



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:03 AM GMT

PDB ID : 2VP6
Title : STRUCTURAL STUDIES OF NUCLEOSIDE ANALOG AND FEEDBACK
INHIBITOR BINDING TO DROSOPHILA MELANOGASTER MULTISUB-
STRATE DEOXYRIBONUCLEOSIDE KINASE
Authors : Mikkelsen, N.E.; Munch-Petersen, B.; Eklund, H.
Deposited on : 2008-02-26
Resolution : 3.00 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

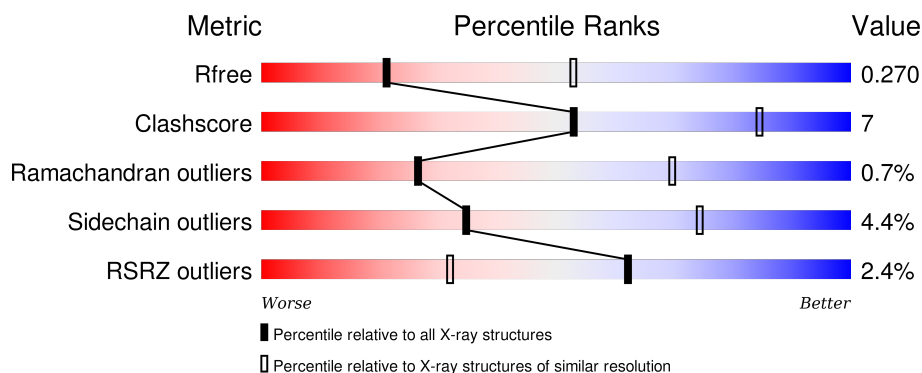
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	230	<div> <div>75%</div> <div>10%</div> <div>14%</div> </div>
1	B	230	<div> <div>69%</div> <div>13%</div> <div>17%</div> </div>
1	C	230	<div> <div>3%</div> <div>65%</div> <div>17%</div> <div>14%</div> </div>
1	D	230	<div> <div>2%</div> <div>70%</div> <div>12%</div> <div>17%</div> </div>
1	E	230	<div> <div>70%</div> <div>13%</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	230	
1	G	230	
1	H	230	

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
2	SO4	B	1209	-	-	X	-
3	5FU	C	1210	-	-	-	X
3	5FU	G	1210	-	-	X	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12918 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 DEOXYNUCLEOSIDE KINASE.

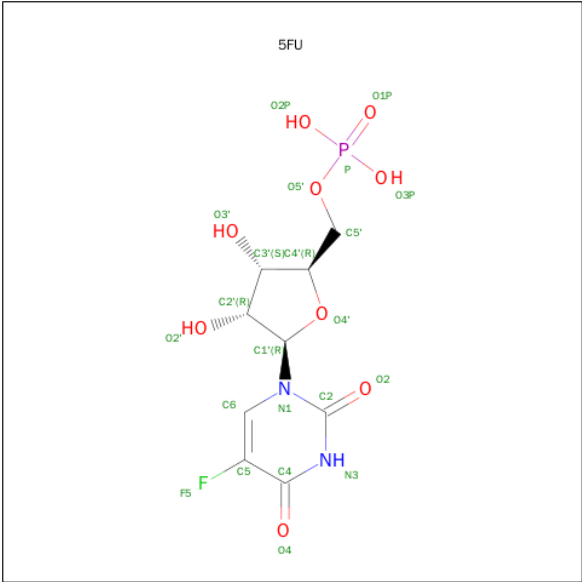
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1640	1046	282	302	10			
1	B	192	Total	C	N	O	S	0	0	0
			1590	1018	267	295	10			
1	C	197	Total	C	N	O	S	0	0	0
			1612	1032	269	301	10			
1	D	191	Total	C	N	O	S	0	0	0
			1569	1007	259	293	10			
1	E	192	Total	C	N	O	S	0	0	0
			1578	1012	261	295	10			
1	F	192	Total	C	N	O	S	0	0	0
			1584	1015	264	295	10			
1	G	192	Total	C	N	O	S	0	0	0
			1574	1010	261	293	10			
1	H	192	Total	C	N	O	S	0	0	0
			1590	1018	267	295	10			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		
2	G	1	Total	O	S	0	0
			5	4	1		
2	H	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is 5-FLUORO-URIDINE-5'-MONOPHOSPHATE (three-letter code: 5FU) (formula: C₉H₁₂FN₂O₉P).

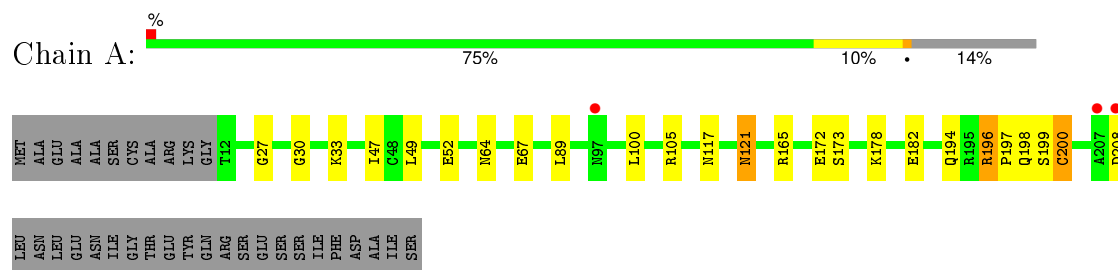


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	0	0
			17	9	1	2	5		
3	B	1	Total	C	F	N	O	0	0
			17	9	1	2	5		
3	C	1	Total	C	F	N	O	0	0
			17	9	1	2	5		
3	D	1	Total	C	F	N	O	0	0
			17	9	1	2	5		
3	E	1	Total	C	F	N	O	0	0
			17	9	1	2	5		
3	F	1	Total	C	F	N	O	0	0
			17	9	1	2	5		
3	G	1	Total	C	F	N	O	0	0
			17	9	1	2	5		
3	H	1	Total	C	F	N	O	0	0
			17	9	1	2	5		

