



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:49 AM GMT

PDB ID : 3Q23
Title : X-ray crystal structure of the N4 mini-VRNAP and P2_7a promoter transcription initiation complex with GMPCPP and Manganese: sustrate complex II
Authors : Gleghorn, M.L.; Murakami, K.S.
Deposited on : 2010-12-19
Resolution : 1.80 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

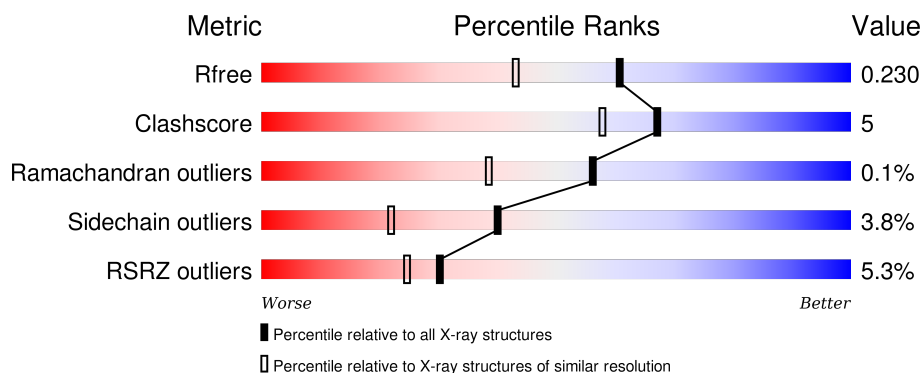
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	1118	<div> <div>5%</div> <div>87%</div> <div>9%</div> <div>• •</div> </div>
1	B	1118	<div> <div>5%</div> <div>87%</div> <div>10%</div> <div>• •</div> </div>
2	C	36	<div> <div>3%</div> <div>47%</div> <div>8%</div> <div>44%</div> </div>
2	D	36	<div> <div>3%</div> <div>56%</div> <div>•</div> <div>42%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 20493 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 Virion RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1095	Total	C	N	O	S	0	0	0
			8454	5306	1435	1672	41			
1	B	1094	Total	C	N	O	S	0	0	0
			8443	5299	1432	1671	41			

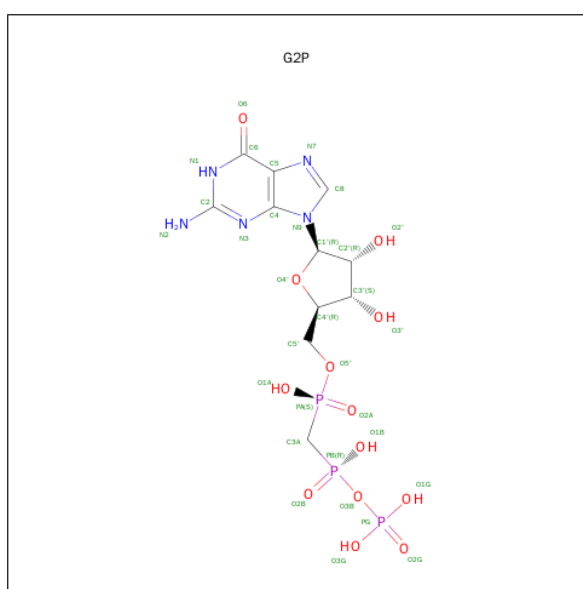
There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	EXPRESSION TAG	UNP Q859P9
A	-10	GLY	-	EXPRESSION TAG	UNP Q859P9
A	-9	GLY	-	EXPRESSION TAG	UNP Q859P9
A	-8	SER	-	EXPRESSION TAG	UNP Q859P9
A	-7	HIS	-	EXPRESSION TAG	UNP Q859P9
A	-6	HIS	-	EXPRESSION TAG	UNP Q859P9
A	-5	HIS	-	EXPRESSION TAG	UNP Q859P9
A	-4	HIS	-	EXPRESSION TAG	UNP Q859P9
A	-3	HIS	-	EXPRESSION TAG	UNP Q859P9
A	-2	HIS	-	EXPRESSION TAG	UNP Q859P9
A	-1	ARG	-	EXPRESSION TAG	UNP Q859P9
A	0	SER	-	EXPRESSION TAG	UNP Q859P9
B	-11	MET	-	EXPRESSION TAG	UNP Q859P9
B	-10	GLY	-	EXPRESSION TAG	UNP Q859P9
B	-9	GLY	-	EXPRESSION TAG	UNP Q859P9
B	-8	SER	-	EXPRESSION TAG	UNP Q859P9
B	-7	HIS	-	EXPRESSION TAG	UNP Q859P9
B	-6	HIS	-	EXPRESSION TAG	UNP Q859P9
B	-5	HIS	-	EXPRESSION TAG	UNP Q859P9
B	-4	HIS	-	EXPRESSION TAG	UNP Q859P9
B	-3	HIS	-	EXPRESSION TAG	UNP Q859P9
B	-2	HIS	-	EXPRESSION TAG	UNP Q859P9
B	-1	ARG	-	EXPRESSION TAG	UNP Q859P9
B	0	SER	-	EXPRESSION TAG	UNP Q859P9

- Molecule 2 is a DNA chain called DNA (5'-D(*TP*GP*CP*CP*TP*CP*CP*CP*AP*GP*GP*CP*AP*TP*CP*CP*AP*AP*AP*AP*GP*AP*AP*GP*CP*GP*GP*AP*GP*CP*TP*TP*CP*TP*TP*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	20	Total	C	N	O	P	0	0	0
			396	185	79	112	20			
2	D	21	Total	C	N	O	P	0	0	0
			432	205	83	123	21			

