Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:11 PM GMT

PDB ID	:	1J3I
Title	:	Wild-type Plasmodium falciparum dihydrofolate reductase-thymidylate synthase (PfDHFR-TS) complexed with WR99210, NADPH, and dUMP
Authors	:	Yuvaniyama, J.; Chitnumsub, P.; Kamchonwongpaisan, S.; Vanichtanankul, J.; Sirawaraporn, W.; Taylor, P.; Walkinshaw, M.; Yuthavong, Y.
Deposited on	:	2003-02-03
Resolution	:	2.33 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

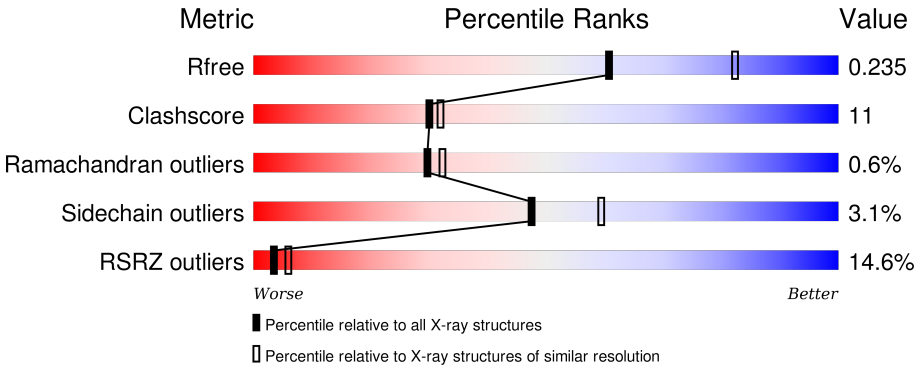
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	1406 (2.36-2.32)
Clashscore	102246	1509 (2.36-2.32)
Ramachandran outliers	100387	1490 (2.36-2.32)
Sidechain outliers	100360	1491 (2.36-2.32)
RSRZ outliers	91569	1412 (2.36-2.32)

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 <=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	280	13% 60% 17% • 20%
1	B	280	30% 47% 33% • 19%
2	C	328	6% 84% 14% • •
2	D	328	6% 83% 16% •

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10135 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 Bifunctional dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1847	1195	297	341	14			
1	B	226	Total	C	N	O	S	0	0	0
			1866	1205	300	348	13			

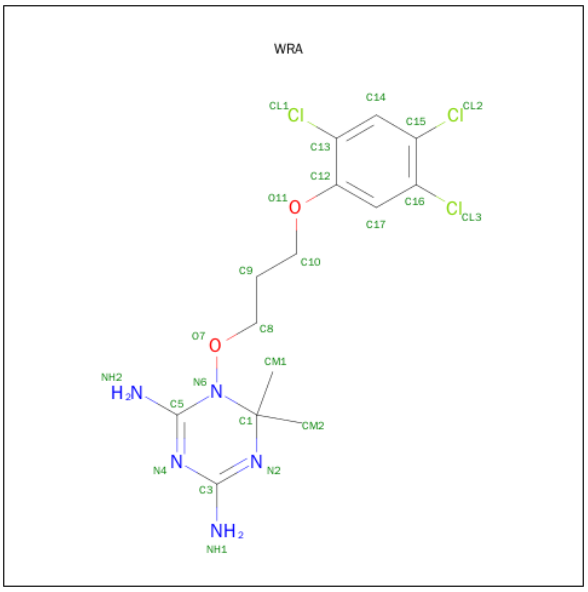
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	CYS	ARG	SEE REMARK 999	UNP P13922
A	108	SER	ASN	SEE REMARK 999	UNP P13922
B	59	CYS	ARG	SEE REMARK 999	UNP P13922
B	108	SER	ASN	SEE REMARK 999	UNP P13922

- Molecule 2 is a protein called Bifunctional dihydrofolate reductase-thymidylate synthase.

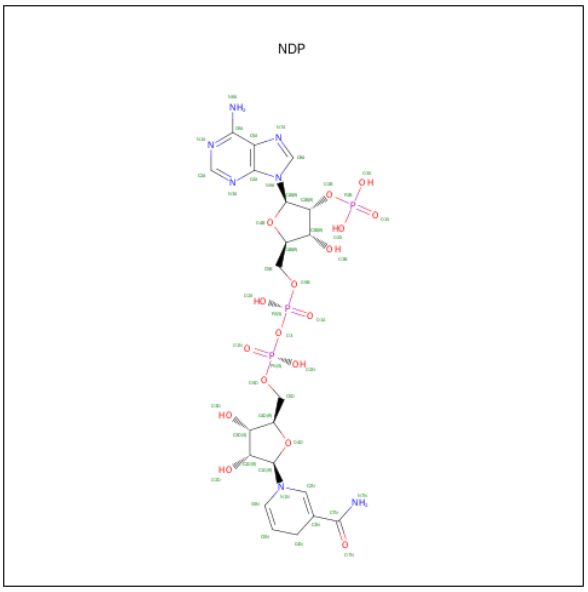
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	327	Total	C	N	O	S	0	0	0
			2721	1751	457	498	15			
2	D	328	Total	C	N	O	S	0	0	0
			2729	1755	458	501	15			

- Molecule 3 is 6,6-DIMETHYL-1-[3-(2,4,5-TRICHLOROPHENOXY)PROPOXY]-1,6-DIHYDRO-1,3,5-TRIAZINE-2,4-DIAMINE (three-letter code: WRA) (formula: $C_{14}H_{18}Cl_3N_5O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	Cl	N	O	0	0
			24	14	3	5	2		
3	B	1	Total	C	Cl	N	O	0	0
			24	14	3	5	2		

- Molecule 4 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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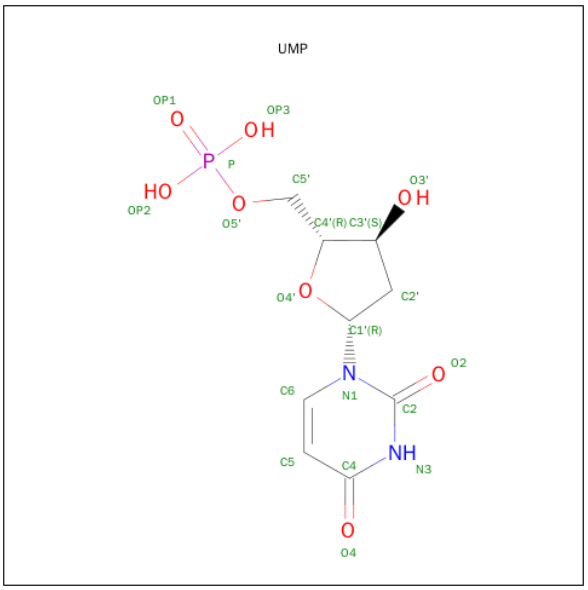
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 is 2'-DEOXYURIDINE 5'-MONOPHOSPHATE (three-letter code: UMP) (formula: $C_9H_{13}N_2O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
5	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

