Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:35 PM GMT

PDB ID	:	1G2V
Title	:	THE STRUCTURAL BASIS OF THE CATALYTIC MECHANISM AND REGULATION OF GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE (RMLA). TTP COMPLEX.
Authors	:	Blankenfeldt, W.; Asuncion, M.; Lam, J.S.; Naismith, J.H.
Deposited on	:	2000-10-21
Resolution	:	2.60 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:

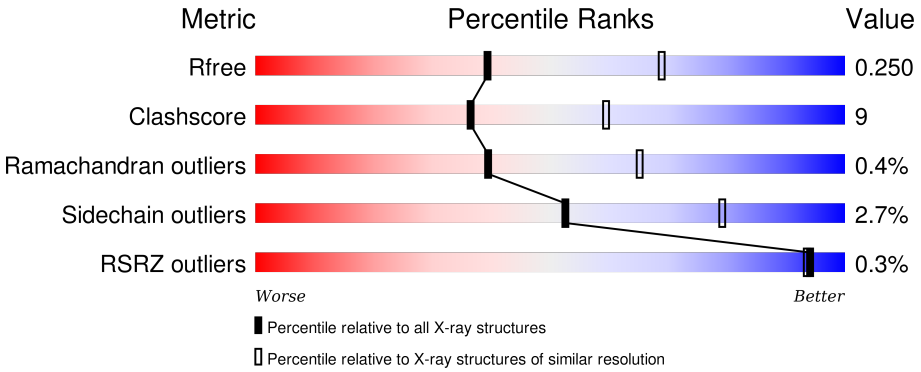
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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	293	80% 17%
1	B	293	77% 20%
1	C	293	% 77% 20%
1	D	293	% 75% 23%
1	E	293	80% 17%

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Mol	Chain	Length	Quality of chain
1	F	293	79% 18%
1	G	293	77% 21%
1	H	293	76% 20%

2 Entry composition (i)

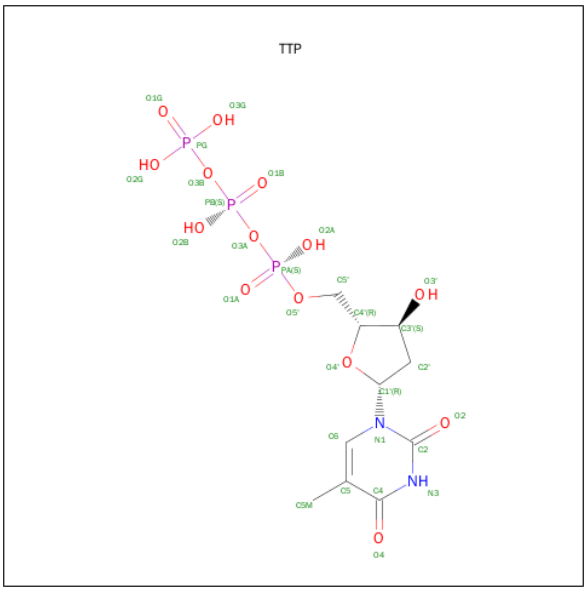
There are 2 unique types of molecules in this entry. The entry contains 18744 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	292	Total	C	N	O	S	0	0	0
			2285	1462	385	434	4			
1	B	292	Total	C	N	O	S	0	0	0
			2285	1462	385	434	4			
1	C	292	Total	C	N	O	S	0	0	0
			2285	1462	385	434	4			
1	D	292	Total	C	N	O	S	0	0	0
			2285	1462	385	434	4			
1	E	292	Total	C	N	O	S	0	0	0
			2285	1462	385	434	4			
1	F	292	Total	C	N	O	S	0	0	0
			2285	1462	385	434	4			
1	G	292	Total	C	N	O	S	0	0	0
			2285	1462	385	434	4			
1	H	292	Total	C	N	O	S	0	0	0
			2285	1462	385	434	4			

- Molecule 2 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: $C_{10}H_{17}N_2O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	A	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	B	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	C	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	C	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	D	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	D	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	E	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	E	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	F	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	F	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	G	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	G	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

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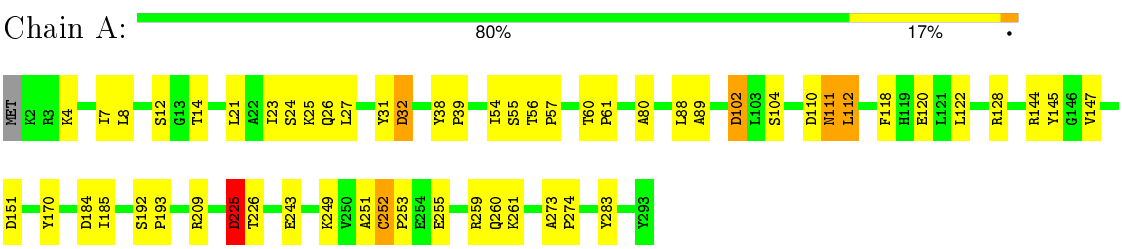
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	H	1	Total	C	N	O	P	0	0
			29	10	2	14	3		
2	H	1	Total	C	N	O	P	0	0
			29	10	2	14	3		

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.

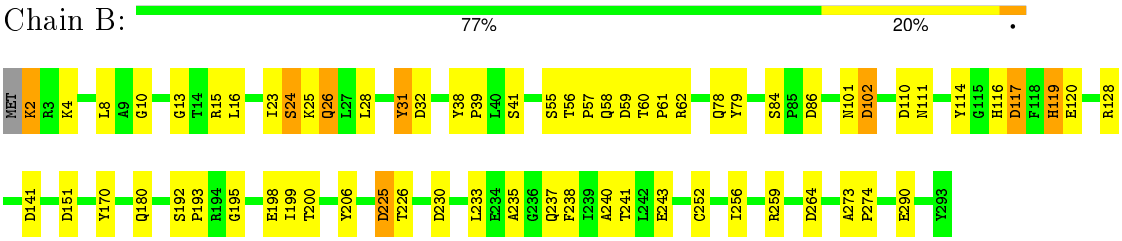
- Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain A:



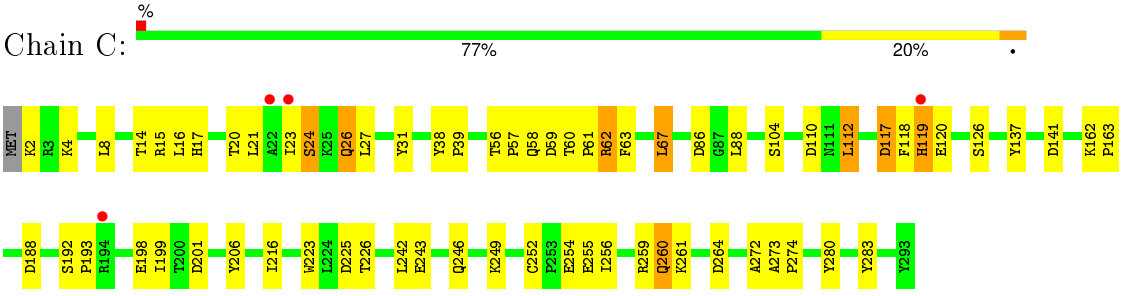
- Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain B:



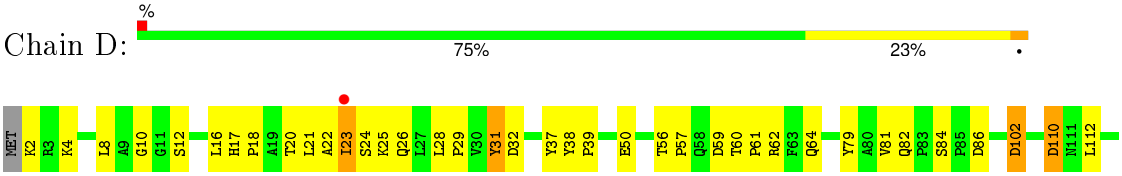
- Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

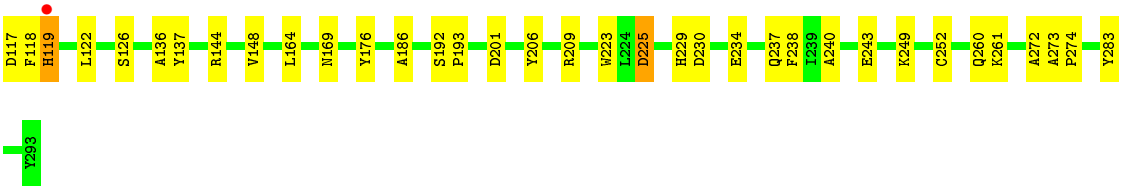
Chain C:



- Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

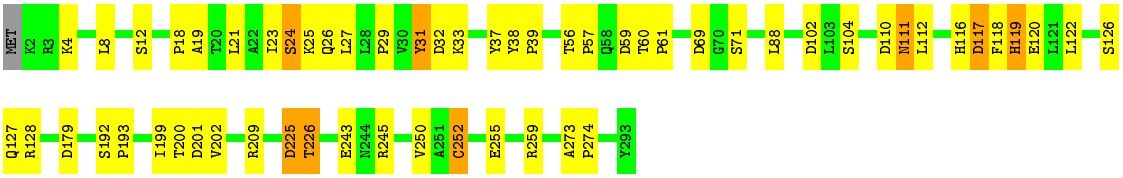
Chain D:





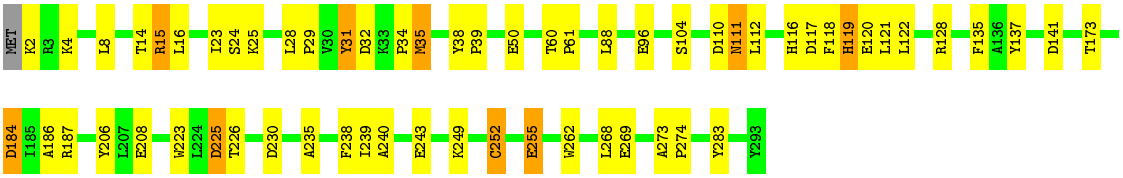
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain E:



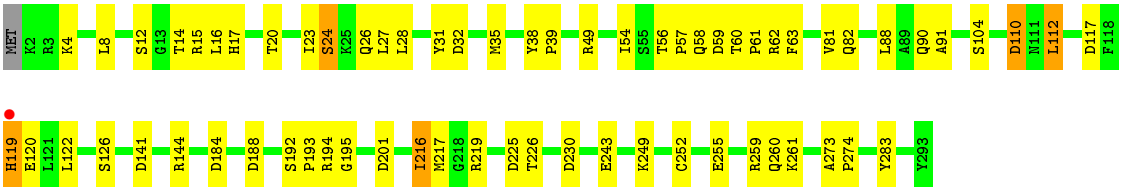
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain F:



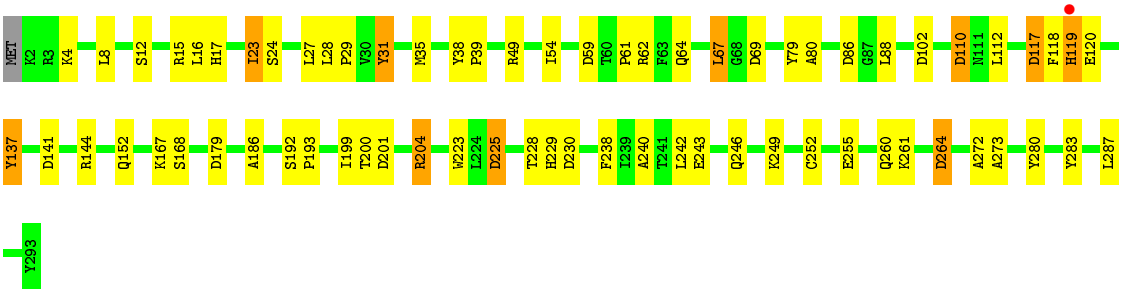
• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain G:



• Molecule 1: GLUCOSE-1-PHOSPHATE THYMIDYLYLTRANSFERASE

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.02Å 134.36Å 140.90Å 90.00° 98.22° 90.00°	Depositor
Resolution (Å)	100.00 – 2.60 50.26 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.4 (100.00-2.60) 91.4 (50.26-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.33 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.215 , 0.242 0.225 , 0.250	Depositor DCC
R_{free} test set	3797 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 26.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Outliers	9 of 75545 reflections (0.012%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	18744	wwPDB-VP
Average B, all atoms (Å^2)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.28 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.6250e-05.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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: TTP

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	1.24	6/2335 (0.3%)	1.16	10/3168 (0.3%)
1	B	1.31	10/2335 (0.4%)	1.20	14/3168 (0.4%)
1	C	1.24	2/2335 (0.1%)	1.17	16/3168 (0.5%)
1	D	1.26	6/2335 (0.3%)	1.18	9/3168 (0.3%)
1	E	1.29	4/2335 (0.2%)	1.15	10/3168 (0.3%)
1	F	1.39	11/2335 (0.5%)	1.19	7/3168 (0.2%)
1	G	1.24	1/2335 (0.0%)	1.19	14/3168 (0.4%)
1	H	1.24	5/2335 (0.2%)	1.21	17/3168 (0.5%)
All	All	1.28	45/18680 (0.2%)	1.18	97/25344 (0.4%)

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	35	MET	SD-CE	-14.80	0.94	1.77
1	F	35	MET	CG-SD	-7.64	1.61	1.81
1	B	206	TYR	CD2-CE2	-7.53	1.28	1.39
1	H	280	TYR	CD2-CE2	-7.50	1.28	1.39
1	D	37	TYR	CD2-CE2	-7.20	1.28	1.39
1	A	89	ALA	CA-CB	-7.06	1.37	1.52
1	A	170	TYR	CD2-CE2	-7.04	1.28	1.39
1	F	235	ALA	CA-CB	-6.80	1.38	1.52
1	B	206	TYR	CD1-CE1	-6.40	1.29	1.39
1	C	206	TYR	CD1-CE1	-6.32	1.29	1.39
1	A	252	CYS	CB-SG	-6.31	1.71	1.82
1	D	186	ALA	CA-CB	-6.22	1.39	1.52
1	B	170	TYR	CD2-CE2	-6.19	1.30	1.39
1	E	252	CYS	CB-SG	-6.11	1.71	1.82
1	D	206	TYR	CD2-CE2	-6.07	1.30	1.39
1	D	148	VAL	CB-CG1	-6.07	1.40	1.52
1	F	96	GLU	CD-OE2	6.07	1.32	1.25
1	G	120	GLU	CG-CD	6.07	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	VAL	CB-CG2	-5.93	1.40	1.52
1	B	24	SER	CB-OG	5.89	1.50	1.42
1	F	255	GLU	CD-OE1	-5.68	1.19	1.25
1	C	198	GLU	CD-OE1	-5.63	1.19	1.25
1	F	186	ALA	CA-CB	-5.63	1.40	1.52
1	B	114	TYR	CD1-CE1	-5.50	1.31	1.39
1	E	37	TYR	CE1-CZ	-5.44	1.31	1.38
1	E	202	VAL	CB-CG1	-5.44	1.41	1.52
1	E	255	GLU	CD-OE2	-5.42	1.19	1.25
1	B	235	ALA	CA-CB	-5.33	1.41	1.52
1	B	2	LYS	CD-CE	5.31	1.64	1.51
1	D	176	TYR	CE1-CZ	-5.31	1.31	1.38
1	D	136	ALA	CA-CB	-5.30	1.41	1.52
1	F	128	ARG	NE-CZ	-5.29	1.26	1.33
1	B	79	TYR	CD2-CE2	-5.29	1.31	1.39
1	H	120	GLU	CG-CD	5.28	1.59	1.51
1	F	208	GLU	CD-OE1	5.27	1.31	1.25
1	H	168	SER	CB-OG	-5.21	1.35	1.42
1	H	186	ALA	CA-CB	-5.20	1.41	1.52
1	A	7	ILE	CA-CB	-5.15	1.43	1.54
1	H	137	TYR	CD2-CE2	-5.15	1.31	1.39
1	B	198	GLU	CD-OE1	-5.11	1.20	1.25
1	A	185	ILE	CA-CB	-5.06	1.43	1.54
1	B	84	SER	CA-CB	-5.04	1.45	1.52
1	F	262	TRP	CG-CD1	-5.03	1.29	1.36
1	F	206	TYR	CD2-CE2	-5.01	1.31	1.39
1	F	252	CYS	CB-SG	-5.01	1.73	1.81

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	15	ARG	NE-CZ-NH1	11.07	125.84	120.30
1	H	86	ASP	CB-CG-OD2	10.98	128.18	118.30
1	H	110	ASP	CB-CG-OD2	10.30	127.57	118.30
1	B	230	ASP	CB-CG-OD2	8.38	125.84	118.30
1	C	201	ASP	CB-CG-OD2	8.33	125.80	118.30
1	G	201	ASP	CB-CG-OD2	8.07	125.57	118.30
1	B	102	ASP	CB-CG-OD2	8.03	125.53	118.30
1	A	128	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	B	128	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	D	225	ASP	CB-CG-OD2	7.65	125.19	118.30
1	C	110	ASP	CB-CG-OD2	7.37	124.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	102	ASP	CB-CG-OD2	7.16	124.74	118.30
1	C	188	ASP	CB-CG-OD1	6.91	124.52	118.30
1	F	141	ASP	CB-CG-OD2	6.90	124.51	118.30
1	A	184	ASP	CB-CG-OD2	6.90	124.51	118.30
1	D	102	ASP	CB-CG-OD2	6.88	124.49	118.30
1	E	59	ASP	CB-CG-OD2	6.82	124.44	118.30
1	G	230	ASP	CB-CG-OD2	6.76	124.39	118.30
1	C	86	ASP	CB-CG-OD2	6.72	124.34	118.30
1	H	230	ASP	CB-CG-OD2	6.71	124.33	118.30
1	H	264	ASP	CB-CG-OD2	6.66	124.30	118.30
1	B	59	ASP	CB-CG-OD2	6.58	124.22	118.30
1	E	128	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	H	117	ASP	CB-CG-OD2	6.50	124.15	118.30
1	D	230	ASP	CB-CG-OD2	6.48	124.13	118.30
1	E	102	ASP	CB-CG-OD2	6.48	124.13	118.30
1	F	184	ASP	CB-CG-OD2	6.47	124.12	118.30
1	G	141	ASP	CB-CG-OD2	6.38	124.04	118.30
1	G	117	ASP	CB-CG-OD2	6.34	124.01	118.30
1	C	141	ASP	CB-CG-OD2	6.31	123.98	118.30
1	D	110	ASP	CB-CG-OD2	6.28	123.95	118.30
1	F	128	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	G	112	LEU	CB-CG-CD2	-6.20	100.46	111.00
1	C	112	LEU	CB-CG-CD2	-6.18	100.50	111.00
1	B	119	HIS	CB-CA-C	6.14	122.69	110.40
1	C	117	ASP	CB-CG-OD1	-6.14	112.77	118.30
1	A	151	ASP	CB-CG-OD1	6.13	123.82	118.30
1	B	259	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	D	86	ASP	CB-CG-OD2	6.08	123.77	118.30
1	H	201	ASP	CB-CG-OD2	6.02	123.71	118.30
1	H	144	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	E	259	ARG	NE-CZ-NH1	-5.90	117.35	120.30
1	C	117	ASP	CB-CG-OD2	5.87	123.58	118.30
1	H	225	ASP	CB-CG-OD2	5.85	123.56	118.30
1	H	69	ASP	CB-CG-OD2	5.82	123.54	118.30
1	H	204	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	A	225	ASP	CB-CA-C	5.78	121.96	110.40
1	H	179	ASP	CB-CG-OD1	5.75	123.47	118.30
1	B	141	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	32	ASP	CB-CG-OD2	5.74	123.47	118.30
1	E	255	GLU	OE1-CD-OE2	-5.74	116.42	123.30
1	B	62	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	G	110	ASP	CB-CG-OD2	5.72	123.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	102	ASP	CB-CG-OD1	-5.68	113.19	118.30
1	B	117	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	112	LEU	CB-CG-CD2	-5.63	101.43	111.00
1	C	67	LEU	CB-CG-CD2	-5.61	101.46	111.00
1	C	110	ASP	OD1-CG-OD2	-5.61	112.64	123.30
1	F	119	HIS	CB-CA-C	5.60	121.60	110.40
1	E	226	THR	OG1-CB-CG2	-5.56	97.21	110.00
1	D	201	ASP	CB-CG-OD2	5.50	123.25	118.30
1	C	201	ASP	OD1-CG-OD2	-5.49	112.87	123.30
1	A	225	ASP	CB-CG-OD2	5.48	123.23	118.30
1	B	86	ASP	CB-CG-OD2	5.45	123.20	118.30
1	G	144	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	B	264	ASP	CB-CG-OD2	5.44	123.19	118.30
1	H	49	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	D	144	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	G	216	ILE	CB-CA-C	-5.35	100.91	111.60
1	G	184	ASP	CB-CG-OD2	5.34	123.11	118.30
1	C	226	THR	OG1-CB-CG2	-5.29	97.83	110.00
1	H	67	LEU	CB-CG-CD2	-5.29	102.01	111.00
1	G	219	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	D	225	ASP	CB-CA-C	5.25	120.90	110.40
1	H	112	LEU	CB-CG-CD2	-5.25	102.08	111.00
1	E	225	ASP	CB-CA-C	5.24	120.88	110.40
1	B	151	ASP	CB-CG-OD1	5.24	123.01	118.30
1	E	201	ASP	CB-CG-OD2	5.21	122.99	118.30
1	G	188	ASP	CB-CG-OD1	5.20	122.98	118.30
1	A	144	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	G	49	ARG	NE-CZ-NH1	-5.17	117.71	120.30
1	H	200	THR	OG1-CB-CG2	-5.17	98.10	110.00
1	B	128	ARG	NH1-CZ-NH2	5.17	125.08	119.40
1	D	112	LEU	CB-CG-CD2	-5.15	102.24	111.00
1	C	254	GLU	OE1-CD-OE2	-5.13	117.15	123.30
1	C	216	ILE	CB-CA-C	-5.12	101.35	111.60
1	F	128	ARG	NH1-CZ-NH2	5.10	125.01	119.40
1	B	225	ASP	CB-CA-C	5.07	120.54	110.40
1	E	119	HIS	CB-CA-C	5.05	120.50	110.40
1	G	194	ARG	CB-CA-C	-5.04	100.32	110.40
1	C	62	ARG	NE-CZ-NH2	-5.03	117.78	120.30
1	G	32	ASP	CB-CG-OD1	5.03	122.83	118.30
1	C	86	ASP	CB-CG-OD1	-5.02	113.78	118.30
1	H	152	GLN	CA-CB-CG	-5.02	102.35	113.40
1	H	141	ASP	CB-CG-OD2	5.02	122.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	245	ARG	NE-CZ-NH2	5.01	122.80	120.30
1	F	225	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2285	0	2272	37	0
1	B	2285	0	2272	40	0
1	C	2285	0	2272	50	0
1	D	2285	0	2272	54	0
1	E	2285	0	2272	34	1
1	F	2285	0	2272	59	0
1	G	2285	0	2272	47	0
1	H	2285	0	2272	46	1
2	A	58	0	26	3	0
2	B	58	0	26	4	0
2	C	58	0	26	3	0
2	D	58	0	26	3	0
2	E	58	0	26	2	0
2	F	58	0	26	3	0
2	G	58	0	26	3	0
2	H	58	0	26	3	0
All	All	18744	0	18384	352	1