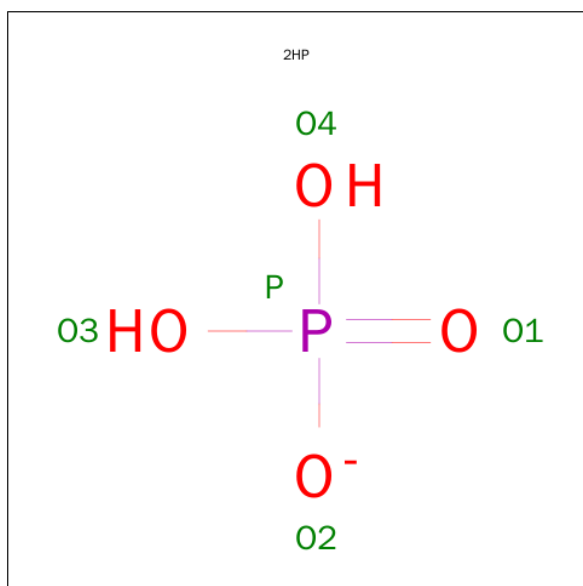
- Molecule 3 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: G2P) (formula: C₁₁H₁₈N₅O₁₃P₃).



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Mn	0	0
			2	2		

- Molecule 5 is DIHYDROGENPHOSPHATE ION (three-letter code: 2HP) (formula: $\text{H}_2\text{O}_4\text{P}$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		

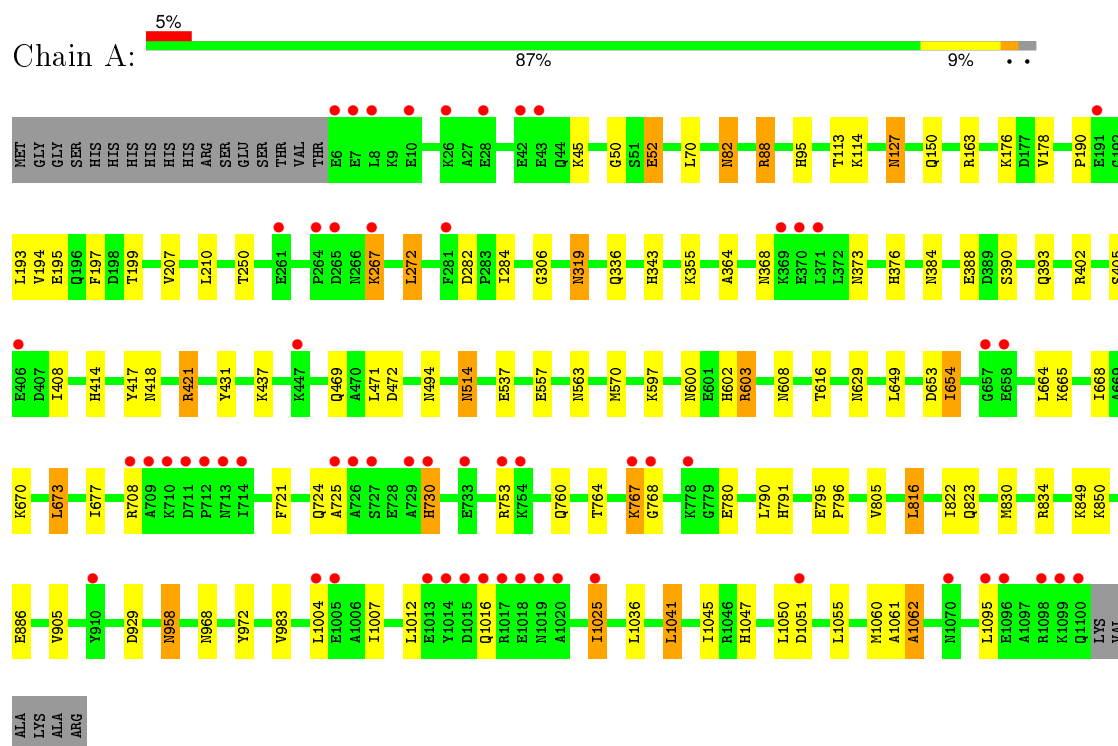
- Molecule 6 is water.

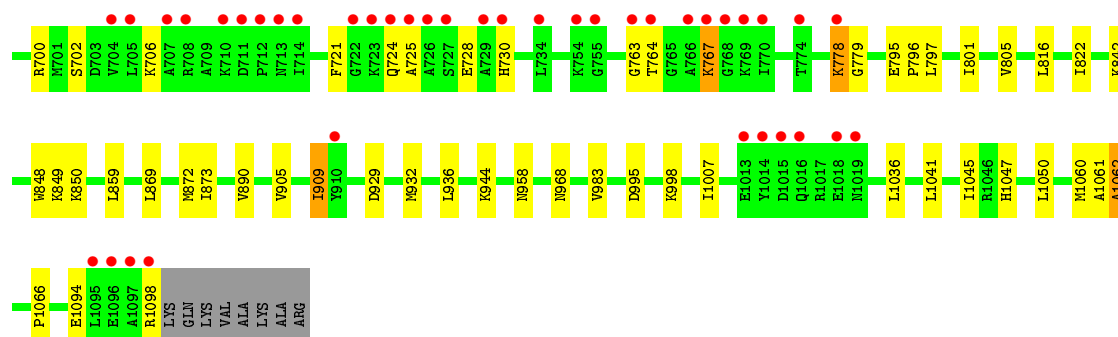
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1187	Total	O	0	0
			1187	1187		
6	C	92	Total	O	0	0
			92	92		
6	B	1240	Total	O	0	0
			1240	1240		
6	D	107	Total	O	0	0
			107	107		

