



Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 11:59 pm BST

PDB ID : 2WQT
Title : Dodecahedral assembly of MhpD
Authors : Montgomery, M.G.; Wood, S.P.
Deposited on : 2009-08-27
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 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 : 2.11
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) : 2.11

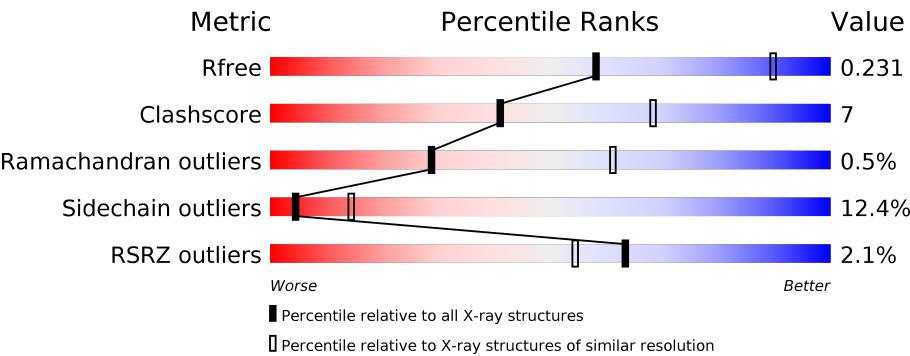
1 Overall quality at a glance i

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 on 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	270	<div><div>2%</div><div>77%</div><div>16%</div><div>.</div><div>.</div></div>
1	B	270	<div><div>%</div><div>77%</div><div>16%</div><div>.</div><div>.</div><div>.</div></div>
1	C	270	<div><div>%</div><div>76%</div><div>16%</div><div>.</div><div>.</div></div>
1	D	270	<div><div>2%</div><div>78%</div><div>15%</div><div>.</div><div>.</div></div>
1	E	270	<div><div>2%</div><div>77%</div><div>16%</div><div>.</div><div>.</div></div>
1	F	270	<div><div>%</div><div>77%</div><div>16%</div><div>.</div><div>.</div><div>.</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	270	
1	H	270	
1	I	270	
1	J	270	
1	K	270	
1	L	270	
1	M	270	
1	N	270	
1	O	270	
1	P	270	
1	Q	270	
1	R	270	
1	S	270	
1	T	270	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	F	1262	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 40183 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 2-KETO-4-PENTENOATE HYDRATASE.

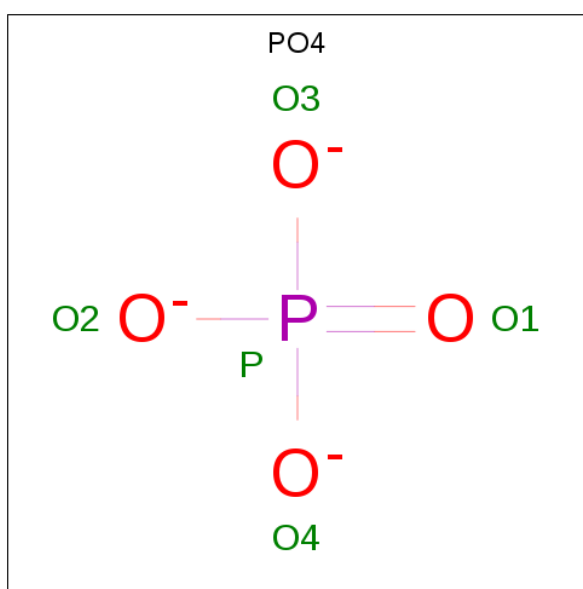
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			1986	1242	357	377	10			
1	B	262	Total	C	N	O	S	0	0	0
			1986	1242	357	377	10			
1	C	262	Total	C	N	O	S	0	0	0
			1986	1242	357	377	10			
1	D	262	Total	C	N	O	S	0	0	0
			1986	1242	357	377	10			
1	E	262	Total	C	N	O	S	0	0	0
			1986	1242	357	377	10			
1	F	262	Total	C	N	O	S	0	0	0
			1986	1242	357	377	10			
1	G	262	Total	C	N	O	S	0	0	0
			1986	1242	357	377	10			
1	H	262	Total	C	N	O	S	0	0	0
			1986	1242	357	377	10			
1	I	262	Total	C	N	O	S	0	0	0
			1986	1242	357	377	10			
1	J	262	Total	C	N	O	S	0	0	0
			1986	1242	357	377	10			
1	K	262	Total	C	N	O	S	0	0	0
			1986	1242	357	377	10			
1	L	262	Total	C	N	O	S	0	0	0
			1986	1242	357	377	10			
1	M	262	Total	C	N	O	S	0	0	0
			1986	1242	357	377	10			
1	N	262	Total	C	N	O	S	0	0	0
			1986	1242	357	377	10			
1	O	262	Total	C	N	O	S	0	0	0
			1986	1242	357	377	10			
1	P	262	Total	C	N	O	S	0	0	0
			1986	1242	357	377	10			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	262	Total	C	N	O	S	0	0	0
			1986	1242	357	377	10			
1	R	262	Total	C	N	O	S	0	0	0
			1986	1242	357	377	10			
1	S	262	Total	C	N	O	S	0	0	0
			1986	1242	357	377	10			
1	T	262	Total	C	N	O	S	0	0	0
			1986	1242	357	377	10			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	G	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		
2	H	1	Total	O	P	0	0
			5	4	1		
2	I	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		
2	J	1	Total	O	P	0	0
			5	4	1		
2	K	1	Total	O	P	0	0
			5	4	1		
2	K	1	Total	O	P	0	0
			5	4	1		
2	K	1	Total	O	P	0	0
			5	4	1		
2	L	1	Total	O	P	0	0
			5	4	1		
2	L	1	Total	O	P	0	0
			5	4	1		
2	M	1	Total	O	P	0	0
			5	4	1		
2	N	1	Total	O	P	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	O	1	Total	O	P	0	0
			5	4	1		
2	P	1	Total	O	P	0	0
			5	4	1		
2	P	1	Total	O	P	0	0
			5	4	1		
2	P	1	Total	O	P	0	0
			5	4	1		
2	Q	1	Total	O	P	0	0
			5	4	1		
2	Q	1	Total	O	P	0	0
			5	4	1		
2	Q	1	Total	O	P	0	0
			5	4	1		
2	R	1	Total	O	P	0	0
			5	4	1		
2	S	1	Total	O	P	0	0
			5	4	1		
2	T	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	P	1	Total	Na	0	0
			1	1		
3	G	1	Total	Na	0	0
			1	1		
3	Q	1	Total	Na	0	0
			1	1		
3	D	1	Total	Na	0	0
			1	1		
3	K	1	Total	Na	0	0
			1	1		
3	E	1	Total	Na	0	0
			1	1		
3	I	1	Total	Na	0	0
			1	1		
3	C	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	T	1	Total 1	Na 1	0	0
3	N	1	Total 1	Na 1	0	0
3	O	2	Total 2	Na 2	0	0
3	R	1	Total 1	Na 1	0	0
3	L	2	Total 2	Na 2	0	0
3	S	2	Total 2	Na 2	0	0
3	F	1	Total 1	Na 1	0	0
3	M	1	Total 1	Na 1	0	0

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	P	1	Total 1	K 1	0	0
4	G	2	Total 2	K 2	0	0
4	Q	2	Total 2	K 2	0	0
4	D	1	Total 1	K 1	0	0
4	K	1	Total 1	K 1	0	0
4	E	1	Total 1	K 1	0	0
4	B	1	Total 1	K 1	0	0
4	I	1	Total 1	K 1	0	0
4	C	1	Total 1	K 1	0	0
4	A	2	Total 2	K 2	0	0
4	T	1	Total 1	K 1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	N	1	Total K 1 1	0	0
4	R	1	Total K 1 1	0	0
4	L	2	Total K 2 2	0	0
4	S	1	Total K 1 1	0	0
4	F	1	Total K 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	10	Total O 10 10	0	0
5	B	9	Total O 9 9	0	0
5	C	13	Total O 13 13	0	0
5	D	12	Total O 12 12	0	0
5	E	10	Total O 10 10	0	0
5	F	14	Total O 14 14	0	0
5	G	11	Total O 11 11	0	0
5	H	12	Total O 12 12	0	0
5	I	11	Total O 11 11	0	0
5	J	13	Total O 13 13	0	0
5	K	14	Total O 14 14	0	0
5	L	17	Total O 17 17	0	0
5	M	10	Total O 10 10	0	0
5	N	11	Total O 11 11	0	0

Continued on next page...

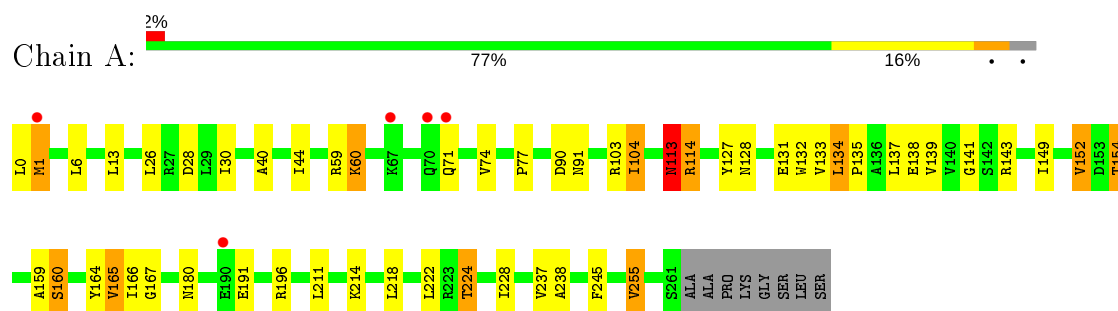
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	O	10	Total 10	O 10	0	0
5	P	11	Total 11	O 11	0	0
5	Q	11	Total 11	O 11	0	0
5	R	12	Total 12	O 12	0	0
5	S	11	Total 11	O 11	0	0
5	T	11	Total 11	O 11	0	0

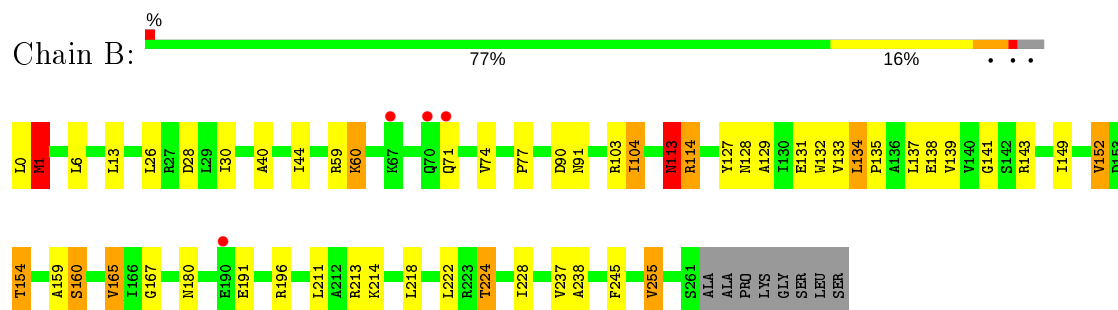
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

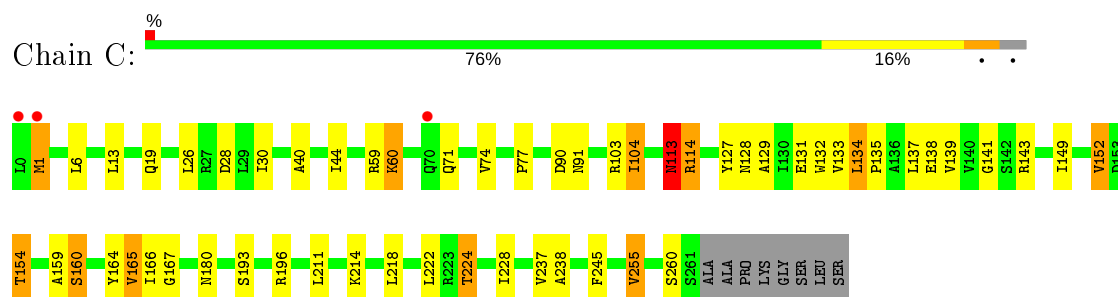
• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



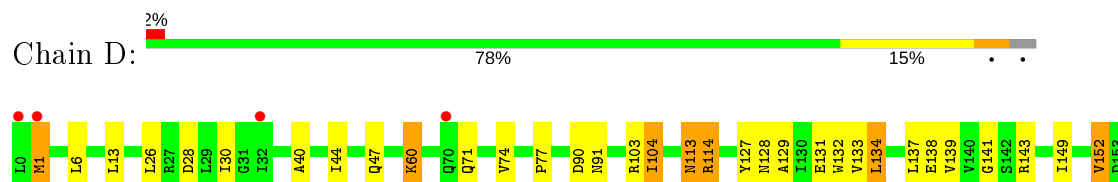
• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE

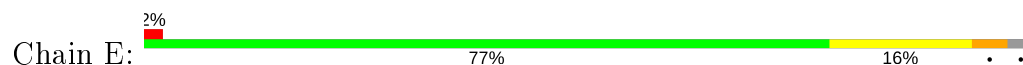


• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE

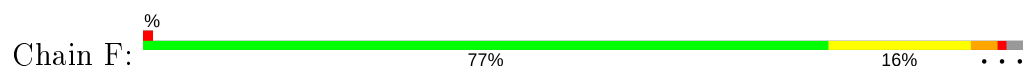




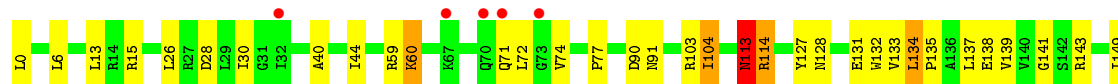
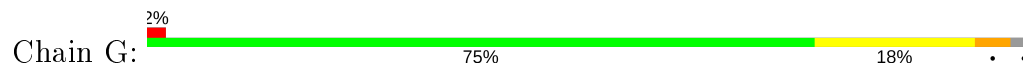
• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



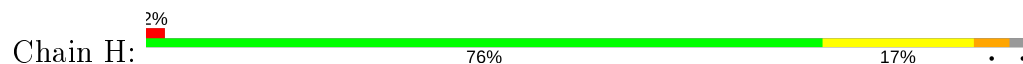
• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



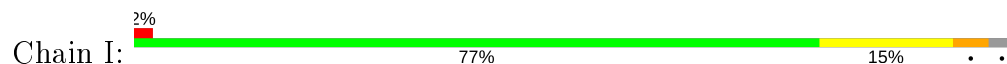
• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE

