



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 7, 2023 – 10:57 AM EST

PDB ID : 6V8W
Title : CDYL2 chromodomain in complex with a synthetic peptide
Authors : Dong, C.; Tempel, W.; James, L.I.; Lamb, K.N.; Bountra, C.; Edwards, A.M.; Arrowsmith, C.H.; Min, J.; Structural Genomics Consortium; Structural Genomics Consortium (SGC)
Deposited on : 2019-12-12
Resolution : 2.80 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 ⓘ 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 ⓘ](#)) 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

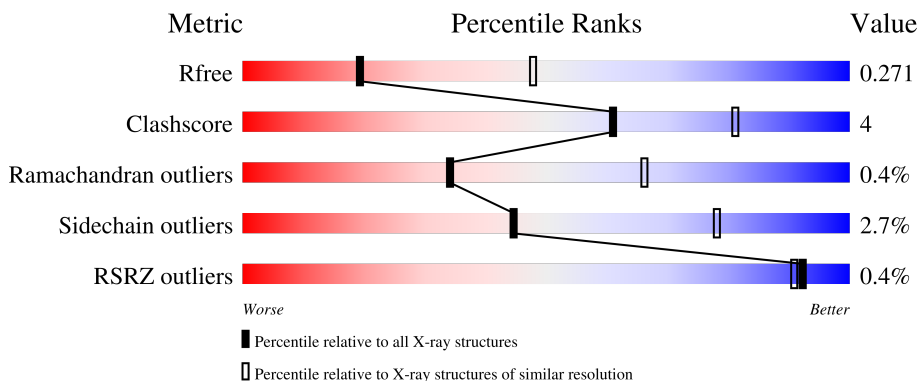
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.











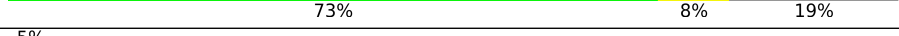

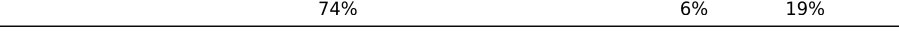
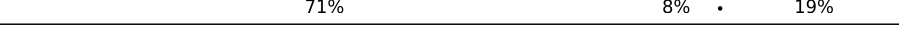

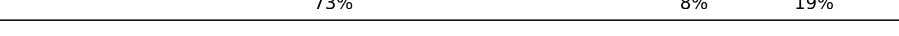


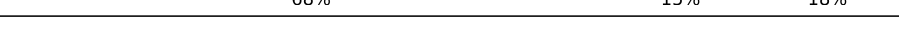

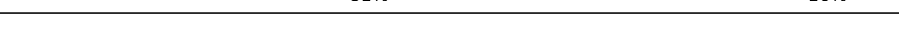






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	62	
1	B	62	
1	C	62	
1	D	62	
1	E	62	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	62	 69% 11% 18%
1	G	62	 74% 6% 19%
1	H	62	 69% 11% 19%
1	I	62	 74% 6% 18%
1	J	62	 71% 11% 18%
1	K	62	 76% 5% 19%
1	L	62	 68% 13% 19%
1	M	62	 2% 68% 15% 18%
1	N	62	 73% 8% 19%
1	O	62	 5% 68% 13% 19%
1	P	62	 74% 6% 19%
1	Q	62	 71% 8% 19%
1	R	62	 60% 21% 19%
1	S	62	 73% 8% 19%
1	T	62	 71% 10% 19%
1	U	62	 71% 10% 19%
1	V	62	 68% 15% 18%
1	W	62	 68% 13% 19%
1	X	62	 3% 81% 6% 16%
1	Y	62	 76% 6% 18%
1	Z	62	 71% 10% 19%
2	AA	7	 100%
2	BB	7	 86% 14%
2	CC	7	 86% 14%
2	DD	7	 71% 29%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	EE	7	100%
2	FF	7	100%
2	GG	7	86% 14%
2	HH	7	71% 29%
2	II	7	71% 29%
2	JJ	7	71% 14% 14%
2	KK	7	57% 43%
2	LL	7	86% 14%
2	MM	7	57% 43%
2	NN	7	86% 14%
2	OO	7	86% 14%
2	PP	7	86% 14%
2	QQ	7	71% 14% 14%
2	RR	7	86% 14%
2	SS	7	57% 43%
2	TT	7	71% 29%
2	UU	7	71% 29%
2	VV	7	86% 14%
2	WW	7	86% 14%
2	XX	7	71% 14% 14%
2	YY	7	71% 29%
2	ZZ	7	86% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	UNX	F	101	-	-	-	X
3	UNX	G	101	-	-	-	X
3	UNX	O	101	-	-	-	X
3	UNX	S	101	-	-	-	X
3	UNX	X	101	-	-	-	X
3	UNX	Y	101	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 12251 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 Chromodomain Y-like protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	50	421	270	71	79	1	0	0	0
1	B	50	419	271	68	79	1	0	0	0
1	C	51	426	275	68	82	1	0	0	0
1	D	50	424	273	71	79	1	0	0	0
1	E	54	438	281	73	83	1	0	0	0
1	F	51	439	281	75	82	1	0	0	0
1	G	50	404	260	65	78	1	0	0	0
1	H	50	418	271	67	79	1	0	0	0
1	I	51	418	271	70	76	1	0	0	0
1	J	51	423	272	70	80	1	0	0	0
1	K	50	416	270	66	79	1	0	0	0
1	L	50	415	265	69	80	1	0	0	0
1	M	51	420	271	69	79	1	0	0	0
1	N	50	419	271	69	78	1	0	0	0
1	O	50	415	268	67	79	1	0	0	0
1	P	50	417	272	69	75	1	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	50	Total	C	N	O	S	0	0	0
			406	264	67	74	1			
1	R	50	Total	C	N	O	S	0	0	0
			418	269	71	77	1			
1	S	50	Total	C	N	O	S	0	0	0
			419	269	70	79	1			
1	T	50	Total	C	N	O	S	0	0	0
			404	264	65	74	1			
1	U	50	Total	C	N	O	S	0	0	0
			410	266	69	74	1			
1	V	51	Total	C	N	O	S	0	0	0
			411	262	68	80	1			
1	W	50	Total	C	N	O	S	0	0	0
			415	266	69	79	1			
1	X	52	Total	C	N	O	S	0	0	0
			413	269	68	75	1			
1	Y	51	Total	C	N	O	S	0	0	0
			420	270	70	79	1			
1	Z	50	Total	C	N	O	S	0	0	0
			408	264	68	75	1			

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP Q8N8U2
B	1	GLY	-	expression tag	UNP Q8N8U2
C	1	GLY	-	expression tag	UNP Q8N8U2
D	1	GLY	-	expression tag	UNP Q8N8U2
E	1	GLY	-	expression tag	UNP Q8N8U2
F	1	GLY	-	expression tag	UNP Q8N8U2
G	1	GLY	-	expression tag	UNP Q8N8U2
H	1	GLY	-	expression tag	UNP Q8N8U2
I	1	GLY	-	expression tag	UNP Q8N8U2
J	1	GLY	-	expression tag	UNP Q8N8U2
K	1	GLY	-	expression tag	UNP Q8N8U2
L	1	GLY	-	expression tag	UNP Q8N8U2
M	1	GLY	-	expression tag	UNP Q8N8U2
N	1	GLY	-	expression tag	UNP Q8N8U2
O	1	GLY	-	expression tag	UNP Q8N8U2
P	1	GLY	-	expression tag	UNP Q8N8U2
Q	1	GLY	-	expression tag	UNP Q8N8U2
R	1	GLY	-	expression tag	UNP Q8N8U2
S	1	GLY	-	expression tag	UNP Q8N8U2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
T	1	GLY	-	expression tag	UNP Q8N8U2
U	1	GLY	-	expression tag	UNP Q8N8U2
V	1	GLY	-	expression tag	UNP Q8N8U2
W	1	GLY	-	expression tag	UNP Q8N8U2
X	1	GLY	-	expression tag	UNP Q8N8U2
Y	1	GLY	-	expression tag	UNP Q8N8U2
Z	1	GLY	-	expression tag	UNP Q8N8U2

