



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:43 PM GMT

PDB ID : 4A6A
Title : A115V variant of dCTP deaminase-dUTPase from Mycobacterium tuberculosis in complex with dTTP
Authors : Lovgreen, M.N.; Ucar, E.; Willemoes, M.; Harris, P.
Deposited on : 2011-11-01
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

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

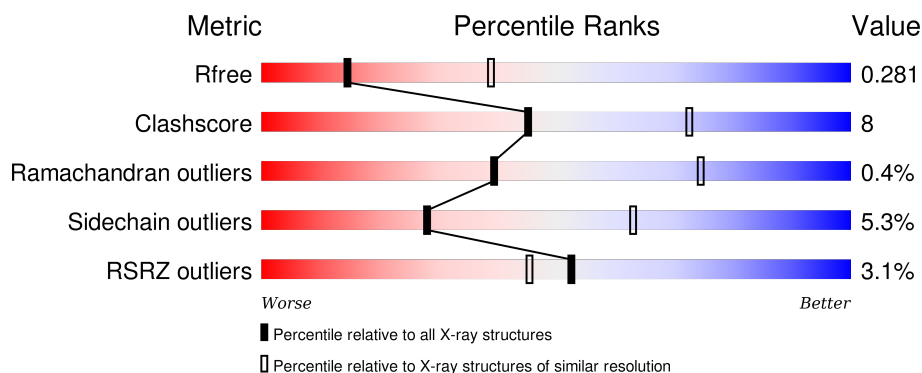
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	190	<div> <div>5%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>
1	B	190	<div> <div>%</div> <div>83%</div> <div>13%</div> <div>..</div> </div>
1	C	190	<div> <div>3%</div> <div>83%</div> <div>14%</div> <div>..</div> </div>
1	D	190	<div> <div>2%</div> <div>85%</div> <div>13%</div> <div>..</div> </div>
1	E	190	<div> <div>7%</div> <div>82%</div> <div>15%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	190	
1	G	190	
1	H	190	
1	I	190	
1	J	190	
1	K	190	
1	L	190	

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	MG	B	203	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17912 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 DEOXYCYTIDINE TRIPHOSPHATE DEAMINASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	189	Total	C	N	O	S	0	0	0
			1464	923	257	279	5			
1	B	188	Total	C	N	O	S	0	0	0
			1458	920	256	277	5			
1	C	189	Total	C	N	O	S	0	0	0
			1464	923	257	279	5			
1	D	188	Total	C	N	O	S	0	0	0
			1458	920	256	277	5			
1	E	188	Total	C	N	O	S	0	0	0
			1458	920	256	277	5			
1	F	189	Total	C	N	O	S	0	0	0
			1464	923	257	279	5			
1	G	189	Total	C	N	O	S	0	0	0
			1464	923	257	279	5			
1	H	189	Total	C	N	O	S	0	0	0
			1464	923	257	279	5			
1	I	189	Total	C	N	O	S	0	0	0
			1464	923	257	279	5			
1	J	188	Total	C	N	O	S	0	0	0
			1458	920	256	277	5			
1	K	188	Total	C	N	O	S	0	0	0
			1458	920	256	277	5			
1	L	189	Total	C	N	O	S	0	0	0
			1464	923	257	279	5			

There are 12 discrepancies between the modelled and reference sequences:

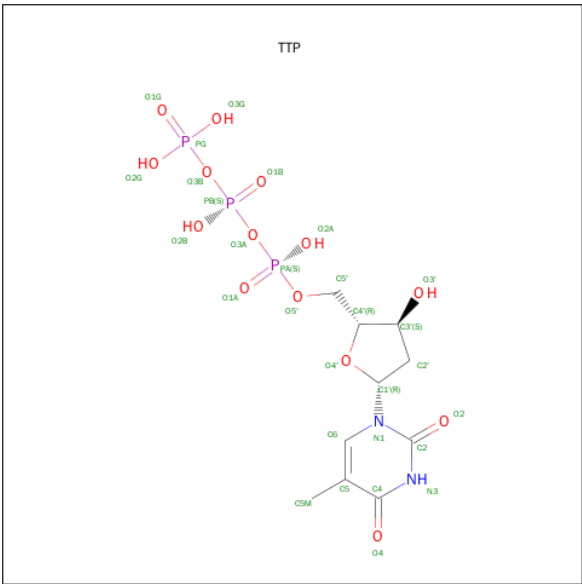
Chain	Residue	Modelled	Actual	Comment	Reference
A	115	VAL	ALA	ENGINEERED MUTATION	UNP O07247
B	115	VAL	ALA	ENGINEERED MUTATION	UNP O07247
C	115	VAL	ALA	ENGINEERED MUTATION	UNP O07247
D	115	VAL	ALA	ENGINEERED MUTATION	UNP O07247
E	115	VAL	ALA	ENGINEERED MUTATION	UNP O07247

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Chain	Residue	Modelled	Actual	Comment	Reference
F	115	VAL	ALA	ENGINEERED MUTATION	UNP O07247
G	115	VAL	ALA	ENGINEERED MUTATION	UNP O07247
H	115	VAL	ALA	ENGINEERED MUTATION	UNP O07247
I	115	VAL	ALA	ENGINEERED MUTATION	UNP O07247
J	115	VAL	ALA	ENGINEERED MUTATION	UNP O07247
K	115	VAL	ALA	ENGINEERED MUTATION	UNP O07247
L	115	VAL	ALA	ENGINEERED MUTATION	UNP O07247

- Molecule 2 is THYMIDINE-5'-TRIPHOSPHATE (three-letter code: TTP) (formula: C₁₀H₁₇N₂O₁₄P₃).



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

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	J	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	K	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	H	2	Total	Mg	0	0
			2	2		
3	B	2	Total	Mg	0	0
			2	2		
3	I	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	L	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

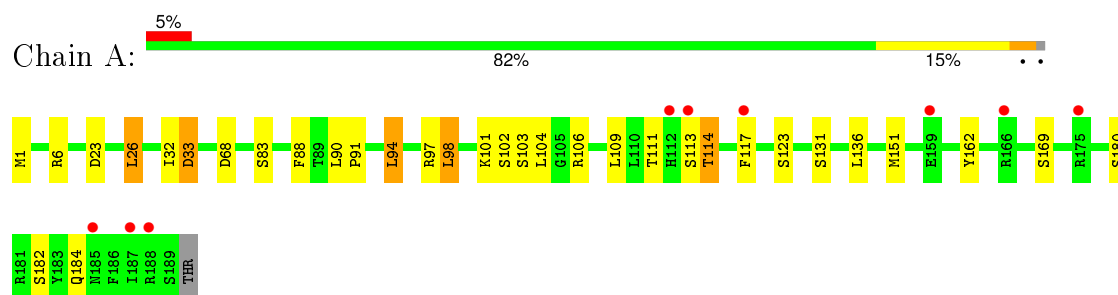
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total 2	O 2	0	0
4	B	1	Total 1	O 1	0	0
4	D	1	Total 1	O 1	0	0
4	G	3	Total 3	O 3	0	0
4	H	2	Total 2	O 2	0	0
4	I	3	Total 3	O 3	0	0

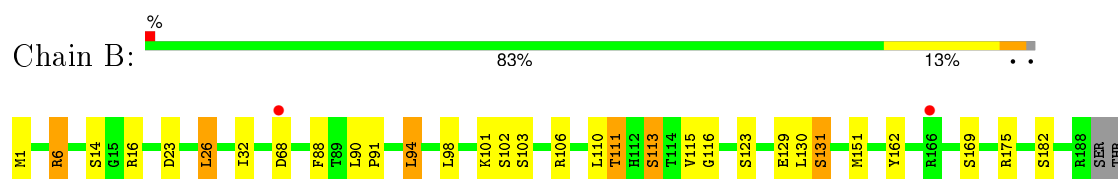
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