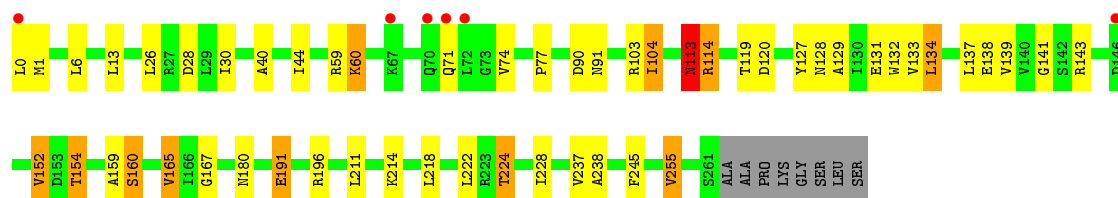


• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE

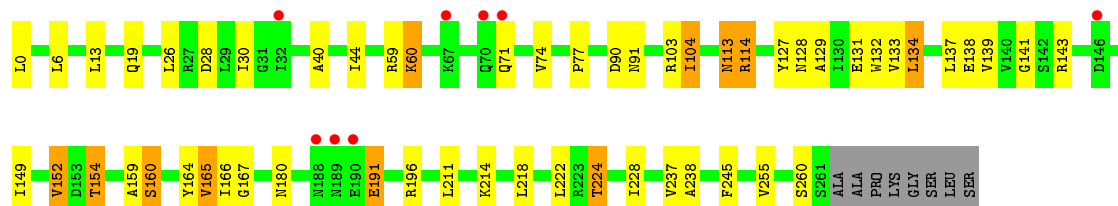
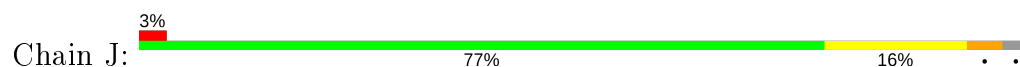


• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE

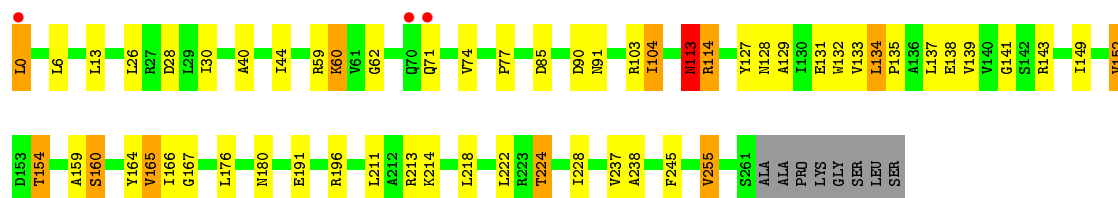
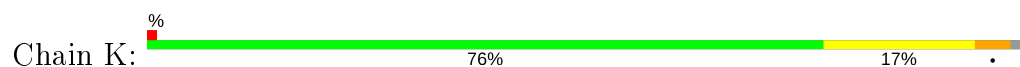




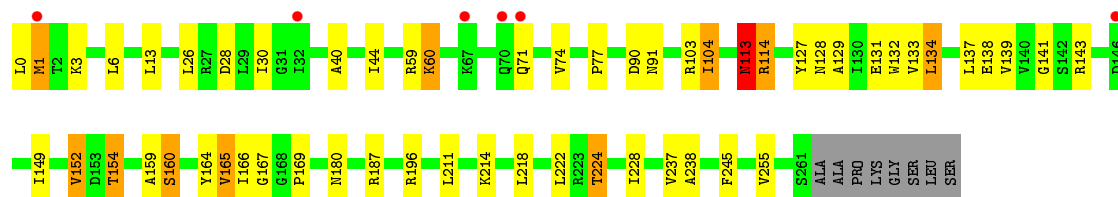
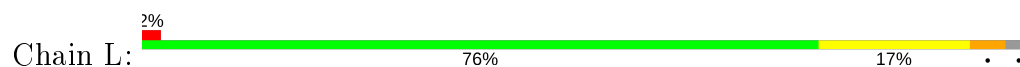
• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



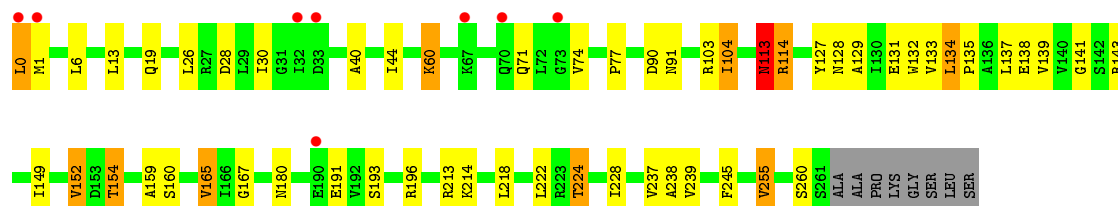
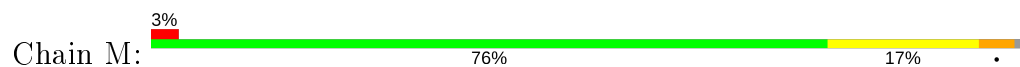
• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



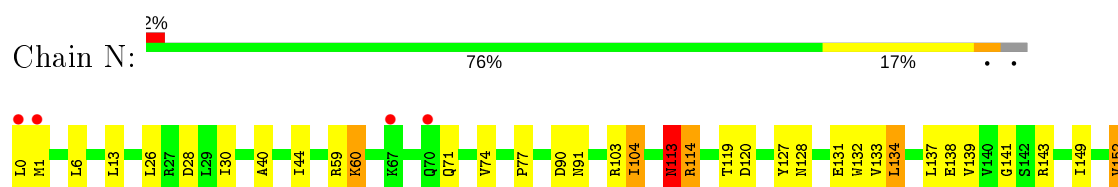
• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



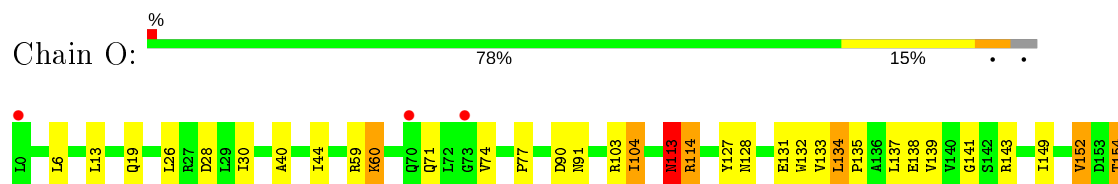
• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



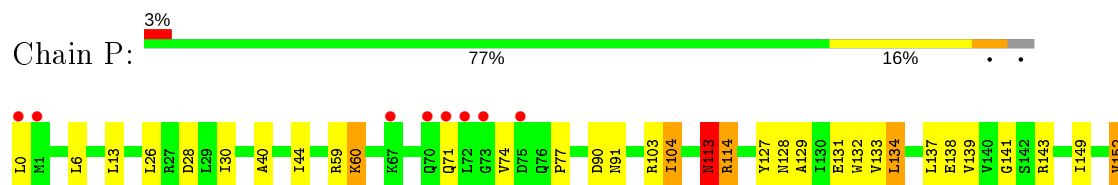
• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



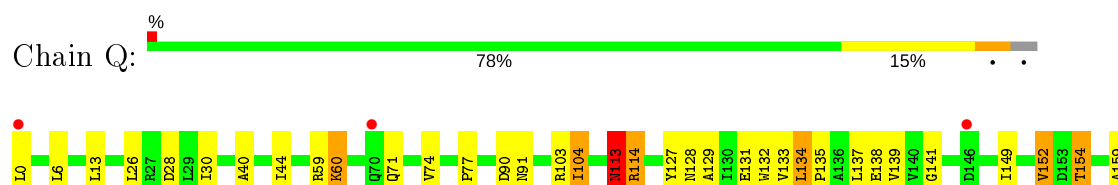
• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



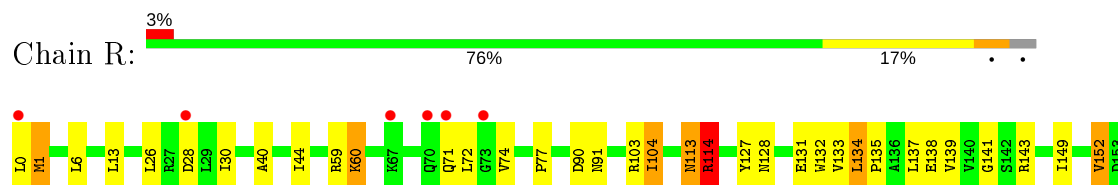
• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE

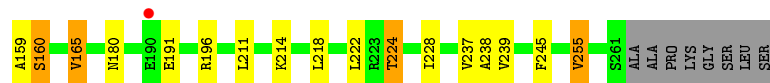
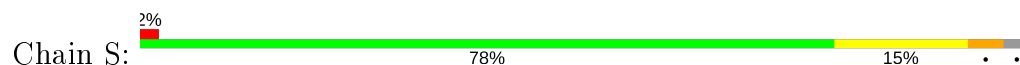


• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE

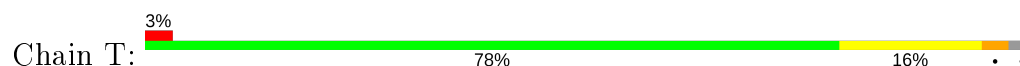




• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



• Molecule 1: 2-KETO-4-PENTENOATE HYDRATASE



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	207.35Å 207.35Å 545.47Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.26 – 2.80 35.26 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.9 (35.26-2.80) 94.8 (35.26-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.87 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.5.0088	Depositor
R, R_{free}	0.222 , 0.234 0.220 , 0.231	Depositor DCC
R_{free} test set	10232 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.010 for -h-k,k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	40183	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: NA, K, PO4

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	0.45	0/2020	0.68	3/2744 (0.1%)
1	B	0.46	0/2020	0.67	3/2744 (0.1%)
1	C	0.54	4/2020 (0.2%)	0.68	2/2744 (0.1%)
1	D	0.47	0/2020	0.68	2/2744 (0.1%)
1	E	0.46	0/2020	0.67	2/2744 (0.1%)
1	F	0.47	0/2020	0.68	3/2744 (0.1%)
1	G	0.46	0/2020	0.68	2/2744 (0.1%)
1	H	0.50	2/2020 (0.1%)	0.67	2/2744 (0.1%)
1	I	0.46	0/2020	0.67	2/2744 (0.1%)
1	J	0.51	2/2020 (0.1%)	0.67	1/2744 (0.0%)
1	K	0.46	0/2020	0.66	2/2744 (0.1%)
1	L	0.47	0/2020	0.71	5/2744 (0.2%)
1	M	0.50	2/2020 (0.1%)	0.67	2/2744 (0.1%)
1	N	0.46	0/2020	0.67	2/2744 (0.1%)
1	O	0.50	2/2020 (0.1%)	0.67	2/2744 (0.1%)
1	P	0.46	0/2020	0.66	2/2744 (0.1%)
1	Q	0.45	0/2020	0.67	2/2744 (0.1%)
1	R	0.47	0/2020	0.84	5/2744 (0.2%)
1	S	0.50	2/2020 (0.1%)	0.68	3/2744 (0.1%)
1	T	0.46	0/2020	0.66	2/2744 (0.1%)
All	All	0.48	14/40400 (0.0%)	0.68	49/54880 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	19	GLN	CD-NE2	-8.03	1.12	1.32
1	M	19	GLN	CD-NE2	-7.82	1.13	1.32
1	J	19	GLN	CD-NE2	-7.79	1.13	1.32
1	O	19	GLN	CD-NE2	-7.78	1.13	1.32
1	C	19	GLN	CD-NE2	-7.55	1.14	1.32
1	S	19	GLN	CD-NE2	-7.47	1.14	1.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	19	GLN	CD-OE1	-7.44	1.07	1.24
1	M	19	GLN	CD-OE1	-7.19	1.08	1.24
1	S	19	GLN	CD-OE1	-7.18	1.08	1.24
1	O	19	GLN	CD-OE1	-7.17	1.08	1.24
1	H	19	GLN	CD-OE1	-7.16	1.08	1.24
1	C	19	GLN	CD-OE1	-7.10	1.08	1.24
1	C	113	ASN	CG-OD1	-6.30	1.10	1.24
1	C	113	ASN	CG-ND2	-6.21	1.17	1.32

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	114	ARG	NE-CZ-NH1	-19.06	110.77	120.30
1	R	114	ARG	NE-CZ-NH2	17.55	129.07	120.30
1	G	134	LEU	CA-CB-CG	8.54	134.94	115.30
1	E	134	LEU	CA-CB-CG	8.48	134.81	115.30
1	D	134	LEU	CA-CB-CG	8.44	134.72	115.30
1	I	134	LEU	CA-CB-CG	8.43	134.69	115.30
1	P	134	LEU	CA-CB-CG	8.43	134.69	115.30
1	B	134	LEU	CA-CB-CG	8.38	134.59	115.30
1	F	134	LEU	CA-CB-CG	8.38	134.56	115.30
1	S	134	LEU	CA-CB-CG	8.37	134.56	115.30
1	A	134	LEU	CA-CB-CG	8.33	134.46	115.30
1	N	134	LEU	CA-CB-CG	8.33	134.46	115.30
1	J	134	LEU	CA-CB-CG	8.30	134.40	115.30
1	Q	134	LEU	CA-CB-CG	8.26	134.29	115.30
1	R	114	ARG	CD-NE-CZ	8.26	135.16	123.60
1	C	134	LEU	CA-CB-CG	8.23	134.24	115.30
1	R	134	LEU	CA-CB-CG	8.21	134.19	115.30
1	M	134	LEU	CA-CB-CG	8.08	133.89	115.30
1	T	134	LEU	CA-CB-CG	8.08	133.88	115.30
1	O	134	LEU	CA-CB-CG	8.06	133.85	115.30
1	K	134	LEU	CA-CB-CG	8.06	133.84	115.30
1	L	134	LEU	CA-CB-CG	7.99	133.67	115.30
1	H	134	LEU	CA-CB-CG	7.86	133.38	115.30
1	L	1	MET	CG-SD-CE	7.55	112.28	100.20
1	A	1	MET	CG-SD-CE	6.96	111.33	100.20
1	L	1	MET	CB-CG-SD	6.41	131.64	112.40
1	S	1	MET	CG-SD-CE	5.88	109.60	100.20
1	D	1	MET	CG-SD-CE	5.76	109.41	100.20
1	L	113	ASN	CB-CA-C	-5.72	98.96	110.40
1	C	1	MET	CG-SD-CE	5.71	109.34	100.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	113	ASN	CB-CA-C	-5.66	99.08	110.40
1	Q	113	ASN	CB-CA-C	-5.60	99.21	110.40
1	M	113	ASN	CB-CA-C	-5.56	99.28	110.40
1	I	113	ASN	CB-CA-C	-5.53	99.35	110.40
1	P	113	ASN	CB-CA-C	-5.48	99.43	110.40
1	E	1	MET	CG-SD-CE	5.46	108.94	100.20
1	O	113	ASN	CB-CA-C	-5.45	99.50	110.40
1	R	113	ASN	CB-CA-C	-5.44	99.52	110.40
1	A	113	ASN	CB-CA-C	-5.43	99.53	110.40
1	T	113	ASN	CB-CA-C	-5.34	99.73	110.40
1	N	113	ASN	CB-CA-C	-5.30	99.80	110.40
1	F	113	ASN	CB-CA-C	-5.29	99.82	110.40
1	F	1	MET	CG-SD-CE	5.27	108.64	100.20
1	H	113	ASN	CB-CA-C	-5.26	99.88	110.40
1	S	113	ASN	CB-CA-C	-5.26	99.88	110.40
1	K	113	ASN	CB-CA-C	-5.19	100.02	110.40
1	B	113	ASN	CB-CA-C	-5.16	100.09	110.40
1	L	1	MET	CA-CB-CG	5.05	121.89	113.30
1	B	1	MET	CG-SD-CE	5.04	108.27	100.20

