Full wwPDB X-ray Structure Validation Report (i)

Feb 5, 2024 – 04:30 AM EST

PDB ID	:	1TRR
Title	:	TANDEM BINDING IN CRYSTALS OF A TRP REPRESSOR/OPERATOR HALF-SITE COMPLEX
Authors	:	Lawson, C.L.; Carey, J.
Deposited on	:	1993-10-21
Resolution	:	2.40 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

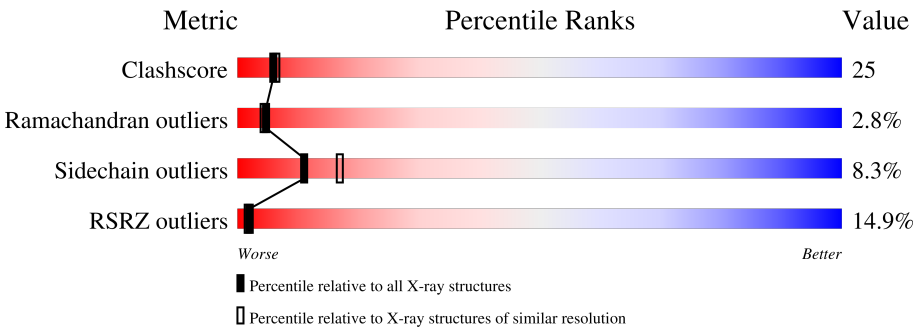
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.40 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))
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	C	16	31% 56% 12%
1	F	16	25% 62% 12%
1	I	16	31% 44% 25%
1	L	16	6% 31% 44% 19%
2	A	107	14% 53% 38% 7% •
2	B	107	12% 54% 36% 6% • •
2	D	107	16% 54% 39% 5% •

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Mol	Chain	Length	Quality of chain
2	E	107	15% 53% 36% 7%
2	G	107	17% 53% 38% 7%
2	H	107	19% 57% 32% 7%
2	J	107	18% 54% 37% 7%
2	K	107	16% 64% 27% 6%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8300 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 DNA chain called DNA (5'-D(*AP*GP*CP*GP*TP*AP*CP*TP*AP*GP*TP*AP*CP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	C	16	325	156	60	94	15	0	0	0
1	F	16	325	156	60	94	15	0	0	0
1	I	16	325	156	60	94	15	0	0	0
1	L	16	325	156	60	94	15	0	0	0

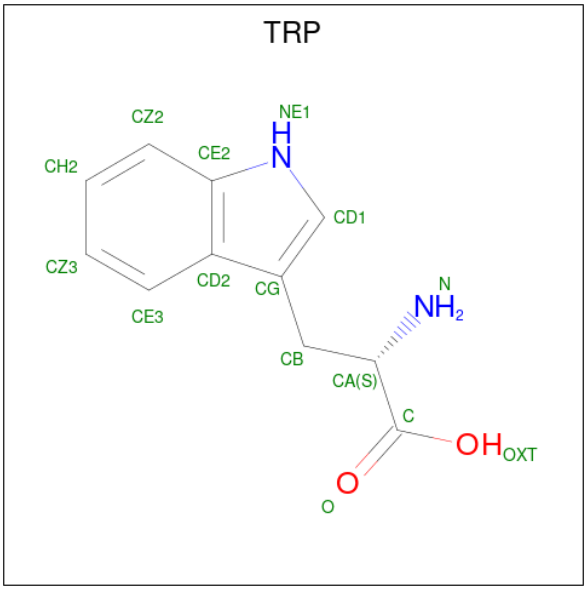
- Molecule 2 is a protein called PROTEIN (TRP REPRESSOR).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	105	836	523	152	158	3	0	0	1
2	B	105	836	523	152	158	3	0	0	1
2	D	105	836	523	152	158	3	0	0	1
2	E	105	836	523	152	158	3	0	0	1
2	G	105	836	523	152	158	3	0	0	1
2	H	105	836	523	152	158	3	0	0	1
2	J	105	836	523	152	158	3	0	0	1
2	K	105	836	523	152	158	3	0	0	1

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	17	GLU	GLN	conflict	UNP P0A881
B	17	GLU	GLN	conflict	UNP P0A881
D	17	GLU	GLN	conflict	UNP P0A881
E	17	GLU	GLN	conflict	UNP P0A881
G	17	GLU	GLN	conflict	UNP P0A881
H	17	GLU	GLN	conflict	UNP P0A881
J	17	GLU	GLN	conflict	UNP P0A881
K	17	GLU	GLN	conflict	UNP P0A881

- Molecule 3 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	15	11	2	2	0	0
			Total	C	N	O		
3	A	1	15	11	2	2	0	0
			Total	C	N	O		
3	D	1	15	11	2	2	0	0
			Total	C	N	O		
3	E	1	15	11	2	2	0	0
			Total	C	N	O		
3	G	1	15	11	2	2	0	0
			Total	C	N	O		
3	H	1	15	11	2	2	0	0
			Total	C	N	O		
3	J	1	15	11	2	2	0	0
			Total	C	N	O		
3	K	1	15	11	2	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	13	Total O 13 13	0	0
4	F	12	Total O 12 12	0	0
4	I	11	Total O 11 11	0	0
4	L	14	Total O 14 14	0	0
4	A	18	Total O 18 18	0	0
4	B	19	Total O 19 19	0	0
4	D	16	Total O 16 16	0	0
4	E	15	Total O 15 15	0	0
4	G	15	Total O 15 15	0	0
4	H	19	Total O 19 19	0	0
4	J	15	Total O 15 15	0	0
4	K	25	Total O 25 25	0	0

3 Residue-property plots (i)

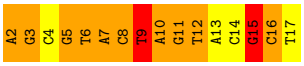
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA (5'-D(*AP*GP*CP*GP*TP*AP*CP*TP*AP*GP*TP*AP*CP*GP*CP*T)-3')

Chain C:

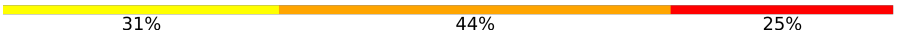
• Molecule 1: DNA (5'-D(*AP*GP*CP*GP*TP*AP*CP*TP*AP*GP*TP*AP*CP*GP*CP*T)-3')

Chain F:



• Molecule 1: DNA (5'-D(*AP*GP*CP*GP*TP*AP*CP*TP*AP*GP*TP*AP*CP*GP*CP*T)-3')

Chain I:

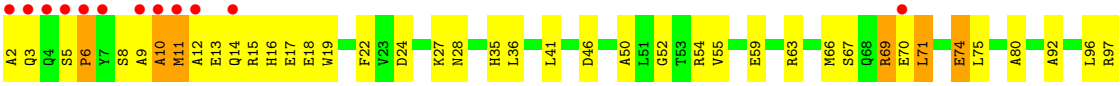


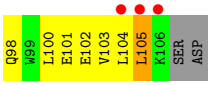
• Molecule 1: DNA (5'-D(*AP*GP*CP*GP*TP*AP*CP*TP*AP*GP*TP*AP*CP*GP*CP*T)-3')

Chain L:

• Molecule 2: PROTEIN (TRP REPRESSOR)

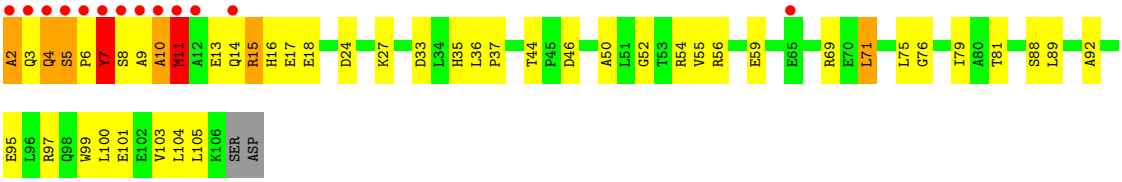
Chain A:





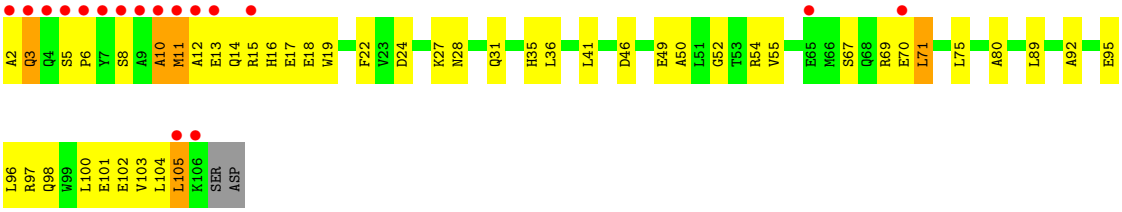
• Molecule 2: PROTEIN (TRP REPRESSOR)

Chain B:



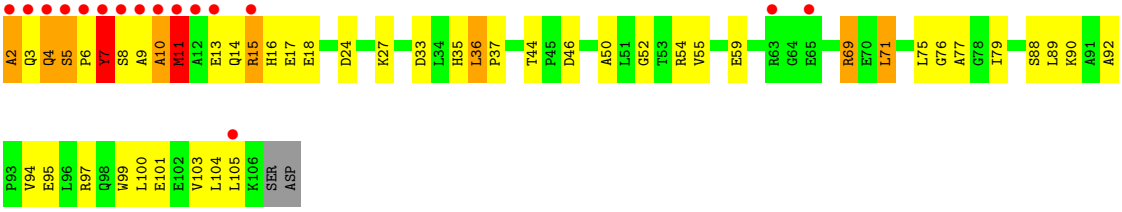
• Molecule 2: PROTEIN (TRP REPRESSOR)

Chain D:



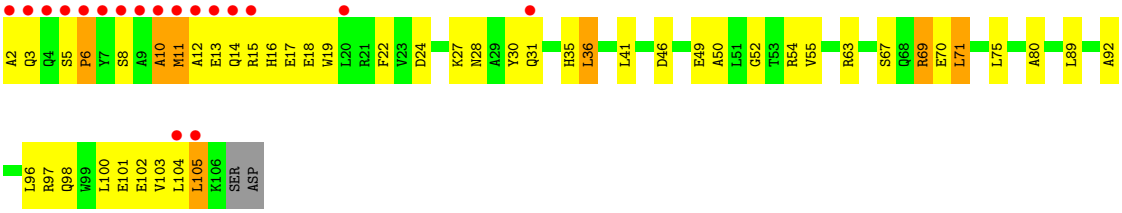
• Molecule 2: PROTEIN (TRP REPRESSOR)

Chain E:



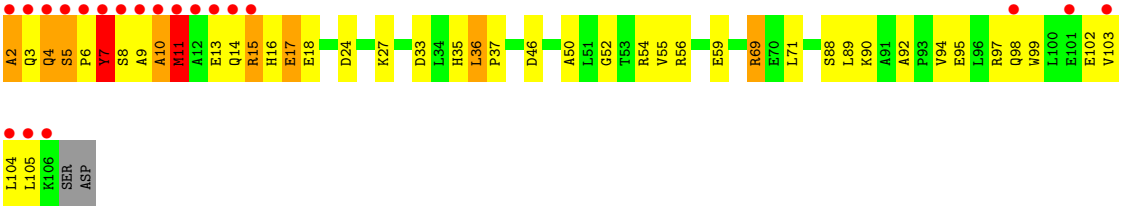
• Molecule 2: PROTEIN (TRP REPRESSOR)