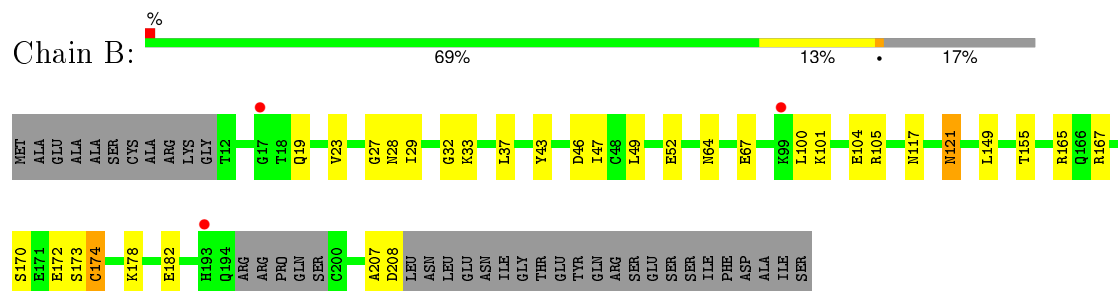
3 Residue-property plots [i](#)

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.

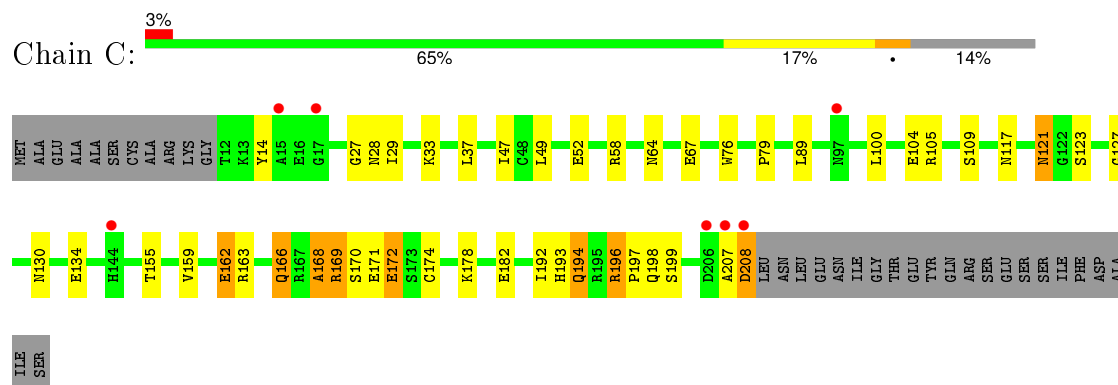
• Molecule 1: DEOXYNUCLEOSIDE KINASE



• Molecule 1: DEOXYNUCLEOSIDE KINASE



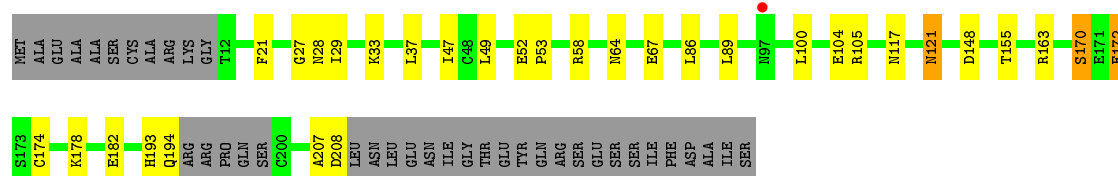
• Molecule 1: DEOXYNUCLEOSIDE KINASE



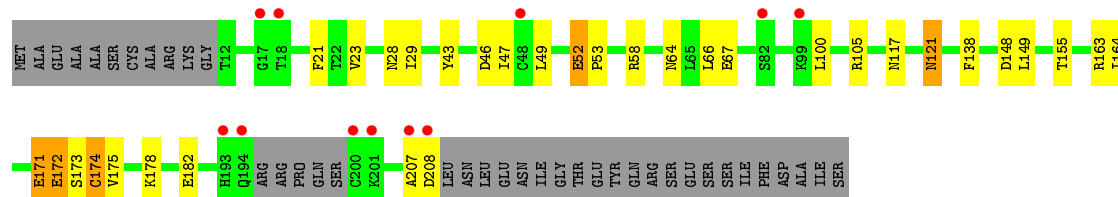
• Molecule 1: DEOXYNUCLEOSIDE KINASE



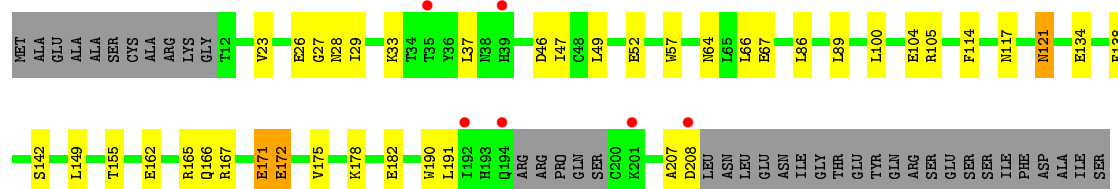
- Molecule 1: DEOXYNUCLEOSIDE KINASE



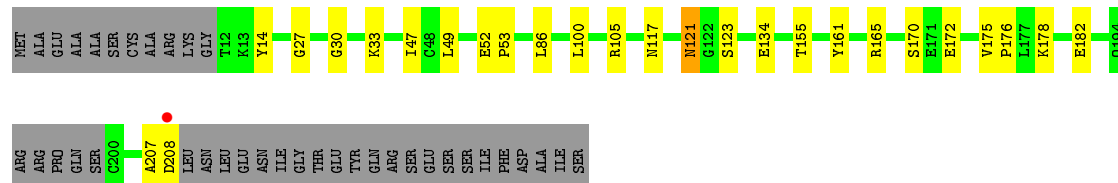
- Molecule 1: DEOXYNUCLEOSIDE KINASE



- Molecule 1: DEOXYNUCLEOSIDE KINASE



- Molecule 1: DEOXYNUCLEOSIDE KINASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.35Å 70.71Å 225.40Å 90.00° 90.29° 90.00°	Depositor
Resolution (Å)	30.00 – 3.00 29.95 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-3.00) 99.0 (29.95-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 3.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.256 , 0.281 0.248 , 0.270	Depositor DCC
R_{free} test set	2232 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	70.4	Xtriage
Anisotropy	0.210	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 44.6	EDS
Estimated twinning fraction	0.002 for -k,-h,-l 0.009 for k,h,-l 0.034 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	1 of 44421 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12918	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.37% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, 5FU

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	0.68	0/1678	0.66	0/2268
1	B	0.60	0/1626	0.64	0/2198
1	C	0.60	0/1650	0.65	1/2235 (0.0%)
1	D	0.66	0/1605	0.63	0/2172
1	E	0.61	0/1614	0.63	0/2184
1	F	0.63	0/1620	0.64	0/2191
1	G	0.65	0/1610	0.65	0/2179
1	H	0.66	0/1626	0.62	0/2198
All	All	0.64	0/13029	0.64	1/17625 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	168	ALA	CB-CA-C	5.39	118.19	110.10

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	1640	0	1629	17	0
1	B	1590	0	1571	19	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1612	0	1579	28	0
1	D	1569	0	1541	17	1
1	E	1578	0	1549	24	0
1	F	1584	0	1560	21	2
1	G	1574	0	1545	31	1
1	H	1590	0	1571	18	0
2	A	10	0	0	1	0
2	B	5	0	0	2	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
2	G	5	0	0	0	0
2	H	5	0	0	1	0
3	A	17	0	8	1	0
3	B	17	0	8	1	0
3	C	17	0	8	3	0
3	D	17	0	8	1	0
3	E	17	0	8	3	0
3	F	17	0	8	1	0
3	G	17	0	8	9	0
3	H	17	0	8	0	0
All	All	12918	0	12609	169	3