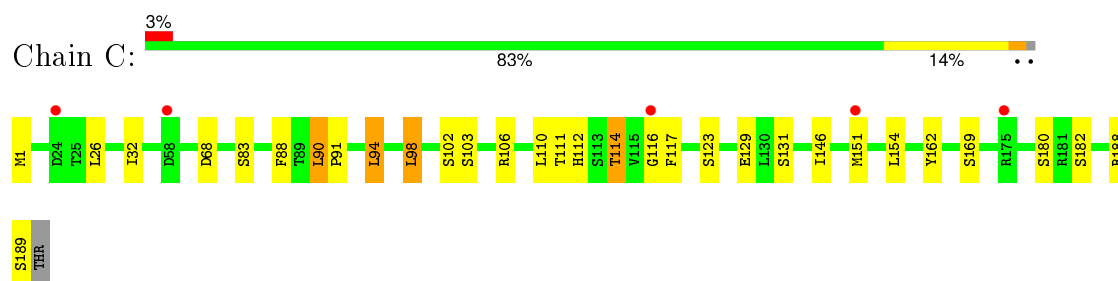
- Molecule 1: DEOXYCYTIDINE TRIPHOSPHATE DEAMINASE



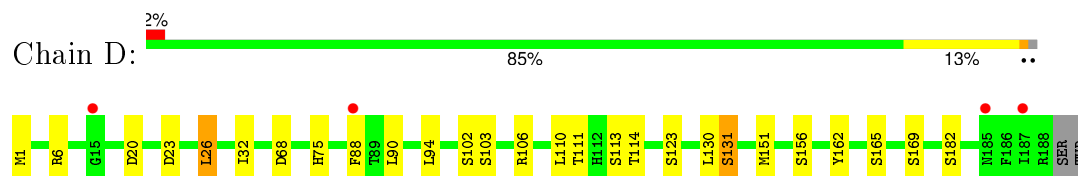
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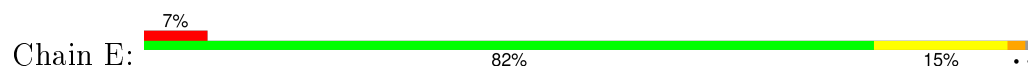
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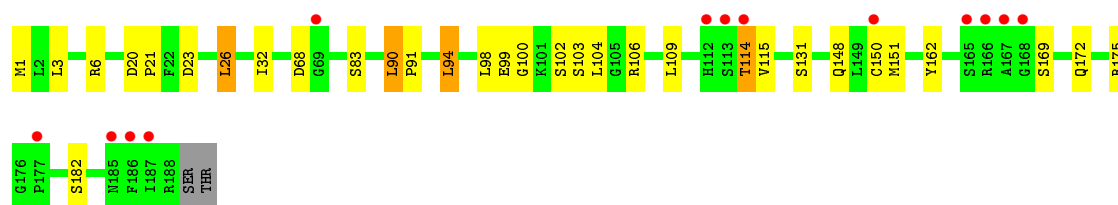


- Molecule 1: DEOXYCYTIDINE TRIPHOSPHATE DEAMINASE

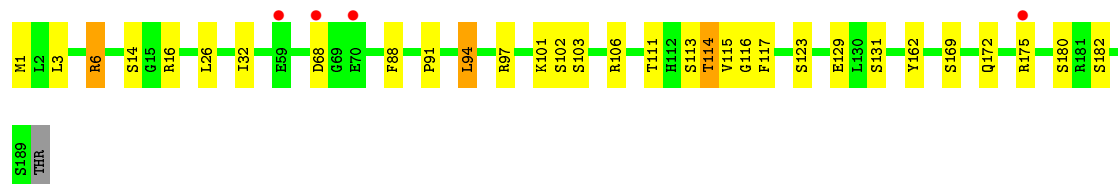
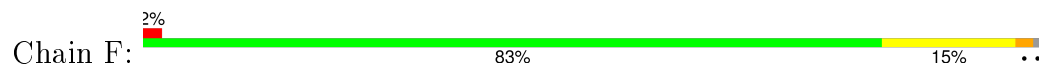


- Molecule 1: DEOXYCYTIDINE TRIPHOSPHATE DEAMINASE

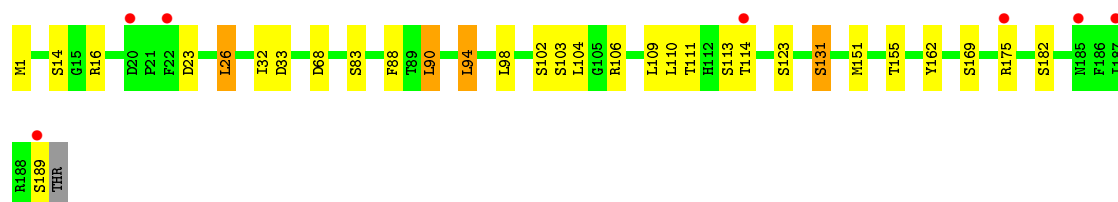
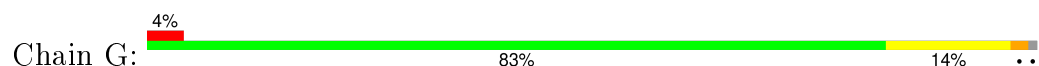




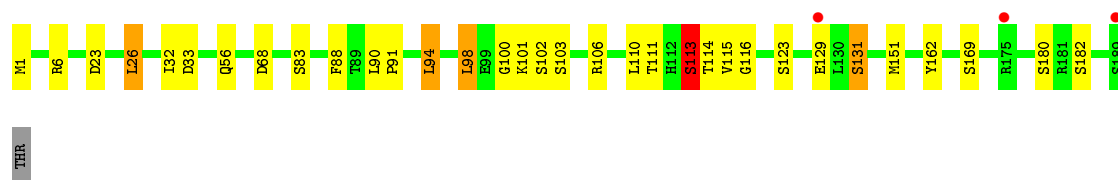
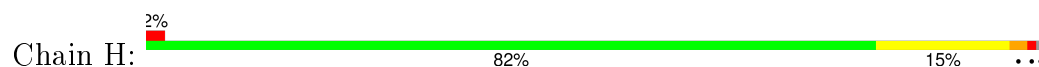
● Molecule 1: DEOXYCYTIDINE TRIPHOSPHATE DEAMINASE



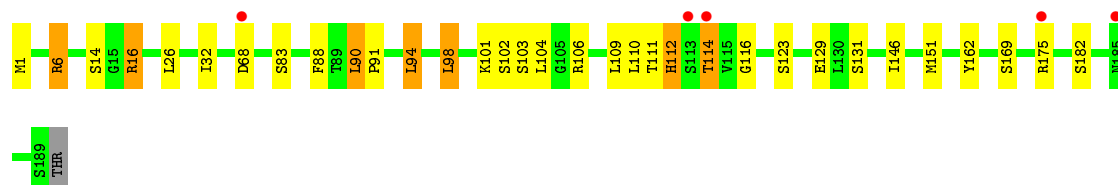
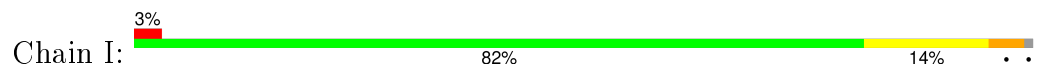
● Molecule 1: DEOXYCYTIDINE TRIPHOSPHATE DEAMINASE



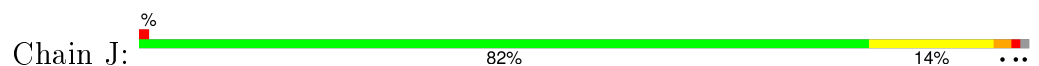
● Molecule 1: DEOXYCYTIDINE TRIPHOSPHATE DEAMINASE

