



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:15 PM GMT

PDB ID : 4KY4
Title : Crystal structure of non-classical TS inhibitor 2 in complex with Toxoplasma gondii TS-DHFR
Authors : Sharma, H.; Anderson, K.S.
Deposited on : 2013-05-28
Resolution : 2.79 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

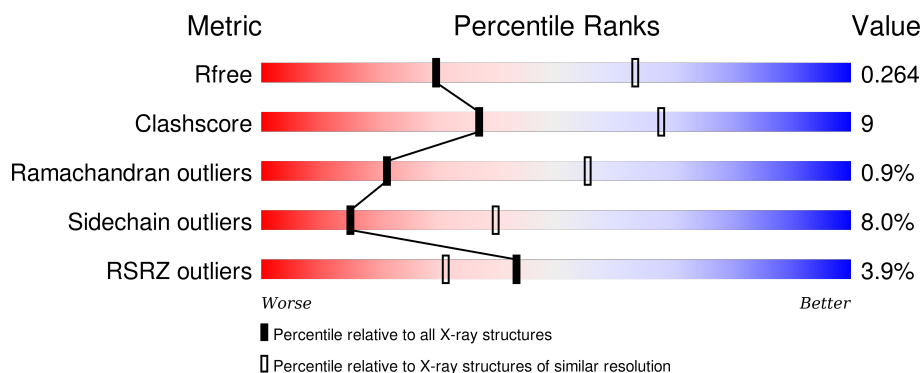
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.79 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	610	
1	B	610	
1	C	610	
1	D	610	
1	E	610	

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Mol	Chain	Length	Quality of chain
1	F	610	
1	G	610	
1	H	610	

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	UMP	D	701	-	-	-	X
2	UMP	F	701	-	-	X	-
3	04J	B	702	-	-	-	X
3	04J	D	702	-	-	-	X
3	04J	H	702	-	-	X	-
5	1UE	A	704	-	-	X	-
5	1UE	B	704	-	-	X	X
5	1UE	C	704	-	-	X	-
5	1UE	D	704	-	-	X	-
5	1UE	E	704	-	-	-	X
5	1UE	F	704	-	-	X	X
5	1UE	G	704	-	-	X	X
5	1UE	H	704	-	-	-	X

2 Entry composition

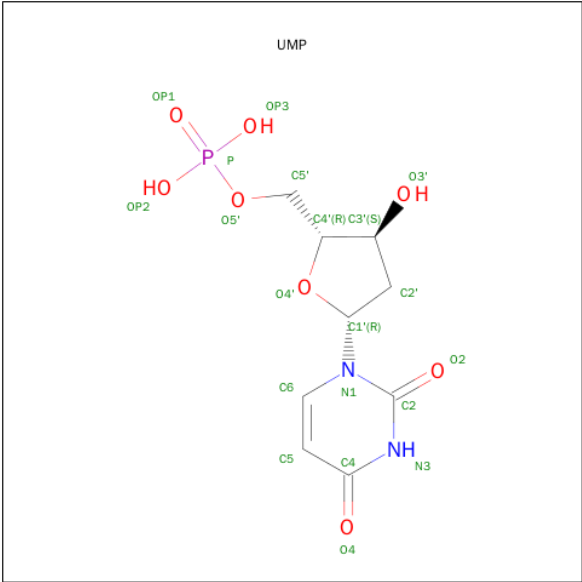
There are 5 unique types of molecules in this entry. The entry contains 32492 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

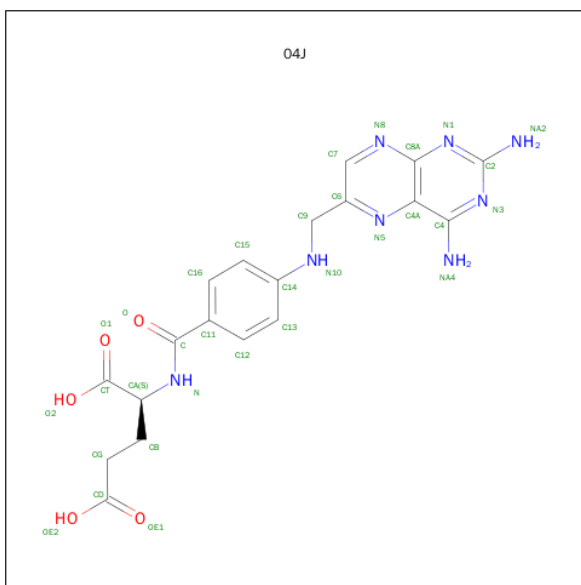
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	489	Total	C	N	O	S	0	1	0
			3931	2522	680	704	25			
1	B	491	Total	C	N	O	S	0	1	0
			3948	2531	682	710	25			
1	C	489	Total	C	N	O	S	0	1	0
			3931	2522	680	704	25			
1	D	491	Total	C	N	O	S	0	1	0
			3948	2531	682	710	25			
1	E	489	Total	C	N	O	S	0	1	0
			3931	2522	680	704	25			
1	F	491	Total	C	N	O	S	0	1	0
			3948	2531	682	710	25			
1	G	489	Total	C	N	O	S	0	1	0
			3931	2522	680	704	25			
1	H	491	Total	C	N	O	S	0	1	0
			3948	2531	682	710	25			

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



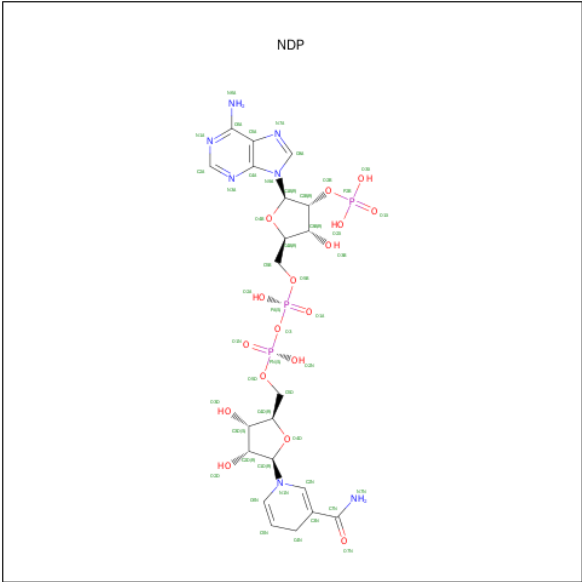
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	B	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	C	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	D	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	E	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	F	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	G	1	Total	C	N	O	P	0	0
			20	9	2	8	1		
2	H	1	Total	C	N	O	P	0	0
			20	9	2	8	1		

- Molecule 3 is AMINOPTERIN (three-letter code: 04J) (formula: C₁₉H₂₀N₈O₅).



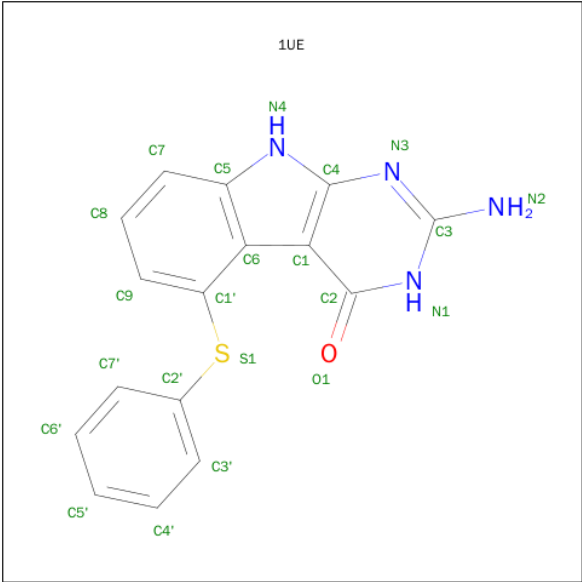
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			32	19	8	5		
3	B	1	Total	C	N	O	0	0
			32	19	8	5		
3	C	1	Total	C	N	O	0	0
			32	19	8	5		
3	D	1	Total	C	N	O	0	0
			32	19	8	5		
3	E	1	Total	C	N	O	0	0
			32	19	8	5		
3	F	1	Total	C	N	O	0	0
			32	19	8	5		
3	G	1	Total	C	N	O	0	0
			32	19	8	5		
3	H	1	Total	C	N	O	0	0
			32	19	8	5		

- Molecule 4 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).



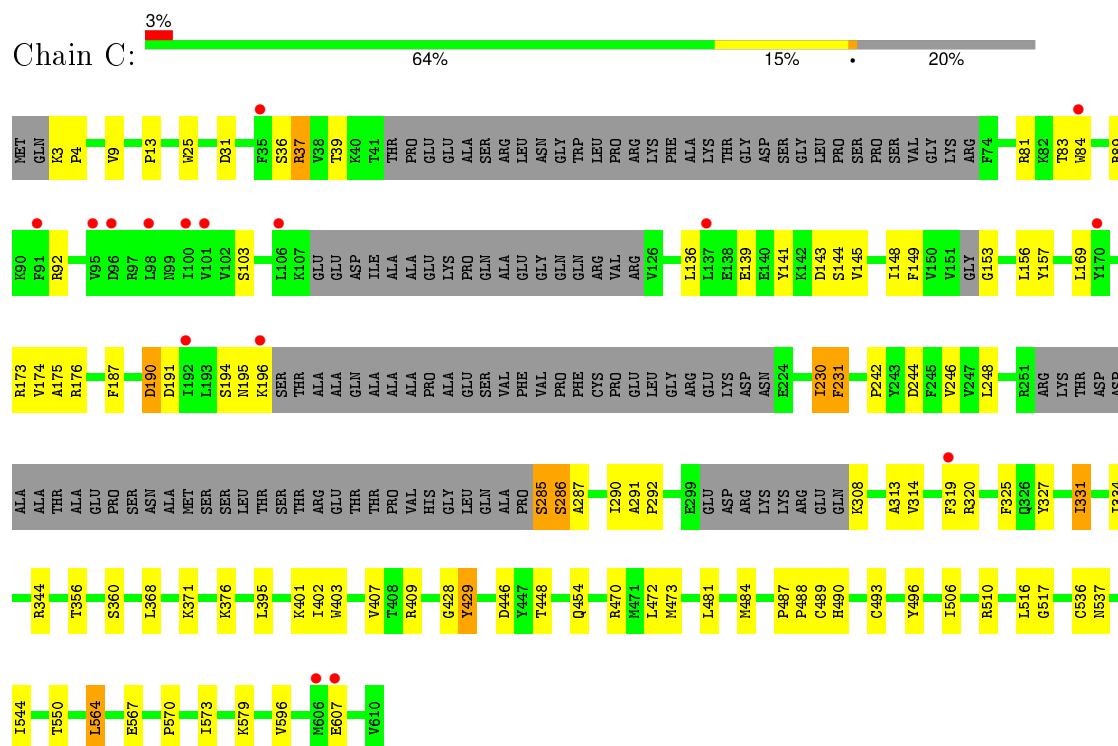
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	E	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	F	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	G	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
4	H	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 5 is 2-AMINO-5-(PHENYLSULFANYL)-3,9-DIHYDRO-4H-PYRIMIDO[4,5-B]IN DOL-4-ONE (three-letter code: 1UE) (formula: C₁₆H₁₂N₄OS).

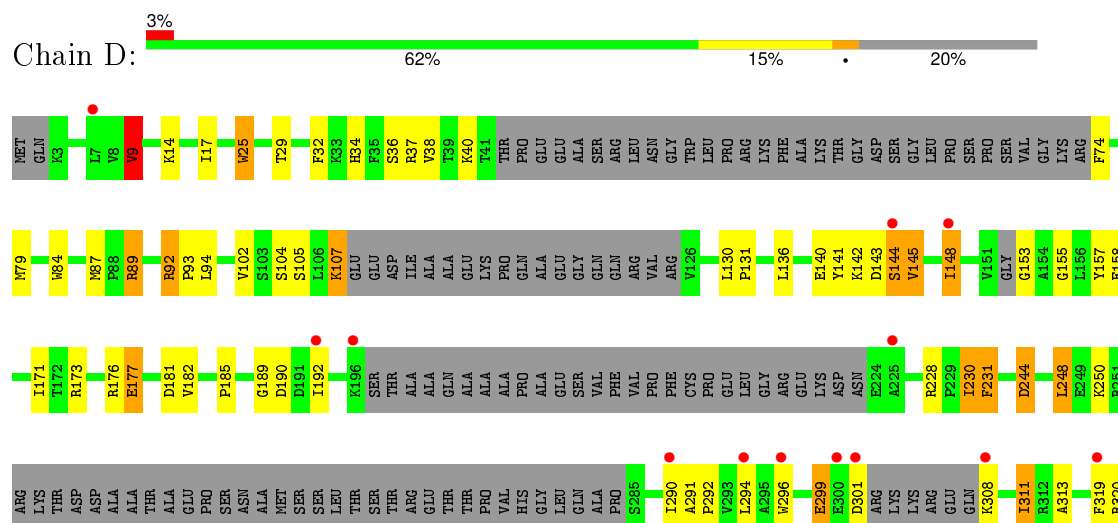


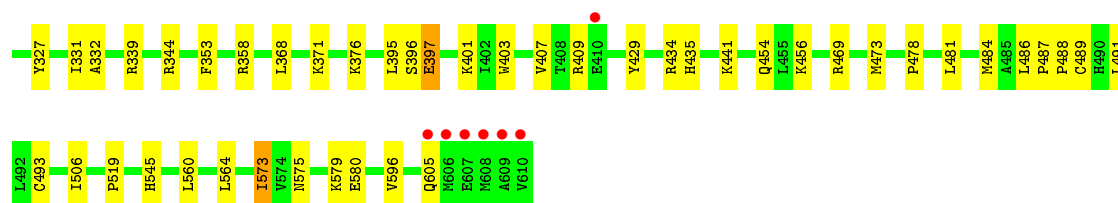
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			22	16	4	1	1		
5	B	1	Total	C	N	O	S	0	0
			22	16	4	1	1		
5	C	1	Total	C	N	O	S	0	0
			22	16	4	1	1		
5	D	1	Total	C	N	O	S	0	0
			22	16	4	1	1		
5	E	1	Total	C	N	O	S	0	0
			22	16	4	1	1		
5	F	1	Total	C	N	O	S	0	0
			22	16	4	1	1		
5	G	1	Total	C	N	O	S	0	0
			22	16	4	1	1		
5	H	1	Total	C	N	O	S	0	0
			22	16	4	1	1		

- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

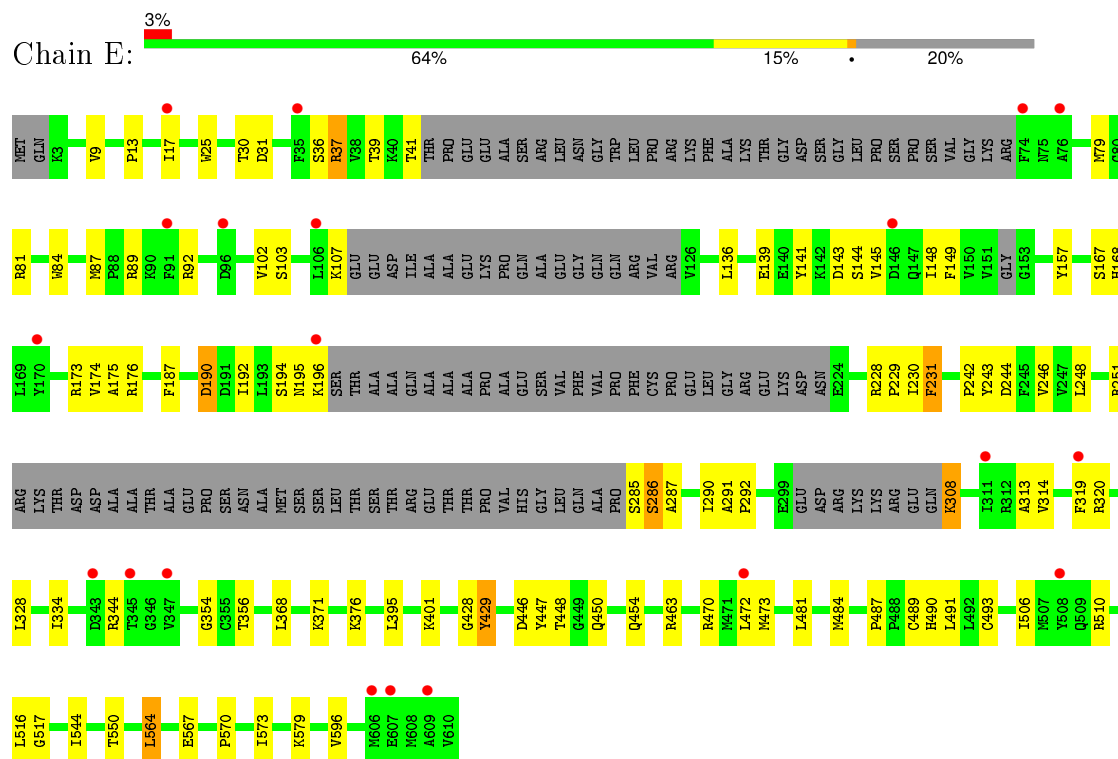


- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

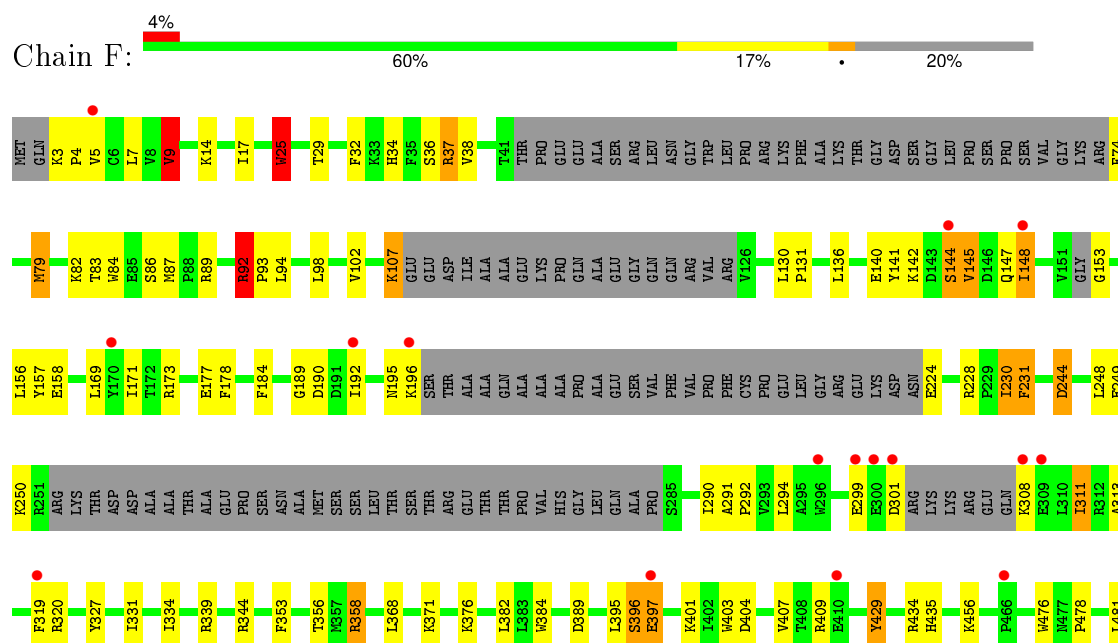




- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

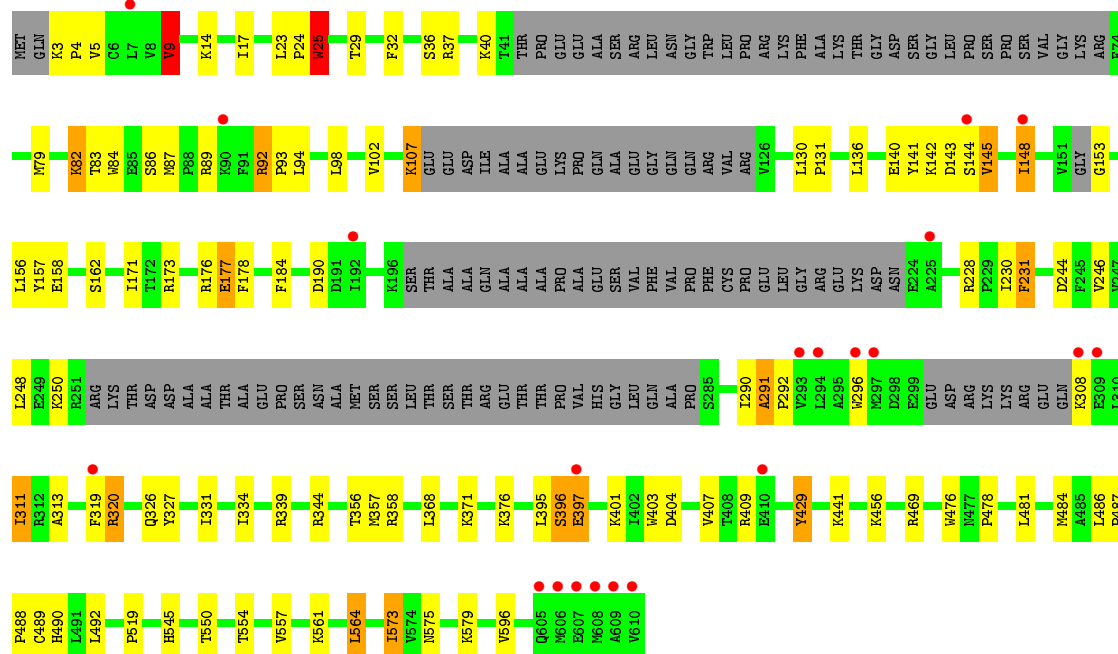


- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

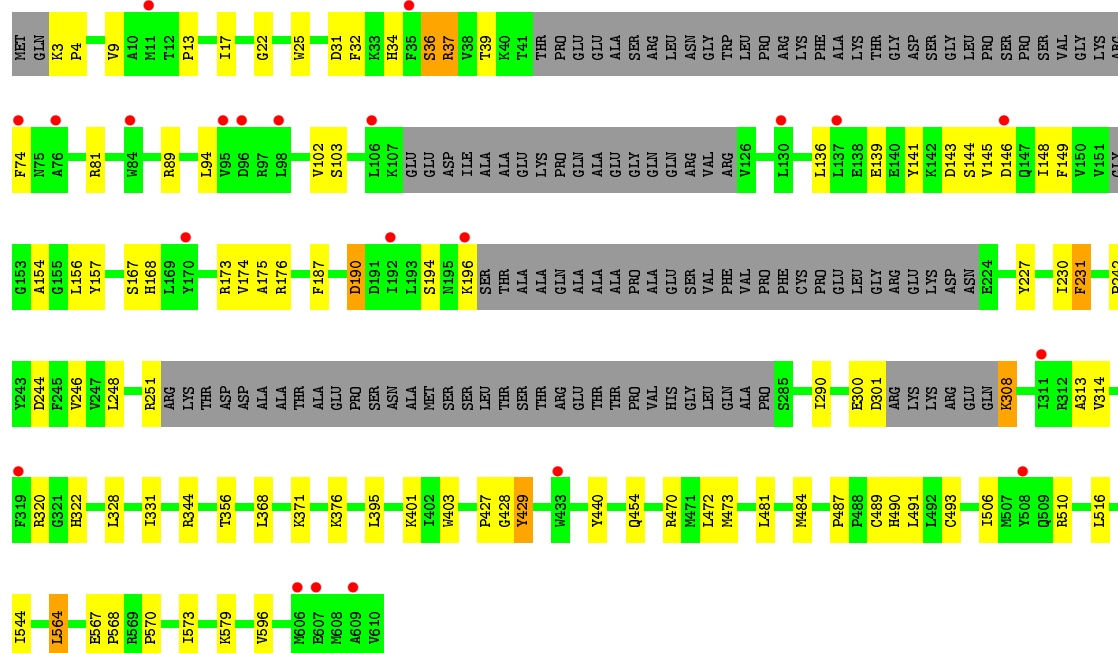




• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	53.54Å 145.12Å 176.16Å 89.97° 89.95° 89.89°	Depositor
Resolution (Å)	48.28 – 2.79 48.37 – 2.79	Depositor EDS
% Data completeness (in resolution range)	97.8 (48.28-2.79) 97.5 (48.37-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.220 , 0.268 0.221 , 0.264	Depositor DCC
R_{free} test set	6476 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	73.2	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 37.2	EDS
Estimated twinning fraction	0.427 for h,-k,-l 0.427 for -h,k,-l 0.439 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 128608 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	32492	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.34% 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: NDP, 1UE, UMP, 04J

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	0.59	0/4026	0.76	3/5450 (0.1%)
1	B	0.67	2/4043 (0.0%)	0.85	4/5473 (0.1%)
1	C	0.58	0/4026	0.76	1/5450 (0.0%)
1	D	0.66	2/4043 (0.0%)	0.84	3/5473 (0.1%)
1	E	0.58	0/4026	0.75	2/5450 (0.0%)
1	F	0.65	2/4043 (0.0%)	0.84	4/5473 (0.1%)
1	G	0.65	3/4026 (0.1%)	0.82	2/5450 (0.0%)
1	H	0.58	0/4043	0.75	1/5473 (0.0%)
All	All	0.62	9/32276 (0.0%)	0.80	20/43692 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	153	GLY	N-CA	6.70	1.56	1.46
1	D	153	GLY	N-CA	6.26	1.55	1.46
1	G	25	TRP	CG-CD1	5.66	1.44	1.36
1	B	25	TRP	CG-CD1	5.46	1.44	1.36
1	G	153	GLY	N-CA	5.45	1.54	1.46
1	F	153	GLY	N-CA	5.38	1.54	1.46
1	G	25	TRP	CD2-CE2	5.30	1.47	1.41
1	F	25	TRP	CG-CD1	5.03	1.43	1.36
1	D	25	TRP	CG-CD1	5.01	1.43	1.36

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	9	VAL	CB-CA-C	-7.17	97.77	111.40
1	D	9	VAL	CB-CA-C	-6.95	98.20	111.40
1	F	358	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	F	9	VAL	CB-CA-C	-6.58	98.89	111.40
1	H	470	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	C	470	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	B	358	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	E	470	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	B	9	VAL	CB-CA-C	-6.08	99.84	111.40
1	B	244	ASP	CB-CA-C	-5.99	98.43	110.40
1	B	92	ARG	C-N-CD	5.59	140.14	128.40
1	F	244	ASP	CB-CA-C	-5.56	99.28	110.40
1	G	358	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	387	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	D	358	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	470	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	F	37	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	A	463	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	D	244	ASP	CB-CA-C	-5.04	100.31	110.40
1	E	463	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	155	GLY	Peptide

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	3931	0	3900	78	0
1	B	3948	0	3910	79	0
1	C	3931	0	3900	78	0
1	D	3948	0	3910	75	0
1	E	3931	0	3900	70	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3948	0	3910	80	0
1	G	3931	0	3900	71	0
1	H	3948	0	3910	70	0
2	A	20	0	11	3	0
2	B	20	0	11	2	0
2	C	20	0	11	5	0
2	D	20	0	11	2	0
2	E	20	0	11	2	0
2	F	20	0	11	7	0
2	G	20	0	11	2	0
2	H	20	0	11	5	0
3	A	32	0	18	5	0
3	B	32	0	18	1	0
3	C	32	0	18	2	0
3	D	32	0	18	3	0
3	E	32	0	18	2	0
3	F	32	0	18	2	0
3	G	32	0	18	2	0
3	H	32	0	18	14	0
4	A	48	0	26	4	0
4	B	48	0	26	2	0
4	C	48	0	26	2	0
4	D	48	0	26	4	0
4	E	48	0	26	3	0
4	F	48	0	26	4	0
4	G	48	0	26	3	0
4	H	48	0	26	15	0
5	A	22	0	12	7	0
5	B	22	0	12	9	0
5	C	22	0	12	7	0
5	D	22	0	12	7	0
5	E	22	0	12	4	0
5	F	22	0	12	7	0
5	G	22	0	12	7	0
5	H	22	0	12	4	0
All	All	32492	0	31776	604	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 9.

