



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:45 PM GMT

PDB ID : 1LVW
Title : Crystal structure of glucose-1-phosphate thymidyltransferase, RmlA, complex with dTDP
Authors : Dong, A.; Christendat, D.; Pai, E.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2002-05-29
Resolution : 1.70 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) : 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

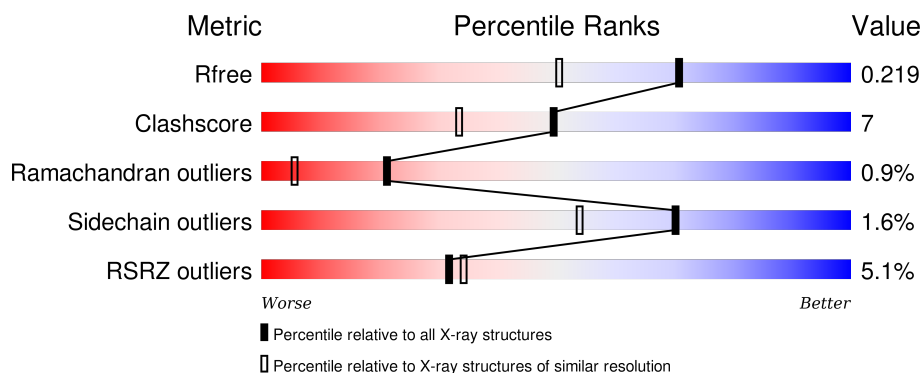
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	3190 (1.70-1.70)
Clashscore	102246	3585 (1.70-1.70)
Ramachandran outliers	100387	3527 (1.70-1.70)
Sidechain outliers	100360	3527 (1.70-1.70)
RSRZ outliers	91569	3200 (1.70-1.70)

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.

Mol	Chain	Length	Quality of chain
1	A	295	<div> <div>3%</div> <div>88%</div> <div>11%</div> <div>.</div> </div>
1	B	295	<div> <div>2%</div> <div>86%</div> <div>12%</div> <div>..</div> </div>
1	C	295	<div> <div>4%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	D	295	<div> <div>11%</div> <div>80%</div> <div>19%</div> <div>.</div> </div>

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
5	GOL	A	2007	-	-	-	X
5	GOL	A	2009	-	-	-	X
5	GOL	B	2008	-	-	-	X
5	GOL	B	2011	-	-	-	X
5	GOL	C	2003	-	-	-	X
5	GOL	D	2006	-	-	-	X

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10472 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 glucose-1-phosphate thymidyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	295	Total	C	N	O	S	0	7	0
			2392	1529	408	447	8			
1	B	292	Total	C	N	O	S	0	7	0
			2376	1521	402	444	9			
1	C	292	Total	C	N	O	S	0	4	0
			2341	1503	397	433	8			
1	D	291	Total	C	N	O	S	0	4	0
			2339	1499	396	436	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	CLONING ARTIFACT	UNP O27819
A	-1	ALA	-	CLONING ARTIFACT	UNP O27819
A	0	HIS	-	CLONING ARTIFACT	UNP O27819
B	-2	GLY	-	CLONING ARTIFACT	UNP O27819
B	-1	ALA	-	CLONING ARTIFACT	UNP O27819
B	0	HIS	-	CLONING ARTIFACT	UNP O27819
C	-2	GLY	-	CLONING ARTIFACT	UNP O27819
C	-1	ALA	-	CLONING ARTIFACT	UNP O27819
C	0	HIS	-	CLONING ARTIFACT	UNP O27819
D	-2	GLY	-	CLONING ARTIFACT	UNP O27819
D	-1	ALA	-	CLONING ARTIFACT	UNP O27819
D	0	HIS	-	CLONING ARTIFACT	UNP O27819

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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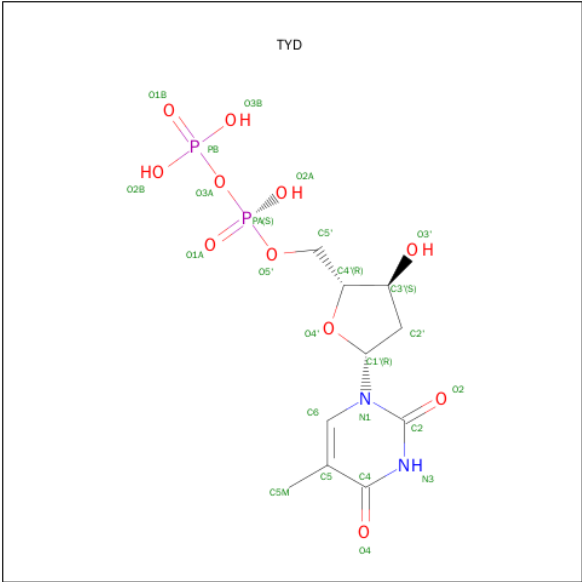
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Cl	0	0
			1	1		
2	C	2	Total	Cl	0	0
			2	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 4 is THYMIDINE-5'-DIPHOSPHATE (three-letter code: TYD) (formula: C₁₀H₁₆N₂O₁₁P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
4	A	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
4	B	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
4	B	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
4	C	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
4	C	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
4	D	1	Total	C	N	O	P	0	0
			25	10	2	11	2		
4	D	1	Total	C	N	O	P	0	0
			25	10	2	11	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	221	Total	O	0	0
			221	221		