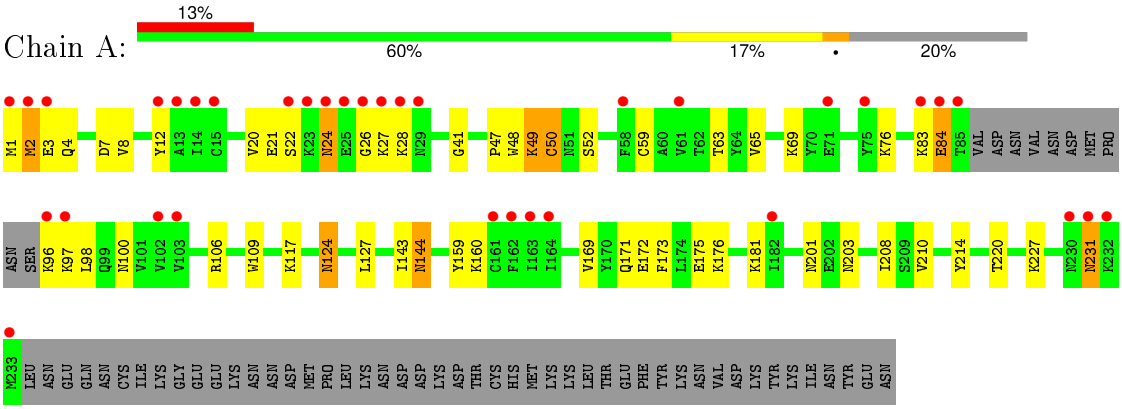
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	156	Total	O	0	0
			156	156		
6	B	51	Total	O	0	0
			51	51		
6	C	289	Total	O	0	0
			289	289		
6	D	292	Total	O	0	0
			292	292		

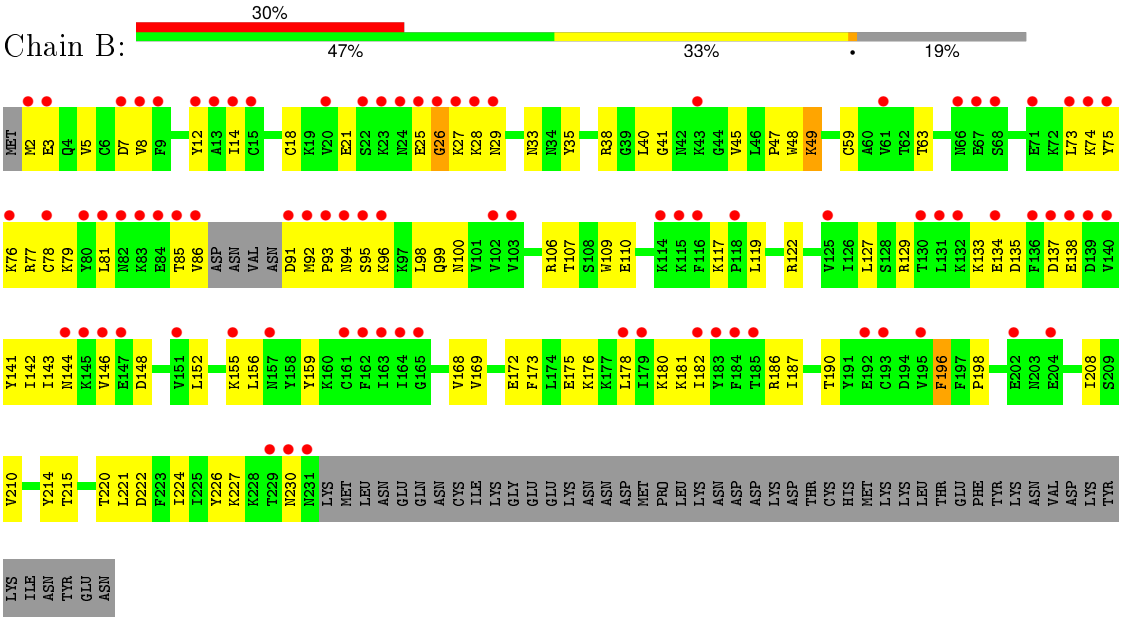
3 Residue-property plots (i)

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.

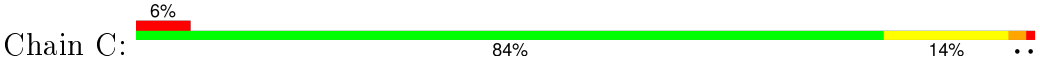
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

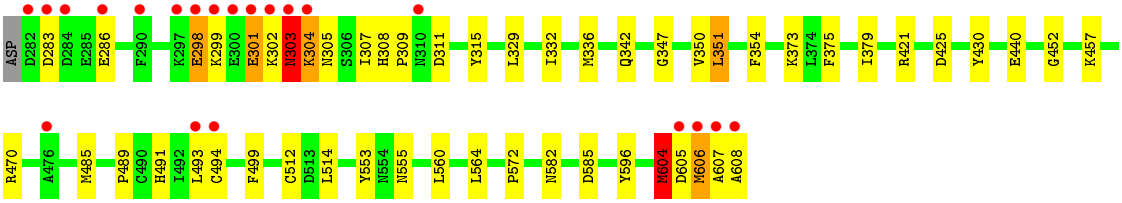


- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



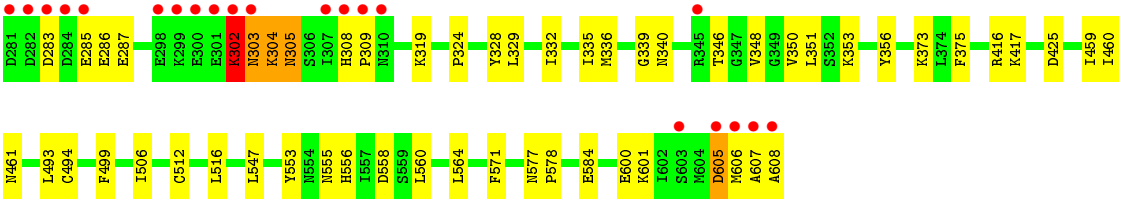
- Molecule 2: Bifunctional dihydrofolate reductase-thymidylate synthase





- Molecule 2: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	59.12Å 157.25Å 165.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.40 – 2.33 29.40 – 2.33	Depositor EDS
% Data completeness (in resolution range)	96.7 (29.40-2.33) 96.8 (29.40-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	3.70 (at 2.34Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.185 , 0.236 0.185 , 0.235	Depositor DCC
R_{free} test set	3211 reflections (4.99%)	DCC
Wilson B-factor (Å^2)	38.2	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 54.9	EDS
Estimated twinning fraction	0.008 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 64375 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10135	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: NDP, UMP, WRA

