



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 09:59 pm GMT

PDB ID : 4ZCM
Title : Crystal Structure of Escherichia coli GTPase BipA/TypA Complexed with ppGpp
Authors : Fan, H.T.; Hahm, J.; Diggs, S.; Blaha, G.
Deposited on : 2015-04-16
Resolution : 3.31 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

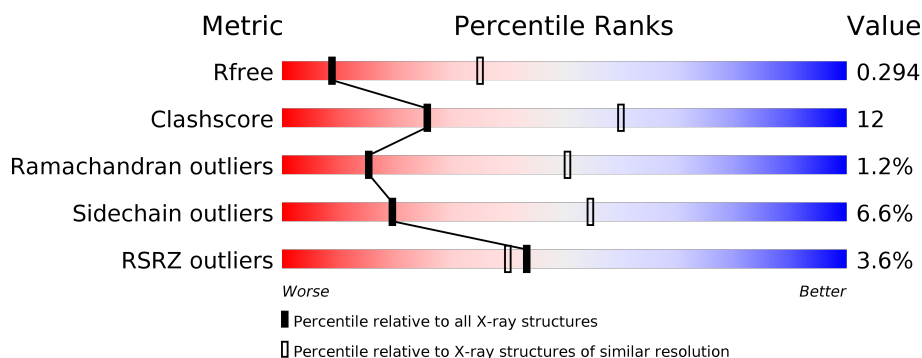
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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}	100719	1002 (3.38-3.26)
Clashscore	112137	1066 (3.38-3.26)
Ramachandran outliers	110173	1048 (3.38-3.26)
Sidechain outliers	110143	1047 (3.38-3.26)
RSRZ outliers	101464	1007 (3.38-3.26)

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	641	<div> <div>3%</div> <div> <div></div> <div>67%</div> <div>19%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	641	<div> <div>3%</div> <div> <div></div> <div>62%</div> <div>22%</div> <div>•</div> <div>12%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8579 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 GTP-binding protein TypA/BipA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	561	Total	C	N	O	S	0	0	0
			4235	2654	745	819	17			
1	B	561	Total	C	N	O	S	0	0	0
			4242	2656	748	821	17			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-33	MET	-	initiating methionine	UNP P32132
A	-32	GLY	-	expression tag	UNP P32132
A	-31	SER	-	expression tag	UNP P32132
A	-30	SER	-	expression tag	UNP P32132
A	-29	HIS	-	expression tag	UNP P32132
A	-28	HIS	-	expression tag	UNP P32132
A	-27	HIS	-	expression tag	UNP P32132
A	-26	HIS	-	expression tag	UNP P32132
A	-25	HIS	-	expression tag	UNP P32132
A	-24	HIS	-	expression tag	UNP P32132
A	-23	SER	-	expression tag	UNP P32132
A	-22	SER	-	expression tag	UNP P32132
A	-21	GLY	-	expression tag	UNP P32132
A	-20	LEU	-	expression tag	UNP P32132
A	-19	VAL	-	expression tag	UNP P32132
A	-18	PRO	-	expression tag	UNP P32132
A	-17	ARG	-	expression tag	UNP P32132
A	-16	GLY	-	expression tag	UNP P32132
A	-15	SER	-	expression tag	UNP P32132
A	-14	HIS	-	expression tag	UNP P32132
A	-13	MET	-	expression tag	UNP P32132
A	-12	ALA	-	expression tag	UNP P32132
A	-11	SER	-	expression tag	UNP P32132
A	-10	MET	-	expression tag	UNP P32132
A	-9	THR	-	expression tag	UNP P32132