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	1986	0	1979	27	0
1	B	1986	0	1979	36	0
1	C	1986	0	1979	28	0
1	D	1986	0	1979	25	0
1	E	1986	0	1979	37	0
1	F	1986	0	1979	37	0
1	G	1986	0	1979	32	0
1	H	1986	0	1979	35	0
1	I	1986	0	1979	34	0
1	J	1986	0	1979	28	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	K	1986	0	1979	35	0
1	L	1986	0	1979	30	0
1	M	1986	0	1979	36	0
1	N	1986	0	1979	34	0
1	O	1986	0	1979	25	0
1	P	1986	0	1979	27	0
1	Q	1986	0	1979	28	0
1	R	1986	0	1979	35	0
1	S	1986	0	1979	25	0
1	T	1986	0	1979	30	0
2	A	15	0	0	1	0
2	B	10	0	0	1	0
2	C	5	0	0	0	0
2	D	15	0	0	1	0
2	E	5	0	0	1	0
2	F	15	0	0	2	0
2	G	15	0	0	2	0
2	H	10	0	0	0	0
2	I	5	0	0	0	0
2	J	10	0	0	0	0
2	K	15	0	0	1	0
2	L	10	0	0	1	0
2	M	5	0	0	0	0
2	N	5	0	0	0	0
2	O	5	0	0	0	0
2	P	15	0	0	1	0
2	Q	15	0	0	1	0
2	R	5	0	0	1	0
2	S	5	0	0	0	0
2	T	5	0	0	1	0
3	A	1	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	I	1	0	0	0	0
3	K	1	0	0	0	0
3	L	2	0	0	0	0
3	M	1	0	0	0	0
3	N	1	0	0	0	0
3	O	2	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	P	1	0	0	0	0
3	Q	1	0	0	0	0
3	R	1	0	0	0	0
3	S	2	0	0	0	0
3	T	1	0	0	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	2	0	0	0	0
4	I	1	0	0	0	0
4	K	1	0	0	0	0
4	L	2	0	0	0	0
4	N	1	0	0	0	0
4	P	1	0	0	0	0
4	Q	2	0	0	0	0
4	R	1	0	0	0	0
4	S	1	0	0	0	0
4	T	1	0	0	0	0
5	A	10	0	0	0	0
5	B	9	0	0	0	0
5	C	13	0	0	1	0
5	D	12	0	0	0	0
5	E	10	0	0	0	0
5	F	14	0	0	0	0
5	G	11	0	0	0	0
5	H	12	0	0	0	0
5	I	11	0	0	1	0
5	J	13	0	0	1	0
5	K	14	0	0	0	0
5	L	17	0	0	0	0
5	M	10	0	0	1	0
5	N	11	0	0	0	0
5	O	10	0	0	0	0
5	P	11	0	0	1	0
5	Q	11	0	0	0	0
5	R	12	0	0	0	0
5	S	11	0	0	0	0
5	T	11	0	0	0	0
All	All	40183	0	39580	565	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 7.