- Molecule 2 is a protein called IVA-PHE-ALA-PHE-5T3-SER-NH2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	AA	7	53	40	7	6	0	0	1
2	BB	7	53	40	7	6	0	0	1
2	CC	7	53	40	7	6	0	0	1
2	DD	7	53	40	7	6	0	0	1
2	EE	7	53	40	7	6	0	0	1
2	FF	7	53	40	7	6	0	0	1
2	GG	7	53	40	7	6	0	0	1
2	HH	7	53	40	7	6	0	0	1
2	II	7	53	40	7	6	0	0	1
2	JJ	7	53	40	7	6	0	0	1
2	KK	7	53	40	7	6	0	0	1
2	LL	7	53	40	7	6	0	0	1
2	MM	7	53	40	7	6	0	0	1
2	NN	7	53	40	7	6	0	0	1
2	OO	7	53	40	7	6	0	0	1
2	PP	7	52	39	7	6	0	0	1

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	QQ	7	Total	C	N	O	0	0	1
			53	40	7	6			
2	RR	7	Total	C	N	O	0	0	1
			53	40	7	6			
2	SS	7	Total	C	N	O	0	0	1
			53	40	7	6			
2	TT	7	Total	C	N	O	0	0	1
			53	40	7	6			
2	UU	5	Total	C	N	O	0	0	0
			47	37	5	5			
2	VV	7	Total	C	N	O	0	0	1
			53	40	7	6			
2	WW	7	Total	C	N	O	0	0	1
			53	40	7	6			
2	XX	6	Total	C	N	O	0	0	1
			49	38	6	5			
2	YY	7	Total	C	N	O	0	0	1
			53	40	7	6			
2	ZZ	7	Total	C	N	O	0	0	1
			53	40	7	6			

- Molecule 3 is UNKNOWN ATOM OR ION (three-letter code: UNX) (formula: X).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	X	0	0
			3	3		
3	C	2	Total	X	0	0
			2	2		
3	D	2	Total	X	0	0
			2	2		
3	F	4	Total	X	0	0
			4	4		
3	G	1	Total	X	0	0
			1	1		
3	H	1	Total	X	0	0
			1	1		
3	I	1	Total	X	0	0
			1	1		
3	J	1	Total	X	0	0
			1	1		
3	K	1	Total	X	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	M	1	Total X 1 1	0	0
3	N	2	Total X 2 2	0	0
3	O	1	Total X 1 1	0	0
3	Q	1	Total X 1 1	0	0
3	S	3	Total X 3 3	0	0
3	T	1	Total X 1 1	0	0
3	X	1	Total X 1 1	0	0
3	Y	1	Total X 1 1	0	0
3	Z	1	Total X 1 1	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: Chromodomain Y-like protein 2

Chain A: 



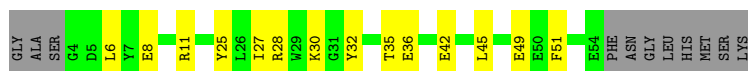
- Molecule 1: Chromodomain Y-like protein 2

Chain B: 



- Molecule 1: Chromodomain Y-like protein 2

Chain C: 




- Molecule 1: Chromodomain Y-like protein 2

Chain D: 



- Molecule 1: Chromodomain Y-like protein 2

Chain E: 



- Molecule 1: Chromodomain Y-like protein 2

Chain F: 



- Molecule 1: Chromodomain Y-like protein 2



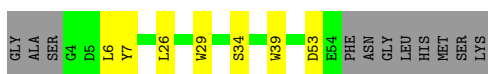
- Molecule 1: Chromodomain Y-like protein 2



- Molecule 1: Chromodomain Y-like protein 2



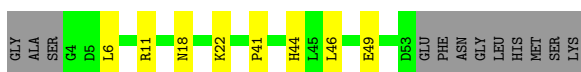
- Molecule 1: Chromodomain Y-like protein 2



- Molecule 1: Chromodomain Y-like protein 2



- Molecule 1: Chromodomain Y-like protein 2



- Molecule 1: Chromodomain Y-like protein 2

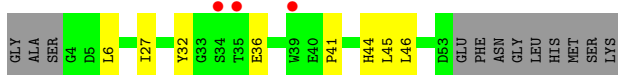




● Molecule 1: Chromodomain Y-like protein 2



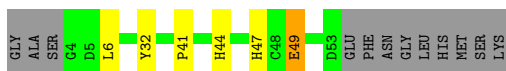
● Molecule 1: Chromodomain Y-like protein 2



● Molecule 1: Chromodomain Y-like protein 2



● Molecule 1: Chromodomain Y-like protein 2



● Molecule 1: Chromodomain Y-like protein 2



● Molecule 1: Chromodomain Y-like protein 2



● Molecule 1: Chromodomain Y-like protein 2





- Molecule 1: Chromodomain Y-like protein 2



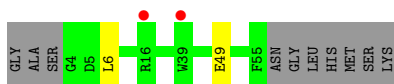
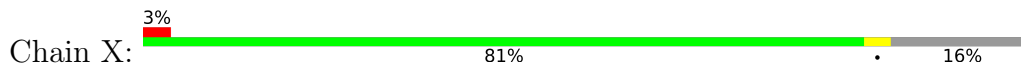
- Molecule 1: Chromodomain Y-like protein 2



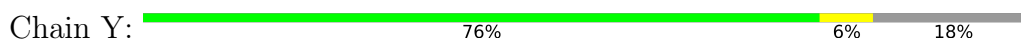
- Molecule 1: Chromodomain Y-like protein 2



- Molecule 1: Chromodomain Y-like protein 2



- Molecule 1: Chromodomain Y-like protein 2



- Molecule 1: Chromodomain Y-like protein 2




- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2




There are no outlier residues recorded for this chain.

- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain BB:  86% 14%



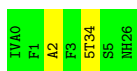
- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain CC:  86% 14%



- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain DD:  71% 29%



- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain EE:  100%


There are no outlier residues recorded for this chain.

- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain FF:  100%

There are no outlier residues recorded for this chain.

- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain GG:  86% 14%



- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain HH:  71% 29%



- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain II:  71% 29%



- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain JJ:  71% 14% 14%




- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain KK:  57% 43%



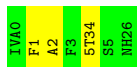
- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain LL:  86% 14%




- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain MM:  57% 43%




- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain NN:  86% 14%




- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain OO:  86% 14%




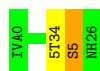
- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain PP:  86% 14%



- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain QQ:  71% 14% 14%



- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain RR: 86% 14%



- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain SS: 57% 43%



- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain TT: 71% 29%



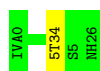
- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain UU: 71% 29%



- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain VV: 86% 14%



- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain WW: 86% 14%



- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain XX: 71% 14% 14%




- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain YY:  71% 29%



- Molecule 2: IVA-PHE-ALA-PHE-5T3-SER-NH2

Chain ZZ:  86% 14%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	88.84Å 82.16Å 128.63Å 90.00° 97.44° 90.00°	Depositor
Resolution (Å)	36.25 – 2.80 36.25 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (36.25-2.80) 99.5 (36.25-2.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.68Å)	Xtrriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.204 , 0.271 0.205 , 0.271	Depositor DCC
R_{free} test set	2506 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	42.5	Xtrriage
Anisotropy	0.020	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	12251	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: IVA, UNX, 5T3, NH2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.52	0/434	0.61	0/588
1	B	0.48	0/432	0.62	0/585
1	C	0.48	0/439	0.62	0/595
1	D	0.58	0/437	0.60	0/591
1	E	0.45	0/451	0.57	0/613
1	F	0.51	0/452	0.62	0/609
1	G	0.40	0/417	0.53	0/568
1	H	0.41	0/431	0.55	0/583
1	I	0.52	0/431	0.62	0/585
1	J	0.44	0/436	0.62	0/591
1	K	0.51	0/429	0.65	0/582
1	L	0.44	0/428	0.57	0/582
1	M	0.42	0/433	0.60	0/588
1	N	0.47	0/432	0.59	0/586
1	O	0.37	0/428	0.59	0/581
1	P	0.37	0/430	0.52	0/581
1	Q	0.40	0/419	0.57	0/569
1	R	0.42	0/431	0.63	0/584
1	S	0.42	0/432	0.60	0/586
1	T	0.42	0/417	0.57	0/567
1	U	0.44	0/423	0.56	0/574
1	V	0.42	0/424	0.57	0/577
1	W	0.38	0/428	0.57	0/582
1	X	0.36	0/426	0.53	0/580
1	Y	0.44	0/433	0.56	0/588
1	Z	0.40	0/421	0.53	0/572
2	AA	0.55	0/32	0.78	0/40
2	BB	0.57	0/32	1.04	0/40
2	CC	0.68	0/32	0.90	0/40
2	DD	0.82	0/32	0.87	0/40
2	EE	0.73	0/32	0.60	0/40
2	FF	0.68	0/32	1.14	0/40