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	0.55	0/1881	0.78	1/2527 (0.0%)
1	B	0.45	0/1901	0.70	0/2558
2	C	0.61	1/2792 (0.0%)	0.85	5/3777 (0.1%)
2	D	0.60	1/2800 (0.0%)	0.85	6/3788 (0.2%)
All	All	0.57	2/9374 (0.0%)	0.81	12/12650 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	494	CYS	CB-SG	-6.37	1.71	1.82
2	D	494	CYS	CB-SG	-5.83	1.72	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	303	ASN	N-CA-C	-10.67	82.20	111.00
2	D	303	ASN	N-CA-C	-10.47	82.73	111.00
2	C	304	LYS	N-CA-C	7.40	130.99	111.00
2	D	305	ASN	N-CA-C	7.07	130.08	111.00
1	A	231	ASN	N-CA-C	6.43	128.37	111.00
2	D	351	LEU	N-CA-C	-6.19	94.28	111.00
2	D	302	LYS	N-CA-C	-6.15	94.40	111.00
2	C	351	LEU	N-CA-C	-5.91	95.04	111.00
2	C	604	MET	N-CA-C	-5.56	96.00	111.00
2	C	301	GLU	CA-CB-CG	-5.47	101.38	113.40
2	D	425	ASP	N-CA-C	-5.10	97.23	111.00
2	D	605	ASP	N-CA-C	5.10	124.76	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1847	0	1881	51	0
1	B	1866	0	1887	68	0
2	C	2721	0	2642	47	0
2	D	2729	0	2646	43	0
3	A	24	0	18	1	0
3	B	24	0	18	1	0
4	A	48	0	26	4	0
4	B	48	0	26	5	0
5	C	20	0	11	1	0
5	D	20	0	11	0	0
6	A	156	0	0	6	0
6	B	51	0	0	3	0
6	C	289	0	0	8	0
6	D	292	0	0	6	0
All	All	10135	0	9166	206	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 11.