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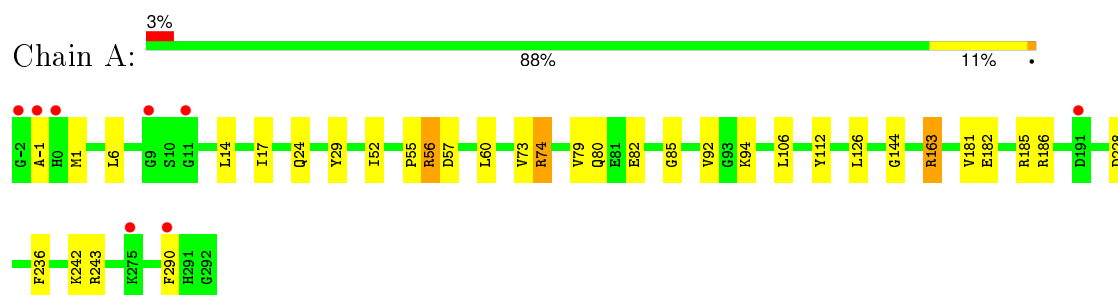
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	218	Total 218	O 218	0	0
6	C	175	Total 175	O 175	0	0
6	D	129	Total 129	O 129	0	0

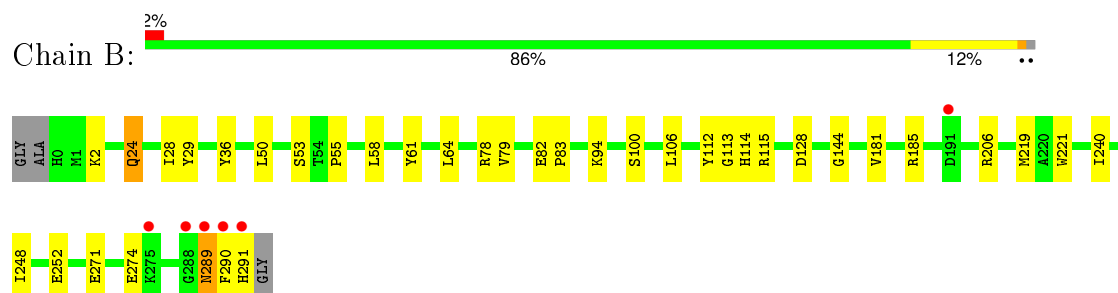
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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.

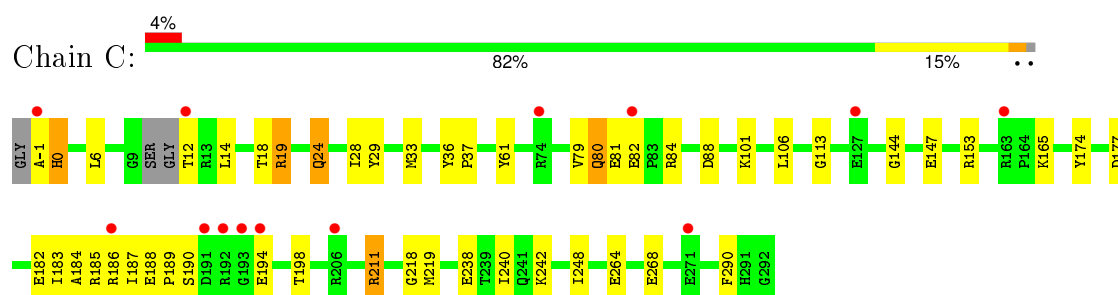
- Molecule 1: glucose-1-phosphate thymidyltransferase



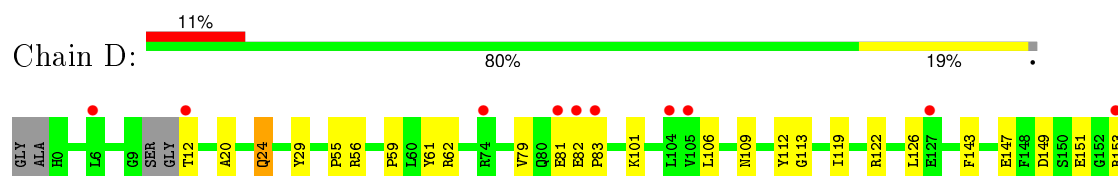
- Molecule 1: glucose-1-phosphate thymidyltransferase