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	GG	0.58	0/32	0.59	0/40
2	HH	0.62	0/32	0.91	0/40
2	II	0.59	0/32	0.82	0/40
2	JJ	0.57	0/32	1.16	1/40 (2.5%)
2	KK	0.58	0/32	0.97	0/40
2	LL	0.62	0/32	0.53	0/40
2	MM	0.39	0/32	0.94	0/40
2	NN	0.58	0/32	0.59	0/40
2	OO	0.62	0/32	0.67	0/40
2	PP	0.56	0/32	0.86	0/40
2	QQ	0.60	0/32	1.23	1/40 (2.5%)
2	RR	0.55	0/32	0.66	0/40
2	SS	0.71	0/32	0.94	0/40
2	TT	0.60	0/32	0.63	0/40
2	UU	0.42	0/28	0.46	0/36
2	VV	0.51	0/32	0.83	0/40
2	WW	0.40	0/32	0.75	0/40
2	XX	0.56	0/29	0.45	0/36
2	YY	0.55	0/32	0.77	0/40
2	ZZ	0.64	0/32	0.67	0/40
All	All	0.46	0/12019	0.60	2/16219 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	QQ	5	SER	N-CA-CB	6.06	119.59	110.50
2	JJ	5	SER	N-CA-CB	5.12	118.18	110.50

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	421	0	370	5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	419	0	367	6	0
1	C	426	0	362	7	0
1	D	424	0	376	7	0
1	E	438	0	369	4	0
1	F	439	0	403	5	0
1	G	404	0	330	2	0
1	H	418	0	359	3	0
1	I	418	0	352	4	0
1	J	423	0	360	5	0
1	K	416	0	355	3	0
1	L	415	0	347	6	0
1	M	420	0	356	7	0
1	N	419	0	359	5	0
1	O	415	0	356	5	0
1	P	417	0	368	2	0
1	Q	406	0	348	3	0
1	R	418	0	368	9	0
1	S	419	0	363	3	0
1	T	404	0	335	4	0
1	U	410	0	349	4	0
1	V	411	0	324	7	0
1	W	415	0	352	6	0
1	X	413	0	339	1	0
1	Y	420	0	353	3	0
1	Z	408	0	344	3	0
2	AA	53	0	34	0	0
2	BB	53	0	34	0	0
2	CC	53	0	34	0	0
2	DD	53	0	34	1	0
2	EE	53	0	34	0	0
2	FF	53	0	34	0	0
2	GG	53	0	34	0	0
2	HH	53	0	34	1	0
2	II	53	0	34	1	0
2	JJ	53	0	34	0	0
2	KK	53	0	34	1	0
2	LL	53	0	34	0	0
2	MM	53	0	34	2	0
2	NN	53	0	34	0	0
2	OO	53	0	34	0	0
2	PP	52	0	34	0	0
2	QQ	53	0	34	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	RR	53	0	34	0	0
2	SS	53	0	34	1	0
2	TT	53	0	34	1	0
2	UU	47	0	32	0	0
2	VV	53	0	34	0	0
2	WW	53	0	34	1	0
2	XX	49	0	33	0	0
2	YY	53	0	34	0	0
2	ZZ	53	0	34	0	0
3	A	3	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	F	4	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
3	K	1	0	0	0	0
3	M	1	0	0	0	0
3	N	2	0	0	0	0
3	O	1	0	0	0	0
3	Q	1	0	0	0	0
3	S	3	0	0	0	0
3	T	1	0	0	0	0
3	X	1	0	0	0	0
3	Y	1	0	0	0	0
3	Z	1	0	0	0	0
All	All	12251	0	10145	100	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 4.