Chain G:



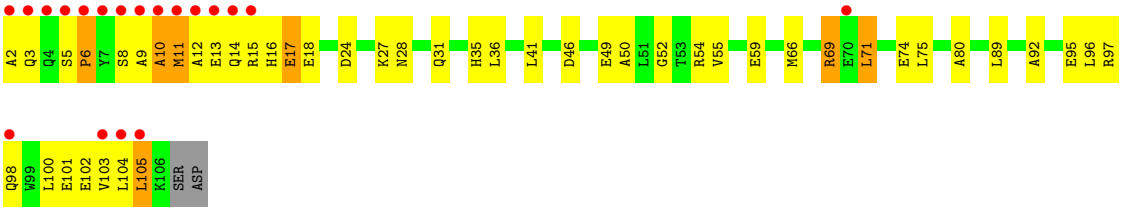
• Molecule 2: PROTEIN (TRP REPRESSOR)

Chain H:



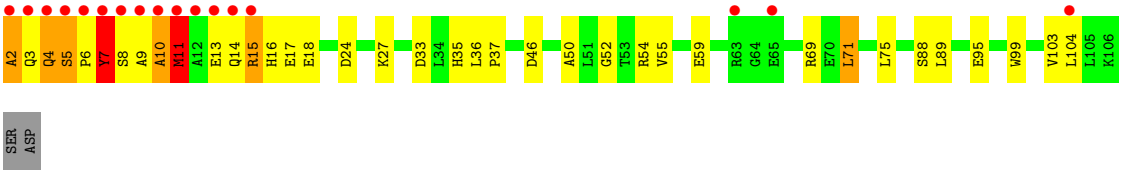
• Molecule 2: PROTEIN (TRP REPRESSOR)

Chain J:



• Molecule 2: PROTEIN (TRP REPRESSOR)

Chain K:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	112.34Å 90.16Å 58.65Å 90.00° 113.92° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.40 34.50 – 2.35	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.40) 58.7 (34.50-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.50 (at 2.36Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.241 , (Not available) 0.265 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	28.8	Xtriage
Anisotropy	0.382	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 48.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	8300	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	C	2.46	17/364 (4.7%)	3.01	57/560 (10.2%)
1	F	2.52	19/364 (5.2%)	3.06	60/560 (10.7%)
1	I	2.49	21/364 (5.8%)	3.09	59/560 (10.5%)
1	L	2.47	17/364 (4.7%)	3.00	52/560 (9.3%)
2	A	0.85	1/848 (0.1%)	0.86	1/1147 (0.1%)
2	B	1.09	3/847 (0.4%)	1.14	5/1144 (0.4%)
2	D	0.83	0/848	0.88	1/1147 (0.1%)
2	E	1.07	3/847 (0.4%)	1.17	5/1144 (0.4%)
2	G	0.84	0/848	0.86	1/1147 (0.1%)
2	H	1.09	4/847 (0.5%)	1.15	5/1144 (0.4%)
2	J	0.90	1/848 (0.1%)	0.88	1/1147 (0.1%)
2	K	1.09	3/847 (0.4%)	1.15	5/1144 (0.4%)
All	All	1.37	89/8236 (1.1%)	1.63	252/11404 (2.2%)

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	C	0	8
1	F	0	8
1	I	0	9
1	L	0	8
2	B	0	2
2	E	0	2
2	H	0	2
2	K	0	2
All	All	0	41

All (89) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	5	SER	C-N	15.68	1.64	1.34
2	B	5	SER	C-N	15.64	1.64	1.34
2	E	5	SER	C-N	15.63	1.64	1.34
2	H	5	SER	C-N	15.63	1.64	1.34
1	F	6	DT	C5-C7	10.53	1.56	1.50
1	C	6	DT	C5-C7	9.45	1.55	1.50
1	F	2	DA	C5'-C4'	8.60	1.60	1.51
1	I	6	DT	C5-C7	8.15	1.54	1.50
1	I	17	DT	P-O5'	-8.02	1.51	1.59
1	C	2	DA	C5'-C4'	7.86	1.59	1.51
1	C	5	DG	P-O5'	-7.60	1.52	1.59
1	L	6	DT	C2'-C1'	-7.46	1.44	1.52
1	L	9	DT	C5-C7	7.45	1.54	1.50
1	L	12	DT	C2'-C1'	-7.20	1.45	1.52
1	L	6	DT	C5-C7	7.05	1.54	1.50
1	I	6	DT	C2'-C1'	-7.00	1.45	1.52
1	F	2	DA	C5-C6	-6.82	1.34	1.41
1	C	6	DT	C2'-C1'	-6.77	1.45	1.52
1	I	2	DA	C5'-C4'	6.66	1.58	1.51
1	I	10	DA	C5'-C4'	6.65	1.58	1.51
1	F	14	DC	P-O5'	-6.50	1.53	1.59
1	L	2	DA	C5'-C4'	6.49	1.58	1.51
1	L	6	DT	C4'-O4'	-6.48	1.38	1.45
1	I	16	DC	P-O5'	-6.45	1.53	1.59
1	I	3	DG	P-O5'	6.40	1.66	1.59
1	F	15	DG	P-O5'	-6.38	1.53	1.59
1	C	9	DT	P-O5'	-6.37	1.53	1.59
1	F	6	DT	C2'-C1'	-6.36	1.45	1.52
1	F	6	DT	C4'-O4'	-6.35	1.38	1.45
1	I	6	DT	P-O5'	-6.35	1.53	1.59
2	E	2	ALA	C-N	-6.13	1.20	1.34
2	B	2	ALA	C-N	-6.13	1.20	1.34
2	H	2	ALA	C-N	-6.13	1.20	1.34
2	K	2	ALA	C-N	-6.10	1.20	1.34
1	C	14	DC	C4'-O4'	-6.10	1.39	1.45
1	I	12	DT	C2'-C1'	-6.09	1.46	1.52
1	L	10	DA	C5'-C4'	6.09	1.58	1.51
1	I	7	DA	C6-N1	-6.08	1.31	1.35
1	I	16	DC	O3'-P	-5.98	1.53	1.61
2	H	17	GLU	CG-CD	5.97	1.60	1.51
1	L	11	DG	C5'-C4'	5.96	1.57	1.51
1	F	16	DC	C4'-C3'	-5.95	1.46	1.52
1	I	9	DT	N3-C4	-5.89	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	16	DC	P-O5'	-5.88	1.53	1.59
1	F	10	DA	C5'-C4'	5.86	1.57	1.51
2	J	95	GLU	CG-CD	5.83	1.60	1.51
1	L	14	DC	P-O5'	-5.83	1.53	1.59
1	F	3	DG	C5-C4	-5.74	1.34	1.38
1	L	14	DC	C4'-O4'	-5.68	1.39	1.45
1	C	16	DC	C4'-C3'	-5.68	1.46	1.52
1	C	12	DT	C2'-C1'	-5.67	1.46	1.52
1	L	10	DA	C5-C6	-5.63	1.35	1.41
1	C	7	DA	C6-N1	-5.62	1.31	1.35
1	F	11	DG	P-O5'	5.61	1.65	1.59
1	I	13	DA	C5-C4	-5.61	1.34	1.38
2	E	11	MET	N-CA	5.53	1.57	1.46
1	C	16	DC	C4'-O4'	-5.50	1.39	1.45
2	K	11	MET	N-CA	5.49	1.57	1.46
2	B	11	MET	N-CA	5.49	1.57	1.46
1	F	16	DC	C4'-O4'	-5.47	1.39	1.45
1	F	12	DT	C2'-C1'	-5.47	1.46	1.52
2	H	11	MET	N-CA	5.46	1.57	1.46
1	C	13	DA	C5-C4	-5.46	1.34	1.38
1	I	3	DG	O3'-P	-5.44	1.54	1.61
1	I	7	DA	P-O5'	-5.44	1.54	1.59
1	I	3	DG	N9-C4	-5.43	1.33	1.38
1	F	4	DC	O3'-P	-5.40	1.54	1.61
2	A	74	GLU	CG-CD	5.40	1.60	1.51
1	L	11	DG	N9-C4	-5.35	1.33	1.38
1	L	5	DG	N9-C8	-5.32	1.34	1.37
1	I	2	DA	C5-C6	-5.32	1.36	1.41
1	I	11	DG	C5-C4	-5.30	1.34	1.38
1	F	3	DG	N9-C4	-5.24	1.33	1.38
1	C	6	DT	C4'-O4'	-5.24	1.39	1.45
1	C	11	DG	C5-C6	-5.22	1.37	1.42
1	F	9	DT	C5-C7	5.19	1.53	1.50
1	F	16	DC	P-O5'	-5.17	1.54	1.59
1	L	3	DG	N9-C4	-5.12	1.33	1.38
1	I	7	DA	C4'-C3'	-5.10	1.47	1.52
1	F	11	DG	N9-C4	-5.10	1.33	1.38
1	C	14	DC	P-O5'	-5.08	1.54	1.59
1	I	15	DG	O3'-P	-5.07	1.55	1.61
1	F	4	DC	P-O5'	-5.05	1.54	1.59
1	L	16	DC	O3'-P	-5.05	1.55	1.61
1	L	13	DA	C5-C4	-5.04	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	15	DG	P-O5'	-5.02	1.54	1.59
1	I	13	DA	C6-N1	-5.02	1.32	1.35
1	C	10	DA	C5'-C4'	5.00	1.56	1.51
1	L	16	DC	P-O5'	-5.00	1.54	1.59

