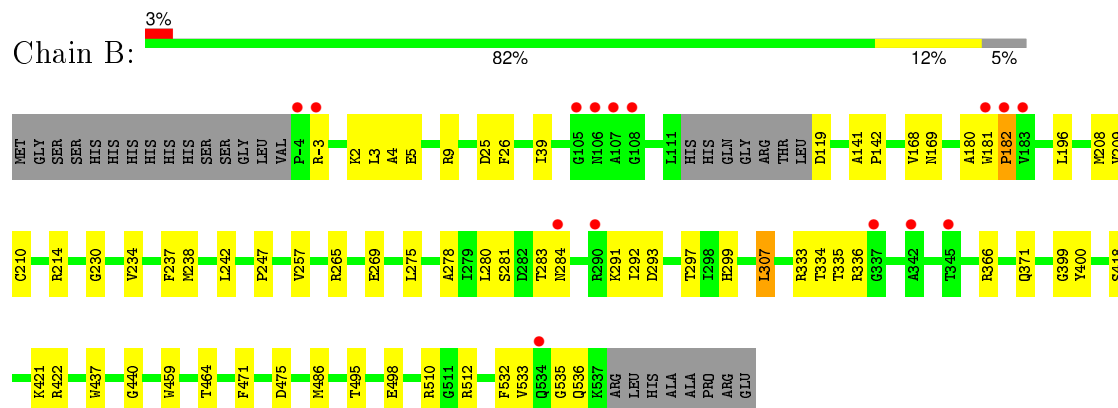
### 3 Residue-property plots [i](#)

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: PHENYLPYRUVATE DECARBOXYLASE



#### • Molecule 1: PHENYLPYRUVATE DECARBOXYLASE





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	99.98Å 179.05Å 120.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.50 – 1.85 32.47 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.4 (32.50-1.85) 98.4 (32.47-1.85)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.08 (at 1.85Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.170 , 0.204 0.171 , 0.204	Depositor DCC
$R_{free}$ test set	4544 reflections (5.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	20.6	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 50.5	EDS
Estimated twinning fraction	0.009 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.017 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 90954 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	9085	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, R1T, S1T, MG, CL

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	0.40	0/4063	0.64	1/5525 (0.0%)
1	B	0.39	0/4042	0.65	2/5496 (0.0%)
All	All	0.40	0/8105	0.64	3/11021 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	307	LEU	CA-CB-CG	6.26	129.70	115.30
1	A	459	TRP	N-CA-C	-5.51	96.12	111.00
1	B	459	TRP	N-CA-C	-5.44	96.32	111.00

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3982	0	3956	37	0
1	B	3961	0	3941	60	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	29	0	20	3	0
4	B	29	0	20	2	0
5	A	29	0	20	1	0
5	B	29	0	20	0	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
7	A	534	0	0	4	0
7	B	476	0	0	6	1
All	All	9085	0	7993	98	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 6.