All (604) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:LEU:HG	5:A:704:1UE:C6'	1.62	1.28
1:C:516:LEU:HG	5:C:704:1UE:C6'	1.70	1.21
4:D:703:NDP:H8A	4:D:703:NDP:H52A	1.25	1.14
1:C:516:LEU:HG	5:C:704:1UE:H11	1.18	1.13
1:A:516:LEU:HG	5:A:704:1UE:H11	1.18	1.11
1:H:510:ARG:NH2	2:H:701:UMP:OP1	1.83	1.11
1:H:102:VAL:O	4:H:703:NDP:H1B	1.55	1.05
1:F:489:CYS:SG	2:F:701:UMP:C6	2.54	1.00
4:F:703:NDP:H52A	4:F:703:NDP:H8A	1.44	0.99
1:A:510:ARG:NH2	2:A:701:UMP:OP1	1.97	0.97
1:B:313:ALA:O	1:B:320:ARG:NH1	1.97	0.96
1:D:313:ALA:O	1:D:320:ARG:NH1	1.99	0.96
4:H:703:NDP:H8A	4:H:703:NDP:H52A	1.46	0.94
1:H:489:CYS:SG	2:H:701:UMP:C6	2.63	0.92
1:A:489:CYS:SG	2:A:701:UMP:C6	2.63	0.91
1:G:403:TRP:CE2	5:G:704:1UE:H2	2.06	0.91
1:C:489:CYS:SG	2:C:701:UMP:C6	2.64	0.90
2:C:701:UMP:OP3	1:D:469:ARG:NH2	2.03	0.90
5:B:704:1UE:C6	5:B:704:1UE:H8	2.03	0.89
1:G:489:CYS:SG	2:G:701:UMP:C6	2.67	0.88
1:B:489:CYS:SG	2:B:701:UMP:C6	2.66	0.88
1:A:517:GLY:HA2	5:A:704:1UE:H12	1.56	0.85
1:H:32:PHE:CE1	3:H:702:04J:C16	2.60	0.85
1:F:17:ILE:O	4:F:703:NDP:H2N	1.77	0.84
1:C:517:GLY:HA2	5:C:704:1UE:H12	1.59	0.84
1:G:313:ALA:O	1:G:320:ARG:NH1	2.10	0.83
1:D:489:CYS:SG	2:D:701:UMP:C6	2.71	0.83
1:C:287:ALA:HB1	1:C:290:ILE:HD12	1.60	0.83
2:G:701:UMP:OP1	2:G:701:UMP:H3'	1.79	0.82
2:D:701:UMP:OP1	2:D:701:UMP:H3'	1.80	0.82
1:F:313:ALA:O	1:F:320:ARG:NH1	2.14	0.81
5:B:704:1UE:H8	5:B:704:1UE:C1	2.11	0.80
5:F:704:1UE:C6	5:F:704:1UE:H8	2.10	0.80
1:C:510:ARG:NH2	2:C:701:UMP:OP1	2.10	0.80
1:A:516:LEU:CG	5:A:704:1UE:H11	2.06	0.79
5:F:704:1UE:C1	5:F:704:1UE:H8	2.13	0.79
5:D:704:1UE:H8	5:D:704:1UE:C6	2.11	0.78
4:H:703:NDP:C8A	4:H:703:NDP:H52A	2.14	0.78
1:C:516:LEU:CG	5:C:704:1UE:H11	2.09	0.77
1:G:17:ILE:O	4:G:703:NDP:H2N	1.84	0.77
1:E:510:ARG:NH2	2:E:701:UMP:OP1	2.13	0.76
1:D:92:ARG:O	1:D:93:PRO:C	2.21	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:32:PHE:CE1	3:H:702:04J:C15	2.69	0.75
1:D:403:TRP:CE2	5:D:704:1UE:H2	2.21	0.75
1:E:313:ALA:O	1:E:320:ARG:NH1	2.19	0.75
5:D:704:1UE:H8	5:D:704:1UE:C1	2.17	0.75
1:A:31:ASP:OD2	3:A:702:04J:N3	2.20	0.75
4:D:703:NDP:C5B	4:D:703:NDP:H8A	2.12	0.74
5:G:704:1UE:C6	5:G:704:1UE:H8	2.17	0.74
1:D:36:SER:HB2	3:D:702:04J:HB	1.70	0.73
5:G:704:1UE:H8	5:G:704:1UE:C1	2.18	0.73
1:G:36:SER:HB2	3:G:702:04J:HB	1.69	0.73
1:E:489:CYS:SG	2:E:701:UMP:C6	2.83	0.72
1:G:397[A]:GLU:O	1:G:397[A]:GLU:HG2	1.90	0.72
1:F:511:SER:HB3	2:F:701:UMP:H5"	1.71	0.72
1:G:82:LYS:HD3	4:G:703:NDP:H51A	1.72	0.71
1:F:403:TRP:CE2	5:F:704:1UE:H2	2.26	0.71
1:C:313:ALA:O	1:C:320:ARG:NH1	2.23	0.71
1:E:313:ALA:HB2	1:E:564:LEU:HD13	1.73	0.70
1:A:32:PHE:CE1	3:A:702:04J:C16	2.75	0.70
1:H:313:ALA:O	1:H:320:ARG:NH1	2.25	0.70
1:H:32:PHE:HE1	3:H:702:04J:C15	2.03	0.69
3:E:702:04J:C7	4:E:703:NDP:H42N	2.22	0.69
1:A:334:ILE:HD11	1:A:550:THR:HG22	1.75	0.68
1:E:173:ARG:HD2	1:E:246:VAL:HG13	1.74	0.68
1:B:173:ARG:NH1	1:B:244:ASP:OD2	2.27	0.68
1:C:402:ILE:HG22	5:C:704:1UE:H9	1.74	0.67
1:H:484:MET:HE3	1:H:487:PRO:HA	1.77	0.67
1:A:230:ILE:HG23	1:B:290:ILE:HD11	1.76	0.67
1:E:516:LEU:HG	5:E:704:1UE:C6'	2.24	0.67
1:A:313:ALA:O	1:A:320:ARG:NH1	2.28	0.66
1:C:9:VAL:HG12	1:C:157:TYR:CZ	2.29	0.66
1:C:484:MET:CE	1:C:487:PRO:HA	2.25	0.66
1:F:195:ASN:O	1:F:196:LYS:C	2.32	0.66
1:D:92:ARG:O	1:D:94:LEU:N	2.29	0.66
1:A:319:PHE:CD1	1:B:290:ILE:HD13	2.30	0.66
1:D:397[A]:GLU:HG2	1:D:397[A]:GLU:O	1.96	0.66
1:G:469:ARG:NE	2:H:701:UMP:OP3	2.27	0.66
1:D:9:VAL:CG1	1:D:157:TYR:CZ	2.79	0.66
1:E:334:ILE:HD11	1:E:550:THR:HG22	1.76	0.65
1:C:319:PHE:CD1	1:D:290:ILE:HD13	2.32	0.65
1:F:511:SER:CB	2:F:701:UMP:H5"	2.26	0.65
1:A:145:VAL:HG13	1:A:145:VAL:O	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:17:ILE:O	4:D:703:NDP:H2N	1.96	0.65
1:A:175:ALA:HB3	1:A:242:PRO:HG2	1.77	0.65
1:C:173:ARG:HD2	1:C:246:VAL:HG13	1.79	0.65
3:C:702:04J:C7	4:C:703:NDP:H42N	2.27	0.65
1:H:145:VAL:HG13	1:H:145:VAL:O	1.97	0.64
1:C:313:ALA:HB2	1:C:564:LEU:HD13	1.80	0.64
1:G:319:PHE:CD1	1:H:290:ILE:HD13	2.33	0.64
1:F:92:ARG:O	1:F:93:PRO:C	2.33	0.64
1:G:92:ARG:O	1:G:93:PRO:C	2.29	0.64
1:E:230:ILE:HG23	1:F:290:ILE:HD11	1.78	0.64
1:C:484:MET:HE3	1:C:487:PRO:HA	1.79	0.64
1:F:173:ARG:NH1	1:F:244:ASP:OD2	2.31	0.64
1:B:403:TRP:CE2	5:B:704:1UE:H2	2.33	0.63
1:G:173:ARG:NH1	1:G:244:ASP:OD2	2.31	0.63
1:D:173:ARG:NH1	1:D:244:ASP:OD2	2.31	0.63
1:F:397[A]:GLU:O	1:F:397[A]:GLU:HG2	1.98	0.63
2:F:701:UMP:H4'	2:F:701:UMP:OP3	1.98	0.63
1:B:107:LYS:O	1:B:107:LYS:NZ	2.27	0.63
1:E:517:GLY:HA2	5:E:704:1UE:H12	1.80	0.63
1:H:516:LEU:HG	5:H:704:1UE:C6'	2.28	0.63
1:G:291:ALA:N	1:G:292:PRO:HD2	2.14	0.63
1:C:244:ASP:HB2	1:C:570:PRO:HG3	1.81	0.62
1:C:230:ILE:HG23	1:D:290:ILE:HD11	1.81	0.62
1:A:285:SER:O	1:A:287:ALA:N	2.32	0.62
1:D:311:ILE:CD1	1:D:564:LEU:HD12	2.30	0.62
1:E:175:ALA:HB3	1:E:242:PRO:HG2	1.82	0.61
1:B:9:VAL:CG1	1:B:157:TYR:CZ	2.83	0.61
1:C:334:ILE:HD11	1:C:550:THR:HG22	1.83	0.61
4:F:703:NDP:H8A	4:F:703:NDP:C5B	2.26	0.61
1:F:489:CYS:SG	2:F:701:UMP:C5	2.94	0.61
1:H:17:ILE:O	4:H:703:NDP:H2N	2.01	0.60
1:G:368:LEU:HD23	1:G:519:PRO:HB3	1.83	0.60
1:F:92:ARG:O	1:F:94:LEU:N	2.35	0.60
1:A:484:MET:HE3	1:A:487:PRO:HA	1.83	0.60
1:D:32:PHE:HE2	3:D:702:04J:C16	2.15	0.60
1:A:313:ALA:HB2	1:A:564:LEU:HD13	1.82	0.60
1:A:290:ILE:HG21	1:B:319:PHE:CE1	2.37	0.60
1:E:484:MET:CE	1:E:487:PRO:HA	2.32	0.60
1:C:287:ALA:CB	1:C:290:ILE:HD12	2.32	0.60
1:A:32:PHE:HE1	3:A:702:04J:C16	2.13	0.60
1:D:148:ILE:O	1:D:148:ILE:HG13	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:244:ASP:HB2	1:H:570:PRO:HG3	1.84	0.60
1:C:83:THR:HG1	1:C:153:GLY:N	1.99	0.60
1:H:484:MET:CE	1:H:487:PRO:HA	2.32	0.60
1:A:287:ALA:HB1	1:A:290:ILE:HD12	1.84	0.60
3:A:702:04J:HGA	3:A:702:04J:O1	2.00	0.60
1:H:173:ARG:HD2	1:H:246:VAL:HG13	1.84	0.60
1:C:37:ARG:HG2	1:D:296:TRP:HB3	1.84	0.59
1:A:9:VAL:HG12	1:A:157:TYR:CZ	2.37	0.59
1:D:84:TRP:CE2	1:D:92:ARG:HD2	2.37	0.59
1:G:9:VAL:CG1	1:G:157:TYR:CZ	2.85	0.59
1:G:403:TRP:CZ2	5:G:704:1UE:H2	2.37	0.59
1:A:517:GLY:CA	5:A:704:1UE:H12	2.30	0.59
1:E:484:MET:HE3	1:E:487:PRO:HA	1.84	0.59
1:B:17:ILE:O	4:B:703:NDP:H2N	2.02	0.59
1:E:187:PHE:O	1:E:190:ASP:HB2	2.01	0.59
1:B:84:TRP:CE2	1:B:92:ARG:HD2	2.37	0.59
1:B:9:VAL:HG13	1:B:157:TYR:CZ	2.37	0.59
1:A:9:VAL:CG1	1:A:157:TYR:CZ	2.86	0.58
1:A:173:ARG:HD2	1:A:246:VAL:HG13	1.85	0.58
1:E:287:ALA:HB1	1:E:290:ILE:HD12	1.84	0.58
1:H:429:TYR:CE1	1:H:490:HIS:CE1	2.91	0.58
1:F:9:VAL:CG1	1:F:157:TYR:CZ	2.86	0.58
1:G:469:ARG:NH2	2:H:701:UMP:OP3	2.37	0.58
1:E:9:VAL:CG1	1:E:157:TYR:CZ	2.87	0.58
1:F:313:ALA:HB2	1:F:564:LEU:HD13	1.84	0.58
1:G:92:ARG:O	1:G:94:LEU:N	2.37	0.58
1:A:469:ARG:NE	2:B:701:UMP:OP3	2.35	0.58
1:F:5:VAL:HG13	1:F:148:ILE:HG13	1.85	0.58
1:G:79:MET:HE3	1:G:83:THR:HG22	1.84	0.58
1:C:290:ILE:HG21	1:D:319:PHE:CE1	2.39	0.57
1:E:429:TYR:CE1	1:E:490:HIS:CE1	2.92	0.57
1:G:9:VAL:HG13	1:G:157:TYR:CZ	2.39	0.57
1:H:9:VAL:HG12	1:H:157:TYR:CZ	2.39	0.57
1:H:81:ARG:NE	4:H:703:NDP:O3X	2.34	0.57
1:D:176:ARG:HD2	1:D:596:VAL:CG1	2.34	0.57
1:C:290:ILE:HG21	1:D:319:PHE:CD1	2.40	0.57
1:A:484:MET:CE	1:A:487:PRO:HA	2.35	0.57
1:E:244:ASP:HB2	1:E:570:PRO:HG3	1.86	0.57
1:C:175:ALA:HB3	1:C:242:PRO:HG2	1.86	0.57
1:G:84:TRP:CE2	1:G:92:ARG:HD2	2.40	0.57
1:G:176:ARG:HD2	1:G:596:VAL:CG1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:VAL:HG13	1:E:145:VAL:O	2.04	0.56
1:B:608:MET:HE2	5:B:704:1UE:H9	1.87	0.56
1:C:9:VAL:CG1	1:C:157:TYR:CZ	2.88	0.56
1:D:231:PHE:C	1:D:231:PHE:CD1	2.78	0.56
1:C:145:VAL:O	1:C:145:VAL:HG13	2.04	0.56
1:H:9:VAL:CG1	1:H:157:TYR:CZ	2.89	0.56
1:G:107:LYS:NZ	1:G:107:LYS:O	2.36	0.56
1:E:285:SER:O	1:E:287:ALA:N	2.38	0.56
1:G:476:TRP:CZ2	1:G:481:LEU:HD11	2.39	0.56
1:G:319:PHE:CE1	1:H:290:ILE:HD13	2.41	0.56
1:B:331:ILE:HD13	1:B:560:LEU:HD22	1.88	0.56
1:F:403:TRP:O	1:F:407:VAL:HG22	2.05	0.56
1:A:328:LEU:HD22	1:A:564:LEU:HD22	1.88	0.56
1:E:491:LEU:HD11	1:F:492:LEU:HD11	1.88	0.56
1:G:573:ILE:HD11	1:G:575:ASN:OD1	2.06	0.55
1:C:517:GLY:CA	5:C:704:1UE:H12	2.32	0.55
1:C:187:PHE:O	1:C:190:ASP:HB2	2.07	0.55
1:E:290:ILE:HD11	1:F:230:ILE:HG23	1.89	0.55
1:B:484:MET:HE3	1:B:487:PRO:HA	1.88	0.55
1:H:39:THR:HA	1:H:149:PHE:CE2	2.42	0.55
1:A:285:SER:O	1:A:286:SER:C	2.45	0.55
1:D:74:PHE:O	1:D:145:VAL:HA	2.06	0.55
1:G:327:TYR:CE2	1:G:331:ILE:HD11	2.42	0.55
3:B:702:04J:C7	4:B:703:NDP:H42N	2.37	0.55
1:C:319:PHE:CE1	1:D:290:ILE:HD13	2.42	0.55
1:C:37:ARG:NH2	1:D:299:GLU:OE1	2.39	0.55
1:B:484:MET:CE	1:B:487:PRO:HA	2.37	0.54
1:H:94:LEU:CD2	3:H:702:04J:O1	2.55	0.54
1:C:285:SER:O	1:C:287:ALA:N	2.40	0.54
1:A:81:ARG:HD3	1:A:103:SER:HG	1.70	0.54
1:C:231:PHE:CD1	1:C:231:PHE:C	2.80	0.54
1:F:32:PHE:HE2	3:F:702:04J:C16	2.19	0.54
1:H:81:ARG:HB3	4:H:703:NDP:H4B	1.89	0.54
1:A:481:LEU:HD23	1:A:484:MET:HE1	1.90	0.54
1:D:368:LEU:HD23	1:D:519:PRO:HB3	1.88	0.54
1:G:484:MET:HE1	1:G:488:PRO:CD	2.38	0.54
1:B:608:MET:CE	5:B:704:1UE:H9	2.38	0.54
1:D:189:GLY:O	1:D:192:ILE:HG13	2.07	0.54
1:G:140:GLU:O	1:G:141:TYR:HB2	2.08	0.54
1:B:140:GLU:O	1:B:141:TYR:HB2	2.07	0.54
1:A:319:PHE:CE1	1:B:290:ILE:HD13	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:TYR:CE1	1:A:490:HIS:CE1	2.96	0.53
1:D:484:MET:CE	1:D:487:PRO:HA	2.38	0.53
1:E:230:ILE:CG2	1:F:290:ILE:HD11	2.37	0.53
1:A:290:ILE:HG21	1:B:319:PHE:CD1	2.42	0.53
1:E:290:ILE:HD11	1:F:230:ILE:CG2	2.38	0.53
1:D:573:ILE:HD11	1:D:575:ASN:OD1	2.07	0.53
1:A:244:ASP:HB2	1:A:570:PRO:HG3	1.90	0.53
1:B:476:TRP:CZ2	1:B:481:LEU:HD11	2.44	0.53
1:B:397[A]:GLU:HG2	1:B:397[A]:GLU:O	2.08	0.53
1:F:334:ILE:HD11	1:F:550:THR:HG22	1.90	0.53
1:C:285:SER:O	1:C:286:SER:C	2.46	0.53
1:E:319:PHE:CD1	1:F:290:ILE:HD13	2.44	0.53
1:H:231:PHE:CD1	1:H:231:PHE:C	2.80	0.53
1:G:484:MET:CE	1:G:488:PRO:HD3	2.39	0.53
1:F:140:GLU:O	1:F:141:TYR:HB2	2.08	0.53
1:C:429:TYR:CE1	1:C:490:HIS:CE1	2.97	0.53
1:B:478:PRO:HA	1:B:481:LEU:HG	1.90	0.53
1:F:244:ASP:OD2	1:F:570:PRO:HD3	2.08	0.52
2:C:701:UMP:OP3	1:D:469:ARG:CZ	2.58	0.52
1:F:573:ILE:HD11	1:F:575:ASN:OD1	2.09	0.52
1:H:313:ALA:HB2	1:H:564:LEU:HD13	1.90	0.52
1:D:9:VAL:HG13	1:D:157:TYR:CZ	2.44	0.52
1:E:102:VAL:O	4:E:703:NDP:H1B	2.08	0.52
1:D:141:TYR:O	1:D:145:VAL:HG12	2.09	0.52
1:D:9:VAL:HG12	1:D:157:TYR:CZ	2.45	0.52
1:H:32:PHE:HE1	3:H:702:04J:C16	2.14	0.52
1:F:84:TRP:CE2	1:F:92:ARG:HD2	2.45	0.52
1:E:447:TYR:HA	1:E:450:GLN:NE2	2.24	0.51
1:F:368:LEU:HD23	1:F:519:PRO:HB3	1.92	0.51
1:E:328:LEU:HD22	1:E:564:LEU:HD22	1.91	0.51
1:G:230:ILE:HG23	1:H:290:ILE:HD11	1.92	0.51
1:A:194:SER:OG	1:A:196:LYS:CD	2.58	0.51
1:A:290:ILE:HD11	1:B:230:ILE:CG2	2.41	0.51
1:E:454:GLN:OE1	1:E:473:MET:HA	2.11	0.51
1:H:32:PHE:CZ	3:H:702:04J:C15	2.93	0.51
1:E:39:THR:HA	1:E:149:PHE:CE2	2.45	0.51
1:G:82:LYS:HB2	4:G:703:NDP:H51A	1.93	0.51
1:G:87:MET:HE1	1:G:94:LEU:HG	1.92	0.51
1:G:484:MET:HE1	1:G:488:PRO:HD3	1.93	0.51
1:E:354:GLY:O	1:F:358:ARG:NH2	2.43	0.51
1:E:167:SER:OG	1:E:168:HIS:CD2	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:GLU:O	1:D:141:TYR:HB2	2.11	0.51
1:H:194:SER:OG	1:H:196:LYS:HD2	2.11	0.51
1:A:30:THR:HB	1:A:243:TYR:OH	2.11	0.51
1:E:231:PHE:CD1	1:E:231:PHE:C	2.84	0.50
1:C:194:SER:OG	1:C:196:LYS:CD	2.59	0.50
1:B:368:LEU:HD23	1:B:519:PRO:HB3	1.93	0.50
1:D:87:MET:HE1	1:D:94:LEU:HG	1.92	0.50
1:G:492:LEU:HD11	1:H:491:LEU:HD11	1.93	0.50
2:C:701:UMP:OP3	1:D:469:ARG:NE	2.43	0.50
1:F:291:ALA:N	1:F:292:PRO:HD2	2.25	0.50
1:H:141:TYR:O	1:H:145:VAL:HG12	2.12	0.50
1:A:167:SER:OG	1:A:168:HIS:CD2	2.65	0.50
1:F:484:MET:HE3	1:F:487:PRO:HA	1.94	0.50
1:F:476:TRP:CZ2	1:F:481:LEU:HD11	2.46	0.50
1:H:187:PHE:O	1:H:190:ASP:HB2	2.12	0.50
1:E:368:LEU:HD22	1:E:368:LEU:N	2.27	0.50
1:A:37:ARG:HG2	1:B:296:TRP:HB3	1.94	0.50
1:C:287:ALA:HB1	1:C:290:ILE:CD1	2.38	0.49
1:A:287:ALA:CB	1:A:290:ILE:HD12	2.42	0.49
1:A:81:ARG:HD3	1:A:103:SER:OG	2.11	0.49
1:G:173:ARG:HD2	1:G:246:VAL:HG13	1.94	0.49
1:A:481:LEU:HA	1:A:484:MET:HE2	1.93	0.49
1:B:189:GLY:O	1:B:192:ILE:HG13	2.13	0.49
1:A:145:VAL:CG1	1:A:145:VAL:O	2.59	0.49
1:A:194:SER:OG	1:A:196:LYS:HD2	2.11	0.49
4:D:703:NDP:C8A	4:D:703:NDP:H52A	2.18	0.49
1:C:368:LEU:N	1:C:368:LEU:HD22	2.28	0.49
1:H:506:ILE:HG12	1:H:544:ILE:HB	1.95	0.49
1:A:141:TYR:O	1:A:145:VAL:HG12	2.12	0.49
1:G:290:ILE:O	1:G:290:ILE:HG22	2.11	0.49
1:B:311:ILE:CD1	1:B:564:LEU:HD12	2.42	0.49
1:D:145:VAL:HG13	1:D:145:VAL:O	2.13	0.49
1:G:25:TRP:HB3	1:G:178:PHE:CE1	2.48	0.49
1:H:194:SER:OG	1:H:196:LYS:CD	2.61	0.49
1:F:9:VAL:HG12	1:F:157:TYR:CZ	2.48	0.49
1:F:327:TYR:CZ	1:F:331:ILE:HD11	2.48	0.49
1:C:506:ILE:HG12	1:C:544:ILE:HB	1.95	0.49
1:H:81:ARG:HD3	1:H:103:SER:OG	2.12	0.49
1:H:94:LEU:HD22	3:H:702:O4J:O1	2.12	0.49
1:H:154:ALA:O	4:H:703:NDP:O1A	2.30	0.49
1:B:92:ARG:O	1:B:93:PRO:C	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:493:CYS:HA	1:E:506:ILE:O	2.12	0.49
1:E:446:ASP:OD2	1:E:448:THR:HG22	2.13	0.49
1:H:32:PHE:CZ	3:H:702:04J:H15	2.48	0.48
1:F:511:SER:OG	2:F:701:UMP:H5"	2.13	0.48
1:G:311:ILE:CD1	1:G:564:LEU:HD12	2.43	0.48
1:E:31:ASP:OD2	3:E:702:04J:N3	2.46	0.48
1:B:231:PHE:C	1:B:231:PHE:CD1	2.86	0.48
1:A:536:CYS:O	1:A:537:ASN:HB2	2.13	0.48
1:E:428:GLY:O	1:E:429:TYR:C	2.51	0.48
1:E:192:ILE:CD1	1:E:248:LEU:HD21	2.43	0.48
3:H:702:04J:C7	4:H:703:NDP:H42N	2.43	0.48
1:B:311:ILE:HD11	1:B:332:ALA:HA	1.95	0.48
1:E:290:ILE:HG21	1:F:319:PHE:CE1	2.47	0.48
1:E:9:VAL:HG12	1:E:157:TYR:CZ	2.48	0.48
1:H:145:VAL:O	1:H:145:VAL:CG1	2.61	0.48
1:E:37:ARG:NH2	1:F:299:GLU:OE1	2.45	0.48
1:B:484:MET:HE1	1:B:488:PRO:HD2	1.95	0.48
1:F:382:LEU:HD23	1:F:527:LEU:HD23	1.94	0.48