All (206) 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)
2:C:301:GLU:O	2:C:301:GLU:HG2	1.61	0.96
2:D:302:LYS:O	2:D:302:LYS:HG3	1.65	0.94
1:A:59:CYS:HB2	6:A:1691:HOH:O	1.66	0.94
1:B:210:VAL:HB	6:B:1248:HOH:O	1.73	0.88
2:D:555:ASN:CB	2:D:607:ALA:HB2	2.06	0.86
1:A:127:LEU:HD23	1:A:143:ILE:HG13	1.59	0.83
1:A:21:GLU:HG2	1:A:21:GLU:O	1.84	0.78
2:C:304:LYS:HD3	6:C:1261:HOH:O	1.86	0.76
2:D:461:ASN:HB3	6:D:1458:HOH:O	1.86	0.75
1:A:59:CYS:SG	6:A:1216:HOH:O	2.43	0.75
2:C:555:ASN:HD22	2:C:606:MET:HA	1.53	0.74
2:C:301:GLU:CG	2:C:301:GLU:O	2.33	0.73
2:D:555:ASN:HB3	2:D:607:ALA:HB2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:ASN:OD1	1:B:159:TYR:HB3	1.90	0.72
1:A:1:MET:HG2	1:A:2:MET:H	1.53	0.72
2:D:555:ASN:HB2	2:D:607:ALA:HB2	1.71	0.72
1:A:48:TRP:O	1:A:49:LYS:HB2	1.90	0.71
1:A:24:ASN:N	1:A:24:ASN:HD22	1.89	0.70
1:B:2:MET:HG2	1:B:3:GLU:H	1.57	0.70
1:B:129:ARG:NH1	1:B:129:ARG:HB2	2.07	0.69
1:B:129:ARG:HH11	1:B:129:ARG:HB2	1.58	0.67
1:B:28:LYS:HG2	1:B:29:ASN:N	2.10	0.67
1:A:106:ARG:HH11	1:A:106:ARG:HG2	1.58	0.67
1:B:12:TYR:CD1	1:B:181:LYS:HB2	2.30	0.66
1:A:41:GLY:HA2	1:A:47:PRO:HD3	1.79	0.65
2:D:558:ASP:OD2	2:D:608:ALA:HB3	1.97	0.65
2:D:493:LEU:C	2:D:493:LEU:HD12	2.18	0.64
2:C:491:HIS:ND1	6:C:1507:HOH:O	2.19	0.64
4:A:610:NDP:H8A	4:A:610:NDP:H52A	1.79	0.64
1:A:20:VAL:HG12	1:A:22:SER:H	1.63	0.64
1:A:210:VAL:HB	6:A:1697:HOH:O	1.98	0.64
1:B:230:ASN:HA	6:B:1010:HOH:O	1.99	0.62
1:B:28:LYS:HG2	1:B:29:ASN:H	1.65	0.62
1:B:168:VAL:HG23	4:B:710:NDP:O2N	2.00	0.62
1:B:48:TRP:O	1:B:49:LYS:HB2	2.00	0.61
2:C:299:LYS:HG3	2:C:301:GLU:H	1.65	0.61
3:B:709:WRA:HH22	3:B:709:WRA:H81	1.66	0.61
2:C:302:LYS:C	2:C:303:ASN:O	2.29	0.61
1:B:92:MET:HG2	1:B:95:SER:H	1.66	0.60
2:C:286:GLU:OE2	2:D:319:LYS:HD3	2.01	0.60
2:C:605:ASP:CG	2:C:608:ALA:HA	2.22	0.60
2:C:604:MET:HA	6:C:1575:HOH:O	2.01	0.60
1:B:98:LEU:HD12	1:B:99:GLN:H	1.67	0.60
1:A:106:ARG:HD3	4:A:610:NDP:O2X	2.02	0.60
2:D:283:ASP:CB	2:D:286:GLU:HG3	2.32	0.59
2:C:347:GLY:O	6:C:1271:HOH:O	2.17	0.59
2:D:283:ASP:HB3	2:D:286:GLU:HG3	1.84	0.59
1:B:146:VAL:HG21	1:B:176:LYS:HE3	1.85	0.59
1:A:24:ASN:N	1:A:24:ASN:ND2	2.49	0.58
2:C:307:ILE:N	2:C:307:ILE:HD12	2.18	0.58
1:A:159:TYR:CE2	1:A:160:LYS:HE3	2.39	0.57
1:B:7:ASP:HA	1:B:180:LYS:HE2	1.86	0.57
1:B:78:CYS:SG	1:B:85:THR:HA	2.45	0.57
1:A:24:ASN:H	1:A:24:ASN:ND2	2.02	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:607:ALA:O	2:C:608:ALA:HB3	2.06	0.56
1:B:8:VAL:HG22	1:B:76:LYS:HE3	1.88	0.56
1:A:106:ARG:NH1	1:A:106:ARG:HG2	2.21	0.55
1:B:109:TRP:CZ2	1:B:117:LYS:HG2	2.40	0.55
1:B:2:MET:HG2	1:B:3:GLU:N	2.20	0.55
2:D:328:TYR:CZ	2:D:332:ILE:HD11	2.41	0.54
2:C:375:PHE:HD1	6:C:1564:HOH:O	1.89	0.54
1:B:59:CYS:O	1:B:63:THR:HG23	2.08	0.54
1:B:129:ARG:CB	1:B:129:ARG:HH11	2.21	0.54
1:B:198:PRO:HD3	6:B:1003:HOH:O	2.08	0.54
2:C:493:LEU:C	2:C:493:LEU:HD12	2.28	0.53
1:B:74:LYS:O	1:B:75:TYR:C	2.43	0.53
2:D:346:THR:OG1	2:D:348:VAL:HG23	2.08	0.53
2:C:342:GLN:HE21	2:D:499:PHE:HD1	1.56	0.53
2:C:572:PRO:HB3	2:C:596:TYR:HA	1.91	0.53
1:B:106:ARG:HE	4:B:710:NDP:P2B	2.31	0.52
2:D:553:TYR:HB3	2:D:555:ASN:OD1	2.10	0.52
1:B:86:VAL:HG21	1:B:155:LYS:C	2.30	0.52
2:D:512:CYS:SG	2:D:547:LEU:HD22	2.50	0.52
1:B:94:ASN:O	1:B:95:SER:HB3	2.10	0.52
2:C:329:LEU:HD22	2:C:564:LEU:HD12	1.92	0.52
2:C:607:ALA:O	2:C:608:ALA:CB	2.58	0.52
1:B:173:PHE:CD1	1:B:178:LEU:HD12	2.44	0.52
2:C:452:GLY:HA2	6:C:1407:HOH:O	2.10	0.52
1:A:21:GLU:O	1:A:22:SER:C	2.47	0.52
2:C:305:ASN:HB2	2:C:307:ILE:HD11	1.92	0.51
1:A:4:GLN:HB3	6:A:1658:HOH:O	2.10	0.51
2:D:584:GLU:HB2	6:D:1464:HOH:O	2.10	0.51
1:A:1:MET:CG	1:A:2:MET:H	2.23	0.51
1:B:41:GLY:HA2	1:B:47:PRO:HD3	1.93	0.51
1:A:1:MET:HG2	1:A:2:MET:N	2.24	0.51
1:A:12:TYR:HD1	1:A:181:LYS:HB2	1.75	0.50
1:B:196:PHE:CD1	1:B:196:PHE:N	2.79	0.50
2:C:308:HIS:O	2:C:311:ASP:HB2	2.12	0.50
1:A:208:ILE:HD13	1:A:227:LYS:HD2	1.92	0.50
2:D:555:ASN:CB	2:D:607:ALA:CB	2.87	0.50
1:A:160:LYS:HE2	2:D:285:GLU:OE1	2.12	0.50
2:D:600:GLU:HG3	6:D:1078:HOH:O	2.12	0.50
1:A:124:ASN:N	1:A:124:ASN:HD22	2.11	0.49
2:D:335:ILE:O	2:D:339:GLY:N	2.38	0.49
2:D:324:PRO:HB2	2:D:571:PHE:HE2	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:152:LEU:O	1:B:156:LEU:HD12	2.12	0.49
2:C:299:LYS:HE3	2:C:301:GLU:HB3	1.95	0.49
2:C:354:PHE:CE2	2:D:506:ILE:HG13	2.47	0.49
1:A:109:TRP:CE2	1:A:117:LYS:HD2	2.48	0.49
1:B:8:VAL:HA	1:B:76:LYS:HE3	1.93	0.49
3:A:609:WRA:H81	3:A:609:WRA:HH22	1.78	0.49
1:B:186:ARG:HB2	1:B:222:ASP:OD1	2.13	0.49
1:B:21:GLU:HB3	1:B:190:THR:HG21	1.94	0.49
1:B:109:TRP:O	1:B:117:LYS:HD2	2.12	0.48
1:B:214:TYR:O	1:B:220:THR:HA	2.14	0.48