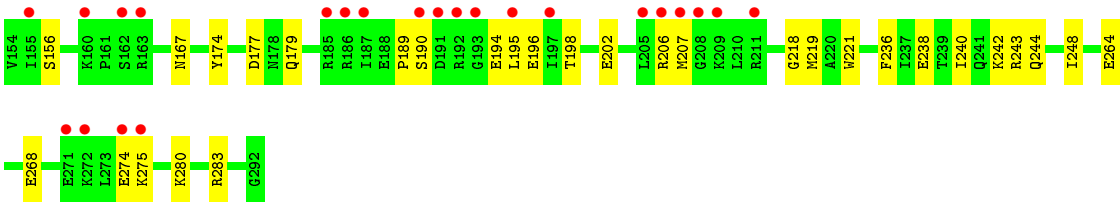


- Molecule 1: glucose-1-phosphate thymidyltransferase



- Molecule 1: glucose-1-phosphate thymidyltransferase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.68Å 115.88Å 116.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.52 – 1.70 31.52 – 1.70	Depositor EDS
% Data completeness (in resolution range)	95.9 (31.52-1.70) 95.6 (31.52-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.34 (at 1.70Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.187 , 0.215 0.193 , 0.219	Depositor DCC
R_{free} test set	8072 reflections (5.01%)	DCC
Wilson B-factor (Å ²)	15.4	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 51.4	EDS
Estimated twinning fraction	0.015 for -h,l,k 0.016 for -l,-k,-h 0.015 for k,h,-l 0.003 for k,l,h 0.003 for l,h,k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 161361 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10472	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹ Intensities estimated from amplitudes.

² 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: TYD, GOL, SO4, 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	0.58	0/2442	0.77	1/3299 (0.0%)
1	B	0.59	0/2425	0.75	1/3275 (0.0%)
1	C	0.56	0/2389	0.73	2/3228 (0.1%)
1	D	0.51	0/2387	0.71	0/3224
All	All	0.56	0/9643	0.74	4/13026 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	144	GLY	N-CA-C	-5.97	98.18	113.10
1	C	144	GLY	N-CA-C	-5.31	99.83	113.10
1	C	80	GLN	N-CA-C	-5.12	97.17	111.00
1	A	144	GLY	N-CA-C	-5.04	100.50	113.10