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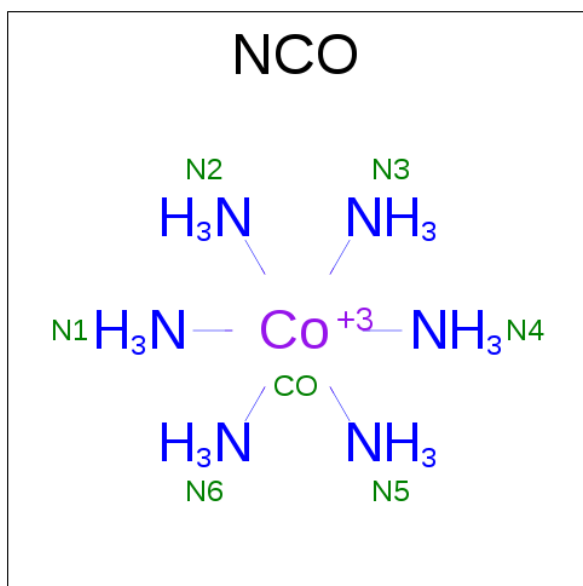
Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	expression tag	UNP P32132
A	-7	GLY	-	expression tag	UNP P32132
A	-6	GLN	-	expression tag	UNP P32132
A	-5	GLN	-	expression tag	UNP P32132
A	-4	MET	-	expression tag	UNP P32132
A	-3	GLY	-	expression tag	UNP P32132
A	-2	ARG	-	expression tag	UNP P32132
A	-1	GLY	-	expression tag	UNP P32132
A	0	SER	-	expression tag	UNP P32132
B	-33	MET	-	initiating methionine	UNP P32132
B	-32	GLY	-	expression tag	UNP P32132
B	-31	SER	-	expression tag	UNP P32132
B	-30	SER	-	expression tag	UNP P32132
B	-29	HIS	-	expression tag	UNP P32132
B	-28	HIS	-	expression tag	UNP P32132
B	-27	HIS	-	expression tag	UNP P32132
B	-26	HIS	-	expression tag	UNP P32132
B	-25	HIS	-	expression tag	UNP P32132
B	-24	HIS	-	expression tag	UNP P32132
B	-23	SER	-	expression tag	UNP P32132
B	-22	SER	-	expression tag	UNP P32132
B	-21	GLY	-	expression tag	UNP P32132
B	-20	LEU	-	expression tag	UNP P32132
B	-19	VAL	-	expression tag	UNP P32132
B	-18	PRO	-	expression tag	UNP P32132
B	-17	ARG	-	expression tag	UNP P32132
B	-16	GLY	-	expression tag	UNP P32132
B	-15	SER	-	expression tag	UNP P32132
B	-14	HIS	-	expression tag	UNP P32132
B	-13	MET	-	expression tag	UNP P32132
B	-12	ALA	-	expression tag	UNP P32132
B	-11	SER	-	expression tag	UNP P32132
B	-10	MET	-	expression tag	UNP P32132
B	-9	THR	-	expression tag	UNP P32132
B	-8	GLY	-	expression tag	UNP P32132
B	-7	GLY	-	expression tag	UNP P32132
B	-6	GLN	-	expression tag	UNP P32132
B	-5	GLN	-	expression tag	UNP P32132
B	-4	MET	-	expression tag	UNP P32132
B	-3	GLY	-	expression tag	UNP P32132
B	-2	ARG	-	expression tag	UNP P32132
B	-1	GLY	-	expression tag	UNP P32132

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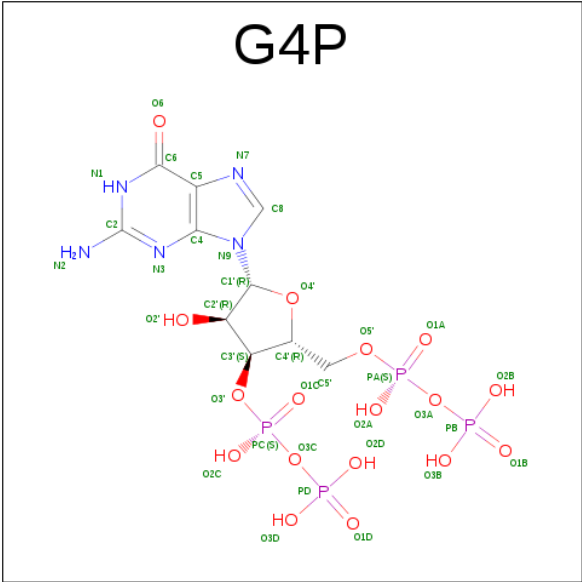
Chain	Residue	Modelled	Actual	Comment	Reference
B	0	SER	-	expression tag	UNP P32132

- Molecule 2 is COBALT HEXAMMINE(III) (three-letter code: NCO) (formula: $\text{CoH}_{18}\text{N}_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Co	N	0	0
			7	1	6		
2	A	1	Total	Co	N	0	0
			7	1	6		
2	B	1	Total	Co	N	0	0
			7	1	6		
2	B	1	Total	Co	N	0	0
			7	1	6		