3 Residue-property plots [i](#)

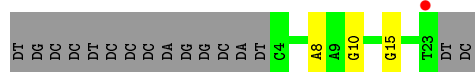
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Virion RNA polymerase





- Molecule 2: DNA (5'-D(*TP*GP*CP*CP*TP*CP*CP*CP*AP*GP*GP*CP*AP*TP*CP*CP*AP*AP*AP*AP*GP*AP*AP*GP*CP*GP*GP*AP*GP*CP*TP*TP*CP*TP*TP*C)-3')



- Molecule 2: DNA (5'-D(*TP*GP*CP*CP*TP*CP*CP*CP*AP*GP*GP*CP*AP*TP*CP*CP*AP*AP*AP*AP*GP*AP*AP*GP*CP*GP*GP*AP*GP*CP*TP*TP*CP*TP*TP*C)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.83Å 111.86Å 276.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.80 42.56 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.0 (50.00-1.80) 99.0 (42.56-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.200 , 0.231 0.198 , 0.230	Depositor DCC
R_{free} test set	11758 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	23.9	Xtriage
Anisotropy	0.288	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 234301 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	20493	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: 2HP, MN, G2P

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	0.35	0/8583	0.51	1/11609 (0.0%)
1	B	0.36	0/8572	0.51	0/11596
2	C	0.61	0/445	1.13	1/685 (0.1%)
2	D	0.61	0/485	1.18	1/746 (0.1%)
All	All	0.37	0/18085	0.57	3/24636 (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	A	673	LEU	CA-CB-CG	5.85	128.75	115.30
2	D	15	DG	P-O3'-C3'	5.32	126.08	119.70
2	C	15	DG	P-O3'-C3'	5.25	126.00	119.70

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	8454	0	8479	84	0
1	B	8443	0	8465	83	0
2	C	396	0	211	2	0
2	D	432	0	236	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	64	0	27	4	0
3	B	64	0	27	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	1	0
6	A	1187	0	0	9	0
6	B	1240	0	0	13	0
6	C	92	0	0	2	0
6	D	107	0	0	1	0
All	All	20493	0	17445	170	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 5.

