Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 08:12 PM EDT

PDB ID	:	5JY7
Title	:	Complex of Mycobacterium smegmatis trehalose synthase with maltokinase
Authors	:	Futterer, K.; Kermani, A.A.; Besra, G.S.
Deposited on	:	2016-05-13
Resolution	:	3.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

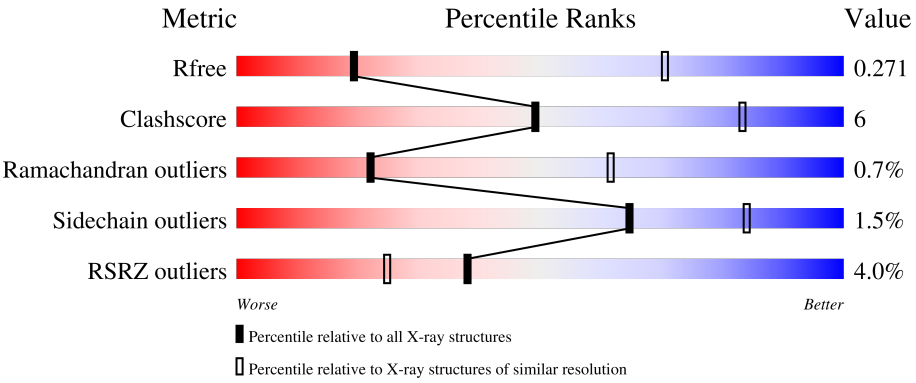
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	593	87% 8% 5%
1	B	593	% 86% 10%
1	C	593	88% 8%
1	D	593	% 87% 9%
1	E	593	2% 83% 10% 7%

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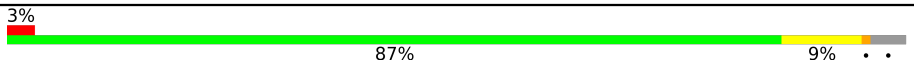
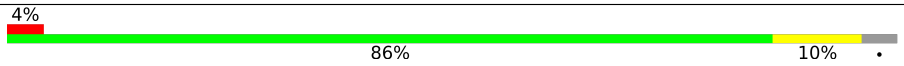
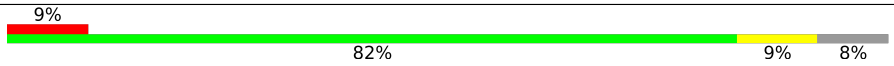
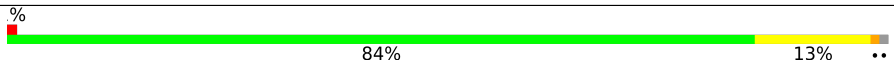
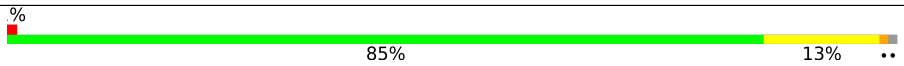
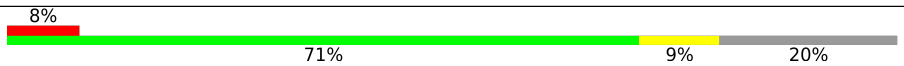
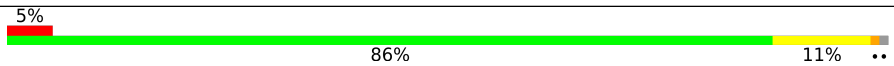
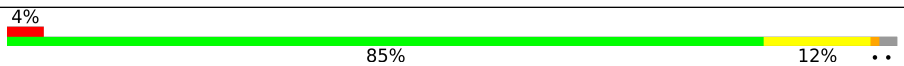
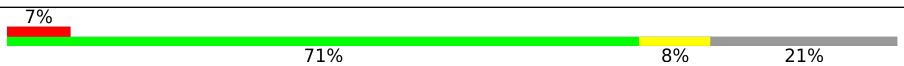
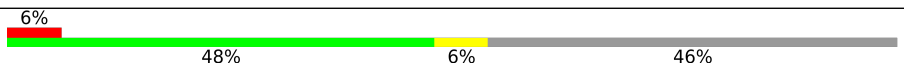
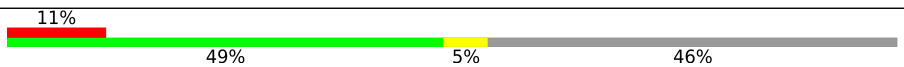
Mol	Chain	Length	Quality of chain
1	F	593	
1	G	593	
1	H	593	
2	I	441	
2	J	441	
2	K	441	
2	L	441	
2	M	441	
2	N	441	
2	O	441	
2	P	441	

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	CA	F	601	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 56343 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 Trehalose synthase/amylase TreS.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	565	Total	C	N	O	S	0	0	0
			4610	2952	788	853	17			
1	B	571	Total	C	N	O	S	0	0	0
			4661	2981	800	863	17			
1	C	569	Total	C	N	O	S	0	0	0
			4630	2964	792	857	17			
1	D	571	Total	C	N	O	S	0	0	0
			4661	2981	800	863	17			
1	E	549	Total	C	N	O	S	0	0	0
			4496	2884	764	831	17			
1	F	571	Total	C	N	O	S	0	0	0
			4661	2981	800	863	17			
1	G	571	Total	C	N	O	S	0	0	0
			4661	2981	800	863	17			
1	H	544	Total	C	N	O	S	0	0	0
			4452	2858	756	821	17			

- Molecule 2 is a protein called Maltokinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	435	Total	C	N	O	S	0	0	0
			2909	1811	523	569	6			
2	J	435	Total	C	N	O	S	0	0	0
			2899	1807	523	563	6			
2	K	353	Total	C	N	O	S	0	0	0
			2380	1481	432	462	5			
2	L	436	Total	C	N	O	S	0	0	0
			2913	1816	524	566	7			
2	M	431	Total	C	N	O	S	0	0	0
			2887	1799	519	563	6			
2	N	349	Total	C	N	O	S	0	0	0
			2347	1459	428	455	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	239	Total	C	N	O	S	0	0	0
			1584	974	291	315	4			
2	P	239	Total	C	N	O	S	0	0	0
			1584	974	291	315	4			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

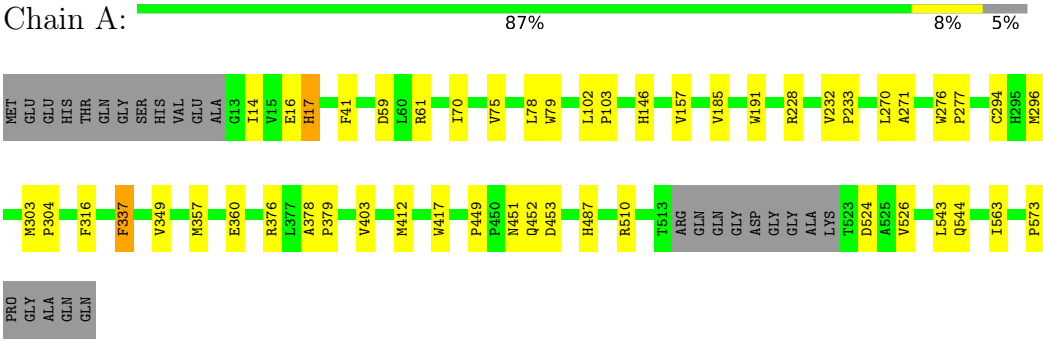
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	E	1	Total	Ca	0	0
			1	1		
3	F	1	Total	Ca	0	0
			1	1		
3	G	1	Total	Ca	0	0
			1	1		
3	H	1	Total	Ca	0	0
			1	1		

3 Residue-property plots (i)

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

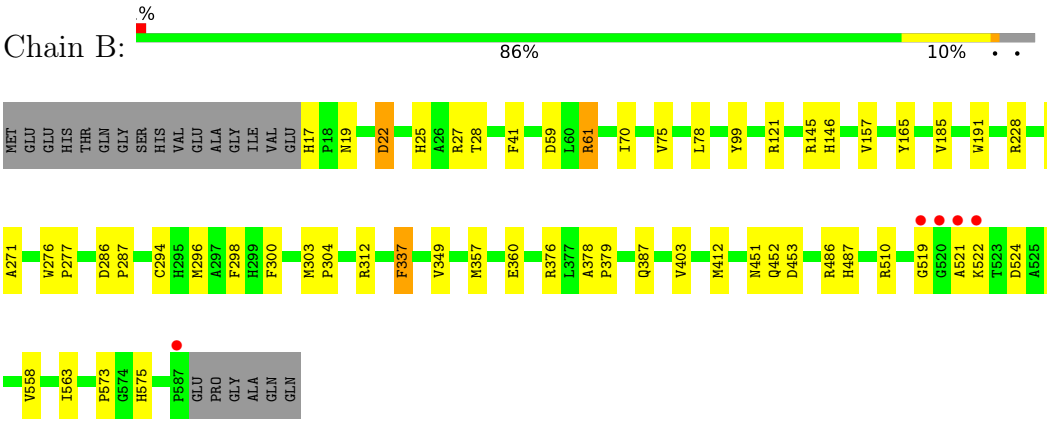
• Molecule 1: Trehalose synthase/amylase TreS