All (100) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LEU:HB2	1:B:6:LEU:HB2	1.70	0.74
1:Y:6:LEU:HB2	1:Z:6:LEU:HB2	1.70	0.73
1:G:6:LEU:HB2	1:H:6:LEU:HB2	1.76	0.67
1:O:6:LEU:HB2	1:P:6:LEU:HB2	1.77	0.66
1:J:53:ASP:HB3	1:M:11:ARG:HD3	1.77	0.65
1:R:41:PRO:HG2	1:R:44:HIS:CD2	2.34	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:32:TYR:HD1	1:R:36:GLU:HG3	1.64	0.62
1:M:6:LEU:HB2	1:N:6:LEU:HB2	1.83	0.61
1:I:6:LEU:HB2	1:J:6:LEU:HB2	1.83	0.60
1:B:18:ASN:HD21	1:B:22:LYS:HB2	1.65	0.60
1:D:11:ARG:NH2	1:E:53:ASP:O	2.37	0.58
1:C:6:LEU:HB2	1:D:6:LEU:HB2	1.84	0.58
1:U:32:TYR:HD2	1:U:36:GLU:HG3	1.70	0.57
1:W:6:LEU:HB2	1:X:6:LEU:HB2	1.86	0.56
1:E:6:LEU:HB2	1:F:6:LEU:HB2	1.88	0.56
1:N:23:TRP:CD1	1:R:15:LYS:HE3	2.41	0.55
1:A:41:PRO:HG2	1:A:44:HIS:CD2	2.41	0.55
1:S:41:PRO:HG2	1:S:44:HIS:CD2	2.43	0.54
1:A:32:TYR:HB3	1:A:36:GLU:HG3	1.89	0.54
1:U:32:TYR:CD2	1:U:36:GLU:HG3	2.43	0.53
1:Y:41:PRO:HG2	1:Y:44:HIS:CD2	2.44	0.53
1:L:11:ARG:HD2	1:V:53:ASP:HB3	1.90	0.52
1:L:41:PRO:HG2	1:L:44:HIS:CD2	2.44	0.52
1:M:41:PRO:HG2	1:M:44:HIS:CD2	2.44	0.52
1:O:6:LEU:HD21	1:O:46:LEU:HD12	1.91	0.52
1:F:26:LEU:HD13	1:F:39:TRP:CD1	2.45	0.52
1:W:41:PRO:HG2	1:W:44:HIS:CD2	2.46	0.51
1:N:26:LEU:HD13	1:N:39:TRP:CD1	2.46	0.51
1:U:6:LEU:HB2	1:V:6:LEU:HB2	1.92	0.51
1:L:6:LEU:HD11	1:L:46:LEU:HD12	1.93	0.51
1:D:9:VAL:HG13	1:D:27:ILE:HG23	1.92	0.50
1:Q:47:HIS:CE1	1:Q:49:GLU:HG2	2.46	0.50
1:S:44:HIS:O	2:SS:2:ALA:HA	2.12	0.50
1:A:26:LEU:HD13	1:A:39:TRP:CD1	2.46	0.50
1:H:44:HIS:O	2:HH:2:ALA:HA	2.12	0.50
1:O:27:ILE:HD11	1:O:45:LEU:HD21	1.94	0.49
1:K:44:HIS:O	2:KK:2:ALA:HA	2.12	0.49
1:E:32:TYR:HD2	1:E:36:GLU:HG3	1.77	0.49
1:B:15:LYS:HB3	1:B:23:TRP:HZ3	1.78	0.49
1:O:41:PRO:HG2	1:O:44:HIS:CD2	2.48	0.48
1:D:26:LEU:HD13	1:D:39:TRP:CD1	2.49	0.48
1:R:28:ARG:NH2	1:R:37:ASP:OD2	2.37	0.48
1:I:32:TYR:HD2	1:I:36:GLU:HG3	1.79	0.48
1:Q:6:LEU:HB2	1:R:6:LEU:HB2	1.95	0.48
1:K:6:LEU:HB2	1:L:6:LEU:HB2	1.96	0.47
1:M:17:LYS:HG3	1:M:23:TRP:CE2	2.50	0.47
1:T:44:HIS:O	2:TT:2:ALA:HA	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:51:PHE:O	1:F:11:ARG:HG3	2.15	0.47
1:B:41:PRO:HG2	1:B:44:HIS:CD2	2.50	0.47
1:W:10:GLU:HB2	1:W:30:LYS:HA	1.98	0.47
1:S:50:GLU:OE1	1:T:43:HIS:HB2	2.15	0.46
1:D:26:LEU:HD13	1:D:39:TRP:NE1	2.30	0.46
1:K:41:PRO:HG2	1:K:44:HIS:CD2	2.51	0.46
1:L:11:ARG:NH2	1:V:53:ASP:O	2.48	0.46
1:N:26:LEU:HD13	1:N:39:TRP:NE1	2.31	0.46
1:J:26:LEU:HD13	1:J:39:TRP:CD1	2.51	0.46
1:P:41:PRO:HG2	1:P:44:HIS:CD2	2.52	0.45
1:Y:6:LEU:HD21	1:Y:46:LEU:HD12	1.99	0.45
1:L:18:ASN:OD1	1:L:22:LYS:N	2.44	0.45
1:V:28:ARG:NH2	1:V:37:ASP:OD2	2.49	0.45
1:C:32:TYR:CD2	1:C:36:GLU:HG3	2.52	0.45
1:W:29:TRP:CZ3	2:WW:2:ALA:HB3	2.53	0.44
1:Z:9:VAL:HG13	1:Z:27:ILE:HG23	1.98	0.44
1:W:26:LEU:HD13	1:W:39:TRP:CD1	2.53	0.44
1:C:25:TYR:HE1	1:C:42:GLU:HG3	1.82	0.43
1:G:41:PRO:HG2	1:G:44:HIS:CD2	2.53	0.43
1:F:13:VAL:HG22	1:F:26:LEU:HB3	2.01	0.43
1:J:7:TYR:HB2	1:J:29:TRP:CZ3	2.54	0.43
1:T:6:LEU:HD11	1:T:46:LEU:HD12	1.99	0.43
1:B:25:TYR:HE1	1:B:42:GLU:HG3	1.84	0.43
1:M:27:ILE:HD11	1:M:45:LEU:HD21	2.00	0.42
1:D:44:HIS:O	2:DD:2:ALA:HA	2.19	0.42
1:E:41:PRO:HG2	1:E:44:HIS:CD2	2.54	0.42
1:J:26:LEU:HD13	1:J:39:TRP:NE1	2.34	0.42
1:D:7:TYR:HB2	1:D:29:TRP:CZ3	2.55	0.42
1:M:6:LEU:HB3	2:MM:1:PHE:HB3	2.01	0.42
1:F:47:HIS:NE2	1:F:49:GLU:HG2	2.35	0.42
1:B:15:LYS:HB3	1:B:23:TRP:CZ3	2.55	0.42
1:C:27:ILE:HD11	1:C:45:LEU:HD21	2.01	0.42
1:V:10:GLU:HB2	1:V:30:LYS:HA	2.02	0.42
1:C:8:GLU:CD	1:C:30:LYS:HD3	2.40	0.41
1:A:12:ILE:HD13	1:A:25:TYR:CD2	2.55	0.41
1:M:44:HIS:O	2:MM:2:ALA:HA	2.20	0.41
1:Z:36:GLU:O	1:Z:38:THR:HG23	2.21	0.41
1:O:32:TYR:HB3	1:O:36:GLU:HG3	2.03	0.41
1:C:11:ARG:HB3	1:C:28:ARG:HB3	2.02	0.41
1:R:6:LEU:HD23	1:R:6:LEU:HA	1.91	0.41
1:R:25:TYR:HE1	1:R:42:GLU:HG3	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:44:HIS:O	2:II:2:ALA:HA	2.20	0.41
1:N:15:LYS:HB2	1:N:23:TRP:HZ3	1.86	0.41
1:H:26:LEU:HD13	1:H:39:TRP:CD1	2.56	0.41
1:U:41:PRO:HG2	1:U:44:HIS:CD2	2.56	0.41
1:V:11:ARG:HB3	1:V:28:ARG:HB3	2.02	0.41
1:I:32:TYR:CD2	1:I:36:GLU:HG3	2.56	0.40
1:Q:41:PRO:HG2	1:Q:44:HIS:CD2	2.56	0.40
1:R:9:VAL:HG13	1:R:27:ILE:HG23	2.04	0.40
1:R:32:TYR:CD1	1:R:36:GLU:HG3	2.50	0.40
1:T:36:GLU:O	1:T:38:THR:HG23	2.21	0.40
1:V:32:TYR:HD1	1:V:36:GLU:HG2	1.86	0.40
1:W:26:LEU:HD12	1:W:26:LEU:HA	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	48/62 (77%)	48 (100%)	0	0	100	100
1	B	48/62 (77%)	48 (100%)	0	0	100	100
1	C	49/62 (79%)	49 (100%)	0	0	100	100
1	D	48/62 (77%)	47 (98%)	1 (2%)	0	100	100
1	E	52/62 (84%)	52 (100%)	0	0	100	100
1	F	49/62 (79%)	49 (100%)	0	0	100	100
1	G	48/62 (77%)	47 (98%)	1 (2%)	0	100	100
1	H	48/62 (77%)	48 (100%)	0	0	100	100
1	I	49/62 (79%)	49 (100%)	0	0	100	100
1	J	49/62 (79%)	49 (100%)	0	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	48/62 (77%)	48 (100%)	0	0	100	100
1	L	48/62 (77%)	48 (100%)	0	0	100	100
1	M	49/62 (79%)	49 (100%)	0	0	100	100
1	N	48/62 (77%)	48 (100%)	0	0	100	100
1	O	48/62 (77%)	48 (100%)	0	0	100	100
1	P	48/62 (77%)	48 (100%)	0	0	100	100
1	Q	48/62 (77%)	48 (100%)	0	0	100	100
1	R	48/62 (77%)	48 (100%)	0	0	100	100
1	S	48/62 (77%)	48 (100%)	0	0	100	100
1	T	48/62 (77%)	48 (100%)	0	0	100	100
1	U	48/62 (77%)	48 (100%)	0	0	100	100
1	V	49/62 (79%)	49 (100%)	0	0	100	100
1	W	48/62 (77%)	48 (100%)	0	0	100	100
1	X	50/62 (81%)	50 (100%)	0	0	100	100
1	Y	49/62 (79%)	48 (98%)	1 (2%)	0	100	100
1	Z	48/62 (77%)	48 (100%)	0	0	100	100
2	AA	4/7 (57%)	3 (75%)	1 (25%)	0	100	100
2	BB	4/7 (57%)	3 (75%)	1 (25%)	0	100	100
2	CC	4/7 (57%)	4 (100%)	0	0	100	100
2	DD	4/7 (57%)	4 (100%)	0	0	100	100
2	EE	4/7 (57%)	3 (75%)	1 (25%)	0	100	100
2	FF	4/7 (57%)	4 (100%)	0	0	100	100
2	GG	4/7 (57%)	4 (100%)	0	0	100	100
2	HH	4/7 (57%)	4 (100%)	0	0	100	100
2	II	4/7 (57%)	4 (100%)	0	0	100	100
2	JJ	4/7 (57%)	3 (75%)	0	1 (25%)	0	0
2	KK	4/7 (57%)	3 (75%)	0	1 (25%)	0	0
2	LL	4/7 (57%)	4 (100%)	0	0	100	100
2	MM	4/7 (57%)	4 (100%)	0	0	100	100
2	NN	4/7 (57%)	3 (75%)	0	1 (25%)	0	0
2	OO	4/7 (57%)	3 (75%)	1 (25%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	PP	4/7 (57%)	4 (100%)	0	0	100	100
2	QQ	4/7 (57%)	3 (75%)	0	1 (25%)	0	0
2	RR	4/7 (57%)	4 (100%)	0	0	100	100
2	SS	4/7 (57%)	3 (75%)	0	1 (25%)	0	0
2	TT	4/7 (57%)	4 (100%)	0	0	100	100
2	UU	3/7 (43%)	3 (100%)	0	0	100	100
2	VV	4/7 (57%)	4 (100%)	0	0	100	100
2	WW	4/7 (57%)	4 (100%)	0	0	100	100
2	XX	3/7 (43%)	3 (100%)	0	0	100	100
2	YY	4/7 (57%)	3 (75%)	0	1 (25%)	0	0
2	ZZ	4/7 (57%)	4 (100%)	0	0	100	100
All	All	1363/1794 (76%)	1350 (99%)	7 (0%)	6 (0%)	34	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	QQ	5	SER
2	YY	5	SER
2	KK	5	SER
2	SS	5	SER
2	JJ	5	SER
2	NN	5	SER