All (170) 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:385:ARG:HG2	1:B:385:ARG:HH11	1.14	1.12
1:B:469:GLN:HE22	1:B:557:GLU:H	1.10	1.00
1:A:469:GLN:HE22	1:A:557:GLU:H	1.13	0.97
1:A:603:ARG:NH1	1:A:608:ASN:OD1	2.06	0.89
1:A:753:ARG:HH11	1:A:753:ARG:HG2	1.41	0.85
1:A:972:TYR:OH	1:A:1051:ASP:OD1	1.95	0.84
1:B:336:GLN:HE21	1:B:417:TYR:H	1.22	0.83
1:A:336:GLN:HE21	1:A:417:TYR:H	1.24	0.82
1:B:673:LEU:HD13	1:B:801:ILE:HG23	1.61	0.81
1:B:385:ARG:NH1	1:B:385:ARG:HG2	1.91	0.79
1:A:767:LYS:HE3	1:A:768:GLY:H	1.47	0.78
1:B:385:ARG:CG	1:B:385:ARG:HH11	1.95	0.77
1:B:932:MET:SD	6:B:2682:HOH:O	2.43	0.76
1:A:603:ARG:HH11	1:A:603:ARG:HB3	1.50	0.73
1:B:721:PHE:HA	1:B:724:GLN:HE21	1.54	0.72
1:A:968:ASN:HD21	1:A:1060:MET:H	1.37	0.72
1:B:654:ILE:HD11	1:B:668:ILE:HG21	1.72	0.71
1:B:616:THR:HG23	1:B:664:LEU:HB2	1.75	0.68
1:B:449:THR:H	1:B:958:ASN:HD21	1.40	0.68
1:A:850:LYS:HB3	6:A:2255:HOH:O	1.93	0.68
1:A:178:VAL:HG21	1:A:194:VAL:HA	1.73	0.68
1:A:721:PHE:HA	1:A:724:GLN:HE21	1.59	0.67
1:A:421:ARG:HD2	6:C:29:HOH:O	1.93	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:ARG:HG2	1:A:753:ARG:NH1	2.08	0.66
1:A:958:ASN:HD22	1:A:958:ASN:H	1.43	0.66
1:B:968:ASN:HD21	1:B:1060:MET:H	1.44	0.66
1:B:995:ASP:OD2	1:B:998:LYS:HG2	1.95	0.65
1:A:418:ASN:HB2	6:A:1738:HOH:O	1.96	0.65
1:A:195:GLU:O	1:A:199:THR:HG23	1.95	0.65
1:A:364:ALA:H	1:A:384:ASN:ND2	1.96	0.64
1:A:402:ARG:HA	1:A:408:ILE:HG22	1.78	0.64
1:A:364:ALA:H	1:A:384:ASN:HD21	1.44	0.64
1:B:795:GLU:HB3	1:B:796:PRO:HD3	1.81	0.63
1:B:364:ALA:H	1:B:384:ASN:HD21	1.47	0.63
1:A:753:ARG:HH21	1:A:760:GLN:HE22	1.47	0.62
1:B:364:ALA:H	1:B:384:ASN:ND2	1.96	0.62
1:B:91:GLU:HG3	6:B:2109:HOH:O	2.00	0.62
1:A:830:MET:O	1:A:834:ARG:HG3	1.99	0.61
1:B:127:ASN:H	1:B:127:ASN:HD22	1.48	0.61
1:A:45:LYS:HE3	6:A:1226:HOH:O	2.02	0.60
1:B:650:PHE:HE2	1:B:700:ARG:HG3	1.67	0.60
1:A:603:ARG:HB3	1:A:603:ARG:NH1	2.17	0.60
1:A:968:ASN:ND2	1:A:1060:MET:H	1.99	0.60
1:A:82:ASN:HD22	1:A:82:ASN:C	2.05	0.59
1:A:670:LYS:NZ	3:A:1108:G2P:H3A1	2.17	0.59
1:A:207:VAL:HG11	1:A:905:VAL:HG21	1.82	0.59
1:B:196:GLN:O	1:B:199:THR:HG22	2.02	0.59
1:B:16:TYR:O	1:B:35:LYS:HE3	2.03	0.58
1:B:13:ASP:HA	1:B:35:LYS:HE2	1.86	0.58
1:A:886:GLU:O	2:C:8:DA:H4'	2.02	0.58
1:B:492:GLU:HG3	6:B:2683:HOH:O	2.03	0.58
1:B:476:HIS:ND1	5:B:1111:2HP:O2	2.32	0.57
1:B:816:LEU:HD13	1:B:983:VAL:HG21	1.86	0.57
1:A:616:THR:CG2	1:A:664:LEU:HB2	2.33	0.57
1:A:469:GLN:NE2	1:A:557:GLU:H	1.94	0.56
1:A:1012:LEU:HD11	1:A:1025:ILE:HG22	1.87	0.56
1:A:790:LEU:O	1:A:795:GLU:HG2	2.07	0.55
1:B:162:TRP:HE1	1:B:209:SER:HB2	1.70	0.55
1:A:597:LYS:NZ	1:A:602:HIS:HD2	2.05	0.54
1:B:597:LYS:NZ	1:B:602:HIS:HD2	2.05	0.54
1:B:616:THR:CG2	1:B:664:LEU:HB2	2.38	0.54
1:A:653:ASP:HB2	1:A:668:ILE:HG23	1.89	0.54
1:A:795:GLU:HB2	1:A:796:PRO:HD3	1.89	0.54
1:B:848:TRP:CH2	1:B:850:LYS:HA	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:LYS:HE2	6:B:1947:HOH:O	2.06	0.54
1:B:469:GLN:HE22	1:B:557:GLU:N	1.93	0.53
1:A:127:ASN:H	1:A:127:ASN:HD22	1.54	0.53
1:B:968:ASN:ND2	1:B:1060:MET:H	2.04	0.53
1:B:520:ASN:HD21	1:B:527:LYS:NZ	2.06	0.53
1:A:822:ILE:HG12	1:A:1007:ILE:HG23	1.91	0.52
1:B:207:VAL:HG11	1:B:905:VAL:HG21	1.92	0.52
1:B:1045:ILE:HD12	1:B:1094:GLU:HG3	1.91	0.52
1:B:309:ILE:HB	6:B:2853:HOH:O	2.09	0.52
1:B:469:GLN:NE2	1:B:557:GLU:H	1.93	0.52
1:A:469:GLN:HE22	1:A:557:GLU:N	1.95	0.51
1:A:150:GLN:HG2	6:A:2213:HOH:O	2.09	0.51
1:A:816:LEU:HD13	1:A:983:VAL:HG21	1.91	0.51
1:A:343:HIS:HE1	1:A:537:GLU:OE2	1.92	0.51
1:A:570:MET:O	1:A:1047:HIS:HE1	1.94	0.51
1:B:178:VAL:HG21	1:B:194:VAL:HA	1.91	0.51
1:A:88:ARG:HD3	1:A:282:ASP:OD1	2.11	0.51
1:A:725:ALA:HB1	1:A:730:HIS:HB3	1.94	0.50
1:A:355:LYS:HD2	1:A:388:GLU:HG3	1.94	0.50
1:A:1047:HIS:HD2	6:A:1227:HOH:O	1.94	0.49
1:B:562:THR:HG22	1:B:612:TYR:CE1	2.47	0.49
1:B:229:GLY:O	1:B:233:GLY:HA3	2.13	0.49
1:B:82:ASN:C	1:B:82:ASN:HD22	2.16	0.49
3:B:1108:G2P:N7	6:B:1719:HOH:O	2.35	0.49