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 (169) 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:G:57:TRP:HZ3	3:G:1210:5FU:H1'	1.28	0.97
1:G:57:TRP:CZ3	3:G:1210:5FU:H1'	2.17	0.78
1:E:52:GLU:OE1	3:E:1210:5FU:O5'	2.05	0.73
1:G:52:GLU:OE2	1:G:105:ARG:NH1	2.23	0.70
1:D:52:GLU:OE2	1:D:105:ARG:NH1	2.25	0.69
1:F:52:GLU:OE2	1:F:105:ARG:NH1	2.26	0.69
1:D:163:ARG:HB2	1:D:163:ARG:HH11	1.59	0.68
1:C:52:GLU:OE2	1:C:105:ARG:NH1	2.25	0.68
1:H:52:GLU:OE2	1:H:105:ARG:NH1	2.29	0.66
1:C:196:ARG:O	1:C:198:GLN:N	2.31	0.64
1:C:121:ASN:HD22	1:C:121:ASN:C	2.00	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:ASN:HD21	1:D:182:GLU:HB3	1.63	0.63
1:A:52:GLU:OE2	1:A:105:ARG:NH1	2.32	0.63
1:B:52:GLU:OE2	1:B:105:ARG:NH1	2.32	0.63
1:G:66:LEU:HD11	3:G:1210:5FU:C2'	2.29	0.62
1:F:173:SER:O	1:F:174:CYS:HB2	1.99	0.62
1:B:173:SER:OG	1:B:174:CYS:N	2.29	0.62
1:E:52:GLU:OE2	1:E:105:ARG:NH1	2.32	0.60
1:B:52:GLU:OE1	3:B:1210:5FU:O5'	2.19	0.60
1:F:117:ASN:HD21	1:F:182:GLU:HB3	1.66	0.60
1:E:117:ASN:HD21	1:E:182:GLU:HB3	1.66	0.60
1:C:27:GLY:O	1:C:33:LYS:HE2	2.01	0.59
1:B:19:GLN:OE1	1:B:101:LYS:NZ	2.27	0.59
1:A:121:ASN:C	1:A:121:ASN:HD22	2.06	0.58
1:A:196:ARG:HG3	1:A:197:PRO:HD2	1.83	0.58
1:G:52:GLU:OE2	1:G:105:ARG:HG3	2.03	0.58
3:D:1210:5FU:O5'	3:D:1210:5FU:H6	2.04	0.57
1:B:121:ASN:C	1:B:121:ASN:HD22	2.07	0.57
1:F:121:ASN:HD22	1:F:121:ASN:C	2.08	0.56
1:G:117:ASN:HD21	1:G:182:GLU:HB3	1.70	0.56
1:H:117:ASN:HD21	1:H:182:GLU:HB3	1.70	0.56
1:G:29:ILE:HG12	3:G:1210:5FU:H5'2	1.88	0.56
1:A:52:GLU:OE1	3:A:1211:5FU:O5'	2.24	0.56
1:G:29:ILE:HG12	3:G:1210:5FU:C5'	2.35	0.56
1:G:86:LEU:HD21	1:H:134:GLU:HB3	1.88	0.55
1:G:27:GLY:O	1:G:33:LYS:HE2	2.06	0.55
1:B:27:GLY:O	1:B:33:LYS:HE2	2.06	0.55
1:E:172:GLU:HB3	3:E:1210:5FU:O3'	2.06	0.55
1:G:29:ILE:HG12	3:G:1210:5FU:O5'	2.07	0.55
1:G:138:PHE:HB2	1:H:86:LEU:HD11	1.89	0.55
1:G:114:PHE:CB	3:G:1210:5FU:O4	2.56	0.54
1:E:121:ASN:HD22	1:E:121:ASN:C	2.10	0.54
1:F:64:ASN:ND2	1:F:67:GLU:HB2	2.21	0.54
1:G:121:ASN:HD22	1:G:121:ASN:C	2.11	0.54
1:G:172:GLU:O	1:G:175:VAL:HG13	2.08	0.53
1:E:86:LEU:HD11	1:F:138:PHE:HB2	1.89	0.53
1:E:64:ASN:ND2	1:E:67:GLU:HB2	2.23	0.53
1:A:30:GLY:N	2:A:1209:SO4:O3	2.38	0.53
1:G:28:ASN:OD1	1:G:29:ILE:N	2.42	0.53
1:E:117:ASN:ND2	1:E:182:GLU:HB3	2.23	0.53
1:A:199:SER:O	1:A:200:CYS:HB3	2.07	0.53
1:G:162:GLU:O	1:G:166:GLN:HG2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:GLY:O	1:D:33:LYS:HE2	2.09	0.53
1:C:121:ASN:C	1:C:121:ASN:ND2	2.62	0.53
1:C:52:GLU:OE1	3:C:1210:5FU:O5'	2.27	0.53