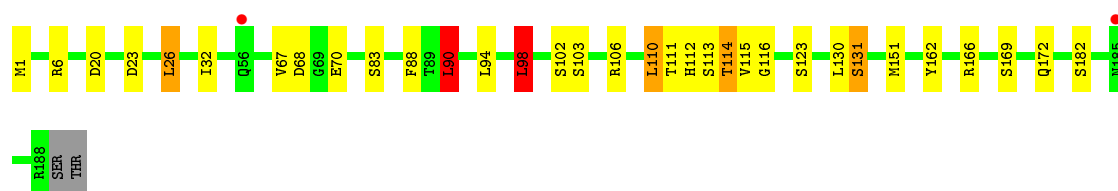


● Molecule 1: DEOXYCYTIDINE TRIPHOSPHATE DEAMINASE



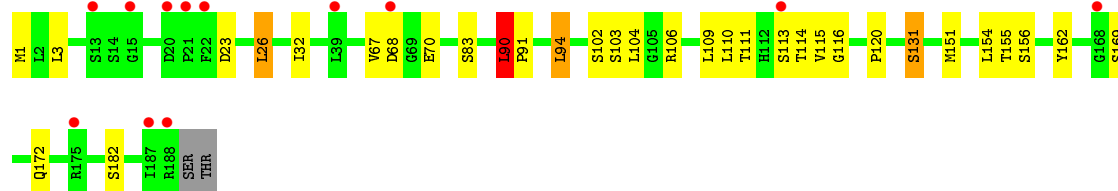
● Molecule 1: DEOXYCYTIDINE TRIPHOSPHATE DEAMINASE





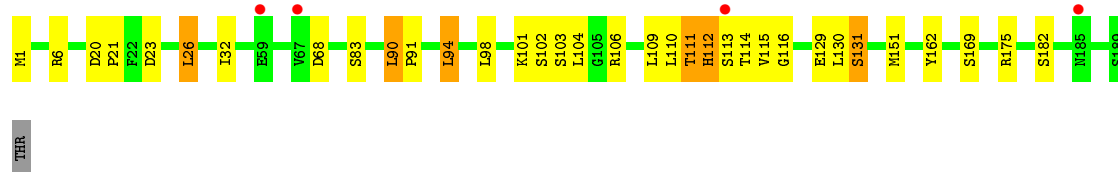
- Molecule 1: DEOXYCYTIDINE TRIPHOSPHATE DEAMINASE

Chain K: 6% 82% 15% ..



- Molecule 1: DEOXYCYTIDINE TRIPHOSPHATE DEAMINASE

Chain L: 2% 82% 15% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.59 Å 179.51 Å 99.81 Å 90.00° 96.28° 90.00°	Depositor
Resolution (Å)	49.42 – 2.90 49.42 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.42-2.90) 98.8 (49.42-2.90)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 2.91 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.253 , 0.290 0.246 , 0.281	Depositor DCC
R_{free} test set	2165 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	43.9	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 26.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 43288 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17912	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.68 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 5.4208e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TTP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.70	0/1497	0.78	3/2032 (0.1%)
1	B	0.75	0/1491	1.06	4/2024 (0.2%)
1	C	0.68	0/1497	0.80	2/2032 (0.1%)
1	D	0.71	0/1491	0.78	1/2024 (0.0%)
1	E	0.67	0/1491	1.03	6/2024 (0.3%)
1	F	0.73	0/1497	0.79	2/2032 (0.1%)
1	G	0.70	0/1497	0.78	2/2032 (0.1%)
1	H	0.70	1/1497 (0.1%)	0.80	3/2032 (0.1%)
1	I	0.72	0/1497	1.08	5/2032 (0.2%)
1	J	0.71	0/1491	0.82	3/2024 (0.1%)
1	K	0.68	0/1491	0.79	2/2024 (0.1%)
1	L	0.69	0/1497	0.80	2/2032 (0.1%)
All	All	0.70	1/17934 (0.0%)	0.87	35/24344 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	33	ASP	CB-CG	5.29	1.62	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	16	ARG	NE-CZ-NH1	22.09	131.34	120.30
1	I	16	ARG	NE-CZ-NH2	-21.56	109.52	120.30
1	B	6	ARG	NE-CZ-NH2	-21.51	109.54	120.30
1	E	6	ARG	NE-CZ-NH1	21.47	131.04	120.30
1	E	6	ARG	NE-CZ-NH2	-20.48	110.06	120.30
1	B	6	ARG	NE-CZ-NH1	20.39	130.50	120.30
1	I	16	ARG	CD-NE-CZ	11.47	139.65	123.60
1	E	6	ARG	CD-NE-CZ	10.42	138.19	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	ARG	CD-NE-CZ	9.83	137.37	123.60
1	C	98	LEU	CA-CB-CG	7.50	132.56	115.30
1	G	98	LEU	CA-CB-CG	6.94	131.27	115.30
1	A	98	LEU	CA-CB-CG	6.93	131.24	115.30
1	H	98	LEU	CA-CB-CG	6.90	131.17	115.30
1	I	98	LEU	CA-CB-CG	6.70	130.70	115.30
1	B	98	LEU	CA-CB-CG	6.47	130.18	115.30
1	E	98	LEU	CA-CB-CG	6.45	130.13	115.30
1	L	6	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	J	98	LEU	CA-CB-CG	5.78	128.59	115.30
1	H	33	ASP	CB-CG-OD1	5.67	123.40	118.30
1	H	6	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	K	3	LEU	CA-CB-CG	5.50	127.96	115.30
1	J	90	LEU	CA-CB-CG	5.46	127.87	115.30
1	D	6	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	L	6	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	F	6	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	K	90	LEU	CA-CB-CG	5.24	127.34	115.30
1	G	33	ASP	CB-CG-OD1	5.22	123.00	118.30
1	J	6	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	6	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	33	ASP	CB-CG-OD1	5.14	122.92	118.30
1	F	3	LEU	CA-CB-CG	5.12	127.07	115.30
1	E	3	LEU	CA-CB-CG	5.10	127.03	115.30
1	I	6	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	C	90	LEU	CA-CB-CG	5.08	126.97	115.30
1	E	90	LEU	CA-CB-CG	5.05	126.93	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1464	0	1456	33	1
1	B	1458	0	1451	31	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1464	0	1456	25	0
1	D	1458	0	1451	34	2
1	E	1458	0	1451	28	0
1	F	1464	0	1456	44	0
1	G	1464	0	1456	26	1
1	H	1464	0	1456	34	1
1	I	1464	0	1456	49	0
1	J	1458	0	1451	32	2
1	K	1458	0	1451	30	0
1	L	1464	0	1456	31	1
2	A	29	0	13	0	0
2	B	29	0	13	2	0
2	C	29	0	13	1	0
2	D	29	0	13	0	0
2	E	29	0	13	1	0
2	F	29	0	13	1	0
2	G	29	0	13	0	0
2	H	29	0	13	2	0
2	I	29	0	13	0	0
2	J	29	0	13	1	0
2	K	29	0	13	1	0
2	L	29	0	13	2	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	2	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	L	1	0	0	0	0
4	A	2	0	0	1	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	G	3	0	0	0	0
4	H	2	0	0	0	0
4	I	3	0	0	1	0
All	All	17912	0	17603	275	4

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 8.