1:A:600:ASN:H	1:A:600:ASN:ND2	2.11	0.49
1:A:52:GLU:CD	1:A:52:GLU:H	2.15	0.48
3:A:1111:G2P:N7	6:A:2285:HOH:O	2.35	0.48
1:A:563:ASN:HD21	1:A:929:ASP:HB3	1.78	0.48
1:B:725:ALA:HB1	1:B:730:HIS:HB3	1.95	0.48
1:B:849:LYS:HE3	6:B:2173:HOH:O	2.13	0.48
1:B:995:ASP:CG	1:B:998:LYS:HG2	2.35	0.47
1:B:822:ILE:HG12	1:B:1007:ILE:HG23	1.97	0.47
6:A:1403:HOH:O	2:C:10:DG:H5'	2.14	0.47
1:A:393:GLN:HG2	1:A:431:TYR:HB2	1.97	0.47
1:B:343:HIS:HE1	1:B:537:GLU:OE2	1.97	0.47
1:A:670:LYS:HZ1	3:A:1108:G2P:H3A1	1.79	0.46
1:B:50:GLY:H	1:B:150:GLN:NE2	2.13	0.46
1:A:849:LYS:HE3	6:A:1340:HOH:O	2.15	0.46
1:B:816:LEU:CD1	1:B:983:VAL:HG21	2.45	0.46
1:A:1012:LEU:HB3	1:A:1016:GLN:HB2	1.97	0.46
1:B:673:LEU:CD1	1:B:801:ILE:HG23	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:GLY:H	1:A:150:GLN:NE2	2.13	0.46
1:B:1061:ALA:O	1:B:1062:ALA:HB2	2.16	0.46
1:B:344:THR:HG23	6:B:2334:HOH:O	2.16	0.46
1:B:91:GLU:HG2	6:B:1977:HOH:O	2.15	0.46
1:B:1047:HIS:HD2	6:B:1777:HOH:O	1.98	0.46
1:A:1061:ALA:O	1:A:1062:ALA:HB2	2.17	0.45
2:D:15:DG:H5''	6:D:2496:HOH:O	2.16	0.45
1:B:763:GLY:HA2	6:B:2238:HOH:O	2.16	0.45
1:A:958:ASN:HD22	1:A:958:ASN:N	2.13	0.45
1:B:764:THR:HG23	6:B:2337:HOH:O	2.16	0.45
1:A:654:ILE:CD1	1:A:668:ILE:HG21	2.47	0.45
1:B:778:LYS:HD3	1:B:779:GLY:H	1.82	0.45
1:B:449:THR:H	1:B:958:ASN:ND2	2.13	0.44
1:A:665:LYS:O	1:A:668:ILE:HG13	2.17	0.44
1:B:1094:GLU:O	1:B:1098:ARG:HG3	2.17	0.44
1:A:306:GLY:O	1:A:414:HIS:HE1	2.00	0.44
1:B:677:ILE:HD11	1:B:805:VAL:HG11	1.99	0.44
1:A:654:ILE:HD11	1:A:668:ILE:HG21	1.98	0.44
1:B:24:ASP:HB3	1:B:27:ALA:HB2	2.00	0.44
1:A:319:ASN:OD1	1:A:421:ARG:HG2	2.18	0.44
1:B:418:ASN:HB2	6:B:2165:HOH:O	2.18	0.44
1:B:267:LYS:HE2	1:B:267:LYS:HA	1.99	0.43
1:A:384:ASN:HD22	1:A:384:ASN:HA	1.65	0.43
1:A:1012:LEU:HD22	1:A:1016:GLN:NE2	2.33	0.43
1:A:421:ARG:CD	6:C:29:HOH:O	2.60	0.43
1:B:842:LYS:HB3	1:B:848:TRP:CD2	2.53	0.43
1:B:890:VAL:HG11	1:B:909:ILE:HD11	1.99	0.43
1:B:597:LYS:HZ1	1:B:602:HIS:HD2	1.66	0.43
1:B:563:ASN:HD21	1:B:929:ASP:HB3	1.83	0.43
1:A:603:ARG:NE	6:A:2211:HOH:O	2.42	0.43
1:A:616:THR:CG2	1:A:664:LEU:CB	2.96	0.43
1:B:520:ASN:HD21	1:B:527:LYS:HZ3	1.67	0.43
1:B:570:MET:O	1:B:1047:HIS:HE1	2.02	0.43
1:B:619:LEU:HD22	1:B:797:LEU:HD13	1.99	0.43
1:A:267:LYS:HB2	1:A:267:LYS:HE2	1.76	0.43
1:A:306:GLY:O	1:A:414:HIS:CE1	2.72	0.43
1:B:50:GLY:H	1:B:150:GLN:HE22	1.66	0.42
1:B:598:THR:HG22	1:B:1066:PRO:HD3	2.01	0.42
1:B:306:GLY:O	1:B:414:HIS:CE1	2.73	0.42
1:B:376:HIS:HD2	1:B:702:SER:OG	2.02	0.42
1:B:89:TYR:CZ	1:B:290:ALA:HB3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:514:ASN:H	1:A:514:ASN:HD22	1.67	0.42
1:A:373:ASN:HD22	1:A:376:HIS:H	1.67	0.42
1:A:190:PRO:HD2	1:A:193:LEU:HD22	2.02	0.42
1:A:1041:LEU:O	1:A:1045:ILE:HG12	2.20	0.42
1:A:603:ARG:HH11	1:A:603:ARG:CB	2.25	0.42
1:B:322:VAL:HG22	1:B:872:MET:CE	2.49	0.42
1:A:319:ASN:HD22	1:A:319:ASN:HA	1.71	0.41
1:B:82:ASN:ND2	1:B:85:VAL:H	2.19	0.41
1:B:650:PHE:CE2	1:B:700:ARG:HG3	2.51	0.41
1:A:791:HIS:HA	1:A:795:GLU:HG3	2.03	0.41
1:B:767:LYS:O	1:B:767:LYS:HE2	2.20	0.41
1:A:600:ASN:H	1:A:600:ASN:HD22	1.68	0.41
1:B:873:ILE:HD13	1:B:983:VAL:HG22	2.02	0.41
1:A:197:PHE:HA	1:A:272:LEU:HD21	2.02	0.41
1:B:612:TYR:CE1	1:B:670:LYS:HG3	2.55	0.41
1:A:677:ILE:HD11	1:A:805:VAL:HG11	2.03	0.41
1:A:267:LYS:N	1:A:267:LYS:HD3	2.37	0.40
1:A:113:THR:HG22	1:A:114:LYS:HG3	2.02	0.40
1:B:654:ILE:CD1	1:B:668:ILE:HG21	2.47	0.40
1:A:95:HIS:HA	1:B:248:GLU:O	2.22	0.40
1:B:127:ASN:N	1:B:127:ASN:HD22	2.15	0.40
1:A:82:ASN:ND2	1:A:82:ASN:C	2.73	0.40
1:A:437:LYS:NZ	3:A:1111:G2P:O1A	2.46	0.40
1:A:823:GLN:HE21	1:A:823:GLN:HB2	1.69	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	1093/1118 (98%)	1072 (98%)	20 (2%)	1 (0%)	56 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	1092/1118 (98%)	1074 (98%)	17 (2%)	1 (0%)	56 38
All	All	2185/2236 (98%)	2146 (98%)	37 (2%)	2 (0%)	56 38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1062	ALA
1	A	1062	ALA