Chain A:



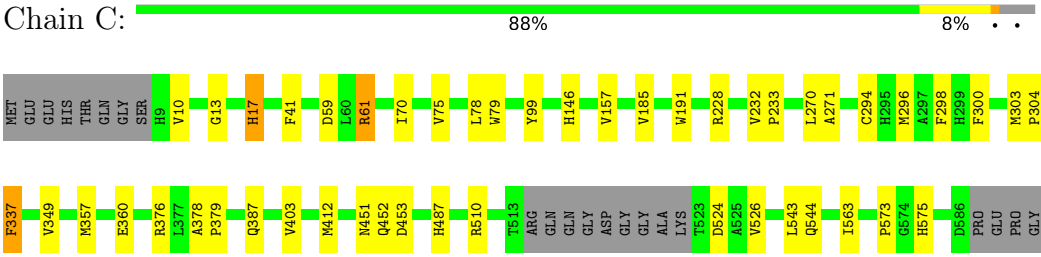
• Molecule 1: Trehalose synthase/amylase TreS

Chain B:



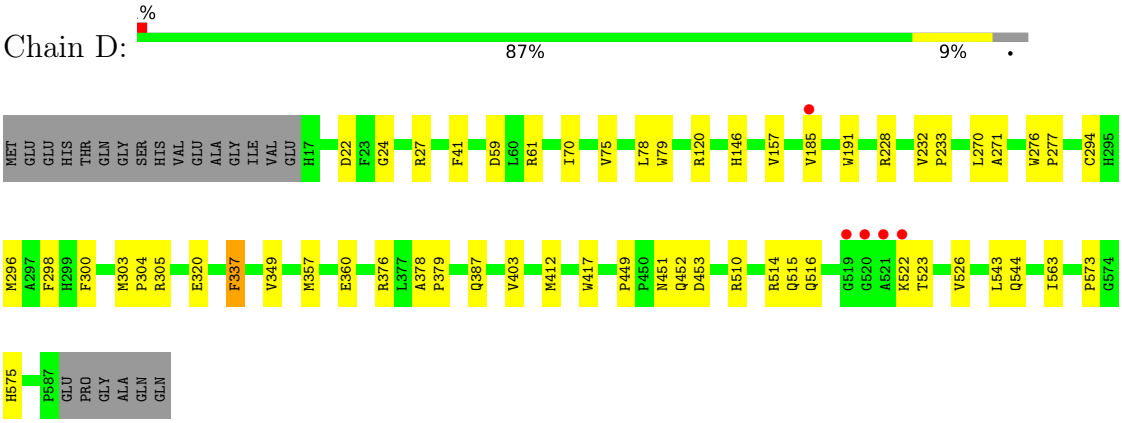
• Molecule 1: Trehalose synthase/amylase TreS

Chain C:



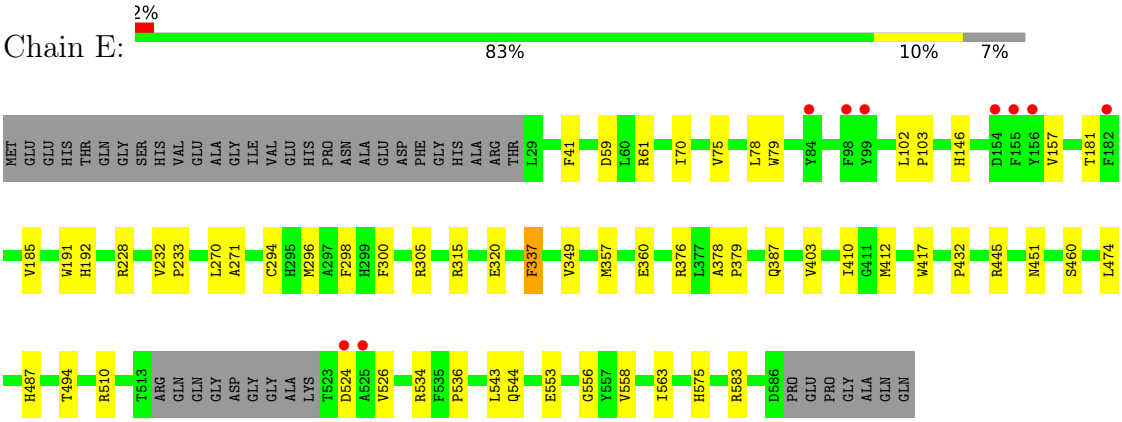
• Molecule 1: Trehalose synthase/amylase TreS

Chain D:



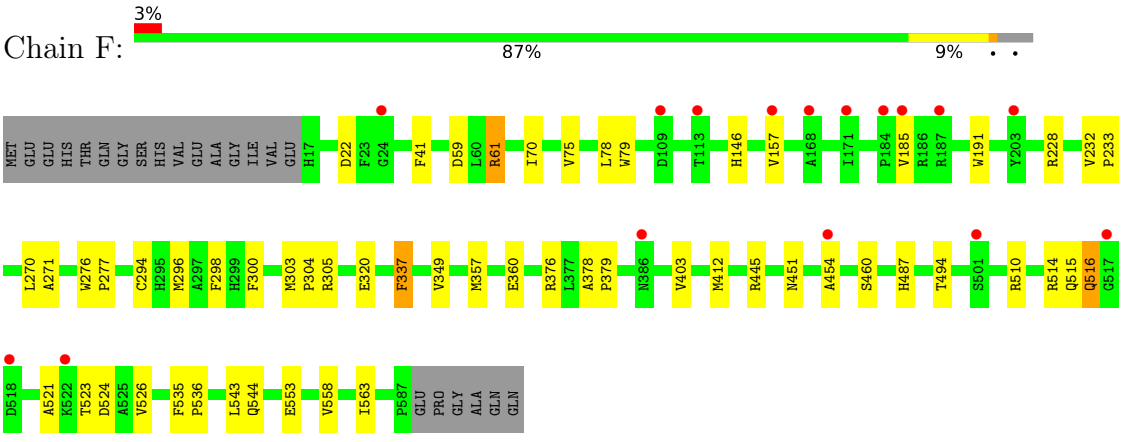
• Molecule 1: Trehalose synthase/amylase TreS

Chain E:



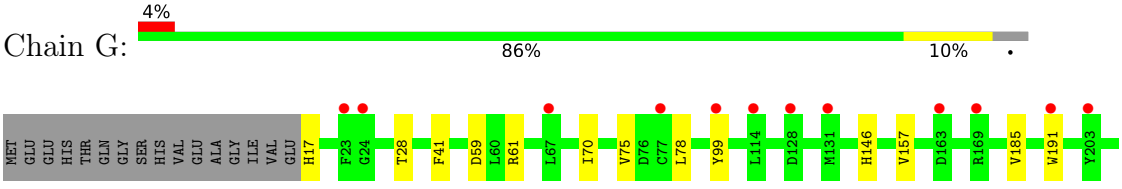
• Molecule 1: Trehalose synthase/amylase TreS

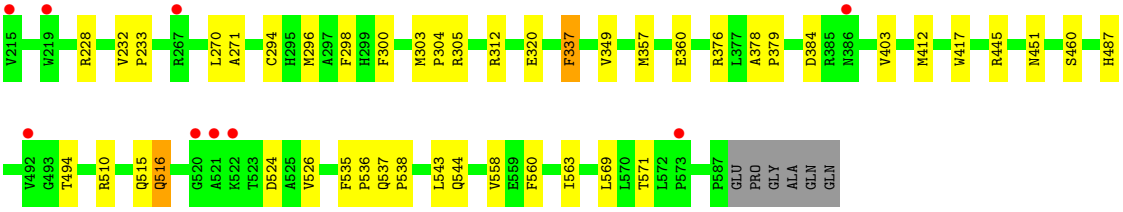
Chain F:



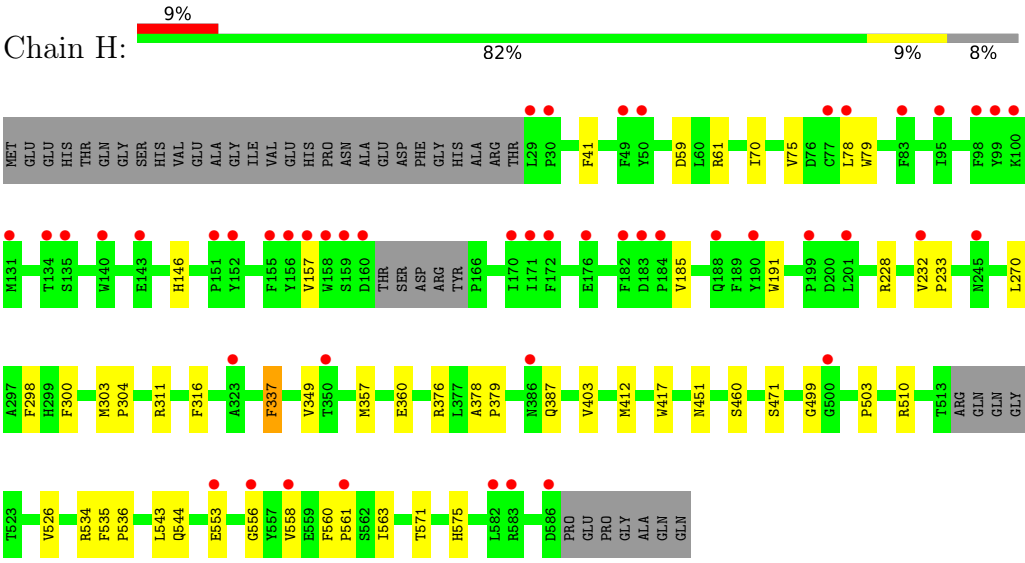
• Molecule 1: Trehalose synthase/amylase TreS

Chain G:

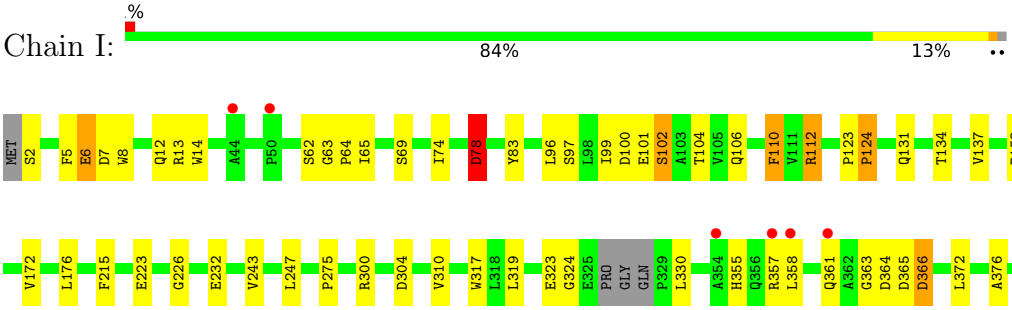




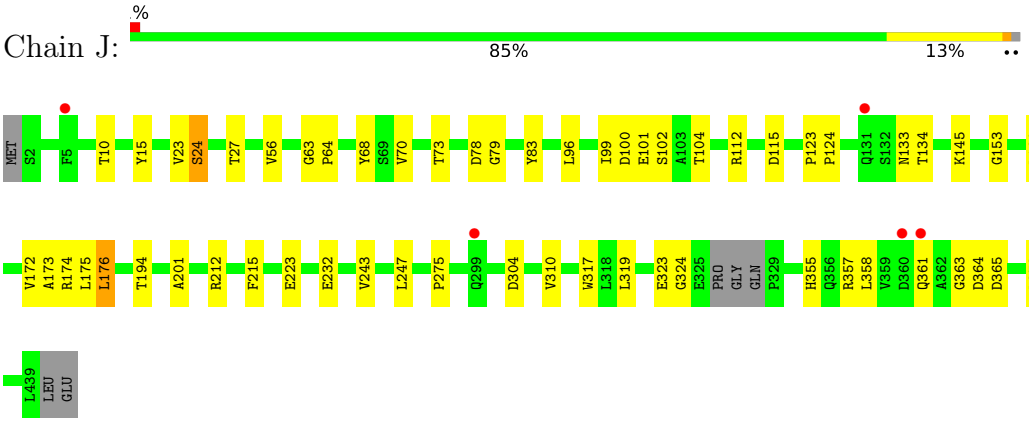
• Molecule 1: Trehalose synthase/amylase TreS



• Molecule 2: Maltokinase

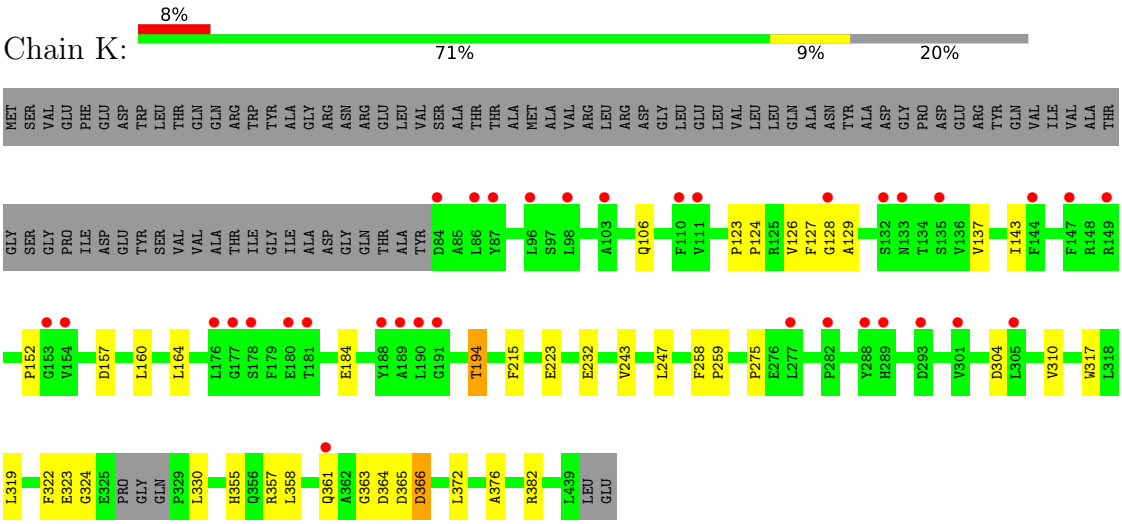


• Molecule 2: Maltokinase



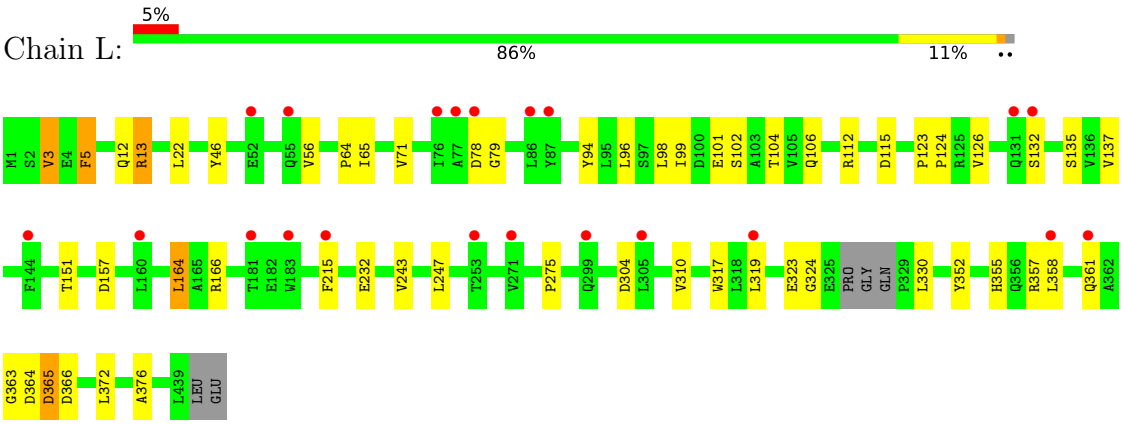
• Molecule 2: Maltokinase

Chain K:



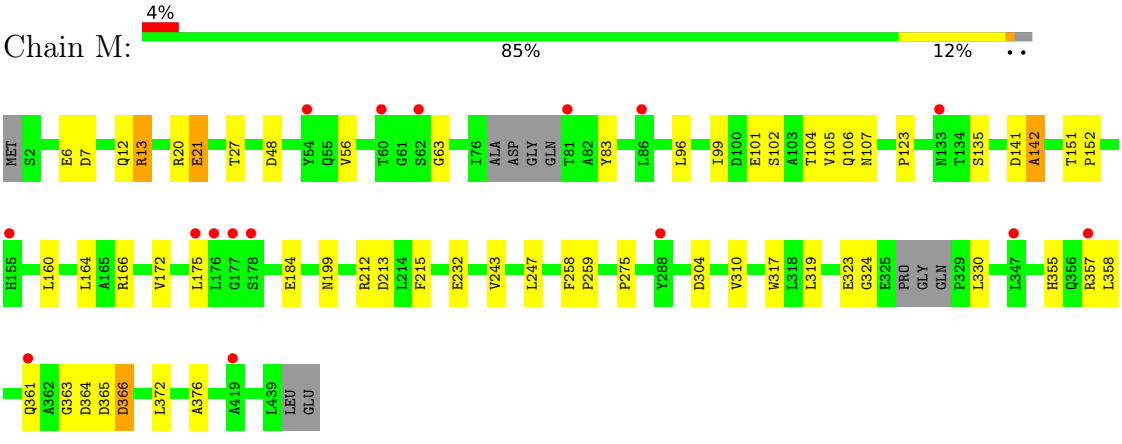
• Molecule 2: Maltokinase

Chain L:



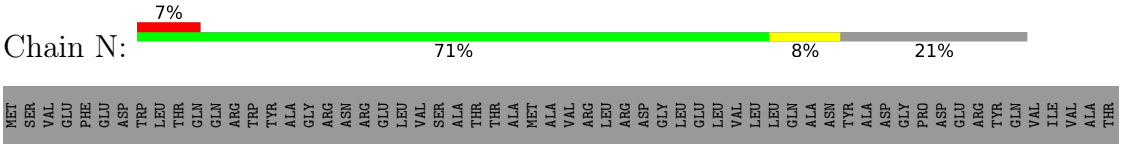
• Molecule 2: Maltokinase

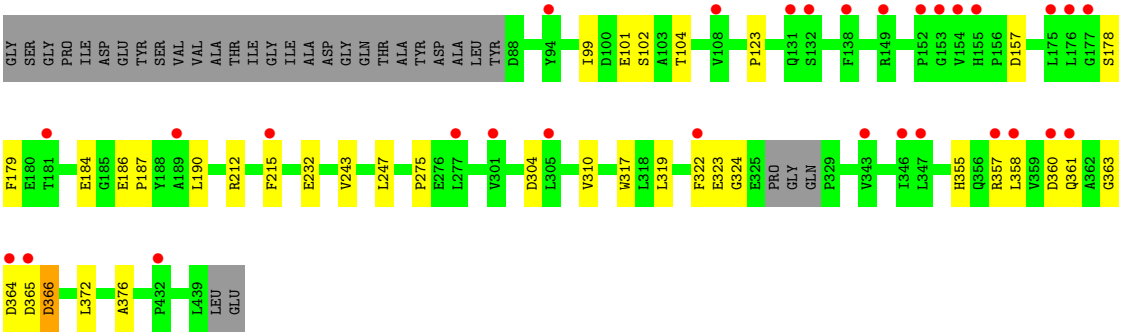
Chain M:



• Molecule 2: Maltokinase

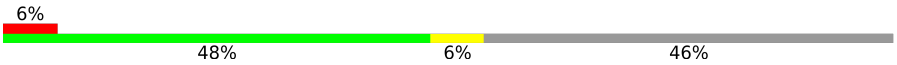
Chain N:

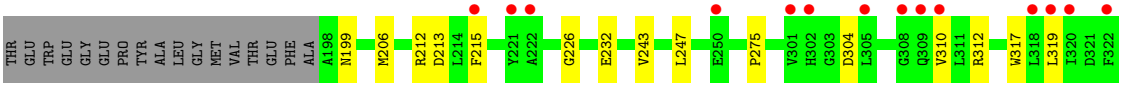


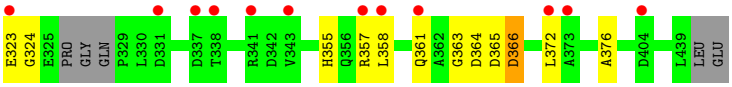


• Molecule 2: Maltokinase

Chain O:

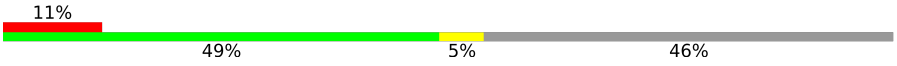


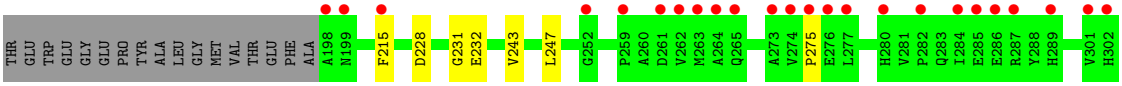


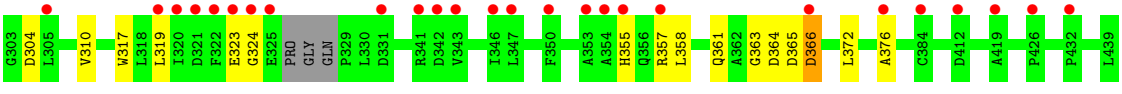


• Molecule 2: Maltokinase

Chain P:







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α, β, γ	315.68Å 315.68Å 124.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.90 – 3.60 49.91 – 3.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.90-3.60) 99.9 (49.91-3.60)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	0.17	Depositor
$< I/\sigma(I) >$ [1]	1.30 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.261 , 0.281 0.254 , 0.271	Depositor DCC
R_{free} test set	7119 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	125.2	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 76.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.036 for h,-k,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	56343	wwPDB-VP
Average B, all atoms (Å^2)	111.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.37	0/4754	0.53	1/6485 (0.0%)
1	B	0.41	0/4807	0.56	1/6556 (0.0%)
1	C	0.38	0/4774	0.54	1/6513 (0.0%)
1	D	0.34	0/4807	0.52	1/6556 (0.0%)
1	E	0.31	0/4636	0.51	1/6324 (0.0%)
1	F	0.36	2/4807 (0.0%)	0.51	1/6556 (0.0%)
1	G	0.29	0/4807	0.51	1/6556 (0.0%)
1	H	0.29	0/4590	0.51	1/6259 (0.0%)
2	I	0.42	0/2973	0.60	0/4091
2	J	0.38	0/2963	0.57	0/4078
2	K	0.32	0/2432	0.52	0/3343
2	L	0.39	2/2977 (0.1%)	0.55	0/4095
2	M	0.33	0/2950	0.54	0/4058
2	N	0.32	0/2398	0.53	0/3296
2	O	0.31	0/1615	0.53	0/2219
2	P	0.32	0/1615	0.53	0/2219
All	All	0.35	4/57905 (0.0%)	0.53	8/79204 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	61	ARG	CZ-NH1	11.18	1.47	1.33
1	F	61	ARG	CD-NE	8.59	1.61	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	352	TYR	C-N	8.42	1.53	1.34
2	L	366	ASP	C-N	7.62	1.51	1.34

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	61	ARG	CG-CD-NE	8.76	130.19	111.80
1	A	61	ARG	CG-CD-NE	7.92	128.42	111.80
1	G	61	ARG	CG-CD-NE	7.85	128.28	111.80
1	H	61	ARG	CG-CD-NE	7.82	128.23	111.80
1	E	61	ARG	CG-CD-NE	7.82	128.23	111.80
1	B	61	ARG	CG-CD-NE	7.81	128.19	111.80
1	D	61	ARG	CG-CD-NE	7.79	128.15	111.80
1	C	61	ARG	CG-CD-NE	7.47	127.48	111.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	365	ASP	Peptide,Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4610	0	4348	32	0
1	B	4661	0	4407	39	0
1	C	4630	0	4359	31	0
1	D	4661	0	4407	36	0
1	E	4496	0	4260	59	0
1	F	4661	0	4407	47	0
1	G	4661	0	4407	74	0
1	H	4452	0	4222	72	0
2	I	2909	0	2344	53	0
2	J	2899	0	2336	51	0
2	K	2380	0	1950	39	0
2	L	2913	0	2356	39	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	M	2887	0	2329	51	0
2	N	2347	0	1921	37	0
2	O	1584	0	1255	43	0
2	P	1584	0	1255	30	0
3	A	1	0	0	0	0
3	B	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	H	1	0	0	0	0
All	All	56343	0	50563	625	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 6.