1:G:64:ASN:ND2	1:G:67:GLU:HB2	2.24	0.52
1:F:66:LEU:HD23	1:F:171:GLU:OE2	2.09	0.52
1:D:28:ASN:OD1	1:D:29:ILE:N	2.42	0.52
1:A:117:ASN:HD21	1:A:182:GLU:HB3	1.74	0.51
1:D:117:ASN:ND2	1:D:182:GLU:HB3	2.24	0.51
1:H:47:ILE:HG12	1:H:100:LEU:HD23	1.92	0.51
1:B:170:SER:HB2	1:B:172:GLU:HG2	1.92	0.51
1:F:117:ASN:ND2	1:F:182:GLU:HB3	2.26	0.51
1:E:170:SER:HB3	1:E:172:GLU:HG3	1.93	0.50
1:C:196:ARG:C	1:C:198:GLN:H	2.13	0.50
1:H:172:GLU:O	1:H:175:VAL:HG13	2.11	0.50
1:D:121:ASN:HD22	1:D:121:ASN:C	2.15	0.50
1:B:117:ASN:HD21	1:B:182:GLU:HB3	1.76	0.50
1:H:121:ASN:HD22	1:H:121:ASN:C	2.14	0.49
1:E:172:GLU:C	1:E:174:CYS:H	2.15	0.49
1:C:162:GLU:HG3	1:C:166:GLN:NE2	2.27	0.49
3:C:1210:5FU:O5'	3:C:1210:5FU:H6	2.12	0.49
1:C:162:GLU:O	1:C:166:GLN:HG2	2.13	0.49
1:B:32:GLY:HA2	2:B:1209:SO4:O4	2.12	0.49
1:E:193:HIS:O	1:E:194:GLN:HB2	2.12	0.49
1:E:47:ILE:HG12	1:E:100:LEU:HD23	1.94	0.49
1:F:52:GLU:OE2	1:F:105:ARG:HG3	2.13	0.48
1:G:134:GLU:HB3	1:H:86:LEU:HD21	1.94	0.48
1:H:117:ASN:ND2	1:H:182:GLU:HB3	2.28	0.48
1:F:23:VAL:HG22	1:F:149:LEU:HB3	1.96	0.48
1:G:47:ILE:HG12	1:G:100:LEU:HD23	1.95	0.48
1:F:58:ARG:HA	1:F:64:ASN:OD1	2.14	0.48
1:C:170:SER:OG	1:C:171:GLU:N	2.47	0.48
1:B:47:ILE:HG12	1:B:100:LEU:HD23	1.95	0.47
1:E:105:ARG:HH12	3:E:1210:5FU:H5'1	1.78	0.47
1:C:47:ILE:HG12	1:C:100:LEU:HD23	1.96	0.47
1:G:142:SER:HB2	1:H:14:TYR:CD2	2.48	0.47
1:G:117:ASN:ND2	1:G:182:GLU:HB3	2.28	0.47
1:B:32:GLY:CA	2:B:1209:SO4:O4	2.63	0.47
1:E:27:GLY:O	1:E:33:LYS:HE2	2.15	0.47
1:C:117:ASN:HD21	1:C:182:GLU:HB3	1.79	0.47
1:G:23:VAL:HG22	1:G:149:LEU:HB3	1.97	0.47
1:A:121:ASN:C	1:A:121:ASN:ND2	2.67	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:161:TYR:HE2	1:H:165:ARG:HH21	1.63	0.46
1:B:23:VAL:HG22	1:B:149:LEU:HB3	1.97	0.46
1:F:28:ASN:OD1	1:F:29:ILE:N	2.48	0.46
1:A:47:ILE:HG12	1:A:100:LEU:HD23	1.96	0.46
1:A:196:ARG:O	1:A:197:PRO:C	2.51	0.46
1:E:193:HIS:O	1:E:194:GLN:CB	2.63	0.46
1:E:58:ARG:HA	1:E:64:ASN:OD1	2.16	0.46
1:E:37:LEU:CD1	1:E:104:GLU:HB2	2.45	0.46
1:F:47:ILE:HG12	1:F:100:LEU:HD23	1.98	0.46
1:D:47:ILE:HG12	1:D:100:LEU:HD23	1.98	0.46
1:A:52:GLU:OE2	1:A:105:ARG:HG3	2.16	0.45
1:C:192:ILE:C	1:C:194:GLN:H	2.20	0.45
1:A:197:PRO:O	1:A:198:GLN:C	2.53	0.45
1:H:155:THR:HG22	1:H:207:ALA:HB3	1.99	0.45
1:D:89:LEU:HA	1:D:89:LEU:HD23	1.76	0.45
1:B:52:GLU:OE2	1:B:105:ARG:HG3	2.16	0.45
1:B:117:ASN:ND2	1:B:182:GLU:HB3	2.32	0.45
1:D:170:SER:HB2	1:D:172:GLU:HG3	1.99	0.45
1:E:28:ASN:OD1	1:E:29:ILE:N	2.49	0.45
1:A:27:GLY:O	1:A:33:LYS:HE2	2.15	0.45
1:C:168:ALA:O	1:C:169:ARG:CB	2.65	0.44
3:G:1210:5FU:O2	3:G:1210:5FU:C2'	2.65	0.44