All (275) 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:L:113:SER:O	1:L:114:THR:HG22	1.29	1.25
1:F:16:ARG:HH11	1:K:156:SER:CB	1.52	1.22
1:F:6:ARG:HD2	1:I:14:SER:HB2	1.33	1.11
1:D:156:SER:CB	1:I:16:ARG:HH21	1.64	1.10
1:F:16:ARG:NH1	1:K:156:SER:HB3	1.65	1.09
1:D:156:SER:HB3	1:I:16:ARG:HE	0.91	1.07
1:F:14:SER:HB2	1:I:6:ARG:HD2	1.34	1.05
1:H:114:THR:HB	1:J:110:LEU:HD13	1.38	1.05
1:D:156:SER:HB3	1:I:16:ARG:NE	1.72	1.03
1:H:113:SER:HB2	1:H:129:GLU:OE1	1.60	1.00
1:F:16:ARG:HH11	1:K:156:SER:HB3	0.81	0.97
1:F:6:ARG:CD	1:I:14:SER:HB2	1.95	0.97
1:G:113:SER:HB3	1:K:110:LEU:HD21	1.48	0.93
1:L:113:SER:O	1:L:114:THR:CG2	2.17	0.91
1:F:14:SER:HB2	1:I:6:ARG:CD	2.01	0.89
1:F:16:ARG:NH1	1:K:156:SER:CB	2.30	0.89
1:H:114:THR:HG21	1:J:111:THR:H	1.35	0.89
1:I:111:THR:O	1:I:129:GLU:O	1.93	0.85
1:A:103:SER:HB3	1:C:182:SER:HB3	1.62	0.82
1:F:14:SER:CB	1:I:6:ARG:HD2	2.09	0.82
1:H:113:SER:CB	1:H:129:GLU:OE1	2.26	0.82
1:B:113:SER:OG	1:B:129:GLU:OE1	1.99	0.81
1:D:156:SER:OG	1:I:16:ARG:NH2	2.14	0.81
1:D:156:SER:HB3	1:I:16:ARG:HH21	1.44	0.81
1:D:156:SER:CB	1:I:16:ARG:HE	1.85	0.79
1:F:6:ARG:HD2	1:I:14:SER:CB	2.12	0.79
1:B:16:ARG:HH12	1:G:14:SER:HB3	1.48	0.79
1:D:156:SER:CB	1:I:16:ARG:NH2	2.46	0.78
1:H:1:MET:H1	1:J:1:MET:N	1.81	0.78
1:G:113:SER:HB3	1:K:110:LEU:CD2	2.14	0.78
1:H:114:THR:HB	1:J:110:LEU:CD1	2.14	0.78
1:G:182:SER:HB3	1:K:103:SER:HB3	1.65	0.77
1:H:1:MET:N	1:J:1:MET:N	2.32	0.77
1:L:98:LEU:HD23	1:L:112:HIS:HD2	1.50	0.76
1:F:113:SER:HB3	1:F:129:GLU:OE1	1.86	0.76
1:G:1:MET:N	1:I:1:MET:H1	1.83	0.76
1:E:102:SER:O	1:E:106:ARG:HG3	1.87	0.75
1:D:156:SER:HB3	1:I:16:ARG:NH2	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:1:MET:H1	1:J:1:MET:H1	1.36	0.73
1:A:1:MET:N	1:C:1:MET:H1	1.86	0.73
1:D:114:THR:HG23	1:D:114:THR:O	1.88	0.73
1:J:102:SER:O	1:J:106:ARG:HG3	1.88	0.73
1:H:115:VAL:HG23	2:H:201:TTP:HM52	1.70	0.72
1:F:6:ARG:CD	1:I:14:SER:CB	2.66	0.72
1:J:114:THR:HG21	1:L:110:LEU:HB3	1.70	0.72
1:A:117:PHE:CE2	1:E:99:GLU:HB2	2.24	0.72
1:I:111:THR:HG23	4:I:2002:HOH:O	1.90	0.72
1:F:14:SER:CB	1:I:6:ARG:CD	2.67	0.70
1:C:1:MET:N	1:E:1:MET:N	2.40	0.70
1:C:103:SER:HB3	1:E:182:SER:HB3	1.74	0.70
1:D:114:THR:HG21	1:F:111:THR:H	1.57	0.69
1:A:1:MET:N	1:C:1:MET:N	2.40	0.69
1:C:1:MET:N	1:E:1:MET:H1	1.91	0.69
1:A:182:SER:HB3	1:E:103:SER:HB3	1.75	0.69
1:G:1:MET:N	1:I:1:MET:N	2.41	0.69
1:H:182:SER:HB3	1:J:103:SER:HB3	1.75	0.69
1:A:1:MET:H2	1:C:1:MET:N	1.91	0.69
1:D:182:SER:HB3	1:F:103:SER:HB3	1.74	0.69
1:H:110:LEU:HB2	1:H:131:SER:HB3	1.75	0.69
1:J:182:SER:HB3	1:L:103:SER:HB3	1.76	0.68
1:J:98:LEU:HD13	1:J:112:HIS:HD2	1.58	0.68
1:K:115:VAL:HB	2:K:201:TTP:HM52	1.75	0.67
1:B:1:MET:H1	1:D:1:MET:N	1.93	0.67
1:B:102:SER:O	1:B:106:ARG:HG3	1.95	0.67
1:H:1:MET:N	1:L:1:MET:H1	1.93	0.67
1:B:182:SER:HB3	1:D:103:SER:HB3	1.77	0.67
1:F:102:SER:O	1:F:106:ARG:HG3	1.94	0.66
1:J:1:MET:H1	1:L:1:MET:N	1.93	0.66
1:B:111:THR:HG23	1:F:114:THR:HG21	1.79	0.65
1:D:1:MET:H1	1:F:1:MET:N	1.95	0.65
1:G:103:SER:HB3	1:I:182:SER:HB3	1.78	0.65
1:H:102:SER:O	1:H:106:ARG:HG3	1.97	0.64
1:B:103:SER:HB3	1:F:182:SER:HB3	1.80	0.64
1:G:1:MET:H1	1:I:1:MET:H1	1.45	0.64
1:H:1:MET:N	1:J:1:MET:H2	1.96	0.64
1:F:114:THR:HG23	1:F:114:THR:O	1.97	0.64
1:B:115:VAL:HG23	2:B:201:TTP:HM52	1.80	0.64
1:F:16:ARG:HD3	1:K:156:SER:HB3	1.80	0.63
1:D:156:SER:HB3	1:I:16:ARG:CZ	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:102:SER:O	1:L:106:ARG:HG3	1.98	0.63
1:H:1:MET:H1	1:L:1:MET:H1	1.47	0.63
1:A:102:SER:O	1:A:106:ARG:HG3	1.99	0.63
1:D:110:LEU:HB2	1:D:131:SER:HB3	1.80	0.62
1:J:1:MET:N	1:L:1:MET:N	2.48	0.61
1:H:103:SER:HB3	1:L:182:SER:HB3	1.82	0.61
1:C:1:MET:H1	1:E:1:MET:H1	1.49	0.60
1:B:1:MET:N	1:D:1:MET:N	2.49	0.60
1:I:103:SER:HB3	1:K:182:SER:HB3	1.83	0.60
1:A:1:MET:H1	1:C:1:MET:H1	1.48	0.60
1:C:1:MET:H2	1:E:1:MET:N	2.00	0.60
1:C:110:LEU:N	1:C:110:LEU:HD23	2.16	0.60
1:I:102:SER:O	1:I:106:ARG:HG3	2.03	0.59
1:H:1:MET:N	1:L:1:MET:N	2.50	0.59
1:F:114:THR:CG2	1:F:114:THR:O	2.51	0.59
1:F:16:ARG:NH1	1:K:156:SER:OG	2.35	0.58
1:B:110:LEU:HB2	1:B:131:SER:HB3	1.85	0.58
1:J:110:LEU:HB2	1:J:131:SER:HB3	1.86	0.57
1:G:162:TYR:CZ	1:G:169:SER:HB3	2.40	0.57
1:D:113:SER:OG	1:D:114:THR:N	2.35	0.57
1:H:115:VAL:CG2	2:H:201:TTP:HM52	2.34	0.57
1:D:162:TYR:CZ	1:D:169:SER:HB3	2.41	0.56
1:J:1:MET:H1	1:L:1:MET:H1	1.52	0.56
1:G:1:MET:H2	1:I:1:MET:N	2.04	0.56
1:F:6:ARG:HD3	1:I:14:SER:CB	2.34	0.55
1:D:1:MET:N	1:F:1:MET:N	2.54	0.55
1:A:162:TYR:CZ	1:A:169:SER:HB3	2.41	0.55
1:C:102:SER:O	1:C:106:ARG:HG3	2.06	0.55
1:I:162:TYR:CZ	1:I:169:SER:HB3	2.42	0.55
1:J:162:TYR:CZ	1:J:169:SER:HB3	2.42	0.55
1:H:100:GLY:CA	1:H:111:THR:HG21	2.36	0.55
1:H:111:THR:HG22	1:L:114:THR:HG21	1.89	0.55
1:E:91:PRO:HG2	1:E:94:LEU:HB2	1.89	0.55
1:E:162:TYR:CZ	1:E:169:SER:HB3	2.42	0.54
1:L:90:LEU:HD13	1:L:151:MET:HE1	1.90	0.54
1:K:102:SER:O	1:K:106:ARG:HG3	2.08	0.54
1:A:1:MET:H1	1:E:1:MET:N	2.04	0.54
1:C:162:TYR:CZ	1:C:169:SER:HB3	2.42	0.54
1:L:113:SER:OG	1:L:129:GLU:OE1	2.21	0.54
1:B:1:MET:N	1:F:1:MET:H1	2.07	0.53
1:A:1:MET:N	1:E:1:MET:N	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:SER:HB3	1:G:16:ARG:HH12	1.74	0.53
1:L:98:LEU:HD23	1:L:112:HIS:CD2	2.36	0.53
1:I:1:MET:N	1:K:1:MET:H1	2.06	0.53
1:I:1:MET:N	1:K:1:MET:N	2.57	0.52
1:K:90:LEU:HD13	1:K:151:MET:CE	2.40	0.52
1:F:14:SER:CB	1:I:6:ARG:HD3	2.40	0.52
1:L:90:LEU:HD13	1:L:151:MET:CE	2.40	0.52
1:L:111:THR:HA	1:L:130:LEU:HD23	1.90	0.52
1:D:102:SER:O	1:D:106:ARG:HG3	2.09	0.52
1:L:115:VAL:HG23	2:L:201:TTP:HM52	1.92	0.52
1:J:1:MET:N	1:L:1:MET:H2	2.08	0.52
1:C:188:ARG:HG3	1:C:189:SER:N	2.24	0.52
1:I:110:LEU:HD23	1:I:110:LEU:N	2.25	0.52
1:D:90:LEU:HD13	1:D:151:MET:HE1	1.91	0.52
1:K:90:LEU:HD13	1:K:151:MET:HE1	1.92	0.52
1:D:114:THR:CG2	1:D:114:THR:O	2.59	0.51
1:C:88:PHE:O	1:C:123:SER:HA	2.10	0.51
1:B:91:PRO:HG2	1:B:94:LEU:HB2	1.93	0.51
1:F:14:SER:HA	1:I:6:ARG:HD3	1.93	0.50
1:H:114:THR:HG21	1:J:111:THR:N	2.15	0.50
1:L:162:TYR:CZ	1:L:169:SER:HB3	2.45	0.50