All (252) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	14	DC	O4'-C1'-C2'	-14.45	94.34	105.90
1	I	14	DC	O4'-C1'-C2'	-14.28	94.47	105.90
1	F	14	DC	O4'-C1'-C2'	-13.46	95.13	105.90
1	C	14	DC	O4'-C1'-C2'	-12.97	95.52	105.90
2	H	7	TYR	O-C-N	-12.89	102.07	122.70
2	E	7	TYR	O-C-N	-12.89	102.07	122.70
2	B	7	TYR	O-C-N	-12.87	102.12	122.70
2	K	7	TYR	O-C-N	-12.85	102.14	122.70
1	L	12	DT	O4'-C4'-C3'	-12.53	98.48	106.00
1	C	12	DT	O4'-C4'-C3'	-11.87	98.88	106.00
1	I	10	DA	O4'-C1'-C2'	-11.83	96.44	105.90
1	I	9	DT	O4'-C1'-N1	11.81	116.27	108.00
1	C	10	DA	O4'-C1'-C2'	-11.80	96.46	105.90
1	L	10	DA	O4'-C1'-C2'	-11.60	96.62	105.90
1	L	13	DA	O4'-C1'-C2'	-11.42	96.77	105.90
1	F	10	DA	O4'-C1'-C2'	-11.37	96.80	105.90
1	F	12	DT	O4'-C4'-C3'	-11.27	99.24	106.00
1	I	13	DA	O4'-C1'-C2'	-11.16	96.97	105.90
1	C	9	DT	O4'-C1'-N1	11.08	115.76	108.00
1	I	8	DC	O4'-C1'-N1	10.99	115.70	108.00
1	I	12	DT	O4'-C4'-C3'	-10.83	99.50	106.00
1	C	8	DC	O4'-C1'-N1	10.68	115.48	108.00
1	C	6	DT	O4'-C1'-C2'	-10.64	97.39	105.90
1	F	9	DT	O4'-C1'-N1	10.61	115.43	108.00
1	F	13	DA	O4'-C1'-C2'	-10.17	97.77	105.90
1	F	8	DC	O4'-C1'-N1	10.13	115.09	108.00
1	I	6	DT	O4'-C1'-C2'	-10.01	97.90	105.90
1	F	12	DT	C6-C5-C7	-9.90	116.96	122.90
1	L	2	DA	O4'-C1'-C2'	-9.83	98.04	105.90
1	L	9	DT	O4'-C1'-N1	9.75	114.82	108.00
1	C	12	DT	C6-C5-C7	-9.74	117.06	122.90
1	F	6	DT	O4'-C1'-C2'	-9.56	98.25	105.90
1	I	2	DA	O4'-C1'-N9	9.56	114.69	108.00
1	C	2	DA	O4'-C1'-C2'	-9.49	98.31	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	14	DC	N3-C2-O2	-9.42	115.30	121.90
1	L	6	DT	O4'-C1'-C2'	-9.37	98.41	105.90
1	F	2	DA	O4'-C1'-N9	9.31	114.52	108.00
1	C	13	DA	O4'-C1'-C2'	-9.30	98.46	105.90
2	K	11	MET	O-C-N	-9.22	107.94	122.70
2	B	11	MET	O-C-N	-9.19	108.00	122.70
2	H	11	MET	O-C-N	-9.19	108.00	122.70
2	E	11	MET	O-C-N	-9.17	108.03	122.70
1	F	14	DC	N1-C2-O2	9.12	124.38	118.90
1	L	2	DA	O4'-C1'-N9	9.02	114.31	108.00
1	I	2	DA	N1-C6-N6	9.00	124.00	118.60
1	L	8	DC	O4'-C1'-N1	8.95	114.27	108.00
1	C	2	DA	O4'-C1'-N9	8.80	114.16	108.00
1	I	14	DC	N3-C2-O2	-8.80	115.74	121.90
1	L	6	DT	C6-C5-C7	-8.78	117.63	122.90
1	C	8	DC	N1-C2-O2	8.77	124.16	118.90
1	I	8	DC	N1-C2-O2	8.76	124.16	118.90
1	I	10	DA	N1-C6-N6	8.71	123.83	118.60
1	L	12	DT	C6-C5-C7	-8.68	117.69	122.90
1	F	2	DA	O4'-C1'-C2'	-8.66	98.97	105.90
1	I	15	DG	P-O3'-C3'	8.53	129.94	119.70
1	C	17	DT	N3-C2-O2	-8.53	117.19	122.30
1	C	6	DT	C6-C5-C7	-8.46	117.83	122.90
1	F	8	DC	N1-C2-O2	8.42	123.95	118.90
1	F	4	DC	P-O3'-C3'	8.31	129.67	119.70
1	I	6	DT	N3-C2-O2	-8.30	117.32	122.30
1	F	2	DA	N1-C6-N6	8.27	123.56	118.60
1	C	2	DA	N1-C6-N6	8.21	123.53	118.60
1	L	4	DC	P-O3'-C3'	8.21	129.55	119.70
1	L	15	DG	P-O3'-C3'	8.19	129.53	119.70
1	C	12	DT	O4'-C1'-C2'	-8.16	99.37	105.90
1	C	14	DC	N3-C2-O2	-8.16	116.19	121.90
1	F	10	DA	N1-C6-N6	8.05	123.43	118.60
1	I	16	DC	N1-C2-O2	8.03	123.72	118.90
1	I	12	DT	C6-C5-C7	-8.03	118.08	122.90
1	L	8	DC	N1-C2-O2	7.92	123.65	118.90
1	I	3	DG	P-O3'-C3'	7.88	129.15	119.70
1	L	8	DC	N3-C2-O2	-7.85	116.41	121.90
1	I	8	DC	N3-C2-O2	-7.84	116.41	121.90
1	I	6	DT	C6-C5-C7	-7.83	118.20	122.90
1	C	4	DC	P-O3'-C3'	7.77	129.03	119.70
1	I	2	DA	O4'-C1'-C2'	-7.73	99.72	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	9	DT	N3-C4-O4	-7.71	115.27	119.90
1	F	6	DT	C6-C5-C7	-7.66	118.31	122.90
1	F	15	DG	P-O3'-C3'	7.65	128.88	119.70
2	H	7	TYR	CA-C-N	7.63	133.99	117.20
2	B	7	TYR	CA-C-N	7.61	133.95	117.20
2	E	7	TYR	CA-C-N	7.61	133.94	117.20
2	K	7	TYR	CA-C-N	7.60	133.92	117.20
1	I	16	DC	O4'-C1'-N1	7.49	113.24	108.00
1	F	17	DT	N3-C2-O2	-7.49	117.81	122.30
1	C	15	DG	P-O3'-C3'	7.46	128.66	119.70
1	F	16	DC	N1-C2-O2	7.46	123.38	118.90
1	F	16	DC	O4'-C1'-N1	7.44	113.21	108.00
1	I	12	DT	C4'-C3'-C2'	-7.40	96.44	103.10
1	L	16	DC	N1-C2-O2	7.39	123.33	118.90
1	L	14	DC	N3-C2-O2	-7.39	116.73	121.90
1	C	12	DT	C4'-C3'-C2'	-7.31	96.52	103.10
1	F	17	DT	O4'-C1'-N1	7.30	113.11	108.00
1	L	17	DT	N3-C2-O2	-7.30	117.92	122.30
1	L	10	DA	N1-C6-N6	7.27	122.96	118.60
1	I	4	DC	P-O3'-C3'	7.20	128.34	119.70
1	L	12	DT	O4'-C1'-C2'	-7.13	100.19	105.90
1	L	4	DC	O4'-C1'-C2'	-7.10	100.22	105.90
1	I	14	DC	N1-C2-O2	7.03	123.12	118.90
1	C	11	DG	O4'-C1'-C2'	-6.97	100.32	105.90
1	F	8	DC	N3-C2-O2	-6.91	117.07	121.90
1	I	9	DT	N3-C2-O2	-6.89	118.16	122.30
1	I	4	DC	O4'-C1'-C2'	-6.89	100.39	105.90
1	I	12	DT	O4'-C1'-C2'	-6.83	100.44	105.90
1	F	3	DG	P-O3'-C3'	6.81	127.87	119.70
1	I	17	DT	N3-C2-O2	-6.80	118.22	122.30
1	I	14	DC	O4'-C1'-N1	6.79	112.75	108.00
1	C	6	DT	N3-C2-O2	-6.78	118.23	122.30
1	I	17	DT	O4'-C1'-N1	6.73	112.71	108.00
1	L	6	DT	N3-C2-O2	-6.73	118.26	122.30
1	L	16	DC	O4'-C1'-N1	6.72	112.71	108.00
1	F	11	DG	O4'-C1'-C2'	-6.70	100.54	105.90
1	L	10	DA	O4'-C1'-N9	6.68	112.68	108.00
1	C	16	DC	N1-C2-O2	6.62	122.88	118.90
1	L	9	DT	N3-C2-O2	-6.62	118.33	122.30
1	C	14	DC	N1-C2-O2	6.62	122.87	118.90
1	L	2	DA	N1-C6-N6	6.61	122.57	118.60
1	L	3	DG	O4'-C1'-C2'	-6.58	100.63	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	10	DA	O4'-C1'-N9	6.58	112.61	108.00
1	F	6	DT	N3-C2-O2	-6.58	118.35	122.30
1	L	3	DG	P-O3'-C3'	6.54	127.54	119.70
1	F	7	DA	C6-N1-C2	6.53	122.52	118.60
1	C	3	DG	N3-C2-N2	-6.52	115.33	119.90
1	C	14	DC	O4'-C1'-N1	6.52	112.56	108.00
1	I	2	DA	C5-C6-N6	-6.49	118.50	123.70
1	I	12	DT	C3'-C2'-C1'	6.47	110.27	102.50
1	F	5	DG	O4'-C1'-N9	-6.44	103.49	108.00
1	I	3	DG	O4'-C1'-C2'	-6.40	100.78	105.90
1	C	11	DG	C5-C6-O6	-6.40	124.76	128.60
1	F	7	DA	C5-C6-N1	-6.38	114.51	117.70
1	F	10	DA	O4'-C1'-N9	6.38	112.47	108.00
1	L	9	DT	N3-C4-O4	-6.38	116.07	119.90
1	I	4	DC	P-O5'-C5'	6.38	131.10	120.90
1	F	4	DC	O4'-C1'-C2'	-6.37	100.81	105.90
1	C	9	DT	P-O5'-C5'	6.36	131.07	120.90
2	K	5	SER	O-C-N	-6.36	109.02	121.10
1	F	2	DA	C5-C6-N6	-6.36	118.61	123.70
1	L	11	DG	O4'-C1'-C2'	-6.36	100.81	105.90
1	L	17	DT	O4'-C1'-N1	6.34	112.44	108.00
2	H	5	SER	O-C-N	-6.33	109.06	121.10
2	B	5	SER	O-C-N	-6.32	109.08	121.10
2	E	5	SER	O-C-N	-6.32	109.09	121.10
1	C	10	DA	N1-C6-N6	6.29	122.37	118.60
1	C	3	DG	P-O3'-C3'	6.28	127.23	119.70
1	C	8	DC	N3-C2-O2	-6.27	117.51	121.90
1	F	16	DC	N3-C2-O2	-6.27	117.51	121.90
1	L	6	DT	N3-C4-O4	-6.22	116.17	119.90
1	C	6	DT	O4'-C1'-N1	6.18	112.33	108.00
1	C	7	DA	O4'-C1'-N9	6.17	112.32	108.00
1	C	4	DC	P-O5'-C5'	6.16	130.75	120.90
1	C	16	DC	O4'-C1'-N1	6.15	112.31	108.00
1	L	6	DT	C5-C4-O4	6.12	129.18	124.90
1	L	12	DT	C4'-C3'-C2'	-6.12	97.60	103.10
2	D	105	LEU	CA-CB-CG	6.08	129.29	115.30
1	F	16	DC	C3'-C2'-C1'	6.06	109.78	102.50
1	F	4	DC	P-O5'-C5'	6.03	130.55	120.90
1	C	4	DC	N1-C2-O2	6.02	122.51	118.90
1	L	14	DC	N1-C2-O2	6.02	122.51	118.90
1	L	16	DC	C4'-C3'-C2'	-6.02	97.68	103.10
1	I	13	DA	P-O3'-C3'	6.00	126.91	119.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	12	DT	C4'-C3'-C2'	-5.99	97.70	103.10
1	L	14	DC	O4'-C1'-N1	5.99	112.19	108.00
1	C	16	DC	N3-C2-O2	-5.98	117.71	121.90
1	I	16	DC	C4'-C3'-C2'	-5.98	97.72	103.10
1	F	12	DT	O4'-C1'-C2'	-5.97	101.12	105.90
1	L	6	DT	O4'-C1'-N1	5.97	112.18	108.00
2	B	11	MET	CG-SD-CE	5.96	109.74	100.20
2	K	11	MET	CG-SD-CE	5.96	109.73	100.20
2	E	11	MET	CG-SD-CE	5.95	109.72	100.20
2	H	11	MET	CG-SD-CE	5.93	109.69	100.20
1	F	11	DG	C5-C6-O6	-5.92	125.05	128.60
1	L	16	DC	C3'-C2'-C1'	5.88	109.56	102.50
1	C	12	DT	C3'-C2'-C1'	5.88	109.55	102.50
1	I	15	DG	O4'-C1'-N9	5.88	112.11	108.00
1	L	12	DT	C4-C5-C6	5.85	121.51	118.00
1	C	4	DC	O4'-C1'-C2'	-5.83	101.23	105.90
1	C	13	DA	P-O5'-C5'	5.82	130.22	120.90
1	F	9	DT	C6-C5-C7	-5.79	119.43	122.90
1	L	13	DA	P-O3'-C3'	5.76	126.62	119.70
1	I	10	DA	O4'-C1'-N9	5.76	112.03	108.00
1	I	9	DT	C5-C4-O4	5.76	128.93	124.90
1	C	6	DT	C5-C4-O4	5.76	128.93	124.90
1	I	9	DT	C6-C5-C7	-5.75	119.45	122.90
1	F	4	DC	N1-C2-O2	5.74	122.34	118.90
1	C	14	DC	P-O3'-C3'	5.74	126.58	119.70
1	F	8	DC	C4'-C3'-C2'	-5.70	97.97	103.10
1	F	6	DT	C5-C4-O4	5.70	128.89	124.90
1	F	6	DT	O4'-C1'-N1	5.70	111.99	108.00
1	F	14	DC	O4'-C1'-N1	5.70	111.99	108.00
1	L	14	DC	P-O3'-C3'	5.68	126.52	119.70
1	L	12	DT	C3'-C2'-C1'	5.67	109.30	102.50
1	C	8	DC	C4'-C3'-C2'	-5.66	98.00	103.10
1	F	14	DC	P-O3'-C3'	5.64	126.47	119.70
1	L	4	DC	P-O5'-C5'	5.62	129.90	120.90
1	L	2	DA	C5-C6-N6	-5.54	119.27	123.70
1	C	10	DA	C3'-C2'-C1'	5.53	109.14	102.50
1	F	7	DA	O4'-C4'-C3'	5.51	109.31	106.00
1	I	7	DA	O4'-C1'-N9	5.51	111.86	108.00
1	C	2	DA	C5-C6-N6	-5.50	119.30	123.70
1	C	9	DT	C6-C5-C7	-5.49	119.60	122.90
1	L	15	DG	O4'-C4'-C3'	5.48	109.29	106.00
1	F	9	DT	P-O5'-C5'	5.48	129.66	120.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	9	DT	N3-C4-O4	-5.43	116.64	119.90
1	I	5	DG	O4'-C1'-N9	-5.38	104.23	108.00
1	I	15	DG	O4'-C1'-C2'	-5.37	101.60	105.90
1	I	8	DC	C3'-C2'-C1'	5.37	108.94	102.50
1	I	14	DC	P-O5'-C5'	5.36	129.47	120.90
2	G	105	LEU	CA-CB-CG	5.35	127.61	115.30
1	I	3	DG	N3-C2-N2	-5.35	116.16	119.90
1	C	8	DC	N3-C4-C5	-5.34	119.77	121.90
1	C	14	DC	P-O5'-C5'	5.33	129.43	120.90
1	F	8	DC	C3'-C2'-C1'	5.33	108.89	102.50
1	F	6	DT	C5-C6-N1	-5.32	120.51	123.70
1	I	11	DG	N3-C2-N2	-5.32	116.17	119.90
1	L	9	DT	C6-C5-C7	-5.32	119.71	122.90
1	F	3	DG	N3-C2-N2	-5.31	116.18	119.90
1	I	12	DT	C4-C5-C6	5.31	121.19	118.00
1	F	5	DG	O4'-C1'-C2'	-5.30	101.66	105.90
1	F	11	DG	P-O3'-C3'	5.30	126.06	119.70
1	C	12	DT	C4-C5-C6	5.27	121.16	118.00
1	C	5	DG	O4'-C1'-C2'	-5.26	101.69	105.90
1	C	7	DA	C5-C6-N1	-5.26	115.07	117.70
1	I	6	DT	O4'-C1'-N1	5.24	111.67	108.00
1	I	16	DC	C3'-C2'-C1'	5.21	108.75	102.50
1	F	16	DC	C4'-C3'-C2'	-5.19	98.43	103.10
1	L	16	DC	N3-C2-O2	-5.19	118.27	121.90
2	J	105	LEU	CA-CB-CG	5.18	127.22	115.30
1	C	9	DT	N3-C4-O4	-5.18	116.79	119.90
1	C	16	DC	C3'-C2'-C1'	5.18	108.72	102.50
1	I	17	DT	C6-C5-C7	-5.18	119.79	122.90
1	C	6	DT	N1-C2-N3	5.16	117.69	114.60
1	I	14	DC	P-O3'-C3'	5.15	125.88	119.70
1	F	13	DA	P-O5'-C5'	5.15	129.13	120.90
1	F	10	DA	C3'-C2'-C1'	5.14	108.67	102.50
1	I	4	DC	N1-C2-O2	5.14	121.99	118.90
1	C	3	DG	C2-N3-C4	-5.13	109.34	111.90
1	I	9	DT	P-O5'-C5'	5.11	129.08	120.90
2	A	105	LEU	CA-CB-CG	5.11	127.05	115.30
1	F	14	DC	P-O5'-C5'	5.10	129.06	120.90
1	L	17	DT	C6-C5-C7	-5.09	119.84	122.90
1	C	11	DG	P-O3'-C3'	5.09	125.80	119.70
1	F	12	DT	C4-C5-C6	5.07	121.04	118.00
1	I	5	DG	O4'-C1'-C2'	-5.07	101.84	105.90
1	L	11	DG	C5-C6-O6	-5.07	125.56	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	4	DC	C2-N3-C4	5.06	122.43	119.90
1	F	15	DG	O4'-C1'-N9	5.06	111.54	108.00
1	L	15	DG	P-O5'-C5'	5.05	128.99	120.90
1	I	13	DA	O4'-C4'-C3'	-5.05	102.48	104.50
1	L	9	DT	P-O5'-C5'	5.05	128.98	120.90
1	I	11	DG	C5-C6-O6	-5.01	125.59	128.60
1	I	6	DT	C5-C4-O4	5.01	128.41	124.90
1	F	13	DA	P-O3'-C3'	5.00	125.71	119.70