All (98) 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:422:ARG:HD2	1:B:510:ARG:HH12	1.27	0.99
1:B:230:GLY:HA2	1:B:333:ARG:NH2	1.90	0.86
1:B:283:THR:HG21	1:B:400:TYR:HA	1.60	0.82
1:A:5:GLU:HG3	1:A:39:ILE:HD11	1.62	0.82
1:B:510:ARG:HD2	7:B:4312:HOH:O	1.79	0.81
1:A:366:ARG:HE	1:A:371:GLN:HE21	1.31	0.79
1:B:180:ALA:C	1:B:182:PRO:HD3	2.02	0.78
1:B:238:MET:HG3	1:B:400:TYR:CE2	2.21	0.76
1:B:464:THR:HG21	1:B:533:VAL:HG21	1.70	0.73
1:B:422:ARG:CD	1:B:510:ARG:HH12	2.02	0.69
1:B:510:ARG:HG2	1:B:510:ARG:HH11	1.57	0.69
1:B:334:THR:HG22	1:B:336:ARG:H	1.57	0.69
1:B:422:ARG:HD2	1:B:510:ARG:NH1	2.05	0.68
1:B:366:ARG:HE	1:B:371:GLN:HE21	1.41	0.68
1:B:214:ARG:HG3	1:B:214:ARG:HH11	1.59	0.68
1:A:230:GLY:HA2	1:A:333:ARG:CZ	2.25	0.66
1:B:293:ASP:O	1:B:297[B]:THR:HG23	1.98	0.64
1:B:278:ALA:O	1:B:299:HIS:HE1	1.82	0.63
1:A:278:ALA:O	1:A:299:HIS:HE1	1.83	0.62
1:B:210:CYS:SG	1:B:278:ALA:HB2	2.41	0.61
1:B:283:THR:HG21	1:B:400:TYR:CA	2.32	0.60
1:A:366:ARG:HE	1:A:371:GLN:NE2	1.98	0.60
1:B:9:ARG:HG3	1:B:39:ILE:HD13	1.84	0.60
1:A:532:PHE:O	1:A:536:GLN:HG2	2.02	0.59
1:A:210:CYS:SG	1:A:278:ALA:HB2	2.42	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:ARG:HE	1:B:371:GLN:NE2	2.01	0.59
1:B:265:ARG:CZ	1:B:269:GLU:OE1	2.50	0.59
1:B:510:ARG:NH1	1:B:510:ARG:HG2	2.20	0.57
1:A:230:GLY:HA2	1:A:333:ARG:NE	2.19	0.57
1:B:230:GLY:HA2	1:B:333:ARG:HH21	1.67	0.56
1:B:237:PHE:CE2	1:B:399:GLY:HA3	2.40	0.56
1:B:238:MET:HG3	1:B:400:TYR:CZ	2.40	0.56
1:A:185:ARG:HB3	1:A:185:ARG:NH1	2.21	0.55
1:B:2:LYS:HD3	1:B:169:ASN:OD1	2.07	0.54
1:B:283:THR:HG23	1:B:284:ASN:OD1	2.07	0.54
1:A:460:GLU:O	1:A:464:THR:HG23	2.07	0.54
1:B:292:ILE:HD12	1:B:297[B]:THR:HG21	1.89	0.53
1:A:5:GLU:HG3	1:A:39:ILE:CD1	2.34	0.53
1:A:230:GLY:HA2	1:A:333:ARG:NH2	2.24	0.53
4:A:2002[A]:S1T:HP23	4:A:2002[A]:S1T:H7'2	1.93	0.51
4:B:2001[A]:S1T:H7'2	4:B:2001[A]:S1T:HP23	1.92	0.51
1:B:247:PRO:O	1:B:334:THR:HG23	2.11	0.51
4:A:2002[A]:S1T:CP2	1:B:25:ASP:H	2.23	0.51
1:B:495:THR:OG1	1:B:498:GLU:HG3	2.11	0.50
1:B:208:MET:HA	1:B:234:VAL:O	2.11	0.50
1:B:214:ARG:NH1	1:B:214:ARG:HG3	2.27	0.50
1:B:283:THR:CG2	1:B:400:TYR:HA	2.38	0.50
1:B:209:VAL:HG12	1:B:242:LEU:HD13	1.93	0.50
1:A:444[B]:ARG:NH1	7:A:4534:HOH:O	2.36	0.49