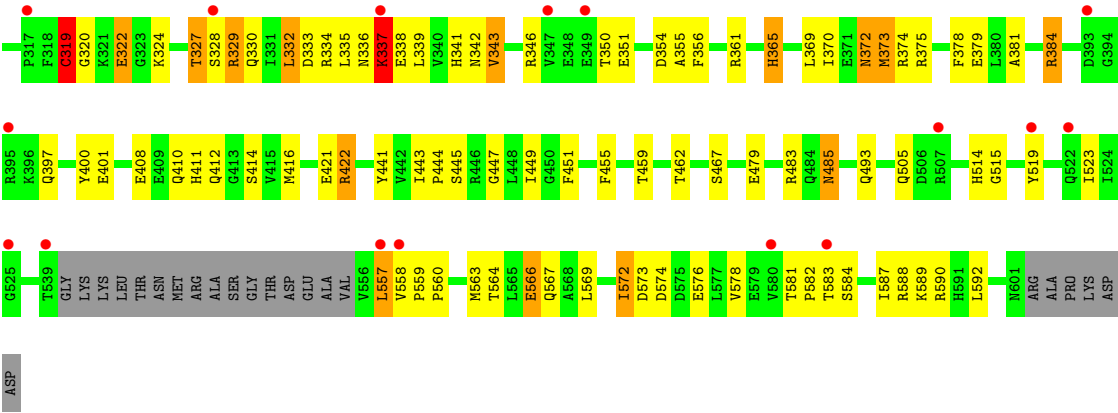
- Molecule 3 is GUANOSINE-5',3'-TETRAPHOSPHATE (three-letter code: G4P) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_5\text{O}_{17}\text{P}_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 36	C 10	N 5	O 17	P 4	0	0
3	B	1	Total 36	C 10	N 5	O 17	P 4	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.82Å 160.12Å 89.72Å 90.00° 98.04° 90.00°	Depositor
Resolution (Å)	48.47 – 3.31 48.47 – 3.31	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.47-3.31) 99.8 (48.47-3.31)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 3.33Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1819)	Depositor
R, R_{free}	0.233 , 0.291 0.235 , 0.294	Depositor DCC
R_{free} test set	1127 reflections (4.78%)	DCC
Wilson B-factor (Å ²)	70.4	Xtriage
Anisotropy	0.791	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 65.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8579	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: G4P, MG, NCO

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	0.24	0/4303	0.49	1/5842 (0.0%)
1	B	0.30	0/4310	0.57	3/5850 (0.1%)
All	All	0.27	0/8613	0.53	4/11692 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	158	LEU	CA-CB-CG	6.42	130.08	115.30
1	B	337	LYS	CD-CE-NZ	6.26	126.09	111.70
1	B	151	LEU	CA-CB-CG	5.71	128.44	115.30
1	A	151	LEU	CA-CB-CG	5.54	128.03	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	337	LYS	Peptide
1	B	372	ASN	Peptide

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	4235	0	4111	79	0
1	B	4242	0	4117	121	0
2	A	14	0	0	1	0
2	B	14	0	0	1	0
3	A	36	0	11	1	0
3	B	36	0	9	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	8579	0	8248	200	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 12.