There are no chirality outliers.

All (41) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	11	MET	Mainchain
2	B	7	TYR	Mainchain
1	C	10	DA	Sidechain
1	C	11	DG	Sidechain
1	C	12	DT	Sidechain
1	C	15	DG	Sidechain
1	C	16	DC	Sidechain
1	C	3	DG	Sidechain
1	C	8	DC	Sidechain
1	C	9	DT	Sidechain
2	E	11	MET	Mainchain
2	E	7	TYR	Mainchain
1	F	10	DA	Sidechain
1	F	11	DG	Sidechain
1	F	12	DT	Sidechain
1	F	15	DG	Sidechain
1	F	16	DC	Sidechain
1	F	3	DG	Sidechain
1	F	8	DC	Sidechain
1	F	9	DT	Sidechain
2	H	11	MET	Mainchain
2	H	7	TYR	Mainchain
1	I	10	DA	Sidechain
1	I	11	DG	Sidechain
1	I	12	DT	Sidechain
1	I	15	DG	Sidechain
1	I	16	DC	Sidechain
1	I	2	DA	Sidechain
1	I	3	DG	Sidechain

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Mol	Chain	Res	Type	Group
1	I	8	DC	Sidechain
1	I	9	DT	Sidechain
2	K	11	MET	Mainchain
2	K	7	TYR	Mainchain
1	L	10	DA	Sidechain
1	L	11	DG	Sidechain
1	L	12	DT	Sidechain
1	L	15	DG	Sidechain
1	L	16	DC	Sidechain
1	L	3	DG	Sidechain
1	L	8	DC	Sidechain
1	L	9	DT	Sidechain

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	C	325	0	182	10	0
1	F	325	0	182	9	0
1	I	325	0	182	11	0
1	L	325	0	182	18	0
2	A	836	0	844	46	0
2	B	836	0	842	52	0
2	D	836	0	844	48	0
2	E	836	0	842	65	0
2	G	836	0	844	49	0
2	H	836	0	842	65	0
2	J	836	0	844	44	0
2	K	836	0	842	44	0
3	A	30	0	18	1	0
3	D	15	0	9	0	0
3	E	15	0	9	0	0
3	G	15	0	9	0	0
3	H	15	0	9	0	0
3	J	15	0	9	0	0
3	K	15	0	9	0	0
4	A	18	0	0	0	0
4	B	19	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	13	0	0	2	0
4	D	16	0	0	1	0
4	E	15	0	0	0	0
4	F	12	0	0	3	0
4	G	15	0	0	1	0
4	H	19	0	0	0	0
4	I	11	0	0	4	0
4	J	15	0	0	1	0
4	K	25	0	0	0	0
4	L	14	0	0	1	0
All	All	8300	0	7544	392	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 25.