1:B:12:TYR:CE1	1:B:180:LYS:HD2	2.49	0.48
1:A:12:TYR:CD1	1:A:181:LYS:HB2	2.49	0.48
2:C:582:ASN:HB3	6:C:1348:HOH:O	2.13	0.48
2:C:298:GLU:HG3	2:C:298:GLU:H	1.29	0.48
2:D:285:GLU:C	2:D:287:GLU:H	2.16	0.47
2:D:350:VAL:HG12	2:D:553:TYR:CD1	2.50	0.47
2:C:350:VAL:HG12	2:C:553:TYR:CD1	2.50	0.47
1:B:172:GLU:HA	1:B:175:GLU:CG	2.45	0.47
2:D:459:ILE:HG13	2:D:460:ILE:N	2.30	0.47
2:C:421:ARG:HD2	2:C:425:ASP:HB3	1.96	0.47
1:A:24:ASN:OD1	1:A:27:LYS:HA	2.15	0.47
1:B:12:TYR:HD1	1:B:181:LYS:HB2	1.77	0.47
2:C:605:ASP:OD2	2:C:608:ALA:HA	2.15	0.47
1:B:8:VAL:HA	1:B:76:LYS:CE	2.45	0.47
1:B:106:ARG:HG2	1:B:110:GLU:OE2	2.16	0.46
1:B:172:GLU:O	1:B:176:LYS:HG3	2.15	0.46
1:B:77:ARG:O	1:B:81:LEU:HG	2.15	0.46
2:C:302:LYS:HA	2:C:302:LYS:HD3	1.70	0.46
1:B:25:GLU:O	1:B:26:GLY:O	2.33	0.46
1:B:40:LEU:O	4:B:710:NDP:H2N	2.15	0.46
1:B:169:VAL:HG23	4:B:710:NDP:O1A	2.15	0.46
2:C:301:GLU:O	2:C:302:LYS:HD3	2.15	0.46
1:B:143:ILE:HG22	1:B:144:ASN:N	2.31	0.45
2:D:373:LYS:HE2	2:D:375:PHE:CE1	2.52	0.45
2:D:373:LYS:NZ	6:D:1715:HOH:O	2.49	0.45
2:D:302:LYS:O	2:D:303:ASN:C	2.52	0.45
2:D:302:LYS:CG	2:D:302:LYS:O	2.49	0.45
2:C:307:ILE:HG13	6:C:1709:HOH:O	2.15	0.45
2:C:332:ILE:CD1	2:C:514:LEU:HB3	2.46	0.45
1:B:73:LEU:O	1:B:76:LYS:HB3	2.16	0.45
1:A:214:TYR:O	1:A:220:THR:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:485:MET:SD	2:C:489:PRO:HD3	2.57	0.45
1:B:208:ILE:HD13	1:B:227:LYS:HB2	1.99	0.45
2:C:336:MET:HE1	2:C:560:LEU:HB2	1.97	0.45
1:B:172:GLU:HA	1:B:175:GLU:HG2	1.99	0.44
2:C:305:ASN:C	2:C:307:ILE:HD12	2.38	0.44
1:A:171:GLN:O	1:A:175:GLU:HG3	2.17	0.44
1:A:8:VAL:HA	1:A:76:LYS:HD3	1.99	0.44
1:B:12:TYR:HE1	1:B:180:LYS:HD2	1.83	0.44
2:D:285:GLU:H	2:D:285:GLU:HG2	1.57	0.44
1:A:3:GLU:OE1	1:A:8:VAL:HG22	2.17	0.44
2:D:416:ARG:O	2:D:417:LYS:HB2	2.18	0.44
1:B:127:LEU:O	4:B:710:NDP:H1B	2.18	0.44
1:A:97:LYS:HG2	6:A:1683:HOH:O	2.16	0.44
2:D:283:ASP:HB2	2:D:286:GLU:HG3	1.98	0.44
1:A:201:ASN:OD1	1:A:203:ASN:HB2	2.18	0.44
1:A:59:CYS:O	1:A:63:THR:HG23	2.18	0.43
1:B:172:GLU:HB2	1:B:176:LYS:HE2	1.99	0.43
1:A:172:GLU:OE2	4:A:610:NDP:N7A	2.51	0.43
1:B:143:ILE:CG2	1:B:144:ASN:N	2.82	0.43
1:A:50:CYS:HA	6:A:1334:HOH:O	2.18	0.43
2:C:301:GLU:O	2:C:302:LYS:CD	2.66	0.43
1:A:2:MET:HG2	1:A:3:GLU:N	2.32	0.43
2:C:315:TYR:HB2	2:C:564:LEU:O	2.18	0.43
1:A:69:LYS:NZ	2:D:285:GLU:HA	2.34	0.43
1:A:24:ASN:C	1:A:26:GLY:H	2.22	0.43
1:B:134:GLU:CD	1:B:134:GLU:H	2.22	0.43
1:A:96:LYS:HB3	1:A:97:LYS:H	1.58	0.42
1:B:119:LEU:HB3	1:B:122:ARG:CZ	2.49	0.42
1:B:182:ILE:HB	1:B:226:TYR:HB2	2.01	0.42
1:B:143:ILE:HG23	1:B:148:ASP:HB2	2.01	0.42
2:C:499:PHE:CE1	2:D:340:ASN:HB3	2.54	0.42
1:B:91:ASP:C	1:B:93:PRO:HD3	2.40	0.42
1:B:133:LYS:HG2	1:B:142:ILE:HB	2.01	0.42
1:A:106:ARG:HE	4:A:610:NDP:P2B	2.42	0.42
1:A:100:ASN:OD1	1:A:159:TYR:HB3	2.19	0.42
2:D:285:GLU:C	2:D:287:GLU:N	2.72	0.42
1:A:83:LYS:O	1:A:84:GLU:HB3	2.20	0.42
1:B:141:TYR:OH	1:B:156:LEU:HD21	2.19	0.42
1:A:159:TYR:CD2	1:A:160:LYS:HG3	2.54	0.42
2:C:491:HIS:CE1	5:C:611:UMP:O4	2.73	0.42
2:C:582:ASN:HB2	2:C:585:ASP:OD2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:421:ARG:CD	2:C:425:ASP:HB3	2.50	0.42
2:C:470:ARG:HD3	6:D:1385:HOH:O	2.20	0.42
1:B:221:LEU:HD23	1:B:221:LEU:N	2.35	0.42
2:D:329:LEU:HD22	2:D:564:LEU:HD12	2.01	0.42
1:A:24:ASN:O	1:A:24:ASN:ND2	2.52	0.41
2:D:353:LYS:HG3	2:D:356:TYR:OH	2.20	0.41
1:A:144:ASN:C	1:A:144:ASN:HD22	2.23	0.41
2:C:373:LYS:HE2	2:C:375:PHE:CE2	2.56	0.41
1:B:14:ILE:HG23	1:B:14:ILE:O	2.20	0.41
2:D:516:LEU:HD12	2:D:556:HIS:CE1	2.55	0.41
2:D:308:HIS:HA	2:D:309:PRO:HD3	1.90	0.41
1:A:172:GLU:O	1:A:176:LYS:HG3	2.20	0.41
1:B:138:GLU:H	1:B:138:GLU:CD	2.22	0.41
1:B:210:VAL:HG12	1:B:224:ILE:HG22	2.02	0.41
2:C:351:LEU:HD23	2:C:351:LEU:HA	1.93	0.41
1:A:65:VAL:HG11	1:A:98:LEU:HB3	2.02	0.41
2:C:305:ASN:ND2	2:C:305:ASN:H	2.18	0.41
1:B:33:ASN:OD1	1:B:35:TYR:HB3	2.21	0.41
2:C:457:LYS:HB2	2:C:457:LYS:HE2	1.88	0.41
1:A:109:TRP:CZ2	1:A:117:LYS:HD2	2.56	0.40
2:D:336:MET:CE	2:D:560:LEU:HB2	2.51	0.40
1:A:169:VAL:O	1:A:173:PHE:HD1	2.04	0.40
2:D:607:ALA:O	2:D:608:ALA:HB2	2.21	0.40
2:D:584:GLU:HG2	6:D:1466:HOH:O	2.21	0.40
1:B:35:TYR:CZ	1:B:38:ARG:HD3	2.57	0.40
1:B:18:CYS:HA	1:B:187:ILE:HB	2.03	0.40
1:B:92:MET:SD	1:B:95:SER:HA	2.62	0.40
2:D:577:ASN:HA	2:D:578:PRO:HD3	1.85	0.40
1:A:26:GLY:C	1:A:28:LYS:N	2.74	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	219/280 (78%)	208 (95%)	9 (4%)	2 (1%)	21	21
1	B	222/280 (79%)	206 (93%)	14 (6%)	2 (1%)	21	21
2	C	325/328 (99%)	307 (94%)	17 (5%)	1 (0%)	46	54
2	D	326/328 (99%)	304 (93%)	20 (6%)	2 (1%)	30	32
All	All	1092/1216 (90%)	1025 (94%)	60 (6%)	7 (1%)	30	32