1:B:291:LYS:HD2	7:B:4372:HOH:O	2.12	0.49
1:A:25:ASP:H	4:B:2001[A]:S1T:CP2	2.26	0.49
1:B:418:SER:HB2	1:B:421:LYS:HB2	1.95	0.48
1:A:283:THR:HB	7:A:4446:HOH:O	2.13	0.48
1:B:512:ARG:HD2	7:B:4236:HOH:O	2.12	0.48
1:A:408:VAL:HB	1:A:409:PRO:HD3	1.96	0.48
1:B:5:GLU:HG3	1:B:39:ILE:HD11	1.95	0.48
1:A:214:ARG:HG3	1:A:214:ARG:HH11	1.79	0.48
1:B:26:PHE:HD1	7:B:4326:HOH:O	1.97	0.48
1:B:275:LEU:HD13	1:B:280:LEU:HD21	1.96	0.47
1:B:299:HIS:HD2	7:B:4154:HOH:O	1.97	0.47
1:B:532:PHE:O	1:B:536:GLN:HG2	2.14	0.47
1:A:437:TRP:CD1	1:B:437:TRP:CD1	3.03	0.47
1:A:307:LEU:HD11	1:A:312:TYR:HE2	1.80	0.46
1:A:308:GLY:O	1:A:309:TYR:HB2	2.16	0.46
1:B:366:ARG:NE	1:B:371:GLN:HE21	2.13	0.46
1:A:340:PRO:O	1:A:341:HIS:HB3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ASP:OD2	1:A:262:GLU:HB2	2.16	0.45
1:A:257:VAL:HG21	1:A:535:GLY:HA3	1.98	0.45
1:A:31:PHE:HB3	1:B:471:PHE:CE2	2.52	0.45
1:A:459:TRP:CD1	4:A:2002[A]:S1T:H61	2.52	0.45
1:B:141:ALA:HB3	1:B:142:PRO:HD3	1.98	0.45
1:A:141:ALA:HB3	1:A:142:PRO:HD3	1.99	0.45
1:A:440:GLY:HA2	1:A:486:MET:HB3	1.97	0.45
1:B:230:GLY:HA2	1:B:333:ARG:CZ	2.47	0.45
1:A:366:ARG:NE	1:A:371:GLN:HE21	2.07	0.44
1:A:134:ARG:NH1	1:A:136:ASP:OD2	2.50	0.44
1:A:372:GLU:HG3	7:A:4432:HOH:O	2.16	0.44
1:B:3:LEU:HD23	1:B:3:LEU:C	2.37	0.44
1:B:214:ARG:NH1	7:B:4472:HOH:O	2.33	0.44
1:A:28:LEU:HB2	1:A:29:PRO:HD3	1.99	0.44
1:B:257:VAL:HG21	1:B:535:GLY:HA3	2.00	0.44
1:A:101:GLY:H	1:A:104:GLU:CD	2.21	0.44
1:B:209:VAL:HG12	1:B:242:LEU:CD1	2.49	0.43
1:B:281:SER:OG	1:B:283:THR:HB	2.19	0.43
1:B:4:ALA:HB2	1:B:168:VAL:HG13	2.01	0.43
1:A:130:VAL:HG11	1:A:157:ARG:HG3	1.99	0.43
1:B:180:ALA:O	1:B:182:PRO:HD3	2.15	0.43
1:B:283:THR:CG2	1:B:284:ASN:N	2.82	0.43
1:B:181:TRP:N	1:B:182:PRO:HD3	2.33	0.42
7:A:4534:HOH:O	1:B:475:ASP:HB2	2.20	0.41
1:A:488:GLY:HA3	1:A:513:PHE:CE2	2.54	0.41
1:A:307:LEU:HD12	1:A:307:LEU:N	2.35	0.41
1:B:464:THR:CG2	1:B:533:VAL:HG21	2.47	0.41
1:A:212:GLU:HB2	1:A:277:GLY:HA3	2.02	0.41
5:A:2004[B]:R1T:OP1	5:A:2004[B]:R1T:N4'	2.47	0.41
1:B:440:GLY:HA2	1:B:486:MET:O	2.21	0.41
1:A:21:GLY:O	1:A:44:THR:HA	2.20	0.41
1:B:334:THR:HG22	1:B:335:THR:N	2.35	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)
7:B:4412:HOH:O	7:B:4412:HOH:O[4_555]	1.96	0.24