All (625) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:215:PHE:CB	2:I:361:GLN:HE22	1.62	1.11
2:O:215:PHE:CB	2:O:361:GLN:HE22	1.64	1.11
2:L:215:PHE:CB	2:L:361:GLN:HE22	1.64	1.10
2:N:215:PHE:CB	2:N:361:GLN:HE22	1.64	1.10
2:K:215:PHE:CB	2:K:361:GLN:HE22	1.64	1.10
2:P:215:PHE:CB	2:P:361:GLN:HE22	1.63	1.10
2:J:215:PHE:CB	2:J:361:GLN:HE22	1.65	1.09
2:M:215:PHE:CB	2:M:361:GLN:HE22	1.64	1.09
2:K:215:PHE:HB3	2:K:361:GLN:HE22	1.16	1.09
2:I:215:PHE:HB3	2:I:361:GLN:HE22	1.17	1.09
2:L:215:PHE:HB3	2:L:361:GLN:HE22	1.16	1.07
2:J:215:PHE:HB3	2:J:361:GLN:HE22	1.19	1.06
2:N:215:PHE:HB3	2:N:361:GLN:HE22	1.17	1.05
2:M:215:PHE:HB3	2:M:361:GLN:HE22	1.17	1.04
2:O:215:PHE:HB3	2:O:361:GLN:HE22	1.17	1.04
2:P:215:PHE:HB3	2:P:361:GLN:NE2	1.73	1.04
2:P:215:PHE:HB3	2:P:361:GLN:HE22	1.16	1.03
2:K:215:PHE:HB3	2:K:361:GLN:NE2	1.73	1.03
2:M:215:PHE:HB3	2:M:361:GLN:NE2	1.73	1.03
2:L:215:PHE:HB3	2:L:361:GLN:NE2	1.72	1.02
2:O:215:PHE:HB3	2:O:361:GLN:NE2	1.73	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:215:PHE:HB3	2:I:361:GLN:NE2	1.72	1.01
2:J:215:PHE:HB3	2:J:361:GLN:NE2	1.74	1.01
2:N:215:PHE:HB3	2:N:361:GLN:NE2	1.74	1.00
1:E:417:TRP:CZ2	1:G:445:ARG:HG2	1.96	1.00
1:G:535:PHE:HD1	1:H:556:GLY:HA2	1.27	0.99
1:G:535:PHE:CD1	1:H:556:GLY:HA2	1.97	0.98
1:E:315:ARG:NH1	2:M:199:ASN:OD1	2.03	0.92
2:M:358:LEU:HD11	2:M:376:ALA:CB	2.01	0.91
2:O:358:LEU:HD11	2:O:376:ALA:CB	2.01	0.91
1:G:536:PRO:HG2	1:H:553:GLU:CG	2.01	0.90
1:G:536:PRO:HG2	1:H:553:GLU:CD	1.92	0.90
2:L:358:LEU:HD11	2:L:376:ALA:CB	2.01	0.90
2:I:215:PHE:CD2	2:I:361:GLN:NE2	2.39	0.90
2:K:358:LEU:HD11	2:K:376:ALA:CB	2.01	0.89
2:L:215:PHE:CD2	2:L:361:GLN:NE2	2.41	0.89
2:J:215:PHE:CD2	2:J:361:GLN:NE2	2.40	0.89
2:M:215:PHE:CD2	2:M:361:GLN:NE2	2.41	0.89
2:O:215:PHE:CD2	2:O:361:GLN:NE2	2.41	0.88
2:P:358:LEU:HD11	2:P:376:ALA:CB	2.02	0.88
1:H:503:PRO:HG3	2:O:206:MET:HA	1.52	0.88
2:I:358:LEU:HD11	2:I:376:ALA:CB	2.02	0.88
2:N:358:LEU:HD11	2:N:376:ALA:CB	2.02	0.88
2:K:215:PHE:CD2	2:K:361:GLN:NE2	2.42	0.88
2:P:215:PHE:CD2	2:P:361:GLN:NE2	2.42	0.88
2:J:358:LEU:HD11	2:J:376:ALA:CB	2.03	0.87
1:G:558:VAL:HG21	1:H:536:PRO:O	1.73	0.87
2:N:215:PHE:CD2	2:N:361:GLN:NE2	2.42	0.86
1:G:538:PRO:HG3	1:H:560:PHE:HA	1.55	0.86
1:C:573:PRO:HG3	1:D:573:PRO:HG3	1.59	0.84
1:E:460:SER:HB3	1:F:460:SER:HB3	1.59	0.84
1:G:535:PHE:CD1	1:H:556:GLY:CA	2.62	0.82
1:H:503:PRO:CB	2:O:206:MET:HG3	2.08	0.82
1:G:536:PRO:O	1:H:558:VAL:HG11	1.81	0.81
1:E:417:TRP:CH2	1:G:445:ARG:HG2	2.17	0.80
2:M:215:PHE:CB	2:M:361:GLN:NE2	2.40	0.80
1:G:535:PHE:HB3	1:H:556:GLY:HA3	1.63	0.79
1:E:445:ARG:HG2	1:G:417:TRP:CZ2	2.17	0.78
2:J:215:PHE:HD2	2:J:361:GLN:NE2	1.81	0.78
1:G:536:PRO:HG2	1:H:553:GLU:HG3	1.66	0.78
1:G:536:PRO:O	1:H:558:VAL:HG21	1.83	0.78
1:G:571:THR:HB	1:H:560:PHE:HE2	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:215:PHE:HD2	2:I:361:GLN:NE2	1.81	0.77
1:G:536:PRO:O	1:H:558:VAL:CB	2.33	0.77
2:M:215:PHE:HD2	2:M:361:GLN:NE2	1.83	0.76
2:K:215:PHE:HD2	2:K:361:GLN:NE2	1.84	0.76
2:O:215:PHE:HD2	2:O:361:GLN:NE2	1.83	0.76
2:N:215:PHE:HD2	2:N:361:GLN:NE2	1.83	0.76
2:O:215:PHE:CB	2:O:361:GLN:NE2	2.39	0.76
1:E:417:TRP:CE2	1:G:445:ARG:HG2	2.20	0.75
1:A:573:PRO:HG3	1:B:573:PRO:HG3	1.69	0.74
1:G:535:PHE:HD1	1:H:556:GLY:CA	2.00	0.74
2:P:215:PHE:HD2	2:P:361:GLN:NE2	1.84	0.74
1:H:535:PHE:CE2	2:O:213:ASP:HA	2.23	0.74
2:P:355:HIS:CD2	2:P:358:LEU:HD12	2.23	0.73
2:I:355:HIS:CD2	2:I:358:LEU:HD12	2.24	0.73
2:L:215:PHE:CB	2:L:361:GLN:NE2	2.39	0.73
2:L:215:PHE:HD2	2:L:361:GLN:NE2	1.83	0.73
2:K:355:HIS:CD2	2:K:358:LEU:HD12	2.23	0.73
2:I:215:PHE:CB	2:I:361:GLN:NE2	2.38	0.73
2:M:164:LEU:HD23	2:M:172:VAL:HG21	1.70	0.73
2:M:358:LEU:HD11	2:M:376:ALA:HB2	1.70	0.73
2:N:355:HIS:CD2	2:N:358:LEU:HD12	2.24	0.72
2:J:361:GLN:HB3	2:J:372:LEU:HD13	1.72	0.72
2:K:358:LEU:HD11	2:K:376:ALA:HB2	1.71	0.72
2:O:358:LEU:HD11	2:O:376:ALA:HB2	1.71	0.72
2:L:355:HIS:CD2	2:L:358:LEU:HD12	2.25	0.72
2:O:355:HIS:CD2	2:O:358:LEU:HD12	2.24	0.72
2:P:358:LEU:HD11	2:P:376:ALA:HB2	1.72	0.72
1:E:553:GLU:HG3	1:F:536:PRO:HG2	1.71	0.72
2:M:355:HIS:CD2	2:M:358:LEU:HD12	2.25	0.72
2:O:361:GLN:HB3	2:O:372:LEU:HD13	1.71	0.72
2:J:215:PHE:CB	2:J:361:GLN:NE2	2.41	0.72
2:J:358:LEU:HD23	2:J:361:GLN:OE1	1.89	0.72
2:M:361:GLN:HB3	2:M:372:LEU:HD13	1.71	0.72
1:E:556:GLY:HA2	1:F:535:PHE:CD1	2.24	0.71
2:N:361:GLN:HB3	2:N:372:LEU:HD13	1.72	0.71
2:M:164:LEU:HD21	2:M:243:VAL:HG23	1.72	0.71
2:J:355:HIS:CD2	2:J:358:LEU:HD12	2.25	0.71
2:L:361:GLN:HB3	2:L:372:LEU:HD13	1.71	0.71
1:G:571:THR:HB	1:H:560:PHE:CE2	2.26	0.71
2:K:361:GLN:HB3	2:K:372:LEU:HD13	1.71	0.71