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 (352) 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:F:35:MET:CG	1:F:35:MET:CE	1.98	1.40
1:F:35:MET:CG	1:F:35:MET:HE2	1.66	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:35:MET:SD	1:F:35:MET:CE	0.95	1.04
1:F:23:ILE:CG2	1:F:28:LEU:HD21	1.87	1.03
1:F:35:MET:SD	1:F:35:MET:HE2	1.56	0.97
1:F:35:MET:HE1	1:F:35:MET:SD	1.56	0.96
1:F:35:MET:SD	1:F:35:MET:HE3	1.56	0.95
1:A:23:ILE:HG13	1:A:24:SER:N	1.80	0.94
1:B:23:ILE:CG2	1:B:28:LEU:HD21	2.02	0.89
1:H:23:ILE:HD11	1:H:62:ARG:HD3	1.54	0.89
1:F:23:ILE:HG23	1:F:28:LEU:HD21	1.55	0.88
1:F:23:ILE:HG21	1:F:28:LEU:CD2	2.05	0.87
1:B:15:ARG:HB2	2:B:3502:TTP:O1G	1.75	0.86
1:A:23:ILE:HD11	1:A:27:LEU:HD12	1.59	0.84
1:F:15:ARG:HB2	2:F:3510:TTP:O1G	1.78	0.84
1:D:2:LYS:NZ	1:D:50:GLU:OE1	2.12	0.83
1:A:23:ILE:HG13	1:A:24:SER:H	1.40	0.82
1:D:119:HIS:HD2	1:D:119:HIS:O	1.60	0.82
1:D:119:HIS:CD2	1:D:119:HIS:O	2.33	0.82
1:B:23:ILE:HG21	1:B:28:LEU:CD2	2.09	0.82
1:F:23:ILE:CG2	1:F:28:LEU:CD2	2.58	0.82
1:D:119:HIS:CD2	1:D:119:HIS:C	2.51	0.81
1:H:23:ILE:HD11	1:H:62:ARG:CD	2.13	0.78
1:B:23:ILE:O	1:B:23:ILE:HG23	1.83	0.75
1:F:23:ILE:HG21	1:F:28:LEU:HD21	1.64	0.75
1:D:4:LYS:NZ	1:D:102:ASP:OD2	2.19	0.75
1:E:8:LEU:HG	2:E:3508:TTP:O2	1.87	0.75
1:G:24:SER:HB2	1:G:59:ASP:OD2	1.86	0.75
1:C:119:HIS:CD2	1:C:119:HIS:C	2.60	0.75
1:D:24:SER:HB2	1:D:59:ASP:OD2	1.87	0.74
1:G:119:HIS:CD2	1:G:119:HIS:C	2.60	0.74
1:H:119:HIS:CD2	1:H:119:HIS:C	2.60	0.74
1:F:35:MET:HE2	1:F:35:MET:HG3	1.69	0.73
1:E:8:LEU:HG	2:E:3508:TTP:C2	2.24	0.73
1:C:256:ILE:O	1:C:260:GLN:HG2	1.91	0.70
1:E:120:GLU:OE1	1:E:120:GLU:N	2.24	0.70
1:F:35:MET:CB	1:F:35:MET:HE2	2.21	0.69
1:B:23:ILE:HG21	1:B:28:LEU:HD21	1.68	0.69
1:D:23:ILE:CG1	1:D:24:SER:H	2.06	0.69
1:H:23:ILE:HG12	1:H:24:SER:H	1.57	0.68
1:B:23:ILE:CG2	1:B:28:LEU:CD2	2.70	0.67
1:F:35:MET:HE1	1:F:226:THR:HG21	1.75	0.67
1:G:14:THR:HA	1:G:17:HIS:ND1	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:ILE:HD12	1:D:23:ILE:HG21	1.77	0.66
1:G:23:ILE:HD12	1:H:23:ILE:HG21	1.76	0.65
1:H:119:HIS:HD2	1:H:119:HIS:O	1.78	0.65
1:E:29:PRO:HD3	1:F:28:LEU:HD22	1.78	0.65
1:E:273:ALA:N	1:E:274:PRO:HD2	2.11	0.64
1:B:23:ILE:O	1:B:23:ILE:CG2	2.47	0.63
1:C:58:GLN:HE21	1:C:62:ARG:HH22	1.45	0.63
1:E:192:SER:HB2	1:E:193:PRO:HD2	1.79	0.63
1:G:119:HIS:HD2	1:G:119:HIS:O	1.82	0.62
1:H:119:HIS:CD2	1:H:119:HIS:O	2.53	0.62
1:B:78:GLN:HG2	1:H:61:PRO:HG3	1.82	0.61
1:H:8:LEU:HG	2:H:3514:TTP:C2	2.34	0.61
1:D:23:ILE:CG1	1:D:24:SER:N	2.63	0.61
1:D:10:GLY:N	2:D:3506:TTP:O2	2.27	0.61
1:B:4:LYS:NZ	1:B:102:ASP:OD2	2.23	0.61
1:A:8:LEU:HG	2:A:3500:TTP:C2	2.36	0.61
1:D:119:HIS:HD2	1:D:119:HIS:C	1.98	0.60
1:G:119:HIS:O	1:G:119:HIS:CD2	2.55	0.60
1:A:8:LEU:HG	2:A:3500:TTP:O2	2.03	0.59
1:E:23:ILE:HG21	1:F:23:ILE:HD12	1.84	0.59
1:B:23:ILE:HG23	1:B:28:LEU:HD21	1.81	0.59
1:G:15:ARG:NE	2:G:3512:TTP:O1G	2.30	0.59
1:H:249:LYS:HD2	1:H:283:TYR:CG	2.38	0.59
1:A:23:ILE:HD11	1:A:27:LEU:CD1	2.29	0.59
1:F:35:MET:CE	1:F:226:THR:HG21	2.33	0.59
1:C:192:SER:HB2	1:C:193:PRO:HD2	1.85	0.58
1:B:110:ASP:HB2	1:B:226:THR:OG1	2.04	0.58
1:G:110:ASP:HB2	1:G:226:THR:OG1	2.04	0.58
1:A:110:ASP:HB2	1:A:226:THR:OG1	2.03	0.58
1:F:35:MET:HG3	1:F:35:MET:CE	2.18	0.57
1:G:27:LEU:HD21	1:G:63:PHE:CE2	2.39	0.57
1:B:23:ILE:HG21	1:B:28:LEU:HD23	1.86	0.57
1:G:27:LEU:HD21	1:G:63:PHE:CD2	2.39	0.57
1:B:192:SER:HB2	1:B:193:PRO:HD2	1.86	0.57
1:D:192:SER:HB2	1:D:193:PRO:HD2	1.86	0.57
1:C:280:TYR:CD1	1:D:18:PRO:HD3	2.38	0.57
1:G:192:SER:HB2	1:G:193:PRO:HD2	1.85	0.57
1:F:23:ILE:HD13	1:F:28:LEU:HD23	1.87	0.57
1:A:111:ASN:HD22	1:A:111:ASN:N	2.01	0.57
1:C:119:HIS:O	1:C:119:HIS:HD2	1.88	0.56
1:H:243:GLU:HG2	1:H:249:LYS:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:14:THR:O	1:G:15:ARG:C	2.39	0.56
1:E:38:TYR:HB2	1:E:39:PRO:HD3	1.87	0.56
1:G:14:THR:HA	1:G:17:HIS:CE1	2.40	0.56
1:E:116:HIS:O	1:E:117:ASP:HB2	2.05	0.56
1:C:38:TYR:HB2	1:C:39:PRO:HD3	1.87	0.56
1:G:38:TYR:HB2	1:G:39:PRO:HD3	1.86	0.56
1:B:273:ALA:N	1:B:274:PRO:HD2	2.20	0.56
1:A:38:TYR:HB2	1:A:39:PRO:HD3	1.87	0.56
1:B:10:GLY:N	2:B:3502:TTP:O2	2.35	0.55
1:C:14:THR:O	1:C:15:ARG:C	2.43	0.55
1:G:27:LEU:CD2	1:G:63:PHE:CE2	2.90	0.55
1:H:119:HIS:HD2	1:H:119:HIS:C	2.07	0.55
1:H:4:LYS:NZ	1:H:102:ASP:OD2	2.28	0.55
1:H:23:ILE:HG12	1:H:24:SER:N	2.20	0.55
1:G:119:HIS:HD2	1:G:119:HIS:C	2.06	0.55
1:D:23:ILE:HG13	1:D:24:SER:H	1.71	0.54
1:D:243:GLU:HG2	1:D:249:LYS:HA	1.90	0.54
1:E:29:PRO:CD	1:F:28:LEU:HD22	2.38	0.54
1:E:31:TYR:OH	1:F:230:ASP:OD1	2.18	0.54
1:F:23:ILE:HG21	1:F:28:LEU:HD23	1.86	0.54
1:C:119:HIS:C	1:C:119:HIS:HD2	2.06	0.54
1:D:8:LEU:HG	2:D:3506:TTP:C2	2.43	0.54
1:B:16:LEU:HD12	1:B:25:LYS:HD3	1.90	0.54
1:G:23:ILE:HG12	1:G:27:LEU:HB2	1.90	0.53
1:F:2:LYS:NZ	1:F:50:GLU:OE1	2.29	0.53
1:B:290:GLU:OE2	1:D:169:ASN:ND2	2.41	0.53
1:C:14:THR:HA	1:C:17:HIS:ND1	2.23	0.53
1:F:112:LEU:C	1:F:112:LEU:HD23	2.28	0.53
1:F:8:LEU:HG	2:F:3510:TTP:C2	2.44	0.53
1:F:8:LEU:HG	2:F:3510:TTP:O2	2.08	0.53
1:C:119:HIS:CD2	1:C:119:HIS:O	2.62	0.53
1:H:38:TYR:HB2	1:H:39:PRO:HD3	1.89	0.53