## 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	535/565 (95%)	521 (97%)	12 (2%)	2 (0%)	39	22
1	B	532/565 (94%)	518 (97%)	12 (2%)	2 (0%)	39	22
All	All	1067/1130 (94%)	1039 (97%)	24 (2%)	4 (0%)	39	22

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	-3	ARG
1	B	182	PRO
1	A	341	HIS
1	A	339	GLU

### 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	394/426 (92%)	392 (100%)	2 (0%)	92	90
1	B	392/426 (92%)	389 (99%)	3 (1%)	86	82
All	All	786/852 (92%)	781 (99%)	5 (1%)	90	87

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	307	LEU
1	A	478	ARG

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Mol	Chain	Res	Type
1	B	119	ASP
1	B	196	LEU
1	B	307	LEU

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	284	ASN
1	A	299	HIS
1	A	371	GLN
1	A	415	GLN
1	A	472	ASN
1	A	536	GLN
1	B	299	HIS
1	B	371	GLN
1	B	415	GLN
1	B	433	GLN
1	B	472	ASN
1	B	536	GLN

### 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 10 ligands modelled in this entry, 4 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
4	S1T	A	2002[A]	2	25,30,30	1.64	6 (24%)	32,45,45	1.88	7 (21%)
5	R1T	A	2004[B]	2	25,30,30	1.52	3 (12%)	32,45,45	1.89	7 (21%)
6	GOL	A	4001	-	5,5,5	0.68	0	5,5,5	0.81	0
4	S1T	B	2001[A]	2	25,30,30	1.69	7 (28%)	32,45,45	1.94	5 (15%)
5	R1T	B	2003[B]	2	25,30,30	1.40	3 (12%)	32,45,45	1.94	6 (18%)
6	GOL	B	4000	-	5,5,5	0.74	0	5,5,5	0.88	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	S1T	A	2002[A]	2	-	0/16/21/21	0/2/2/2
5	R1T	A	2004[B]	2	-	0/16/21/21	0/2/2/2
6	GOL	A	4001	-	-	0/4/4/4	0/0/0/0
4	S1T	B	2001[A]	2	-	0/16/21/21	0/2/2/2
5	R1T	B	2003[B]	2	-	0/16/21/21	0/2/2/2
6	GOL	B	4000	-	-	0/4/4/4	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2002[A]	S1T	C2-S1	-3.11	1.68	1.74
4	B	2001[A]	S1T	C2-S1	-2.46	1.69	1.74
4	A	2002[A]	S1T	CM4-C4	2.04	1.55	1.51
4	A	2002[A]	S1T	C7'-C3	2.06	1.57	1.52
4	B	2001[A]	S1T	C6'-C5'	2.13	1.42	1.37
4	B	2001[A]	S1T	C7'-C3	2.22	1.57	1.52
5	B	2003[B]	R1T	C4'-N3'	2.44	1.38	1.35
4	B	2001[A]	S1T	C5-S1	2.56	1.78	1.74
4	A	2002[A]	S1T	C7'-C5'	2.65	1.57	1.52
4	B	2001[A]	S1T	C4'-N3'	2.72	1.39	1.35
5	A	2004[B]	R1T	C7'-C5'	2.72	1.57	1.52
5	B	2003[B]	R1T	C7'-C5'	2.75	1.57	1.52
5	B	2003[B]	R1T	C2-CP1	2.83	1.54	1.51
5	A	2004[B]	R1T	C4'-N3'	2.88	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2002[A]	S1T	C2-CP1	3.29	1.54	1.51
4	A	2002[A]	S1T	C4'-N3'	3.35	1.40	1.35
4	B	2001[A]	S1T	C7'-C5'	3.41	1.58	1.52
5	A	2004[B]	R1T	C2-CP1	3.59	1.55	1.51
4	B	2001[A]	S1T	C2-CP1	3.81	1.55	1.51