1:C:454:GLN:HB2	1:C:473:MET:HG3	1.95	0.48
1:A:402:ILE:HG22	5:A:704:1UE:H9	1.95	0.48
1:B:176:ARG:HD2	1:B:596:VAL:CG1	2.43	0.48
1:D:84:TRP:CZ2	1:D:92:ARG:HD2	2.48	0.48
1:F:429:TYR:CE1	1:F:490:HIS:CE1	3.02	0.48
1:D:403:TRP:O	1:D:407:VAL:HG22	2.13	0.48
1:G:32:PHE:HE2	3:G:702:04J:C16	2.27	0.48
1:G:231:PHE:CD1	1:G:231:PHE:C	2.86	0.48
1:G:334:ILE:HD11	1:G:550:THR:HG22	1.95	0.48
1:C:481:LEU:HA	1:C:484:MET:HE2	1.96	0.47
1:G:327:TYR:O	1:G:331:ILE:HG13	2.14	0.47
1:C:194:SER:OG	1:C:196:LYS:HD2	2.13	0.47
1:G:296:TRP:HB3	1:H:37:ARG:HG2	1.96	0.47
1:A:308:LYS:HE3	1:A:308:LYS:HA	1.96	0.47
1:C:145:VAL:O	1:C:145:VAL:CG1	2.61	0.47
1:G:481:LEU:HA	1:G:484:MET:HE2	1.95	0.47
5:B:704:1UE:C3'	5:B:704:1UE:C2	2.92	0.47
1:E:173:ARG:HD2	1:E:246:VAL:CG1	2.41	0.47
1:D:484:MET:HE3	1:D:487:PRO:HA	1.96	0.47
1:C:39:THR:HA	1:C:149:PHE:CE2	2.49	0.47
1:C:446:ASP:OD2	1:C:448:THR:HG22	2.15	0.47
1:C:319:PHE:CE2	1:D:294:LEU:HD11	2.49	0.47
1:C:81:ARG:HD3	1:C:103:SER:HG	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:VAL:HG11	1:B:184:PHE:CD1	2.49	0.47
1:E:313:ALA:O	1:E:314:VAL:C	2.53	0.47
1:H:74:PHE:O	1:H:145:VAL:HA	2.14	0.47
1:E:481:LEU:HD23	1:E:484:MET:HE1	1.97	0.47
1:C:141:TYR:O	1:C:145:VAL:HG12	2.15	0.47
1:B:327:TYR:CZ	1:B:331:ILE:HD11	2.50	0.47
1:F:484:MET:CE	1:F:488:PRO:HD3	2.45	0.47
1:A:391:ASN:OD1	1:A:393:ASN:HB2	2.14	0.47
1:D:327:TYR:CE2	1:D:331:ILE:HD11	2.50	0.47
1:D:34:HIS:O	1:D:38:VAL:HG23	2.15	0.47
1:A:102:VAL:O	4:A:703:NDP:H1B	2.15	0.47
3:A:702:04J:C7	4:A:703:NDP:H42N	2.45	0.47
1:E:285:SER:O	1:E:286:SER:C	2.52	0.47
1:E:145:VAL:CG1	1:E:145:VAL:O	2.62	0.47
1:D:145:VAL:CG1	1:D:145:VAL:O	2.63	0.47
5:G:704:1UE:H8	5:G:704:1UE:C2	2.45	0.47
1:F:327:TYR:CE2	1:F:331:ILE:HD11	2.50	0.46
1:A:84:TRP:CE2	1:A:92:ARG:HD2	2.49	0.46
1:E:141:TYR:O	1:E:145:VAL:HG12	2.16	0.46
1:E:84:TRP:CE2	1:E:92:ARG:HD2	2.50	0.46
1:D:291:ALA:N	1:D:292:PRO:HD2	2.30	0.46
1:A:81:ARG:HB3	4:A:703:NDP:H4B	1.98	0.46
1:B:9:VAL:CG1	1:B:157:TYR:CE2	2.97	0.46
1:B:327:TYR:CE2	1:B:331:ILE:HD11	2.51	0.46
1:E:81:ARG:HD3	1:E:103:SER:OG	2.15	0.46
1:D:434:ARG:HB2	1:D:435:HIS:CD2	2.51	0.46
5:F:704:1UE:C2	5:F:704:1UE:C3'	2.93	0.46
5:F:704:1UE:C2	5:F:704:1UE:H8	2.46	0.46
1:B:320:ARG:HB3	1:B:325:PHE:CD2	2.50	0.46
1:B:173:ARG:HB2	1:B:244:ASP:HB2	1.98	0.46
1:A:313:ALA:O	1:A:314:VAL:C	2.52	0.46
1:H:368:LEU:N	1:H:368:LEU:HD22	2.31	0.46
1:H:81:ARG:HD3	1:H:103:SER:HG	1.80	0.46
1:A:354:GLY:O	1:B:358:ARG:NH2	2.48	0.46
1:F:79:MET:HE2	1:F:83:THR:HG22	1.98	0.46
1:G:9:VAL:HG11	1:G:184:PHE:CD2	2.50	0.46
1:F:189:GLY:O	1:F:192:ILE:HG13	2.16	0.46
1:F:231:PHE:C	1:F:231:PHE:CD1	2.89	0.46
1:A:326:GLN:HB3	1:A:357:MET:HG2	1.98	0.46
1:D:79:MET:HE1	1:D:87:MET:SD	2.56	0.46
1:G:403:TRP:O	1:G:407:VAL:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:MET:HE1	1:B:94:LEU:HG	1.97	0.46
1:B:484:MET:CE	1:B:488:PRO:HD3	2.46	0.46
1:F:551:HIS:CE1	2:F:701:UMP:H3'	2.51	0.46
2:A:701:UMP:OP3	1:B:469:ARG:NH2	2.41	0.46
1:C:290:ILE:HD13	1:D:319:PHE:CE1	2.50	0.46
1:F:87:MET:HE1	1:F:94:LEU:HG	1.97	0.46
1:G:84:TRP:CZ2	1:G:92:ARG:HD2	2.50	0.46
1:E:287:ALA:CB	1:E:290:ILE:HD12	2.46	0.46
1:G:5:VAL:HG13	1:G:148:ILE:HG13	1.98	0.46
1:H:81:ARG:HD3	4:H:703:NDP:O1X	2.15	0.45
4:H:703:NDP:O3X	4:H:703:NDP:O3B	2.32	0.45
1:A:230:ILE:CG2	1:B:290:ILE:HD11	2.46	0.45
1:B:484:MET:HE1	1:B:488:PRO:CD	2.46	0.45
1:D:484:MET:HE1	1:D:488:PRO:CD	2.46	0.45
1:E:454:GLN:HB2	1:E:473:MET:HG3	1.98	0.45
1:E:506:ILE:HG12	1:E:544:ILE:HB	1.98	0.45
1:A:231:PHE:C	1:A:231:PHE:CD1	2.88	0.45
1:B:145:VAL:CG1	1:B:145:VAL:O	2.64	0.45
1:D:181:ASP:OD1	1:D:182:VAL:HG23	2.16	0.45
1:C:156:LEU:HD12	1:C:156:LEU:HA	1.85	0.45
1:B:403:TRP:O	1:B:407:VAL:HG22	2.16	0.45
1:H:175:ALA:HB3	1:H:242:PRO:HG2	1.97	0.45
1:B:34:HIS:O	1:B:38:VAL:HG23	2.16	0.45
1:C:3:LYS:N	1:C:4:PRO:HD3	2.31	0.45
1:G:326:GLN:HB3	1:G:357:MET:HG2	1.98	0.45
1:B:79:MET:HE1	1:B:87:MET:SD	2.56	0.45
1:A:195:ASN:O	1:A:196:LYS:C	2.55	0.45
1:G:429:TYR:CE1	1:G:490:HIS:CE1	3.05	0.45
1:C:536:CYS:O	1:C:537:ASN:HB2	2.15	0.45
4:H:703:NDP:N3A	4:H:703:NDP:H2B	2.31	0.45
1:H:328:LEU:HD22	1:H:564:LEU:HD22	1.97	0.45
1:F:3:LYS:N	1:F:4:PRO:HD3	2.32	0.45
1:G:396:SER:HG	1:G:404:ASP:CG	2.20	0.45
1:F:311:ILE:CD1	1:F:564:LEU:HD12	2.47	0.45
1:A:37:ARG:NH2	1:B:299:GLU:OE1	2.49	0.45
1:F:14:LYS:HD2	1:F:177:GLU:HG2	1.99	0.45
1:F:9:VAL:HG13	1:F:157:TYR:CZ	2.51	0.44
1:G:140:GLU:O	1:G:141:TYR:CB	2.64	0.44
1:B:192:ILE:HD13	1:B:248:LEU:HD11	1.98	0.44
1:G:296:TRP:CZ2	1:H:34:HIS:HB2	2.52	0.44
1:D:327:TYR:CZ	1:D:331:ILE:HD11	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:506:ILE:HG12	1:A:544:ILE:HB	1.99	0.44
1:H:403:TRP:CE2	5:H:704:1UE:H2	2.52	0.44
1:F:478:PRO:HA	1:F:481:LEU:HG	1.98	0.44
1:A:39:THR:HA	1:A:149:PHE:CE2	2.51	0.44
1:F:7:LEU:HD12	1:F:169:LEU:HD22	1.99	0.44
5:D:704:1UE:C3'	5:D:704:1UE:C2	2.95	0.44
1:F:145:VAL:CG1	1:F:145:VAL:O	2.65	0.44
1:H:176:ARG:HD2	1:H:596:VAL:CG1	2.47	0.44
1:F:107:LYS:NZ	1:F:107:LYS:O	2.39	0.44
1:E:290:ILE:HD13	1:F:319:PHE:CE1	2.52	0.44
1:C:13:PRO:HD3	1:C:174:VAL:O	2.18	0.44
4:H:703:NDP:HO3A	4:H:703:NDP:P2B	2.40	0.44
1:H:493:CYS:HA	1:H:506:ILE:O	2.18	0.44
1:F:384:TRP:CD1	1:F:389:ASP:HB3	2.52	0.44
1:E:176:ARG:HD2	1:E:596:VAL:CG1	2.47	0.44
1:D:478:PRO:HA	1:D:481:LEU:HG	1.99	0.44
1:D:89:ARG:HA	1:D:92:ARG:HG3	2.00	0.44
1:D:484:MET:CE	1:D:488:PRO:HD3	2.47	0.44
1:E:192:ILE:HD12	1:E:248:LEU:HD21	1.99	0.44
1:B:358:ARG:HD3	1:B:542:GLU:OE1	2.18	0.44
1:E:13:PRO:HD3	1:E:174:VAL:O	2.18	0.44
1:C:290:ILE:HD11	1:D:230:ILE:CG2	2.47	0.44
1:B:169:LEU:HD12	1:B:248:LEU:HD23	1.99	0.44
1:C:368:LEU:HD22	1:C:368:LEU:H	1.81	0.44
1:F:327:TYR:O	1:F:331:ILE:HG13	2.18	0.44
1:H:454:GLN:CB	1:H:473:MET:HG3	2.48	0.44
1:G:327:TYR:CZ	1:G:331:ILE:HD11	2.51	0.44
1:F:484:MET:CE	1:F:487:PRO:HA	2.48	0.44
1:G:171:ILE:HD12	1:G:248:LEU:HD22	2.00	0.44
1:G:3:LYS:N	1:G:4:PRO:HD3	2.33	0.44
1:C:81:ARG:HD3	1:C:103:SER:OG	2.18	0.43
1:F:9:VAL:HG11	1:F:184:PHE:CD1	2.52	0.43
1:A:493:CYS:HA	1:A:506:ILE:O	2.18	0.43
1:B:130:LEU:HB3	1:B:131:PRO:HD3	2.00	0.43
1:B:313:ALA:HB2	1:B:564:LEU:HD13	2.00	0.43
1:F:173:ARG:HB2	1:F:244:ASP:HB2	2.00	0.43
1:B:140:GLU:O	1:B:141:TYR:CB	2.66	0.43
1:C:454:GLN:CB	1:C:473:MET:HG3	2.47	0.43
1:B:156:LEU:HA	1:B:156:LEU:HD12	1.72	0.43
1:D:130:LEU:HB3	1:D:131:PRO:HD3	2.00	0.43
1:B:334:ILE:HD11	1:B:550:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:130:LEU:HB3	1:G:131:PRO:HD3	2.00	0.43
1:C:291:ALA:N	1:C:292:PRO:HD2	2.32	0.43
1:C:176:ARG:HD2	1:C:596:VAL:CG1	2.48	0.43
1:C:313:ALA:O	1:C:314:VAL:C	2.57	0.43
1:B:84:TRP:O	1:B:92:ARG:HD3	2.18	0.43
1:F:368:LEU:HD22	1:F:368:LEU:H	1.82	0.43
1:C:195:ASN:O	1:C:196:LYS:O	2.36	0.43
4:F:703:NDP:C8A	4:F:703:NDP:H52A	2.32	0.43
5:H:704:1UE:H8	5:H:704:1UE:C6	2.47	0.43
1:D:491:LEU:C	1:D:491:LEU:HD12	2.39	0.43
1:B:367:LEU:HD12	1:B:367:LEU:HA	1.88	0.43
1:E:17:ILE:O	4:E:703:NDP:H2N	2.19	0.43
1:D:311:ILE:HD11	1:D:332:ALA:HA	2.00	0.43
1:D:484:MET:HE1	1:D:488:PRO:HD2	1.99	0.43
1:B:175:ALA:HB3	1:B:242:PRO:HG2	2.01	0.43
1:H:13:PRO:HD3	1:H:174:VAL:O	2.16	0.43
1:C:31:ASP:OD2	3:C:702:04J:N3	2.52	0.43
1:B:145:VAL:HG13	1:B:145:VAL:O	2.18	0.43
1:D:14:LYS:HD2	1:D:177:GLU:HG2	2.00	0.43
1:F:396:SER:OG	1:F:404:ASP:OD2	2.36	0.43
1:H:308:LYS:HA	1:H:308:LYS:HE3	2.01	0.43
1:B:321:GLY:O	1:B:322:HIS:C	2.55	0.43
1:H:22:GLY:N	4:H:703:NDP:O3D	2.52	0.43
1:H:36:SER:OG	3:H:702:04J:O2	2.36	0.43
1:A:290:ILE:HD11	1:B:230:ILE:HG21	2.00	0.43
1:H:428:GLY:O	1:H:429:TYR:C	2.56	0.43
1:G:557:VAL:HG12	1:G:561:LYS:HD2	2.00	0.43
1:D:454:GLN:OE1	1:D:473:MET:HA	2.18	0.43
1:G:484:MET:HE1	1:G:488:PRO:HD2	2.01	0.43
1:D:140:GLU:O	1:D:141:TYR:CB	2.66	0.42
1:B:74:PHE:O	1:B:145:VAL:HA	2.19	0.42
1:G:14:LYS:HD2	1:G:177:GLU:HG2	2.01	0.42
1:C:84:TRP:CE2	1:C:92:ARG:HD2	2.54	0.42
1:H:167:SER:OG	1:H:168:HIS:CD2	2.73	0.42
1:A:298:ASP:OD1	1:A:299:GLU:N	2.51	0.42
1:D:79:MET:CE	1:D:87:MET:SD	3.07	0.42
1:A:173:ARG:HD2	1:A:246:VAL:CG1	2.49	0.42
1:F:74:PHE:O	1:F:145:VAL:HA	2.19	0.42
1:H:32:PHE:HZ	3:H:702:04J:H15	1.85	0.42
1:H:322:HIS:CD2	1:H:568:PRO:HB2	2.54	0.42
1:G:469:ARG:CZ	2:H:701:UMP:OP3	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:704:1UE:C2	5:G:704:1UE:C3'	2.97	0.42
1:E:192:ILE:HD11	1:E:229:PRO:HD3	2.00	0.42
5:B:704:1UE:H8	5:B:704:1UE:C2	2.47	0.42
1:C:320:ARG:HB3	1:C:325:PHE:CD2	2.54	0.42
1:B:9:VAL:HG12	1:B:157:TYR:CE2	2.55	0.42
1:G:484:MET:CE	1:G:487:PRO:HA	2.50	0.42
1:E:291:ALA:N	1:E:292:PRO:HD2	2.34	0.42
1:E:319:PHE:CE2	1:F:294:LEU:HD11	2.55	0.42
1:D:74:PHE:N	1:D:144:SER:O	2.52	0.42
1:H:454:GLN:HB3	1:H:473:MET:HG3	2.01	0.42
1:G:23:LEU:HA	1:G:24:PRO:HD3	1.87	0.42
1:H:156:LEU:HD12	1:H:156:LEU:HA	1.82	0.42
5:D:704:1UE:H8	5:D:704:1UE:C2	2.50	0.42
5:E:704:1UE:S1	5:E:704:1UE:O1	2.78	0.42
1:B:84:TRP:CZ2	1:B:92:ARG:HD2	2.55	0.42
1:G:368:LEU:H	1:G:368:LEU:HD22	1.85	0.42
1:E:290:ILE:HG21	1:F:319:PHE:CD1	2.54	0.42
1:E:30:THR:HB	1:E:243:TYR:OH	2.19	0.42
1:C:290:ILE:HD13	1:D:319:PHE:HE1	1.84	0.42
1:F:195:ASN:O	1:F:196:LYS:O	2.38	0.42
1:A:368:LEU:N	1:A:368:LEU:HD22	2.35	0.42
1:C:81:ARG:HB3	4:C:703:NDP:H4B	2.02	0.42
1:E:319:PHE:CE1	1:F:290:ILE:HD13	2.54	0.42
1:B:3:LYS:N	1:B:4:PRO:HD3	2.35	0.42
1:H:227:TYR:HB3	1:H:248:LEU:HD23	2.01	0.42
5:B:704:1UE:C3'	5:B:704:1UE:C1	2.91	0.41
1:H:481:LEU:HD23	1:H:484:MET:HE1	2.01	0.41
5:H:704:1UE:S1	5:H:704:1UE:O1	2.78	0.41
1:G:396:SER:OG	1:G:404:ASP:OD2	2.37	0.41
1:A:12:THR:HB	1:A:13:PRO:CD	2.49	0.41
1:B:300:GLU:HA	1:B:301:ASP:HA	1.84	0.41
1:D:9:VAL:CG1	1:D:157:TYR:CE2	3.03	0.41
1:C:496:TYR:HB2	1:D:353:PHE:CE1	2.55	0.41
5:C:704:1UE:S1	5:C:704:1UE:O1	2.78	0.41
1:C:481:LEU:HD23	1:C:484:MET:HE1	2.02	0.41
1:B:92:ARG:O	1:B:94:LEU:N	2.53	0.41
1:F:358:ARG:HD3	1:F:542:GLU:OE1	2.19	0.41
1:G:145:VAL:O	1:G:145:VAL:CG1	2.67	0.41
1:C:195:ASN:O	1:C:196:LYS:C	2.58	0.41
1:C:169:LEU:HB2	1:C:248:LEU:HB2	2.02	0.41
1:B:491:LEU:HD12	1:B:491:LEU:C	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:ILE:O	4:A:703:NDP:H2N	2.20	0.41
1:C:484:MET:HE1	1:C:487:PRO:HA	2.01	0.41
1:F:5:VAL:HG13	1:F:148:ILE:CG1	2.50	0.41
1:F:331:ILE:HD13	1:F:560:LEU:HD22	2.02	0.41
1:D:331:ILE:HD13	1:D:560:LEU:HD22	2.02	0.41
1:F:34:HIS:O	1:F:38:VAL:HG23	2.20	0.41
1:D:171:ILE:HD12	1:D:248:LEU:HD22	2.02	0.41
1:H:31:ASP:OD2	3:H:702:04J:N3	2.53	0.41
1:F:36:SER:HB2	3:F:702:04J:HB	2.03	0.41
1:B:429:TYR:CE1	1:B:490:HIS:CE1	3.08	0.41
1:F:130:LEU:HB3	1:F:131:PRO:HD3	2.03	0.41
1:H:3:LYS:N	1:H:4:PRO:HD3	2.36	0.41
1:B:9:VAL:HG11	1:B:184:PHE:CE1	2.55	0.41
1:C:493:CYS:HA	1:C:506:ILE:O	2.20	0.41
1:B:291:ALA:N	1:B:292:PRO:HD2	2.36	0.41
1:A:192:ILE:HD11	1:A:229:PRO:HD3	2.02	0.41
1:A:79:MET:HE1	1:A:87:MET:SD	2.61	0.41
1:E:195:ASN:O	1:E:196:LYS:O	2.39	0.41
1:C:173:ARG:NH1	1:C:570:PRO:HD3	2.35	0.41
1:E:506:ILE:HD12	1:F:353:PHE:CZ	2.56	0.41
1:H:427:PRO:HB3	1:H:440:TYR:HB2	2.03	0.41
5:A:704:1UE:S1	5:A:704:1UE:O1	2.78	0.41
5:G:704:1UE:O1	5:G:704:1UE:S1	2.78	0.41
5:B:704:1UE:O1	5:B:704:1UE:S1	2.78	0.41
1:D:403:TRP:CZ2	5:D:704:1UE:H2	2.54	0.41
5:D:704:1UE:O1	5:D:704:1UE:S1	2.79	0.41
1:F:79:MET:HE1	1:F:87:MET:SD	2.61	0.41
1:G:156:LEU:HA	1:G:156:LEU:HD12	1.84	0.41
1:F:171:ILE:HD12	1:F:248:LEU:HD22	2.02	0.41
1:F:434:ARG:HB2	1:F:435:HIS:CD2	2.56	0.41
3:H:702:04J:C6	4:H:703:NDP:H42N	2.51	0.41
1:H:313:ALA:O	1:H:314:VAL:C	2.57	0.41
1:E:516:LEU:HG	5:E:704:1UE:H11	2.00	0.41
1:G:173:ARG:HD2	1:G:246:VAL:CG1	2.51	0.41
1:A:290:ILE:HG23	1:B:231:PHE:HD2	1.86	0.41
1:D:327:TYR:O	1:D:331:ILE:HG13	2.20	0.41
5:F:704:1UE:O1	5:F:704:1UE:S1	2.78	0.40
1:H:9:VAL:HG12	1:H:157:TYR:CE2	2.56	0.40
1:G:478:PRO:HA	1:G:481:LEU:HG	2.03	0.40
1:C:428:GLY:O	1:C:429:TYR:C	2.59	0.40
1:E:194:SER:OG	1:E:196:LYS:CD	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:TYR:HA	1:A:450:GLN:NE2	2.36	0.40
1:H:300:GLU:HA	1:H:301:ASP:HA	1.72	0.40
4:H:703:NDP:C5B	4:H:703:NDP:C8A	2.92	0.40
1:A:80:GLY:O	1:A:81:ARG:C	2.59	0.40
1:A:319:PHE:CE2	1:B:294:LEU:HD11	2.56	0.40
1:G:173:ARG:HD3	1:G:244:ASP:HB2	2.03	0.40
1:A:291:ALA:N	1:A:292:PRO:HD2	2.35	0.40
1:F:25:TRP:HB3	1:F:178:PHE:CE2	2.57	0.40
1:E:481:LEU:HA	1:E:484:MET:HE2	2.04	0.40
1:A:368:LEU:HD22	1:A:368:LEU:H	1.87	0.40
1:C:403:TRP:O	1:C:407:VAL:HG22	2.21	0.40
1:D:493:CYS:HA	1:D:506:ILE:O	2.21	0.40
1:B:454:GLN:OE1	1:B:473:MET:HA	2.22	0.40
1:E:308:LYS:HE3	1:E:308:LYS:HA	2.02	0.40
1:H:32:PHE:CZ	3:H:702:04J:C16	3.05	0.40
1:G:313:ALA:HB2	1:G:564:LEU:HD13	2.03	0.40
1:C:290:ILE:HG23	1:D:231:PHE:HD2	1.87	0.40
1:C:484:MET:CE	1:C:488:PRO:HD3	2.52	0.40
1:A:9:VAL:HG12	1:A:157:TYR:CE2	2.56	0.40
1:C:194:SER:OG	1:C:196:LYS:HD3	2.21	0.40
1:E:79:MET:CE	1:E:87:MET:SD	3.09	0.40
1:F:156:LEU:HD12	1:F:156:LEU:HA	1.71	0.40
1:D:107:LYS:O	1:D:107:LYS:NZ	2.45	0.40
1:B:493:CYS:HA	1:B:506:ILE:O	2.22	0.40
5:F:704:1UE:O1	5:F:704:1UE:C3'	2.70	0.40
1:D:36:SER:HB2	3:D:702:04J:CB	2.45	0.40
1:C:327:TYR:CZ	1:C:331:ILE:HD11	2.57	0.40
1:B:13:PRO:HD3	1:B:174:VAL:O	2.22	0.40
1:A:3:LYS:N	1:A:4:PRO:HD3	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	476/610 (78%)	448 (94%)	23 (5%)	5 (1%)	17	50
1	B	478/610 (78%)	454 (95%)	21 (4%)	3 (1%)	30	65
1	C	476/610 (78%)	444 (93%)	28 (6%)	4 (1%)	24	58
1	D	478/610 (78%)	451 (94%)	22 (5%)	5 (1%)	19	52
1	E	476/610 (78%)	448 (94%)	24 (5%)	4 (1%)	24	58
1	F	478/610 (78%)	456 (95%)	18 (4%)	4 (1%)	24	58
1	G	476/610 (78%)	450 (94%)	22 (5%)	4 (1%)	24	58
1	H	478/610 (78%)	451 (94%)	23 (5%)	4 (1%)	24	58
All	All	3816/4880 (78%)	3602 (94%)	181 (5%)	33 (1%)	21	55