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	2392	0	2367	32	0
1	B	2376	0	2359	35	0
1	C	2341	0	2324	38	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2339	0	2311	42	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	2	0	0	1	0
2	D	1	0	0	1	0
3	A	5	0	0	0	0
3	D	5	0	0	0	0
4	A	50	0	26	4	0
4	B	50	0	26	2	0
4	C	50	0	26	2	0
4	D	50	0	26	3	0
5	A	18	0	24	0	0
5	B	18	0	24	1	0
5	C	18	0	24	0	0
5	D	12	0	16	2	0
6	A	221	0	0	0	0
6	B	218	0	0	2	0
6	C	175	0	0	1	0
6	D	129	0	0	2	0
All	All	10472	0	9553	137	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (137) 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:82:GLU:HG3	1:B:83:PRO:HD2	1.31	1.07
1:B:82:GLU:HG3	1:B:83:PRO:CD	2.12	0.80
1:C:19:ARG:HH11	1:C:19:ARG:CG	1.93	0.80
1:C:12:THR:HG22	1:C:14:LEU:H	1.45	0.80
1:B:55:PRO:HG3	1:B:79:VAL:HG11	1.65	0.77
1:D:280:LYS:HE3	1:D:283:ARG:HH22	1.52	0.73
1:A:236:PHE:HE1	1:C:240:ILE:HD11	1.54	0.73
1:B:94:LYS:HE3	1:B:185:ARG:NH2	2.03	0.73
1:A:182:GLU:HG3	1:A:186:ARG:NH1	2.06	0.71
1:B:94:LYS:HE3	1:B:185:ARG:HH22	1.56	0.70
1:C:81:GLU:HB2	1:C:84:ARG:HH21	1.56	0.70
1:A:242:LYS:CE	1:A:243:ARG:HH12	2.06	0.69
1:B:78:ARG:HH11	1:B:78:ARG:HB3	1.58	0.69
1:B:291:HIS:HB2	1:D:167:ASN:OD1	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ARG:NH1	1:B:78:ARG:HB3	2.09	0.67
1:A:182:GLU:HG3	1:A:186:ARG:CZ	2.24	0.67
1:C:198:THR:HG22	2:C:4003:CL:CL	2.32	0.67
1:A:163:ARG:HH11	1:A:163:ARG:HB3	1.61	0.65
1:D:280:LYS:HG3	1:D:283:ARG:NH2	2.11	0.64
1:C:190:SER:OG	1:C:194:GLU:HG2	1.98	0.64
1:C:153:ARG:HB2	1:C:211:ARG:NH2	2.13	0.63
1:B:113:GLY:HA3	1:B:219[A]:MET:HE2	1.80	0.61
1:D:20:ALA:C	1:D:56:ARG:HH12	2.03	0.61
1:C:147:GLU:OE1	1:C:165:LYS:HD3	2.02	0.60
1:C:19:ARG:HH11	1:C:19:ARG:HG3	1.65	0.60
1:A:242:LYS:HE2	1:A:243:ARG:HH12	1.66	0.60
1:B:55:PRO:HG3	1:B:79:VAL:CG1	2.31	0.60
5:B:2011:GOL:H11	1:D:221:TRP:O	2.01	0.59
1:B:113:GLY:HA3	1:B:219[A]:MET:CE	2.32	0.59
1:C:240:ILE:HG21	1:C:248[B]:ILE:HD11	1.83	0.59
1:D:143:PHE:HE1	5:D:2006:GOL:H32	1.68	0.59
1:C:19:ARG:HH11	1:C:19:ARG:HG2	1.66	0.58
1:B:94:LYS:HG3	1:B:181:VAL:HG11	1.86	0.58
1:C:-1:ALA:O	1:C:0:HIS:O	2.20	0.58
1:A:56:ARG:HH12	1:A:60:LEU:HD11	1.67	0.58
1:D:280:LYS:HE3	1:D:283:ARG:NH2	2.18	0.58
1:B:113:GLY:HA3	1:B:219[B]:MET:SD	2.44	0.58
1:B:206:ARG:NE	6:B:1671:HOH:O	2.36	0.58
1:A:106:LEU:HB3	4:A:3001:TYD:H4'	1.86	0.57
1:C:101:LYS:HG2	1:C:177:ASP:HA	1.86	0.57
1:B:252:GLU:HG2	6:B:1430:HOH:O	2.04	0.57
1:D:198:THR:HG22	2:D:4004:CL:CL	2.42	0.57
1:D:238[A]:GLU:OE2	1:D:242:LYS:HE3	2.06	0.56
1:D:190:SER:HB3	1:D:196:GLU:OE2	2.04	0.56
1:D:147:GLU:HB3	1:D:156:SER:HB3	1.86	0.56
1:A:74:ARG:N	1:A:74:ARG:HD3	2.20	0.55
1:D:112:TYR:CE2	1:D:240:ILE:HD13	2.42	0.55
1:A:73:VAL:C	1:A:74:ARG:HD3	2.27	0.55
1:D:143:PHE:CE1	5:D:2006:GOL:H32	2.42	0.54
1:D:149:ASP:OD2	1:D:153:ARG:HB3	2.08	0.54
1:A:185:ARG:HB3	1:A:185:ARG:NH1	2.22	0.54
1:C:12:THR:HG21	1:C:18:THR:OG1	2.08	0.54
1:B:64:LEU:HA	1:C:19:ARG:HD3	1.90	0.54
1:C:84:ARG:HD2	1:C:88:ASP:OD2	2.09	0.53
1:B:112:TYR:OH	1:D:218:GLY:HA2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:GLU:O	1:C:268:GLU:HG3	2.10	0.52
1:D:12:THR:N	6:D:1133:HOH:O	2.42	0.52
1:A:56:ARG:NH2	1:A:57:ASP:OD1	2.42	0.52
1:D:106:LEU:HB3	4:D:3007:TYD:H4'	1.92	0.52
1:B:24:GLN:HB2	1:B:61:TYR:OH	2.09	0.51
1:D:206:ARG:O	1:D:206:ARG:HG3	2.11	0.51
1:C:113:GLY:HA3	1:C:219:MET:SD	2.51	0.51
1:A:112:TYR:OH	1:C:218:GLY:HA2	2.11	0.51
1:D:113:GLY:HA3	1:D:219:MET:SD	2.51	0.50