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	41/55 (74%)	39 (95%)	2 (5%)	25	57
1	B	40/55 (73%)	39 (98%)	1 (2%)	47	80
1	C	40/55 (73%)	38 (95%)	2 (5%)	24	56
1	D	41/55 (74%)	39 (95%)	2 (5%)	25	57

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	39/55 (71%)	38 (97%)	1 (3%)	46	79
1	F	45/55 (82%)	43 (96%)	2 (4%)	28	61
1	G	36/55 (66%)	35 (97%)	1 (3%)	43	77
1	H	38/55 (69%)	35 (92%)	3 (8%)	12	34
1	I	36/55 (66%)	34 (94%)	2 (6%)	21	51
1	J	39/55 (71%)	38 (97%)	1 (3%)	46	79
1	K	38/55 (69%)	38 (100%)	0	100	100
1	L	39/55 (71%)	38 (97%)	1 (3%)	46	79
1	M	38/55 (69%)	37 (97%)	1 (3%)	46	79
1	N	38/55 (69%)	38 (100%)	0	100	100
1	O	39/55 (71%)	39 (100%)	0	100	100
1	P	38/55 (69%)	37 (97%)	1 (3%)	46	79
1	Q	36/55 (66%)	34 (94%)	2 (6%)	21	51
1	R	40/55 (73%)	39 (98%)	1 (2%)	47	80
1	S	40/55 (73%)	38 (95%)	2 (5%)	24	56
1	T	34/55 (62%)	34 (100%)	0	100	100
1	U	36/55 (66%)	35 (97%)	1 (3%)	43	77
1	V	36/55 (66%)	36 (100%)	0	100	100
1	W	39/55 (71%)	39 (100%)	0	100	100
1	X	34/55 (62%)	33 (97%)	1 (3%)	42	76
1	Y	38/55 (69%)	38 (100%)	0	100	100
1	Z	36/55 (66%)	35 (97%)	1 (3%)	43	77
2	AA	2/3 (67%)	2 (100%)	0	100	100
2	BB	2/3 (67%)	2 (100%)	0	100	100
2	CC	2/3 (67%)	2 (100%)	0	100	100
2	DD	2/3 (67%)	2 (100%)	0	100	100
2	EE	2/3 (67%)	2 (100%)	0	100	100
2	FF	2/3 (67%)	2 (100%)	0	100	100
2	GG	2/3 (67%)	2 (100%)	0	100	100
2	HH	2/3 (67%)	2 (100%)	0	100	100
2	II	2/3 (67%)	2 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	JJ	2/3 (67%)	2 (100%)	0	100	100
2	KK	2/3 (67%)	2 (100%)	0	100	100
2	LL	2/3 (67%)	2 (100%)	0	100	100
2	MM	2/3 (67%)	2 (100%)	0	100	100
2	NN	2/3 (67%)	2 (100%)	0	100	100
2	OO	2/3 (67%)	2 (100%)	0	100	100
2	PP	2/3 (67%)	2 (100%)	0	100	100
2	QQ	2/3 (67%)	2 (100%)	0	100	100
2	RR	2/3 (67%)	2 (100%)	0	100	100
2	SS	2/3 (67%)	2 (100%)	0	100	100
2	TT	2/3 (67%)	2 (100%)	0	100	100
2	UU	2/3 (67%)	2 (100%)	0	100	100
2	VV	2/3 (67%)	2 (100%)	0	100	100
2	WW	2/3 (67%)	2 (100%)	0	100	100
2	XX	2/3 (67%)	2 (100%)	0	100	100
2	YY	2/3 (67%)	2 (100%)	0	100	100
2	ZZ	2/3 (67%)	2 (100%)	0	100	100
All	All	1046/1508 (69%)	1018 (97%)	28 (3%)	44	78

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	TYR
1	A	34	SER
1	B	34	SER
1	C	35	THR
1	C	49	GLU
1	D	19	LYS
1	D	34	SER
1	E	32	TYR
1	F	13	VAL
1	F	35	THR
1	G	50	GLU
1	H	34	SER
1	H	35	THR
1	H	49	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	13	VAL
1	I	32	TYR
1	J	34	SER
1	L	49	GLU
1	M	35	THR
1	P	50	GLU
1	Q	32	TYR
1	Q	49	GLU
1	R	49	GLU
1	S	11	ARG
1	S	35	THR
1	U	10	GLU
1	X	49	GLU
1	Z	32	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	G	44	HIS
1	I	44	HIS
1	N	44	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

26 non-standard protein/DNA/RNA residues 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	5T3	VV	4	2	12,13,14	0.73	1 (8%)	9,15,17	1.52	2 (22%)
2	5T3	UU	4	2	12,13,14	0.61	0	9,15,17	0.72	0
2	5T3	HH	4	2	12,13,14	0.36	0	9,15,17	1.72	1 (11%)
2	5T3	TT	4	2	12,13,14	0.70	1 (8%)	9,15,17	2.84	2 (22%)
2	5T3	JJ	4	2	12,13,14	0.86	1 (8%)	9,15,17	1.31	2 (22%)
2	5T3	CC	4	2	12,13,14	0.40	0	9,15,17	1.68	2 (22%)
2	5T3	ZZ	4	2	12,13,14	0.30	0	9,15,17	1.59	1 (11%)
2	5T3	KK	4	2	12,13,14	0.28	0	9,15,17	1.81	2 (22%)
2	5T3	OO	4	2	12,13,14	0.29	0	9,15,17	1.16	1 (11%)
2	5T3	PP	4	2	10,12,14	0.46	0	9,14,17	1.05	1 (11%)
2	5T3	EE	4	2	12,13,14	0.64	0	9,15,17	0.71	0
2	5T3	XX	4	2	12,13,14	0.50	0	9,15,17	1.56	2 (22%)
2	5T3	NN	4	2	12,13,14	0.52	0	9,15,17	0.83	0
2	5T3	YY	4	2	12,13,14	0.56	0	9,15,17	1.85	1 (11%)
2	5T3	GG	4	2	12,13,14	0.26	0	9,15,17	1.04	1 (11%)
2	5T3	AA	4	2	12,13,14	0.39	0	9,15,17	0.90	0
2	5T3	BB	4	2	12,13,14	0.32	0	9,15,17	0.81	1 (11%)
2	5T3	SS	4	2	12,13,14	0.65	1 (8%)	9,15,17	1.01	1 (11%)
2	5T3	QQ	4	2	12,13,14	0.53	0	9,15,17	1.07	1 (11%)
2	5T3	LL	4	2	12,13,14	0.53	0	9,15,17	1.64	1 (11%)
2	5T3	RR	4	2	12,13,14	0.22	0	9,15,17	1.38	2 (22%)
2	5T3	FF	4	2	12,13,14	0.23	0	9,15,17	0.82	0
2	5T3	II	4	2	12,13,14	0.65	1 (8%)	9,15,17	1.74	3 (33%)
2	5T3	DD	4	2	12,13,14	0.29	0	9,15,17	1.56	2 (22%)
2	5T3	WW	4	2	12,13,14	0.28	0	9,15,17	0.66	0
2	5T3	MM	4	2	12,13,14	0.70	1 (8%)	9,15,17	0.99	1 (11%)