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	916/935 (98%)	876 (96%)	40 (4%)	35 17
1	B	915/935 (98%)	886 (97%)	29 (3%)	46 29
All	All	1831/1870 (98%)	1762 (96%)	69 (4%)	40 22

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	GLU
1	A	70	LEU
1	A	82	ASN
1	A	88	ARG
1	A	127	ASN
1	A	163	ARG
1	A	176	LYS
1	A	210	LEU
1	A	250	THR
1	A	267	LYS
1	A	272	LEU
1	A	284	ILE
1	A	319	ASN
1	A	368	ASN

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Mol	Chain	Res	Type
1	A	390	SER
1	A	405	SER
1	A	421	ARG
1	A	471	LEU
1	A	472	ASP
1	A	494	ASN
1	A	514	ASN
1	A	603	ARG
1	A	629	ASN
1	A	649	LEU
1	A	654	ILE
1	A	673	LEU
1	A	708	ARG
1	A	730	HIS
1	A	764	THR
1	A	767	LYS
1	A	780	GLU
1	A	816	LEU
1	A	958	ASN
1	A	1004	LEU
1	A	1025	ILE
1	A	1036	LEU
1	A	1041	LEU
1	A	1050	LEU
1	A	1055	LEU
1	A	1095	LEU
1	B	8	LEU
1	B	52	GLU
1	B	70	LEU
1	B	82	ASN
1	B	124	THR
1	B	127	ASN
1	B	163	ARG
1	B	319	ASN
1	B	368	ASN
1	B	385	ARG
1	B	427	MET
1	B	514	ASN
1	B	520	ASN
1	B	623	LEU
1	B	649	LEU
1	B	656	LEU

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Mol	Chain	Res	Type
1	B	673	LEU
1	B	706	LYS
1	B	728	GLU
1	B	767	LYS
1	B	778	LYS
1	B	859	LEU
1	B	869	LEU
1	B	909	ILE
1	B	936	LEU
1	B	944	LYS
1	B	1036	LEU
1	B	1041	LEU
1	B	1050	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	127	ASN
1	A	140	GLN
1	A	150	GLN
1	A	212	GLN
1	A	316	GLN
1	A	319	ASN
1	A	324	ASN
1	A	336	GLN
1	A	343	HIS
1	A	348	GLN
1	A	368	ASN
1	A	373	ASN
1	A	375	ASN
1	A	384	ASN
1	A	414	HIS
1	A	426	GLN
1	A	455	GLN
1	A	457	ASN
1	A	469	GLN
1	A	494	ASN
1	A	514	ASN
1	A	563	ASN
1	A	600	ASN
1	A	602	HIS

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Mol	Chain	Res	Type
1	A	613	GLN
1	A	629	ASN
1	A	639	GLN
1	A	724	GLN
1	A	760	GLN
1	A	781	GLN
1	A	815	GLN
1	A	817	GLN
1	A	823	GLN
1	A	833	GLN
1	A	863	GLN
1	A	878	GLN
1	A	954	ASN
1	A	958	ASN
1	A	968	ASN
1	A	1035	ASN
1	A	1038	ASN
1	A	1047	HIS
1	A	1059	GLN
1	B	82	ASN
1	B	127	ASN
1	B	150	GLN
1	B	196	GLN
1	B	255	ASN
1	B	314	ASN
1	B	316	GLN
1	B	319	ASN
1	B	324	ASN
1	B	336	GLN
1	B	343	HIS
1	B	348	GLN
1	B	368	ASN
1	B	376	HIS
1	B	384	ASN
1	B	393	GLN
1	B	414	HIS
1	B	469	GLN
1	B	506	ASN
1	B	514	ASN
1	B	520	ASN
1	B	563	ASN
1	B	602	HIS

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Mol	Chain	Res	Type
1	B	629	ASN
1	B	639	GLN
1	B	724	GLN
1	B	786	GLN
1	B	815	GLN
1	B	817	GLN
1	B	833	GLN
1	B	878	GLN
1	B	893	GLN
1	B	914	GLN
1	B	954	ASN
1	B	958	ASN
1	B	968	ASN
1	B	1035	ASN
1	B	1047	HIS
1	B	1059	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
3	G2P	A	1108	4	26,34,34	1.28	3 (11%)	33,54,54	2.14	12 (36%)
5	2HP	A	1110	-	4,4,4	4.22	2 (50%)	6,6,6	0.61	0
3	G2P	A	1111	4	26,34,34	1.30	4 (15%)	33,54,54	1.81	8 (24%)
3	G2P	B	1108	4	26,34,34	1.31	4 (15%)	33,54,54	1.79	9 (27%)
3	G2P	B	1109	4	26,34,34	1.42	5 (19%)	33,54,54	2.14	9 (27%)
5	2HP	B	1111	-	4,4,4	4.28	2 (50%)	6,6,6	0.74	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
3	G2P	A	1108	4	-	0/15/38/38	0/3/3/3
5	2HP	A	1110	-	-	0/0/0/0	0/0/0/0
3	G2P	A	1111	4	-	0/15/38/38	0/3/3/3
3	G2P	B	1108	4	-	0/15/38/38	0/3/3/3
3	G2P	B	1109	4	-	0/15/38/38	0/3/3/3
5	2HP	B	1111	-	-	0/0/0/0	0/0/0/0