All (565) 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:P:128:ASN:HD22	1:Q:132:TRP:HE1	1.05	1.00
1:B:128:ASN:HD22	1:E:132:TRP:HE1	1.02	0.99
1:P:132:TRP:HE1	1:S:128:ASN:HD22	1.04	0.98
1:F:132:TRP:HE1	1:I:128:ASN:HD22	1.02	0.96
1:K:132:TRP:HE1	1:N:128:ASN:HD22	1.01	0.96
1:A:132:TRP:HE1	1:D:128:ASN:HD22	1.15	0.95
1:A:128:ASN:HD22	1:B:132:TRP:HE1	1.02	0.94
1:Q:128:ASN:HD22	1:T:132:TRP:HE1	1.11	0.94
1:F:128:ASN:HD22	1:G:132:TRP:HE1	1.14	0.93
1:H:128:ASN:HD22	1:I:132:TRP:HE1	1.03	0.93
1:M:132:TRP:HE1	1:O:128:ASN:HD22	1.15	0.93
1:R:128:ASN:HD22	1:S:132:TRP:HE1	1.09	0.92
1:M:128:ASN:HD22	1:N:132:TRP:HE1	1.02	0.92
1:H:132:TRP:HE1	1:J:128:ASN:HD22	1.15	0.92
1:C:132:TRP:HE1	1:E:128:ASN:HD22	1.12	0.91
1:C:128:ASN:HD22	1:D:132:TRP:HE1	1.19	0.89
1:H:213:ARG:NH1	1:R:1:MET:HE3	1.89	0.88
1:K:128:ASN:HD22	1:L:132:TRP:HE1	1.21	0.88
1:R:132:TRP:HE1	1:T:128:ASN:HD22	1.17	0.88
1:G:60:LYS:NZ	2:G:1263:PO4:O1	2.11	0.83
1:B:1:MET:HE3	1:F:213:ARG:NH1	1.96	0.80
1:H:213:ARG:NH1	1:R:1:MET:CE	2.44	0.80
1:E:60:LYS:NZ	2:E:1262:PO4:O3	2.16	0.78
1:F:104:ILE:HD11	1:F:245:PHE:CE2	2.20	0.77
1:Q:114:ARG:HA	1:Q:224:THR:HB	1.69	0.75
1:L:114:ARG:HA	1:L:224:THR:HB	1.68	0.75
1:G:128:ASN:HD22	1:J:132:TRP:HE1	1.34	0.74
1:C:114:ARG:HA	1:C:224:THR:HB	1.69	0.74
1:R:60:LYS:NZ	2:R:1262:PO4:O3	2.22	0.73
1:C:104:ILE:HD11	1:C:245:PHE:CE2	2.24	0.73
1:A:114:ARG:HA	1:A:224:THR:HB	1.70	0.73
1:G:114:ARG:HA	1:G:224:THR:HB	1.71	0.73
1:F:114:ARG:HA	1:F:224:THR:HB	1.71	0.72
1:G:104:ILE:HD11	1:G:245:PHE:CE2	2.24	0.72
1:I:119:THR:OG1	1:N:0:LEU:HD12	1.90	0.72
1:B:1:MET:CE	1:F:213:ARG:NH1	2.53	0.72
1:Q:154:THR:HG23	1:Q:160:SER:OG	1.91	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:114:ARG:HA	1:J:224:THR:HB	1.73	0.71
1:I:114:ARG:HA	1:I:224:THR:HB	1.72	0.71
1:N:154:THR:HG23	1:N:160:SER:OG	1.91	0.70
1:T:114:ARG:HA	1:T:224:THR:HB	1.73	0.70
1:J:104:ILE:HD11	1:J:245:PHE:CE2	2.27	0.70
1:K:114:ARG:HA	1:K:224:THR:HB	1.74	0.70
1:M:154:THR:HG23	1:M:160:SER:OG	1.92	0.70
1:E:114:ARG:HA	1:E:224:THR:HB	1.73	0.69
1:L:128:ASN:HD22	1:O:132:TRP:HE1	1.38	0.69
1:B:114:ARG:HA	1:B:224:THR:HB	1.74	0.69
1:H:114:ARG:HA	1:H:224:THR:HB	1.74	0.69
1:D:154:THR:HG23	1:D:160:SER:OG	1.93	0.69
1:A:154:THR:HG23	1:A:160:SER:OG	1.93	0.69
1:D:114:ARG:HA	1:D:224:THR:HB	1.73	0.69
1:K:0:LEU:HD13	1:T:119:THR:OG1	1.93	0.69
1:S:114:ARG:HA	1:S:224:THR:HB	1.73	0.69
1:D:40:ALA:O	1:D:44:ILE:HG12	1.92	0.69
1:S:40:ALA:O	1:S:44:ILE:HG12	1.93	0.69
1:N:114:ARG:HA	1:N:224:THR:HB	1.72	0.69
1:O:114:ARG:HA	1:O:224:THR:HB	1.75	0.68
1:H:40:ALA:O	1:H:44:ILE:HG12	1.94	0.68
1:M:114:ARG:HA	1:M:224:THR:HB	1.74	0.68
1:P:154:THR:HG23	1:P:160:SER:OG	1.93	0.68
1:A:40:ALA:O	1:A:44:ILE:HG12	1.94	0.68
1:O:154:THR:HG23	1:O:160:SER:OG	1.94	0.67
1:C:40:ALA:O	1:C:44:ILE:HG12	1.94	0.67
1:A:60:LYS:NZ	2:A:1264:PO4:O1	2.28	0.67
1:E:154:THR:HG23	1:E:160:SER:OG	1.95	0.67
1:J:154:THR:HG23	1:J:160:SER:OG	1.94	0.67
1:K:154:THR:HG23	1:K:160:SER:OG	1.93	0.67
1:I:154:THR:HG23	1:I:160:SER:OG	1.95	0.67
1:Q:104:ILE:HD11	1:Q:245:PHE:CE2	2.28	0.67
1:B:154:THR:HG23	1:B:160:SER:OG	1.95	0.67
1:K:40:ALA:O	1:K:44:ILE:HG12	1.95	0.66
1:F:154:THR:HG23	1:F:160:SER:OG	1.96	0.66
1:L:154:THR:HG23	1:L:160:SER:OG	1.95	0.66
1:R:40:ALA:O	1:R:44:ILE:HG12	1.94	0.66
1:C:104:ILE:HD11	1:C:245:PHE:CZ	2.31	0.66
1:I:0:LEU:HD12	1:N:119:THR:OG1	1.96	0.66
1:K:132:TRP:HE1	1:N:128:ASN:ND2	1.85	0.65
1:R:154:THR:HG23	1:R:160:SER:OG	1.96	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:THR:HG23	1:C:160:SER:OG	1.96	0.65
1:E:1:MET:CE	1:M:213:ARG:NH1	2.60	0.65
1:I:40:ALA:O	1:I:44:ILE:HG12	1.97	0.65
1:P:114:ARG:HA	1:P:224:THR:HB	1.78	0.65
1:T:154:THR:HG23	1:T:160:SER:OG	1.97	0.65
1:B:213:ARG:NH1	1:F:1:MET:HE3	2.12	0.65
1:H:154:THR:HG23	1:H:160:SER:OG	1.95	0.65
1:P:60:LYS:NZ	2:P:1263:PO4:O2	2.29	0.65
1:M:40:ALA:O	1:M:44:ILE:HG12	1.97	0.65
1:Q:40:ALA:O	1:Q:44:ILE:HG12	1.97	0.65
1:B:40:ALA:O	1:B:44:ILE:HG12	1.97	0.65
1:F:104:ILE:HD11	1:F:245:PHE:CZ	2.32	0.64
1:E:40:ALA:O	1:E:44:ILE:HG12	1.96	0.64
1:F:40:ALA:O	1:F:44:ILE:HG12	1.97	0.64
1:N:40:ALA:O	1:N:44:ILE:HG12	1.97	0.64
1:B:154:THR:CG2	1:B:160:SER:OG	2.45	0.64
1:R:114:ARG:HA	1:R:224:THR:HB	1.80	0.64
1:J:40:ALA:O	1:J:44:ILE:HG12	1.97	0.64
1:B:213:ARG:NH1	1:F:1:MET:CE	2.60	0.64
1:K:104:ILE:HD11	1:K:245:PHE:CE2	2.32	0.63
1:S:154:THR:HG23	1:S:160:SER:OG	1.98	0.63
1:T:40:ALA:O	1:T:44:ILE:HG12	1.98	0.63
1:L:40:ALA:O	1:L:44:ILE:HG12	1.98	0.63
1:E:104:ILE:HD11	1:E:245:PHE:CE2	2.33	0.63
1:P:40:ALA:O	1:P:44:ILE:HG12	1.99	0.63
1:Q:104:ILE:HD11	1:Q:245:PHE:CZ	2.34	0.63
1:O:40:ALA:O	1:O:44:ILE:HG12	1.99	0.62
1:B:60:LYS:NZ	2:B:1263:PO4:O3	2.33	0.62
1:Q:154:THR:CG2	1:Q:160:SER:OG	2.47	0.62
1:J:104:ILE:HD11	1:J:245:PHE:CZ	2.34	0.62
1:E:1:MET:HE2	1:M:213:ARG:NH1	2.14	0.62
1:N:104:ILE:HD11	1:N:245:PHE:CE2	2.34	0.62
1:T:60:LYS:NZ	2:T:1262:PO4:O3	2.33	0.62
1:J:154:THR:CG2	1:J:160:SER:OG	2.48	0.61
1:G:40:ALA:O	1:G:44:ILE:HG12	1.99	0.61
1:S:104:ILE:HD11	1:S:245:PHE:CE2	2.36	0.61
1:N:154:THR:CG2	1:N:160:SER:OG	2.49	0.61
1:G:30:ILE:HD11	1:G:152:VAL:HG13	1.82	0.61
1:S:30:ILE:HD11	1:S:152:VAL:HG13	1.82	0.61
1:B:104:ILE:HD11	1:B:245:PHE:CE2	2.36	0.61
1:E:30:ILE:HD11	1:E:152:VAL:HG13	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:113:ASN:HD22	1:G:114:ARG:HH11	1.47	0.61
1:G:154:THR:HG23	1:G:160:SER:OG	2.01	0.61
1:L:104:ILE:HD11	1:L:245:PHE:CE2	2.36	0.60
1:D:104:ILE:HD11	1:D:245:PHE:CE2	2.36	0.60
1:I:154:THR:CG2	1:I:160:SER:OG	2.49	0.60
1:O:104:ILE:HD11	1:O:245:PHE:CE2	2.36	0.60
1:K:154:THR:CG2	1:K:160:SER:OG	2.48	0.60
1:R:30:ILE:HD11	1:R:152:VAL:HG13	1.82	0.60
1:I:191:GLU:OE1	5:I:2008:HOH:O	2.16	0.60
1:F:132:TRP:HE1	1:I:128:ASN:ND2	1.87	0.60
1:P:104:ILE:HD11	1:P:245:PHE:CE2	2.37	0.59
1:I:30:ILE:HD11	1:I:152:VAL:HG13	1.84	0.59
1:T:30:ILE:HD11	1:T:152:VAL:HG13	1.84	0.59
1:F:30:ILE:HD11	1:F:152:VAL:HG13	1.84	0.59
1:K:213:ARG:NH1	1:T:1:MET:CE	2.64	0.59
1:P:191:GLU:OE1	5:P:2007:HOH:O	2.17	0.59
1:F:154:THR:CG2	1:F:160:SER:OG	2.51	0.59
1:K:104:ILE:HD11	1:K:245:PHE:CZ	2.36	0.59
1:O:113:ASN:HD22	1:O:114:ARG:HH11	1.51	0.59
1:H:154:THR:CG2	1:H:160:SER:OG	2.50	0.59
1:D:154:THR:CG2	1:D:160:SER:OG	2.51	0.59
1:M:154:THR:CG2	1:M:160:SER:OG	2.51	0.59
1:A:30:ILE:HD11	1:A:152:VAL:HG13	1.84	0.59
1:A:154:THR:CG2	1:A:160:SER:OG	2.50	0.59
1:G:104:ILE:HD11	1:G:245:PHE:CZ	2.37	0.59
1:K:30:ILE:HD11	1:K:152:VAL:HG13	1.85	0.59
1:P:30:ILE:HD11	1:P:152:VAL:HG13	1.85	0.59
1:N:30:ILE:HD11	1:N:152:VAL:HG13	1.84	0.58
1:I:104:ILE:HD11	1:I:245:PHE:CE2	2.38	0.58
1:S:154:THR:CG2	1:S:160:SER:OG	2.52	0.58
1:M:104:ILE:HD11	1:M:245:PHE:CE2	2.38	0.58
1:O:30:ILE:HD11	1:O:152:VAL:HG13	1.83	0.58
1:B:113:ASN:OD1	1:B:129:ALA:O	2.22	0.58
1:C:154:THR:CG2	1:C:160:SER:OG	2.52	0.58
1:O:154:THR:CG2	1:O:160:SER:OG	2.51	0.58
1:S:113:ASN:HD22	1:S:114:ARG:HH11	1.52	0.58
1:E:104:ILE:HD11	1:E:245:PHE:CZ	2.39	0.57
1:T:154:THR:CG2	1:T:160:SER:OG	2.52	0.57
1:J:30:ILE:HD11	1:J:152:VAL:HG13	1.87	0.57
1:N:113:ASN:HD22	1:N:114:ARG:HH11	1.52	0.57
1:Q:30:ILE:HD11	1:Q:152:VAL:HG13	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:30:ILE:HD11	1:L:152:VAL:HG13	1.84	0.57
1:A:104:ILE:HD11	1:A:245:PHE:CE2	2.39	0.57
1:P:104:ILE:HG23	1:P:139:VAL:HG22	1.85	0.57
1:P:154:THR:CG2	1:P:160:SER:OG	2.52	0.57
1:R:104:ILE:H	1:R:104:ILE:HD12	1.70	0.57
1:R:104:ILE:HD11	1:R:245:PHE:CE2	2.39	0.57
1:H:104:ILE:HD11	1:H:245:PHE:CE2	2.38	0.57
1:E:104:ILE:HG23	1:E:139:VAL:HG22	1.87	0.57
1:M:104:ILE:HG23	1:M:139:VAL:HG22	1.87	0.57
1:N:104:ILE:HG23	1:N:139:VAL:HG22	1.86	0.57
1:O:104:ILE:HD11	1:O:245:PHE:CZ	2.40	0.57
1:E:104:ILE:H	1:E:104:ILE:HD12	1.70	0.57
1:E:154:THR:CG2	1:E:160:SER:OG	2.53	0.57
1:B:104:ILE:HD11	1:B:245:PHE:CZ	2.40	0.56
1:D:104:ILE:HG23	1:D:139:VAL:HG22	1.87	0.56
1:H:104:ILE:HD12	1:H:104:ILE:H	1.71	0.56
1:M:128:ASN:ND2	1:N:132:TRP:HE1	1.87	0.56
1:S:104:ILE:HD11	1:S:245:PHE:CZ	2.40	0.56
1:B:104:ILE:HG23	1:B:139:VAL:HG22	1.87	0.56
1:B:30:ILE:HD11	1:B:152:VAL:HG13	1.86	0.56
1:L:154:THR:CG2	1:L:160:SER:OG	2.53	0.56
1:N:104:ILE:HD11	1:N:245:PHE:CZ	2.41	0.56
1:M:104:ILE:H	1:M:104:ILE:HD12	1.71	0.56
1:R:104:ILE:HG23	1:R:139:VAL:HG22	1.86	0.56
1:A:104:ILE:HG23	1:A:139:VAL:HG22	1.88	0.56
1:H:30:ILE:HD11	1:H:152:VAL:HG13	1.88	0.56
1:I:104:ILE:H	1:I:104:ILE:HD12	1.70	0.55
1:Q:104:ILE:HG23	1:Q:139:VAL:HG22	1.88	0.55
1:C:30:ILE:HD11	1:C:152:VAL:HG13	1.89	0.55
1:D:113:ASN:OD1	1:D:129:ALA:C	2.45	0.55
1:F:104:ILE:HG23	1:F:139:VAL:HG22	1.88	0.55
1:K:62:GLY:HA3	2:K:1264:PO4:O3	2.06	0.55
1:T:113:ASN:HD22	1:T:114:ARG:HH11	1.53	0.55
1:F:113:ASN:HD22	1:F:114:ARG:HH11	1.54	0.55
1:D:30:ILE:HD11	1:D:152:VAL:HG13	1.87	0.55
1:R:104:ILE:HD11	1:R:245:PHE:CZ	2.41	0.55
1:M:30:ILE:HD11	1:M:152:VAL:HG13	1.87	0.55
1:M:104:ILE:HD11	1:M:245:PHE:CZ	2.41	0.55
1:O:104:ILE:HD12	1:O:104:ILE:H	1.72	0.55
1:K:113:ASN:HD22	1:K:114:ARG:HH11	1.55	0.55
1:C:104:ILE:HG23	1:C:139:VAL:HG22	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:113:ASN:HD22	1:Q:114:ARG:HH11	1.55	0.54
1:K:104:ILE:HG23	1:K:139:VAL:HG22	1.89	0.54
1:N:104:ILE:H	1:N:104:ILE:HD12	1.72	0.54
1:B:131:GLU:HG2	1:B:132:TRP:CD1	2.42	0.54
1:T:104:ILE:HG23	1:T:139:VAL:HG22	1.89	0.54
1:H:104:ILE:HG23	1:H:139:VAL:HG22	1.89	0.54
1:K:60:LYS:HE3	1:K:159:ALA:O	2.07	0.54
1:P:104:ILE:HD11	1:P:245:PHE:CZ	2.41	0.54
1:E:60:LYS:HE3	1:E:159:ALA:O	2.08	0.54
1:J:104:ILE:H	1:J:104:ILE:HD12	1.71	0.54
1:P:104:ILE:HD12	1:P:104:ILE:H	1.73	0.54
1:R:154:THR:CG2	1:R:160:SER:OG	2.56	0.54
1:H:213:ARG:NH1	1:R:1:MET:HE2	2.21	0.54
1:P:113:ASN:HD22	1:P:114:ARG:HH11	1.57	0.53
1:E:1:MET:HE3	1:M:213:ARG:NH1	2.23	0.53
1:M:113:ASN:HD22	1:M:114:ARG:HH11	1.56	0.53
1:G:104:ILE:HG23	1:G:139:VAL:HG22	1.91	0.53
1:I:60:LYS:HE2	1:I:138:GLU:OE2	2.09	0.53
1:L:113:ASN:HD22	1:L:114:ARG:HH11	1.55	0.53
1:O:60:LYS:HE3	1:O:159:ALA:O	2.09	0.53
1:B:113:ASN:OD1	1:B:129:ALA:C	2.47	0.53
1:S:104:ILE:HG23	1:S:139:VAL:HG22	1.91	0.53
1:H:104:ILE:HD11	1:H:245:PHE:CZ	2.44	0.53
1:Q:131:GLU:HG2	1:Q:132:TRP:CD1	2.44	0.53
1:I:113:ASN:HD22	1:I:114:ARG:HH11	1.57	0.53
1:G:104:ILE:H	1:G:104:ILE:HD12	1.74	0.53
1:O:104:ILE:HG23	1:O:139:VAL:HG22	1.91	0.53
1:H:213:ARG:HH11	1:R:1:MET:CE	2.20	0.53
1:D:104:ILE:H	1:D:104:ILE:HD12	1.74	0.52
1:S:131:GLU:HG2	1:S:132:TRP:CD1	2.43	0.52
1:A:104:ILE:HD11	1:A:245:PHE:CZ	2.45	0.52
1:I:104:ILE:HD11	1:I:245:PHE:CZ	2.44	0.52
1:E:131:GLU:HG2	1:E:132:TRP:CD1	2.44	0.52
1:L:104:ILE:HG23	1:L:139:VAL:HG22	1.91	0.52
1:L:103:ARG:HG3	1:L:238:ALA:HA	1.91	0.52
1:A:60:LYS:HE2	1:A:138:GLU:OE2	2.09	0.52
1:H:113:ASN:HD22	1:H:114:ARG:HH11	1.56	0.52
1:I:131:GLU:HG2	1:I:132:TRP:CD1	2.45	0.52
1:K:104:ILE:HD12	1:K:104:ILE:H	1.74	0.52
1:T:104:ILE:HD11	1:T:245:PHE:CE2	2.45	0.52
1:H:1:MET:HE3	1:R:213:ARG:NH1	2.25	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ILE:H	1:B:104:ILE:HD12	1.74	0.52
1:C:104:ILE:HD12	1:C:104:ILE:H	1.74	0.52
1:D:104:ILE:HD11	1:D:245:PHE:CZ	2.44	0.52
1:F:103:ARG:HG3	1:F:238:ALA:HA	1.91	0.52
1:L:104:ILE:HD12	1:L:104:ILE:H	1.75	0.52
1:A:131:GLU:HG2	1:A:132:TRP:CD1	2.45	0.52
1:J:131:GLU:HG2	1:J:132:TRP:CD1	2.45	0.52
1:O:131:GLU:HG2	1:O:132:TRP:CD1	2.45	0.52
1:P:60:LYS:HE3	1:P:159:ALA:O	2.09	0.52
1:Q:60:LYS:HE3	1:Q:159:ALA:O	2.10	0.52
1:B:60:LYS:HE2	1:B:138:GLU:OE2	2.10	0.52
1:F:60:LYS:HE3	1:F:159:ALA:O	2.09	0.52
1:C:60:LYS:HE3	1:C:159:ALA:O	2.10	0.51
1:J:104:ILE:HG23	1:J:139:VAL:HG22	1.90	0.51
1:D:131:GLU:HG2	1:D:132:TRP:CD1	2.45	0.51
1:I:104:ILE:HG23	1:I:139:VAL:HG22	1.91	0.51
1:R:60:LYS:HE3	1:R:159:ALA:O	2.09	0.51
1:T:104:ILE:H	1:T:104:ILE:HD12	1.75	0.51
1:C:103:ARG:HG3	1:C:238:ALA:HA	1.91	0.51
1:E:113:ASN:OD1	1:E:129:ALA:O	2.28	0.51
1:H:141:GLY:O	1:H:160:SER:HB3	2.10	0.51
1:K:213:ARG:NH1	1:T:1:MET:HE2	2.25	0.51
1:T:60:LYS:HE2	1:T:138:GLU:OE2	2.11	0.51
1:G:141:GLY:O	1:G:160:SER:HB3	2.10	0.51
1:K:103:ARG:HG3	1:K:238:ALA:HA	1.93	0.51
1:K:213:ARG:NH1	1:T:1:MET:HE3	2.26	0.51
1:S:104:ILE:HD12	1:S:104:ILE:H	1.74	0.51
1:F:60:LYS:HE2	1:F:138:GLU:OE2	2.11	0.51
1:G:60:LYS:HE3	1:G:159:ALA:O	2.10	0.51
1:C:113:ASN:OD1	1:C:129:ALA:HA	2.11	0.51
1:G:154:THR:CG2	1:G:160:SER:OG	2.59	0.51
1:K:131:GLU:HG2	1:K:132:TRP:CD1	2.45	0.51
1:M:60:LYS:HE2	1:M:138:GLU:OE2	2.10	0.51
1:N:60:LYS:HE2	1:N:138:GLU:OE2	2.10	0.51
1:T:131:GLU:HG2	1:T:132:TRP:CD1	2.46	0.51
1:J:113:ASN:OD1	1:J:129:ALA:C	2.49	0.50
1:K:60:LYS:HE2	1:K:138:GLU:OE2	2.11	0.50
1:N:131:GLU:HG2	1:N:132:TRP:CD1	2.45	0.50
1:F:104:ILE:CD1	1:F:245:PHE:CE2	2.93	0.50
1:D:113:ASN:OD1	1:D:129:ALA:O	2.29	0.50
1:C:114:ARG:CA	1:C:224:THR:HB	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:60:LYS:HE3	1:J:159:ALA:O	2.12	0.50
1:L:60:LYS:HE2	1:L:138:GLU:OE2	2.12	0.50
1:H:60:LYS:HE3	1:H:159:ALA:O	2.11	0.50
1:T:60:LYS:HE3	1:T:159:ALA:O	2.12	0.50
1:E:119:THR:OG1	1:M:0:LEU:HG	2.11	0.49
1:F:131:GLU:HG2	1:F:132:TRP:CD1	2.47	0.49
1:J:60:LYS:HE2	1:J:138:GLU:OE2	2.12	0.49
1:F:85:ASP:HA	1:N:1:MET:SD	2.51	0.49
1:P:131:GLU:HG2	1:P:132:TRP:CD1	2.46	0.49
1:Q:104:ILE:H	1:Q:104:ILE:HD12	1.77	0.49