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	139	GLU
1	A	286	SER
1	A	429	TYR
1	B	190	ASP
1	B	429	TYR
1	C	139	GLU
1	C	286	SER
1	C	429	TYR
1	D	92	ARG
1	D	190	ASP
1	D	429	TYR
1	E	139	GLU
1	E	286	SER
1	E	429	TYR
1	F	190	ASP
1	F	429	TYR
1	G	190	ASP
1	G	429	TYR
1	H	139	GLU
1	H	429	TYR
1	A	144	SER
1	B	299	GLU
1	C	144	SER
1	E	144	SER
1	H	144	SER
1	A	146	ASP
1	D	299	GLU

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Mol	Chain	Res	Type
1	D	580	GLU
1	F	144	SER
1	G	92	ARG
1	H	146	ASP
1	F	92	ARG
1	G	291	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	429/525 (82%)	405 (94%)	24 (6%)	26	59
1	B	431/525 (82%)	389 (90%)	42 (10%)	10	29
1	C	429/525 (82%)	401 (94%)	28 (6%)	21	52
1	D	431/525 (82%)	387 (90%)	44 (10%)	9	26
1	E	429/525 (82%)	404 (94%)	25 (6%)	25	57
1	F	431/525 (82%)	385 (89%)	46 (11%)	8	24
1	G	429/525 (82%)	384 (90%)	45 (10%)	8	24
1	H	431/525 (82%)	407 (94%)	24 (6%)	26	59
All	All	3440/4200 (82%)	3162 (92%)	278 (8%)	15	39

All (278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	25	TRP
1	A	36	SER
1	A	37	ARG
1	A	41	THR
1	A	89	ARG
1	A	136	LEU
1	A	148	ILE
1	A	162	SER

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Mol	Chain	Res	Type
1	A	165	VAL
1	A	190	ASP
1	A	228	ARG
1	A	285	SER
1	A	308	LYS
1	A	331	ILE
1	A	344	ARG
1	A	356	THR
1	A	371	LYS
1	A	376	LYS
1	A	395	LEU
1	A	401	LYS
1	A	564	LEU
1	A	573	ILE
1	A	579	LYS
1	B	9	VAL
1	B	25	TRP
1	B	29	THR
1	B	37	ARG
1	B	77	VAL
1	B	86	SER
1	B	89	ARG
1	B	102	VAL
1	B	105	SER
1	B	107	LYS
1	B	136	LEU
1	B	142	LYS
1	B	144	SER
1	B	145	VAL
1	B	147	GLN
1	B	148	ILE
1	B	158	GLU
1	B	224	GLU
1	B	228	ARG
1	B	230	ILE
1	B	231	PHE
1	B	249	GLU
1	B	250	LYS
1	B	301	ASP
1	B	308	LYS
1	B	311	ILE
1	B	320	ARG

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Mol	Chain	Res	Type
1	B	339	ARG
1	B	344	ARG
1	B	371	LYS
1	B	376	LYS
1	B	395	LEU
1	B	396	SER
1	B	401	LYS
1	B	414	SER
1	B	456	LYS
1	B	472	LEU
1	B	486	LEU
1	B	545	HIS
1	B	564	LEU
1	B	573	ILE
1	B	579	LYS
1	C	25	TRP
1	C	36	SER
1	C	37	ARG
1	C	89	ARG
1	C	136	LEU
1	C	143	ASP
1	C	148	ILE
1	C	190	ASP
1	C	191	ASP
1	C	230	ILE
1	C	231	PHE
1	C	285	SER
1	C	308	LYS
1	C	331	ILE
1	C	344	ARG
1	C	356	THR
1	C	360	SER
1	C	371	LYS
1	C	376	LYS
1	C	395	LEU
1	C	401	LYS
1	C	409	ARG
1	C	472	LEU
1	C	564	LEU
1	C	567	GLU
1	C	573	ILE
1	C	579	LYS