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2001[A]	S1T	PA-O3A-PB	-5.28	114.96	132.67
5	B	2003[B]	R1T	PA-O3A-PB	-5.23	115.13	132.67
4	A	2002[A]	S1T	PA-O3A-PB	-4.85	116.41	132.67
5	A	2004[B]	R1T	PA-O3A-PB	-4.81	116.55	132.67
4	B	2001[A]	S1T	N1'-C2'-N3'	-2.43	121.10	125.60
5	B	2003[B]	R1T	N1'-C2'-N3'	-2.41	121.14	125.60
5	A	2004[B]	R1T	N1'-C2'-N3'	-2.41	121.14	125.60
4	A	2002[A]	S1T	N1'-C2'-N3'	-2.41	121.14	125.60
5	A	2004[B]	R1T	C7'-C5'-C6'	-2.17	118.50	121.72
5	B	2003[B]	R1T	C7'-C5'-C6'	-2.13	118.56	121.72
4	A	2002[A]	S1T	C7'-C5'-C6'	-2.03	118.71	121.72
4	A	2002[A]	S1T	C7'-C5'-C4'	2.04	124.81	122.21
5	A	2004[B]	R1T	C7'-C5'-C4'	2.34	125.20	122.21
4	B	2001[A]	S1T	C6'-N1'-C2'	3.25	121.45	115.77
5	B	2003[B]	R1T	C6'-N1'-C2'	3.27	121.49	115.77
4	A	2002[A]	S1T	C6'-N1'-C2'	3.30	121.54	115.77
5	A	2004[B]	R1T	C6'-N1'-C2'	3.40	121.70	115.77
4	A	2002[A]	S1T	C6-C5-S1	4.10	125.97	120.24
5	A	2004[B]	R1T	O3A-PA-O7	4.18	114.02	102.94
5	A	2004[B]	R1T	C6-C5-S1	4.19	126.10	120.24
5	B	2003[B]	R1T	C6-C5-S1	4.20	126.11	120.24
4	A	2002[A]	S1T	O3A-PA-O7	4.20	114.07	102.94
4	B	2001[A]	S1T	O3A-PA-O7	4.30	114.36	102.94
4	B	2001[A]	S1T	C6-C5-S1	4.39	126.38	120.24
5	B	2003[B]	R1T	O3A-PA-O7	4.51	114.89	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2002[A]	S1T	3	0
5	A	2004[B]	R1T	1	0
4	B	2001[A]	S1T	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	538/565 (95%)	-0.23	20 (3%) 45 43	11, 20, 39, 57	0
1	B	535/565 (94%)	-0.06	15 (2%) 56 54	11, 21, 43, 65	0
All	All	1073/1130 (94%)	-0.15	35 (3%) 50 47	11, 20, 41, 65	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	107	ALA	8.4
1	A	309	TYR	6.7
1	B	182	PRO	6.5
1	A	107	ALA	6.3
1	A	-5	VAL	6.2
1	B	106	ASN	5.2
1	A	111	LEU	4.3
1	A	105	GLY	4.3
1	A	308	GLY	4.2
1	B	-3	ARG	4.2
1	B	181	TRP	4.1
1	A	-4	PRO	3.9
1	B	105	GLY	3.8
1	A	340	PRO	3.8
1	A	103	THR	3.8
1	A	118	LEU	3.6
1	B	-4	PRO	3.5
1	A	108	GLY	3.3
1	A	310	HIS	3.0
1	A	117	THR	3.0
1	B	337	GLY	2.7
1	B	345	THR	2.6
1	B	183	VAL	2.4
1	B	290	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	106	ASN	2.3
1	B	284	ASN	2.3
1	A	-2	GLY	2.3
1	A	185	ARG	2.3
1	A	307	LEU	2.3
1	A	0	HIS	2.3
1	A	-3	ARG	2.2
1	B	108	GLY	2.1
1	A	341	HIS	2.1
1	B	342	ALA	2.1
1	B	534	GLN	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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
6	GOL	A	4001	6/6	0.90	0.15	9.13	28,32,33,35	0
6	GOL	B	4000	6/6	0.95	0.11	1.28	25,33,35,37	0
4	S1T	A	2002[A]	29/29	0.98	0.10	0.71	8,11,17,18	29
5	R1T	A	2004[B]	29/29	0.98	0.10	0.58	9,13,22,27	29
4	S1T	B	2001[A]	29/29	0.97	0.10	0.36	10,15,20,22	29
5	R1T	B	2003[B]	29/29	0.97	0.10	0.02	12,16,19,23	29
2	MG	B	3001	1/1	0.95	0.07	-1.19	19,19,19,19	0
2	MG	A	3002	1/1	0.99	0.07	-1.33	15,15,15,15	0
3	CL	A	3004	1/1	1.00	0.05	-1.80	17,17,17,17	0
3	CL	B	3003	1/1	1.00	0.04	-3.74	17,17,17,17	0

## 6.5 Other polymers

There are no such residues in this entry.