2:I:361:GLN:HB3	2:I:372:LEU:HD13	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:358:LEU:HD11	2:J:376:ALA:HB2	1.72	0.71
2:P:361:GLN:HB3	2:P:372:LEU:HD13	1.71	0.71
2:I:358:LEU:HD11	2:I:376:ALA:HB2	1.71	0.71
2:N:358:LEU:HD11	2:N:376:ALA:HB2	1.71	0.71
2:L:358:LEU:HD11	2:L:376:ALA:HB2	1.71	0.70
2:K:215:PHE:CB	2:K:361:GLN:NE2	2.40	0.70
1:E:417:TRP:CZ2	1:G:445:ARG:CG	2.73	0.70
1:H:503:PRO:CG	2:O:206:MET:HG3	2.22	0.70
2:I:164:LEU:HD21	2:I:243:VAL:HG23	1.71	0.70
2:P:215:PHE:CB	2:P:361:GLN:NE2	2.40	0.70
1:C:17:HIS:CD2	1:C:99:TYR:CE2	2.79	0.70
1:G:535:PHE:HB3	1:H:558:VAL:HG23	1.73	0.69
2:I:358:LEU:HD23	2:I:361:GLN:OE1	1.91	0.69
2:M:358:LEU:HD23	2:M:361:GLN:OE1	1.92	0.69
1:E:556:GLY:CA	1:F:535:PHE:CD1	2.74	0.69
2:O:358:LEU:HD23	2:O:361:GLN:OE1	1.91	0.69
2:L:358:LEU:HD23	2:L:361:GLN:OE1	1.92	0.69
2:K:358:LEU:HD23	2:K:361:GLN:OE1	1.92	0.69
2:N:215:PHE:CB	2:N:361:GLN:NE2	2.40	0.69
1:E:460:SER:HB3	1:F:460:SER:CB	2.23	0.69
1:E:460:SER:CB	1:F:460:SER:HB3	2.22	0.69
2:N:358:LEU:HD23	2:N:361:GLN:OE1	1.93	0.68
1:G:536:PRO:O	1:H:558:VAL:CG1	2.41	0.68
2:P:358:LEU:HD23	2:P:361:GLN:OE1	1.94	0.68
1:G:536:PRO:O	1:H:558:VAL:CG2	2.43	0.67
1:H:535:PHE:HE2	2:O:213:ASP:HA	1.58	0.67
1:E:558:VAL:HG22	2:N:212:ARG:HD3	1.76	0.67
1:H:503:PRO:HG3	2:O:206:MET:HG3	1.77	0.66
1:B:121:ARG:HA	2:M:48:ASP:CB	2.26	0.65
1:F:515:GLN:O	1:F:516:GLN:HB2	1.95	0.65
1:G:538:PRO:CB	1:H:561:PRO:HD3	2.26	0.65
2:N:357:ARG:O	2:N:361:GLN:HG3	1.97	0.65
1:D:146:HIS:CD2	1:D:185:VAL:HG11	2.32	0.64
2:L:94:TYR:CE2	2:L:98:LEU:HD11	2.32	0.64
1:G:535:PHE:CB	1:H:558:VAL:CG2	2.76	0.64
2:L:12:GLN:O	2:L:13:ARG:CB	2.46	0.64
2:M:12:GLN:O	2:M:13:ARG:CB	2.46	0.64
1:B:146:HIS:CD2	1:B:185:VAL:HG11	2.33	0.64
1:C:146:HIS:CD2	1:C:185:VAL:HG11	2.32	0.64
1:G:146:HIS:CD2	1:G:185:VAL:HG11	2.34	0.63
1:H:503:PRO:HG3	2:O:206:MET:CA	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:151:THR:CB	2:L:330:LEU:HD11	2.29	0.63
2:M:357:ARG:O	2:M:361:GLN:HG3	1.98	0.63
1:E:445:ARG:HG2	1:G:417:TRP:CH2	2.33	0.63
2:K:357:ARG:O	2:K:361:GLN:HG3	1.99	0.63
1:H:146:HIS:CD2	1:H:185:VAL:HG11	2.33	0.63
2:J:112:ARG:NH2	2:J:115:ASP:O	2.33	0.62
2:I:152:PRO:O	2:I:330:LEU:HD13	1.99	0.62
1:G:535:PHE:HB2	1:H:558:VAL:CG2	2.30	0.62
2:P:357:ARG:O	2:P:361:GLN:HG3	1.99	0.62
1:F:146:HIS:CD2	1:F:185:VAL:HG11	2.34	0.62
2:L:357:ARG:O	2:L:361:GLN:HG3	1.99	0.62
2:O:357:ARG:O	2:O:361:GLN:HG3	1.98	0.62
1:A:146:HIS:CD2	1:A:185:VAL:HG11	2.34	0.62
1:E:146:HIS:CD2	1:E:185:VAL:HG11	2.34	0.62
2:I:357:ARG:O	2:I:361:GLN:HG3	2.01	0.61
2:K:164:LEU:HD21	2:K:243:VAL:HG23	1.82	0.61
1:A:453:ASP:HA	1:D:452:GLN:HE22	1.65	0.60
1:G:535:PHE:CB	1:H:556:GLY:HA3	2.32	0.60
1:G:460:SER:HB3	1:H:460:SER:HB3	1.84	0.60
1:G:460:SER:HB3	1:H:460:SER:CB	2.32	0.60
2:J:96:LEU:O	2:J:99:ILE:HG22	2.02	0.59
2:J:357:ARG:O	2:J:361:GLN:HG3	2.02	0.59
1:E:271:ALA:HB2	1:E:294:CYS:SG	2.43	0.58
2:I:365:ASP:HB3	2:I:366:ASP:CG	2.24	0.58
1:C:17:HIS:CD2	1:C:99:TYR:CZ	2.91	0.57
1:B:519:GLY:HA2	1:B:522:LYS:HB2	1.86	0.57
2:I:358:LEU:HA	2:I:361:GLN:HB2	1.87	0.57
2:I:361:GLN:HB3	2:I:372:LEU:CD1	2.35	0.57
2:K:160:LEU:O	2:K:164:LEU:HB2	2.05	0.56
1:B:17:HIS:HD2	1:B:99:TYR:CE2	2.24	0.56
1:E:553:GLU:CG	1:F:536:PRO:HG2	2.35	0.56
1:F:271:ALA:HB2	1:F:294:CYS:SG	2.45	0.56
1:G:536:PRO:CG	1:H:553:GLU:HG3	2.35	0.56
1:G:558:VAL:HG22	2:O:212:ARG:HD3	1.88	0.56
2:I:358:LEU:CD2	2:I:372:LEU:HB3	2.35	0.56
1:H:499:GLY:HA3	2:O:199:ASN:HA	1.86	0.56
2:I:14:TRP:HA	2:I:131:GLN:HA	1.87	0.56
1:E:534:ARG:HH22	2:M:213:ASP:CG	2.09	0.56
2:K:358:LEU:HA	2:K:361:GLN:HB2	1.88	0.56
2:J:358:LEU:CD2	2:J:372:LEU:HB3	2.36	0.56
2:N:358:LEU:HA	2:N:361:GLN:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:ARG:NH1	1:D:120:ARG:HG2	2.21	0.56
2:I:63:GLY:HA2	2:I:83:TYR:CZ	2.40	0.56
2:I:357:ARG:O	2:I:361:GLN:N	2.39	0.56
2:O:358:LEU:HA	2:O:361:GLN:HB2	1.88	0.56
1:E:556:GLY:HA3	1:F:535:PHE:CD1	2.41	0.55
1:G:535:PHE:HB3	1:H:558:VAL:CG2	2.35	0.55
1:E:417:TRP:CH2	1:G:445:ARG:CG	2.89	0.55
2:O:361:GLN:HB3	2:O:372:LEU:CD1	2.37	0.55
1:B:521:ALA:HB3	2:J:363:GLY:O	2.07	0.55
2:P:357:ARG:O	2:P:361:GLN:N	2.40	0.55
2:M:357:ARG:O	2:M:361:GLN:N	2.39	0.55
1:G:537:GLN:HA	1:H:558:VAL:HG11	1.88	0.55
2:K:361:GLN:HB3	2:K:372:LEU:CD1	2.37	0.55
2:L:358:LEU:HA	2:L:361:GLN:HB2	1.88	0.55
1:G:536:PRO:HG2	1:H:553:GLU:OE1	2.07	0.55
2:I:78:ASP:CG	2:I:78:ASP:O	2.45	0.55
2:P:361:GLN:HB3	2:P:372:LEU:CD1	2.37	0.55
1:E:378:ALA:HB3	1:E:379:PRO:HD3	1.89	0.55
1:F:378:ALA:HB3	1:F:379:PRO:HD3	1.89	0.55
2:J:63:GLY:N	2:J:64:PRO:HD3	2.21	0.55
1:G:536:PRO:O	1:H:558:VAL:HB	2.06	0.55