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	5T3	VV	4	2	-	7/14/15/17	-
2	5T3	UU	4	2	-	8/14/15/17	-
2	5T3	HH	4	2	-	6/14/15/17	-
2	5T3	TT	4	2	-	9/14/15/17	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	5T3	JJ	4	2	-	5/14/15/17	-
2	5T3	CC	4	2	-	6/14/15/17	-
2	5T3	ZZ	4	2	-	7/14/15/17	-
2	5T3	KK	4	2	-	4/14/15/17	-
2	5T3	OO	4	2	-	7/14/15/17	-
2	5T3	PP	4	2	-	6/12/13/17	-
2	5T3	EE	4	2	-	4/14/15/17	-
2	5T3	XX	4	2	-	6/14/15/17	-
2	5T3	NN	4	2	-	6/14/15/17	-
2	5T3	YY	4	2	-	7/14/15/17	-
2	5T3	GG	4	2	-	7/14/15/17	-
2	5T3	AA	4	2	-	8/14/15/17	-
2	5T3	BB	4	2	-	7/14/15/17	-
2	5T3	SS	4	2	-	5/14/15/17	-
2	5T3	QQ	4	2	-	6/14/15/17	-
2	5T3	LL	4	2	-	7/14/15/17	-
2	5T3	RR	4	2	-	7/14/15/17	-
2	5T3	FF	4	2	-	7/14/15/17	-
2	5T3	II	4	2	-	3/14/15/17	-
2	5T3	DD	4	2	-	3/14/15/17	-
2	5T3	WW	4	2	-	7/14/15/17	-
2	5T3	MM	4	2	-	7/14/15/17	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	JJ	4	5T3	CB-CA	2.83	1.57	1.53
2	VV	4	5T3	CB-CA	2.34	1.56	1.53
2	MM	4	5T3	CB-CA	-2.25	1.50	1.53
2	TT	4	5T3	CB-CA	2.15	1.56	1.53
2	II	4	5T3	CB-CA	2.05	1.56	1.53
2	SS	4	5T3	CB-CA	-2.01	1.50	1.53

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	TT	4	5T3	CE-NZ-CH1	7.73	124.02	113.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	YY	4	5T3	CE-NZ-CH1	5.00	120.25	113.33
2	KK	4	5T3	CE-NZ-CH1	4.47	119.52	113.33
2	HH	4	5T3	CE-NZ-CH1	4.37	119.38	113.33
2	CC	4	5T3	CE-NZ-CH1	4.12	119.03	113.33
2	LL	4	5T3	CE-NZ-CH1	4.08	118.97	113.33
2	ZZ	4	5T3	CE-NZ-CH1	3.96	118.82	113.33
2	XX	4	5T3	CE-NZ-CH1	3.78	118.56	113.33
2	VV	4	5T3	CE-NZ-CH1	3.55	118.25	113.33
2	II	4	5T3	CE-NZ-CH1	-3.48	108.51	113.33
2	OO	4	5T3	CE-NZ-CH1	3.37	117.99	113.33
2	DD	4	5T3	CE-NZ-CH1	3.27	117.86	113.33
2	KK	4	5T3	CH2-NZ-CE	2.88	121.73	113.20
2	SS	4	5T3	CE-NZ-CH1	2.83	117.24	113.33
2	DD	4	5T3	CD-CE-NZ	-2.76	106.33	113.88
2	MM	4	5T3	CE-NZ-CH1	2.76	117.15	113.33
2	JJ	4	5T3	CD-CE-NZ	-2.65	106.62	113.88
2	RR	4	5T3	CH2-NZ-CE	2.62	120.95	113.20
2	II	4	5T3	CH2-NZ-CE	2.58	120.82	113.20
2	VV	4	5T3	CH2-NZ-CE	2.53	120.69	113.20
2	CC	4	5T3	CH2-NZ-CE	2.52	120.67	113.20
2	PP	4	5T3	CH2-NZ-CE	2.47	114.17	110.53
2	GG	4	5T3	CE-NZ-CH1	2.37	116.61	113.33
2	QQ	4	5T3	CE-NZ-CH1	2.33	116.56	113.33
2	II	4	5T3	CD-CE-NZ	-2.28	107.63	113.88
2	XX	4	5T3	CH2-NZ-CE	2.26	119.88	113.20
2	BB	4	5T3	CH2-NZ-CE	2.23	119.79	113.20
2	RR	4	5T3	CE-NZ-CH1	2.14	116.29	113.33
2	JJ	4	5T3	CE-NZ-CH1	2.08	116.20	113.33
2	TT	4	5T3	CD-CE-NZ	-2.02	108.34	113.88

There are no chirality outliers.