1:K:162:TYR:CZ	1:K:169:SER:HB3	2.46	0.50
1:I:111:THR:HG21	1:I:146:ILE:O	2.11	0.50
1:H:91:PRO:HG2	1:H:94:LEU:HB2	1.94	0.50
1:B:90:LEU:HD13	1:B:151:MET:CE	2.41	0.50
1:I:91:PRO:HG2	1:I:94:LEU:HB2	1.94	0.50
1:G:110:LEU:HB2	1:G:131:SER:HB3	1.93	0.50
1:C:110:LEU:HA	1:E:114:THR:HG21	1.93	0.50
1:E:90:LEU:HD13	1:E:151:MET:CE	2.42	0.50
1:I:88:PHE:O	1:I:123:SER:HA	2.11	0.50
1:B:16:ARG:NH1	1:G:14:SER:HB3	2.21	0.50
1:F:113:SER:O	1:F:114:THR:HB	2.10	0.50
1:G:102:SER:O	1:G:106:ARG:HG3	2.12	0.50
1:H:100:GLY:HA3	1:H:111:THR:HG21	1.93	0.50
1:E:23:ASP:HB3	1:E:26:LEU:HD22	1.94	0.49
1:G:1:MET:H1	1:K:1:MET:N	2.10	0.49
1:H:111:THR:H	1:L:114:THR:HG21	1.76	0.49
1:I:146:ILE:O	1:I:146:ILE:HG13	2.12	0.49
1:H:162:TYR:CZ	1:H:169:SER:HB3	2.47	0.49
1:K:110:LEU:HB2	1:K:131:SER:HB3	1.95	0.49
1:H:90:LEU:HD13	1:H:151:MET:CE	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:6:ARG:HD3	1:I:14:SER:HA	1.94	0.49
1:B:1:MET:H1	1:D:1:MET:H1	1.57	0.49
1:A:33:ASP:OD2	4:A:2001:HOH:O	2.20	0.49
1:G:88:PHE:O	1:G:123:SER:HA	2.13	0.48
1:K:104:LEU:HB3	1:K:109:LEU:HD23	1.95	0.48
1:L:91:PRO:HG2	1:L:94:LEU:HB2	1.94	0.48
1:H:111:THR:HG22	1:L:114:THR:CG2	2.42	0.48
1:B:88:PHE:O	1:B:123:SER:HA	2.14	0.48
1:A:1:MET:H1	1:E:1:MET:H1	1.61	0.48
1:A:117:PHE:CE2	1:E:148:GLN:HG3	2.49	0.48
1:F:162:TYR:CZ	1:F:169:SER:HB3	2.47	0.48
1:L:23:ASP:HB3	1:L:26:LEU:HD22	1.95	0.48
1:K:23:ASP:HB3	1:K:26:LEU:HD22	1.96	0.48
1:L:110:LEU:HB2	1:L:131:SER:HB3	1.96	0.48
1:A:97:ARG:CZ	1:A:117:PHE:HD1	2.26	0.48
1:B:14:SER:HB2	1:G:14:SER:HB2	1.95	0.47
1:L:115:VAL:CG2	2:L:201:TTP:HM52	2.44	0.47
1:J:111:THR:HA	1:J:130:LEU:HD23	1.94	0.47
1:B:162:TYR:CZ	1:B:169:SER:HB3	2.49	0.47
1:F:91:PRO:HG2	1:F:94:LEU:HB2	1.96	0.47
1:B:1:MET:N	1:F:1:MET:N	2.63	0.47
1:D:111:THR:HA	1:D:130:LEU:HD23	1.96	0.47
1:A:117:PHE:HE2	1:E:148:GLN:HG3	1.79	0.47
1:B:115:VAL:CG2	2:B:201:TTP:HM52	2.43	0.47
1:I:90:LEU:HD13	1:I:151:MET:HE1	1.97	0.47
1:G:90:LEU:HD13	1:G:151:MET:HE1	1.97	0.47
1:H:23:ASP:HB3	1:H:26:LEU:HD22	1.96	0.47
1:A:88:PHE:O	1:A:123:SER:HA	2.15	0.47
1:A:23:ASP:HB3	1:A:26:LEU:HD22	1.97	0.47
1:D:1:MET:N	1:F:1:MET:H2	2.13	0.47
1:H:1:MET:H2	1:J:1:MET:H2	1.63	0.46
1:E:90:LEU:HD13	1:E:151:MET:HE1	1.97	0.46
1:D:1:MET:H1	1:F:1:MET:H1	1.62	0.46
1:H:90:LEU:HD13	1:H:151:MET:HE1	1.97	0.46
1:F:172:GLN:HA	1:F:172:GLN:OE1	2.16	0.46
1:B:1:MET:N	1:D:1:MET:H2	2.13	0.46
1:B:1:MET:H1	1:F:1:MET:H1	1.63	0.45
1:H:100:GLY:HA2	1:H:111:THR:HG21	1.98	0.45
1:E:104:LEU:HB3	1:E:109:LEU:HD23	1.98	0.45
1:J:112:HIS:ND1	1:J:112:HIS:C	2.69	0.45
1:A:114:THR:HG23	1:E:100:GLY:HA3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:111:THR:OG1	1:I:112:HIS:N	2.49	0.45
1:A:1:MET:HE3	1:C:154:LEU:O	2.16	0.45
1:G:90:LEU:HD13	1:G:151:MET:CE	2.47	0.45
1:G:110:LEU:HD22	1:I:114:THR:HB	2.00	0.44
1:C:91:PRO:HG2	1:C:94:LEU:HB2	1.99	0.44
1:K:91:PRO:HG2	1:K:94:LEU:HB2	1.99	0.44
1:K:172:GLN:OE1	1:K:172:GLN:HA	2.18	0.44
1:A:90:LEU:HD13	1:A:151:MET:CE	2.48	0.44
1:A:1:MET:N	1:E:1:MET:H2	2.16	0.44
1:H:88:PHE:O	1:H:123:SER:HA	2.17	0.44
1:A:117:PHE:HE1	1:E:150:CYS:HG	1.61	0.44
1:I:1:MET:H2	1:K:1:MET:N	2.15	0.44
1:I:102:SER:HA	1:K:115:VAL:HG11	1.99	0.43
1:A:136:LEU:HD21	1:D:75:HIS:CD2	2.53	0.43
1:F:113:SER:O	1:F:114:THR:CB	2.65	0.43
1:B:106:ARG:HB2	1:F:180:SER:HB2	2.00	0.43
1:I:90:LEU:HD13	1:I:151:MET:CE	2.48	0.43
1:G:1:MET:CA	1:I:1:MET:H1	2.31	0.43
1:D:90:LEU:HD13	1:D:151:MET:CE	2.49	0.43
1:A:111:THR:HG22	1:C:114:THR:HG21	2.00	0.43
1:E:115:VAL:HG23	2:E:201:TTP:HM52	2.00	0.43
1:H:114:THR:HG21	1:J:110:LEU:HA	2.00	0.43
1:J:90:LEU:HD13	1:J:151:MET:CE	2.49	0.43
1:J:88:PHE:O	1:J:123:SER:HA	2.19	0.43
1:J:98:LEU:HD13	1:J:112:HIS:CD2	2.46	0.43
1:C:146:ILE:HG13	1:C:146:ILE:O	2.19	0.43
1:C:117:PHE:O	2:C:201:TTP:HM51	2.18	0.43
1:J:67:VAL:O	1:J:70:GLU:HB2	2.19	0.42
1:G:23:ASP:HB3	1:G:26:LEU:HD22	2.00	0.42
1:L:104:LEU:HB3	1:L:109:LEU:HD23	2.01	0.42
1:I:112:HIS:ND1	1:I:112:HIS:C	2.73	0.42
1:L:175:ARG:HA	1:L:175:ARG:HD3	1.76	0.42
1:B:90:LEU:HD13	1:B:151:MET:HE3	2.01	0.42
1:D:23:ASP:HB3	1:D:26:LEU:HD22	2.01	0.42
1:C:90:LEU:HD13	1:C:151:MET:CE	2.50	0.42
1:F:175:ARG:HA	1:F:175:ARG:HD3	1.81	0.42
1:J:23:ASP:HB3	1:J:26:LEU:HD22	2.02	0.42
1:D:88:PHE:O	1:D:123:SER:HA	2.19	0.42
1:A:111:THR:HG22	1:C:114:THR:CG2	2.49	0.42
1:J:90:LEU:HD13	1:J:151:MET:HE1	2.01	0.42
1:E:172:GLN:OE1	1:E:172:GLN:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:PRO:HG2	1:A:94:LEU:HB2	2.02	0.42
1:G:1:MET:N	1:K:1:MET:N	2.68	0.42
1:F:97:ARG:CZ	1:F:117:PHE:CD1	3.03	0.42
1:J:172:GLN:OE1	1:J:172:GLN:HA	2.19	0.41
1:C:111:THR:O	1:C:129:GLU:O	2.38	0.41
1:A:106:ARG:HB2	1:C:180:SER:HB2	2.02	0.41
1:I:104:LEU:HB3	1:I:109:LEU:HD23	2.01	0.41
1:B:1:MET:H1	1:D:1:MET:CA	2.34	0.41
1:K:67:VAL:O	1:K:70:GLU:HB2	2.20	0.41
1:F:16:ARG:HD3	1:K:155:THR:O	2.20	0.41
1:G:104:LEU:HB3	1:G:109:LEU:HD23	2.02	0.41
1:B:111:THR:HA	1:B:130:LEU:HD23	2.02	0.41
1:B:90:LEU:HD13	1:B:151:MET:HE1	2.03	0.41
1:A:136:LEU:CD2	1:D:75:HIS:HD2	2.34	0.41
1:F:88:PHE:O	1:F:123:SER:HA	2.20	0.41
1:B:175:ARG:HD3	1:B:175:ARG:HA	1.90	0.41
1:B:6:ARG:NH2	1:G:155:THR:O	2.53	0.41
1:J:115:VAL:HB	2:J:201:TTP:HM52	2.03	0.41
1:I:1:MET:CA	1:K:1:MET:H1	2.33	0.41
1:A:90:LEU:HD13	1:A:151:MET:HE1	2.02	0.41
1:L:20:ASP:HA	1:L:21:PRO:HA	1.95	0.41
1:F:115:VAL:HB	2:F:201:TTP:HM52	2.02	0.40
1:K:120:PRO:HG2	1:K:154:LEU:HD11	2.03	0.40
1:I:175:ARG:HA	1:I:175:ARG:HD3	1.88	0.40
1:B:23:ASP:HB3	1:B:26:LEU:HD22	2.03	0.40
1:A:97:ARG:CZ	1:A:117:PHE:CD1	3.04	0.40
1:H:180:SER:HB2	1:J:106:ARG:HB2	2.03	0.40
1:E:175:ARG:HA	1:E:175:ARG:HD3	1.89	0.40
1:A:180:SER:HB2	1:E:106:ARG:HB2	2.03	0.40
1:E:20:ASP:HA	1:E:21:PRO:HA	1.98	0.40
1:G:94:LEU:HB3	1:G:151:MET:CE	2.52	0.40
1:A:104:LEU:HB3	1:A:109:LEU:HD23	2.04	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:56:GLN:OE1	1:L:175:ARG:NE[1_455]	1.87	0.33
1:D:20:ASP:OD2	1:J:20:ASP:OD2[2_645]	2.05	0.15
1:A:184:GLN:CG	1:G:175:ARG:CG[2_646]	2.07	0.13
1:D:165:SER:OG	1:J:166:ARG:CD[2_745]	2.15	0.05