1:F:23:ILE:HG23	1:F:28:LEU:CD2	2.32	0.52
1:F:273:ALA:N	1:F:274:PRO:HD2	2.24	0.52
1:E:110:ASP:HB2	1:E:226:THR:OG1	2.10	0.52
1:A:273:ALA:HB3	1:A:274:PRO:CD	2.39	0.52
1:B:101:ASN:O	1:B:180:GLN:NE2	2.43	0.52
1:F:35:MET:HE1	1:F:226:THR:CG2	2.40	0.52
1:D:249:LYS:HD2	1:D:283:TYR:CG	2.44	0.52
1:A:4:LYS:O	1:A:104:SER:HA	2.10	0.52
1:D:137:TYR:CE2	1:D:223:TRP:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:23:ILE:CG2	1:G:28:LEU:CD2	2.88	0.52
1:D:22:ALA:O	1:D:23:ILE:HB	2.09	0.51
1:H:192:SER:HB2	1:H:193:PRO:HD2	1.92	0.51
1:H:137:TYR:CE2	1:H:223:TRP:HB3	2.46	0.51
1:F:110:ASP:HB2	1:F:226:THR:OG1	2.11	0.51
1:F:35:MET:CE	1:F:226:THR:OG1	2.58	0.51
1:C:8:LEU:HG	2:C:3504:TTP:O2	2.11	0.51
1:D:23:ILE:HD11	1:D:62:ARG:HD3	1.91	0.50
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.93	0.50
1:H:23:ILE:CD1	1:H:62:ARG:HD3	2.35	0.50
1:A:192:SER:HB2	1:A:193:PRO:HD2	1.92	0.50
1:G:58:GLN:CD	1:G:58:GLN:H	2.15	0.50
1:C:243:GLU:HG2	1:C:249:LYS:HA	1.92	0.50
1:B:38:TYR:HB2	1:B:39:PRO:HD3	1.93	0.50
1:F:38:TYR:HB2	1:F:39:PRO:HD3	1.93	0.50
1:A:112:LEU:C	1:A:112:LEU:HD23	2.32	0.50
1:C:56:THR:HB	1:C:57:PRO:HD2	1.93	0.50
1:E:69:ASP:OD1	1:E:71:SER:OG	2.18	0.50
1:D:23:ILE:CD1	1:D:62:ARG:HD3	2.41	0.50
1:H:8:LEU:HG	2:H:3514:TTP:O2	2.12	0.50
1:A:118:PHE:CE2	1:A:122:LEU:HD11	2.47	0.50
1:E:179:ASP:C	1:E:179:ASP:OD1	2.49	0.50
1:C:26:GLN:NE2	1:C:26:GLN:H	2.10	0.50
1:D:23:ILE:HG12	1:D:24:SER:N	2.27	0.50
1:G:255:GLU:O	1:G:259:ARG:HG3	2.12	0.50
1:F:60:THR:N	1:F:61:PRO:CD	2.75	0.49
1:C:242:LEU:O	1:C:246:GLN:HG3	2.12	0.49
1:E:23:ILE:HD11	1:E:27:LEU:CD1	2.42	0.49
1:F:16:LEU:HD12	1:F:25:LYS:HD3	1.95	0.49
1:G:243:GLU:HG2	1:G:249:LYS:HA	1.93	0.49
1:D:60:THR:HB	1:D:61:PRO:HD3	1.94	0.49
1:H:23:ILE:CG1	1:H:24:SER:H	2.22	0.49
1:E:56:THR:HB	1:E:57:PRO:HD2	1.94	0.49
1:D:23:ILE:HG12	1:D:24:SER:H	1.78	0.49
1:A:4:LYS:NZ	1:A:102:ASP:OD2	2.22	0.49
1:B:8:LEU:HG	2:B:3502:TTP:C2	2.47	0.49
1:C:255:GLU:O	1:C:259:ARG:HG3	2.12	0.49
1:D:273:ALA:HB3	1:D:274:PRO:CD	2.42	0.49
1:D:260:GLN:O	1:D:261:LYS:HB2	2.13	0.49
1:E:23:ILE:HG12	1:E:24:SER:N	2.28	0.49
1:C:23:ILE:HG12	1:C:27:LEU:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:14:THR:O	1:G:16:LEU:N	2.46	0.48
1:H:255:GLU:OE1	1:H:283:TYR:OH	2.25	0.48
1:D:16:LEU:HA	1:D:229:HIS:CE1	2.48	0.48
1:F:238:PHE:CE1	1:H:238:PHE:CE1	3.01	0.48
1:F:4:LYS:O	1:F:104:SER:HA	2.13	0.48
1:C:8:LEU:HG	2:C:3504:TTP:C2	2.47	0.48
1:D:38:TYR:HB2	1:D:39:PRO:HD3	1.94	0.48
1:A:273:ALA:N	1:A:274:PRO:HD2	2.29	0.48
1:G:59:ASP:OD1	1:G:62:ARG:NH1	2.44	0.48
1:G:216:ILE:HG22	1:G:217:MET:N	2.26	0.48
1:A:25:LYS:HE3	1:A:26:GLN:HE22	1.79	0.48
1:C:24:SER:HB2	1:C:59:ASP:OD2	2.14	0.48
1:E:111:ASN:N	1:E:111:ASN:HD22	2.10	0.48
1:D:81:VAL:HG12	1:D:82:GLN:N	2.28	0.48
1:E:18:PRO:O	1:E:19:ALA:C	2.51	0.47
1:A:25:LYS:HE3	1:A:26:GLN:NE2	2.28	0.47
1:D:31:TYR:CD1	1:D:240:ALA:HB2	2.50	0.47
1:C:8:LEU:HD23	1:C:88:LEU:HD22	1.96	0.47
1:C:112:LEU:C	1:C:112:LEU:HD23	2.34	0.47
1:G:8:LEU:HG	2:G:3512:TTP:C2	2.49	0.47
1:C:27:LEU:HD21	1:C:63:PHE:CE2	2.50	0.47
1:D:249:LYS:HD2	1:D:283:TYR:CD2	2.49	0.47
1:F:273:ALA:HB3	1:F:274:PRO:HD3	1.95	0.47
1:H:31:TYR:CD1	1:H:240:ALA:HB2	2.49	0.47
1:B:120:GLU:N	1:B:120:GLU:OE1	2.47	0.47
1:C:60:THR:HB	1:C:61:PRO:HD3	1.96	0.47
1:G:23:ILE:CG2	1:G:28:LEU:HD23	2.45	0.47
1:B:237:GLN:HG2	1:D:237:GLN:HG2	1.97	0.47
1:H:260:GLN:O	1:H:261:LYS:HB2	2.15	0.47
1:A:56:THR:HB	1:A:57:PRO:HD2	1.97	0.47
1:G:112:LEU:C	1:G:112:LEU:HD23	2.35	0.47
1:B:111:ASN:N	1:B:111:ASN:HD22	2.11	0.46
1:C:14:THR:O	1:C:16:LEU:N	2.48	0.46
1:A:60:THR:HB	1:A:61:PRO:HD3	1.98	0.46
1:D:82:GLN:HG2	1:D:84:SER:O	2.14	0.46
1:G:14:THR:HG22	1:G:17:HIS:HE1	1.79	0.46
1:H:264:ASP:OD1	1:H:264:ASP:C	2.54	0.46
1:B:241:THR:HA	1:D:234:GLU:OE1	2.15	0.46
1:G:81:VAL:HG12	1:G:82:GLN:N	2.31	0.46
1:G:260:GLN:O	1:G:261:LYS:CB	2.62	0.46
1:G:23:ILE:CG2	1:G:28:LEU:HD21	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:GLN:O	1:D:261:LYS:CB	2.61	0.46
1:D:25:LYS:NZ	1:D:110:ASP:OD2	2.40	0.46
1:D:16:LEU:HD23	1:D:16:LEU:N	2.27	0.46
1:G:8:LEU:HD23	1:G:88:LEU:HD22	1.98	0.45
1:A:255:GLU:O	1:A:259:ARG:HG3	2.17	0.45
1:F:255:GLU:OE1	1:F:283:TYR:OH	2.14	0.45
1:D:272:ALA:O	1:D:273:ALA:C	2.55	0.45
1:H:67:LEU:HA	1:H:67:LEU:HD23	1.70	0.45
1:G:8:LEU:HG	2:G:3512:TTP:O2	2.15	0.45
1:A:21:LEU:HA	1:A:21:LEU:HD23	1.83	0.45
1:C:14:THR:HA	1:C:17:HIS:CE1	2.52	0.45
1:F:111:ASN:N	1:F:111:ASN:HD22	2.13	0.45
1:E:199:ILE:CG2	1:E:200:THR:N	2.78	0.45
1:D:8:LEU:HA	1:D:8:LEU:HD12	1.75	0.45
1:H:260:GLN:O	1:H:261:LYS:CB	2.64	0.45
1:F:173:THR:HB	1:F:223:TRP:CE2	2.51	0.45
1:D:273:ALA:HB3	1:D:274:PRO:HD3	1.98	0.45
1:A:120:GLU:OE1	1:A:120:GLU:N	2.50	0.45
1:A:260:GLN:O	1:A:261:LYS:CB	2.65	0.45
1:C:272:ALA:O	1:C:273:ALA:C	2.55	0.45
1:C:273:ALA:HB3	1:C:274:PRO:CD	2.47	0.45
1:B:2:LYS:HG3	1:B:2:LYS:O	2.16	0.45
1:H:8:LEU:HD23	1:H:88:LEU:HD22	1.99	0.44
1:E:32:ASP:OD2	1:E:243:GLU:OE1	2.34	0.44
1:H:204:ARG:HH11	1:H:204:ARG:HD2	1.63	0.44
1:F:120:GLU:N	1:F:120:GLU:OE1	2.51	0.44
1:G:260:GLN:O	1:G:261:LYS:HB2	2.17	0.44
1:A:145:TYR:OH	1:A:225:ASP:OD2	2.28	0.44