All (162) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AA	4	5T3	O-C-CA-CB
2	AA	4	5T3	CT1-CH1-NZ-CH2
2	AA	4	5T3	CT3-CH1-NZ-CH2
2	AA	4	5T3	CT2-CH2-NZ-CH1
2	BB	4	5T3	CT1-CH1-NZ-CH2
2	BB	4	5T3	CT3-CH1-NZ-CH2
2	CC	4	5T3	O-C-CA-CB
2	CC	4	5T3	CT1-CH1-NZ-CE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	CC	4	5T3	CT3-CH1-NZ-CE
2	CC	4	5T3	CT2-CH2-NZ-CH1
2	DD	4	5T3	CT1-CH1-NZ-CH2
2	DD	4	5T3	CT3-CH1-NZ-CH2
2	EE	4	5T3	CD-CE-NZ-CH1
2	EE	4	5T3	CT2-CH2-NZ-CE
2	FF	4	5T3	CT1-CH1-NZ-CH2
2	FF	4	5T3	CT3-CH1-NZ-CH2
2	GG	4	5T3	CT1-CH1-NZ-CH2
2	GG	4	5T3	CT3-CH1-NZ-CH2
2	HH	4	5T3	CT1-CH1-NZ-CH2
2	HH	4	5T3	CT3-CH1-NZ-CH2
2	II	4	5T3	CT2-CH2-NZ-CE
2	II	4	5T3	CT2-CH2-NZ-CH1
2	JJ	4	5T3	CT1-CH1-NZ-CH2
2	LL	4	5T3	CT1-CH1-NZ-CH2
2	LL	4	5T3	CT3-CH1-NZ-CH2
2	LL	4	5T3	CT2-CH2-NZ-CH1
2	MM	4	5T3	O-C-CA-CB
2	MM	4	5T3	N-CA-CB-CG
2	MM	4	5T3	C-CA-CB-CG
2	MM	4	5T3	CD-CE-NZ-CH1
2	MM	4	5T3	CT2-CH2-NZ-CH1
2	NN	4	5T3	CT3-CH1-NZ-CE
2	NN	4	5T3	CT1-CH1-NZ-CH2
2	NN	4	5T3	CT3-CH1-NZ-CH2
2	OO	4	5T3	CT3-CH1-NZ-CE
2	OO	4	5T3	CT1-CH1-NZ-CH2
2	OO	4	5T3	CT3-CH1-NZ-CH2
2	OO	4	5T3	CT2-CH2-NZ-CE
2	PP	4	5T3	O-C-CA-CB
2	PP	4	5T3	CD-CE-NZ-CH2
2	QQ	4	5T3	CT1-CH1-NZ-CH2
2	QQ	4	5T3	CT3-CH1-NZ-CH2
2	RR	4	5T3	O-C-CA-CB
2	RR	4	5T3	CT1-CH1-NZ-CH2
2	RR	4	5T3	CT3-CH1-NZ-CH2
2	SS	4	5T3	CD-CE-NZ-CH2
2	TT	4	5T3	N-CA-CB-CG
2	TT	4	5T3	C-CA-CB-CG
2	TT	4	5T3	CD-CE-NZ-CH2
2	TT	4	5T3	CT1-CH1-NZ-CH2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	TT	4	5T3	CT3-CH1-NZ-CH2
2	TT	4	5T3	CT2-CH2-NZ-CH1
2	UU	4	5T3	O-C-CA-CB
2	UU	4	5T3	CT1-CH1-NZ-CH2
2	UU	4	5T3	CT3-CH1-NZ-CH2
2	UU	4	5T3	CT2-CH2-NZ-CE
2	VV	4	5T3	O-C-CA-CB
2	VV	4	5T3	CT1-CH1-NZ-CH2
2	VV	4	5T3	CT3-CH1-NZ-CH2
2	WW	4	5T3	O-C-CA-CB
2	WW	4	5T3	CT1-CH1-NZ-CH2
2	WW	4	5T3	CT3-CH1-NZ-CH2
2	XX	4	5T3	CT1-CH1-NZ-CH2
2	XX	4	5T3	CT3-CH1-NZ-CH2
2	XX	4	5T3	CT2-CH2-NZ-CH1
2	YY	4	5T3	CT1-CH1-NZ-CH2
2	YY	4	5T3	CT3-CH1-NZ-CH2
2	ZZ	4	5T3	O-C-CA-CB
2	ZZ	4	5T3	CT1-CH1-NZ-CH2
2	ZZ	4	5T3	CT3-CH1-NZ-CH2
2	AA	4	5T3	CE-CD-CG-CB
2	GG	4	5T3	CE-CD-CG-CB
2	SS	4	5T3	CE-CD-CG-CB
2	ZZ	4	5T3	CE-CD-CG-CB
2	HH	4	5T3	CE-CD-CG-CB
2	OO	4	5T3	CE-CD-CG-CB
2	QQ	4	5T3	CE-CD-CG-CB
2	RR	4	5T3	CE-CD-CG-CB
2	TT	4	5T3	CE-CD-CG-CB
2	WW	4	5T3	CE-CD-CG-CB
2	YY	4	5T3	CE-CD-CG-CB
2	FF	4	5T3	CE-CD-CG-CB
2	KK	4	5T3	CE-CD-CG-CB
2	VV	4	5T3	CE-CD-CG-CB
2	BB	4	5T3	CE-CD-CG-CB
2	DD	4	5T3	CE-CD-CG-CB
2	XX	4	5T3	CE-CD-CG-CB
2	UU	4	5T3	CG-CD-CE-NZ
2	LL	4	5T3	CE-CD-CG-CB
2	NN	4	5T3	CE-CD-CG-CB
2	II	4	5T3	CE-CD-CG-CB
2	UU	4	5T3	CA-CB-CG-CD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	BB	4	5T3	CT1-CH1-NZ-CE
2	BB	4	5T3	CT3-CH1-NZ-CE
2	EE	4	5T3	CT3-CH1-NZ-CH2
2	GG	4	5T3	CT3-CH1-NZ-CE
2	HH	4	5T3	CT3-CH1-NZ-CE
2	JJ	4	5T3	CT3-CH1-NZ-CH2
2	MM	4	5T3	CT1-CH1-NZ-CH2
2	QQ	4	5T3	CT3-CH1-NZ-CE
2	WW	4	5T3	CT3-CH1-NZ-CE
2	YY	4	5T3	CD-CE-NZ-CH2
2	AA	4	5T3	CT1-CH1-NZ-CE
2	AA	4	5T3	CT3-CH1-NZ-CE
2	FF	4	5T3	CT1-CH1-NZ-CE
2	GG	4	5T3	CT1-CH1-NZ-CE
2	HH	4	5T3	CT1-CH1-NZ-CE
2	LL	4	5T3	CT1-CH1-NZ-CE
2	NN	4	5T3	CT1-CH1-NZ-CE
2	OO	4	5T3	CT1-CH1-NZ-CE
2	PP	4	5T3	CT1-CH1-NZ-CE
2	QQ	4	5T3	CT1-CH1-NZ-CE
2	RR	4	5T3	CT1-CH1-NZ-CE
2	VV	4	5T3	CT1-CH1-NZ-CE
2	VV	4	5T3	CT3-CH1-NZ-CE
2	WW	4	5T3	CT1-CH1-NZ-CE
2	YY	4	5T3	CT1-CH1-NZ-CE
2	ZZ	4	5T3	CT1-CH1-NZ-CE
2	ZZ	4	5T3	CT3-CH1-NZ-CE
2	FF	4	5T3	CD-CE-NZ-CH1
2	KK	4	5T3	CD-CE-NZ-CH1
2	VV	4	5T3	CD-CE-NZ-CH1
2	XX	4	5T3	CD-CE-NZ-CH1
2	CC	4	5T3	CE-CD-CG-CB
2	SS	4	5T3	CT2-CH2-NZ-CE
2	JJ	4	5T3	CE-CD-CG-CB
2	EE	4	5T3	CT1-CH1-NZ-CH2
2	SS	4	5T3	CT2-CH2-NZ-CH1
2	PP	4	5T3	CT1-CH1-NZ-CH2
2	AA	4	5T3	CD-CE-NZ-CH2
2	NN	4	5T3	CD-CE-NZ-CH2
2	FF	4	5T3	CT3-CH1-NZ-CE
2	LL	4	5T3	CT3-CH1-NZ-CE
2	RR	4	5T3	CT3-CH1-NZ-CE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	YY	4	5T3	CT3-CH1-NZ-CE
2	TT	4	5T3	CT2-CH2-NZ-CE
2	PP	4	5T3	CG-CD-CE-NZ
2	YY	4	5T3	C-CA-CB-CG
2	BB	4	5T3	CD-CE-NZ-CH2
2	FF	4	5T3	CD-CE-NZ-CH2
2	GG	4	5T3	CD-CE-NZ-CH2
2	KK	4	5T3	CD-CE-NZ-CH2
2	MM	4	5T3	CD-CE-NZ-CH2
2	WW	4	5T3	CD-CE-NZ-CH2
2	ZZ	4	5T3	CD-CE-NZ-CH2
2	JJ	4	5T3	CT1-CH1-NZ-CE
2	PP	4	5T3	CT3-CH1-NZ-CE
2	TT	4	5T3	CT1-CH1-NZ-CE
2	UU	4	5T3	CT1-CH1-NZ-CE
2	XX	4	5T3	CT1-CH1-NZ-CE
2	BB	4	5T3	CD-CE-NZ-CH1
2	CC	4	5T3	CD-CE-NZ-CH1
2	GG	4	5T3	CD-CE-NZ-CH1
2	HH	4	5T3	CD-CE-NZ-CH1
2	LL	4	5T3	CD-CE-NZ-CH1
2	QQ	4	5T3	CD-CE-NZ-CH1
2	RR	4	5T3	CD-CE-NZ-CH1
2	SS	4	5T3	CD-CE-NZ-CH1
2	JJ	4	5T3	CT2-CH2-NZ-CH1
2	KK	4	5T3	CT2-CH2-NZ-CH1
2	OO	4	5T3	CT2-CH2-NZ-CH1
2	UU	4	5T3	CT2-CH2-NZ-CH1