1:A:452:GLN:HE22	1:D:453:ASP:HA	1.72	0.54
1:B:378:ALA:HB3	1:B:379:PRO:HD3	1.89	0.54
2:M:358:LEU:CD2	2:M:372:LEU:HB3	2.37	0.54
2:J:358:LEU:HA	2:J:361:GLN:HB2	1.88	0.54
2:J:361:GLN:HB3	2:J:372:LEU:CD1	2.36	0.54
2:P:358:LEU:HA	2:P:361:GLN:HB2	1.88	0.54
1:H:271:ALA:HB2	1:H:294:CYS:SG	2.47	0.54
1:G:378:ALA:HB3	1:G:379:PRO:HD3	1.88	0.54
1:H:316:PHE:CE1	2:O:312:ARG:HG2	2.42	0.54
1:H:378:ALA:HB3	1:H:379:PRO:HD3	1.89	0.54
2:M:358:LEU:HA	2:M:361:GLN:HB2	1.88	0.54
1:B:19:ASN:O	1:B:22:ASP:HB3	2.07	0.54
2:L:3:VAL:O	2:L:5:PHE:N	2.41	0.54
2:O:358:LEU:CD2	2:O:372:LEU:HB3	2.38	0.54
2:K:357:ARG:O	2:K:361:GLN:N	2.41	0.54
2:M:361:GLN:HB3	2:M:372:LEU:CD1	2.37	0.53
2:J:160:LEU:HD12	2:J:247:LEU:HD21	1.90	0.53
2:J:164:LEU:HD21	2:J:243:VAL:HG23	1.91	0.53
2:L:358:LEU:CD2	2:L:372:LEU:HB3	2.37	0.53
1:D:378:ALA:HB3	1:D:379:PRO:HD3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:449:PRO:HD3	1:D:417:TRP:CG	2.44	0.53
1:C:378:ALA:HB3	1:C:379:PRO:HD3	1.89	0.53
1:E:417:TRP:CZ2	1:G:445:ARG:CD	2.92	0.53
1:H:534:ARG:NH1	2:O:213:ASP:OD1	2.41	0.53
2:J:357:ARG:O	2:J:361:GLN:N	2.41	0.53
1:A:378:ALA:HB3	1:A:379:PRO:HD3	1.90	0.53
2:O:357:ARG:O	2:O:361:GLN:N	2.41	0.53
2:P:358:LEU:CD2	2:P:372:LEU:HB3	2.39	0.53
1:D:228:ARG:HD2	1:D:298:PHE:HE2	1.73	0.53
2:I:164:LEU:HD21	2:I:243:VAL:CG2	2.35	0.53
2:L:357:ARG:O	2:L:361:GLN:N	2.41	0.53
2:N:179:PHE:CZ	2:N:190:LEU:HB3	2.44	0.53
2:N:357:ARG:O	2:N:361:GLN:N	2.42	0.53
2:L:361:GLN:HB3	2:L:372:LEU:CD1	2.37	0.53
1:G:384:ASP:HA	1:H:471:SER:CB	2.39	0.53
2:K:358:LEU:CD2	2:K:372:LEU:HB3	2.38	0.53
1:B:486:ARG:CD	2:J:365:ASP:O	2.58	0.52
2:M:164:LEU:HD21	2:M:243:VAL:CG2	2.40	0.52
2:I:8:TRP:HE3	2:I:12:GLN:OE1	1.93	0.52
1:E:460:SER:CB	1:F:460:SER:CB	2.86	0.52
1:B:270:LEU:HG	1:B:296:MET:HB2	1.92	0.52
1:D:271:ALA:HB2	1:D:294:CYS:SG	2.50	0.52
1:E:558:VAL:HA	2:N:212:ARG:HE	1.74	0.52
2:L:22:LEU:HA	2:L:46:TYR:HA	1.92	0.52
1:A:228:ARG:HD2	1:A:298:PHE:HE2	1.75	0.52
2:N:358:LEU:CD2	2:N:372:LEU:HB3	2.39	0.52
1:D:270:LEU:HG	1:D:296:MET:HB2	1.92	0.52
1:C:270:LEU:HG	1:C:296:MET:HB2	1.91	0.52
1:C:228:ARG:HD2	1:C:298:PHE:HE2	1.75	0.52
1:E:270:LEU:HG	1:E:296:MET:HB2	1.92	0.51
1:G:271:ALA:HB2	1:G:294:CYS:SG	2.49	0.51
1:G:360:GLU:OE2	2:P:231:GLY:HA3	2.10	0.51
1:D:514:ARG:HA	1:D:523:THR:HG21	1.93	0.51
1:H:270:LEU:HG	1:H:296:MET:HB2	1.91	0.51
2:M:160:LEU:HD12	2:M:247:LEU:HD11	1.93	0.51
2:N:361:GLN:HB3	2:N:372:LEU:CD1	2.38	0.51
1:F:270:LEU:HG	1:F:296:MET:HB2	1.92	0.51
1:G:270:LEU:HG	1:G:296:MET:HB2	1.92	0.50
2:N:101:GLU:N	2:N:102:SER:HA	2.26	0.50
1:H:228:ARG:HD2	1:H:298:PHE:HE2	1.75	0.50
2:I:8:TRP:CD1	2:I:74:ILE:HA	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:96:LEU:O	2:L:99:ILE:HG22	2.10	0.50
1:B:271:ALA:HB2	1:B:294:CYS:SG	2.51	0.50
1:F:228:ARG:HD2	1:F:298:PHE:HE2	1.77	0.50
2:I:12:GLN:O	2:I:13:ARG:CB	2.59	0.50
2:I:124:PRO:HD2	2:I:137:VAL:O	2.12	0.50
1:E:228:ARG:HD2	1:E:298:PHE:HE2	1.76	0.49
2:J:363:GLY:N	2:J:364:ASP:CB	2.75	0.49
1:A:270:LEU:HG	1:A:296:MET:HB2	1.93	0.49
2:P:304:ASP:HB2	2:P:324:GLY:O	2.12	0.49
2:L:101:GLU:N	2:L:102:SER:HA	2.26	0.49
2:L:304:ASP:HB2	2:L:324:GLY:O	2.13	0.49
2:O:363:GLY:N	2:O:364:ASP:CB	2.76	0.49
2:I:160:LEU:HD12	2:I:247:LEU:HD11	1.95	0.49
2:M:20:ARG:O	2:M:21:GLU:CB	2.60	0.49
1:B:312:ARG:HD3	2:I:226:GLY:O	2.13	0.49
1:E:534:ARG:NH1	2:M:213:ASP:OD1	2.44	0.49
2:N:365:ASP:HB3	2:N:366:ASP:CG	2.33	0.49
2:M:304:ASP:HB2	2:M:324:GLY:O	2.12	0.49
1:E:445:ARG:HG2	1:G:417:TRP:CE2	2.47	0.48
1:B:376:ARG:HH12	1:B:412:MET:CE	2.27	0.48
2:I:5:PHE:O	2:I:6:GLU:C	2.51	0.48
2:M:105:VAL:O	2:M:107:ASN:N	2.47	0.48
2:N:157:ASP:HA	2:N:322:PHE:HB2	1.96	0.48
2:O:304:ASP:HB2	2:O:324:GLY:O	2.12	0.48
1:E:536:PRO:HG2	1:F:553:GLU:HG3	1.95	0.48
1:G:228:ARG:HD2	1:G:298:PHE:HE2	1.78	0.48
1:A:271:ALA:HB2	1:A:294:CYS:SG	2.53	0.48
2:J:23:VAL:O	2:J:24:SER:C	2.51	0.48
2:O:243:VAL:HG11	2:O:319:LEU:HD22	1.96	0.48
1:C:271:ALA:HB2	1:C:294:CYS:SG	2.53	0.48
1:F:514:ARG:HA	1:F:523:THR:HG21	1.96	0.48
2:M:96:LEU:O	2:M:99:ILE:HG22	2.13	0.48
2:O:365:ASP:HB3	2:O:366:ASP:CG	2.34	0.48
2:N:304:ASP:HB2	2:N:324:GLY:O	2.13	0.48
2:I:8:TRP:O	2:I:12:GLN:HG2	2.13	0.48
2:M:243:VAL:HG11	2:M:319:LEU:HD22	1.96	0.48
1:E:41:PHE:HB2	1:E:403:VAL:HG22	1.95	0.48
2:I:215:PHE:CD2	2:I:361:GLN:CD	2.88	0.48
2:K:243:VAL:HG11	2:K:319:LEU:HD22	1.96	0.48
1:C:41:PHE:HB2	1:C:403:VAL:HG22	1.96	0.47
2:I:62:SER:C	2:I:64:PRO:HD3	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:243:VAL:HG11	2:I:319:LEU:HD22	1.96	0.47
2:M:152:PRO:HG2	2:M:330:LEU:HD12	1.96	0.47
2:P:365:ASP:HB3	2:P:366:ASP:CG	2.34	0.47
2:J:101:GLU:N	2:J:102:SER:HA	2.28	0.47