1:C:60:LYS:HE2	1:C:138:GLU:OE2	2.12	0.49
1:G:131:GLU:HG2	1:G:132:TRP:CD1	2.47	0.49
1:G:103:ARG:HG3	1:G:238:ALA:HA	1.92	0.49
1:I:60:LYS:HE3	1:I:159:ALA:O	2.12	0.49
1:M:131:GLU:HG2	1:M:132:TRP:CD1	2.47	0.49
1:R:71:GLN:O	1:R:71:GLN:HG2	2.12	0.49
1:B:60:LYS:HE3	1:B:159:ALA:O	2.12	0.49
1:C:131:GLU:HG2	1:C:132:TRP:CD1	2.47	0.49
1:E:71:GLN:HG2	1:E:71:GLN:O	2.12	0.49
1:T:104:ILE:HD11	1:T:245:PHE:CZ	2.48	0.49
1:D:60:LYS:HE3	1:D:159:ALA:O	2.12	0.49
1:M:60:LYS:HE3	1:M:159:ALA:O	2.13	0.49
1:N:60:LYS:HE3	1:N:159:ALA:O	2.11	0.49
1:A:104:ILE:HD12	1:A:104:ILE:H	1.77	0.49
1:Q:103:ARG:HG3	1:Q:238:ALA:HA	1.95	0.49
1:R:180:ASN:HD22	1:R:196:ARG:HH21	1.61	0.49
1:B:213:ARG:NH1	1:F:1:MET:HE2	2.27	0.49
1:L:180:ASN:HD22	1:L:196:ARG:HH21	1.60	0.49
1:Q:114:ARG:CA	1:Q:224:THR:HB	2.40	0.49
1:L:141:GLY:O	1:L:160:SER:HB3	2.13	0.49
1:S:71:GLN:HG2	1:S:71:GLN:O	2.13	0.49
1:L:131:GLU:HG2	1:L:132:TRP:CD1	2.48	0.49
1:P:60:LYS:HE2	1:P:138:GLU:OE2	2.12	0.49
1:E:113:ASN:OD1	1:E:129:ALA:C	2.52	0.49
1:F:104:ILE:H	1:F:104:ILE:HD12	1.78	0.49
1:G:180:ASN:HD22	1:G:196:ARG:HH21	1.61	0.49
1:A:114:ARG:CA	1:A:224:THR:HB	2.41	0.48
1:I:141:GLY:O	1:I:160:SER:HB3	2.12	0.48
1:T:71:GLN:O	1:T:71:GLN:HG2	2.13	0.48
1:A:113:ASN:OD1	1:A:113:ASN:N	2.47	0.48
1:P:103:ARG:HG3	1:P:238:ALA:HA	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:60:LYS:HE2	1:G:138:GLU:OE2	2.12	0.48
1:H:60:LYS:HE2	1:H:138:GLU:OE2	2.14	0.48
1:O:180:ASN:HD22	1:O:196:ARG:HH21	1.61	0.48
1:A:137:LEU:HB2	1:A:165:VAL:HG13	1.96	0.48
1:D:60:LYS:HE2	1:D:138:GLU:OE2	2.12	0.48
1:H:131:GLU:HG2	1:H:132:TRP:CD1	2.48	0.48
1:J:141:GLY:O	1:J:160:SER:HB3	2.14	0.48
1:K:176:LEU:O	1:L:169:PRO:HB3	2.13	0.48
1:L:71:GLN:HG2	1:L:71:GLN:O	2.13	0.48
1:F:141:GLY:O	1:F:160:SER:HB3	2.14	0.48
1:G:71:GLN:O	1:G:71:GLN:HG2	2.13	0.48
1:E:113:ASN:OD1	1:E:113:ASN:N	2.47	0.48
1:O:60:LYS:HE2	1:O:138:GLU:OE2	2.13	0.48
1:Q:222:LEU:HD13	1:Q:228:ILE:HD11	1.96	0.48
1:R:131:GLU:HG2	1:R:132:TRP:CD1	2.49	0.48
1:B:222:LEU:HD13	1:B:228:ILE:HD11	1.94	0.48
1:H:71:GLN:O	1:H:71:GLN:HG2	2.13	0.48
1:K:71:GLN:HG2	1:K:71:GLN:O	2.14	0.48
1:L:60:LYS:HE3	1:L:159:ALA:O	2.13	0.48
1:Q:71:GLN:HG2	1:Q:71:GLN:O	2.12	0.48
1:J:71:GLN:HG2	1:J:71:GLN:O	2.14	0.48
1:L:104:ILE:HD11	1:L:245:PHE:CZ	2.48	0.48
1:R:141:GLY:O	1:R:160:SER:HB3	2.13	0.48
1:S:60:LYS:HE2	1:S:138:GLU:OE2	2.14	0.48
1:D:71:GLN:O	1:D:71:GLN:HG2	2.14	0.47
1:H:1:MET:CE	1:R:213:ARG:NH1	2.78	0.47
1:H:128:ASN:ND2	1:I:132:TRP:HE1	1.88	0.47
1:N:137:LEU:HB2	1:N:165:VAL:HG13	1.96	0.47
1:T:137:LEU:HB2	1:T:165:VAL:HG13	1.97	0.47
1:C:141:GLY:O	1:C:160:SER:HB3	2.14	0.47
1:H:137:LEU:HB2	1:H:165:VAL:HG13	1.96	0.47
1:I:103:ARG:HG3	1:I:238:ALA:HA	1.96	0.47
1:F:71:GLN:O	1:F:71:GLN:HG2	2.13	0.47
1:G:104:ILE:CD1	1:G:245:PHE:CE2	2.95	0.47
1:L:114:ARG:CA	1:L:224:THR:HB	2.41	0.47
1:E:213:ARG:NH1	1:M:1:MET:CE	2.77	0.47
1:O:71:GLN:O	1:O:71:GLN:HG2	2.13	0.47
1:F:114:ARG:CA	1:F:224:THR:HB	2.44	0.47
1:P:180:ASN:HD22	1:P:196:ARG:HH21	1.63	0.47
1:R:59:ARG:HB2	1:R:211:LEU:HD21	1.96	0.47
1:A:71:GLN:HG2	1:A:71:GLN:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:LYS:HE3	1:A:159:ALA:O	2.14	0.47
1:D:103:ARG:HG3	1:D:238:ALA:HA	1.96	0.47
1:I:71:GLN:HG2	1:I:71:GLN:O	2.14	0.47
1:K:59:ARG:HB2	1:K:211:LEU:HD21	1.97	0.47
1:T:0:LEU:HA	1:T:3:LYS:HB2	1.96	0.47
1:C:104:ILE:CD1	1:C:245:PHE:CE2	2.97	0.47
1:E:1:MET:HE2	1:M:213:ARG:HH11	1.80	0.47
1:I:1:MET:SD	1:K:85:ASP:HA	2.55	0.47
1:F:187:ARG:HB2	1:F:245:PHE:CE2	2.50	0.47
1:M:71:GLN:HG2	1:M:71:GLN:O	2.15	0.47
1:P:71:GLN:HG2	1:P:71:GLN:O	2.14	0.47
1:A:141:GLY:O	1:A:160:SER:HB3	2.15	0.46
1:B:213:ARG:HH11	1:F:1:MET:CE	2.27	0.46
1:G:137:LEU:HB2	1:G:165:VAL:HG13	1.96	0.46
1:B:213:ARG:HH11	1:F:1:MET:HE2	1.80	0.46
1:E:60:LYS:HE2	1:E:138:GLU:OE2	2.15	0.46
1:N:71:GLN:HG2	1:N:71:GLN:O	2.14	0.46
1:O:141:GLY:O	1:O:160:SER:HB3	2.16	0.46
1:J:113:ASN:OD1	1:J:129:ALA:O	2.33	0.46
1:B:71:GLN:O	1:B:71:GLN:HG2	2.15	0.46
1:A:135:PRO:HB2	1:A:255:VAL:HG22	1.97	0.46
1:O:103:ARG:HG3	1:O:238:ALA:HA	1.97	0.46
1:Q:60:LYS:HE2	1:Q:138:GLU:OE2	2.15	0.46
1:R:114:ARG:CA	1:R:224:THR:HB	2.45	0.46
1:T:180:ASN:HD22	1:T:196:ARG:HH21	1.64	0.46
1:I:180:ASN:HD22	1:I:196:ARG:HH21	1.62	0.46
1:M:141:GLY:O	1:M:160:SER:HB3	2.16	0.46
1:B:1:MET:HE2	1:F:213:ARG:NH1	2.30	0.46
1:H:90:ASP:HB2	1:H:167:GLY:HA2	1.98	0.46
1:K:141:GLY:O	1:K:160:SER:HB3	2.16	0.46
1:S:60:LYS:HE3	1:S:159:ALA:O	2.16	0.46
1:A:59:ARG:HB2	1:A:211:LEU:HD21	1.96	0.46
1:G:114:ARG:CA	1:G:224:THR:HB	2.42	0.45
1:J:103:ARG:HG3	1:J:238:ALA:HA	1.97	0.45
1:M:103:ARG:HG3	1:M:238:ALA:HA	1.97	0.45
1:L:59:ARG:HB2	1:L:211:LEU:HD21	1.98	0.45
1:N:180:ASN:HD22	1:N:196:ARG:HH21	1.63	0.45
1:Q:137:LEU:HB2	1:Q:165:VAL:HG13	1.98	0.45
1:B:103:ARG:HG3	1:B:238:ALA:HA	1.98	0.45
1:H:103:ARG:HG3	1:H:238:ALA:HA	1.98	0.45
1:K:137:LEU:HB2	1:K:165:VAL:HG13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:180:ASN:HD22	1:E:196:ARG:HH21	1.63	0.45
1:J:104:ILE:CD1	1:J:245:PHE:CE2	2.98	0.45
1:J:191:GLU:OE1	5:J:2011:HOH:O	2.21	0.45
1:P:90:ASP:HB2	1:P:167:GLY:HA2	1.99	0.45
1:T:141:GLY:O	1:T:160:SER:HB3	2.16	0.45
1:C:71:GLN:O	1:C:71:GLN:HG2	2.15	0.45
1:F:137:LEU:HB2	1:F:165:VAL:HG13	1.99	0.45
1:J:180:ASN:HD22	1:J:196:ARG:HH21	1.63	0.45
1:N:141:GLY:O	1:N:160:SER:HB3	2.16	0.45
1:Q:90:ASP:HB2	1:Q:167:GLY:HA2	1.99	0.45
1:R:60:LYS:HE2	1:R:138:GLU:OE2	2.16	0.45
1:D:141:GLY:O	1:D:160:SER:HB3	2.16	0.45
1:D:180:ASN:HD22	1:D:196:ARG:HH21	1.64	0.45
1:E:103:ARG:HG3	1:E:238:ALA:HA	1.98	0.45
1:B:137:LEU:HB2	1:B:165:VAL:HG13	1.97	0.45
1:O:90:ASP:HB2	1:O:167:GLY:HA2	1.99	0.45
1:T:222:LEU:HD13	1:T:228:ILE:HD11	1.98	0.45
1:B:180:ASN:HD22	1:B:196:ARG:HH21	1.64	0.45
1:D:114:ARG:CA	1:D:224:THR:HB	2.46	0.45
1:R:137:LEU:HB2	1:R:165:VAL:HG13	1.98	0.45
1:S:222:LEU:HD13	1:S:228:ILE:HD11	1.99	0.45
1:C:137:LEU:HB2	1:C:165:VAL:HG13	1.97	0.44
1:D:137:LEU:HB2	1:D:165:VAL:HG13	1.98	0.44
1:M:222:LEU:HD13	1:M:228:ILE:HD11	1.99	0.44
1:S:103:ARG:HG3	1:S:238:ALA:HA	1.99	0.44
1:A:90:ASP:HB2	1:A:167:GLY:HA2	1.99	0.44
1:G:187:ARG:HB2	1:G:245:PHE:CE2	2.51	0.44
1:R:222:LEU:HD13	1:R:228:ILE:HD11	2.00	0.44
1:S:141:GLY:O	1:S:160:SER:HB3	2.17	0.44
1:S:114:ARG:CA	1:S:224:THR:HB	2.43	0.44
1:B:135:PRO:HB2	1:B:255:VAL:HG22	2.00	0.44
1:J:137:LEU:HB2	1:J:165:VAL:HG13	2.00	0.44
1:E:141:GLY:O	1:E:160:SER:HB3	2.18	0.44
1:N:103:ARG:HG3	1:N:238:ALA:HA	2.00	0.44
1:G:222:LEU:HD13	1:G:228:ILE:HD11	1.99	0.44
1:J:222:LEU:HD13	1:J:228:ILE:HD11	1.99	0.44
1:N:90:ASP:HB2	1:N:167:GLY:HA2	1.98	0.44
1:O:135:PRO:HB2	1:O:255:VAL:HG22	2.00	0.44
1:T:114:ARG:CA	1:T:224:THR:HB	2.45	0.44
1:H:114:ARG:CA	1:H:224:THR:HB	2.46	0.44
1:K:114:ARG:CA	1:K:224:THR:HB	2.46	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:222:LEU:HD13	1:N:228:ILE:HD11	2.00	0.44
1:P:222:LEU:HD13	1:P:228:ILE:HD11	2.00	0.44
1:H:180:ASN:HD22	1:H:196:ARG:HH21	1.64	0.44
1:H:135:PRO:HB2	1:H:255:VAL:HG22	2.00	0.44
1:I:222:LEU:HD13	1:I:228:ILE:HD11	2.00	0.44
1:L:137:LEU:HB2	1:L:165:VAL:HG13	1.99	0.44
1:I:114:ARG:CA	1:I:224:THR:HB	2.44	0.44
1:I:0:LEU:HB3	1:N:120:ASP:HB3	1.98	0.44
1:N:114:ARG:CA	1:N:224:THR:HB	2.44	0.44
1:P:141:GLY:O	1:P:160:SER:HB3	2.17	0.44
1:H:113:ASN:ND2	1:H:129:ALA:HA	2.33	0.43
1:R:90:ASP:HB2	1:R:167:GLY:HA2	1.99	0.43
1:C:222:LEU:HD13	1:C:228:ILE:HD11	1.99	0.43
1:D:90:ASP:HB2	1:D:167:GLY:HA2	2.00	0.43
1:A:180:ASN:HD22	1:A:196:ARG:HH21	1.66	0.43
1:B:128:ASN:ND2	1:E:132:TRP:HE1	1.87	0.43
1:F:222:LEU:HD13	1:F:228:ILE:HD11	2.00	0.43
1:J:114:ARG:CA	1:J:224:THR:HB	2.45	0.43
1:O:137:LEU:HB2	1:O:165:VAL:HG13	1.99	0.43
1:Q:104:ILE:CD1	1:Q:245:PHE:CE2	3.00	0.43
1:L:60:LYS:NZ	2:L:1262:PO4:O2	2.51	0.43
1:Q:113:ASN:ND2	1:Q:129:ALA:HA	2.34	0.43
1:Q:141:GLY:O	1:Q:160:SER:HB3	2.17	0.43
1:S:180:ASN:HD22	1:S:196:ARG:HH21	1.66	0.43
1:I:113:ASN:ND2	1:I:129:ALA:HA	2.33	0.43
1:M:180:ASN:HD22	1:M:196:ARG:HH21	1.65	0.43
1:M:114:ARG:CA	1:M:224:THR:HB	2.46	0.43
1:O:59:ARG:HB2	1:O:211:LEU:HD21	2.01	0.43
1:Q:180:ASN:HD22	1:Q:196:ARG:HH21	1.67	0.43
1:I:120:ASP:HB3	1:N:0:LEU:HB3	1.99	0.43
1:J:164:TYR:HE2	1:J:166:ILE:CD1	2.32	0.43
1:K:180:ASN:HD22	1:K:196:ARG:HH21	1.66	0.43
1:R:104:ILE:HG13	1:R:239:VAL:CG2	2.49	0.43
1:B:59:ARG:HB2	1:B:211:LEU:HD21	2.00	0.43
1:D:222:LEU:HD13	1:D:228:ILE:HD11	1.99	0.43
1:L:222:LEU:HD13	1:L:228:ILE:HD11	2.01	0.43
1:S:59:ARG:HB2	1:S:211:LEU:HD21	2.01	0.43
1:T:135:PRO:HB2	1:T:255:VAL:HG22	2.01	0.43
1:B:141:GLY:O	1:B:160:SER:HB3	2.18	0.42
1:E:222:LEU:HD13	1:E:228:ILE:HD11	2.01	0.42
1:G:90:ASP:HB2	1:G:167:GLY:HA2	2.00	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:193:SER:HA	5:M:2008:HOH:O	2.19	0.42
1:R:164:TYR:HE2	1:R:166:ILE:CD1	2.32	0.42
1:S:137:LEU:HB2	1:S:165:VAL:HG13	2.00	0.42
1:L:90:ASP:HB2	1:L:167:GLY:HA2	2.01	0.42
1:N:104:ILE:HG13	1:N:239:VAL:CG2	2.49	0.42
1:M:90:ASP:HB2	1:M:167:GLY:HA2	2.02	0.42
1:T:187:ARG:HB2	1:T:245:PHE:CE2	2.55	0.42
1:B:167:GLY:HA3	1:B:255:VAL:HG13	2.02	0.42
1:I:90:ASP:HB2	1:I:167:GLY:HA2	2.01	0.42
1:E:1:MET:CE	1:M:213:ARG:HH11	2.33	0.42
1:F:15:ARG:NH1	2:F:1262:PO4:O3	2.53	0.42
1:R:103:ARG:HG3	1:R:238:ALA:HA	2.01	0.42
1:G:59:ARG:HB2	1:G:211:LEU:HD21	2.01	0.42
1:T:103:ARG:HG3	1:T:238:ALA:HA	2.01	0.42
1:B:90:ASP:HB2	1:B:167:GLY:HA2	2.02	0.42
1:G:71:GLN:O	1:G:72:LEU:HD12	2.20	0.42
1:I:137:LEU:HB2	1:I:165:VAL:HG13	2.02	0.42
1:K:90:ASP:HB2	1:K:167:GLY:HA2	2.01	0.42
1:C:180:ASN:HD22	1:C:196:ARG:HH21	1.67	0.42
1:E:59:ARG:HB2	1:E:211:LEU:HD21	2.01	0.42
1:G:104:ILE:HG13	1:G:239:VAL:CG2	2.50	0.42
1:H:222:LEU:HD13	1:H:228:ILE:HD11	2.02	0.42
1:S:135:PRO:HB2	1:S:255:VAL:HG22	2.02	0.42
1:F:180:ASN:HD22	1:F:196:ARG:HH21	1.68	0.42
1:J:59:ARG:HB2	1:J:211:LEU:HD21	2.01	0.42
1:O:114:ARG:CA	1:O:224:THR:HB	2.47	0.42
1:P:137:LEU:HB2	1:P:165:VAL:HG13	2.02	0.42
1:L:113:ASN:ND2	1:L:129:ALA:HA	2.35	0.41
1:O:222:LEU:HD13	1:O:228:ILE:HD11	2.02	0.41
1:E:90:ASP:HB2	1:E:167:GLY:HA2	2.02	0.41
1:I:59:ARG:HB2	1:I:211:LEU:HD21	2.02	0.41
1:R:71:GLN:O	1:R:72:LEU:HD12	2.20	0.41
1:Q:60:LYS:NZ	2:Q:1262:PO4:O2	2.53	0.41
1:E:137:LEU:HB2	1:E:165:VAL:HG13	2.02	0.41
1:M:137:LEU:HB2	1:M:165:VAL:HG13	2.03	0.41
1:M:135:PRO:HB2	1:M:255:VAL:HG22	2.03	0.41
1:C:135:PRO:HB2	1:C:255:VAL:HG22	2.03	0.41
1:I:167:GLY:HA3	1:I:255:VAL:HG13	2.03	0.41
1:P:113:ASN:ND2	1:P:129:ALA:HA	2.36	0.41
1:A:103:ARG:HG3	1:A:238:ALA:HA	2.02	0.41
1:E:114:ARG:CA	1:E:224:THR:HB	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:59:ARG:HB2	1:Q:211:LEU:HD21	2.03	0.41
1:F:164:TYR:HE2	1:F:166:ILE:CD1	2.34	0.41
1:C:193:SER:HA	5:C:2010:HOH:O	2.19	0.41
1:G:135:PRO:HB2	1:G:255:VAL:HG22	2.02	0.41
1:J:90:ASP:HB2	1:J:167:GLY:HA2	2.03	0.41
1:G:246:GLU:HG3	1:G:256:ALA:HB2	2.02	0.41
1:Q:135:PRO:HB2	1:Q:255:VAL:HG22	2.02	0.41
1:A:222:LEU:HD13	1:A:228:ILE:HD11	2.03	0.41
1:C:90:ASP:HB2	1:C:167:GLY:HA2	2.03	0.41
1:F:15:ARG:HD3	2:F:1262:PO4:O2	2.20	0.41
1:H:59:ARG:HB2	1:H:211:LEU:HD21	2.03	0.41
1:K:135:PRO:HB2	1:K:255:VAL:HG22	2.03	0.41
1:K:164:TYR:HE2	1:K:166:ILE:CD1	2.34	0.41
1:E:164:TYR:HE2	1:E:166:ILE:CD1	2.34	0.41
1:N:104:ILE:CD1	1:N:245:PHE:CE2	3.04	0.41
1:P:104:ILE:HG13	1:P:239:VAL:CG2	2.51	0.41
1:C:59:ARG:HB2	1:C:211:LEU:HD21	2.02	0.40
1:D:60:LYS:NZ	2:D:1263:PO4:O4	2.54	0.40
1:H:213:ARG:CZ	1:R:1:MET:HE2	2.51	0.40
1:M:113:ASN:ND2	1:M:129:ALA:HA	2.36	0.40
1:M:104:ILE:HG13	1:M:239:VAL:CG2	2.51	0.40
1:R:135:PRO:HB2	1:R:255:VAL:HG22	2.03	0.40
1:L:164:TYR:HE2	1:L:166:ILE:CD1	2.34	0.40
1:L:187:ARG:HB2	1:L:245:PHE:CE2	2.56	0.40
1:N:59:ARG:HB2	1:N:211:LEU:HD21	2.03	0.40
1:S:104:ILE:HG13	1:S:239:VAL:CG2	2.51	0.40
1:N:164:TYR:HE2	1:N:166:ILE:CD1	2.34	0.40
1:A:164:TYR:HE2	1:A:166:ILE:CD1	2.34	0.40
1:G:15:ARG:HD3	2:G:1262:PO4:O2	2.22	0.40
1:L:0:LEU:HD22	1:L:3:LYS:HD2	2.03	0.40
1:P:59:ARG:HB2	1:P:211:LEU:HD21	2.04	0.40
1:C:164:TYR:HE2	1:C:166:ILE:CD1	2.34	0.40
1:E:213:ARG:NH1	1:M:1:MET:HE3	2.37	0.40
1:H:164:TYR:HE2	1:H:166:ILE:CD1	2.33	0.40
1:K:113:ASN:ND2	1:K:129:ALA:HA	2.37	0.40
1:K:222:LEU:HD13	1:K:228:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	260/270 (96%)	250 (96%)	9 (4%)	1 (0%)	34	66
1	B	260/270 (96%)	250 (96%)	9 (4%)	1 (0%)	34	66
1	C	260/270 (96%)	253 (97%)	5 (2%)	2 (1%)	19	49
1	D	260/270 (96%)	251 (96%)	7 (3%)	2 (1%)	19	49
1	E	260/270 (96%)	252 (97%)	7 (3%)	1 (0%)	34	66
1	F	260/270 (96%)	251 (96%)	8 (3%)	1 (0%)	34	66
1	G	260/270 (96%)	251 (96%)	7 (3%)	2 (1%)	19	49
1	H	260/270 (96%)	252 (97%)	7 (3%)	1 (0%)	34	66
1	I	260/270 (96%)	251 (96%)	8 (3%)	1 (0%)	34	66
1	J	260/270 (96%)	252 (97%)	6 (2%)	2 (1%)	19	49
1	K	260/270 (96%)	251 (96%)	8 (3%)	1 (0%)	34	66
1	L	260/270 (96%)	251 (96%)	8 (3%)	1 (0%)	34	66
1	M	260/270 (96%)	252 (97%)	6 (2%)	2 (1%)	19	49
1	N	260/270 (96%)	252 (97%)	7 (3%)	1 (0%)	34	66
1	O	260/270 (96%)	251 (96%)	8 (3%)	1 (0%)	34	66
1	P	260/270 (96%)	251 (96%)	7 (3%)	2 (1%)	19	49
1	Q	260/270 (96%)	252 (97%)	7 (3%)	1 (0%)	34	66
1	R	260/270 (96%)	251 (96%)	7 (3%)	2 (1%)	19	49
1	S	260/270 (96%)	253 (97%)	6 (2%)	1 (0%)	34	66
1	T	260/270 (96%)	252 (97%)	7 (3%)	1 (0%)	34	66
All	All	5200/5400 (96%)	5029 (97%)	144 (3%)	27 (0%)	29	61