1:A:55:PRO:HG3	1:A:79:VAL:HG11	1.93	0.50
1:D:244:GLN:HB3	6:D:1059:HOH:O	2.10	0.50
1:C:182:GLU:OE2	1:C:185:ARG:NE	2.45	0.50
1:D:240:ILE:HG21	1:D:248[A]:ILE:HD11	1.93	0.49
1:B:94:LYS:CE	1:B:185:ARG:NH2	2.73	0.49
1:C:19:ARG:HG3	1:C:19:ARG:NH1	2.27	0.49
1:B:106:LEU:HD13	4:B:3003:TYD:H5'1	1.94	0.49
1:C:81:GLU:H	1:C:84:ARG:NH2	2.10	0.49
1:A:182:GLU:CG	1:A:186:ARG:CZ	2.91	0.48
1:A:55:PRO:HG3	1:A:79:VAL:CG1	2.43	0.48
1:D:119:ILE:HG22	1:D:122:ARG:NH2	2.28	0.48
1:B:289:ASN:O	1:B:290:PHE:HB2	2.13	0.48
1:A:80:GLN:HG2	1:A:82:GLU:O	2.14	0.48
1:B:53[A]:SER:OG	1:B:58:LEU:CD1	2.62	0.48
1:D:106:LEU:HD13	4:D:3007:TYD:H5'1	1.95	0.47
1:B:106:LEU:HB3	4:B:3003:TYD:H4'	1.96	0.47
1:A:182:GLU:CG	1:A:186:ARG:NH2	2.77	0.47
1:A:242:LYS:HE2	1:A:243:ARG:HH22	1.79	0.47
1:B:271:GLU:O	1:B:274:GLU:HG2	2.15	0.47
1:B:221:TRP:O	1:D:243[B]:ARG:HG2	2.15	0.46
1:D:59:PRO:HA	1:D:62:ARG:HD2	1.98	0.46
1:C:211:ARG:HD3	6:C:1477:HOH:O	2.16	0.46
1:D:236:PHE:CZ	1:D:240:ILE:HD11	2.50	0.46
1:C:12:THR:HG22	1:C:14:LEU:N	2.23	0.45
1:C:79[A]:VAL:CG1	1:C:80:GLN:N	2.79	0.45
1:D:198:THR:O	1:D:202:GLU:HG2	2.17	0.45
1:C:6:LEU:HG	4:C:3005:TYD:C2	2.47	0.45
1:A:85:GLY:HA2	4:A:3001:TYD:H52	1.98	0.45
1:C:106:LEU:HB3	4:C:3005:TYD:H4'	1.99	0.45
1:C:238:GLU:OE2	1:C:242:LYS:HE3	2.16	0.44
1:C:82:GLU:O	1:C:84:ARG:HG3	2.18	0.44
1:A:163:ARG:CB	1:A:163:ARG:HH11	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228[B]:ASP:OD1	1:D:238[B]:GLU:OE2	2.34	0.44
1:B:112:TYR:CZ	1:D:218:GLY:HA2	2.53	0.44
1:C:183:ILE:O	1:C:187:ILE:HG23	2.16	0.44
1:B:78:ARG:HH11	1:B:78:ARG:CB	2.29	0.44
1:D:106:LEU:HD13	4:D:3007:TYD:C5'	2.47	0.44
1:B:114:HIS:CD2	1:B:115:ARG:HG3	2.53	0.43
1:D:24:GLN:HB2	1:D:61:TYR:OH	2.18	0.43
1:C:24:GLN:HB2	1:C:61:TYR:OH	2.19	0.43
1:D:55:PRO:HG3	1:D:79:VAL:HG21	2.00	0.43
1:A:112:TYR:CZ	1:C:218:GLY:HA2	2.54	0.43
1:B:53[A]:SER:OG	1:B:58:LEU:HD13	2.18	0.43
1:D:177:ASP:OD1	1:D:179:GLN:HB2	2.18	0.43
1:B:240:ILE:HG21	1:B:248:ILE:HD11	2.02	0.42
1:D:81:GLU:C	1:D:82:GLU:HG3	2.39	0.42
1:D:81:GLU:O	1:D:82:GLU:HG3	2.20	0.42
1:A:106:LEU:HD13	4:A:3001:TYD:C5'	2.50	0.42
1:A:14:LEU:O	1:A:17:ILE:HG12	2.20	0.42
1:B:50:LEU:HD11	1:B:78:ARG:HG2	2.01	0.42
1:D:202:GLU:O	1:D:206:ARG:HG2	2.20	0.41
1:C:184:ALA:O	1:C:187:ILE:HG12	2.20	0.41
1:C:33:MET:O	1:C:37:PRO:HD2	2.20	0.41
1:A:163:ARG:HH11	1:A:163:ARG:CG	2.33	0.41
1:A:56:ARG:HH12	1:A:60:LEU:CD1	2.32	0.41
1:B:2[A]:LYS:HE3	1:B:100:SER:OG	2.19	0.41
1:D:149:ASP:OD1	1:D:151:GLU:N	2.50	0.41
1:A:1:MET:CE	1:A:126[A]:LEU:HD21	2.50	0.41
1:B:64:LEU:HD12	1:C:19:ARG:HD3	2.03	0.41
1:D:274:GLU:O	1:D:275:LYS:CB	2.68	0.41
1:A:6:LEU:HG	4:A:3001:TYD:O2	2.21	0.41
1:A:52:ILE:HD13	1:A:92[B]:VAL:CG2	2.51	0.41
1:C:182:GLU:HG3	1:C:186:ARG:CZ	2.51	0.41
1:D:101:LYS:HG2	1:D:177:ASP:HA	2.03	0.41
1:D:190:SER:OG	1:D:194:GLU:HB2	2.21	0.40
1:B:28:ILE:HB	1:B:36:TYR:CE1	2.57	0.40
1:C:188:GLU:HA	1:C:189:PRO:HD3	1.94	0.40
1:B:289:ASN:HD22	1:B:289:ASN:HA	1.61	0.40
1:A:94:LYS:HG3	1:A:181:VAL:HG11	2.03	0.40
1:A:185:ARG:HH11	1:A:185:ARG:CB	2.35	0.40
1:D:82:GLU:HA	1:D:83:PRO:HD3	1.91	0.40
1:D:264:GLU:OE2	1:D:268:GLU:HG3	2.22	0.40
1:C:28:ILE:HB	1:C:36:TYR:CE1	2.56	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	300/295 (102%)	294 (98%)	3 (1%)	3 (1%)	19	4
1	B	297/295 (101%)	290 (98%)	6 (2%)	1 (0%)	46	26
1	C	292/295 (99%)	283 (97%)	6 (2%)	3 (1%)	19	4
1	D	291/295 (99%)	281 (97%)	7 (2%)	3 (1%)	19	4
All	All	1180/1180 (100%)	1148 (97%)	22 (2%)	10 (1%)	21	7