All (392) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4:GLN:O	2:H:6:PRO:HD3	1.51	1.10
2:E:4:GLN:O	2:E:6:PRO:HD3	1.51	1.09
2:K:4:GLN:O	2:K:6:PRO:HD3	1.51	1.07
2:B:4:GLN:O	2:B:6:PRO:HD3	1.51	1.06
1:I:15:DG:H21	2:A:2:ALA:HB1	1.23	1.01
1:L:15:DG:H21	2:D:2:ALA:HB1	1.29	0.98
1:C:13:DA:H62	2:E:69:ARG:HH22	1.01	0.98
1:C:13:DA:H62	2:E:69:ARG:NH2	1.61	0.97
1:L:13:DA:H62	2:H:69:ARG:NH2	1.64	0.96
2:H:4:GLN:O	2:H:4:GLN:HG3	1.65	0.95
2:B:4:GLN:O	2:B:4:GLN:HG3	1.65	0.95
1:L:13:DA:N7	2:H:69:ARG:NH1	2.14	0.94
2:K:4:GLN:O	2:K:4:GLN:HG3	1.65	0.93
2:E:4:GLN:O	2:E:4:GLN:HG3	1.65	0.93
2:K:6:PRO:O	2:K:8:SER:N	2.02	0.92
1:L:13:DA:H62	2:H:69:ARG:HH22	1.05	0.92
2:B:6:PRO:O	2:B:8:SER:N	2.02	0.92
2:E:6:PRO:O	2:E:8:SER:N	2.02	0.91
2:H:6:PRO:O	2:H:8:SER:N	2.02	0.90
1:L:15:DG:N2	2:D:2:ALA:HB1	1.87	0.89
1:I:15:DG:N2	2:A:2:ALA:HB1	1.87	0.88
2:A:11:MET:SD	2:A:14:GLN:N	2.47	0.88
2:J:104:LEU:O	2:J:105:LEU:HD23	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:11:MET:SD	2:E:14:GLN:HB2	2.16	0.86
1:F:15:DG:H21	2:J:2:ALA:HB1	1.40	0.86
2:B:11:MET:SD	2:B:14:GLN:HB2	2.15	0.86
2:K:11:MET:SD	2:K:14:GLN:HB2	2.15	0.86
2:H:11:MET:SD	2:H:14:GLN:HB2	2.15	0.85
2:D:11:MET:SD	2:D:14:GLN:N	2.50	0.85
2:K:11:MET:SD	2:K:14:GLN:N	2.50	0.85
1:C:15:DG:H21	2:G:2:ALA:HB1	1.41	0.84
2:B:11:MET:SD	2:B:14:GLN:N	2.50	0.84
2:K:6:PRO:O	2:K:7:TYR:C	2.14	0.84
2:G:11:MET:SD	2:G:14:GLN:N	2.50	0.84
2:B:6:PRO:O	2:B:7:TYR:C	2.14	0.84
2:E:11:MET:SD	2:E:14:GLN:N	2.50	0.84
2:H:11:MET:SD	2:H:14:GLN:N	2.49	0.84
2:G:11:MET:SD	2:G:14:GLN:HB2	2.19	0.83
2:H:11:MET:SD	2:H:14:GLN:CB	2.69	0.81
2:K:11:MET:SD	2:K:14:GLN:CB	2.69	0.81
2:H:6:PRO:O	2:H:7:TYR:C	2.14	0.81
2:E:6:PRO:O	2:E:7:TYR:C	2.14	0.81
2:B:11:MET:SD	2:B:14:GLN:CB	2.69	0.80
2:E:11:MET:SD	2:E:14:GLN:CB	2.69	0.80
2:J:11:MET:SD	2:J:14:GLN:N	2.55	0.80
1:C:13:DA:N7	2:E:69:ARG:NH1	2.29	0.80
2:K:14:GLN:O	2:K:18:GLU:HG3	1.83	0.78
2:D:104:LEU:O	2:D:105:LEU:HD23	1.83	0.78
2:G:11:MET:SD	2:G:14:GLN:CB	2.72	0.77
2:G:104:LEU:O	2:G:105:LEU:HD23	1.83	0.77
2:B:2:ALA:O	2:B:3:GLN:CG	2.33	0.77
2:E:2:ALA:O	2:E:3:GLN:CG	2.33	0.77
2:H:2:ALA:O	2:H:3:GLN:CG	2.33	0.76
2:A:104:LEU:O	2:A:105:LEU:HD23	1.84	0.76
1:I:15:DG:H21	2:A:2:ALA:CB	1.98	0.76
2:K:2:ALA:O	2:K:3:GLN:CG	2.33	0.76
1:F:5:DG:OP2	4:F:7207:HOH:O	2.03	0.75
1:I:2:DA:H2'	4:I:4403:HOH:O	1.86	0.75
2:E:2:ALA:O	2:E:3:GLN:HG2	1.87	0.74
2:K:2:ALA:O	2:K:3:GLN:HG2	1.87	0.74
1:L:15:DG:H21	2:D:2:ALA:CB	2.01	0.74
2:B:2:ALA:O	2:B:3:GLN:HG2	1.87	0.74
2:H:2:ALA:O	2:H:3:GLN:HG2	1.87	0.73
2:B:14:GLN:O	2:B:18:GLU:HG3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:ARG:C	2:B:16:HIS:N	2.41	0.73
2:E:14:GLN:O	2:E:18:GLU:HG3	1.89	0.73
2:E:9:ALA:O	2:E:13:GLU:OE1	2.07	0.73
2:H:14:GLN:O	2:H:18:GLU:HG3	1.89	0.73
2:H:9:ALA:O	2:H:13:GLU:OE1	2.07	0.72
2:B:9:ALA:O	2:B:13:GLU:OE1	2.07	0.72
1:L:13:DA:N6	2:H:69:ARG:NH2	2.37	0.72
2:K:9:ALA:O	2:K:13:GLU:OE1	2.07	0.72
1:I:2:DA:H5'	1:L:17:DT:O3'	1.90	0.71
2:D:6:PRO:HB2	2:D:8:SER:HB3	1.70	0.71
1:C:15:DG:N2	2:G:2:ALA:HB1	2.05	0.71
1:C:13:DA:N6	2:E:69:ARG:NH2	2.35	0.71
2:E:15:ARG:C	2:E:16:HIS:N	2.44	0.71
2:J:11:MET:SD	2:J:14:GLN:HB2	2.29	0.71
2:H:52:GLY:O	2:H:55:VAL:HG22	1.91	0.70
1:C:5:DG:OP2	4:C:5207:HOH:O	2.09	0.69
2:K:52:GLY:O	2:K:55:VAL:HG22	1.92	0.69
2:G:52:GLY:O	2:G:55:VAL:HG22	1.93	0.69
2:A:11:MET:SD	2:A:14:GLN:HB2	2.33	0.69
2:J:6:PRO:C	2:J:8:SER:H	1.96	0.69
1:F:15:DG:N2	2:J:2:ALA:HB1	2.06	0.69
2:E:9:ALA:O	2:E:13:GLU:CD	2.32	0.68
2:E:4:GLN:O	2:E:6:PRO:CD	2.37	0.68
2:K:15:ARG:C	2:K:16:HIS:N	2.46	0.68
2:D:11:MET:SD	2:D:11:MET:O	2.52	0.68
2:H:9:ALA:O	2:H:13:GLU:CD	2.32	0.67
2:B:9:ALA:O	2:B:13:GLU:CD	2.32	0.67
2:K:9:ALA:O	2:K:13:GLU:CD	2.32	0.67
2:B:9:ALA:O	2:B:13:GLU:OE2	2.13	0.67
2:K:9:ALA:O	2:K:13:GLU:OE2	2.13	0.67
2:E:9:ALA:O	2:E:13:GLU:OE2	2.13	0.66
2:K:4:GLN:O	2:K:6:PRO:CD	2.37	0.66
2:H:9:ALA:O	2:H:13:GLU:OE2	2.13	0.66
2:E:52:GLY:O	2:E:55:VAL:HG22	1.96	0.66
2:D:15:ARG:HA	2:D:18:GLU:HG3	1.78	0.66
2:K:2:ALA:C	2:K:3:GLN:HG3	2.17	0.66
2:E:2:ALA:C	2:E:3:GLN:CG	2.65	0.65
2:H:15:ARG:C	2:H:16:HIS:N	2.49	0.65
2:K:2:ALA:C	2:K:3:GLN:CG	2.65	0.65
2:H:2:ALA:C	2:H:3:GLN:CG	2.65	0.65
1:L:13:DA:OP2	4:L:6207:HOH:O	2.15	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:52:GLY:O	2:A:55:VAL:HG22	1.97	0.65
2:B:2:ALA:C	2:B:3:GLN:HG3	2.17	0.64
2:H:2:ALA:C	2:H:3:GLN:HG3	2.17	0.64
2:H:95:GLU:H	2:H:95:GLU:CD	2.01	0.64
2:D:6:PRO:C	2:D:8:SER:H	1.99	0.64
2:H:59:GLU:HB2	2:H:104:LEU:HD13	1.80	0.64
2:B:81:THR:OG1	4:B:1204:HOH:O	2.11	0.64
2:D:6:PRO:HB2	2:D:8:SER:CB	2.27	0.64
2:J:6:PRO:HB2	2:J:8:SER:HB3	1.77	0.64
2:D:100:LEU:O	2:D:104:LEU:HB2	1.98	0.64
2:B:4:GLN:O	2:B:6:PRO:CD	2.37	0.63
2:D:11:MET:SD	2:D:14:GLN:HB2	2.37	0.63
2:E:2:ALA:C	2:E:3:GLN:HG3	2.17	0.63
2:H:4:GLN:O	2:H:6:PRO:CD	2.37	0.63
2:J:52:GLY:O	2:J:55:VAL:HG22	1.98	0.63
1:F:2:DA:H2'	4:F:6403:HOH:O	1.99	0.63
2:A:100:LEU:O	2:A:104:LEU:HB2	1.97	0.63
2:D:96:LEU:HD22	2:E:37:PRO:HB2	1.81	0.63
2:J:11:MET:SD	2:J:14:GLN:CB	2.86	0.63
2:B:3:GLN:HB3	2:B:15:ARG:NH2	2.14	0.62
2:K:95:GLU:CD	2:K:95:GLU:H	2.02	0.62
2:B:52:GLY:O	2:B:55:VAL:HG22	2.00	0.62
2:E:95:GLU:CD	2:E:95:GLU:H	2.03	0.62
2:A:6:PRO:C	2:A:8:SER:H	2.00	0.62
2:D:11:MET:SD	2:D:14:GLN:CB	2.88	0.62
2:B:2:ALA:C	2:B:3:GLN:CG	2.65	0.62
2:H:3:GLN:HB3	2:H:15:ARG:NH2	2.14	0.62
2:J:11:MET:SD	2:J:11:MET:O	2.58	0.62
2:E:3:GLN:HB3	2:E:15:ARG:NH2	2.14	0.61
2:E:71:LEU:HD22	2:E:75:LEU:HD22	1.82	0.61
2:J:50:ALA:O	2:J:54:ARG:HG3	2.00	0.61
1:L:17:DT:H3'	2:E:76:GLY:O	2.01	0.61
2:K:3:GLN:HB3	2:K:15:ARG:NH2	2.14	0.61
2:G:50:ALA:O	2:G:54:ARG:HG3	2.00	0.61
2:A:6:PRO:HB2	2:A:8:SER:HB3	1.82	0.60
2:E:90:LYS:HG2	2:H:7:TYR:HD1	1.67	0.60
2:G:71:LEU:HD22	2:G:75:LEU:HD22	1.84	0.60
2:J:27:LYS:O	2:J:31:GLN:HG3	2.02	0.59
2:G:49:GLU:HG3	4:G:7502:HOH:O	2.02	0.59
2:G:100:LEU:O	2:G:104:LEU:HB2	2.01	0.59
2:B:95:GLU:CD	2:B:95:GLU:H	2.06	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:96:LEU:HD22	2:B:37:PRO:HB2	1.84	0.59
2:G:6:PRO:C	2:G:8:SER:H	2.04	0.58
2:D:71:LEU:HD22	2:D:75:LEU:HD22	1.86	0.58
2:D:101:GLU:HA	2:D:105:LEU:HG	1.86	0.58
2:G:98:GLN:O	2:G:102:GLU:HG3	2.04	0.58
1:I:5:DG:OP2	4:I:1207:HOH:O	2.17	0.58
2:H:50:ALA:O	2:H:54:ARG:HG3	2.04	0.58
1:C:15:DG:H21	2:G:2:ALA:CB	2.14	0.58
2:J:6:PRO:C	2:J:8:SER:N	2.56	0.58
2:J:49:GLU:HG3	4:J:5502:HOH:O	2.04	0.57
2:E:7:TYR:HD1	2:H:90:LYS:HG2	1.68	0.57
2:B:6:PRO:C	2:B:8:SER:N	2.58	0.57
1:F:5:DG:C8	1:F:6:DT:H72	2.40	0.57
2:D:52:GLY:O	2:D:55:VAL:HG22	2.04	0.57
2:G:96:LEU:HD22	2:H:37:PRO:HB2	1.86	0.57
2:D:6:PRO:C	2:D:8:SER:N	2.57	0.57
2:A:6:PRO:C	2:A:8:SER:N	2.58	0.56
2:A:15:ARG:HA	2:A:18:GLU:HG3	1.87	0.56
2:K:6:PRO:C	2:K:8:SER:N	2.58	0.56
2:H:6:PRO:C	2:H:8:SER:N	2.58	0.56
2:A:6:PRO:HB2	2:A:8:SER:CB	2.35	0.56
2:E:6:PRO:C	2:E:8:SER:N	2.58	0.56
2:G:11:MET:SD	2:G:11:MET:O	2.63	0.56
2:B:71:LEU:HD22	2:B:75:LEU:HD22	1.88	0.56
2:J:14:GLN:O	2:J:17:GLU:N	2.37	0.56
1:F:15:DG:H21	2:J:2:ALA:CB	2.16	0.56
2:B:59:GLU:HB2	2:B:104:LEU:HD13	1.86	0.56
2:J:6:PRO:HB2	2:J:8:SER:CB	2.35	0.56
2:D:49:GLU:HG3	4:D:3502:HOH:O	2.05	0.56
2:H:4:GLN:O	2:H:4:GLN:CG	2.46	0.56
2:A:11:MET:SD	2:A:14:GLN:CB	2.93	0.56
2:A:24:ASP:O	2:A:27:LYS:HB3	2.06	0.55
2:A:11:MET:SD	2:A:11:MET:O	2.65	0.55
4:F:7207:HOH:O	2:J:69:ARG:NH1	2.40	0.55
2:G:2:ALA:N	2:H:46:ASP:OD1	2.40	0.55
2:E:90:LYS:HG2	2:H:7:TYR:CD1	2.42	0.55
2:G:6:PRO:HB2	2:G:8:SER:CB	2.37	0.55
2:G:8:SER:HB2	2:G:10:ALA:HB3	1.88	0.54
2:J:96:LEU:HD22	2:K:37:PRO:HB2	1.89	0.54
2:D:28:ASN:HB3	2:E:99:TRP:HZ2	1.72	0.54
2:G:6:PRO:HB2	2:G:8:SER:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:94:VAL:CG2	2:H:9:ALA:HB2	2.37	0.54
2:E:50:ALA:O	2:E:54:ARG:HG3	2.07	0.54
2:K:8:SER:C	2:K:10:ALA:N	2.61	0.54
2:A:2:ALA:N	2:B:46:ASP:OD1	2.41	0.54
2:J:59:GLU:HB2	2:J:104:LEU:HD13	1.88	0.54
2:D:89:LEU:O	2:D:97:ARG:HD3	2.06	0.54
2:J:12:ALA:O	2:J:16:HIS:HB2	2.08	0.53
1:L:13:DA:N7	2:H:69:ARG:CZ	2.71	0.53
2:A:71:LEU:HD22	2:A:75:LEU:HD22	1.90	0.53
2:G:6:PRO:C	2:G:8:SER:N	2.62	0.53
2:A:101:GLU:HA	2:A:105:LEU:HG	1.90	0.53
2:E:35:HIS:H	2:E:35:HIS:CD2	2.26	0.53
2:H:8:SER:C	2:H:10:ALA:N	2.61	0.53
2:J:15:ARG:HA	2:J:18:GLU:HG3	1.90	0.53
2:K:50:ALA:O	2:K:54:ARG:HG3	2.08	0.53
2:B:24:ASP:O	2:B:27:LYS:HB3	2.09	0.53