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	187/190 (98%)	180 (96%)	7 (4%)	0	100	100
1	B	186/190 (98%)	178 (96%)	6 (3%)	2 (1%)	17	51
1	C	187/190 (98%)	178 (95%)	8 (4%)	1 (0%)	34	71
1	D	186/190 (98%)	178 (96%)	8 (4%)	0	100	100
1	E	186/190 (98%)	179 (96%)	7 (4%)	0	100	100
1	F	187/190 (98%)	179 (96%)	7 (4%)	1 (0%)	34	71
1	G	187/190 (98%)	179 (96%)	8 (4%)	0	100	100
1	H	187/190 (98%)	177 (95%)	8 (4%)	2 (1%)	17	51
1	I	187/190 (98%)	178 (95%)	8 (4%)	1 (0%)	34	71
1	J	186/190 (98%)	180 (97%)	5 (3%)	1 (0%)	34	71
1	K	186/190 (98%)	180 (97%)	5 (3%)	1 (0%)	34	71
1	L	187/190 (98%)	178 (95%)	8 (4%)	1 (0%)	34	71
All	All	2239/2280 (98%)	2144 (96%)	85 (4%)	10 (0%)	39	74

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	113	SER
1	I	116	GLY
1	L	116	GLY
1	B	116	GLY
1	K	116	GLY
1	H	113	SER
1	F	116	GLY
1	H	116	GLY
1	J	116	GLY
1	C	116	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	166/167 (99%)	156 (94%)	10 (6%)	24	57
1	B	165/167 (99%)	158 (96%)	7 (4%)	36	73
1	C	166/167 (99%)	157 (95%)	9 (5%)	27	62
1	D	165/167 (99%)	160 (97%)	5 (3%)	48	83
1	E	165/167 (99%)	158 (96%)	7 (4%)	36	73
1	F	166/167 (99%)	159 (96%)	7 (4%)	36	73
1	G	166/167 (99%)	156 (94%)	10 (6%)	24	57
1	H	166/167 (99%)	157 (95%)	9 (5%)	27	62
1	I	166/167 (99%)	155 (93%)	11 (7%)	21	51
1	J	165/167 (99%)	154 (93%)	11 (7%)	20	50
1	K	165/167 (99%)	155 (94%)	10 (6%)	23	56
1	L	166/167 (99%)	156 (94%)	10 (6%)	24	57
All	All	1987/2004 (99%)	1881 (95%)	106 (5%)	28	63