1:F:184:ASP:HA	1:F:187:ARG:HG3	2.00	0.44
1:C:27:LEU:HD21	1:C:63:PHE:CD2	2.53	0.44
1:C:58:GLN:HE21	1:C:62:ARG:HH12	1.66	0.44
1:A:54:ILE:HA	1:A:80:ALA:O	2.18	0.44
1:G:192:SER:O	1:G:195:GLY:N	2.44	0.44
1:C:120:GLU:N	1:C:120:GLU:OE1	2.51	0.44
1:H:117:ASP:O	1:H:118:PHE:C	2.55	0.43
1:C:58:GLN:HE21	1:C:62:ARG:NH2	2.13	0.43
1:G:255:GLU:OE1	1:G:283:TYR:OH	2.31	0.43
1:D:56:THR:HB	1:D:57:PRO:HD2	2.00	0.43
1:A:14:THR:N	2:A:3500:TTP:O2G	2.52	0.43
1:E:19:ALA:HA	1:F:34:PRO:HG3	1.99	0.43
1:A:249:LYS:HD2	1:A:283:TYR:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:14:THR:C	1:G:16:LEU:N	2.69	0.43
1:H:15:ARG:HG3	2:H:3514:TTP:O1G	2.19	0.43
1:D:118:PHE:CE2	1:D:122:LEU:HD11	2.54	0.43
1:E:192:SER:HB2	1:E:193:PRO:CD	2.45	0.43
1:B:56:THR:HB	1:B:57:PRO:HD2	2.00	0.43
1:C:67:LEU:HD23	1:C:67:LEU:HA	1.76	0.43
1:B:41:SER:HB2	1:B:256:ILE:CD1	2.49	0.43
1:C:58:GLN:NE2	1:C:62:ARG:HH12	2.17	0.43
1:E:33:LYS:NZ	1:E:250:VAL:O	2.52	0.43
1:F:32:ASP:OD2	1:F:243:GLU:OE1	2.36	0.43
1:G:4:LYS:O	1:G:104:SER:HA	2.19	0.42
1:G:60:THR:N	1:G:61:PRO:CD	2.82	0.42
1:C:4:LYS:O	1:C:104:SER:HA	2.20	0.42
1:G:90:GLN:O	1:G:91:ALA:C	2.57	0.42
1:C:137:TYR:CE2	1:C:223:TRP:HB3	2.54	0.42
1:B:32:ASP:OD2	1:B:243:GLU:OE1	2.37	0.42
1:C:17:HIS:CD2	1:C:21:LEU:CD2	3.02	0.42
1:F:118:PHE:CE2	1:F:122:LEU:HD11	2.54	0.42
1:C:2:LYS:HG3	1:C:2:LYS:O	2.20	0.42
1:B:26:GLN:NE2	1:B:26:GLN:H	2.18	0.42
1:E:118:PHE:CE2	1:E:122:LEU:HD11	2.54	0.42
1:A:23:ILE:HG21	1:B:23:ILE:HD12	2.02	0.42
1:D:137:TYR:CD2	1:D:223:TRP:HE3	2.38	0.42
1:C:249:LYS:HD2	1:C:283:TYR:CD2	2.54	0.42
1:B:31:TYR:CD1	1:B:240:ALA:HB2	2.54	0.42
1:F:121:LEU:HD11	1:F:135:PHE:HE2	1.84	0.42
1:H:54:ILE:HA	1:H:80:ALA:O	2.19	0.42
1:G:23:ILE:HG21	1:G:28:LEU:HD23	1.99	0.42
1:F:8:LEU:HD21	1:F:88:LEU:HA	2.01	0.42
1:H:249:LYS:HD2	1:H:283:TYR:CD2	2.54	0.42
1:E:199:ILE:HG23	1:E:200:THR:N	2.34	0.42
1:A:260:GLN:O	1:A:261:LYS:HB2	2.18	0.42
1:H:228:THR:O	1:H:229:HIS:C	2.57	0.42
1:F:28:LEU:HA	1:F:29:PRO:HD3	1.81	0.42
1:G:56:THR:HB	1:G:57:PRO:HD2	2.01	0.42
1:G:122:LEU:HD23	1:G:122:LEU:HA	1.79	0.42
1:H:242:LEU:O	1:H:246:GLN:HG3	2.19	0.42
1:F:35:MET:HB2	1:F:35:MET:HE2	1.97	0.42
1:A:27:LEU:HA	1:A:27:LEU:HD23	1.86	0.42
1:B:13:GLY:HA2	2:B:3502:TTP:O3B	2.19	0.42
1:E:112:LEU:HD23	1:E:112:LEU:C	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:59:ASP:OD1	1:H:62:ARG:NH1	2.48	0.42
1:D:23:ILE:HD11	1:D:62:ARG:CD	2.49	0.42
1:E:273:ALA:N	1:E:274:PRO:CD	2.83	0.42
1:C:88:LEU:HB2	1:C:199:ILE:HB	2.02	0.42
1:H:64:GLN:HA	1:H:79:TYR:CZ	2.55	0.42
1:C:264:ASP:OD1	1:C:264:ASP:C	2.58	0.42
1:B:58:GLN:CD	1:B:58:GLN:H	2.22	0.42
1:F:116:HIS:O	1:F:117:ASP:HB2	2.19	0.41
1:B:238:PHE:CE1	1:D:238:PHE:CE1	3.08	0.41
1:E:4:LYS:O	1:E:104:SER:HA	2.20	0.41
1:B:192:SER:O	1:B:195:GLY:N	2.47	0.41
1:D:25:LYS:HE3	1:D:26:GLN:NE2	2.35	0.41
1:B:55:SER:OG	1:B:56:THR:N	2.54	0.41
1:F:110:ASP:OD1	1:F:110:ASP:C	2.58	0.41
1:C:8:LEU:HD23	1:C:88:LEU:CD2	2.50	0.41
1:F:137:TYR:CE2	1:F:223:TRP:HB3	2.55	0.41
1:F:243:GLU:HG2	1:F:249:LYS:HA	2.00	0.41
1:H:16:LEU:O	1:H:17:HIS:C	2.57	0.41
1:B:60:THR:N	1:B:61:PRO:CD	2.83	0.41
1:D:64:GLN:HA	1:D:79:TYR:CZ	2.55	0.41
1:E:8:LEU:HD21	1:E:88:LEU:HA	2.02	0.41
1:C:15:ARG:NE	2:C:3504:TTP:O1G	2.41	0.41
1:H:272:ALA:O	1:H:273:ALA:C	2.59	0.41
1:C:162:LYS:N	1:C:163:PRO:CD	2.83	0.41
1:E:21:LEU:HD23	1:E:21:LEU:HA	1.89	0.41
1:F:31:TYR:CD1	1:F:240:ALA:HB2	2.56	0.41
1:G:273:ALA:N	1:G:274:PRO:HD2	2.35	0.41
1:H:28:LEU:HA	1:H:29:PRO:HD3	1.85	0.41
1:H:35:MET:SD	1:H:110:ASP:HA	2.60	0.41
1:C:280:TYR:CG	1:D:18:PRO:HD3	2.56	0.41
1:A:55:SER:OG	1:A:56:THR:N	2.53	0.41
1:H:199:ILE:HA	1:H:199:ILE:HD12	1.92	0.41
1:G:24:SER:CB	1:G:59:ASP:OD2	2.63	0.41
1:C:27:LEU:HD23	1:C:27:LEU:HA	1.93	0.41
1:D:32:ASP:OD2	1:D:243:GLU:OE1	2.38	0.41
1:D:17:HIS:NE2	1:D:21:LEU:HD23	2.36	0.41
1:F:268:LEU:O	1:F:269:GLU:C	2.58	0.41
1:E:60:THR:HB	1:E:61:PRO:HD3	2.03	0.41
1:F:35:MET:SD	1:F:110:ASP:HA	2.61	0.41
1:E:23:ILE:HD11	1:E:27:LEU:HD13	2.02	0.41
1:A:8:LEU:HD21	1:A:88:LEU:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:LEU:HB2	1:H:79:TYR:OH	2.21	0.41
1:B:199:ILE:CG2	1:B:200:THR:N	2.83	0.41
1:E:25:LYS:HE3	1:E:26:GLN:HE22	1.85	0.41
1:F:14:THR:C	1:F:16:LEU:N	2.75	0.40
1:H:287:LEU:HD23	1:H:287:LEU:HA	1.87	0.40
1:A:32:ASP:OD2	1:A:243:GLU:OE1	2.37	0.40
1:C:260:GLN:O	1:C:261:LYS:CB	2.67	0.40
1:C:14:THR:C	1:C:16:LEU:N	2.72	0.40
1:A:249:LYS:HD2	1:A:283:TYR:CG	2.55	0.40
1:F:239:ILE:HA	1:F:239:ILE:HD13	1.82	0.40
1:B:116:HIS:O	1:B:117:ASP:HB2	2.20	0.40
1:G:35:MET:SD	1:G:110:ASP:HA	2.61	0.40
1:D:16:LEU:O	1:D:229:HIS:HE1	2.04	0.40
1:H:31:TYR:CE1	1:H:240:ALA:HB2	2.56	0.40
1:B:233:LEU:HD12	1:B:233:LEU:HA	1.76	0.40
1:H:27:LEU:HA	1:H:27:LEU:HD23	1.80	0.40
1:C:117:ASP:O	1:C:118:PHE:C	2.58	0.40
1:D:28:LEU:HA	1:D:29:PRO:HD3	1.84	0.40
2:D:3506:TTP:H2'2	2:D:3506:TTP:O1B	2.22	0.40
1:G:54:ILE:HD13	1:G:54:ILE:HG21	1.88	0.40
1:D:117:ASP:O	1:D:118:PHE:C	2.59	0.40
1:A:251:ALA:O	1:A:253:PRO:HD3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:127:GLN:OE1	1:H:167:LYS:NZ[2_647]	2.19	0.01