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	26	GLY
1	A	231	ASN
1	B	5	VAL
2	D	304	LYS
1	A	49	LYS
2	C	430	TYR
2	D	605	ASP

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	212/268 (79%)	204 (96%)	8 (4%)	40	51
1	B	215/268 (80%)	205 (95%)	10 (5%)	32	40
2	C	301/302 (100%)	292 (97%)	9 (3%)	48	61
2	D	302/302 (100%)	297 (98%)	5 (2%)	68	80
All	All	1030/1140 (90%)	998 (97%)	32 (3%)	47	59

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	MET
1	A	7	ASP
1	A	24	ASN
1	A	50	CYS

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Mol	Chain	Res	Type
1	A	52	SER
1	A	84	GLU
1	A	124	ASN
1	A	144	ASN
1	B	27	LYS
1	B	45	VAL
1	B	49	LYS
1	B	79	LYS
1	B	96	LYS
1	B	107	THR
1	B	135	ASP
1	B	137	ASP
1	B	196	PHE
1	B	215	THR
2	C	283	ASP
2	C	298	GLU
2	C	303	ASN
2	C	309	PRO
2	C	379	ILE
2	C	440	GLU
2	C	512	CYS
2	C	604	MET
2	C	606	MET
2	D	302	LYS
2	D	304	LYS
2	D	305	ASN
2	D	601	LYS
2	D	606	MET

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	24	ASN
1	A	144	ASN
1	B	29	ASN
1	B	121	ASN
2	C	303	ASN
2	C	316	ASN
2	C	342	GLN
2	C	394	ASN
2	C	424	ASN
2	D	394	ASN

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Mol	Chain	Res	Type
2	D	424	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

6 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	$\#\|Z\| > 2$
3	WRA	A	609	-	22,25,25	2.61	10 (45%)	28,36,36	1.96	5 (17%)
4	NDP	A	610	-	42,52,52	2.64	17 (40%)	55,80,80	2.51	22 (40%)
3	WRA	B	709	-	22,25,25	2.79	11 (50%)	28,36,36	1.72	4 (14%)
4	NDP	B	710	-	42,52,52	2.78	18 (42%)	55,80,80	2.29	22 (40%)
5	UMP	C	611	-	16,21,21	2.10	5 (31%)	23,31,31	3.21	8 (34%)
5	UMP	D	711	-	16,21,21	2.24	7 (43%)	23,31,31	3.27	7 (30%)

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	WRA	A	609	-	-	0/7/27/27	0/2/2/2
4	NDP	A	610	-	-	0/30/77/77	0/5/5/5
3	WRA	B	709	-	-	0/7/27/27	0/2/2/2
4	NDP	B	710	-	-	0/30/77/77	0/5/5/5
5	UMP	C	611	-	-	0/6/22/22	0/2/2/2
5	UMP	D	711	-	-	0/6/22/22	0/2/2/2

All (68) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	710	NDP	O4B-C1B	-8.81	1.30	1.41
4	A	610	NDP	P2B-O2X	-4.60	1.38	1.54
4	B	710	NDP	C2D-C3D	-4.07	1.42	1.53
4	B	710	NDP	P2B-O2X	-4.03	1.40	1.54
4	B	710	NDP	C4N-C5N	-3.84	1.40	1.49
4	A	610	NDP	C2D-C3D	-3.68	1.43	1.53
4	A	610	NDP	P2B-O2B	-3.30	1.50	1.60
4	B	710	NDP	PN-O2N	-3.14	1.41	1.54
4	A	610	NDP	C4N-C5N	-2.93	1.42	1.49
5	D	711	UMP	P-OP3	-2.87	1.44	1.54
5	D	711	UMP	P-OP2	-2.83	1.44	1.54
5	C	611	UMP	P-OP3	-2.53	1.45	1.54
5	C	611	UMP	P-O5'	-2.49	1.51	1.60
5	D	711	UMP	P-OP1	-2.47	1.43	1.51
5	C	611	UMP	P-OP2	-2.40	1.46	1.54
5	D	711	UMP	P-O5'	-2.39	1.52	1.60
4	B	710	NDP	PA-O2A	-2.13	1.45	1.54
4	A	610	NDP	C5A-N7A	-2.11	1.32	1.39
3	B	709	WRA	C3-NH1	-2.10	1.29	1.34
4	A	610	NDP	O4D-C4D	-2.07	1.40	1.45
4	A	610	NDP	C8A-N7A	-2.05	1.30	1.34
4	B	710	NDP	C3B-C4B	2.12	1.58	1.53
5	D	711	UMP	O3'-C3'	2.14	1.48	1.43
3	A	609	WRA	C9-C10	2.25	1.61	1.50
3	A	609	WRA	C1-N6	2.27	1.51	1.48
4	B	710	NDP	C2A-N3A	2.28	1.36	1.32
3	B	709	WRA	O11-C12	2.32	1.42	1.37
4	A	610	NDP	C6N-N1N	2.35	1.44	1.37
3	B	709	WRA	C16-CL3	2.41	1.79	1.73
3	B	709	WRA	C15-CL2	2.43	1.79	1.73
4	A	610	NDP	O3D-C3D	2.59	1.49	1.43
4	B	710	NDP	O3B-C3B	2.77	1.49	1.43
4	B	710	NDP	O3D-C3D	2.77	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	710	NDP	PN-O5D	2.80	1.71	1.59
4	A	610	NDP	C5D-C4D	2.88	1.60	1.51
3	A	609	WRA	C14-C13	3.13	1.43	1.38
4	B	710	NDP	C6N-N1N	3.26	1.47	1.37
4	B	710	NDP	O4D-C1D	3.29	1.50	1.42
3	B	709	WRA	O7-C8	3.35	1.50	1.45
4	A	610	NDP	C2A-N1A	3.35	1.40	1.33
4	B	710	NDP	C2A-N1A	3.47	1.40	1.33
3	A	609	WRA	O11-C12	3.59	1.44	1.37
3	A	609	WRA	C16-C15	3.65	1.48	1.39
3	B	709	WRA	C16-C15	3.84	1.48	1.39
5	D	711	UMP	O4'-C1'	3.85	1.51	1.42
3	A	609	WRA	C12-C13	3.86	1.46	1.39
4	A	610	NDP	O4D-C1D	3.88	1.51	1.42
3	B	709	WRA	C12-C13	3.90	1.46	1.39
5	C	611	UMP	O4'-C1'	3.91	1.51	1.42
3	A	609	WRA	O7-C8	3.98	1.51	1.45
3	A	609	WRA	C17-C12	4.05	1.46	1.38
3	A	609	WRA	C14-C15	4.15	1.45	1.38
4	B	710	NDP	C4A-N3A	4.36	1.42	1.35
4	A	610	NDP	O4B-C4B	4.36	1.55	1.45
4	B	710	NDP	C6N-C5N	4.38	1.41	1.33
3	B	709	WRA	C14-C13	4.47	1.46	1.38
5	C	611	UMP	C4-N3	4.68	1.41	1.33
3	B	709	WRA	C14-C15	4.76	1.46	1.38
3	A	609	WRA	C17-C16	4.77	1.46	1.38
3	B	709	WRA	C17-C16	4.78	1.46	1.38
4	A	610	NDP	C2N-C3N	4.83	1.46	1.34
4	A	610	NDP	C4A-N3A	4.87	1.42	1.35
3	B	709	WRA	C17-C12	4.88	1.47	1.38
4	A	610	NDP	C6N-C5N	4.93	1.42	1.33
5	D	711	UMP	C4-N3	5.12	1.42	1.33
4	B	710	NDP	C5D-C4D	5.28	1.68	1.51
4	B	710	NDP	C2N-C3N	5.73	1.48	1.34
4	A	610	NDP	O4B-C1B	8.04	1.51	1.41