All (200) 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:A:150:ASN:O	1:A:152:ASP:N	2.01	0.94
1:B:78:HIS:O	1:B:78:HIS:CD2	2.35	0.79
1:A:422:ARG:NH1	1:A:447:GLY:O	2.18	0.76
1:A:374:ARG:NH1	1:A:581:THR:O	2.20	0.75
1:B:338:GLU:HA	1:B:341:HIS:CD2	2.22	0.74
1:A:576:GLU:HG2	1:A:589:LYS:HD3	1.69	0.74
1:B:337:LYS:NZ	1:B:369:LEU:HD11	2.03	0.74
1:A:253:LYS:HD2	1:A:277:THR:HG21	1.71	0.71
1:B:215:ASN:HB3	1:B:218:VAL:HG12	1.73	0.71
1:A:215:ASN:HB3	1:A:218:VAL:HG12	1.72	0.71
1:B:322:GLU:OE1	1:B:583:THR:OG1	2.09	0.70
1:A:314:ASN:HD21	1:A:316:SER:HB3	1.57	0.69
1:B:576:GLU:HG2	1:B:589:LYS:HD3	1.73	0.69
1:B:334:ARG:HG3	1:B:337:LYS:HE2	1.75	0.68
1:B:208:GLN:HB3	1:B:297:LEU:HD12	1.78	0.66
1:B:158:LEU:O	1:B:160:PHE:N	2.30	0.65
1:B:422:ARG:HH11	1:B:422:ARG:HG2	1.61	0.65
1:B:581:THR:OG1	1:B:584:SER:O	2.15	0.65
1:B:422:ARG:NH1	1:B:447:GLY:O	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:159:ASP:OD1	2:B:1002:NCO:N4	2.32	0.62
1:A:505:GLN:HE22	1:A:558:VAL:H	1.47	0.62
1:B:372:ASN:CG	1:B:375:ARG:HB2	2.20	0.62
1:B:374:ARG:NH1	1:B:581:THR:O	2.33	0.62
1:B:563:MET:HA	1:B:567:GLN:HE21	1.64	0.62
1:B:337:LYS:HZ2	1:B:369:LEU:HD11	1.63	0.61
1:A:128:ASN:OD1	1:A:129:LYS:N	2.33	0.61
1:A:314:ASN:ND2	1:A:316:SER:HB3	2.16	0.61
1:A:154:THR:HG22	1:A:158:LEU:HG	1.83	0.61
1:A:149:VAL:O	1:A:149:VAL:HG22	2.00	0.60
1:B:588:ARG:HH21	1:B:592:LEU:HD21	1.66	0.60
1:A:300:LEU:HD23	1:A:300:LEU:H	1.66	0.60
1:A:326:VAL:N	1:A:330:GLN:OE1	2.35	0.59
1:B:302:VAL:HG22	1:B:304:GLU:HG2	1.85	0.59
1:B:337:LYS:HD2	1:B:338:GLU:HB2	1.84	0.58
1:A:401:GLU:OE1	1:A:467:SER:OG	2.19	0.58
1:B:384:ARG:HB3	1:B:572:ILE:HG22	1.86	0.57
1:A:150:ASN:O	1:A:151:LEU:C	2.43	0.57
1:B:334:ARG:HG3	1:B:337:LYS:CE	2.34	0.57
1:B:337:LYS:HZ2	1:B:369:LEU:CD1	2.18	0.57
1:A:201:LEU:O	1:A:230:LYS:NZ	2.38	0.57
1:B:338:GLU:HA	1:B:341:HIS:HD2	1.68	0.56
1:B:128:ASN:OD1	1:B:129:LYS:N	2.36	0.56
1:B:108:GLN:N	1:B:108:GLN:OE1	2.39	0.56
1:B:337:LYS:CD	1:B:338:GLU:HB2	2.36	0.56
1:A:327:THR:HG22	1:A:328:SER:H	1.71	0.56
1:B:15:ASP:N	3:B:1003:G4P:O2B	2.37	0.56
1:B:208:GLN:OE1	1:B:300:LEU:HD21	2.05	0.56
1:B:401:GLU:OE1	1:B:467:SER:OG	2.22	0.56
1:A:12:ALA:HB2	1:A:98:VAL:HB	1.89	0.55
1:B:150:ASN:O	1:B:152:ASP:N	2.40	0.55
1:A:108:GLN:OE1	1:A:108:GLN:N	2.41	0.54
1:B:337:LYS:HZ1	1:B:369:LEU:HD11	1.73	0.54
1:A:159:ASP:OD1	2:A:1002:NCO:N4	2.41	0.54
1:A:336:ASN:HD22	1:A:339:LEU:HD11	1.72	0.53
1:B:338:GLU:HG3	1:B:342:ASN:ND2	2.24	0.53
1:A:332:LEU:HD12	1:A:356:PHE:CZ	2.43	0.53
1:A:85:VAL:O	1:A:89:MET:HG2	2.09	0.52
1:A:147:LEU:C	1:A:149:VAL:H	2.13	0.52
1:B:84:GLU:HA	1:B:87:ARG:HD2	1.91	0.52
1:B:12:ALA:HB2	1:B:98:VAL:HB	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:THR:OG1	1:B:355:ALA:O	2.23	0.52
1:B:493:GLN:HA	1:B:519:TYR:HA	1.91	0.52
1:A:416:MET:HG2	1:A:441:TYR:OH	2.09	0.52
1:A:378:PHE:O	1:A:582:PRO:HD3	2.10	0.51
1:A:451:PHE:CD1	1:A:455:PHE:HB2	2.46	0.51
1:A:327:THR:N	1:A:330:GLN:OE1	2.43	0.51