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	290/293 (99%)	285 (98%)	4 (1%)	1 (0%)	46	72
1	B	290/293 (99%)	282 (97%)	7 (2%)	1 (0%)	46	72
1	C	290/293 (99%)	280 (97%)	9 (3%)	1 (0%)	46	72
1	D	290/293 (99%)	283 (98%)	5 (2%)	2 (1%)	26	51
1	E	290/293 (99%)	282 (97%)	7 (2%)	1 (0%)	46	72
1	F	290/293 (99%)	284 (98%)	5 (2%)	1 (0%)	46	72
1	G	290/293 (99%)	281 (97%)	8 (3%)	1 (0%)	46	72
1	H	290/293 (99%)	283 (98%)	5 (2%)	2 (1%)	26	51
All	All	2320/2344 (99%)	2260 (97%)	50 (2%)	10 (0%)	39	65

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	23	ILE
1	C	31	TYR
1	A	31	TYR
1	B	31	TYR
1	D	31	TYR
1	E	31	TYR
1	F	31	TYR
1	G	31	TYR
1	H	31	TYR
1	H	23	ILE

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	239/240 (100%)	234 (98%)	5 (2%)	61	85
1	B	239/240 (100%)	234 (98%)	5 (2%)	61	85
1	C	239/240 (100%)	231 (97%)	8 (3%)	45	73
1	D	239/240 (100%)	231 (97%)	8 (3%)	45	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	239/240 (100%)	230 (96%)	9 (4%)	40 68
1	F	239/240 (100%)	234 (98%)	5 (2%)	61 85
1	G	239/240 (100%)	231 (97%)	8 (3%)	45 73
1	H	239/240 (100%)	235 (98%)	4 (2%)	68 88
All	All	1912/1920 (100%)	1860 (97%)	52 (3%)	52 79

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	SER
1	A	111	ASN
1	A	209	ARG
1	A	225	ASP
1	A	252	CYS
1	B	24	SER
1	B	26	GLN
1	B	119	HIS
1	B	225	ASP
1	B	252	CYS
1	C	20	THR
1	C	24	SER
1	C	26	GLN
1	C	119	HIS
1	C	126	SER
1	C	225	ASP
1	C	252	CYS
1	C	260	GLN
1	D	12	SER
1	D	20	THR
1	D	119	HIS
1	D	126	SER
1	D	164	LEU
1	D	209	ARG
1	D	225	ASP
1	D	252	CYS
1	E	12	SER
1	E	24	SER
1	E	111	ASN
1	E	117	ASP
1	E	119	HIS
1	E	126	SER

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Mol	Chain	Res	Type
1	E	209	ARG
1	E	225	ASP
1	E	252	CYS
1	F	24	SER
1	F	111	ASN
1	F	119	HIS
1	F	225	ASP
1	F	252	CYS
1	G	12	SER
1	G	20	THR
1	G	24	SER
1	G	26	GLN
1	G	119	HIS
1	G	126	SER
1	G	225	ASP
1	G	252	CYS
1	H	12	SER
1	H	119	HIS
1	H	225	ASP
1	H	252	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	26	GLN
1	A	111	ASN
1	B	26	GLN
1	B	111	ASN
1	C	17	HIS
1	C	26	GLN
1	C	58	GLN
1	C	119	HIS
1	D	26	GLN
1	D	119	HIS
1	D	229	HIS
1	E	26	GLN
1	E	111	ASN
1	E	119	HIS
1	F	26	GLN
1	F	111	ASN
1	F	229	HIS
1	G	17	HIS

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Mol	Chain	Res	Type
1	G	119	HIS
1	H	26	GLN
1	H	119	HIS

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

16 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	TTP	A	3500	-	21,30,30	2.45	6 (28%)	31,47,47	1.97	8 (25%)
2	TTP	A	3501	-	21,30,30	2.28	7 (33%)	31,47,47	2.02	9 (29%)
2	TTP	B	3502	-	21,30,30	2.27	7 (33%)	31,47,47	2.51	9 (29%)
2	TTP	B	3503	-	21,30,30	2.46	7 (33%)	31,47,47	2.19	9 (29%)
2	TTP	C	3504	-	21,30,30	2.22	7 (33%)	31,47,47	2.08	7 (22%)
2	TTP	C	3505	-	21,30,30	2.53	5 (23%)	31,47,47	2.95	9 (29%)
2	TTP	D	3506	-	21,30,30	2.21	7 (33%)	31,47,47	2.17	9 (29%)
2	TTP	D	3507	-	21,30,30	2.25	6 (28%)	31,47,47	2.59	8 (25%)
2	TTP	E	3508	-	21,30,30	2.17	8 (38%)	31,47,47	2.16	9 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	TTP	E	3509	-	21,30,30	2.24	6 (28%)	31,47,47	2.12	8 (25%)
2	TTP	F	3510	-	21,30,30	2.29	6 (28%)	31,47,47	2.00	10 (32%)
2	TTP	F	3511	-	21,30,30	2.32	5 (23%)	31,47,47	2.25	10 (32%)
2	TTP	G	3512	-	21,30,30	2.19	6 (28%)	31,47,47	2.25	7 (22%)
2	TTP	G	3513	-	21,30,30	2.16	5 (23%)	31,47,47	2.65	9 (29%)
2	TTP	H	3514	-	21,30,30	2.27	8 (38%)	31,47,47	2.11	9 (29%)
2	TTP	H	3515	-	21,30,30	2.26	6 (28%)	31,47,47	2.52	9 (29%)

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	TTP	A	3500	-	-	0/18/34/34	0/2/2/2
2	TTP	A	3501	-	-	0/18/34/34	0/2/2/2
2	TTP	B	3502	-	-	0/18/34/34	0/2/2/2
2	TTP	B	3503	-	-	0/18/34/34	0/2/2/2
2	TTP	C	3504	-	-	0/18/34/34	0/2/2/2
2	TTP	C	3505	-	-	0/18/34/34	0/2/2/2
2	TTP	D	3506	-	-	0/18/34/34	0/2/2/2
2	TTP	D	3507	-	-	0/18/34/34	0/2/2/2
2	TTP	E	3508	-	-	0/18/34/34	0/2/2/2
2	TTP	E	3509	-	-	0/18/34/34	0/2/2/2
2	TTP	F	3510	-	-	0/18/34/34	0/2/2/2
2	TTP	F	3511	-	-	0/18/34/34	0/2/2/2
2	TTP	G	3512	-	-	0/18/34/34	0/2/2/2
2	TTP	G	3513	-	-	0/18/34/34	0/2/2/2
2	TTP	H	3514	-	-	0/18/34/34	0/2/2/2
2	TTP	H	3515	-	-	0/18/34/34	0/2/2/2