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	260	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	260	SER
1	A	77	PRO
1	C	260	SER
1	D	260	SER
1	F	77	PRO
1	G	77	PRO
1	H	77	PRO
1	I	77	PRO
1	L	77	PRO
1	M	260	SER
1	N	77	PRO
1	P	260	SER
1	R	77	PRO
1	R	260	SER
1	S	77	PRO
1	B	77	PRO
1	C	77	PRO
1	D	77	PRO
1	E	77	PRO
1	J	77	PRO
1	K	77	PRO
1	M	77	PRO
1	O	77	PRO
1	P	77	PRO
1	Q	77	PRO
1	T	77	PRO

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	207/212 (98%)	180 (87%)	27 (13%)	4	13
1	B	207/212 (98%)	180 (87%)	27 (13%)	4	13
1	C	207/212 (98%)	182 (88%)	25 (12%)	5	15
1	D	207/212 (98%)	181 (87%)	26 (13%)	4	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	207/212 (98%)	181 (87%)	26 (13%)	4	14
1	F	207/212 (98%)	180 (87%)	27 (13%)	4	13
1	G	207/212 (98%)	180 (87%)	27 (13%)	4	13
1	H	207/212 (98%)	182 (88%)	25 (12%)	5	15
1	I	207/212 (98%)	183 (88%)	24 (12%)	5	17
1	J	207/212 (98%)	181 (87%)	26 (13%)	4	14
1	K	207/212 (98%)	181 (87%)	26 (13%)	4	14
1	L	207/212 (98%)	182 (88%)	25 (12%)	5	15
1	M	207/212 (98%)	182 (88%)	25 (12%)	5	15
1	N	207/212 (98%)	182 (88%)	25 (12%)	5	15
1	O	207/212 (98%)	182 (88%)	25 (12%)	5	15
1	P	207/212 (98%)	181 (87%)	26 (13%)	4	14
1	Q	207/212 (98%)	182 (88%)	25 (12%)	5	15
1	R	207/212 (98%)	181 (87%)	26 (13%)	4	14
1	S	207/212 (98%)	180 (87%)	27 (13%)	4	13
1	T	207/212 (98%)	182 (88%)	25 (12%)	5	15
All	All	4140/4240 (98%)	3625 (88%)	515 (12%)	4	14