2:J:8:SER:HB2	2:J:10:ALA:HB3	1.89	0.53
2:E:8:SER:C	2:E:10:ALA:N	2.61	0.52
2:A:28:ASN:HB3	2:B:99:TRP:HZ2	1.74	0.52
2:G:12:ALA:O	2:G:16:HIS:HB2	2.10	0.52
2:D:92:ALA:O	2:D:97:ARG:NH1	2.42	0.52
2:J:28:ASN:HB3	2:K:99:TRP:HZ2	1.74	0.52
2:J:2:ALA:N	2:K:46:ASP:OD1	2.42	0.52
2:K:71:LEU:HD22	2:K:75:LEU:HD22	1.92	0.52
2:A:50:ALA:O	2:A:54:ARG:HG3	2.10	0.52
2:A:67:SER:OG	2:A:70:GLU:HG3	2.10	0.52
2:A:35:HIS:H	2:A:35:HIS:CD2	2.27	0.51
2:G:97:ARG:O	2:G:101:GLU:HG3	2.09	0.51
2:E:97:ARG:NH2	2:H:7:TYR:O	2.43	0.51
2:D:103:VAL:HG23	2:D:104:LEU:N	2.26	0.51
2:B:8:SER:C	2:B:10:ALA:N	2.61	0.51
2:D:50:ALA:O	2:D:54:ARG:HG3	2.11	0.51
2:J:101:GLU:HA	2:J:105:LEU:HG	1.92	0.51
2:B:4:GLN:O	2:B:4:GLN:CG	2.46	0.50
2:J:92:ALA:O	2:J:97:ARG:NH1	2.45	0.50
2:A:9:ALA:O	2:A:13:GLU:OE1	2.30	0.50
2:B:35:HIS:CD2	2:B:35:HIS:H	2.29	0.50
2:G:28:ASN:HB3	2:H:99:TRP:HZ2	1.76	0.50
2:J:100:LEU:O	2:J:104:LEU:HB2	2.10	0.50
2:A:8:SER:HB2	2:A:10:ALA:HB3	1.94	0.49
2:G:8:SER:C	2:G:10:ALA:N	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:3:GLN:HB3	2:K:15:ARG:HH21	1.77	0.49
1:C:17:DT:O3'	1:F:2:DA:H5'	2.12	0.49
2:D:2:ALA:N	2:E:46:ASP:OD1	2.46	0.49
1:L:13:DA:N6	2:H:69:ARG:HH22	1.89	0.49
2:J:98:GLN:O	2:J:102:GLU:HG3	2.13	0.49
2:D:67:SER:OG	2:D:70:GLU:HG3	2.12	0.49
2:G:89:LEU:O	2:G:97:ARG:HD3	2.12	0.49
2:K:11:MET:CE	2:K:11:MET:HA	2.43	0.49
1:I:17:DT:H3'	2:B:76:GLY:O	2.13	0.49
2:A:66:MET:SD	2:A:74:GLU:OE1	2.71	0.49
2:J:71:LEU:HD22	2:J:75:LEU:HD22	1.95	0.48
2:H:3:GLN:HB3	2:H:15:ARG:HH21	1.77	0.48
2:B:8:SER:C	2:B:10:ALA:H	2.16	0.48
2:B:92:ALA:O	2:B:97:ARG:NH1	2.46	0.48
2:D:49:GLU:HG2	2:E:15:ARG:HB2	1.95	0.48
2:J:89:LEU:O	2:J:97:ARG:HD3	2.13	0.48
2:K:8:SER:C	2:K:10:ALA:H	2.17	0.48
2:D:35:HIS:CD2	2:D:35:HIS:H	2.29	0.48
2:J:24:ASP:O	2:J:27:LYS:HB3	2.12	0.48
2:B:3:GLN:HB3	2:B:15:ARG:HH21	1.77	0.48
2:G:67:SER:OG	2:G:70:GLU:HG3	2.13	0.48
2:K:103:VAL:HG23	2:K:104:LEU:N	2.29	0.48
1:F:9:DT:H72	2:D:80:ALA:HB3	1.96	0.48
1:L:17:DT:OP1	2:D:15:ARG:NH2	2.47	0.48
2:E:3:GLN:HB3	2:E:15:ARG:HH21	1.76	0.48
1:L:16:DC:H4'	2:D:3:GLN:HG3	1.95	0.48
2:A:41:LEU:HD12	2:B:88:SER:HB3	1.95	0.48
2:B:50:ALA:O	2:B:54:ARG:HG3	2.14	0.48
2:D:11:MET:C	2:D:13:GLU:H	2.16	0.48
2:G:13:GLU:O	2:G:16:HIS:HB3	2.14	0.48
2:H:104:LEU:O	2:H:105:LEU:HD23	2.14	0.48
2:A:8:SER:C	2:A:10:ALA:N	2.65	0.48
2:J:66:MET:SD	2:J:74:GLU:OE1	2.72	0.48
2:D:12:ALA:O	2:D:16:HIS:HB2	2.14	0.47
2:D:27:LYS:O	2:D:31:GLN:HG3	2.14	0.47
2:H:35:HIS:H	2:H:35:HIS:CD2	2.32	0.47
1:I:2:DA:O5'	4:I:4403:HOH:O	2.20	0.47
2:A:103:VAL:HG23	2:A:104:LEU:N	2.30	0.47
2:A:11:MET:C	2:A:13:GLU:H	2.18	0.47
2:A:98:GLN:O	2:A:102:GLU:HG3	2.14	0.47
2:D:24:ASP:O	2:D:27:LYS:HB3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:8:SER:C	2:E:10:ALA:H	2.16	0.47
2:H:8:SER:C	2:H:10:ALA:H	2.17	0.47
2:J:41:LEU:HD12	2:K:88:SER:HB3	1.96	0.47
2:J:50:ALA:HB2	2:K:3:GLN:OE1	2.14	0.47
2:A:97:ARG:O	2:A:101:GLU:HG3	2.14	0.47
3:A:109:TRP:HB3	2:B:44:THR:HG22	1.96	0.47
2:B:11:MET:HA	2:B:11:MET:CE	2.43	0.47
2:D:8:SER:C	2:D:10:ALA:N	2.67	0.47
2:J:8:SER:C	2:J:10:ALA:N	2.66	0.47
2:K:8:SER:O	2:K:8:SER:OG	2.33	0.47
2:A:11:MET:SD	2:A:11:MET:C	2.92	0.47
2:E:4:GLN:O	2:E:4:GLN:CG	2.46	0.47
2:E:11:MET:HA	2:E:11:MET:CE	2.43	0.47
2:E:92:ALA:O	2:E:97:ARG:NH1	2.48	0.47
2:G:15:ARG:HA	2:G:18:GLU:HG3	1.96	0.46
2:E:100:LEU:O	2:E:104:LEU:HB2	2.15	0.46
2:K:2:ALA:O	2:K:3:GLN:HG3	2.12	0.46
1:C:9:DT:H72	2:A:80:ALA:HB3	1.98	0.46
2:G:35:HIS:CD2	2:G:35:HIS:H	2.33	0.46
2:J:11:MET:HA	2:J:11:MET:CE	2.46	0.46
2:K:95:GLU:CD	2:K:95:GLU:N	2.68	0.46
2:D:11:MET:O	2:D:13:GLU:N	2.49	0.46
2:J:103:VAL:HG23	2:J:104:LEU:N	2.30	0.46
2:B:8:SER:O	2:B:8:SER:OG	2.33	0.46
2:H:11:MET:HA	2:H:11:MET:CE	2.43	0.46
2:A:11:MET:C	2:A:13:GLU:N	2.67	0.46
2:H:8:SER:O	2:H:8:SER:OG	2.33	0.45
2:H:55:VAL:HG23	2:H:56:ARG:N	2.31	0.45
2:G:50:ALA:HB2	2:H:3:GLN:OE1	2.17	0.45
2:G:92:ALA:O	2:G:97:ARG:NH1	2.50	0.45
2:A:92:ALA:O	2:A:97:ARG:NH1	2.49	0.45
2:D:41:LEU:HD12	2:E:88:SER:HB3	1.97	0.45
2:J:11:MET:SD	2:J:11:MET:C	2.92	0.45
4:C:5207:HOH:O	2:G:69:ARG:NH1	2.47	0.45
2:A:50:ALA:HB2	2:B:3:GLN:OE1	2.16	0.45
2:D:103:VAL:CG2	2:D:104:LEU:N	2.79	0.45
2:E:103:VAL:HG23	2:E:104:LEU:N	2.32	0.45
2:E:59:GLU:HB2	2:E:104:LEU:HD13	1.99	0.44
2:G:11:MET:C	2:G:13:GLU:H	2.21	0.44
2:G:11:MET:HA	2:G:11:MET:CE	2.47	0.44
2:G:36:LEU:HD12	2:G:36:LEU:HA	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:35:HIS:CD2	2:J:35:HIS:H	2.33	0.44
2:K:35:HIS:H	2:K:35:HIS:CD2	2.35	0.44
2:B:89:LEU:HD12	2:B:89:LEU:HA	1.84	0.44
2:E:36:LEU:HD12	2:E:36:LEU:HA	1.87	0.44
2:G:63:ARG:NH1	2:G:63:ARG:HG2	2.31	0.44
1:L:17:DT:P	2:E:77:ALA:HA	2.58	0.44
2:D:50:ALA:HB2	2:E:3:GLN:OE1	2.17	0.44
2:H:59:GLU:HA	2:H:104:LEU:HD13	1.99	0.44
2:H:95:GLU:CD	2:H:95:GLU:N	2.65	0.44
2:D:19:TRP:O	2:D:22:PHE:HB3	2.17	0.44
2:G:24:ASP:O	2:G:27:LYS:HB3	2.18	0.44
1:I:3:DG:O6	2:E:79:ILE:HG22	2.18	0.44
1:I:9:DT:H72	2:G:80:ALA:HB3	2.00	0.44
2:G:101:GLU:HA	2:G:105:LEU:HG	2.00	0.44
2:B:100:LEU:O	2:B:104:LEU:HB2	2.18	0.43
2:G:41:LEU:HD12	2:H:88:SER:HB3	2.00	0.43
2:B:11:MET:SD	2:B:14:GLN:HB3	2.58	0.43
2:D:13:GLU:O	2:D:16:HIS:HB3	2.19	0.43
2:E:95:GLU:CD	2:E:95:GLU:N	2.71	0.43
2:H:92:ALA:O	2:H:97:ARG:NH1	2.51	0.43
2:D:11:MET:C	2:D:13:GLU:N	2.71	0.43
2:D:98:GLN:O	2:D:102:GLU:HG3	2.19	0.43
2:J:13:GLU:O	2:J:16:HIS:HB3	2.19	0.43
2:B:103:VAL:HG23	2:B:104:LEU:N	2.34	0.43
2:E:89:LEU:HD12	2:E:89:LEU:HA	1.91	0.43
2:A:103:VAL:CG2	2:A:104:LEU:N	2.82	0.43
2:H:24:ASP:O	2:H:27:LYS:HB3	2.18	0.43
2:H:36:LEU:HD12	2:H:36:LEU:HA	1.90	0.43
2:H:59:GLU:CB	2:H:104:LEU:HD13	2.49	0.43
2:K:4:GLN:O	2:K:4:GLN:CG	2.46	0.43
2:K:6:PRO:C	2:K:8:SER:H	2.22	0.43
2:K:59:GLU:HB2	2:K:104:LEU:HD13	2.00	0.43
1:L:9:DT:H72	2:J:80:ALA:HB3	1.99	0.43
2:D:11:MET:SD	2:D:11:MET:C	2.95	0.43
2:E:11:MET:SD	2:E:14:GLN:HB3	2.58	0.42
2:B:79:ILE:HG23	4:B:1209:HOH:O	2.19	0.42
2:G:19:TRP:O	2:G:22:PHE:HB3	2.19	0.42
1:I:2:DA:H5'	1:L:17:DT:HO3'	1.83	0.42
2:A:12:ALA:O	2:A:16:HIS:HB2	2.18	0.42
2:A:19:TRP:O	2:A:22:PHE:HB3	2.20	0.42
2:B:15:ARG:H	2:B:15:ARG:HG2	1.65	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:15:ARG:H	2:H:15:ARG:HG2	1.65	0.42
2:H:103:VAL:HG23	2:H:104:LEU:N	2.35	0.42
2:K:24:ASP:O	2:K:27:LYS:HB3	2.19	0.42
2:A:13:GLU:O	2:A:16:HIS:HB3	2.19	0.42
2:A:59:GLU:HB2	2:A:104:LEU:HD13	2.01	0.42
2:E:7:TYR:HD1	2:H:90:LYS:CG	2.32	0.42
2:E:101:GLU:HA	2:E:105:LEU:HG	2.02	0.42
2:E:2:ALA:O	2:E:3:GLN:HG3	2.12	0.42
2:J:103:VAL:CG2	2:J:104:LEU:N	2.83	0.42
2:G:2:ALA:N	2:H:46:ASP:OD2	2.53	0.42
2:B:6:PRO:C	2:B:8:SER:H	2.22	0.41
2:G:103:VAL:HG23	2:G:104:LEU:N	2.35	0.41
2:H:59:GLU:CA	2:H:104:LEU:HD13	2.50	0.41
2:K:89:LEU:HD12	2:K:89:LEU:HA	1.92	0.41
4:I:1207:HOH:O	2:A:69:ARG:NH1	2.52	0.41
2:B:11:MET:SD	2:B:14:GLN:CA	3.09	0.41
2:E:6:PRO:C	2:E:8:SER:H	2.22	0.41
2:H:11:MET:SD	2:H:14:GLN:HB3	2.58	0.41
2:G:30:TYR:HA	2:G:35:HIS:CD2	2.54	0.41
2:K:3:GLN:HE21	2:K:15:ARG:HH21	1.68	0.41
2:K:11:MET:SD	2:K:14:GLN:CA	3.09	0.41
2:G:11:MET:C	2:G:13:GLU:N	2.74	0.41
2:H:6:PRO:C	2:H:8:SER:H	2.22	0.41
2:D:95:GLU:H	2:D:95:GLU:CD	2.24	0.41
2:E:24:ASP:O	2:E:27:LYS:HB3	2.20	0.41
1:F:7:DA:H5"	2:E:44:THR:HG21	2.03	0.41
2:E:3:GLN:HE21	2:E:15:ARG:HH21	1.68	0.41
2:G:18:GLU:OE2	2:H:56:ARG:HG3	2.21	0.41
2:H:89:LEU:HD12	2:H:89:LEU:HA	1.90	0.41
2:A:63:ARG:NH1	2:A:63:ARG:HG2	2.35	0.41
2:H:98:GLN:O	2:H:102:GLU:HG3	2.21	0.41
2:B:101:GLU:HA	2:B:105:LEU:HG	2.02	0.41
2:G:11:MET:SD	2:G:14:GLN:CA	3.08	0.41
2:G:27:LYS:O	2:G:31:GLN:HG3	2.20	0.41
2:B:2:ALA:O	2:B:3:GLN:HG3	2.12	0.40
2:J:9:ALA:O	2:J:13:GLU:OE1	2.38	0.40
1:L:15:DG:N2	2:D:2:ALA:CB	2.70	0.40
2:D:2:ALA:N	2:E:46:ASP:OD2	2.54	0.40
2:E:11:MET:SD	2:E:14:GLN:CA	3.09	0.40
2:A:18:GLU:OE2	2:B:56:ARG:HG3	2.21	0.40
2:E:9:ALA:HB2	2:H:94:VAL:HG22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	103/107 (96%)	93 (90%)	7 (7%)	3 (3%)	4 4
2	B	101/107 (94%)	93 (92%)	5 (5%)	3 (3%)	4 3
2	D	103/107 (96%)	92 (89%)	9 (9%)	2 (2%)	8 10
2	E	101/107 (94%)	93 (92%)	5 (5%)	3 (3%)	4 3
2	G	103/107 (96%)	93 (90%)	7 (7%)	3 (3%)	4 4
2	H	101/107 (94%)	92 (91%)	6 (6%)	3 (3%)	4 3
2	J	103/107 (96%)	91 (88%)	9 (9%)	3 (3%)	4 4
2	K	101/107 (94%)	93 (92%)	5 (5%)	3 (3%)	4 3
All	All	816/856 (95%)	740 (91%)	53 (6%)	23 (3%)	5 4