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	0	HIS
1	D	207	MET
1	A	-1	ALA
1	D	29	TYR
1	A	290	PHE
1	B	29	TYR
1	C	29	TYR
1	A	29	TYR
1	C	290	PHE
1	D	189	PRO

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	252/248 (102%)	248 (98%)	4 (2%)	70	54
1	B	252/248 (102%)	249 (99%)	3 (1%)	78	65
1	C	245/248 (99%)	241 (98%)	4 (2%)	70	54
1	D	245/248 (99%)	240 (98%)	5 (2%)	63	44
All	All	994/992 (100%)	978 (98%)	16 (2%)	70	54

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	56	ARG
1	A	74	ARG
1	A	163	ARG
1	B	24	GLN
1	B	128	ASP
1	B	289	ASN
1	C	19	ARG
1	C	24	GLN
1	C	174	TYR
1	C	211	ARG
1	D	24	GLN
1	D	109	ASN
1	D	126	LEU
1	D	174	TYR
1	D	195	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	289	ASN
1	D	201	ASN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 5 are monoatomic - leaving 21 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$
5	GOL	A	2005	-	5,5,5	0.30	0	5,5,5	0.23	0
5	GOL	A	2007	-	5,5,5	0.23	0	5,5,5	0.25	0
5	GOL	A	2009	-	5,5,5	0.29	0	5,5,5	0.31	0
4	TYD	A	3001	-	19,26,26	1.91	7 (36%)	27,40,40	3.25	3 (11%)
4	TYD	A	3002	-	19,26,26	1.93	6 (31%)	27,40,40	3.11	2 (7%)
3	SO4	A	5001	-	4,4,4	0.27	0	6,6,6	0.14	0
5	GOL	B	2002	-	5,5,5	0.31	0	5,5,5	0.21	0
5	GOL	B	2008	-	5,5,5	0.37	0	5,5,5	0.23	0
5	GOL	B	2011	-	5,5,5	0.11	0	5,5,5	0.21	0
4	TYD	B	3003	-	19,26,26	1.82	7 (36%)	27,40,40	3.21	3 (11%)
4	TYD	B	3004	-	19,26,26	1.86	7 (36%)	27,40,40	3.18	3 (11%)
5	GOL	C	2001	-	5,5,5	0.21	0	5,5,5	0.26	0
5	GOL	C	2003	-	5,5,5	0.29	0	5,5,5	0.20	0
5	GOL	C	2010	-	5,5,5	0.16	0	5,5,5	0.26	0
4	TYD	C	3005	-	19,26,26	1.93	8 (42%)	27,40,40	3.28	3 (11%)
4	TYD	C	3006	-	19,26,26	1.95	6 (31%)	27,40,40	3.14	3 (11%)
5	GOL	D	2004	-	5,5,5	0.18	0	5,5,5	0.21	0
5	GOL	D	2006	-	5,5,5	0.28	0	5,5,5	0.36	0
4	TYD	D	3007	-	19,26,26	1.95	8 (42%)	27,40,40	3.17	3 (11%)
4	TYD	D	3008	-	19,26,26	1.92	6 (31%)	27,40,40	3.20	3 (11%)
3	SO4	D	5002	-	4,4,4	0.44	0	6,6,6	0.23	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
5	GOL	A	2005	-	-	0/4/4/4	0/0/0/0
5	GOL	A	2007	-	-	0/4/4/4	0/0/0/0
5	GOL	A	2009	-	-	0/4/4/4	0/0/0/0
4	TYD	A	3001	-	-	0/12/28/28	0/2/2/2
4	TYD	A	3002	-	-	0/12/28/28	0/2/2/2
3	SO4	A	5001	-	-	0/0/0/0	0/0/0/0
5	GOL	B	2002	-	-	0/4/4/4	0/0/0/0
5	GOL	B	2008	-	-	0/4/4/4	0/0/0/0
5	GOL	B	2011	-	-	0/4/4/4	0/0/0/0
4	TYD	B	3003	-	-	0/12/28/28	0/2/2/2
4	TYD	B	3004	-	-	0/12/28/28	0/2/2/2
5	GOL	C	2001	-	-	0/4/4/4	0/0/0/0
5	GOL	C	2003	-	-	0/4/4/4	0/0/0/0
5	GOL	C	2010	-	-	0/4/4/4	0/0/0/0
4	TYD	C	3005	-	-	0/12/28/28	0/2/2/2
4	TYD	C	3006	-	-	0/12/28/28	0/2/2/2
5	GOL	D	2004	-	-	0/4/4/4	0/0/0/0
5	GOL	D	2006	-	-	0/4/4/4	0/0/0/0
4	TYD	D	3007	-	-	0/12/28/28	0/2/2/2
4	TYD	D	3008	-	-	0/12/28/28	0/2/2/2
3	SO4	D	5002	-	-	0/0/0/0	0/0/0/0