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	32	ILE
1	A	68	ASP
1	A	83	SER
1	A	94	LEU
1	A	98	LEU
1	A	101	LYS
1	A	113	SER
1	A	114	THR
1	A	131	SER
1	B	26	LEU
1	B	32	ILE
1	B	68	ASP
1	B	94	LEU

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Mol	Chain	Res	Type
1	B	101	LYS
1	B	111	THR
1	B	131	SER
1	C	26	LEU
1	C	32	ILE
1	C	68	ASP
1	C	83	SER
1	C	94	LEU
1	C	98	LEU
1	C	112	HIS
1	C	114	THR
1	C	131	SER
1	D	26	LEU
1	D	32	ILE
1	D	68	ASP
1	D	94	LEU
1	D	131	SER
1	E	26	LEU
1	E	32	ILE
1	E	68	ASP
1	E	83	SER
1	E	94	LEU
1	E	114	THR
1	E	131	SER
1	F	26	LEU
1	F	32	ILE
1	F	68	ASP
1	F	94	LEU
1	F	101	LYS
1	F	114	THR
1	F	131	SER
1	G	26	LEU
1	G	32	ILE
1	G	68	ASP
1	G	83	SER
1	G	90	LEU
1	G	94	LEU
1	G	111	THR
1	G	114	THR
1	G	131	SER
1	G	189	SER
1	H	26	LEU

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Mol	Chain	Res	Type
1	H	32	ILE
1	H	68	ASP
1	H	83	SER
1	H	94	LEU
1	H	98	LEU
1	H	101	LYS
1	H	113	SER
1	H	131	SER
1	I	26	LEU
1	I	32	ILE
1	I	68	ASP
1	I	83	SER
1	I	90	LEU
1	I	94	LEU
1	I	98	LEU
1	I	101	LYS
1	I	112	HIS
1	I	114	THR
1	I	131	SER
1	J	26	LEU
1	J	32	ILE
1	J	68	ASP
1	J	83	SER
1	J	90	LEU
1	J	94	LEU
1	J	98	LEU
1	J	110	LEU
1	J	113	SER
1	J	114	THR
1	J	131	SER
1	K	26	LEU
1	K	32	ILE
1	K	68	ASP
1	K	83	SER
1	K	90	LEU
1	K	94	LEU
1	K	111	THR
1	K	113	SER
1	K	114	THR
1	K	131	SER
1	L	26	LEU
1	L	32	ILE

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Mol	Chain	Res	Type
1	L	68	ASP
1	L	83	SER
1	L	90	LEU
1	L	94	LEU
1	L	101	LYS
1	L	111	THR
1	L	112	HIS
1	L	131	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	HIS
1	B	75	HIS
1	C	75	HIS
1	D	75	HIS
1	E	75	HIS
1	F	75	HIS
1	H	75	HIS
1	I	75	HIS
1	J	75	HIS
1	K	75	HIS
1	L	75	HIS
1	L	112	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 26 ligands modelled in this entry, 14 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	TTP	A	201	3	21,30,30	0.67	0	31,47,47	2.07	4 (12%)
2	TTP	B	201	3	21,30,30	0.62	0	31,47,47	1.97	4 (12%)
2	TTP	C	201	3	21,30,30	0.58	0	31,47,47	2.18	4 (12%)
2	TTP	D	201	3	21,30,30	0.63	0	31,47,47	2.21	4 (12%)
2	TTP	E	201	3	21,30,30	0.53	0	31,47,47	2.07	4 (12%)
2	TTP	F	201	3	21,30,30	0.68	0	31,47,47	1.87	4 (12%)
2	TTP	G	201	3	21,30,30	0.60	0	31,47,47	2.33	5 (16%)
2	TTP	H	201	3	21,30,30	0.48	0	31,47,47	2.02	5 (16%)
2	TTP	I	201	3	21,30,30	0.66	0	31,47,47	2.12	4 (12%)
2	TTP	J	201	3	21,30,30	0.57	0	31,47,47	2.24	4 (12%)
2	TTP	K	201	3	21,30,30	0.56	0	31,47,47	2.22	4 (12%)
2	TTP	L	201	3	21,30,30	0.77	1 (4%)	31,47,47	1.99	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TTP	A	201	3	-	0/18/34/34	0/2/2/2
2	TTP	B	201	3	-	0/18/34/34	0/2/2/2
2	TTP	C	201	3	-	0/18/34/34	0/2/2/2
2	TTP	D	201	3	-	0/18/34/34	0/2/2/2
2	TTP	E	201	3	-	0/18/34/34	0/2/2/2
2	TTP	F	201	3	-	0/18/34/34	0/2/2/2
2	TTP	G	201	3	-	0/18/34/34	0/2/2/2
2	TTP	H	201	3	-	0/18/34/34	0/2/2/2
2	TTP	I	201	3	-	0/18/34/34	0/2/2/2
2	TTP	J	201	3	-	0/18/34/34	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TTP	K	201	3	-	0/18/34/34	0/2/2/2
2	TTP	L	201	3	-	0/18/34/34	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	201	TTP	PA-O2A	-2.10	1.46	1.54