1:B:201:LEU:O	1:B:230:LYS:NZ	2.43	0.51
1:A:84:GLU:HA	1:A:87:ARG:HD2	1.93	0.51
1:B:213:ASP:HB3	1:B:221:ILE:HB	1.92	0.50
1:A:17:GLY:N	3:A:1003:G4P:O1A	2.40	0.50
1:B:451:PHE:CD1	1:B:455:PHE:HB2	2.46	0.50
1:B:557:LEU:H	1:B:557:LEU:HD22	1.76	0.50
1:B:459:THR:O	1:B:462:THR:HG22	2.12	0.50
1:A:588:ARG:HG2	1:A:589:LYS:O	2.13	0.49
1:B:215:ASN:HB3	1:B:218:VAL:CG1	2.42	0.49
1:B:334:ARG:HG2	1:B:378:PHE:CZ	2.47	0.49
1:B:337:LYS:NZ	1:B:369:LEU:CD1	2.74	0.49
1:B:412:GLN:O	1:B:416:MET:HB2	2.12	0.49
1:A:459:THR:O	1:A:462:THR:HG22	2.12	0.49
1:A:215:ASN:HB3	1:A:218:VAL:CG1	2.42	0.49
1:B:338:GLU:HG3	1:B:342:ASN:HD21	1.78	0.49
1:B:85:VAL:O	1:B:89:MET:HG2	2.12	0.49
1:A:519:TYR:OH	1:A:588:ARG:HD3	2.12	0.49
1:B:79:ALA:HB3	1:B:81:PHE:CE1	2.48	0.49
1:A:483:ARG:HH12	1:A:576:GLU:CD	2.17	0.49
1:A:150:ASN:C	1:A:152:ASP:N	2.62	0.48
1:A:443:ILE:HG13	1:A:444:PRO:HD2	1.95	0.48
1:B:351:GLU:N	1:B:351:GLU:OE1	2.46	0.48
1:B:78:HIS:O	1:B:78:HIS:CG	2.65	0.48
1:A:373:MET:O	1:A:378:PHE:HB2	2.13	0.48
1:B:336:ASN:HD22	1:B:339:LEU:HD11	1.79	0.48
1:A:12:ALA:HB3	1:A:18:LYS:HB3	1.95	0.48
1:B:445:SER:O	1:B:449:ILE:HG13	2.13	0.48
1:B:483:ARG:NH1	1:B:576:GLU:OE1	2.46	0.48
1:B:329:ARG:O	1:B:333:ASP:N	2.29	0.48
1:B:422:ARG:HG2	1:B:422:ARG:NH1	2.23	0.48
1:B:400:TYR:HA	1:B:444:PRO:HA	1.94	0.48
1:A:313:VAL:HG22	1:A:354:ASP:HB3	1.96	0.47
1:A:483:ARG:NH1	1:A:576:GLU:OE1	2.46	0.47
1:B:372:ASN:HD22	1:B:375:ARG:NH1	2.12	0.47
1:B:483:ARG:HD2	1:B:485:ASN:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:GLU:OE1	1:A:351:GLU:N	2.47	0.47
1:A:384:ARG:HB3	1:A:572:ILE:HG22	1.95	0.47
1:B:365:HIS:CD2	1:B:365:HIS:C	2.88	0.47
1:A:445:SER:O	1:A:449:ILE:HG13	2.15	0.47
1:B:147:LEU:C	1:B:149:VAL:H	2.17	0.47
1:B:443:ILE:HG13	1:B:444:PRO:HD2	1.96	0.47
1:B:338:GLU:O	1:B:342:ASN:ND2	2.47	0.47
1:B:416:MET:HG2	1:B:441:TYR:OH	2.15	0.47
1:B:572:ILE:HD11	1:B:587:ILE:HG23	1.97	0.47
1:B:374:ARG:HH11	1:B:581:THR:C	2.18	0.46
1:B:378:PHE:O	1:B:379:GLU:HG3	2.16	0.46
1:B:213:ASP:OD1	1:B:214:TYR:N	2.46	0.46
1:A:137:PRO:HA	1:A:140:VAL:HG22	1.98	0.46
1:A:284:ILE:O	1:A:285:SER:HB2	2.16	0.46
1:A:493:GLN:HA	1:A:519:TYR:HA	1.98	0.46
1:B:284:ILE:O	1:B:285:SER:HB2	2.16	0.46
1:B:337:LYS:HB3	1:B:338:GLU:HB2	1.98	0.46
1:B:253:LYS:H	1:B:277:THR:HB	1.81	0.45
1:A:370:ILE:O	1:A:374:ARG:N	2.41	0.45
1:A:392:ILE:O	1:A:395:ARG:HG3	2.16	0.45
1:A:505:GLN:NE2	1:A:558:VAL:HG22	2.31	0.45
1:B:313:VAL:HG22	1:B:354:ASP:HB3	1.99	0.45
1:A:379:GLU:HG3	1:A:581:THR:HG22	1.99	0.45
1:A:13:HIS:O	1:A:16:HIS:HB2	2.17	0.45
1:B:327:THR:HG22	1:B:328:SER:H	1.81	0.45
1:A:26:LEU:O	1:A:29:SER:OG	2.27	0.45
1:B:6:ARG:HD2	1:B:194:VAL:HB	1.99	0.45
1:B:483:ARG:HH12	1:B:576:GLU:CD	2.20	0.45
1:A:265:THR:HG22	1:A:267:LEU:H	1.82	0.45
1:A:581:THR:OG1	1:A:584:SER:O	2.20	0.45
1:B:15:ASP:O	1:B:129:LYS:NZ	2.50	0.45
1:A:566:GLU:CD	1:A:566:GLU:H	2.21	0.44
1:B:422:ARG:NE	1:B:451:PHE:HD2	2.16	0.44
1:B:572:ILE:HG12	1:B:578:VAL:HG13	2.00	0.44
1:A:232:LYS:HG2	1:A:266:ASP:O	2.18	0.44