1:C:14:TYR:HB2	1:D:14:TYR:HB2	1.98	0.44
1:B:121:ASN:ND2	1:B:121:ASN:C	2.71	0.44
1:D:21:PHE:HA	1:D:148:ASP:OD2	2.18	0.44
1:C:117:ASN:ND2	1:C:182:GLU:HB3	2.33	0.44
1:B:28:ASN:OD1	1:B:29:ILE:N	2.51	0.44
1:C:121:ASN:ND2	1:C:123:SER:OG	2.51	0.44
1:C:28:ASN:OD1	1:C:29:ILE:N	2.51	0.44
1:D:155:THR:HG22	1:D:207:ALA:HB3	1.99	0.43
1:E:86:LEU:HD11	1:F:138:PHE:CB	2.49	0.43
1:C:64:ASN:ND2	1:C:67:GLU:HB2	2.34	0.43
1:A:64:ASN:ND2	1:A:67:GLU:HB2	2.34	0.43
1:H:52:GLU:HA	1:H:53:PRO:HD3	1.90	0.43
1:F:155:THR:HG22	1:F:207:ALA:HB3	2.01	0.43
1:C:89:LEU:HA	1:C:89:LEU:HD23	1.78	0.43
1:A:117:ASN:ND2	1:A:182:GLU:HB3	2.32	0.43
1:F:121:ASN:C	1:F:121:ASN:ND2	2.71	0.43
1:C:76:TRP:C	1:C:79:PRO:HD2	2.39	0.43
1:E:155:THR:HG22	1:E:207:ALA:HB3	2.01	0.43
1:G:121:ASN:ND2	1:G:121:ASN:C	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:142:SER:HB2	1:H:14:TYR:CE2	2.55	0.42
1:B:64:ASN:ND2	1:B:67:GLU:HB2	2.34	0.42
1:D:52:GLU:OE2	1:D:105:ARG:HG3	2.19	0.42
1:D:52:GLU:HA	1:D:53:PRO:HD3	1.91	0.42
1:F:172:GLU:HB3	3:F:1210:5FU:O3'	2.20	0.42
1:H:175:VAL:HA	1:H:176:PRO:HD3	1.62	0.42
1:G:26:GLU:HG3	1:G:190:TRP:CH2	2.55	0.42
1:E:121:ASN:C	1:E:121:ASN:ND2	2.72	0.42
1:H:121:ASN:ND2	1:H:123:SER:OG	2.52	0.42
1:C:37:LEU:CD1	1:C:104:GLU:HB2	2.49	0.42
1:C:155:THR:HG22	1:C:207:ALA:HB3	2.02	0.42
1:C:172:GLU:HB3	3:C:1210:5FU:O3'	2.20	0.42
1:F:52:GLU:HA	1:F:53:PRO:HD3	1.87	0.41
1:E:21:PHE:HA	1:E:148:ASP:OD2	2.20	0.41
1:C:130:ASN:O	1:C:134:GLU:HG2	2.20	0.41
1:B:37:LEU:CD1	1:B:104:GLU:HB2	2.51	0.41
1:G:37:LEU:CD1	1:G:104:GLU:HB2	2.50	0.41
1:E:52:GLU:HA	1:E:53:PRO:HD3	1.95	0.41
1:H:30:GLY:N	2:H:1209:SO4:O3	2.47	0.41
1:C:127:GLY:HA3	1:D:76:TRP:CZ3	2.56	0.41
1:H:27:GLY:O	1:H:33:LYS:HE2	2.21	0.41
1:G:89:LEU:HA	1:G:89:LEU:HD23	1.75	0.41
1:F:171:GLU:N	1:F:171:GLU:OE1	2.37	0.41
1:F:29:ILE:HG22	1:F:164:ILE:HD11	2.03	0.41
1:B:155:THR:HG22	1:B:207:ALA:HB3	2.02	0.41
1:D:162:GLU:O	1:D:166:GLN:HG2	2.21	0.41
1:G:155:THR:HG22	1:G:207:ALA:HB3	2.03	0.41
1:A:198:GLN:HE21	1:A:199:SER:C	2.24	0.40
1:G:191:LEU:HD23	1:G:191:LEU:HA	1.83	0.40
1:C:58:ARG:HA	1:C:64:ASN:OD1	2.21	0.40
1:A:89:LEU:HD23	1:A:89:LEU:HA	1.81	0.40
1:C:159:VAL:HG21	1:C:208:ASP:OD2	2.21	0.40
1:G:114:PHE:CG	3:G:1210:5FU:O4	2.74	0.40
1:E:89:LEU:HA	1:E:89:LEU:HD23	1.78	0.40
1:F:21:PHE:HA	1:F:148:ASP:OD2	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:ASP:OD1	1:F:43:TYR:OH[2_546]	1.73	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:TYR:OH	1:G:46:ASP:OD1[2_746]	2.12	0.08
1:B:43:TYR:OH	1:F:46:ASP:OD1[2_546]	2.13	0.07