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	10	ALA
2	B	5	SER
2	B	7	TYR
2	D	10	ALA
2	E	5	SER
2	E	7	TYR
2	G	10	ALA
2	H	5	SER
2	H	7	TYR
2	J	10	ALA
2	K	5	SER
2	K	7	TYR
2	D	5	SER
2	A	6	PRO

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Mol	Chain	Res	Type
2	B	10	ALA
2	E	10	ALA
2	G	5	SER
2	H	10	ALA
2	J	5	SER
2	J	6	PRO
2	K	10	ALA
2	A	5	SER
2	G	6	PRO

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
2	A	89/92 (97%)	82 (92%)	7 (8%)	12 19
2	B	89/92 (97%)	81 (91%)	8 (9%)	9 14
2	D	89/92 (97%)	82 (92%)	7 (8%)	12 19
2	E	89/92 (97%)	81 (91%)	8 (9%)	9 14
2	G	89/92 (97%)	82 (92%)	7 (8%)	12 19
2	H	89/92 (97%)	81 (91%)	8 (9%)	9 14
2	J	89/92 (97%)	82 (92%)	7 (8%)	12 19
2	K	89/92 (97%)	81 (91%)	8 (9%)	9 14
All	All	712/736 (97%)	652 (92%)	60 (8%)	11 16

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	3	GLN
2	A	11	MET
2	A	17	GLU
2	A	36	LEU
2	A	46	ASP
2	A	69	ARG

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Mol	Chain	Res	Type
2	A	71	LEU
2	B	4	GLN
2	B	11	MET
2	B	15	ARG
2	B	17	GLU
2	B	33	ASP
2	B	36	LEU
2	B	69	ARG
2	B	71	LEU
2	D	3	GLN
2	D	11	MET
2	D	17	GLU
2	D	36	LEU
2	D	46	ASP
2	D	69	ARG
2	D	71	LEU
2	E	4	GLN
2	E	11	MET
2	E	15	ARG
2	E	17	GLU
2	E	33	ASP
2	E	36	LEU
2	E	69	ARG
2	E	71	LEU
2	G	3	GLN
2	G	11	MET
2	G	17	GLU
2	G	36	LEU
2	G	46	ASP
2	G	69	ARG
2	G	71	LEU
2	H	4	GLN
2	H	11	MET
2	H	15	ARG
2	H	17	GLU
2	H	33	ASP
2	H	36	LEU
2	H	69	ARG
2	H	71	LEU
2	J	3	GLN
2	J	11	MET
2	J	17	GLU