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	201	TTP	C5-C4-N3	-7.12	117.21	125.14
2	K	201	TTP	C5-C4-N3	-6.45	117.96	125.14
2	C	201	TTP	C5-C4-N3	-6.39	118.02	125.14
2	A	201	TTP	C5-C4-N3	-6.37	118.04	125.14
2	E	201	TTP	C5-C4-N3	-6.22	118.22	125.14
2	H	201	TTP	C5-C4-N3	-5.94	118.52	125.14
2	D	201	TTP	C5-C4-N3	-5.82	118.66	125.14
2	L	201	TTP	C5-C4-N3	-5.73	118.76	125.14
2	B	201	TTP	C5-C4-N3	-5.63	118.87	125.14
2	F	201	TTP	C5-C4-N3	-5.57	118.93	125.14
2	J	201	TTP	C5-C4-N3	-5.37	119.16	125.14
2	I	201	TTP	C5-C4-N3	-5.37	119.16	125.14
2	J	201	TTP	PB-O3A-PA	-4.83	119.16	132.73
2	E	201	TTP	PB-O3A-PA	-4.43	120.28	132.73
2	I	201	TTP	PB-O3A-PA	-4.41	120.35	132.73
2	B	201	TTP	PB-O3A-PA	-4.20	120.93	132.73
2	K	201	TTP	PB-O3A-PA	-4.20	120.94	132.73
2	H	201	TTP	PB-O3A-PA	-4.09	121.24	132.73
2	L	201	TTP	PB-O3A-PA	-3.93	121.69	132.73
2	D	201	TTP	PB-O3A-PA	-3.87	121.85	132.73
2	A	201	TTP	PB-O3A-PA	-3.65	122.48	132.73
2	D	201	TTP	PB-O3B-PG	-3.59	120.62	132.67
2	C	201	TTP	PB-O3A-PA	-3.49	122.92	132.73
2	F	201	TTP	PB-O3A-PA	-3.46	123.02	132.73
2	G	201	TTP	PB-O3A-PA	-3.44	123.06	132.73
2	J	201	TTP	PB-O3B-PG	-3.37	121.36	132.67
2	C	201	TTP	PB-O3B-PG	-3.19	121.99	132.67
2	I	201	TTP	PB-O3B-PG	-3.13	122.18	132.67
2	H	201	TTP	PB-O3B-PG	-2.92	122.87	132.67
2	K	201	TTP	PB-O3B-PG	-2.72	123.53	132.67
2	A	201	TTP	PB-O3B-PG	-2.69	123.64	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	201	TTP	PB-O3B-PG	-2.58	124.00	132.67
2	F	201	TTP	PB-O3B-PG	-2.54	124.16	132.67
2	E	201	TTP	PB-O3B-PG	-2.50	124.27	132.67
2	L	201	TTP	PB-O3B-PG	-2.38	124.68	132.67
2	G	201	TTP	PB-O3B-PG	-2.28	125.00	132.67
2	L	201	TTP	O2B-PB-O3A	2.17	114.96	105.09
2	H	201	TTP	O4'-C1'-N1	2.25	111.61	107.72
2	G	201	TTP	O4'-C1'-N1	3.08	113.06	107.72
2	H	201	TTP	C4-N3-C2	6.48	120.85	115.25
2	F	201	TTP	C4-N3-C2	6.50	120.87	115.25
2	B	201	TTP	C4-N3-C2	7.06	121.35	115.25
2	L	201	TTP	C4-N3-C2	7.08	121.37	115.25
2	E	201	TTP	C4-N3-C2	7.19	121.46	115.25
2	A	201	TTP	C4-N3-C2	7.45	121.69	115.25
2	I	201	TTP	C4-N3-C2	7.86	122.04	115.25
2	K	201	TTP	C4-N3-C2	7.95	122.12	115.25
2	D	201	TTP	C4-N3-C2	8.07	122.23	115.25
2	C	201	TTP	C4-N3-C2	8.21	122.34	115.25
2	J	201	TTP	C4-N3-C2	8.44	122.54	115.25
2	G	201	TTP	C4-N3-C2	8.49	122.58	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	201	TTP	2	0
2	C	201	TTP	1	0
2	E	201	TTP	1	0
2	F	201	TTP	1	0
2	H	201	TTP	2	0
2	J	201	TTP	1	0
2	K	201	TTP	1	0
2	L	201	TTP	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	189/190 (99%)	0.42	9 (4%) 34 28	31, 46, 69, 82	0
1	B	188/190 (98%)	0.08	2 (1%) 82 80	26, 39, 61, 72	0
1	C	189/190 (99%)	0.31	5 (2%) 59 54	30, 46, 71, 87	0
1	D	188/190 (98%)	0.09	4 (2%) 67 62	27, 40, 62, 75	0
1	E	188/190 (98%)	0.51	13 (6%) 20 14	35, 49, 72, 86	0
1	F	189/190 (99%)	0.13	4 (2%) 67 62	29, 41, 64, 73	0
1	G	189/190 (99%)	0.26	7 (3%) 45 38	29, 44, 66, 79	0
1	H	189/190 (99%)	0.16	3 (1%) 74 72	28, 41, 64, 73	0
1	I	189/190 (99%)	0.24	5 (2%) 59 54	28, 42, 65, 86	0
1	J	188/190 (98%)	0.14	2 (1%) 82 80	26, 41, 64, 79	0
1	K	188/190 (98%)	0.46	12 (6%) 23 16	31, 45, 67, 79	0
1	L	189/190 (99%)	0.14	4 (2%) 67 62	28, 41, 66, 76	0
All	All	2263/2280 (99%)	0.24	70 (3%) 52 45	26, 43, 68, 87	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	185	ASN	5.3
1	C	24	ASP	4.8
1	A	187	ILE	4.6
1	K	39	LEU	4.4
1	G	187	ILE	4.3
1	E	165	SER	4.0
1	E	187	ILE	3.7
1	K	187	ILE	3.7
1	G	185	ASN	3.6
1	E	113	SER	3.6
1	K	68	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	166	ARG	3.6
1	K	22	PHE	3.6
1	L	67	VAL	3.4
1	E	167	ALA	3.3
1	K	113	SER	3.2
1	I	175	ARG	3.2
1	I	68	ASP	3.1
1	B	166	ARG	3.1
1	D	187	ILE	3.1
1	C	175	ARG	3.1
1	K	175	ARG	3.0
1	K	21	PRO	3.0
1	J	185	ASN	3.0
1	G	22	PHE	2.9
1	E	185	ASN	2.9
1	D	185	ASN	2.9
1	E	168	GLY	2.8
1	F	59	GLU	2.8
1	E	69	GLY	2.8
1	H	175	ARG	2.7
1	G	175	ARG	2.7
1	A	166	ARG	2.7
1	D	88	PHE	2.7
1	E	112	HIS	2.6
1	E	114	THR	2.6
1	K	13	SER	2.6
1	C	58	ASP	2.6
1	A	112	HIS	2.5
1	L	59	GLU	2.5
1	F	70	GLU	2.4
1	K	15	GLY	2.4
1	K	20	ASP	2.4
1	A	159	GLU	2.4
1	E	150	CYS	2.4
1	A	175	ARG	2.4
1	G	114	THR	2.3
1	I	113	SER	2.3
1	A	117	PHE	2.3
1	E	186	PHE	2.3
1	L	185	ASN	2.2
1	I	114	THR	2.2
1	A	113	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	G	189	SER	2.2
1	K	168	GLY	2.2
1	F	68	ASP	2.1
1	C	116	GLY	2.1
1	K	188	ARG	2.1
1	E	177	PRO	2.1
1	B	68	ASP	2.1
1	A	188	ARG	2.1
1	H	189	SER	2.1
1	I	185	ASN	2.1
1	C	151	MET	2.1
1	D	15	GLY	2.1
1	H	129	GLU	2.0
1	F	175	ARG	2.0
1	J	56	GLN	2.0
1	L	113	SER	2.0
1	G	20	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MG	B	203	1/1	0.81	0.34	4.13	44,44,44,44	0
2	TTP	G	201	29/29	0.92	0.17	-0.51	31,37,43,44	0
2	TTP	I	201	29/29	0.95	0.16	-0.60	29,35,41,42	0
2	TTP	A	201	29/29	0.93	0.17	-0.79	34,39,46,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	TTP	E	201	29/29	0.93	0.14	-0.97	36,42,48,49	0
2	TTP	H	201	29/29	0.95	0.14	-1.07	25,31,39,40	0
2	TTP	D	201	29/29	0.95	0.14	-1.08	25,32,38,40	0
2	TTP	F	201	29/29	0.94	0.14	-1.12	25,31,40,41	0
2	TTP	B	201	29/29	0.97	0.13	-1.25	24,30,38,39	0
2	TTP	C	201	29/29	0.92	0.16	-1.26	32,39,44,45	0
2	TTP	L	201	29/29	0.95	0.12	-1.26	25,31,39,40	0
2	TTP	J	201	29/29	0.94	0.13	-1.68	27,33,39,41	0
2	TTP	K	201	29/29	0.95	0.12	-1.70	30,36,43,44	0
3	MG	J	202	1/1	0.94	0.14	-	23,23,23,23	0
3	MG	A	202	1/1	0.85	0.08	-	29,29,29,29	0
3	MG	H	203	1/1	0.90	0.24	-	42,42,42,42	0
3	MG	L	202	1/1	0.96	0.10	-	20,20,20,20	0
3	MG	B	202	1/1	0.96	0.12	-	19,19,19,19	0
3	MG	H	202	1/1	0.95	0.10	-	20,20,20,20	0
3	MG	E	202	1/1	0.78	0.10	-	31,31,31,31	0
3	MG	D	202	1/1	0.94	0.11	-	21,21,21,21	0
3	MG	K	202	1/1	0.92	0.10	-	25,25,25,25	0
3	MG	G	202	1/1	0.89	0.13	-	26,26,26,26	0
3	MG	C	202	1/1	0.85	0.15	-	28,28,28,28	0
3	MG	F	202	1/1	0.94	0.24	-	19,19,19,19	0
3	MG	I	202	1/1	0.97	0.22	-	25,25,25,25	0

6.5 Other polymers

There are no such residues in this entry.