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	195/230 (85%)	178 (91%)	15 (8%)	2 (1%)	19	61
1	B	188/230 (82%)	167 (89%)	20 (11%)	1 (0%)	34	76
1	C	195/230 (85%)	171 (88%)	20 (10%)	4 (2%)	9	40
1	D	187/230 (81%)	171 (91%)	16 (9%)	0	100	100
1	E	188/230 (82%)	172 (92%)	16 (8%)	0	100	100
1	F	188/230 (82%)	168 (89%)	19 (10%)	1 (0%)	34	76
1	G	188/230 (82%)	170 (90%)	16 (8%)	2 (1%)	17	58
1	H	188/230 (82%)	176 (94%)	12 (6%)	0	100	100
All	All	1517/1840 (82%)	1373 (90%)	134 (9%)	10 (1%)	26	70

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	174	CYS
1	G	171	GLU
1	A	194	GLN
1	A	200	CYS
1	C	169	ARG
1	C	193	HIS
1	B	167	ARG
1	C	197	PRO
1	C	194	GLN
1	G	167	ARG

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	182/208 (88%)	174 (96%)	8 (4%)	35	74
1	B	176/208 (85%)	170 (97%)	6 (3%)	44	81
1	C	177/208 (85%)	165 (93%)	12 (7%)	20	56
1	D	173/208 (83%)	165 (95%)	8 (5%)	33	73
1	E	174/208 (84%)	167 (96%)	7 (4%)	38	77
1	F	175/208 (84%)	166 (95%)	9 (5%)	29	69
1	G	173/208 (83%)	166 (96%)	7 (4%)	38	77
1	H	176/208 (85%)	171 (97%)	5 (3%)	51	84
All	All	1406/1664 (84%)	1344 (96%)	62 (4%)	35	74

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	LEU
1	A	121	ASN
1	A	165	ARG
1	A	172	GLU
1	A	173	SER
1	A	178	LYS
1	A	196	ARG
1	A	208	ASP
1	B	49	LEU
1	B	121	ASN
1	B	165	ARG
1	B	174	CYS
1	B	178	LYS
1	B	208	ASP
1	C	49	LEU
1	C	109	SER
1	C	121	ASN
1	C	162	GLU
1	C	163	ARG

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Mol	Chain	Res	Type
1	C	166	GLN
1	C	172	GLU
1	C	174	CYS
1	C	178	LYS
1	C	196	ARG
1	C	199	SER
1	C	208	ASP
1	D	49	LEU
1	D	121	ASN
1	D	163	ARG
1	D	170	SER
1	D	171	GLU
1	D	175	VAL
1	D	178	LYS
1	D	208	ASP
1	E	49	LEU
1	E	121	ASN
1	E	163	ARG
1	E	170	SER
1	E	172	GLU
1	E	178	LYS
1	E	208	ASP
1	F	49	LEU
1	F	52	GLU
1	F	121	ASN
1	F	163	ARG
1	F	171	GLU
1	F	172	GLU
1	F	175	VAL
1	F	178	LYS
1	F	208	ASP
1	G	49	LEU
1	G	121	ASN
1	G	165	ARG
1	G	171	GLU
1	G	172	GLU
1	G	178	LYS
1	G	208	ASP
1	H	49	LEU
1	H	121	ASN
1	H	170	SER
1	H	178	LYS

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Mol	Chain	Res	Type
1	H	208	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	121	ASN
1	A	198	GLN
1	B	117	ASN
1	B	121	ASN
1	B	194	GLN
1	C	117	ASN
1	C	121	ASN
1	D	117	ASN
1	D	121	ASN
1	D	166	GLN
1	E	117	ASN
1	E	121	ASN
1	F	117	ASN
1	F	121	ASN
1	G	81	GLN
1	G	117	ASN
1	G	121	ASN
1	H	117	ASN
1	H	121	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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

17 ligands are modelled in this entry.