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 28 are unknown - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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 [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	A	50/62 (80%)	-0.59	0 100 100	18, 28, 45, 54	0
1	B	50/62 (80%)	-0.54	0 100 100	20, 30, 39, 45	0
1	C	51/62 (82%)	-0.52	0 100 100	16, 26, 52, 58	0
1	D	50/62 (80%)	-0.59	0 100 100	14, 21, 36, 42	0
1	E	54/62 (87%)	-0.53	0 100 100	14, 29, 51, 54	0
1	F	51/62 (82%)	-0.45	0 100 100	16, 26, 42, 45	0
1	G	50/62 (80%)	-0.38	0 100 100	29, 47, 66, 68	0
1	H	50/62 (80%)	-0.39	0 100 100	31, 38, 51, 70	0
1	I	51/62 (82%)	-0.49	0 100 100	23, 31, 40, 56	0
1	J	51/62 (82%)	-0.23	0 100 100	23, 37, 51, 62	0
1	K	50/62 (80%)	-0.69	0 100 100	19, 26, 41, 50	0
1	L	50/62 (80%)	-0.51	0 100 100	24, 39, 60, 64	0
1	M	51/62 (82%)	-0.21	1 (1%) 65 56	24, 34, 69, 87	0
1	N	50/62 (80%)	-0.46	0 100 100	26, 34, 49, 61	0
1	O	50/62 (80%)	0.01	3 (6%) 21 14	34, 49, 64, 66	0
1	P	50/62 (80%)	-0.13	0 100 100	37, 55, 68, 73	0
1	Q	50/62 (80%)	-0.17	0 100 100	33, 51, 85, 90	0
1	R	50/62 (80%)	-0.38	0 100 100	27, 38, 59, 70	0
1	S	50/62 (80%)	-0.54	0 100 100	20, 28, 49, 60	0
1	T	50/62 (80%)	-0.41	0 100 100	26, 36, 70, 77	0
1	U	50/62 (80%)	-0.27	0 100 100	35, 47, 67, 77	0
1	V	51/62 (82%)	0.06	0 100 100	39, 57, 81, 82	0
1	W	50/62 (80%)	-0.20	0 100 100	31, 43, 63, 70	0
1	X	52/62 (83%)	0.11	2 (3%) 40 30	33, 49, 75, 89	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9		
1	Y	51/62 (82%)	-0.16	0	100	100	24, 45, 57, 62	0
1	Z	50/62 (80%)	-0.29	0	100	100	26, 39, 61, 66	0
2	AA	4/7 (57%)	-0.14	0	100	100	18, 22, 27, 45	0
2	BB	4/7 (57%)	-0.31	0	100	100	19, 22, 25, 38	0
2	CC	4/7 (57%)	-0.57	0	100	100	17, 18, 19, 30	0
2	DD	4/7 (57%)	-0.68	0	100	100	16, 17, 19, 30	0
2	EE	4/7 (57%)	-0.36	0	100	100	20, 22, 24, 36	0
2	FF	4/7 (57%)	-0.56	0	100	100	19, 20, 20, 40	0
2	GG	4/7 (57%)	-0.50	0	100	100	31, 32, 38, 50	0
2	HH	4/7 (57%)	-0.46	0	100	100	32, 33, 33, 40	0
2	II	4/7 (57%)	-0.07	0	100	100	22, 24, 25, 40	0
2	JJ	4/7 (57%)	-0.21	0	100	100	25, 25, 27, 47	0
2	KK	4/7 (57%)	-0.35	0	100	100	20, 23, 23, 40	0
2	LL	4/7 (57%)	-0.20	0	100	100	24, 30, 31, 38	0
2	MM	4/7 (57%)	-0.60	0	100	100	26, 27, 30, 40	0
2	NN	4/7 (57%)	-0.51	0	100	100	26, 27, 30, 37	0
2	OO	4/7 (57%)	-0.28	0	100	100	35, 39, 42, 62	0
2	PP	4/7 (57%)	-0.30	0	100	100	34, 39, 49, 56	0
2	QQ	4/7 (57%)	-0.34	0	100	100	34, 37, 37, 59	0
2	RR	4/7 (57%)	-0.73	0	100	100	32, 35, 37, 39	0
2	SS	4/7 (57%)	-0.37	0	100	100	21, 22, 23, 34	0
2	TT	4/7 (57%)	-0.55	0	100	100	24, 26, 27, 38	0
2	UU	3/7 (42%)	-0.22	0	100	100	41, 41, 43, 43	0
2	VV	4/7 (57%)	-0.51	0	100	100	42, 45, 48, 57	0
2	WW	4/7 (57%)	-0.28	0	100	100	33, 33, 37, 61	0
2	XX	4/7 (57%)	-0.17	0	100	100	36, 40, 45, 62	0
2	YY	4/7 (57%)	-0.56	0	100	100	30, 33, 39, 51	0
2	ZZ	4/7 (57%)	-0.33	0	100	100	27, 31, 32, 43	0
All	All	1416/1794 (78%)	-0.35	6 (0%)	92	91	14, 38, 64, 90	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	39	TRP	3.6
1	X	16	ARG	3.0
1	O	39	TRP	2.5
1	O	34	SER	2.2
1	O	35	THR	2.2
1	M	20	LYS	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	5T3	QQ	4	14/15	0.85	0.29	46,58,74,77	0
2	5T3	XX	4	14/15	0.85	0.32	46,55,65,67	0
2	5T3	WW	4	14/15	0.86	0.27	41,54,63,71	0
2	5T3	PP	4	13/15	0.88	0.23	48,55,63,67	0
2	5T3	UU	4	14/15	0.88	0.26	48,56,63,67	0
2	5T3	OO	4	14/15	0.89	0.27	43,58,67,73	0
2	5T3	GG	4	14/15	0.89	0.36	44,53,63,68	0
2	5T3	YY	4	14/15	0.89	0.19	44,50,59,63	0
2	5T3	VV	4	14/15	0.90	0.25	46,57,70,71	0
2	5T3	JJ	4	14/15	0.91	0.32	33,40,54,58	0
2	5T3	LL	4	14/15	0.91	0.23	33,37,50,58	0
2	5T3	ZZ	4	14/15	0.91	0.24	36,43,66,66	0
2	5T3	HH	4	14/15	0.92	0.21	33,43,55,58	0
2	5T3	DD	4	14/15	0.92	0.23	17,25,37,40	0
2	5T3	TT	4	14/15	0.92	0.25	26,34,43,50	0
2	5T3	II	4	14/15	0.93	0.21	27,34,44,52	0
2	5T3	MM	4	14/15	0.93	0.20	28,35,44,45	0
2	5T3	SS	4	14/15	0.93	0.23	24,29,36,38	0
2	5T3	NN	4	14/15	0.93	0.23	28,33,47,48	0
2	5T3	AA	4	14/15	0.93	0.21	31,37,45,49	0
2	5T3	EE	4	14/15	0.94	0.20	23,31,40,45	0
2	5T3	FF	4	14/15	0.94	0.23	27,32,41,43	0
2	5T3	KK	4	14/15	0.94	0.21	21,26,34,40	0
2	5T3	RR	4	14/15	0.94	0.23	32,40,47,53	0
2	5T3	BB	4	14/15	0.95	0.24	25,31,46,48	0
2	5T3	CC	4	14/15	0.96	0.20	17,26,38,39	0

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	UNX	X	101	1/1	0.00	0.42	61,61,61,61	0
3	UNX	O	101	1/1	0.51	0.53	41,41,41,41	0
3	UNX	G	101	1/1	0.52	0.40	47,47,47,47	0
3	UNX	D	101	1/1	0.53	0.35	27,27,27,27	0
3	UNX	S	101	1/1	0.57	0.71	36,36,36,36	0
3	UNX	Q	101	1/1	0.67	0.18	45,45,45,45	0
3	UNX	N	102	1/1	0.75	0.28	31,31,31,31	0
3	UNX	A	103	1/1	0.77	0.35	22,22,22,22	0
3	UNX	F	101	1/1	0.78	0.41	22,22,22,22	0
3	UNX	Y	101	1/1	0.80	0.45	41,41,41,41	0
3	UNX	Z	101	1/1	0.83	0.77	26,26,26,26	0
3	UNX	J	101	1/1	0.86	0.47	27,27,27,27	0
3	UNX	F	103	1/1	0.87	0.30	16,16,16,16	0
3	UNX	M	101	1/1	0.88	0.92	41,41,41,41	0
3	UNX	S	103	1/1	0.91	0.18	23,23,23,23	0
3	UNX	A	102	1/1	0.93	0.36	19,19,19,19	0
3	UNX	D	102	1/1	0.94	0.43	25,25,25,25	0
3	UNX	S	102	1/1	0.94	0.22	20,20,20,20	0
3	UNX	N	101	1/1	0.95	0.17	26,26,26,26	0
3	UNX	C	102	1/1	0.96	0.26	18,18,18,18	0
3	UNX	F	102	1/1	0.96	0.14	20,20,20,20	0
3	UNX	H	101	1/1	0.96	0.12	21,21,21,21	0
3	UNX	T	101	1/1	0.97	0.26	32,32,32,32	0
3	UNX	C	101	1/1	0.97	0.30	17,17,17,17	0
3	UNX	F	104	1/1	0.97	0.18	17,17,17,17	0
3	UNX	I	101	1/1	0.97	0.26	16,16,16,16	0
3	UNX	A	101	1/1	0.98	0.22	13,13,13,13	0
3	UNX	K	101	1/1	0.99	0.23	18,18,18,18	0

6.5 Other polymers [i](#)

There are no such residues in this entry.