1:A:326:VAL:HG12	1:A:379:GLU:HB3	1.99	0.44
1:B:372:ASN:HD22	1:B:375:ARG:HH11	1.64	0.44
1:B:410:GLN:HG3	1:B:411:HIS:CD2	2.52	0.44
1:B:149:VAL:HG22	1:B:149:VAL:O	2.17	0.44
1:B:209:ILE:HD13	1:B:286:ASP:HB2	1.99	0.44
1:A:213:ASP:HB3	1:A:221:ILE:HB	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:SER:HB2	1:A:64:LYS:O	2.17	0.43
1:A:6:ARG:HD2	1:A:194:VAL:HB	1.99	0.43
1:B:129:LYS:O	1:B:132:ARG:HG2	2.18	0.43
1:B:564:THR:H	1:B:567:GLN:NE2	2.15	0.43
1:B:422:ARG:HH11	1:B:422:ARG:CG	2.31	0.43
1:B:154:THR:O	1:B:158:LEU:N	2.46	0.43
1:B:408:GLU:OE2	1:B:462:THR:HG21	2.18	0.43
1:B:137:PRO:HA	1:B:140:VAL:HG22	2.01	0.43
1:B:218:VAL:HG23	1:B:277:THR:HG23	2.00	0.43
1:A:456:MET:O	1:A:460:SER:N	2.52	0.43
1:A:572:ILE:HD11	1:A:587:ILE:HG23	1.99	0.43
1:A:327:THR:HG22	1:A:328:SER:N	2.34	0.42
1:A:107:PRO:O	1:A:110:ARG:HB2	2.19	0.42
1:A:405:LEU:O	1:A:438:ARG:HA	2.19	0.42
1:A:350:THR:OG1	1:A:355:ALA:O	2.22	0.42
1:B:370:ILE:O	1:B:373:MET:N	2.50	0.42
1:B:100:ASP:OD1	1:B:129:LYS:HD3	2.19	0.42
1:B:559:PRO:HA	1:B:560:PRO:HD3	1.86	0.42
1:B:79:ALA:HB3	1:B:81:PHE:HE1	1.82	0.42
1:B:149:VAL:HG13	1:B:149:VAL:O	2.19	0.42
1:A:201:LEU:HD21	1:A:269:GLU:HB2	2.00	0.42
1:B:131:ASP:N	1:B:131:ASP:OD1	2.48	0.42
1:A:473:ASP:OD1	1:A:474:ASP:N	2.53	0.42
1:B:306:THR:OG1	1:B:361:ARG:O	2.37	0.42
1:A:332:LEU:HD23	1:A:336:ASN:OD1	2.20	0.42
1:A:312:CYS:N	1:A:381:ALA:O	2.51	0.42
1:B:505:GLN:HE22	1:B:558:VAL:H	1.66	0.42
1:B:566:GLU:H	1:B:566:GLU:CD	2.21	0.42
1:A:29:SER:OG	1:A:31:THR:HG22	2.20	0.42
1:B:208:GLN:HE21	1:B:297:LEU:HB2	1.84	0.41
1:B:330:GLN:O	1:B:378:PHE:HE2	2.03	0.41
1:B:505:GLN:NE2	1:B:558:VAL:HG22	2.35	0.41
1:B:483:ARG:NH1	1:B:573:ASP:HB2	2.35	0.41
1:B:564:THR:H	1:B:567:GLN:HE21	1.67	0.41
1:B:150:ASN:C	1:B:152:ASP:N	2.74	0.41
1:B:107:PRO:O	1:B:110:ARG:HB2	2.21	0.41
1:B:483:ARG:O	1:B:485:ASN:N	2.47	0.41
1:B:29:SER:OG	1:B:31:THR:HG22	2.21	0.41
1:B:333:ASP:C	1:B:335:LEU:H	2.24	0.41
1:B:332:LEU:HG	1:B:356:PHE:CZ	2.56	0.41
1:B:96:LEU:HD11	1:B:126:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:310:PHE:O	1:A:382:VAL:HA	2.21	0.41
1:A:385:PRO:HD3	1:A:569:LEU:CD2	2.50	0.41
1:B:12:ALA:HB3	1:B:18:LYS:HB3	2.03	0.41
1:A:213:ASP:OD1	1:A:214:TYR:N	2.54	0.40
1:A:319:CYS:HB3	1:A:320:GLY:H	1.74	0.40
1:B:232:LYS:HG2	1:B:266:ASP:O	2.20	0.40
1:B:319:CYS:HB3	1:B:320:GLY:H	1.74	0.40
1:B:581:THR:O	1:B:584:SER:N	2.54	0.40
1:A:422:ARG:HG2	1:A:422:ARG:HH11	1.86	0.40
1:B:312:CYS:HB2	1:B:381:ALA:HB3	2.02	0.40
1:B:372:ASN:ND2	1:B:375:ARG:HH11	2.19	0.40
1:B:523:ILE:HB	1:B:587:ILE:HG22	2.02	0.40
1:A:379:GLU:HA	1:A:580:VAL:O	2.21	0.40
1:B:574:ASP:O	1:B:590:ARG:NH1	2.55	0.40
1:B:13:HIS:O	1:B:16:HIS:HB2	2.21	0.40
1:B:343:VAL:O	1:B:346:ARG:NH2	2.44	0.40
1:B:370:ILE:HA	1:B:373:MET:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	555/641 (87%)	507 (91%)	45 (8%)	3 (0%)	32	67
1	B	555/641 (87%)	507 (91%)	38 (7%)	10 (2%)	10	42
All	All	1110/1282 (87%)	1014 (91%)	83 (8%)	13 (1%)	15	50