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	SO4	A	1209	-	4,4,4	0.24	0	6,6,6	0.25	0
2	SO4	A	1210	-	4,4,4	0.29	0	6,6,6	0.51	0
3	5FU	A	1211	-	14,18,23	1.90	1 (7%)	15,26,35	2.33	4 (26%)
2	SO4	B	1209	-	4,4,4	0.38	0	6,6,6	0.62	0
3	5FU	B	1210	-	14,18,23	1.56	1 (7%)	15,26,35	2.48	3 (20%)
2	SO4	C	1209	-	4,4,4	0.19	0	6,6,6	0.43	0
3	5FU	C	1210	-	14,18,23	2.35	1 (7%)	15,26,35	2.55	5 (33%)
2	SO4	D	1209	-	4,4,4	0.18	0	6,6,6	0.54	0
3	5FU	D	1210	-	14,18,23	2.03	1 (7%)	15,26,35	2.72	4 (26%)
2	SO4	E	1209	-	4,4,4	0.44	0	6,6,6	0.49	0
3	5FU	E	1210	-	14,18,23	2.31	1 (7%)	15,26,35	2.48	5 (33%)
2	SO4	F	1209	-	4,4,4	0.21	0	6,6,6	0.49	0
3	5FU	F	1210	-	14,18,23	2.37	1 (7%)	15,26,35	2.35	4 (26%)
2	SO4	G	1209	-	4,4,4	0.20	0	6,6,6	0.56	0
3	5FU	G	1210	-	14,18,23	2.18	1 (7%)	15,26,35	2.29	3 (20%)
2	SO4	H	1209	-	4,4,4	0.76	0	6,6,6	0.52	0
3	5FU	H	1210	-	14,18,23	1.70	1 (7%)	15,26,35	2.05	5 (33%)

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	SO4	A	1209	-	-	0/0/0/0	0/0/0/0
2	SO4	A	1210	-	-	0/0/0/0	0/0/0/0
3	5FU	A	1211	-	-	0/2/18/26	0/2/2/2
2	SO4	B	1209	-	-	0/0/0/0	0/0/0/0
3	5FU	B	1210	-	-	0/2/18/26	0/2/2/2
2	SO4	C	1209	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	5FU	C	1210	-	-	0/2/18/26	0/2/2/2
2	SO4	D	1209	-	-	0/0/0/0	0/0/0/0
3	5FU	D	1210	-	-	0/2/18/26	0/2/2/2
2	SO4	E	1209	-	-	0/0/0/0	0/0/0/0
3	5FU	E	1210	-	-	0/2/18/26	0/2/2/2
2	SO4	F	1209	-	-	0/0/0/0	0/0/0/0
3	5FU	F	1210	-	-	0/2/18/26	0/2/2/2
2	SO4	G	1209	-	-	0/0/0/0	0/0/0/0
3	5FU	G	1210	-	-	0/2/18/26	0/2/2/2
2	SO4	H	1209	-	-	0/0/0/0	0/0/0/0
3	5FU	H	1210	-	-	0/2/18/26	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1210	5FU	C4-C5	5.49	1.45	1.38
3	H	1210	5FU	C4-C5	5.70	1.45	1.38
3	A	1211	5FU	C4-C5	6.64	1.46	1.38
3	D	1210	5FU	C4-C5	7.12	1.47	1.38
3	G	1210	5FU	C4-C5	7.92	1.48	1.38
3	E	1210	5FU	C4-C5	8.30	1.48	1.38
3	C	1210	5FU	C4-C5	8.53	1.49	1.38
3	F	1210	5FU	C4-C5	8.66	1.49	1.38