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1109	G2P	PA-O1A	-2.22	1.50	1.56
3	B	1108	G2P	PA-O1A	-2.10	1.51	1.56
3	A	1108	G2P	PA-O1A	-2.07	1.51	1.56
3	B	1109	G2P	PB-O1B	-2.03	1.51	1.56
3	A	1111	G2P	PA-O1A	-2.03	1.51	1.56
3	B	1108	G2P	O4'-C1'	2.09	1.43	1.41
3	A	1111	G2P	O4'-C1'	2.33	1.44	1.41
3	B	1109	G2P	C5'-C4'	2.60	1.60	1.51
3	B	1108	G2P	PB-O3B	2.90	1.61	1.58
3	A	1111	G2P	PB-O3B	2.99	1.61	1.58
3	A	1108	G2P	PB-O3B	3.19	1.62	1.58
3	B	1109	G2P	PB-O3B	3.25	1.62	1.58
3	A	1111	G2P	PA-O5'	3.68	1.61	1.57
3	A	1108	G2P	PA-O5'	3.87	1.61	1.57
3	B	1108	G2P	PA-O5'	3.88	1.61	1.57
3	B	1109	G2P	PA-O5'	3.92	1.61	1.57
5	A	1110	2HP	P-O4	5.96	1.78	1.55
5	A	1110	2HP	P-O3	5.97	1.78	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1111	2HP	P-O3	6.01	1.78	1.55
5	B	1111	2HP	P-O4	6.08	1.78	1.55

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1109	G2P	C2'-C1'-N9	-6.94	103.69	114.29
3	A	1108	G2P	C2'-C1'-N9	-6.69	104.08	114.29
3	A	1108	G2P	N3-C2-N1	-4.63	120.40	127.44
3	B	1108	G2P	N3-C2-N1	-4.48	120.62	127.44
3	A	1111	G2P	N3-C2-N1	-4.38	120.78	127.44
3	B	1109	G2P	N3-C2-N1	-4.37	120.80	127.44
3	A	1111	G2P	O5'-PA-O2A	-3.77	103.97	113.98
3	B	1109	G2P	C5-C6-N1	-3.50	118.81	123.59
3	B	1108	G2P	O5'-PA-O2A	-3.45	104.81	113.98
3	B	1108	G2P	C5-C6-N1	-3.37	118.98	123.59
3	A	1108	G2P	C5-C6-N1	-3.29	119.09	123.59
3	A	1111	G2P	C5-C6-N1	-3.29	119.09	123.59
3	B	1109	G2P	C4-C5-N7	-2.89	106.82	109.48
3	A	1111	G2P	C4-C5-N7	-2.70	106.99	109.48
3	A	1108	G2P	C1'-N9-C4	-2.70	122.87	126.94
3	B	1108	G2P	C4-C5-N7	-2.63	107.06	109.48
3	A	1108	G2P	PG-O3B-PB	-2.49	124.33	132.67
3	B	1109	G2P	PG-O3B-PB	-2.48	124.35	132.67
3	A	1108	G2P	C4-C5-N7	-2.40	107.27	109.48
3	A	1111	G2P	C2'-C1'-N9	-2.36	110.69	114.29
3	A	1108	G2P	C6-C5-C4	-2.26	118.19	120.90
3	B	1108	G2P	C2'-C1'-N9	-2.13	111.04	114.29
3	A	1108	G2P	O1A-PA-O2A	2.07	116.62	110.12
3	A	1108	G2P	N2-C2-N1	2.07	120.62	117.20
3	B	1109	G2P	O1B-PB-O2B	2.09	116.69	110.12
3	B	1108	G2P	N2-C2-N1	2.11	120.69	117.20
3	A	1108	G2P	O1B-PB-O2B	2.13	116.81	110.12
3	A	1108	G2P	O4'-C1'-N9	2.23	112.77	108.10
3	B	1108	G2P	O1A-PA-O2A	2.27	117.27	110.12
3	B	1109	G2P	N2-C2-N1	2.32	121.04	117.20
3	B	1108	G2P	O1B-PB-O2B	2.53	118.07	110.12
3	A	1111	G2P	O1B-PB-O2B	2.63	118.38	110.12
3	B	1109	G2P	O1A-PA-O2A	2.68	118.56	110.12
3	A	1111	G2P	O1A-PA-O2A	2.75	118.76	110.12
3	A	1111	G2P	C6-N1-C2	3.43	120.70	115.94
3	B	1108	G2P	C6-N1-C2	3.56	120.88	115.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1109	G2P	C6-N1-C2	3.60	120.94	115.94
3	A	1108	G2P	C6-N1-C2	4.11	121.65	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1108	G2P	2	0
3	A	1111	G2P	2	0
3	B	1108	G2P	1	0
5	B	1111	2HP	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	1095/1118 (97%)	0.19	58 (5%)	30	25	13, 25, 47, 75	0
1	B	1094/1118 (97%)	0.21	58 (5%)	30	25	14, 23, 44, 71	0
2	C	20/36 (55%)	-0.30	1 (5%)	32	27	19, 29, 50, 55	0
2	D	21/36 (58%)	-0.09	1 (4%)	34	28	21, 25, 43, 75	0
All	All	2230/2308 (96%)	0.19	118 (5%)	30	25	13, 24, 46, 75	0