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	3008	TYD	PB-O1B	-2.86	1.41	1.51
4	B	3004	TYD	PB-O2B	-2.84	1.44	1.54
4	A	3002	TYD	PB-O1B	-2.84	1.41	1.51
4	B	3004	TYD	PB-O1B	-2.75	1.42	1.51
4	A	3002	TYD	PB-O2B	-2.74	1.44	1.54
4	C	3006	TYD	PB-O2B	-2.68	1.45	1.54
4	C	3006	TYD	PB-O1B	-2.67	1.42	1.51
4	D	3007	TYD	PB-O1B	-2.60	1.42	1.51
4	C	3005	TYD	C6-C5	-2.58	1.33	1.40
4	B	3004	TYD	PA-O2A	-2.57	1.44	1.54
4	A	3002	TYD	C6-C5	-2.56	1.33	1.40
4	C	3006	TYD	C6-C5	-2.54	1.33	1.40
4	D	3008	TYD	PA-O2A	-2.54	1.44	1.54
4	D	3007	TYD	C6-C5	-2.51	1.33	1.40
4	B	3003	TYD	C6-C5	-2.50	1.33	1.40
4	D	3007	TYD	O4-C4	-2.46	1.18	1.24
4	D	3008	TYD	PB-O2B	-2.45	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	3006	TYD	PA-O2A	-2.43	1.44	1.54
4	D	3008	TYD	C6-C5	-2.39	1.33	1.40
4	A	3001	TYD	PB-O1B	-2.37	1.43	1.51
4	A	3001	TYD	PA-O2A	-2.31	1.45	1.54
4	C	3005	TYD	PB-O2B	-2.29	1.46	1.54
4	D	3007	TYD	PB-O2B	-2.28	1.46	1.54
4	C	3005	TYD	O4-C4	-2.27	1.19	1.24
4	A	3001	TYD	PB-O2B	-2.26	1.46	1.54
4	B	3003	TYD	PA-O2A	-2.22	1.45	1.54
4	B	3004	TYD	C6-C5	-2.21	1.34	1.40
4	D	3007	TYD	PA-O2A	-2.18	1.45	1.54
4	A	3001	TYD	C6-C5	-2.17	1.34	1.40
4	C	3005	TYD	PA-O2A	-2.16	1.45	1.54
4	C	3005	TYD	PB-O1B	-2.11	1.44	1.51
4	A	3002	TYD	PA-O2A	-2.07	1.46	1.54
4	B	3003	TYD	PB-O2B	-2.06	1.47	1.54
4	B	3003	TYD	PB-O1B	-2.00	1.44	1.51
4	B	3004	TYD	PB-O3B	2.37	1.63	1.54
4	C	3005	TYD	PB-O3B	2.37	1.63	1.54
4	B	3003	TYD	PB-O3B	2.42	1.63	1.54
4	A	3001	TYD	PB-O3B	2.57	1.64	1.54
4	D	3007	TYD	PB-O3B	2.73	1.64	1.54
4	B	3004	TYD	C4-N3	3.06	1.38	1.33
4	C	3005	TYD	C4-N3	3.69	1.40	1.33
4	D	3008	TYD	C4-N3	3.69	1.40	1.33
4	D	3007	TYD	C4-N3	3.70	1.40	1.33
4	B	3003	TYD	C4-N3	3.74	1.40	1.33
4	C	3006	TYD	C6-N1	3.80	1.40	1.35
4	A	3001	TYD	C4-N3	3.93	1.40	1.33
4	B	3004	TYD	C6-N1	3.93	1.40	1.35
4	A	3002	TYD	C4-N3	3.94	1.40	1.33
4	B	3003	TYD	C6-N1	4.01	1.41	1.35
4	D	3007	TYD	C6-N1	4.33	1.41	1.35
4	A	3002	TYD	C6-N1	4.36	1.41	1.35
4	D	3008	TYD	C6-N1	4.50	1.41	1.35
4	C	3006	TYD	C4-N3	4.53	1.41	1.33
4	A	3001	TYD	C6-N1	4.59	1.41	1.35
4	C	3005	TYD	C6-N1	4.66	1.42	1.35

All (23) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3001	TYD	C5-C4-N3	-7.95	116.29	125.14
4	D	3008	TYD	C5-C4-N3	-7.71	116.55	125.14
4	C	3006	TYD	C5-C4-N3	-7.60	116.67	125.14
4	A	3002	TYD	C5-C4-N3	-7.52	116.77	125.14
4	B	3003	TYD	C5-C4-N3	-7.42	116.88	125.14
4	C	3005	TYD	C5-C4-N3	-7.38	116.92	125.14
4	B	3004	TYD	C5-C4-N3	-7.33	116.98	125.14
4	D	3007	TYD	C5-C4-N3	-7.13	117.20	125.14
4	B	3004	TYD	C5M-C5-C6	2.04	122.73	118.62
4	C	3006	TYD	C5M-C5-C6	2.11	122.86	118.62
4	A	3001	TYD	C5M-C5-C6	2.12	122.88	118.62
4	D	3008	TYD	C5M-C5-C6	2.23	123.11	118.62
4	D	3007	TYD	C5M-C5-C6	2.30	123.24	118.62
4	C	3005	TYD	C5M-C5-C6	2.30	123.25	118.62
4	B	3003	TYD	C5M-C5-C6	2.39	123.44	118.62
4	A	3002	TYD	C4-N3-C2	13.83	127.20	115.25
4	C	3006	TYD	C4-N3-C2	13.90	127.27	115.25
4	D	3008	TYD	C4-N3-C2	14.16	127.49	115.25
4	B	3003	TYD	C4-N3-C2	14.19	127.51	115.25
4	B	3004	TYD	C4-N3-C2	14.24	127.56	115.25
4	D	3007	TYD	C4-N3-C2	14.26	127.58	115.25
4	A	3001	TYD	C4-N3-C2	14.31	127.61	115.25
4	C	3005	TYD	C4-N3-C2	14.76	128.00	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3001	TYD	4	0
5	B	2011	GOL	1	0
4	B	3003	TYD	2	0
4	C	3005	TYD	2	0
5	D	2006	GOL	2	0
4	D	3007	TYD	3	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 ⓘ