All (515) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	LEU
1	A	1	MET
1	A	6	LEU
1	A	13	LEU
1	A	26	LEU
1	A	28	ASP
1	A	60	LYS
1	A	74	VAL
1	A	91	ASN
1	A	104	ILE
1	A	113	ASN
1	A	114	ARG
1	A	127	TYR
1	A	133	VAL
1	A	134	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	143	ARG
1	A	149	ILE
1	A	152	VAL
1	A	154	THR
1	A	160	SER
1	A	165	VAL
1	A	191	GLU
1	A	214	LYS
1	A	218	LEU
1	A	224	THR
1	A	237	VAL
1	A	255	VAL
1	B	0	LEU
1	B	1	MET
1	B	6	LEU
1	B	13	LEU
1	B	26	LEU
1	B	28	ASP
1	B	60	LYS
1	B	74	VAL
1	B	91	ASN
1	B	104	ILE
1	B	113	ASN
1	B	114	ARG
1	B	127	TYR
1	B	133	VAL
1	B	134	LEU
1	B	143	ARG
1	B	149	ILE
1	B	152	VAL
1	B	154	THR
1	B	160	SER
1	B	165	VAL
1	B	191	GLU
1	B	214	LYS
1	B	218	LEU
1	B	224	THR
1	B	237	VAL
1	B	255	VAL
1	C	1	MET
1	C	6	LEU
1	C	13	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	26	LEU
1	C	28	ASP
1	C	60	LYS
1	C	74	VAL
1	C	91	ASN
1	C	104	ILE
1	C	113	ASN
1	C	114	ARG
1	C	127	TYR
1	C	133	VAL
1	C	134	LEU
1	C	143	ARG
1	C	149	ILE
1	C	152	VAL
1	C	154	THR
1	C	160	SER
1	C	165	VAL
1	C	214	LYS
1	C	218	LEU
1	C	224	THR
1	C	237	VAL
1	C	255	VAL
1	D	1	MET
1	D	6	LEU
1	D	13	LEU
1	D	26	LEU
1	D	28	ASP
1	D	47	GLN
1	D	60	LYS
1	D	74	VAL
1	D	91	ASN
1	D	104	ILE
1	D	113	ASN
1	D	114	ARG
1	D	127	TYR
1	D	133	VAL
1	D	134	LEU
1	D	143	ARG
1	D	149	ILE
1	D	152	VAL
1	D	154	THR
1	D	165	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	191	GLU
1	D	214	LYS
1	D	218	LEU
1	D	224	THR
1	D	237	VAL
1	D	255	VAL
1	E	1	MET
1	E	6	LEU
1	E	13	LEU
1	E	26	LEU
1	E	28	ASP
1	E	60	LYS
1	E	74	VAL
1	E	91	ASN
1	E	104	ILE
1	E	113	ASN
1	E	114	ARG
1	E	127	TYR
1	E	133	VAL
1	E	134	LEU
1	E	143	ARG
1	E	149	ILE
1	E	152	VAL
1	E	154	THR
1	E	160	SER
1	E	165	VAL
1	E	191	GLU
1	E	214	LYS
1	E	218	LEU
1	E	224	THR
1	E	237	VAL
1	E	255	VAL
1	F	1	MET
1	F	6	LEU
1	F	13	LEU
1	F	26	LEU
1	F	28	ASP
1	F	60	LYS
1	F	74	VAL
1	F	91	ASN
1	F	104	ILE
1	F	113	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	114	ARG
1	F	127	TYR
1	F	133	VAL
1	F	134	LEU
1	F	143	ARG
1	F	149	ILE
1	F	152	VAL
1	F	154	THR
1	F	165	VAL
1	F	191	GLU
1	F	192	VAL
1	F	214	LYS
1	F	218	LEU
1	F	224	THR
1	F	237	VAL
1	F	244	ARG
1	F	255	VAL
1	G	0	LEU
1	G	6	LEU
1	G	13	LEU
1	G	26	LEU
1	G	28	ASP
1	G	60	LYS
1	G	74	VAL
1	G	91	ASN
1	G	104	ILE
1	G	113	ASN
1	G	114	ARG
1	G	127	TYR
1	G	133	VAL
1	G	134	LEU
1	G	143	ARG
1	G	149	ILE
1	G	152	VAL
1	G	154	THR
1	G	160	SER
1	G	165	VAL
1	G	184	LYS
1	G	191	GLU
1	G	214	LYS
1	G	218	LEU
1	G	224	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	237	VAL
1	G	255	VAL
1	H	6	LEU
1	H	13	LEU
1	H	26	LEU
1	H	28	ASP
1	H	60	LYS
1	H	74	VAL
1	H	91	ASN
1	H	104	ILE
1	H	113	ASN
1	H	114	ARG
1	H	127	TYR
1	H	133	VAL
1	H	134	LEU
1	H	143	ARG
1	H	149	ILE
1	H	152	VAL
1	H	154	THR
1	H	160	SER
1	H	165	VAL
1	H	191	GLU
1	H	214	LYS
1	H	218	LEU
1	H	224	THR
1	H	237	VAL
1	H	255	VAL
1	I	6	LEU
1	I	13	LEU
1	I	26	LEU
1	I	28	ASP
1	I	60	LYS
1	I	74	VAL
1	I	91	ASN
1	I	104	ILE
1	I	113	ASN
1	I	114	ARG
1	I	127	TYR
1	I	133	VAL
1	I	134	LEU
1	I	143	ARG
1	I	152	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	154	THR
1	I	160	SER
1	I	165	VAL
1	I	191	GLU
1	I	214	LYS
1	I	218	LEU
1	I	224	THR
1	I	237	VAL
1	I	255	VAL
1	J	0	LEU
1	J	6	LEU
1	J	13	LEU
1	J	26	LEU
1	J	28	ASP
1	J	60	LYS
1	J	74	VAL
1	J	91	ASN
1	J	104	ILE
1	J	113	ASN
1	J	114	ARG
1	J	127	TYR
1	J	133	VAL
1	J	134	LEU
1	J	143	ARG
1	J	149	ILE
1	J	152	VAL
1	J	154	THR
1	J	160	SER
1	J	165	VAL
1	J	191	GLU
1	J	214	LYS
1	J	218	LEU
1	J	224	THR
1	J	237	VAL
1	J	255	VAL
1	K	0	LEU
1	K	6	LEU
1	K	13	LEU
1	K	26	LEU
1	K	28	ASP
1	K	60	LYS
1	K	74	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	91	ASN
1	K	104	ILE
1	K	113	ASN
1	K	114	ARG
1	K	127	TYR
1	K	133	VAL
1	K	134	LEU
1	K	143	ARG
1	K	149	ILE
1	K	152	VAL
1	K	154	THR
1	K	160	SER
1	K	165	VAL
1	K	191	GLU
1	K	214	LYS
1	K	218	LEU
1	K	224	THR
1	K	237	VAL
1	K	255	VAL
1	L	1	MET
1	L	6	LEU
1	L	13	LEU
1	L	26	LEU
1	L	28	ASP
1	L	60	LYS
1	L	74	VAL
1	L	91	ASN
1	L	104	ILE
1	L	113	ASN
1	L	114	ARG
1	L	127	TYR
1	L	133	VAL
1	L	134	LEU
1	L	143	ARG
1	L	149	ILE
1	L	152	VAL
1	L	154	THR
1	L	160	SER
1	L	165	VAL
1	L	214	LYS
1	L	218	LEU
1	L	224	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	237	VAL
1	L	255	VAL
1	M	0	LEU
1	M	6	LEU
1	M	13	LEU
1	M	26	LEU
1	M	28	ASP
1	M	60	LYS
1	M	74	VAL
1	M	91	ASN
1	M	104	ILE
1	M	113	ASN
1	M	114	ARG
1	M	127	TYR
1	M	133	VAL
1	M	134	LEU
1	M	143	ARG
1	M	149	ILE
1	M	152	VAL
1	M	154	THR
1	M	165	VAL
1	M	191	GLU
1	M	214	LYS
1	M	218	LEU
1	M	224	THR
1	M	237	VAL
1	M	255	VAL
1	N	6	LEU
1	N	13	LEU
1	N	26	LEU
1	N	28	ASP
1	N	60	LYS
1	N	74	VAL
1	N	91	ASN
1	N	104	ILE
1	N	113	ASN
1	N	114	ARG
1	N	127	TYR
1	N	133	VAL
1	N	134	LEU
1	N	143	ARG
1	N	149	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	N	152	VAL
1	N	154	THR
1	N	160	SER
1	N	165	VAL
1	N	191	GLU
1	N	214	LYS
1	N	218	LEU
1	N	224	THR
1	N	237	VAL
1	N	255	VAL
1	O	6	LEU
1	O	13	LEU
1	O	26	LEU
1	O	28	ASP
1	O	60	LYS
1	O	74	VAL
1	O	91	ASN
1	O	104	ILE
1	O	113	ASN
1	O	114	ARG
1	O	127	TYR
1	O	133	VAL
1	O	134	LEU
1	O	143	ARG
1	O	149	ILE
1	O	152	VAL
1	O	154	THR
1	O	160	SER
1	O	165	VAL
1	O	191	GLU
1	O	214	LYS
1	O	218	LEU
1	O	224	THR
1	O	237	VAL
1	O	255	VAL
1	P	0	LEU
1	P	6	LEU
1	P	13	LEU
1	P	26	LEU
1	P	28	ASP
1	P	60	LYS
1	P	74	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	P	91	ASN
1	P	104	ILE
1	P	113	ASN
1	P	114	ARG
1	P	127	TYR
1	P	133	VAL
1	P	134	LEU
1	P	143	ARG
1	P	149	ILE
1	P	152	VAL
1	P	154	THR
1	P	160	SER
1	P	165	VAL
1	P	191	GLU
1	P	214	LYS
1	P	218	LEU
1	P	224	THR
1	P	237	VAL
1	P	255	VAL
1	Q	0	LEU
1	Q	6	LEU
1	Q	13	LEU
1	Q	26	LEU
1	Q	28	ASP
1	Q	60	LYS
1	Q	74	VAL
1	Q	91	ASN
1	Q	104	ILE
1	Q	113	ASN
1	Q	114	ARG
1	Q	127	TYR
1	Q	133	VAL
1	Q	134	LEU
1	Q	149	ILE
1	Q	152	VAL
1	Q	154	THR
1	Q	160	SER
1	Q	165	VAL
1	Q	191	GLU
1	Q	214	LYS
1	Q	218	LEU
1	Q	224	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	Q	237	VAL
1	Q	255	VAL
1	R	0	LEU
1	R	1	MET
1	R	6	LEU
1	R	13	LEU
1	R	26	LEU
1	R	28	ASP
1	R	60	LYS
1	R	74	VAL
1	R	91	ASN
1	R	104	ILE
1	R	113	ASN
1	R	114	ARG
1	R	127	TYR
1	R	133	VAL
1	R	134	LEU
1	R	143	ARG
1	R	149	ILE
1	R	152	VAL
1	R	154	THR
1	R	165	VAL
1	R	191	GLU
1	R	214	LYS
1	R	218	LEU
1	R	224	THR
1	R	237	VAL
1	R	255	VAL
1	S	0	LEU
1	S	1	MET
1	S	6	LEU
1	S	13	LEU
1	S	26	LEU
1	S	28	ASP
1	S	60	LYS
1	S	74	VAL
1	S	91	ASN
1	S	104	ILE
1	S	113	ASN
1	S	114	ARG
1	S	127	TYR
1	S	133	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S	134	LEU
1	S	143	ARG
1	S	149	ILE
1	S	152	VAL
1	S	154	THR
1	S	160	SER
1	S	165	VAL
1	S	191	GLU
1	S	214	LYS
1	S	218	LEU
1	S	224	THR
1	S	237	VAL
1	S	255	VAL
1	T	6	LEU
1	T	13	LEU
1	T	26	LEU
1	T	28	ASP
1	T	47	GLN
1	T	60	LYS
1	T	74	VAL
1	T	91	ASN
1	T	104	ILE
1	T	113	ASN
1	T	114	ARG
1	T	127	TYR
1	T	133	VAL
1	T	134	LEU
1	T	143	ARG
1	T	149	ILE
1	T	152	VAL
1	T	154	THR
1	T	165	VAL
1	T	191	GLU
1	T	214	LYS
1	T	218	LEU
1	T	224	THR
1	T	237	VAL
1	T	255	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (99) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	91	ASN
1	A	128	ASN
1	A	180	ASN
1	B	69	GLN
1	B	91	ASN
1	B	128	ASN
1	B	180	ASN
1	C	19	GLN
1	C	69	GLN
1	C	91	ASN
1	C	128	ASN
1	C	180	ASN
1	D	69	GLN
1	D	91	ASN
1	D	128	ASN
1	D	180	ASN
1	E	69	GLN
1	E	91	ASN
1	E	128	ASN
1	E	180	ASN
1	F	69	GLN
1	F	91	ASN
1	F	113	ASN
1	F	128	ASN
1	G	69	GLN
1	G	91	ASN
1	G	113	ASN
1	G	128	ASN
1	G	180	ASN
1	H	19	GLN
1	H	69	GLN
1	H	91	ASN
1	H	113	ASN
1	H	128	ASN
1	H	180	ASN
1	I	69	GLN
1	I	91	ASN
1	I	113	ASN
1	I	128	ASN
1	I	180	ASN
1	J	19	GLN
1	J	69	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	91	ASN
1	J	128	ASN
1	J	180	ASN
1	K	69	GLN
1	K	91	ASN
1	K	113	ASN
1	K	128	ASN
1	K	180	ASN
1	L	69	GLN
1	L	91	ASN
1	L	113	ASN
1	L	128	ASN
1	L	180	ASN
1	M	19	GLN
1	M	69	GLN
1	M	91	ASN
1	M	113	ASN
1	M	128	ASN
1	M	180	ASN
1	N	69	GLN
1	N	91	ASN
1	N	113	ASN
1	N	128	ASN
1	N	180	ASN
1	O	19	GLN
1	O	69	GLN
1	O	91	ASN
1	O	113	ASN
1	O	128	ASN
1	O	180	ASN
1	P	69	GLN
1	P	91	ASN
1	P	113	ASN
1	P	128	ASN
1	P	180	ASN
1	Q	69	GLN
1	Q	91	ASN
1	Q	113	ASN
1	Q	128	ASN
1	Q	180	ASN
1	R	69	GLN
1	R	91	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	R	113	ASN
1	R	128	ASN
1	R	180	ASN
1	S	19	GLN
1	S	69	GLN
1	S	91	ASN
1	S	113	ASN
1	S	128	ASN
1	S	180	ASN
1	T	69	GLN
1	T	91	ASN
1	T	113	ASN
1	T	128	ASN
1	T	180	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 78 ligands modelled in this entry, 40 are monoatomic - leaving 38 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	PO4	P	1264	-	4,4,4	1.30	1 (25%)	6,6,6	0.41	0
2	PO4	H	1262	-	4,4,4	0.87	0	6,6,6	0.62	0
2	PO4	A	1262	-	4,4,4	0.89	0	6,6,6	0.60	0
2	PO4	D	1262	-	4,4,4	0.92	0	6,6,6	0.41	0
2	PO4	C	1262	-	4,4,4	0.84	0	6,6,6	0.60	0
2	PO4	J	1262	-	4,4,4	0.92	0	6,6,6	0.46	0
2	PO4	I	1262	-	4,4,4	0.81	0	6,6,6	0.47	0
2	PO4	L	1262	-	4,4,4	0.97	0	6,6,6	0.61	0
2	PO4	A	1263	-	4,4,4	1.04	0	6,6,6	0.48	0
2	PO4	R	1262	-	4,4,4	0.94	0	6,6,6	0.54	0
2	PO4	G	1263	-	4,4,4	0.98	0	6,6,6	0.68	0
2	PO4	G	1262	-	4,4,4	0.83	0	6,6,6	0.58	0
2	PO4	B	1262	-	4,4,4	1.08	0	6,6,6	0.51	0
2	PO4	M	1262	-	4,4,4	0.91	0	6,6,6	0.47	0
2	PO4	F	1264	-	4,4,4	0.86	0	6,6,6	0.67	0
2	PO4	O	1262	-	4,4,4	0.99	0	6,6,6	0.62	0
2	PO4	B	1263	-	4,4,4	0.91	0	6,6,6	0.55	0
2	PO4	H	1263	-	4,4,4	0.93	0	6,6,6	0.44	0
2	PO4	T	1262	-	4,4,4	0.85	0	6,6,6	0.46	0
2	PO4	J	1263	-	4,4,4	0.82	0	6,6,6	0.60	0
2	PO4	P	1263	-	4,4,4	0.95	0	6,6,6	0.61	0
2	PO4	F	1262	-	4,4,4	0.82	0	6,6,6	0.67	0
2	PO4	E	1262	-	4,4,4	0.85	0	6,6,6	0.68	0
2	PO4	Q	1263	-	4,4,4	0.94	0	6,6,6	0.43	0
2	PO4	N	1262	-	4,4,4	0.90	0	6,6,6	0.53	0
2	PO4	K	1264	-	4,4,4	0.93	0	6,6,6	0.48	0
2	PO4	G	1264	-	4,4,4	0.87	0	6,6,6	0.56	0
2	PO4	Q	1264	-	4,4,4	0.72	0	6,6,6	0.73	0
2	PO4	K	1263	-	4,4,4	0.80	0	6,6,6	0.48	0
2	PO4	D	1263	-	4,4,4	0.85	0	6,6,6	0.55	0
2	PO4	P	1262	-	4,4,4	0.89	0	6,6,6	0.42	0
2	PO4	F	1263	-	4,4,4	0.96	0	6,6,6	0.47	0
2	PO4	K	1262	-	4,4,4	0.78	0	6,6,6	0.52	0
2	PO4	L	1263	-	4,4,4	1.04	0	6,6,6	0.50	0
2	PO4	A	1264	-	4,4,4	0.80	0	6,6,6	0.59	0
2	PO4	D	1264	-	4,4,4	0.87	0	6,6,6	0.41	0
2	PO4	Q	1262	-	4,4,4	0.88	0	6,6,6	0.55	0
2	PO4	S	1262	-	4,4,4	0.74	0	6,6,6	0.71	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	P	1264	PO4	P-O1	2.30	1.56	1.50