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Mol	Chain	Res	Type
1	C	607	GLU
1	D	9	VAL
1	D	25	TRP
1	D	29	THR
1	D	37	ARG
1	D	40	LYS
1	D	89	ARG
1	D	102	VAL
1	D	104	SER
1	D	105	SER
1	D	107	LYS
1	D	136	LEU
1	D	142	LYS
1	D	143	ASP
1	D	144	SER
1	D	145	VAL
1	D	148	ILE
1	D	158	GLU
1	D	177	GLU
1	D	185	PRO
1	D	228	ARG
1	D	230	ILE
1	D	231	PHE
1	D	248	LEU
1	D	250	LYS
1	D	301	ASP
1	D	308	LYS
1	D	311	ILE
1	D	339	ARG
1	D	344	ARG
1	D	371	LYS
1	D	376	LYS
1	D	395	LEU
1	D	396	SER
1	D	397[A]	GLU
1	D	397[B]	GLU
1	D	401	LYS
1	D	409	ARG
1	D	441	LYS
1	D	456	LYS
1	D	486	LEU
1	D	545	HIS

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Mol	Chain	Res	Type
1	D	573	ILE
1	D	579	LYS
1	D	605	GLN
1	E	25	TRP
1	E	36	SER
1	E	37	ARG
1	E	41	THR
1	E	89	ARG
1	E	107	LYS
1	E	136	LEU
1	E	143	ASP
1	E	148	ILE
1	E	190	ASP
1	E	228	ARG
1	E	231	PHE
1	E	251	ARG
1	E	308	LYS
1	E	344	ARG
1	E	356	THR
1	E	371	LYS
1	E	376	LYS
1	E	395	LEU
1	E	401	LYS
1	E	472	LEU
1	E	564	LEU
1	E	567	GLU
1	E	573	ILE
1	E	579	LYS
1	F	9	VAL
1	F	25	TRP
1	F	29	THR
1	F	37	ARG
1	F	79	MET
1	F	82	LYS
1	F	86	SER
1	F	89	ARG
1	F	92	ARG
1	F	98	LEU
1	F	102	VAL
1	F	107	LYS
1	F	136	LEU
1	F	142	LYS

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Mol	Chain	Res	Type
1	F	144	SER
1	F	145	VAL
1	F	147	GLN
1	F	148	ILE
1	F	158	GLU
1	F	224	GLU
1	F	228	ARG
1	F	230	ILE
1	F	231	PHE
1	F	249	GLU
1	F	250	LYS
1	F	301	ASP
1	F	308	LYS
1	F	311	ILE
1	F	339	ARG
1	F	344	ARG
1	F	356	THR
1	F	371	LYS
1	F	376	LYS
1	F	395	LEU
1	F	396	SER
1	F	397[A]	GLU
1	F	397[B]	GLU
1	F	401	LYS
1	F	409	ARG
1	F	456	LYS
1	F	486	LEU
1	F	545	HIS
1	F	554	THR
1	F	564	LEU
1	F	573	ILE
1	F	579	LYS
1	G	9	VAL
1	G	25	TRP
1	G	29	THR
1	G	37	ARG
1	G	40	LYS
1	G	82	LYS
1	G	86	SER
1	G	89	ARG
1	G	98	LEU
1	G	102	VAL

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Mol	Chain	Res	Type
1	G	107	LYS
1	G	136	LEU
1	G	142	LYS
1	G	143	ASP
1	G	144	SER
1	G	145	VAL
1	G	148	ILE
1	G	158	GLU
1	G	162	SER
1	G	177	GLU
1	G	228	ARG
1	G	231	PHE
1	G	250	LYS
1	G	308	LYS
1	G	311	ILE
1	G	320	ARG
1	G	339	ARG
1	G	344	ARG
1	G	356	THR
1	G	371	LYS
1	G	376	LYS
1	G	395	LEU
1	G	396	SER
1	G	397[A]	GLU
1	G	397[B]	GLU
1	G	401	LYS
1	G	409	ARG
1	G	441	LYS
1	G	456	LYS
1	G	486	LEU
1	G	545	HIS
1	G	554	THR
1	G	564	LEU
1	G	573	ILE
1	G	579	LYS
1	H	25	TRP
1	H	36	SER
1	H	37	ARG
1	H	89	ARG
1	H	136	LEU
1	H	143	ASP
1	H	148	ILE

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Mol	Chain	Res	Type
1	H	190	ASP
1	H	230	ILE
1	H	231	PHE
1	H	251	ARG
1	H	308	LYS
1	H	331	ILE
1	H	344	ARG
1	H	356	THR
1	H	371	LYS
1	H	376	LYS
1	H	395	LEU
1	H	401	LYS
1	H	472	LEU
1	H	564	LEU
1	H	567	GLU
1	H	573	ILE
1	H	579	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	HIS
1	A	450	GLN
1	A	545	HIS
1	B	435	HIS
1	B	450	GLN
1	B	545	HIS
1	C	168	HIS
1	C	450	GLN
1	D	435	HIS
1	D	450	GLN
1	D	545	HIS
1	E	168	HIS
1	E	450	GLN
1	F	168	HIS
1	F	416	ASN
1	F	435	HIS
1	F	450	GLN
1	F	545	HIS
1	G	99	ASN
1	G	168	HIS
1	G	435	HIS

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Mol	Chain	Res	Type
1	G	545	HIS
1	H	168	HIS
1	H	450	GLN
1	H	545	HIS

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](#)

32 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	UMP	A	701	-	16,21,21	1.52	4 (25%)	23,31,31	2.01	5 (21%)
3	04J	A	702	-	26,34,34	2.00	4 (15%)	29,47,47	1.73	6 (20%)
4	NDP	A	703	-	42,52,52	1.76	7 (16%)	55,80,80	2.19	5 (9%)
5	1UE	A	704	-	24,25,25	2.48	9 (37%)	25,36,36	1.77	4 (16%)
2	UMP	B	701	-	16,21,21	1.61	5 (31%)	23,31,31	1.86	6 (26%)
3	04J	B	702	-	26,34,34	1.95	3 (11%)	29,47,47	1.42	4 (13%)
4	NDP	B	703	-	42,52,52	1.72	7 (16%)	55,80,80	2.37	9 (16%)
5	1UE	B	704	-	24,25,25	2.46	9 (37%)	25,36,36	1.86	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	UMP	C	701	-	16,21,21	1.52	4 (25%)	23,31,31	2.03	5 (21%)
3	04J	C	702	-	26,34,34	1.96	3 (11%)	29,47,47	1.68	6 (20%)
4	NDP	C	703	-	42,52,52	1.73	7 (16%)	55,80,80	2.28	7 (12%)
5	1UE	C	704	-	24,25,25	2.38	9 (37%)	25,36,36	1.76	5 (20%)
2	UMP	D	701	-	16,21,21	1.70	6 (37%)	23,31,31	1.88	6 (26%)
3	04J	D	702	-	26,34,34	1.99	4 (15%)	29,47,47	1.42	4 (13%)
4	NDP	D	703	-	42,52,52	1.71	11 (26%)	55,80,80	2.29	7 (12%)
5	1UE	D	704	-	24,25,25	2.36	9 (37%)	25,36,36	1.80	5 (20%)
2	UMP	E	701	-	16,21,21	1.70	5 (31%)	23,31,31	1.84	5 (21%)
3	04J	E	702	-	26,34,34	1.91	3 (11%)	29,47,47	1.52	5 (17%)
4	NDP	E	703	-	42,52,52	1.76	7 (16%)	55,80,80	2.22	3 (5%)
5	1UE	E	704	-	24,25,25	2.29	9 (37%)	25,36,36	1.78	4 (16%)
2	UMP	F	701	-	16,21,21	1.61	5 (31%)	23,31,31	1.61	2 (8%)
3	04J	F	702	-	26,34,34	1.99	4 (15%)	29,47,47	1.45	5 (17%)
4	NDP	F	703	-	42,52,52	1.75	13 (30%)	55,80,80	2.30	9 (16%)
5	1UE	F	704	-	24,25,25	2.44	10 (41%)	25,36,36	1.91	4 (16%)
2	UMP	G	701	-	16,21,21	1.67	5 (31%)	23,31,31	1.85	5 (21%)
3	04J	G	702	-	26,34,34	1.96	4 (15%)	29,47,47	1.51	5 (17%)
4	NDP	G	703	-	42,52,52	1.73	11 (26%)	55,80,80	2.27	7 (12%)
5	1UE	G	704	-	24,25,25	2.55	9 (37%)	25,36,36	1.88	4 (16%)
2	UMP	H	701	-	16,21,21	1.53	4 (25%)	23,31,31	2.14	5 (21%)
3	04J	H	702	-	26,34,34	1.90	4 (15%)	29,47,47	1.60	5 (17%)
4	NDP	H	703	-	42,52,52	1.69	7 (16%)	55,80,80	2.33	8 (14%)
5	1UE	H	704	-	24,25,25	2.31	10 (41%)	25,36,36	1.83	4 (16%)

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	UMP	A	701	-	-	0/6/22/22	0/2/2/2
3	04J	A	702	-	-	0/16/22/22	0/3/3/3
4	NDP	A	703	-	-	0/30/77/77	0/5/5/5
5	1UE	A	704	-	-	0/4/4/4	0/4/4/4
2	UMP	B	701	-	-	0/6/22/22	0/2/2/2
3	04J	B	702	-	-	0/16/22/22	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NDP	B	703	-	-	0/30/77/77	0/5/5/5
5	1UE	B	704	-	-	0/4/4/4	0/4/4/4
2	UMP	C	701	-	-	0/6/22/22	0/2/2/2
3	04J	C	702	-	-	0/16/22/22	0/3/3/3
4	NDP	C	703	-	-	0/30/77/77	0/5/5/5
5	1UE	C	704	-	-	0/4/4/4	0/4/4/4
2	UMP	D	701	-	-	0/6/22/22	0/2/2/2
3	04J	D	702	-	-	0/16/22/22	0/3/3/3
4	NDP	D	703	-	-	0/30/77/77	0/5/5/5
5	1UE	D	704	-	-	0/4/4/4	0/4/4/4
2	UMP	E	701	-	-	0/6/22/22	0/2/2/2
3	04J	E	702	-	-	0/16/22/22	0/3/3/3
4	NDP	E	703	-	-	0/30/77/77	0/5/5/5
5	1UE	E	704	-	-	0/4/4/4	0/4/4/4
2	UMP	F	701	-	-	0/6/22/22	0/2/2/2
3	04J	F	702	-	-	0/16/22/22	0/3/3/3
4	NDP	F	703	-	-	0/30/77/77	0/5/5/5
5	1UE	F	704	-	-	0/4/4/4	0/4/4/4
2	UMP	G	701	-	-	0/6/22/22	0/2/2/2
3	04J	G	702	-	-	0/16/22/22	0/3/3/3
4	NDP	G	703	-	-	0/30/77/77	0/5/5/5
5	1UE	G	704	-	-	0/4/4/4	0/4/4/4
2	UMP	H	701	-	-	0/6/22/22	0/2/2/2
3	04J	H	702	-	-	0/16/22/22	0/3/3/3
4	NDP	H	703	-	-	0/30/77/77	0/5/5/5
5	1UE	H	704	-	-	0/4/4/4	0/4/4/4