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Mol	Chain	Res	Type
2	J	36	LEU
2	J	46	ASP
2	J	69	ARG
2	J	71	LEU
2	K	4	GLN
2	K	11	MET
2	K	15	ARG
2	K	17	GLU
2	K	33	ASP
2	K	36	LEU
2	K	69	ARG
2	K	71	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	4	GLN
2	A	14	GLN
2	A	35	HIS
2	A	98	GLN
2	B	4	GLN
2	B	35	HIS
2	B	98	GLN
2	D	4	GLN
2	D	14	GLN
2	D	35	HIS
2	D	98	GLN
2	E	4	GLN
2	E	14	GLN
2	E	35	HIS
2	E	98	GLN
2	G	4	GLN
2	G	14	GLN
2	G	35	HIS
2	G	98	GLN
2	H	4	GLN
2	H	35	HIS
2	H	98	GLN
2	J	4	GLN
2	J	14	GLN
2	J	35	HIS
2	J	98	GLN

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Mol	Chain	Res	Type
2	K	4	GLN
2	K	35	HIS
2	K	98	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

8 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	TRP	E	109	-	14,16,16	1.09	1 (7%)	16,22,22	0.98	1 (6%)
3	TRP	J	109	-	14,16,16	0.97	0	16,22,22	0.90	0
3	TRP	A	110	-	14,16,16	1.13	1 (7%)	16,22,22	1.00	1 (6%)
3	TRP	D	109	-	14,16,16	1.07	1 (7%)	16,22,22	0.97	1 (6%)
3	TRP	G	109	-	14,16,16	0.98	1 (7%)	16,22,22	0.94	1 (6%)
3	TRP	A	109	-	14,16,16	1.12	1 (7%)	16,22,22	1.01	1 (6%)
3	TRP	K	109	-	14,16,16	1.04	1 (7%)	16,22,22	0.95	1 (6%)
3	TRP	H	109	-	14,16,16	0.99	0	16,22,22	0.89	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRP	E	109	-	-	0/7/8/8	0/2/2/2
3	TRP	J	109	-	-	0/7/8/8	0/2/2/2
3	TRP	A	110	-	-	0/7/8/8	0/2/2/2
3	TRP	D	109	-	-	0/7/8/8	0/2/2/2
3	TRP	G	109	-	-	0/7/8/8	0/2/2/2
3	TRP	A	109	-	-	0/7/8/8	0/2/2/2
3	TRP	K	109	-	-	0/7/8/8	0/2/2/2
3	TRP	H	109	-	-	0/7/8/8	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	109	TRP	CB-CG	-2.66	1.44	1.51
3	A	110	TRP	CB-CG	-2.59	1.44	1.51
3	K	109	TRP	CB-CG	-2.39	1.44	1.51
3	G	109	TRP	CB-CG	-2.09	1.45	1.51
3	D	109	TRP	CB-CG	-2.03	1.45	1.51
3	E	109	TRP	CB-CG	-2.03	1.45	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	E	109	TRP	CH2-CZ2-CE2	-2.13	117.02	120.08
3	D	109	TRP	CH2-CZ2-CE2	-2.10	117.07	120.08
3	A	110	TRP	CH2-CZ2-CE2	-2.08	117.08	120.08
3	A	109	TRP	CH2-CZ2-CE2	-2.05	117.13	120.08
3	K	109	TRP	CH2-CZ2-CE2	-2.05	117.14	120.08
3	G	109	TRP	CH2-CZ2-CE2	-2.03	117.17	120.08

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	109	TRP	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	3
2	K	3
2	E	3
2	B	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	15:ARG	C	16:HIS	N	2.49
1	K	15:ARG	C	16:HIS	N	2.46
1	E	15:ARG	C	16:HIS	N	2.44
1	B	15:ARG	C	16:HIS	N	2.41
1	B	5:SER	C	6:PRO	N	1.64
1	K	5:SER	C	6:PRO	N	1.64
1	E	5:SER	C	6:PRO	N	1.63
1	H	5:SER	C	6:PRO	N	1.63
1	B	2:ALA	C	3:GLN	N	1.20
1	H	2:ALA	C	3:GLN	N	1.20
1	K	2:ALA	C	3:GLN	N	1.20
1	E	2:ALA	C	3:GLN	N	1.19

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	C	16/16 (100%)	-0.39	0	100	100	25, 25, 25, 25	16 (100%)
1	F	16/16 (100%)	-0.18	0	100	100	25, 25, 25, 25	16 (100%)
1	I	16/16 (100%)	-0.27	0	100	100	25, 25, 25, 25	16 (100%)
1	L	16/16 (100%)	-0.27	0	100	100	25, 25, 25, 25	16 (100%)
2	A	105/107 (98%)	0.80	15 (14%)	2	2	25, 25, 25, 25	105 (100%)
2	B	105/107 (98%)	0.74	13 (12%)	4	3	25, 25, 25, 25	105 (100%)
2	D	105/107 (98%)	1.18	17 (16%)	1	1	25, 25, 25, 25	105 (100%)
2	E	105/107 (98%)	1.15	16 (15%)	2	1	25, 25, 25, 25	105 (100%)
2	G	105/107 (98%)	0.98	18 (17%)	1	1	25, 25, 25, 25	105 (100%)
2	H	105/107 (98%)	1.40	20 (19%)	1	1	25, 25, 25, 25	105 (100%)
2	J	105/107 (98%)	1.28	19 (18%)	1	1	25, 25, 25, 25	105 (100%)
2	K	105/107 (98%)	1.01	17 (16%)	1	1	25, 25, 25, 25	105 (100%)
All	All	904/920 (98%)	0.97	135 (14%)	2	2	25, 25, 25, 25	904 (100%)

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	3	GLN	11.7
2	H	6	PRO	11.4
2	J	6	PRO	10.9
2	K	2	ALA	10.5
2	J	5	SER	10.5
2	H	5	SER	10.3
2	H	4	GLN	9.9
2	D	4	GLN	9.8
2	E	4	GLN	9.3
2	J	4	GLN	9.3
2	E	2	ALA	9.3

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Mol	Chain	Res	Type	RSRZ
2	E	9	ALA	9.2
2	D	9	ALA	9.0
2	K	3	GLN	9.0
2	J	3	GLN	8.8
2	G	3	GLN	8.8
2	G	2	ALA	8.4
2	E	3	GLN	8.3
2	B	6	PRO	8.2
2	E	6	PRO	8.1
2	D	2	ALA	8.0
2	E	8	SER	8.0
2	A	4	GLN	8.0
2	B	4	GLN	7.9
2	D	5	SER	7.9
2	J	10	ALA	7.8
2	D	3	GLN	7.8
2	J	104	LEU	7.6
2	D	105	LEU	7.3
2	A	6	PRO	7.3
2	E	7	TYR	7.3
2	E	12	ALA	7.2
2	J	2	ALA	7.2
2	H	10	ALA	7.2
2	E	5	SER	7.2
2	D	8	SER	7.1
2	D	6	PRO	7.1
2	H	2	ALA	7.0
2	D	12	ALA	7.0
2	D	7	TYR	7.0
2	H	104	LEU	6.8
2	B	5	SER	6.8
2	A	5	SER	6.7
2	B	3	GLN	6.7
2	H	8	SER	6.6
2	E	105	LEU	6.5
2	J	8	SER	6.5
2	K	12	ALA	6.5
2	K	6	PRO	6.5
2	G	12	ALA	6.5
2	K	7	TYR	6.3
2	A	2	ALA	6.2
2	H	106	LYS	5.9

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Mol	Chain	Res	Type	RSRZ
2	K	4	GLN	5.8
2	H	15	ARG	5.7
2	J	9	ALA	5.7
2	G	7	TYR	5.7
2	B	9	ALA	5.7
2	G	5	SER	5.6
2	J	11	MET	5.5
2	B	10	ALA	5.4
2	G	4	GLN	5.4
2	A	9	ALA	5.4
2	K	5	SER	5.4
2	J	105	LEU	5.4
2	H	7	TYR	5.4
2	K	11	MET	5.3
2	A	3	GLN	5.3
2	G	11	MET	5.3
2	B	7	TYR	5.3
2	J	15	ARG	5.3
2	K	10	ALA	5.2
2	H	105	LEU	5.2
2	K	9	ALA	5.1
2	K	15	ARG	5.1
2	G	9	ALA	5.1
2	H	11	MET	5.1
2	G	6	PRO	5.0
2	A	7	TYR	4.9
2	A	10	ALA	4.9
2	H	12	ALA	4.7
2	J	12	ALA	4.7
2	J	7	TYR	4.6
2	D	11	MET	4.5
2	A	11	MET	4.2
2	G	8	SER	4.2
2	E	13	GLU	4.1
2	G	15	ARG	4.1
2	D	10	ALA	4.1
2	E	10	ALA	4.1
2	A	106	LYS	4.0
2	D	13	GLU	4.0
2	B	2	ALA	4.0
2	E	11	MET	3.9
2	G	20	LEU	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	11	MET	3.8
2	H	9	ALA	3.7
2	K	13	GLU	3.7
2	J	14	GLN	3.7
2	K	104	LEU	3.7
2	K	8	SER	3.6
2	H	14	GLN	3.6
2	G	10	ALA	3.6
2	A	104	LEU	3.5
2	H	103	VAL	3.4
2	G	104	LEU	3.4
2	A	105	LEU	3.3
2	G	13	GLU	3.2
2	E	15	ARG	3.1
2	H	98	GLN	3.0
2	B	65	GLU	2.9
2	J	70	GLU	2.9
2	K	63	ARG	2.9
2	D	15	ARG	2.8
2	J	98	GLN	2.7
2	D	65	GLU	2.6
2	E	65	GLU	2.6
2	G	14	GLN	2.6
2	K	14	GLN	2.6
2	H	13	GLU	2.6
2	H	101	GLU	2.5
2	A	70	GLU	2.4
2	B	14	GLN	2.3
2	A	14	GLN	2.3
2	J	13	GLU	2.3
2	D	70	GLU	2.2
2	E	63	ARG	2.2
2	G	105	LEU	2.1
2	D	106	LYS	2.1
2	J	103	VAL	2.1
2	B	12	ALA	2.1
2	G	31	GLN	2.1
2	K	65	GLU	2.1
2	A	12	ALA	2.0
2	B	8	SER	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides 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. 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	B-factors(Å^2)	Q<0.9
3	TRP	G	109	15/15	0.94	0.19	25,25,25,25	15
3	TRP	J	109	15/15	0.94	0.17	25,25,25,25	15
3	TRP	K	109	15/15	0.94	0.19	25,25,25,25	15
3	TRP	H	109	15/15	0.95	0.17	25,25,25,25	15
3	TRP	E	109	15/15	0.95	0.19	25,25,25,25	15
3	TRP	A	110	15/15	0.95	0.14	25,25,25,25	15
3	TRP	D	109	15/15	0.96	0.18	25,25,25,25	15
3	TRP	A	109	15/15	0.96	0.15	25,25,25,25	15

6.5 Other polymers (i)

There are no such residues in this entry.