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

13 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	1262	PO4	1	0
2	R	1262	PO4	1	0
2	G	1263	PO4	1	0
2	G	1262	PO4	1	0
2	B	1263	PO4	1	0
2	T	1262	PO4	1	0
2	P	1263	PO4	1	0
2	F	1262	PO4	2	0
2	E	1262	PO4	1	0
2	K	1264	PO4	1	0
2	D	1263	PO4	1	0
2	A	1264	PO4	1	0
2	Q	1262	PO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	262/270 (97%)	-0.22	5 (1%) 66 59	23, 33, 53, 71	0
1	B	262/270 (97%)	-0.23	4 (1%) 73 68	23, 33, 53, 71	0
1	C	262/270 (97%)	-0.24	3 (1%) 80 75	23, 33, 53, 71	0
1	D	262/270 (97%)	-0.31	6 (2%) 60 51	23, 33, 53, 71	0
1	E	262/270 (97%)	-0.15	5 (1%) 66 59	23, 33, 53, 71	0
1	F	262/270 (97%)	-0.19	4 (1%) 73 68	23, 33, 53, 71	0
1	G	262/270 (97%)	-0.19	5 (1%) 66 59	23, 33, 53, 71	0
1	H	262/270 (97%)	-0.20	5 (1%) 66 59	23, 33, 53, 71	0
1	I	262/270 (97%)	-0.20	6 (2%) 60 51	23, 33, 53, 71	0
1	J	262/270 (97%)	-0.19	8 (3%) 49 39	23, 33, 53, 71	0
1	K	262/270 (97%)	-0.26	3 (1%) 80 75	23, 33, 53, 71	0
1	L	262/270 (97%)	-0.19	6 (2%) 60 51	23, 33, 53, 71	0
1	M	262/270 (97%)	-0.23	8 (3%) 49 39	23, 33, 53, 71	0
1	N	262/270 (97%)	-0.16	6 (2%) 60 51	23, 33, 53, 71	0
1	O	262/270 (97%)	-0.21	3 (1%) 80 75	23, 33, 53, 71	0
1	P	262/270 (97%)	-0.16	9 (3%) 45 35	23, 33, 53, 71	0
1	Q	262/270 (97%)	-0.26	3 (1%) 80 75	23, 33, 53, 71	0
1	R	262/270 (97%)	-0.20	7 (2%) 54 44	23, 33, 53, 71	0
1	S	262/270 (97%)	-0.21	5 (1%) 66 59	23, 33, 53, 71	0
1	T	262/270 (97%)	-0.22	7 (2%) 54 44	23, 33, 53, 71	0
All	All	5240/5400 (97%)	-0.21	108 (2%) 63 54	23, 33, 53, 71	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	70	GLN	4.8
1	R	70	GLN	4.8
1	E	70	GLN	4.7
1	P	70	GLN	4.5
1	O	0	LEU	4.4
1	M	70	GLN	4.4
1	L	70	GLN	4.2
1	C	70	GLN	4.2
1	O	70	GLN	4.1
1	F	70	GLN	4.1
1	B	70	GLN	4.0
1	I	70	GLN	3.8
1	T	70	GLN	3.7
1	P	1	MET	3.7
1	J	70	GLN	3.7
1	G	67	LYS	3.6
1	D	70	GLN	3.5
1	G	71	GLN	3.5
1	K	70	GLN	3.3
1	P	71	GLN	3.2
1	G	73	GLY	3.2
1	S	70	GLN	3.2
1	A	190	GLU	3.2
1	M	190	GLU	3.1
1	R	67	LYS	3.1
1	H	70	GLN	3.1
1	G	70	GLN	3.1
1	R	73	GLY	3.1
1	P	190	GLU	3.1
1	R	190	GLU	3.1
1	O	73	GLY	3.0
1	T	189	ASN	2.9
1	T	190	GLU	2.9
1	Q	70	GLN	2.9
1	K	0	LEU	2.8
1	C	1	MET	2.8
1	N	1	MET	2.8
1	I	71	GLN	2.8
1	F	67	LYS	2.8
1	A	71	GLN	2.8
1	E	75	ASP	2.7
1	T	146	ASP	2.7
1	B	71	GLN	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	R	28	ASP	2.7
1	N	70	GLN	2.7
1	P	67	LYS	2.7
1	E	1	MET	2.6
1	I	67	LYS	2.6
1	K	71	GLN	2.6
1	H	67	LYS	2.6
1	N	190	GLU	2.6
1	M	67	LYS	2.6
1	F	71	GLN	2.5
1	S	1	MET	2.5
1	D	0	LEU	2.5
1	B	190	GLU	2.5
1	P	0	LEU	2.5
1	I	146	ASP	2.5
1	N	67	LYS	2.5
1	E	0	LEU	2.5
1	D	190	GLU	2.4
1	L	67	LYS	2.4
1	G	32	ILE	2.4
1	S	71	GLN	2.3
1	B	67	LYS	2.3
1	M	73	GLY	2.3
1	P	73	GLY	2.3
1	Q	146	ASP	2.3
1	H	190	GLU	2.3
1	J	32	ILE	2.3
1	L	146	ASP	2.3
1	A	1	MET	2.3
1	L	71	GLN	2.3
1	P	75	ASP	2.3
1	R	71	GLN	2.3
1	S	190	GLU	2.3
1	D	1	MET	2.3
1	S	0	LEU	2.3
1	N	189	ASN	2.2
1	C	0	LEU	2.2
1	I	72	LEU	2.2
1	N	0	LEU	2.2
1	M	0	LEU	2.2
1	E	190	GLU	2.2
1	T	71	GLN	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	71	GLN	2.2
1	H	189	ASN	2.2
1	M	32	ILE	2.2
1	T	1	MET	2.2
1	J	189	ASN	2.2
1	J	67	LYS	2.2
1	I	0	LEU	2.2
1	P	72	LEU	2.2
1	R	0	LEU	2.1
1	M	1	MET	2.1
1	A	67	LYS	2.1
1	J	146	ASP	2.1
1	D	189	ASN	2.1
1	M	33	ASP	2.1
1	H	33	ASP	2.1
1	D	32	ILE	2.1
1	F	32	ILE	2.1
1	L	32	ILE	2.1
1	T	33	ASP	2.1
1	J	190	GLU	2.0
1	Q	0	LEU	2.0
1	L	1	MET	2.0
1	J	188	ASN	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. 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.

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	NA	I	1306	1/1	0.87	0.26	32,32,32,32	0
2	PO4	B	1263	5/5	0.89	0.19	73,73,73,73	0
3	NA	F	1312	1/1	0.90	0.32	26,26,26,26	0
3	NA	Q	1302	1/1	0.91	0.23	11,11,11,11	0
3	NA	G	1313	1/1	0.92	0.43	18,18,18,18	0
2	PO4	D	1263	5/5	0.92	0.18	62,63,64,64	0
4	K	N	1263	1/1	0.93	0.21	46,46,46,46	0
2	PO4	M	1262	5/5	0.93	0.15	56,56,57,57	0
3	NA	M	1307	1/1	0.94	0.34	31,31,31,31	0
4	K	I	1263	1/1	0.94	0.23	57,57,57,57	0
2	PO4	R	1262	5/5	0.94	0.15	61,61,62,62	0
2	PO4	I	1262	5/5	0.94	0.12	55,55,56,56	0
2	PO4	F	1264	5/5	0.94	0.16	45,46,46,47	0
2	PO4	Q	1264	5/5	0.94	0.23	52,52,52,53	0
4	K	Q	1416	1/1	0.94	0.22	46,46,46,46	0
2	PO4	L	1262	5/5	0.94	0.14	42,43,44,44	0
2	PO4	A	1264	5/5	0.94	0.16	53,53,53,53	0
3	NA	L	1314	1/1	0.95	0.40	21,21,21,21	0
2	PO4	J	1263	5/5	0.95	0.13	54,55,55,55	0
2	PO4	O	1262	5/5	0.95	0.15	53,53,54,54	0
3	NA	P	1317	1/1	0.95	0.41	19,19,19,19	0
3	NA	N	1315	1/1	0.95	0.41	24,24,24,24	0
2	PO4	H	1263	5/5	0.95	0.18	53,53,54,54	0
3	NA	A	1265	1/1	0.96	0.34	22,22,22,22	0
2	PO4	B	1262	5/5	0.96	0.18	54,54,55,55	0
3	NA	L	1319	1/1	0.96	0.30	18,18,18,18	0
4	K	Q	1412	1/1	0.96	0.16	40,40,40,40	0
2	PO4	K	1264	5/5	0.96	0.14	42,43,44,44	0
2	PO4	C	1262	5/5	0.96	0.13	52,53,53,53	0
2	PO4	T	1262	5/5	0.96	0.14	57,58,58,58	0
3	NA	T	1303	1/1	0.96	0.25	29,29,29,29	0
2	PO4	K	1263	5/5	0.96	0.23	65,65,65,65	0
4	K	F	1265	1/1	0.96	0.22	47,47,47,47	0
3	NA	O	1301	1/1	0.96	0.32	26,26,26,26	0
2	PO4	F	1263	5/5	0.96	0.24	69,69,69,69	0
2	PO4	P	1263	5/5	0.96	0.16	65,65,66,66	0
2	PO4	S	1262	5/5	0.96	0.11	53,53,53,54	0
4	K	T	1263	1/1	0.97	0.19	42,42,42,42	0
2	PO4	D	1262	5/5	0.97	0.09	52,52,52,52	5
4	K	A	1401	1/1	0.97	0.14	42,42,42,42	0
3	NA	R	1318	1/1	0.97	0.27	15,15,15,15	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PO4	G	1264	5/5	0.97	0.24	55,55,56,56	0
2	PO4	Q	1263	5/5	0.97	0.18	57,57,57,57	0
4	K	A	1266	1/1	0.97	0.21	49,49,49,49	0
4	K	S	1413	1/1	0.97	0.22	47,47,47,47	0
3	NA	S	1320	1/1	0.97	0.41	27,27,27,27	0
3	NA	K	1305	1/1	0.97	0.28	21,21,21,21	0
4	K	G	1265	1/1	0.97	0.22	43,43,43,43	0
2	PO4	G	1263	5/5	0.97	0.10	48,48,50,50	0
2	PO4	N	1262	5/5	0.97	0.13	57,58,59,59	0
2	PO4	L	1263	5/5	0.97	0.19	53,54,54,54	0
4	K	G	1408	1/1	0.97	0.23	39,39,39,39	0
2	PO4	D	1264	5/5	0.97	0.25	47,47,48,48	5
2	PO4	Q	1262	5/5	0.97	0.10	44,45,45,45	0
4	K	L	1415	1/1	0.97	0.21	41,41,41,41	0
4	K	E	1263	1/1	0.98	0.26	45,45,45,45	0
2	PO4	G	1262	5/5	0.98	0.08	38,39,39,40	0
2	PO4	A	1263	5/5	0.98	0.15	51,51,52,52	0
3	NA	C	1310	1/1	0.98	0.37	24,24,24,24	0
4	K	R	1263	1/1	0.98	0.24	44,44,44,44	0
3	NA	D	1304	1/1	0.98	0.28	18,18,18,18	0
2	PO4	J	1262	5/5	0.98	0.09	35,35,36,37	0
2	PO4	P	1264	5/5	0.98	0.13	57,57,57,57	5
2	PO4	H	1262	5/5	0.98	0.08	46,46,46,47	0
2	PO4	P	1262	5/5	0.98	0.10	51,51,51,51	5
2	PO4	F	1262	5/5	0.98	0.11	40,41,41,41	0
2	PO4	K	1262	5/5	0.98	0.07	44,45,46,46	0
3	NA	O	1316	1/1	0.98	0.35	21,21,21,21	0
2	PO4	E	1262	5/5	0.98	0.10	44,44,45,45	0
3	NA	E	1311	1/1	0.98	0.32	17,17,17,17	0
4	K	C	1263	1/1	0.98	0.18	42,42,42,42	0
3	NA	S	1308	1/1	0.98	0.42	30,30,30,30	0
4	K	D	1265	1/1	0.99	0.22	42,42,42,42	0
2	PO4	A	1262	5/5	0.99	0.07	39,39,39,39	0
4	K	B	1264	1/1	0.99	0.24	48,48,48,48	0
4	K	P	1265	1/1	0.99	0.18	46,46,46,46	0
4	K	K	1265	1/1	0.99	0.24	46,46,46,46	0
4	K	L	1264	1/1	0.99	0.25	42,42,42,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.