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	151	LEU

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Mol	Chain	Res	Type
1	B	151	LEU
1	B	159	ASP
1	B	582	PRO
1	B	514	HIS
1	A	319	CYS
1	B	319	CYS
1	B	515	GLY
1	B	557	LEU
1	B	337	LYS
1	B	324	LYS
1	B	2	ILE
1	A	2	ILE

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	446/545 (82%)	418 (94%)	28 (6%)	21	56
1	B	447/545 (82%)	416 (93%)	31 (7%)	18	53
All	All	893/1090 (82%)	834 (93%)	59 (7%)	19	54

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	THR
1	A	78	HIS
1	A	151	LEU
1	A	171	ILE
1	A	201	LEU
1	A	211	GLN
1	A	237	VAL
1	A	247	ARG
1	A	251	VAL
1	A	277	THR
1	A	292	GLN

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Mol	Chain	Res	Type
1	A	300	LEU
1	A	314	ASN
1	A	319	CYS
1	A	334	ARG
1	A	358	VAL
1	A	384	ARG
1	A	393	ASP
1	A	395	ARG
1	A	397	GLN
1	A	422	ARG
1	A	479	GLU
1	A	514	HIS
1	A	566	GLU
1	A	569	LEU
1	A	583	THR
1	A	584	SER
1	A	594	GLU
1	B	76	PRO
1	B	78	HIS
1	B	151	LEU
1	B	157	GLN
1	B	178	ASP
1	B	201	LEU
1	B	208	GLN
1	B	237	VAL
1	B	242	SER
1	B	247	ARG
1	B	251	VAL
1	B	314	ASN
1	B	319	CYS
1	B	322	GLU
1	B	327	THR
1	B	329	ARG
1	B	332	LEU
1	B	337	LYS
1	B	343	VAL
1	B	365	HIS
1	B	373	MET
1	B	384	ARG
1	B	397	GLN
1	B	414	SER
1	B	421	GLU

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Mol	Chain	Res	Type
1	B	422	ARG
1	B	479	GLU
1	B	485	ASN
1	B	566	GLU
1	B	569	LEU
1	B	572	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	HIS
1	A	314	ASN
1	A	505	GLN
1	B	13	HIS
1	B	78	HIS
1	B	208	GLN
1	B	342	ASN
1	B	365	HIS
1	B	372	ASN
1	B	505	GLN
1	B	567	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 8 ligands modelled in this entry, 2 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
2	NCO	A	1001	-	6,6,6	0.36	0	0,15,15	0.00	-
2	NCO	A	1002	-	6,6,6	0.37	0	0,15,15	0.00	-
3	G4P	A	1003	-	32,38,38	4.22	15 (46%)	35,61,61	1.96	9 (25%)
2	NCO	B	1001	-	6,6,6	0.37	0	0,15,15	0.00	-
2	NCO	B	1002	-	6,6,6	0.36	0	0,15,15	0.00	-
3	G4P	B	1003	-	32,38,38	4.22	15 (46%)	35,61,61	1.89	8 (22%)

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
2	NCO	A	1001	-	-	0/0/0/0	0/0/0/0
2	NCO	A	1002	-	-	0/0/0/0	0/0/0/0
3	G4P	A	1003	-	-	0/23/43/43	0/3/3/3
2	NCO	B	1001	-	-	0/0/0/0	0/0/0/0
2	NCO	B	1002	-	-	0/0/0/0	0/0/0/0
3	G4P	B	1003	-	-	0/23/43/43	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003	G4P	C2'-C3'	-12.77	1.24	1.53
3	B	1003	G4P	C2'-C3'	-12.54	1.25	1.53
3	A	1003	G4P	O4'-C4'	-6.16	1.31	1.45
3	B	1003	G4P	O4'-C4'	-6.14	1.31	1.45
3	A	1003	G4P	O6-C6	-2.28	1.18	1.24
3	B	1003	G4P	O6-C6	-2.22	1.19	1.24
3	A	1003	G4P	C2-N3	2.22	1.46	1.35
3	B	1003	G4P	C2-N3	2.25	1.46	1.35
3	A	1003	G4P	PD-O3C	3.17	1.65	1.60
3	B	1003	G4P	PD-O3C	3.28	1.65	1.60
3	A	1003	G4P	PB-O3A	3.37	1.65	1.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1003	G4P	O2'-C2'	3.37	1.50	1.43
3	B	1003	G4P	PB-O3A	3.43	1.65	1.60
3	B	1003	G4P	O2'-C2'	3.46	1.50	1.43
3	B	1003	G4P	C2'-C1'	4.83	1.61	1.53
3	A	1003	G4P	C2'-C1'	4.94	1.61	1.53
3	B	1003	G4P	C2-N1	5.01	1.44	1.35
3	A	1003	G4P	C2-N1	5.04	1.44	1.35
3	A	1003	G4P	C3'-C4'	5.22	1.67	1.52
3	B	1003	G4P	C3'-C4'	5.36	1.67	1.52
3	A	1003	G4P	C2-N2	5.65	1.45	1.34
3	B	1003	G4P	C2-N2	5.67	1.45	1.34
3	A	1003	G4P	C6-N1	5.75	1.43	1.33
3	B	1003	G4P	C6-N1	5.78	1.43	1.33
3	B	1003	G4P	C6-C5	6.56	1.53	1.41
3	A	1003	G4P	C6-C5	6.59	1.53	1.41
3	A	1003	G4P	O4'-C1'	7.13	1.51	1.41
3	B	1003	G4P	O4'-C1'	7.23	1.51	1.41
3	A	1003	G4P	C4-N3	8.63	1.49	1.35
3	B	1003	G4P	C4-N3	8.79	1.50	1.35