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	610	NDP	C4B-O4B-C1B	-5.42	103.77	109.72
4	A	610	NDP	C1D-N1N-C2N	-4.97	112.25	120.91
4	B	710	NDP	N3A-C2A-N1A	-4.71	125.29	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	710	NDP	O4B-C4B-C5B	-4.50	93.23	109.32
4	B	710	NDP	O3X-P2B-O1X	-4.49	96.14	110.58
4	A	610	NDP	N3A-C2A-N1A	-4.37	125.55	128.89
4	B	710	NDP	C3N-C2N-N1N	-4.00	117.41	123.14
4	B	710	NDP	C1D-N1N-C2N	-3.95	114.03	120.91
3	A	609	WRA	N4-C3-N2	-3.63	120.72	126.51
4	A	610	NDP	O4B-C4B-C5B	-3.58	96.52	109.32
5	D	711	UMP	O4'-C1'-C2'	-3.48	99.34	106.27
4	A	610	NDP	C3N-C2N-N1N	-3.46	118.19	123.14
4	B	710	NDP	O5B-PA-O1A	-3.42	96.34	109.62
3	B	709	WRA	N4-C3-N2	-3.20	121.42	126.51
4	A	610	NDP	O5B-C5B-C4B	-3.15	97.49	109.12
4	A	610	NDP	O3D-C3D-C4D	-3.15	101.61	111.05
4	A	610	NDP	O3X-P2B-O1X	-2.93	101.15	110.58
5	D	711	UMP	C5-C4-N3	-2.87	115.75	123.12
5	C	611	UMP	C5-C4-N3	-2.83	115.85	123.12
5	C	611	UMP	O4'-C1'-C2'	-2.77	100.76	106.27
4	A	610	NDP	O3X-P2B-O2X	-2.75	96.91	107.38
4	A	610	NDP	O5D-C5D-C4D	-2.68	99.25	109.12
4	B	710	NDP	O3D-C3D-C4D	-2.67	103.05	111.05
4	B	710	NDP	O7N-C7N-N7N	-2.66	116.16	122.76
4	A	610	NDP	C4N-C5N-C6N	-2.58	118.32	122.58
4	B	710	NDP	O3X-P2B-O2X	-2.53	97.73	107.38
5	D	711	UMP	O4'-C4'-C3'	-2.45	99.51	105.67
4	B	710	NDP	C4B-O4B-C1B	-2.43	107.04	109.72
4	A	610	NDP	O3-PA-O5B	-2.35	96.69	102.94
4	A	610	NDP	O7N-C7N-N7N	-2.35	116.93	122.76
5	C	611	UMP	O4'-C4'-C3'	-2.34	99.78	105.67
4	B	710	NDP	C2D-C1D-N1N	-2.34	107.02	113.34
4	B	710	NDP	C4N-C5N-C6N	-2.19	118.97	122.58
4	B	710	NDP	C2B-C3B-C4B	-2.08	96.92	101.85
3	A	609	WRA	CM2-C1-CM1	-2.04	107.86	110.69
4	A	610	NDP	O3B-C3B-C4B	-2.00	105.05	111.05
5	C	611	UMP	C2'-C3'-C4'	2.22	107.38	102.77
4	A	610	NDP	O2B-C2B-C3B	2.33	120.58	111.51
4	A	610	NDP	C5B-C4B-C3B	2.41	124.77	115.21
3	A	609	WRA	NH1-C3-N4	2.55	119.90	116.56
4	B	710	NDP	O3B-C3B-C4B	2.61	118.89	111.05
3	B	709	WRA	NH1-C3-N4	2.62	119.99	116.56
3	B	709	WRA	C5-N4-C3	2.64	121.43	116.13
4	B	710	NDP	O2B-C2B-C3B	2.77	122.27	111.51
5	D	711	UMP	C4'-O4'-C1'	2.81	116.57	109.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	C	611	UMP	C2'-C1'-N1	2.86	121.12	114.16
4	B	710	NDP	C2D-C3D-C4D	2.86	108.50	102.61
4	B	710	NDP	C5B-C4B-C3B	2.88	126.65	115.21
5	C	611	UMP	C4'-O4'-C1'	2.89	116.76	109.47
4	B	710	NDP	P2B-O2B-C2B	2.91	128.54	121.56
3	A	609	WRA	C5-N4-C3	3.01	122.17	116.13
4	A	610	NDP	C2D-C3D-C4D	3.37	109.54	102.61
5	D	711	UMP	C2'-C1'-N1	3.41	122.44	114.16
4	A	610	NDP	C5N-C4N-C3N	3.56	122.32	112.52
4	B	710	NDP	O4B-C1B-C2B	3.61	113.14	106.60
4	B	710	NDP	O3-PN-O5D	3.86	113.17	102.94
4	B	710	NDP	C5N-C4N-C3N	3.88	123.20	112.52
5	C	611	UMP	O4'-C1'-N1	3.97	114.60	107.72
5	D	711	UMP	O4'-C1'-N1	4.45	115.42	107.72
4	A	610	NDP	O2X-P2B-O1X	4.76	125.91	110.58
4	B	710	NDP	O2X-P2B-O1X	4.82	126.08	110.58
4	A	610	NDP	P2B-O2B-C2B	4.89	133.29	121.56
4	A	610	NDP	O4B-C1B-N9A	5.25	119.09	108.10
4	A	610	NDP	O3-PN-O5D	5.37	117.19	102.94
3	B	709	WRA	C8-O7-N6	6.70	119.64	110.49
3	A	609	WRA	C8-O7-N6	7.88	121.26	110.49
5	D	711	UMP	C4-N3-C2	12.81	126.83	114.14
5	C	611	UMP	C4-N3-C2	12.95	126.97	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	609	WRA	1	0
4	A	610	NDP	4	0
3	B	709	WRA	1	0
4	B	710	NDP	5	0
5	C	611	UMP	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, 95^{th} 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	223/280 (79%)	0.81	35 (15%) 3 5	24, 44, 94, 96	0
1	B	226/280 (80%)	1.91	84 (37%) 0 0	31, 79, 96, 96	0
2	C	327/328 (99%)	0.21	21 (6%) 23 33	21, 33, 94, 96	0
2	D	328/328 (100%)	0.18	21 (6%) 23 33	21, 33, 94, 96	0
All	All	1104/1216 (90%)	0.67	161 (14%) 3 6	21, 39, 95, 96	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	85	THR	10.9
2	D	607	ALA	10.8
1	A	233	MET	10.5
1	B	2	MET	9.7
2	D	282	ASP	9.5
1	B	95	SER	9.2
1	B	91	ASP	9.0
1	B	92	MET	9.0
2	C	606	MET	9.0
1	B	94	ASN	9.0
1	A	2	MET	8.8
1	A	1	MET	8.6
1	A	85	THR	8.4
2	D	608	ALA	8.3
2	C	608	ALA	8.2
1	B	231	ASN	8.0
2	C	302	LYS	7.8
1	A	231	ASN	7.7
2	C	607	ALA	7.5
2	C	303	ASN	7.4
2	D	606	MET	7.1