All (211) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	704	1UE	C2'-S1	-6.37	1.65	1.77
5	A	704	1UE	C2'-S1	-6.23	1.65	1.77
5	B	704	1UE	C2'-S1	-6.02	1.66	1.77
3	A	702	04J	C11-C	-5.71	1.38	1.50
3	A	702	04J	C9-C6	-5.44	1.40	1.51
3	D	702	04J	C9-C6	-5.41	1.40	1.51
5	G	704	1UE	C7-C5	-5.39	1.32	1.41
5	F	704	1UE	C2'-S1	-5.39	1.67	1.77
3	G	702	04J	C11-C	-5.37	1.38	1.50
3	F	702	04J	C9-C6	-5.36	1.40	1.51
3	D	702	04J	C11-C	-5.33	1.38	1.50
3	F	702	04J	C11-C	-5.28	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	704	1UE	C7-C5	-5.25	1.32	1.41
5	F	704	1UE	C7-C5	-5.24	1.32	1.41
5	H	704	1UE	C7-C5	-5.23	1.32	1.41
5	B	704	1UE	C7-C5	-5.21	1.32	1.41
5	A	704	1UE	C7-C5	-5.20	1.32	1.41
3	H	702	04J	C11-C	-5.19	1.39	1.50
5	C	704	1UE	C7-C5	-5.17	1.32	1.41
5	E	704	1UE	C7-C5	-5.13	1.32	1.41
5	C	704	1UE	C2'-S1	-5.12	1.67	1.77
5	D	704	1UE	C2'-S1	-5.08	1.68	1.77
3	G	702	04J	C9-C6	-5.07	1.41	1.51
3	H	702	04J	C9-C6	-4.85	1.41	1.51
4	H	703	NDP	C4N-C5N	-4.70	1.38	1.49
3	C	702	04J	C11-C	-4.55	1.40	1.50
4	F	703	NDP	C4N-C5N	-4.51	1.39	1.49
4	G	703	NDP	C4N-C5N	-4.47	1.39	1.49
4	D	703	NDP	C4N-C5N	-4.45	1.39	1.49
3	E	702	04J	C9-C6	-4.39	1.42	1.51
4	A	703	NDP	C4N-C5N	-4.33	1.39	1.49
4	C	703	NDP	C4N-C5N	-4.30	1.39	1.49
4	E	703	NDP	C4N-C5N	-4.30	1.39	1.49
3	E	702	04J	C11-C	-4.26	1.41	1.50
3	C	702	04J	C9-C6	-4.21	1.42	1.51
5	C	704	1UE	C2-C1	-4.21	1.34	1.41
5	A	704	1UE	C2-C1	-4.21	1.34	1.41
5	H	704	1UE	C2-C1	-4.15	1.34	1.41
4	B	703	NDP	C4N-C5N	-4.14	1.40	1.49
5	E	704	1UE	C2-C1	-4.14	1.34	1.41
3	B	702	04J	C11-C	-4.07	1.41	1.50
5	E	704	1UE	C2'-S1	-4.05	1.70	1.77
5	F	704	1UE	C2-C1	-3.88	1.35	1.41
5	B	704	1UE	C2-C1	-3.86	1.35	1.41
5	D	704	1UE	C2-C1	-3.82	1.35	1.41
5	H	704	1UE	C2'-S1	-3.81	1.70	1.77
5	D	704	1UE	C1'-C6	-3.79	1.34	1.43
5	G	704	1UE	C1'-C6	-3.75	1.35	1.43
5	F	704	1UE	C1'-C6	-3.75	1.35	1.43
5	G	704	1UE	C2-C1	-3.73	1.35	1.41
5	B	704	1UE	C1'-C6	-3.73	1.35	1.43
5	H	704	1UE	C1'-C6	-3.64	1.35	1.43
5	A	704	1UE	C1'-C6	-3.64	1.35	1.43
5	E	704	1UE	C1'-C6	-3.60	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	704	1UE	C1'-C6	-3.59	1.35	1.43
3	B	702	04J	C9-C6	-3.50	1.44	1.51
4	F	703	NDP	C5A-C4A	-3.38	1.32	1.40
5	E	704	1UE	C1-C4	-3.35	1.34	1.43
5	C	704	1UE	C1-C4	-3.34	1.34	1.43
4	D	703	NDP	C5A-C4A	-3.32	1.33	1.40
4	G	703	NDP	C5A-C4A	-3.32	1.33	1.40
5	A	704	1UE	C1-C4	-3.31	1.34	1.43
5	H	704	1UE	C1-C4	-3.31	1.34	1.43
4	H	703	NDP	C5A-C4A	-3.24	1.33	1.40
5	D	704	1UE	C1-C4	-3.20	1.34	1.43
5	G	704	1UE	C1-C4	-3.18	1.34	1.43
5	F	704	1UE	C1-C6	-3.15	1.35	1.43
5	B	704	1UE	C1-C4	-3.14	1.34	1.43
5	D	704	1UE	C1-C6	-3.11	1.35	1.43
5	B	704	1UE	C1-C6	-3.11	1.35	1.43
5	G	704	1UE	C1-C6	-3.08	1.35	1.43
5	A	704	1UE	C1-C6	-3.08	1.35	1.43
5	F	704	1UE	C1-C4	-3.07	1.34	1.43
5	C	704	1UE	C1-C6	-3.07	1.35	1.43
5	F	704	1UE	C1'-S1	-3.07	1.68	1.79
2	B	701	UMP	P-O5'	-3.05	1.50	1.60
5	E	704	1UE	C1-C6	-3.04	1.36	1.43
5	E	704	1UE	C1'-S1	-3.03	1.68	1.79
5	G	704	1UE	C1'-S1	-3.01	1.68	1.79
5	H	704	1UE	C1-C6	-3.01	1.36	1.43
4	A	703	NDP	C5A-C4A	-2.86	1.34	1.40
4	E	703	NDP	C5A-C4A	-2.83	1.34	1.40
5	H	704	1UE	C1'-S1	-2.83	1.69	1.79
5	C	704	1UE	C1'-S1	-2.80	1.69	1.79
3	D	702	04J	C8A-N8	-2.76	1.32	1.37
3	H	702	04J	C8A-N8	-2.75	1.32	1.37
4	C	703	NDP	C5A-C4A	-2.74	1.34	1.40
3	G	702	04J	C8A-N8	-2.70	1.32	1.37
2	C	701	UMP	P-OP2	-2.68	1.45	1.54
2	D	701	UMP	P-O5'	-2.68	1.51	1.60
2	F	701	UMP	P-OP2	-2.67	1.45	1.54
4	B	703	NDP	C5A-C4A	-2.67	1.34	1.40
2	E	701	UMP	P-OP2	-2.65	1.45	1.54
5	B	704	1UE	C1'-S1	-2.63	1.69	1.79
2	A	701	UMP	P-OP2	-2.63	1.45	1.54
2	H	701	UMP	P-OP2	-2.59	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	04J	C8A-N8	-2.58	1.33	1.37
2	B	701	UMP	P-OP2	-2.57	1.45	1.54
3	F	702	04J	C8A-N8	-2.56	1.33	1.37
2	G	701	UMP	P-OP2	-2.53	1.45	1.54
2	F	701	UMP	P-O5'	-2.52	1.51	1.60
2	G	701	UMP	P-O5'	-2.51	1.51	1.60
2	D	701	UMP	P-OP2	-2.49	1.45	1.54
5	D	704	1UE	C1'-S1	-2.49	1.70	1.79
2	F	701	UMP	P-OP3	-2.47	1.45	1.54
4	D	703	NDP	P2B-O3X	-2.44	1.46	1.54
4	F	703	NDP	P2B-O2B	-2.41	1.52	1.60
4	G	703	NDP	P2B-O2X	-2.39	1.46	1.54
4	G	703	NDP	P2B-O3X	-2.39	1.46	1.54
4	D	703	NDP	P2B-O2X	-2.38	1.46	1.54
4	F	703	NDP	P2B-O3X	-2.37	1.46	1.54
4	F	703	NDP	P2B-O2X	-2.36	1.46	1.54
4	D	703	NDP	C3B-C2B	-2.36	1.47	1.53
5	A	704	1UE	C1'-S1	-2.32	1.70	1.79
2	A	701	UMP	P-OP3	-2.31	1.46	1.54
2	E	701	UMP	P-O5'	-2.30	1.52	1.60
2	E	701	UMP	P-OP3	-2.28	1.46	1.54
2	B	701	UMP	P-OP3	-2.26	1.46	1.54
2	H	701	UMP	P-OP3	-2.26	1.46	1.54
2	C	701	UMP	P-OP3	-2.26	1.46	1.54
4	H	703	NDP	P2B-O2X	-2.24	1.46	1.54
4	G	703	NDP	PA-O2A	-2.22	1.45	1.54
2	G	701	UMP	P-OP3	-2.19	1.46	1.54
2	D	701	UMP	P-OP3	-2.18	1.46	1.54
4	F	703	NDP	PA-O2A	-2.16	1.45	1.54
5	G	704	1UE	C5-N4	-2.15	1.31	1.39
5	D	704	1UE	C5-N4	-2.15	1.31	1.39
5	H	704	1UE	C5-N4	-2.14	1.31	1.39
5	C	704	1UE	C5-N4	-2.12	1.31	1.39
5	A	704	1UE	C5-N4	-2.11	1.32	1.39
4	G	703	NDP	C5A-N7A	-2.11	1.32	1.39
5	E	704	1UE	C5-N4	-2.08	1.32	1.39
4	F	703	NDP	PN-O2N	-2.07	1.46	1.54
4	D	703	NDP	PA-O2A	-2.07	1.46	1.54
5	B	704	1UE	C5-N4	-2.06	1.32	1.39
4	D	703	NDP	C5A-N7A	-2.03	1.32	1.39
2	D	701	UMP	O4'-C4'	-2.03	1.40	1.45
4	F	703	NDP	C5A-N7A	-2.03	1.32	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	704	1UE	C5-N4	-2.02	1.32	1.39
4	D	703	NDP	PN-O2N	-2.02	1.46	1.54
4	F	703	NDP	C3B-C2B	-2.02	1.48	1.53
4	G	703	NDP	PN-O2N	-2.00	1.46	1.54
5	F	704	1UE	C3-N1	2.02	1.39	1.35
4	F	703	NDP	O4B-C1B	2.10	1.43	1.41
4	A	703	NDP	C2N-C3N	2.13	1.39	1.34
4	E	703	NDP	C2N-C3N	2.15	1.39	1.34
4	C	703	NDP	C2N-C3N	2.18	1.40	1.34
5	H	704	1UE	C3-N1	2.19	1.39	1.35
2	B	701	UMP	C6-N1	2.22	1.38	1.35
4	G	703	NDP	O4B-C1B	2.40	1.44	1.41
4	B	703	NDP	O4D-C1D	2.56	1.48	1.42
2	C	701	UMP	C6-N1	2.61	1.39	1.35
2	F	701	UMP	C6-N1	2.63	1.39	1.35
2	A	701	UMP	C6-N1	2.65	1.39	1.35
4	F	703	NDP	C6N-C5N	2.70	1.38	1.33
2	B	701	UMP	C4-N3	2.72	1.38	1.33
4	H	703	NDP	O4B-C1B	2.74	1.44	1.41
2	H	701	UMP	C6-N1	2.75	1.39	1.35
2	D	701	UMP	C4-N3	2.76	1.38	1.33
2	C	701	UMP	C4-N3	2.82	1.38	1.33
4	G	703	NDP	C6N-C5N	2.82	1.38	1.33
4	D	703	NDP	C2A-N1A	2.82	1.39	1.33
4	F	703	NDP	C2A-N1A	2.84	1.39	1.33
2	F	701	UMP	C4-N3	2.86	1.38	1.33
4	D	703	NDP	C6N-C5N	2.86	1.38	1.33
2	H	701	UMP	C4-N3	2.90	1.38	1.33
4	G	703	NDP	C2A-N1A	2.93	1.39	1.33
2	G	701	UMP	C4-N3	2.93	1.38	1.33
4	H	703	NDP	C6N-C5N	2.95	1.39	1.33
4	B	703	NDP	C6N-C5N	2.96	1.39	1.33
2	G	701	UMP	C6-N1	2.98	1.40	1.35
2	A	701	UMP	C4-N3	3.00	1.38	1.33
2	E	701	UMP	C6-N1	3.08	1.40	1.35
5	C	704	1UE	C2-N1	3.10	1.38	1.33
2	D	701	UMP	C6-N1	3.13	1.40	1.35
4	H	703	NDP	C2A-N1A	3.21	1.40	1.33
5	E	704	1UE	C2-N1	3.22	1.39	1.33
2	E	701	UMP	C4-N3	3.22	1.39	1.33
4	C	703	NDP	C6N-C5N	3.32	1.39	1.33
5	A	704	1UE	C2-N1	3.33	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	704	1UE	C2-N1	3.41	1.39	1.33
4	E	703	NDP	C2A-N1A	3.43	1.40	1.33
5	D	704	1UE	C2-N1	3.44	1.39	1.33
4	E	703	NDP	C6N-C5N	3.44	1.40	1.33
4	C	703	NDP	C2A-N1A	3.46	1.40	1.33
5	H	704	1UE	C2-N1	3.47	1.39	1.33
4	A	703	NDP	C2A-N1A	3.51	1.40	1.33
4	A	703	NDP	C6N-C5N	3.58	1.40	1.33
4	B	703	NDP	O4B-C1B	3.61	1.45	1.41
5	G	704	1UE	C2-N1	3.75	1.40	1.33
4	B	703	NDP	C2A-N1A	3.75	1.41	1.33
5	F	704	1UE	C2-N1	3.76	1.40	1.33
4	D	703	NDP	C2A-N3A	3.93	1.39	1.32
4	G	703	NDP	C2A-N3A	4.12	1.39	1.32
4	F	703	NDP	C2A-N3A	4.15	1.39	1.32
4	A	703	NDP	O4B-C1B	4.33	1.46	1.41
4	H	703	NDP	C2A-N3A	4.36	1.39	1.32
3	A	702	04J	C7-N8	4.39	1.39	1.31
4	E	703	NDP	O4B-C1B	4.52	1.46	1.41
3	H	702	04J	C7-N8	4.52	1.39	1.31
4	C	703	NDP	O4B-C1B	4.57	1.47	1.41
3	D	702	04J	C7-N8	4.65	1.39	1.31
3	G	702	04J	C7-N8	4.80	1.40	1.31
4	B	703	NDP	C2A-N3A	4.91	1.40	1.32
4	A	703	NDP	C2A-N3A	4.91	1.40	1.32
4	C	703	NDP	C2A-N3A	4.98	1.41	1.32
3	F	702	04J	C7-N8	5.00	1.40	1.31
4	E	703	NDP	C2A-N3A	5.04	1.41	1.32
3	E	702	04J	C7-N8	5.91	1.41	1.31
3	C	702	04J	C7-N8	6.42	1.42	1.31
3	B	702	04J	C7-N8	6.54	1.43	1.31

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	703	NDP	N3A-C2A-N1A	-14.36	117.90	128.89
4	B	703	NDP	N3A-C2A-N1A	-14.30	117.95	128.89
4	C	703	NDP	N3A-C2A-N1A	-14.12	118.08	128.89
4	F	703	NDP	N3A-C2A-N1A	-14.02	118.16	128.89
4	D	703	NDP	N3A-C2A-N1A	-13.99	118.18	128.89
4	A	703	NDP	N3A-C2A-N1A	-13.97	118.20	128.89
4	G	703	NDP	N3A-C2A-N1A	-13.94	118.22	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	703	NDP	N3A-C2A-N1A	-13.77	118.35	128.89
5	H	704	1UE	N3-C3-N1	-6.04	118.24	127.44
5	E	704	1UE	N3-C3-N1	-5.97	118.36	127.44
5	A	704	1UE	N3-C3-N1	-5.90	118.46	127.44
5	F	704	1UE	N3-C3-N1	-5.86	118.51	127.44
5	C	704	1UE	N3-C3-N1	-5.86	118.52	127.44
5	B	704	1UE	N3-C3-N1	-5.85	118.53	127.44
5	G	704	1UE	N3-C3-N1	-5.76	118.67	127.44
5	D	704	1UE	N3-C3-N1	-5.74	118.70	127.44
5	F	704	1UE	C1-C2-N1	-5.58	119.96	124.19
5	G	704	1UE	C1-C2-N1	-5.49	120.03	124.19
5	B	704	1UE	C1-C2-N1	-5.13	120.30	124.19
5	D	704	1UE	C1-C2-N1	-4.90	120.48	124.19
5	H	704	1UE	C1-C2-N1	-4.66	120.66	124.19
4	H	703	NDP	C1B-N9A-C4A	-4.46	120.21	126.94
3	E	702	04J	N1-C2-N3	-4.38	120.78	127.44
3	C	702	04J	N1-C2-N3	-4.37	120.79	127.44
5	A	704	1UE	C1-C2-N1	-4.34	120.90	124.19
5	C	704	1UE	C1-C2-N1	-4.28	120.95	124.19
5	E	704	1UE	C1-C2-N1	-4.24	120.98	124.19
2	C	701	UMP	C4'-O4'-C1'	-4.07	99.17	109.47
3	H	702	04J	N1-C2-N3	-4.07	121.25	127.44
2	H	701	UMP	C4'-O4'-C1'	-4.06	99.21	109.47
3	A	702	04J	N1-C2-N3	-4.06	121.27	127.44
2	A	701	UMP	C4'-O4'-C1'	-4.00	99.35	109.47
3	B	702	04J	N1-C2-N3	-3.90	121.50	127.44
3	G	702	04J	N1-C2-N3	-3.85	121.58	127.44
3	F	702	04J	N1-C2-N3	-3.76	121.72	127.44
3	A	702	04J	C11-C-N	-3.73	110.29	116.93
4	G	703	NDP	PN-O3-PA	-3.67	122.44	132.73
3	D	702	04J	N1-C2-N3	-3.65	121.89	127.44
4	D	703	NDP	PN-O3-PA	-3.58	122.67	132.73
4	H	703	NDP	PN-O3-PA	-3.54	122.78	132.73
4	F	703	NDP	PN-O3-PA	-3.06	124.14	132.73
2	H	701	UMP	O4'-C1'-C2'	-3.03	100.24	106.27
2	B	701	UMP	C4'-O4'-C1'	-2.96	101.98	109.47
2	A	701	UMP	O4'-C1'-C2'	-2.95	100.40	106.27
3	C	702	04J	CG-CB-CA	-2.93	107.04	112.99
4	A	703	NDP	C1B-N9A-C4A	-2.91	122.56	126.94
4	B	703	NDP	C1B-N9A-C4A	-2.89	122.59	126.94
2	C	701	UMP	O4'-C1'-C2'	-2.78	100.73	106.27
4	B	703	NDP	C4B-O4B-C1B	-2.70	106.75	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	703	NDP	O2B-P2B-O1X	-2.67	100.43	107.11
4	H	703	NDP	C4D-O4D-C1D	-2.66	103.66	109.52
2	C	701	UMP	O5'-P-OP1	-2.64	100.42	107.14
2	B	701	UMP	O4'-C1'-C2'	-2.61	101.07	106.27
4	H	703	NDP	C4B-O4B-C1B	-2.60	106.86	109.72
2	A	701	UMP	O5'-P-OP1	-2.59	100.54	107.14
2	H	701	UMP	O5'-P-OP1	-2.58	100.58	107.14
4	F	703	NDP	C3N-C2N-N1N	-2.56	119.47	123.14
2	E	701	UMP	O5'-P-OP1	-2.54	100.67	107.14
4	F	703	NDP	O4D-C1D-C2D	-2.54	100.69	106.58
4	H	703	NDP	O4D-C1D-C2D	-2.48	100.82	106.58
4	D	703	NDP	C4B-O4B-C1B	-2.46	107.02	109.72
2	G	701	UMP	O4'-C1'-C2'	-2.44	101.41	106.27
2	B	701	UMP	O5'-P-OP1	-2.42	100.99	107.14
4	F	703	NDP	O4D-C4D-C5D	-2.39	100.78	109.32
2	E	701	UMP	OP3-P-O5'	-2.37	99.73	106.56
4	C	703	NDP	C4D-O4D-C1D	-2.37	104.30	109.52
4	G	703	NDP	C3N-C2N-N1N	-2.35	119.77	123.14
3	H	702	04J	C9-C6-C7	-2.35	117.01	121.18
3	C	702	04J	CB-CG-CD	-2.34	103.48	113.02
2	D	701	UMP	O4'-C1'-C2'	-2.30	101.68	106.27
2	E	701	UMP	O4'-C1'-C2'	-2.29	101.71	106.27
3	E	702	04J	CG-CB-CA	-2.28	108.36	112.99
4	D	703	NDP	O4D-C1D-C2D	-2.27	101.31	106.58
4	G	703	NDP	O4D-C1D-C2D	-2.25	101.37	106.58
3	F	702	04J	C11-C-N	-2.23	112.95	116.93
4	F	703	NDP	C4B-O4B-C1B	-2.23	107.27	109.72
2	E	701	UMP	O4'-C4'-C5'	-2.23	101.35	109.32
3	G	702	04J	C9-C6-C7	-2.23	117.23	121.18
4	B	703	NDP	O5B-C5B-C4B	-2.22	100.92	109.12
2	D	701	UMP	OP3-P-O5'	-2.22	100.18	106.56
3	A	702	04J	C9-C6-C7	-2.21	117.25	121.18
4	D	703	NDP	C3N-C2N-N1N	-2.20	119.98	123.14
2	D	701	UMP	C4'-O4'-C1'	-2.18	103.95	109.47
4	C	703	NDP	O2B-P2B-O1X	-2.17	101.69	107.11
3	G	702	04J	C11-C-N	-2.17	113.06	116.93
3	E	702	04J	CB-CG-CD	-2.15	104.24	113.02
4	B	703	NDP	C1D-N1N-C2N	-2.15	117.16	120.91
4	C	703	NDP	O4D-C1D-N1N	-2.14	103.56	108.07
3	B	702	04J	CB-CG-CD	-2.13	104.35	113.02
5	C	704	1UE	C7-C8-C9	-2.11	117.46	120.96
3	D	702	04J	C9-C6-C7	-2.10	117.45	121.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	701	UMP	O5'-P-OP1	-2.08	101.85	107.14
3	C	702	04J	C15-C14-N10	-2.08	117.08	121.06
5	D	704	1UE	C7-C8-C9	-2.07	117.52	120.96
2	G	701	UMP	C4'-O4'-C1'	-2.06	104.26	109.47
4	G	703	NDP	O4D-C1D-N1N	-2.05	103.74	108.07
4	F	703	NDP	C4A-C5A-N7A	-2.05	107.60	109.48
4	H	703	NDP	O2B-P2B-O1X	-2.02	102.06	107.11
4	C	703	NDP	O4D-C1D-C2D	-2.02	101.91	106.58
2	G	701	UMP	OP3-P-O5'	-2.01	100.78	106.56
3	H	702	04J	C11-C-N	-2.01	113.35	116.93
2	F	701	UMP	OP2-P-OP1	2.03	117.11	110.58
3	F	702	04J	NA4-C4-N3	2.06	123.33	116.45
4	E	703	NDP	O3X-P2B-O2X	2.08	115.30	107.38
5	D	704	1UE	N2-C3-N1	2.10	120.67	117.20
2	G	701	UMP	OP3-P-OP2	2.12	115.45	107.38
3	B	702	04J	N8-C8A-N1	2.13	119.19	116.14
2	D	701	UMP	OP3-P-OP2	2.13	115.49	107.38
4	G	703	NDP	O3X-P2B-O2X	2.14	115.55	107.38
4	D	703	NDP	O3X-P2B-O2X	2.15	115.55	107.38
4	A	703	NDP	O3X-P2B-O2X	2.16	115.61	107.38
2	B	701	UMP	O4'-C1'-N1	2.16	111.46	107.72
5	E	704	1UE	N2-C3-N1	2.17	120.79	117.20
2	B	701	UMP	OP3-P-OP2	2.17	115.64	107.38
4	C	703	NDP	O3X-P2B-O2X	2.18	115.68	107.38
5	A	704	1UE	C2-N1-C3	2.19	118.98	115.94
5	C	704	1UE	C2-N1-C3	2.20	119.00	115.94
5	A	704	1UE	N2-C3-N1	2.22	120.87	117.20
3	G	702	04J	N8-C8A-N1	2.25	119.36	116.14
3	C	702	04J	C9-N10-C14	2.26	128.29	122.15
5	C	704	1UE	N2-C3-N1	2.27	120.96	117.20
3	D	702	04J	N8-C8A-N1	2.29	119.41	116.14
5	H	704	1UE	C2-N1-C3	2.29	119.11	115.94
3	A	702	04J	O-C-N	2.31	126.61	122.44
4	F	703	NDP	O3X-P2B-O2X	2.32	116.20	107.38
5	E	704	1UE	C2-N1-C3	2.35	119.20	115.94
5	D	704	1UE	C2-N1-C3	2.35	119.20	115.94
5	B	704	1UE	N2-C3-N1	2.35	121.10	117.20
5	G	704	1UE	C2-N1-C3	2.36	119.22	115.94
5	F	704	1UE	N2-C3-N1	2.37	121.12	117.20
4	A	703	NDP	O4B-C1B-N9A	2.40	113.13	108.10
5	B	704	1UE	C2-N1-C3	2.43	119.32	115.94
5	G	704	1UE	N2-C3-N1	2.44	121.24	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	703	NDP	O3X-P2B-O2X	2.47	116.78	107.38
3	H	702	04J	N8-C8A-N1	2.50	119.72	116.14
5	F	704	1UE	C2-N1-C3	2.52	119.44	115.94
3	F	702	04J	N8-C8A-N1	2.60	119.86	116.14
5	H	704	1UE	N2-C3-N1	2.65	121.59	117.20
4	H	703	NDP	C5N-C4N-C3N	2.70	119.97	112.52
3	A	702	04J	N8-C8A-N1	2.76	120.09	116.14
3	E	702	04J	C9-C6-N5	2.79	122.10	116.81
2	C	701	UMP	O4'-C1'-N1	2.83	112.62	107.72
4	A	703	NDP	C5N-C4N-C3N	2.84	120.36	112.52
3	E	702	04J	N8-C8A-N1	2.92	120.32	116.14
4	B	703	NDP	O4B-C1B-N9A	2.92	114.22	108.10
4	G	703	NDP	C5N-C4N-C3N	2.96	120.69	112.52
4	C	703	NDP	C5N-C4N-C3N	3.01	120.80	112.52
4	D	703	NDP	C5N-C4N-C3N	3.03	120.88	112.52
4	F	703	NDP	C5N-C4N-C3N	3.06	120.94	112.52
4	E	703	NDP	C5N-C4N-C3N	3.09	121.05	112.52
2	A	701	UMP	O4'-C1'-N1	3.18	113.22	107.72
4	B	703	NDP	C5N-C4N-C3N	3.21	121.37	112.52
3	C	702	04J	N8-C8A-N1	3.28	120.83	116.14
3	B	702	04J	C9-C6-N5	3.46	123.37	116.81
2	H	701	UMP	O4'-C1'-N1	3.48	113.73	107.72
3	A	702	04J	C9-C6-N5	3.62	123.68	116.81
3	F	702	04J	C9-C6-N5	3.63	123.69	116.81
3	D	702	04J	C9-C6-N5	3.78	123.98	116.81
3	G	702	04J	C9-C6-N5	4.04	124.47	116.81
3	H	702	04J	C9-C6-N5	4.17	124.72	116.81
2	F	701	UMP	C4-N3-C2	5.53	119.62	114.14
2	B	701	UMP	C4-N3-C2	5.57	119.66	114.14
2	A	701	UMP	C4-N3-C2	5.83	119.92	114.14
2	C	701	UMP	C4-N3-C2	6.04	120.12	114.14
2	E	701	UMP	C4-N3-C2	6.05	120.13	114.14
2	G	701	UMP	C4-N3-C2	6.08	120.16	114.14
2	H	701	UMP	C4-N3-C2	6.14	120.22	114.14
2	D	701	UMP	C4-N3-C2	6.24	120.32	114.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