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3505	TTP	C3'-C4'	-5.85	1.36	1.53
2	F	3510	TTP	C3'-C4'	-5.71	1.36	1.53
2	F	3511	TTP	C3'-C4'	-5.61	1.37	1.53
2	D	3507	TTP	C3'-C4'	-5.45	1.37	1.53
2	B	3503	TTP	C3'-C4'	-5.40	1.37	1.53
2	B	3503	TTP	C2'-C1'	-5.34	1.37	1.52
2	C	3505	TTP	C2'-C3'	-5.26	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3505	TTP	C2'-C1'	-5.16	1.37	1.52
2	A	3500	TTP	C3'-C4'	-5.15	1.38	1.53
2	D	3506	TTP	C3'-C4'	-5.11	1.38	1.53
2	A	3501	TTP	C2'-C1'	-5.08	1.38	1.52
2	G	3513	TTP	C3'-C4'	-5.08	1.38	1.53
2	F	3511	TTP	C2'-C1'	-5.02	1.38	1.52
2	H	3515	TTP	C3'-C4'	-4.98	1.38	1.53
2	A	3500	TTP	C2'-C1'	-4.94	1.38	1.52
2	A	3501	TTP	C3'-C4'	-4.86	1.39	1.53
2	E	3509	TTP	C2'-C1'	-4.80	1.38	1.52
2	G	3512	TTP	C2'-C3'	-4.75	1.40	1.52
2	H	3514	TTP	C2'-C3'	-4.75	1.40	1.52
2	D	3507	TTP	C2'-C1'	-4.73	1.39	1.52
2	B	3502	TTP	C3'-C4'	-4.68	1.39	1.53
2	G	3513	TTP	C2'-C3'	-4.65	1.40	1.52
2	C	3504	TTP	C2'-C3'	-4.64	1.40	1.52
2	E	3508	TTP	C2'-C1'	-4.63	1.39	1.52
2	F	3510	TTP	C2'-C1'	-4.62	1.39	1.52
2	G	3512	TTP	C2'-C1'	-4.60	1.39	1.52
2	H	3515	TTP	C2'-C1'	-4.53	1.39	1.52
2	E	3509	TTP	C3'-C4'	-4.52	1.40	1.53
2	F	3511	TTP	C2'-C3'	-4.51	1.40	1.52
2	B	3503	TTP	C2'-C3'	-4.43	1.40	1.52
2	D	3506	TTP	C2'-C1'	-4.41	1.39	1.52
2	D	3506	TTP	C2'-C3'	-4.41	1.40	1.52
2	A	3500	TTP	C2'-C3'	-4.41	1.40	1.52
2	B	3502	TTP	C2'-C1'	-4.39	1.40	1.52
2	H	3515	TTP	C2'-C3'	-4.36	1.41	1.52
2	C	3504	TTP	C2'-C1'	-4.31	1.40	1.52
2	A	3500	TTP	C6-N1	-4.19	1.28	1.35
2	G	3513	TTP	C2'-C1'	-4.15	1.40	1.52
2	E	3508	TTP	C3'-C4'	-4.13	1.41	1.53
2	D	3507	TTP	C2'-C3'	-4.05	1.41	1.52
2	E	3508	TTP	C2'-C3'	-4.02	1.42	1.52
2	E	3509	TTP	C2'-C3'	-4.01	1.42	1.52
2	C	3504	TTP	C3'-C4'	-4.00	1.41	1.53
2	H	3514	TTP	C2'-C1'	-3.92	1.41	1.52
2	G	3512	TTP	C3'-C4'	-3.89	1.42	1.53
2	B	3502	TTP	C5'-C4'	-3.88	1.39	1.51
2	A	3501	TTP	C2'-C3'	-3.84	1.42	1.52
2	F	3510	TTP	C2'-C3'	-3.77	1.42	1.52
2	H	3514	TTP	C3'-C4'	-3.74	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3502	TTP	C2'-C3'	-3.74	1.42	1.52
2	B	3503	TTP	C5'-C4'	-3.68	1.39	1.51
2	G	3512	TTP	C6-N1	-3.58	1.29	1.35
2	F	3510	TTP	C5'-C4'	-3.57	1.40	1.51
2	C	3505	TTP	O4'-C4'	-3.53	1.36	1.45
2	D	3507	TTP	C5'-C4'	-3.49	1.40	1.51
2	H	3514	TTP	C5'-C4'	-3.47	1.40	1.51
2	B	3502	TTP	C6-N1	-3.45	1.29	1.35
2	D	3506	TTP	C5'-C4'	-3.42	1.40	1.51
2	H	3515	TTP	C5'-C4'	-3.42	1.40	1.51
2	A	3500	TTP	C5'-C4'	-3.34	1.40	1.51
2	C	3505	TTP	C5'-C4'	-3.26	1.41	1.51
2	H	3515	TTP	O4'-C4'	-3.22	1.37	1.45
2	D	3507	TTP	O4'-C4'	-3.21	1.37	1.45
2	E	3508	TTP	C5'-C4'	-3.19	1.41	1.51
2	G	3513	TTP	C5'-C4'	-3.18	1.41	1.51
2	H	3514	TTP	C6-N1	-3.17	1.30	1.35
2	F	3510	TTP	C6-N1	-3.10	1.30	1.35
2	C	3504	TTP	C5'-C4'	-3.01	1.41	1.51
2	G	3512	TTP	C5'-C4'	-2.98	1.42	1.51
2	C	3504	TTP	C6-N1	-2.98	1.30	1.35
2	A	3501	TTP	C5'-C4'	-2.95	1.42	1.51
2	B	3503	TTP	C6-N1	-2.94	1.30	1.35
2	F	3511	TTP	C5'-C4'	-2.92	1.42	1.51
2	E	3509	TTP	C5'-C4'	-2.88	1.42	1.51
2	C	3504	TTP	PG-O3G	-2.77	1.44	1.54
2	A	3501	TTP	C6-N1	-2.73	1.30	1.35
2	E	3509	TTP	PA-O2A	-2.72	1.43	1.54
2	B	3502	TTP	PG-O3G	-2.69	1.45	1.54
2	F	3511	TTP	PB-O2B	-2.68	1.43	1.54
2	A	3500	TTP	PG-O3G	-2.65	1.45	1.54
2	G	3513	TTP	O4'-C4'	-2.65	1.38	1.45
2	D	3506	TTP	C6-N1	-2.62	1.31	1.35
2	F	3510	TTP	PG-O2G	-2.61	1.45	1.54
2	E	3508	TTP	PB-O2B	-2.59	1.43	1.54
2	B	3502	TTP	PG-O2G	-2.54	1.45	1.54
2	B	3503	TTP	PA-O1A	-2.42	1.42	1.51
2	H	3515	TTP	PB-O2B	-2.38	1.44	1.54
2	E	3508	TTP	C6-N1	-2.35	1.31	1.35
2	A	3501	TTP	PA-O2A	-2.32	1.45	1.54
2	H	3514	TTP	PG-O3G	-2.30	1.46	1.54
2	D	3507	TTP	PB-O2B	-2.28	1.45	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	3508	TTP	PG-O1G	-2.22	1.43	1.51
2	D	3506	TTP	PG-O3G	-2.09	1.47	1.54
2	B	3503	TTP	PB-O2B	-2.09	1.46	1.54
2	E	3508	TTP	PG-O3G	-2.04	1.47	1.54
2	C	3504	TTP	PG-O2G	-2.03	1.47	1.54
2	D	3506	TTP	C4-N3	2.22	1.37	1.33
2	G	3512	TTP	C4-N3	2.23	1.37	1.33
2	H	3514	TTP	O4'-C1'	2.38	1.47	1.42
2	A	3501	TTP	C4-N3	2.77	1.38	1.33
2	E	3509	TTP	C4-N3	2.84	1.38	1.33
2	H	3514	TTP	C4-N3	3.32	1.39	1.33