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	G4P	N3-C2-N1	-5.09	120.03	127.46
3	B	1003	G4P	N3-C2-N1	-5.00	120.16	127.46
3	A	1003	G4P	C1'-N9-C4	-4.12	119.51	126.64
3	B	1003	G4P	C1'-N9-C4	-3.36	120.82	126.64
3	B	1003	G4P	C5-C6-N1	-2.45	120.00	123.48
3	A	1003	G4P	C5-C6-N1	-2.45	120.00	123.48
3	A	1003	G4P	C4'-O4'-C1'	-2.00	107.64	109.77
3	B	1003	G4P	C6-N1-C2	2.42	119.53	116.06
3	A	1003	G4P	C6-N1-C2	2.50	119.66	116.06
3	A	1003	G4P	C2'-C3'-C4'	2.81	108.27	103.23
3	B	1003	G4P	C2'-C3'-C4'	3.22	108.99	103.23
3	B	1003	G4P	C3'-C2'-C1'	3.40	107.58	99.95
3	A	1003	G4P	C3'-C2'-C1'	3.44	107.68	99.95
3	A	1003	G4P	C2-N3-C4	4.32	120.21	115.16
3	B	1003	G4P	C2-N3-C4	4.36	120.25	115.16
3	B	1003	G4P	O3C-PC-O3'	4.41	109.93	102.05
3	A	1003	G4P	O3C-PC-O3'	4.46	110.01	102.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1002	NCO	1	0
3	A	1003	G4P	1	0
2	B	1002	NCO	1	0
3	B	1003	G4P	1	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, 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	561/641 (87%)	0.21	20 (3%) 43 40	42, 88, 166, 210	0
1	B	561/641 (87%)	0.28	20 (3%) 43 40	60, 105, 170, 248	0
All	All	1122/1282 (87%)	0.24	40 (3%) 43 40	42, 100, 169, 248	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	394	GLY	5.4
1	B	317	PRO	4.5
1	A	557	LEU	3.5
1	A	519	TYR	3.4
1	B	82	GLY	3.4
1	B	78	HIS	3.3
1	A	522	GLN	3.2
1	A	503	GLY	3.0
1	B	328	SER	3.0
1	A	563	MET	3.0
1	A	502	PHE	2.9
1	A	78	HIS	2.9
1	A	30	GLY	2.9
1	B	539	THR	2.9
1	B	347	VAL	2.8
1	A	568	ALA	2.8
1	A	501	LEU	2.8
1	B	558	VAL	2.8
1	A	317	PRO	2.7
1	B	522	GLN	2.7
1	B	580	VAL	2.6
1	A	393	ASP	2.5
1	B	583	THR	2.5
1	B	519	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	81	PHE	2.4
1	B	395	ARG	2.4
1	B	525	GLY	2.4
1	B	507	ARG	2.3
1	A	31	THR	2.3
1	A	507	ARG	2.3
1	A	157	GLN	2.2
1	B	266	ASP	2.2
1	B	337	LYS	2.1
1	B	393	ASP	2.1
1	B	31	THR	2.1
1	A	351	GLU	2.1
1	B	557	LEU	2.1
1	A	82	GLY	2.0
1	A	490	SER	2.0
1	B	349	GLU	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
2	NCO	B	1001	7/7	0.97	0.31	1.51	66,75,103,109	0
2	NCO	A	1001	7/7	0.94	0.27	1.50	114,121,133,133	0
3	G4P	A	1003	36/36	0.89	0.23	0.07	60,93,119,143	0
2	NCO	B	1002	7/7	0.92	0.22	-0.10	114,115,128,143	0
2	NCO	A	1002	7/7	0.94	0.17	-0.79	80,95,118,137	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	G4P	B	1003	36/36	0.88	0.21	-0.93	71,109,126,144	0
4	MG	B	1004	1/1	0.69	0.30	-	62,62,62,62	0
4	MG	A	1004	1/1	0.96	0.42	-	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.