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1210	5FU	C5-C4-N3	-4.55	117.27	122.34
3	A	1211	5FU	C5'-C4'-C3'	-3.35	105.87	114.80
3	F	1210	5FU	C5-C4-N3	-3.33	118.63	122.34
3	D	1210	5FU	C5-C4-N3	-3.29	118.68	122.34
3	H	1210	5FU	O3'-C3'-C4'	-2.86	98.50	110.05
3	G	1210	5FU	C5'-C4'-C3'	-2.75	107.47	114.80
3	E	1210	5FU	C5'-C4'-C3'	-2.71	107.58	114.80
3	C	1210	5FU	C5-C4-N3	-2.69	119.34	122.34
3	D	1210	5FU	O3'-C3'-C4'	-2.58	99.64	110.05
3	B	1210	5FU	C2'-C1'-N1	-2.55	107.96	114.16
3	C	1210	5FU	C5'-C4'-C3'	-2.46	108.25	114.80
3	F	1210	5FU	C5'-C4'-C3'	-2.45	108.27	114.80
3	C	1210	5FU	C2'-C1'-N1	-2.44	108.23	114.16
3	E	1210	5FU	O5'-C5'-C4'	-2.07	104.48	111.33
3	A	1211	5FU	C2'-C3'-C4'	2.09	107.10	102.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	1210	5FU	C2'-C3'-C4'	2.17	107.26	102.77
3	H	1210	5FU	C4-N3-C2	2.29	117.23	115.25
3	H	1210	5FU	C4'-O4'-C1'	2.93	116.88	109.47
3	E	1210	5FU	O4'-C1'-N1	3.40	113.61	107.72
3	C	1210	5FU	O4'-C1'-N1	3.56	113.88	107.72
3	F	1210	5FU	O4'-C1'-N1	3.74	114.19	107.72
3	A	1211	5FU	O4'-C1'-N1	3.86	114.39	107.72
3	D	1210	5FU	O4'-C1'-N1	4.13	114.86	107.72
3	H	1210	5FU	O4'-C1'-N1	4.86	116.13	107.72
3	B	1210	5FU	O4'-C1'-N1	5.00	116.37	107.72
3	G	1210	5FU	O4'-C1'-N1	5.27	116.84	107.72
3	G	1210	5FU	C4-N3-C2	5.45	119.96	115.25
3	A	1211	5FU	C4-N3-C2	6.22	120.63	115.25
3	F	1210	5FU	C4-N3-C2	6.49	120.86	115.25
3	E	1210	5FU	C4-N3-C2	6.84	121.16	115.25
3	B	1210	5FU	C4-N3-C2	6.86	121.17	115.25
3	C	1210	5FU	C4-N3-C2	7.25	121.51	115.25
3	D	1210	5FU	C4-N3-C2	7.95	122.12	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1209	SO4	1	0
3	A	1211	5FU	1	0
2	B	1209	SO4	2	0
3	B	1210	5FU	1	0
3	C	1210	5FU	3	0
3	D	1210	5FU	1	0
3	E	1210	5FU	3	0
3	F	1210	5FU	1	0
3	G	1210	5FU	9	0
2	H	1209	SO4	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	197/230 (85%)	0.16	3 (1%) 76 49	43, 60, 84, 102	0
1	B	192/230 (83%)	-0.10	3 (1%) 74 47	42, 62, 84, 102	0
1	C	197/230 (85%)	0.01	7 (3%) 46 20	43, 62, 87, 102	0
1	D	191/230 (83%)	0.09	5 (2%) 59 29	43, 62, 84, 102	0
1	E	192/230 (83%)	-0.09	1 (0%) 91 76	43, 62, 84, 102	0
1	F	192/230 (83%)	0.11	11 (5%) 27 10	43, 62, 84, 102	0
1	G	192/230 (83%)	0.04	6 (3%) 52 24	43, 62, 84, 102	0
1	H	192/230 (83%)	0.08	1 (0%) 91 76	43, 60, 84, 102	0
All	All	1545/1840 (83%)	0.04	37 (2%) 62 32	42, 62, 84, 102	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	207	ALA	5.8
1	A	208	ASP	5.1
1	C	208	ASP	3.7
1	B	17	GLY	3.4
1	C	17	GLY	3.3
1	C	207	ALA	3.3
1	D	208	ASP	3.3
1	F	17	GLY	3.3
1	D	17	GLY	3.2
1	G	39	HIS	3.0
1	F	193	HIS	2.9
1	F	208	ASP	2.9
1	G	208	ASP	2.7
1	G	35	THR	2.7
1	F	48	CYS	2.6
1	F	200	CYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	97	ASN	2.4
1	F	201	LYS	2.4
1	D	166	GLN	2.4
1	C	144	HIS	2.3
1	E	97	ASN	2.3
1	C	15	ALA	2.3
1	F	18	THR	2.3
1	F	99	LYS	2.3
1	H	208	ASP	2.3
1	C	206	ASP	2.2
1	F	194	GLN	2.2
1	G	194	GLN	2.2
1	F	82	SER	2.1
1	D	99	LYS	2.1
1	A	97	ASN	2.1
1	F	207	ALA	2.1
1	G	201	LYS	2.1
1	B	99	LYS	2.1
1	D	18	THR	2.0
1	B	193	HIS	2.0
1	G	192	ILE	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
3	5FU	C	1210	17/22	0.93	0.43	3.23	62,65,66,66	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	5FU	G	1210	17/22	0.82	0.38	2.82	82,84,88,90	0
3	5FU	F	1210	17/22	0.96	0.23	0.60	47,50,57,58	0
3	5FU	E	1210	17/22	0.96	0.22	0.38	43,44,51,51	0
3	5FU	D	1210	17/22	0.95	0.21	0.15	53,58,60,62	0
3	5FU	H	1210	17/22	0.96	0.23	-0.40	26,31,39,43	0
2	SO4	E	1209	5/5	0.97	0.17	-0.54	58,58,62,63	0
3	5FU	B	1210	17/22	0.96	0.18	-0.67	46,48,55,57	0
3	5FU	A	1211	17/22	0.96	0.22	-0.72	35,36,45,45	0
2	SO4	D	1209	5/5	0.96	0.14	-1.02	60,61,63,64	0
2	SO4	G	1209	5/5	0.96	0.15	-1.18	67,68,70,70	0
2	SO4	C	1209	5/5	0.98	0.10	-1.44	57,58,59,59	0
2	SO4	F	1209	5/5	0.95	0.13	-1.71	55,58,60,62	0
2	SO4	B	1209	5/5	0.98	0.11	-1.79	41,43,45,46	0
2	SO4	H	1209	5/5	0.99	0.10	-3.04	16,19,24,25	0
2	SO4	A	1209	5/5	0.98	0.10	-3.37	29,30,32,33	0
2	SO4	A	1210	5/5	0.97	0.23	-	54,56,56,59	0

6.5 Other polymers

There are no such residues in this entry.