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Mol	Chain	Res	Type	RSRZ
2	C	301	GLU	6.8
1	B	75	TYR	6.8
1	B	14	ILE	6.7
1	B	26	GLY	6.7
1	A	23	LYS	6.6
1	B	28	LYS	6.5
2	D	281	ASP	6.5
2	D	300	GLU	6.3
1	A	24	ASN	6.1
2	D	284	ASP	6.0
1	B	82	ASN	5.9
1	A	75	TYR	5.9
1	B	86	VAL	5.8
2	C	300	GLU	5.8
1	B	96	LYS	5.8
1	A	25	GLU	5.8
1	A	22	SER	5.8
1	A	26	GLY	5.7
1	B	73	LEU	5.7
2	C	282	ASP	5.7
2	D	299	LYS	5.5
1	B	80	TYR	5.5
2	C	283	ASP	5.4
1	B	84	GLU	5.3
1	A	232	LYS	5.3
1	B	93	PRO	5.3
1	B	162	PHE	5.2
2	D	283	ASP	5.1
2	D	301	GLU	5.1
1	A	230	ASN	5.0
1	B	164	ILE	4.9
2	D	303	ASN	4.8
1	B	130	THR	4.8
1	B	151	VAL	4.7
1	B	163	ILE	4.7
1	A	28	LYS	4.6
1	B	138	GLU	4.5
1	B	81	LEU	4.5
1	B	3	GLU	4.5
2	C	299	LYS	4.4
2	D	302	LYS	4.4
1	A	14	ILE	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	27	LYS	4.4
1	B	78	CYS	4.4
1	B	24	ASN	4.3
2	D	298	GLU	4.2
1	B	144	ASN	4.2
1	B	13	ALA	4.1
2	D	285	GLU	4.1
1	B	182	ILE	4.0
2	C	284	ASP	4.0
1	B	116	PHE	4.0
1	B	134	GLU	4.0
1	B	15	CYS	4.0
1	B	27	LYS	3.9
2	D	309	PRO	3.9
1	A	163	ILE	3.8
1	B	23	LYS	3.7
2	D	605	ASP	3.6
1	A	96	LYS	3.6
2	D	307	ILE	3.6
1	B	12	TYR	3.6
1	B	29	ASN	3.6
1	A	164	ILE	3.5
1	B	146	VAL	3.5
1	B	230	ASN	3.5
1	B	195	VAL	3.4
1	A	162	PHE	3.4
1	B	184	PHE	3.4
1	A	84	GLU	3.4
1	B	25	GLU	3.4
2	C	298	GLU	3.4
1	B	145	LYS	3.3
1	B	192	GLU	3.3
1	B	8	VAL	3.2
1	A	13	ALA	3.2
1	B	68	SER	3.2
1	B	76	LYS	3.1
1	A	29	ASN	3.1
2	C	297	LYS	3.1
1	B	71	GLU	3.0
1	A	182	ILE	3.0
1	B	74	LYS	3.0
1	B	115	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	157	ASN	3.0
1	B	102	VAL	3.0
1	B	183	TYR	2.9
1	B	137	ASP	2.9
1	B	7	ASP	2.9
1	A	3	GLU	2.9
1	B	61	VAL	2.9
1	A	83	LYS	2.9
1	A	102	VAL	2.8
1	B	43	LYS	2.8
1	A	161	CYS	2.8
1	B	139	ASP	2.8
1	B	131	LEU	2.8
2	C	304	LYS	2.8
1	A	12	TYR	2.7
1	B	136	PHE	2.7
1	B	155	LYS	2.7
2	D	345	ARG	2.6
1	B	185	THR	2.6
1	B	9	PHE	2.6
2	C	605	ASP	2.6
1	B	22	SER	2.6
1	B	83	LYS	2.5
1	B	66	ASN	2.5
1	B	147	GLU	2.5
1	A	71	GLU	2.4
1	B	202	GLU	2.4
1	B	193	CYS	2.4
1	B	118	PRO	2.4
1	B	20	VAL	2.3
1	A	97	LYS	2.3
2	C	494	CYS	2.3
1	B	204	GLU	2.3
2	C	310	ASN	2.3
2	C	290	PHE	2.2
2	D	308	HIS	2.2
1	A	103	VAL	2.2
1	B	165	GLY	2.2
2	C	493	LEU	2.2
1	B	125	VAL	2.1
1	B	132	LYS	2.1
1	B	103	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	114	LYS	2.1
1	A	61	VAL	2.1
1	B	178	LEU	2.1
1	A	15	CYS	2.1
1	A	58	PHE	2.1
1	B	179	ILE	2.1
2	D	603	SER	2.1
1	B	67	GLU	2.1
1	B	140	VAL	2.1
1	B	161	CYS	2.0
1	B	229	THR	2.0
2	C	286	GLU	2.0
2	D	310	ASN	2.0
2	C	476	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	WRA	A	609	24/24	0.67	0.28	1.33	29,35,44,45	0
3	WRA	B	709	24/24	0.61	0.32	0.96	56,65,67,68	0
5	UMP	C	611	20/20	0.97	0.15	0.32	38,48,55,55	0
5	UMP	D	711	20/20	0.97	0.15	0.12	39,54,62,62	0
4	NDP	B	710	48/48	0.83	0.21	-0.34	74,90,95,95	0
4	NDP	A	610	48/48	0.96	0.10	-0.73	35,42,49,52	0

6.5 Other polymers (i)

There are no such residues in this entry.