32 monomers are involved in 142 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	UMP	3	0
3	A	702	04J	5	0
4	A	703	NDP	4	0
5	A	704	1UE	7	0
2	B	701	UMP	2	0
3	B	702	04J	1	0
4	B	703	NDP	2	0
5	B	704	1UE	9	0
2	C	701	UMP	5	0
3	C	702	04J	2	0
4	C	703	NDP	2	0
5	C	704	1UE	7	0
2	D	701	UMP	2	0
3	D	702	04J	3	0
4	D	703	NDP	4	0
5	D	704	1UE	7	0
2	E	701	UMP	2	0
3	E	702	04J	2	0
4	E	703	NDP	3	0
5	E	704	1UE	4	0
2	F	701	UMP	7	0
3	F	702	04J	2	0
4	F	703	NDP	4	0
5	F	704	1UE	7	0
2	G	701	UMP	2	0
3	G	702	04J	2	0
4	G	703	NDP	3	0
5	G	704	1UE	7	0
2	H	701	UMP	5	0
3	H	702	04J	14	0
4	H	703	NDP	15	0
5	H	704	1UE	4	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	489/610 (80%)	0.34	15 (3%)	52	40	51, 71, 125, 144	0
1	B	491/610 (80%)	0.44	18 (3%)	45	33	48, 69, 118, 180	0
1	C	489/610 (80%)	0.32	16 (3%)	50	38	51, 71, 125, 148	0
1	D	491/610 (80%)	0.41	20 (4%)	41	29	50, 70, 119, 180	0
1	E	489/610 (80%)	0.31	20 (4%)	41	29	53, 72, 125, 146	0
1	F	491/610 (80%)	0.38	22 (4%)	37	26	48, 70, 120, 178	0
1	G	489/610 (80%)	0.37	21 (4%)	39	27	50, 70, 117, 170	0
1	H	491/610 (80%)	0.31	22 (4%)	37	26	53, 72, 126, 144	0
All	All	3920/4880 (80%)	0.36	154 (3%)	43	31	48, 71, 124, 180	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	300	GLU	11.3
1	B	610	VAL	9.1
1	F	300	GLU	7.9
1	D	300	GLU	7.6
1	B	308	LYS	6.9
1	G	610	VAL	6.8
1	F	610	VAL	6.2
1	D	610	VAL	6.0
1	D	308	LYS	5.8
1	D	319	PHE	5.6
1	G	308	LYS	5.6
1	G	144	SER	5.5
1	G	319	PHE	5.5
1	F	308	LYS	5.5
1	B	319	PHE	5.4
1	F	319	PHE	5.4

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Mol	Chain	Res	Type	RSRZ
1	B	301	ASP	4.8
1	C	170	TYR	4.8
1	B	607	GLU	4.7
1	B	144	SER	4.7
1	B	606	MET	4.6
1	A	106	LEU	4.5
1	F	607	GLU	4.5
1	C	606	MET	4.5
1	H	170	TYR	4.5
1	G	607	GLU	4.4
1	D	607	GLU	4.2
1	F	301	ASP	4.2
1	A	606	MET	4.2
1	D	301	ASP	4.1
1	B	296	TRP	4.1
1	F	299	GLU	4.1
1	E	606	MET	4.1
1	H	106	LEU	4.0
1	C	607	GLU	4.0
1	B	609	ALA	4.0
1	B	604	ILE	3.8
1	F	296	TRP	3.7
1	F	606	MET	3.7
1	G	609	ALA	3.7
1	G	606	MET	3.6
1	C	96	ASP	3.6
1	A	76	ALA	3.5
1	E	170	TYR	3.5
1	A	74	PHE	3.5
1	E	91	PHE	3.3
1	C	95	VAL	3.3
1	H	98	LEU	3.3
1	D	144	SER	3.3
1	F	608	MET	3.3
1	H	76	ALA	3.2
1	E	76	ALA	3.2
1	C	106	LEU	3.1
1	D	196	LYS	3.1
1	A	91	PHE	3.1
1	F	144	SER	3.1
1	E	607	GLU	3.0
1	A	311	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	299	GLU	3.0
1	D	296	TRP	3.0
1	G	410	GLU	3.0
1	H	196	LYS	3.0
1	E	472	LEU	3.0
1	D	606	MET	3.0
1	A	607	GLU	3.0
1	D	608	MET	2.9
1	A	170	TYR	2.9
1	B	196	LYS	2.9
1	B	608	MET	2.9
1	C	319	PHE	2.9
1	B	605	GLN	2.8
1	D	609	ALA	2.8
1	H	319	PHE	2.8
1	G	293	VAL	2.8
1	B	475	ALA	2.8
1	H	137	LEU	2.8
1	H	606	MET	2.8
1	E	319	PHE	2.8
1	G	225	ALA	2.7
1	H	74	PHE	2.7
1	H	607	GLU	2.7
1	H	311	ILE	2.7
1	E	196	LYS	2.7
1	G	309	GLU	2.7
1	G	296	TRP	2.7
1	H	35	PHE	2.7
1	H	130	LEU	2.7
1	A	95	VAL	2.7
1	E	35	PHE	2.7
1	D	294	LEU	2.6
1	H	146	ASP	2.6
1	C	196	LYS	2.6
1	E	311	ILE	2.6
1	G	608	MET	2.5
1	A	319	PHE	2.5
1	G	192	ILE	2.5
1	E	146	ASP	2.5
1	C	98	LEU	2.5
1	D	225	ALA	2.5
1	E	106	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	137	LEU	2.5
1	E	347	VAL	2.4
1	A	508	TYR	2.4
1	A	148	ILE	2.4
1	F	192	ILE	2.4
1	G	294	LEU	2.4
1	F	196	LYS	2.4
1	H	95	VAL	2.4
1	E	96	ASP	2.4
1	F	309	GLU	2.4
1	F	609	ALA	2.4
1	D	290	ILE	2.4
1	H	96	ASP	2.4
1	A	137	LEU	2.4
1	G	605	GLN	2.3
1	F	170	TYR	2.3
1	A	96	ASP	2.3
1	F	604	ILE	2.3
1	C	35	PHE	2.3
1	E	74	PHE	2.3
1	H	433	TRP	2.3
1	G	297	MET	2.3
1	H	609	ALA	2.3
1	C	84	TRP	2.3
1	D	148	ILE	2.2
1	D	410	GLU	2.2
1	F	148	ILE	2.2
1	H	192	ILE	2.2
1	E	508	TYR	2.2
1	H	84	TRP	2.2
1	D	7	LEU	2.2
1	F	397[A]	GLU	2.2
1	G	90	LYS	2.2
1	C	101	VAL	2.1
1	E	345	THR	2.1
1	F	5	VAL	2.1
1	G	7	LEU	2.1
1	C	100	ILE	2.1
1	E	609	ALA	2.1
1	F	410	GLU	2.1
1	C	91	PHE	2.1
1	C	192	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	508	TYR	2.1
1	G	397[A]	GLU	2.1
1	B	74	PHE	2.0
1	E	17	ILE	2.0
1	B	397[A]	GLU	2.0
1	H	11	MET	2.0
1	D	605	GLN	2.0
1	D	192	ILE	2.0
1	G	148	ILE	2.0
1	A	246	VAL	2.0
1	E	343	ASP	2.0
1	F	466	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	1UE	F	704	22/22	0.69	0.51	4.08	127,153,164,169	0
5	1UE	E	704	22/22	0.73	0.39	3.59	115,130,146,151	0
2	UMP	D	701	20/20	0.88	0.29	2.51	114,125,138,148	0
5	1UE	G	704	22/22	0.71	0.42	2.50	120,150,162,169	0
5	1UE	H	704	22/22	0.78	0.34	2.39	117,133,144,149	0
3	04J	B	702	32/32	0.87	0.32	2.22	96,128,152,156	0
3	04J	D	702	32/32	0.86	0.31	2.19	98,122,153,155	0
5	1UE	B	704	22/22	0.79	0.41	2.11	112,144,163,169	0
5	1UE	D	704	22/22	0.77	0.36	1.96	110,153,164,166	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	04J	E	702	32/32	0.90	0.39	1.95	89,134,162,165	0
2	UMP	H	701	20/20	0.87	0.24	1.82	107,132,138,138	0
5	1UE	C	704	22/22	0.80	0.28	1.64	106,130,152,161	0
3	04J	C	702	32/32	0.89	0.39	1.54	101,142,157,165	0
3	04J	A	702	32/32	0.89	0.33	1.42	95,139,161,161	0
2	UMP	G	701	20/20	0.83	0.25	1.36	110,127,134,138	0
3	04J	F	702	32/32	0.87	0.28	1.33	95,122,152,157	0
2	UMP	B	701	20/20	0.90	0.25	1.18	106,122,134,136	0
5	1UE	A	704	22/22	0.77	0.26	1.14	110,125,139,154	0
3	04J	G	702	32/32	0.88	0.26	1.04	94,122,156,162	0
2	UMP	F	701	20/20	0.88	0.23	1.00	113,125,142,151	0
2	UMP	E	701	20/20	0.93	0.24	0.94	95,120,129,130	0
3	04J	H	702	32/32	0.90	0.32	0.92	98,136,154,156	0
4	NDP	B	703	48/48	0.94	0.23	0.84	81,120,132,139	0
2	UMP	A	701	20/20	0.91	0.21	0.44	103,124,135,135	0
4	NDP	E	703	48/48	0.93	0.21	0.28	112,149,190,194	0
2	UMP	C	701	20/20	0.90	0.18	0.13	93,116,131,135	0
4	NDP	G	703	48/48	0.94	0.19	0.13	91,123,130,133	0
4	NDP	A	703	48/48	0.94	0.20	0.09	118,149,185,188	0
4	NDP	F	703	48/48	0.94	0.19	0.06	87,120,132,135	0
4	NDP	D	703	48/48	0.93	0.19	-0.00	93,117,133,137	0
4	NDP	H	703	48/48	0.91	0.18	-0.11	116,151,181,187	0
4	NDP	C	703	48/48	0.93	0.18	-0.14	117,144,185,186	0

6.5 Other polymers

There are no such residues in this entry.