All (118) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	725	ALA	7.4
1	A	1018	GLU	6.3
1	A	1014	TYR	5.9
1	A	1016	GLN	5.9
1	A	1019	ASN	5.5
2	D	23	DT	5.2
1	A	8	LEU	5.0
1	A	726	ALA	4.9
1	A	7	GLU	4.8
1	A	1020	ALA	4.8
1	B	264	PRO	4.7
1	A	1099	LYS	4.5
1	B	1014	TYR	4.5
1	B	730	HIS	4.4
1	B	722	GLY	4.4
1	A	1017	ARG	4.3
1	A	1100	GLN	4.2
1	B	708	ARG	4.2
1	B	726	ALA	4.1
1	A	729	ALA	4.1
1	A	725	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	1095	LEU	3.9
1	A	1098	ARG	3.9
1	A	264	PRO	3.9
1	A	28	GLU	3.8
1	B	281	PHE	3.7
1	A	10	GLU	3.6
1	A	267	LYS	3.6
1	B	729	ALA	3.6
1	B	755	GLY	3.6
1	B	42	GLU	3.5
1	B	713	ASN	3.5
1	B	1098	ARG	3.4
1	A	658	GLU	3.4
1	B	1018	GLU	3.4
1	A	730	HIS	3.4
1	B	5	THR	3.4
1	A	767	LYS	3.4
1	A	281	PHE	3.3
1	A	713	ASN	3.3
1	B	707	ALA	3.2
1	A	710	LYS	3.2
1	A	1015	ASP	3.2
1	A	1096	GLU	3.2
1	A	42	GLU	3.2
1	A	406	GLU	3.2
1	A	714	ILE	3.2
1	A	265	ASP	3.1
1	B	6	GLU	3.1
1	B	723	LYS	3.1
1	A	708	ARG	3.1
1	B	191	GLU	3.1
1	B	1019	ASN	3.0
1	B	769	LYS	3.0
1	B	910	TYR	2.9
1	B	727	SER	2.9
1	A	910	TYR	2.9
1	A	727	SER	2.8
1	B	710	LYS	2.8
1	A	6	GLU	2.8
1	B	767	LYS	2.8
1	B	768	GLY	2.8
1	B	712	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	191	GLU	2.7
1	B	1015	ASP	2.7
1	B	8	LEU	2.7
1	A	709	ALA	2.6
1	B	763	GLY	2.6
1	A	370	GLU	2.6
1	B	754	LYS	2.6
1	A	753	ARG	2.6
1	B	265	ASP	2.6
1	A	733	GLU	2.5
2	C	23	DT	2.5
1	B	1013	GLU	2.5
1	B	1097	ALA	2.5
1	B	267	LYS	2.4
1	A	754	LYS	2.4
1	B	1095	LEU	2.4
1	B	704	VAL	2.4
1	A	778	LYS	2.4
1	B	711	ASP	2.4
1	A	657	GLY	2.4
1	A	768	GLY	2.4
1	B	724	GLN	2.3
1	A	1004	LEU	2.3
1	B	75	GLU	2.3
1	B	764	THR	2.3
1	B	654	ILE	2.3
1	A	712	PRO	2.3
1	A	1005	GLU	2.3
1	B	371	LEU	2.3
1	B	26	LYS	2.3
1	B	7	GLU	2.3
1	B	406	GLU	2.2
1	B	545	GLU	2.2
1	B	774	THR	2.2
1	B	766	ALA	2.2
1	B	1096	GLU	2.2
1	B	734	LEU	2.2
1	B	28	GLU	2.1
1	B	770	ILE	2.1
1	A	1070	ASN	2.1
1	A	711	ASP	2.1
1	B	714	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	371	LEU	2.1
1	B	705	LEU	2.1
1	A	26	LYS	2.1
1	A	1025	ILE	2.1
1	A	43	GLU	2.1
1	B	111	LEU	2.1
1	B	778	LYS	2.1
1	A	369	LYS	2.0
1	A	447	LYS	2.0
1	A	261	GLU	2.0
1	A	1013	GLU	2.0
1	B	1016	GLN	2.0
1	A	1051	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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	2HP	B	1111	5/5	0.95	0.13	1.93	33,33,34,34	0
5	2HP	A	1110	5/5	0.96	0.12	1.51	30,30,31,31	0
3	G2P	B	1108	32/32	0.93	0.11	-0.35	21,24,34,34	0
3	G2P	A	1108	32/32	0.97	0.10	-0.71	15,17,18,19	0
3	G2P	B	1109	32/32	0.97	0.10	-0.75	17,19,22,22	0
3	G2P	A	1111	32/32	0.95	0.10	-1.17	18,20,27,28	0
4	MN	A	1109	1/1	0.99	0.07	-1.80	17,17,17,17	0
4	MN	B	1110	1/1	1.00	0.04	-5.35	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	MN	A	1107	1/1	1.00	0.05	-	16,16,16,16	0
4	MN	B	1107	1/1	1.00	0.05	-	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.