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3505	TTP	C5-C4-N3	-8.29	115.91	125.14
2	G	3512	TTP	C5-C4-N3	-7.02	117.32	125.14
2	D	3507	TTP	C5-C4-N3	-6.94	117.41	125.14
2	B	3502	TTP	C5-C4-N3	-6.86	117.50	125.14
2	E	3509	TTP	C5-C4-N3	-6.25	118.18	125.14
2	G	3513	TTP	C5-C4-N3	-6.15	118.28	125.14
2	C	3504	TTP	C5-C4-N3	-6.05	118.40	125.14
2	E	3508	TTP	C5-C4-N3	-5.99	118.47	125.14
2	D	3506	TTP	C5-C4-N3	-5.92	118.54	125.14
2	A	3500	TTP	C5-C4-N3	-5.87	118.60	125.14
2	H	3515	TTP	C5-C4-N3	-5.86	118.62	125.14
2	H	3514	TTP	C5-C4-N3	-5.80	118.68	125.14
2	F	3511	TTP	C5-C4-N3	-5.46	119.05	125.14
2	F	3510	TTP	C5-C4-N3	-5.34	119.19	125.14
2	B	3503	TTP	C5-C4-N3	-5.33	119.20	125.14
2	C	3505	TTP	PB-O3B-PG	-5.17	115.35	132.67
2	C	3505	TTP	PB-O3A-PA	-5.10	118.40	132.73
2	A	3501	TTP	PB-O3A-PA	-4.94	118.84	132.73
2	G	3513	TTP	PB-O3B-PG	-4.88	116.30	132.67
2	G	3513	TTP	PB-O3A-PA	-4.64	119.71	132.73
2	D	3507	TTP	PB-O3B-PG	-4.63	117.13	132.67
2	H	3515	TTP	PB-O3B-PG	-4.45	117.75	132.67
2	B	3503	TTP	PB-O3A-PA	-4.43	120.28	132.73
2	H	3515	TTP	PB-O3A-PA	-4.42	120.32	132.73
2	A	3501	TTP	C5-C4-N3	-4.26	120.39	125.14
2	D	3507	TTP	PB-O3A-PA	-4.12	121.15	132.73
2	D	3506	TTP	PB-O3B-PG	-3.97	119.37	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3504	TTP	PB-O3B-PG	-3.94	119.45	132.67
2	A	3500	TTP	PB-O3A-PA	-3.87	121.87	132.73
2	H	3514	TTP	PB-O3A-PA	-3.70	122.34	132.73
2	F	3511	TTP	PB-O3A-PA	-3.54	122.79	132.73
2	E	3509	TTP	PB-O3A-PA	-3.40	123.19	132.73
2	F	3510	TTP	PB-O3A-PA	-3.39	123.22	132.73
2	C	3504	TTP	PB-O3A-PA	-3.35	123.33	132.73
2	E	3508	TTP	PB-O3A-PA	-3.26	123.58	132.73
2	B	3502	TTP	PB-O3A-PA	-3.22	123.69	132.73
2	G	3512	TTP	PB-O3B-PG	-3.22	121.88	132.67
2	F	3511	TTP	C5M-C5-C4	-3.17	115.96	120.05
2	A	3500	TTP	PB-O3B-PG	-3.03	122.50	132.67
2	H	3514	TTP	C5M-C5-C4	-2.94	116.26	120.05
2	D	3506	TTP	O3'-C3'-C4'	-2.81	98.71	110.05
2	H	3514	TTP	PB-O3B-PG	-2.76	123.42	132.67
2	D	3507	TTP	C5M-C5-C4	-2.69	116.58	120.05
2	E	3508	TTP	C5M-C5-C4	-2.66	116.62	120.05
2	E	3509	TTP	PB-O3B-PG	-2.57	124.06	132.67
2	A	3500	TTP	O4'-C1'-C2'	-2.54	101.20	106.27
2	E	3508	TTP	PB-O3B-PG	-2.52	124.21	132.67
2	G	3512	TTP	PB-O3A-PA	-2.48	125.75	132.73
2	F	3510	TTP	PB-O3B-PG	-2.48	124.34	132.67
2	F	3510	TTP	O4'-C1'-C2'	-2.47	101.34	106.27
2	B	3502	TTP	PB-O3B-PG	-2.41	124.58	132.67
2	H	3515	TTP	C2'-C1'-N1	-2.31	108.53	114.16
2	A	3501	TTP	PB-O3B-PG	-2.29	124.98	132.67
2	F	3511	TTP	PB-O3B-PG	-2.28	125.04	132.67
2	D	3506	TTP	PB-O3A-PA	-2.26	126.37	132.73
2	B	3503	TTP	O2B-PB-O3B	-2.08	95.68	105.09
2	F	3510	TTP	O3'-C3'-C4'	-2.05	101.77	110.05
2	B	3503	TTP	O5'-C5'-C4'	2.06	116.70	109.12
2	E	3508	TTP	O3G-PG-O3B	2.06	114.44	105.09
2	A	3500	TTP	C2'-C3'-C4'	2.06	107.04	102.77
2	A	3500	TTP	O3G-PG-O2G	2.07	115.24	107.38
2	B	3502	TTP	O2B-PB-O3A	2.07	114.47	105.09
2	B	3502	TTP	C2'-C3'-C4'	2.07	107.07	102.77
2	F	3510	TTP	O3'-C3'-C2'	2.09	117.67	110.74
2	B	3502	TTP	O3A-PA-O5'	2.12	108.57	102.94
2	B	3503	TTP	C2'-C3'-C4'	2.13	107.19	102.77
2	B	3502	TTP	C5M-C5-C6	2.14	122.92	118.62
2	H	3515	TTP	C5M-C5-C6	2.14	122.93	118.62
2	C	3504	TTP	C3'-C2'-C1'	2.15	107.56	102.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	3505	TTP	O2B-PB-O1B	2.15	124.17	112.53
2	C	3505	TTP	O3G-PG-O2G	2.18	115.67	107.38
2	F	3511	TTP	O2A-PA-O3A	2.19	115.02	105.09
2	H	3514	TTP	O3A-PA-O5'	2.19	108.74	102.94
2	F	3511	TTP	C2'-C3'-C4'	2.19	107.32	102.77
2	E	3509	TTP	C2'-C3'-C4'	2.20	107.33	102.77
2	D	3506	TTP	C2'-C3'-C4'	2.26	107.45	102.77
2	G	3513	TTP	O3G-PG-O2G	2.28	116.06	107.38
2	B	3502	TTP	O3G-PG-O2G	2.28	116.06	107.38
2	D	3507	TTP	O2B-PB-O1B	2.28	124.91	112.53
2	D	3506	TTP	O3G-PG-O2G	2.29	116.10	107.38
2	A	3500	TTP	O2B-PB-O1B	2.29	124.95	112.53
2	B	3503	TTP	C5M-C5-C6	2.30	123.24	118.62
2	A	3501	TTP	O5'-C5'-C4'	2.31	117.65	109.12
2	E	3508	TTP	O3G-PG-O2G	2.32	116.20	107.38
2	F	3511	TTP	O4'-C4'-C5'	2.35	117.74	109.32
2	E	3509	TTP	O3'-C3'-C2'	2.45	118.85	110.74
2	G	3513	TTP	O2B-PB-O1B	2.47	125.92	112.53
2	F	3510	TTP	O4'-C1'-N1	2.47	112.00	107.72
2	F	3510	TTP	C2'-C3'-C4'	2.59	108.14	102.77
2	A	3501	TTP	O3'-C3'-C2'	2.60	119.36	110.74
2	C	3505	TTP	O5'-C5'-C4'	2.65	118.90	109.12
2	D	3506	TTP	C3'-C2'-C1'	2.66	108.80	102.40
2	H	3515	TTP	O2B-PB-O1B	2.69	127.12	112.53
2	F	3511	TTP	O5'-C5'-C4'	2.69	119.05	109.12
2	A	3501	TTP	O4'-C4'-C5'	2.71	119.03	109.32
2	A	3501	TTP	C2'-C3'-C4'	2.73	108.43	102.77
2	G	3512	TTP	O3G-PG-O3B	2.74	117.52	105.09
2	H	3514	TTP	O3G-PG-O2G	2.78	117.97	107.38
2	G	3512	TTP	C2'-C3'-C4'	2.80	108.58	102.77
2	B	3503	TTP	O2B-PB-O3A	2.81	117.83	105.09
2	B	3503	TTP	O4'-C1'-N1	2.85	112.66	107.72
2	E	3509	TTP	O5'-C5'-C4'	2.85	119.64	109.12
2	F	3510	TTP	O3G-PG-O2G	2.91	118.45	107.38
2	G	3513	TTP	O5'-C5'-C4'	2.97	120.06	109.12
2	H	3515	TTP	C2'-C3'-C4'	3.03	109.05	102.77
2	C	3504	TTP	C2'-C3'-C4'	3.04	109.08	102.77
2	H	3514	TTP	C2'-C3'-C4'	3.05	109.10	102.77
2	E	3508	TTP	O3A-PA-O5'	3.10	111.17	102.94
2	A	3501	TTP	O4'-C1'-N1	3.32	113.46	107.72
2	C	3505	TTP	O4'-C1'-N1	3.37	113.55	107.72
2	E	3508	TTP	C2'-C3'-C4'	3.37	109.76	102.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	3512	TTP	O4'-C1'-N1	3.38	113.57	107.72
2	D	3507	TTP	O4'-C1'-N1	3.57	113.90	107.72
2	F	3511	TTP	O4'-C1'-N1	3.58	113.92	107.72
2	H	3514	TTP	O4'-C1'-N1	3.59	113.93	107.72
2	H	3514	TTP	C4-N3-C2	3.69	118.44	115.25
2	G	3513	TTP	O4'-C1'-N1	3.72	114.16	107.72
2	C	3504	TTP	O4'-C1'-N1	3.73	114.18	107.72
2	F	3510	TTP	C4-N3-C2	3.80	118.53	115.25
2	G	3513	TTP	C2'-C3'-C4'	3.81	110.68	102.77
2	D	3506	TTP	O4'-C1'-N1	3.92	114.50	107.72
2	A	3500	TTP	C4-N3-C2	4.03	118.73	115.25
2	E	3509	TTP	O4'-C1'-N1	4.11	114.83	107.72
2	A	3501	TTP	C4-N3-C2	4.16	118.84	115.25
2	D	3507	TTP	C2'-C3'-C4'	4.16	111.40	102.77
2	E	3509	TTP	C4-N3-C2	4.16	118.85	115.25
2	C	3505	TTP	C2'-C3'-C4'	4.46	112.02	102.77
2	C	3504	TTP	C4-N3-C2	4.53	119.17	115.25
2	D	3506	TTP	C4-N3-C2	4.70	119.31	115.25
2	E	3508	TTP	C4-N3-C2	5.10	119.65	115.25
2	H	3515	TTP	O4'-C1'-N1	5.29	116.88	107.72
2	G	3512	TTP	C4-N3-C2	6.31	120.70	115.25
2	B	3503	TTP	C4-N3-C2	6.50	120.86	115.25
2	D	3507	TTP	C4-N3-C2	6.72	121.06	115.25
2	H	3515	TTP	C4-N3-C2	6.94	121.25	115.25
2	F	3511	TTP	C4-N3-C2	6.94	121.25	115.25
2	G	3513	TTP	C4-N3-C2	8.12	122.26	115.25
2	C	3505	TTP	C4-N3-C2	8.92	122.96	115.25
2	B	3502	TTP	C4-N3-C2	9.53	123.49	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 24 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	3500	TTP	3	0
2	B	3502	TTP	4	0
2	C	3504	TTP	3	0
2	D	3506	TTP	3	0
2	E	3508	TTP	2	0
2	F	3510	TTP	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	3512	TTP	3	0
2	H	3514	TTP	3	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	292/293 (99%)	-0.48	0 100 100	6, 12, 23, 33	0
1	B	292/293 (99%)	-0.40	0 100 100	6, 12, 23, 33	0
1	C	292/293 (99%)	-0.32	4 (1%) 78 74	5, 12, 23, 39	0
1	D	292/293 (99%)	-0.28	2 (0%) 89 87	5, 12, 24, 33	0
1	E	292/293 (99%)	-0.45	0 100 100	5, 12, 23, 35	0
1	F	292/293 (99%)	-0.44	0 100 100	5, 12, 24, 34	0
1	G	292/293 (99%)	-0.34	1 (0%) 94 93	6, 12, 23, 33	0
1	H	292/293 (99%)	-0.36	1 (0%) 94 93	6, 12, 25, 32	0
All	All	2336/2344 (99%)	-0.38	8 (0%) 94 93	5, 12, 24, 39	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	22	ALA	4.3
1	D	119	HIS	3.1
1	H	119	HIS	2.9
1	C	23	ILE	2.8
1	C	119	HIS	2.7
1	G	119	HIS	2.6
1	C	194	ARG	2.5
1	D	23	ILE	2.2

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 (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
2	TTP	D	3506	29/29	0.89	0.20	1.37	25,33,45,49	0
2	TTP	A	3500	29/29	0.94	0.16	1.07	20,30,41,42	0
2	TTP	C	3504	29/29	0.95	0.15	0.96	22,30,37,41	0
2	TTP	F	3511	29/29	0.93	0.17	0.76	8,22,39,41	0
2	TTP	A	3501	29/29	0.93	0.16	0.56	12,20,43,46	0
2	TTP	B	3503	29/29	0.94	0.16	0.48	6,20,29,33	0
2	TTP	H	3514	29/29	0.93	0.15	0.48	26,31,38,43	0
2	TTP	E	3508	29/29	0.95	0.15	0.39	19,27,36,43	0
2	TTP	F	3510	29/29	0.94	0.15	0.38	15,29,38,41	0
2	TTP	G	3512	29/29	0.93	0.14	0.32	13,29,40,44	0
2	TTP	B	3502	29/29	0.93	0.16	0.27	18,30,43,46	0
2	TTP	E	3509	29/29	0.94	0.15	0.13	10,20,40,42	0
2	TTP	C	3505	29/29	0.94	0.15	0.05	11,26,46,47	0
2	TTP	D	3507	29/29	0.94	0.15	-0.15	11,21,43,45	0
2	TTP	G	3513	29/29	0.93	0.14	-0.20	9,24,41,47	0
2	TTP	H	3515	29/29	0.94	0.15	-0.21	10,22,42,47	0

6.5 Other polymers (i)

There are no such residues in this entry.