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	295/295 (100%)	-0.07	8 (2%) 58 62	9, 15, 34, 50	0
1	B	292/295 (98%)	-0.03	6 (2%) 67 71	8, 16, 34, 65	0
1	C	292/295 (98%)	0.17	13 (4%) 37 41	9, 19, 40, 59	0
1	D	291/295 (98%)	0.49	33 (11%) 7 7	9, 24, 47, 60	0
All	All	1170/1180 (99%)	0.14	60 (5%) 32 34	8, 18, 40, 65	0

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	290	PHE	10.8
1	A	-2	GLY	10.7
1	C	-1	ALA	7.4
1	B	291	HIS	7.4
1	A	-1	ALA	7.0
1	B	289	ASN	6.9
1	C	192	ARG	6.5
1	D	192	ARG	5.9
1	C	191	ASP	5.5
1	D	193	GLY	4.4
1	C	193	GLY	4.3
1	D	191	ASP	4.0
1	D	163	ARG	3.7
1	A	11	GLY	3.4
1	D	186	ARG	3.4
1	A	0	HIS	3.3
1	B	191	ASP	3.2
1	C	206	ARG	3.2
1	D	206	ARG	3.2
1	D	271	GLU	3.1
1	D	105	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	12	THR	3.0
1	D	12	THR	3.0
1	D	187	ILE	2.9
1	A	9	GLY	2.8
1	B	288	GLY	2.8
1	D	160	LYS	2.8
1	D	83	PRO	2.8
1	C	194	GLU	2.7
1	D	127	GLU	2.7
1	D	185	ARG	2.7
1	C	127	GLU	2.7
1	C	163	ARG	2.6
1	D	155	ILE	2.6
1	D	74	ARG	2.4
1	C	186	ARG	2.4
1	D	211	ARG	2.4
1	A	191	ASP	2.4
1	A	275	LYS	2.3
1	B	275	LYS	2.3
1	D	82	GLU	2.3
1	D	104	LEU	2.3
1	C	74	ARG	2.3
1	A	290	PHE	2.3
1	D	207	MET	2.3
1	D	6	LEU	2.3
1	D	195	LEU	2.3
1	D	197	ILE	2.3
1	D	209	LYS	2.2
1	D	190	SER	2.2
1	D	208	GLY	2.1
1	D	275	LYS	2.1
1	D	153	ARG	2.1
1	D	162	SER	2.1
1	D	272	LYS	2.1
1	C	82	GLU	2.1
1	C	271	GLU	2.0
1	D	81	GLU	2.0
1	D	274	GLU	2.0
1	D	205	LEU	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, 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	LLDF	B-factors(Å ²)	Q<0.9
5	GOL	B	2011	6/6	0.88	0.14	5.45	23,28,30,34	0
5	GOL	A	2007	6/6	0.86	0.18	5.23	24,31,33,38	0
5	GOL	B	2008	6/6	0.76	0.20	4.24	28,37,41,42	0
5	GOL	A	2009	6/6	0.88	0.14	3.83	22,31,33,35	0
5	GOL	C	2003	6/6	0.87	0.14	3.62	17,24,28,32	0
5	GOL	D	2006	6/6	0.91	0.15	2.77	20,29,31,32	0
5	GOL	D	2004	6/6	0.91	0.10	1.42	19,26,30,35	0
5	GOL	A	2005	6/6	0.95	0.09	1.21	13,18,21,24	0
4	TYD	D	3007	25/25	0.65	0.22	1.14	36,48,57,57	0
4	TYD	A	3001	25/25	0.83	0.15	1.09	21,30,54,55	0
5	GOL	B	2002	6/6	0.95	0.11	0.96	15,19,22,27	0
5	GOL	C	2010	6/6	0.92	0.10	0.86	18,20,22,23	0
4	TYD	C	3005	25/25	0.84	0.15	0.47	26,34,47,48	0
4	TYD	B	3003	25/25	0.84	0.13	0.44	18,25,51,53	0
4	TYD	A	3002	25/25	0.98	0.08	-0.29	9,12,25,26	0
5	GOL	C	2001	6/6	0.97	0.07	-0.44	17,22,24,27	0
4	TYD	B	3004	25/25	0.97	0.08	-0.61	11,13,32,34	0
4	TYD	D	3008	25/25	0.97	0.06	-0.69	13,16,27,31	0
4	TYD	C	3006	25/25	0.98	0.06	-1.09	10,12,27,30	0
2	CL	D	4004	1/1	0.91	0.07	-1.85	44,44,44,44	0
2	CL	C	4003	1/1	0.98	0.04	-1.95	26,26,26,26	0
2	CL	A	4001	1/1	1.00	0.04	-2.21	17,17,17,17	0
2	CL	B	4002	1/1	1.00	0.04	-2.94	16,16,16,16	0
3	SO4	A	5001	5/5	0.91	0.23	-	52,53,53,54	0
2	CL	C	4005	1/1	0.99	0.04	-	24,24,24,24	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	SO4	D	5002	5/5	0.96	0.11	-	29,30,31,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.