1:B:357:MET:HA	1:B:360:GLU:HG3	1.96	0.47
1:G:312:ARG:NH1	2:P:228:ASP:O	2.46	0.47
1:G:515:GLN:O	1:G:516:GLN:HB2	2.14	0.47
2:J:164:LEU:HD21	2:J:243:VAL:CG2	2.44	0.47
1:F:376:ARG:HH12	1:F:412:MET:CE	2.27	0.47
2:J:63:GLY:HA2	2:J:83:TYR:CZ	2.50	0.47
2:L:164:LEU:HD11	2:L:243:VAL:HG23	1.96	0.47
2:L:243:VAL:HG11	2:L:319:LEU:HD22	1.95	0.47
2:M:358:LEU:HD11	2:M:376:ALA:HB3	1.93	0.47
2:N:243:VAL:HG11	2:N:319:LEU:HD22	1.96	0.47
2:O:215:PHE:CD2	2:O:361:GLN:CD	2.88	0.47
2:P:363:GLY:N	2:P:364:ASP:CB	2.78	0.47
2:K:164:LEU:HD13	2:K:247:LEU:CD1	2.45	0.47
2:K:363:GLY:N	2:K:364:ASP:CB	2.77	0.47
2:N:215:PHE:CD2	2:N:361:GLN:CD	2.88	0.47
1:A:70:ILE:HG21	1:A:78:LEU:HD11	1.97	0.47
2:K:304:ASP:HB2	2:K:324:GLY:O	2.13	0.47
2:M:141:ASP:O	2:M:142:ALA:HB2	2.14	0.47
1:C:376:ARG:HH12	1:C:412:MET:CE	2.28	0.47
1:F:544:GLN:OE1	1:F:544:GLN:N	2.47	0.47
2:J:323:GLU:N	2:J:324:GLY:HA2	2.30	0.47
2:N:323:GLU:N	2:N:324:GLY:HA2	2.30	0.47
2:N:363:GLY:N	2:N:364:ASP:CB	2.78	0.47
1:B:228:ARG:HD2	1:B:298:PHE:HE2	1.79	0.46
1:B:558:VAL:HG22	2:J:212:ARG:NE	2.30	0.46
2:N:186:GLU:CB	2:N:187:PRO:HD2	2.44	0.46
2:P:243:VAL:HG11	2:P:319:LEU:HD22	1.96	0.46
2:J:304:ASP:HB2	2:J:324:GLY:O	2.16	0.46
2:M:363:GLY:N	2:M:364:ASP:CB	2.78	0.46
1:F:445:ARG:HG2	1:H:417:TRP:CE2	2.50	0.46
1:G:544:GLN:OE1	1:G:544:GLN:N	2.48	0.46
1:H:376:ARG:HH12	1:H:412:MET:CE	2.28	0.46
2:I:363:GLY:N	2:I:364:ASP:CB	2.78	0.46
2:J:361:GLN:CB	2:J:372:LEU:HD13	2.45	0.46
2:M:63:GLY:HA2	2:M:83:TYR:CZ	2.50	0.46
2:L:323:GLU:N	2:L:324:GLY:HA2	2.31	0.46
1:B:337:PHE:HB3	1:B:403:VAL:HB	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:41:PHE:HB2	1:G:403:VAL:HG22	1.98	0.46
2:I:304:ASP:HB2	2:I:324:GLY:O	2.16	0.46
1:C:544:GLN:OE1	1:C:544:GLN:N	2.47	0.46
1:E:376:ARG:HH12	1:E:412:MET:CE	2.28	0.46
2:J:215:PHE:CD2	2:J:361:GLN:CD	2.88	0.46
2:M:215:PHE:CD2	2:M:361:GLN:CD	2.89	0.46
1:D:514:ARG:HD2	1:D:523:THR:HB	1.97	0.46
1:F:157:VAL:HB	1:F:191:TRP:HB3	1.98	0.46
2:I:101:GLU:N	2:I:102:SER:HA	2.31	0.46
2:I:361:GLN:CB	2:I:372:LEU:HD13	2.43	0.46
2:P:215:PHE:CD2	2:P:361:GLN:CD	2.89	0.46
1:C:510:ARG:HB2	1:C:526:VAL:HG22	1.98	0.46
1:D:376:ARG:HH12	1:D:412:MET:CE	2.28	0.46
1:G:70:ILE:HG21	1:G:78:LEU:HD11	1.98	0.46
1:G:569:LEU:CD1	1:H:561:PRO:HG2	2.44	0.46
2:M:323:GLU:N	2:M:324:GLY:HA2	2.31	0.46
1:D:27:ARG:NH2	1:D:120:ARG:HD3	2.30	0.46
1:F:558:VAL:HG22	2:M:212:ARG:HD3	1.98	0.46
1:G:376:ARG:HH12	1:G:412:MET:CE	2.29	0.46
1:G:510:ARG:HB2	1:G:526:VAL:HG22	1.98	0.46
2:J:243:VAL:HG11	2:J:319:LEU:HD22	1.97	0.46
2:L:215:PHE:CD2	2:L:361:GLN:CD	2.89	0.46
1:E:487:HIS:ND1	1:E:524:ASP:OD2	2.49	0.46
1:H:41:PHE:HB2	1:H:403:VAL:HG22	1.98	0.46
2:K:323:GLU:N	2:K:324:GLY:HA2	2.31	0.46
2:K:157:ASP:HA	2:K:322:PHE:HB2	1.98	0.45
2:L:64:PRO:CB	2:L:65:ILE:HA	2.46	0.45
2:L:112:ARG:NH2	2:L:115:ASP:O	2.48	0.45
2:N:358:LEU:HD11	2:N:376:ALA:HB3	1.94	0.45
2:K:215:PHE:CD2	2:K:361:GLN:CD	2.90	0.45
2:K:361:GLN:CB	2:K:372:LEU:HD13	2.45	0.45
1:E:157:VAL:HB	1:E:191:TRP:HB3	1.98	0.45
1:H:157:VAL:HB	1:H:191:TRP:HB3	1.98	0.45
2:I:164:LEU:HG	2:I:172:VAL:HG21	1.98	0.45
2:O:323:GLU:N	2:O:324:GLY:HA2	2.31	0.45
1:E:300:PHE:HB3	1:E:349:VAL:HG11	1.98	0.45
1:H:544:GLN:OE1	1:H:544:GLN:N	2.48	0.45
2:L:363:GLY:N	2:L:364:ASP:CB	2.79	0.45
1:A:357:MET:HA	1:A:360:GLU:HG3	1.98	0.45
1:A:544:GLN:OE1	1:A:544:GLN:N	2.48	0.45
1:C:543:LEU:HB2	1:C:563:ILE:HG21	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:558:VAL:CG2	1:F:535:PHE:HB3	2.46	0.45
1:H:70:ILE:HG21	1:H:78:LEU:HD11	1.99	0.45
1:H:510:ARG:HB2	1:H:526:VAL:HG22	1.99	0.45
1:B:70:ILE:HG21	1:B:78:LEU:HD11	1.98	0.45
1:D:157:VAL:HB	1:D:191:TRP:HB3	1.98	0.45
2:M:232:GLU:HG3	2:M:317:TRP:HZ2	1.81	0.45
1:B:453:ASP:HA	1:C:452:GLN:HE22	1.81	0.45
1:D:510:ARG:HB2	1:D:526:VAL:HG22	1.99	0.45
2:J:361:GLN:O	2:J:364:ASP:O	2.34	0.45
1:B:543:LEU:HB2	1:B:563:ILE:HG21	1.99	0.45
1:F:337:PHE:HB3	1:F:403:VAL:HB	1.98	0.45
1:G:300:PHE:HB3	1:G:349:VAL:HG11	1.99	0.45
1:A:300:PHE:HB3	1:A:349:VAL:HG11	1.98	0.45
1:B:487:HIS:ND1	1:B:524:ASP:OD2	2.50	0.45
1:E:510:ARG:HB2	1:E:526:VAL:HG22	1.99	0.45
1:E:553:GLU:CD	1:F:536:PRO:HG2	2.37	0.45
1:H:300:PHE:HB3	1:H:349:VAL:HG11	1.99	0.45
2:M:164:LEU:CD2	2:M:172:VAL:HG21	2.41	0.45
1:D:70:ILE:HG21	1:D:78:LEU:HD11	1.99	0.45
1:F:521:ALA:HB3	2:M:364:ASP:H	1.82	0.45
2:J:232:GLU:HG3	2:J:317:TRP:HZ2	1.81	0.45
1:A:157:VAL:HB	1:A:191:TRP:HB3	1.99	0.44
1:D:41:PHE:HB2	1:D:403:VAL:HG22	1.98	0.44
1:G:157:VAL:HB	1:G:191:TRP:HB3	1.98	0.44
1:G:535:PHE:HB3	1:H:556:GLY:CA	2.41	0.44
2:J:358:LEU:HD11	2:J:376:ALA:HB3	1.95	0.44
2:O:363:GLY:H	2:O:364:ASP:CB	2.30	0.44
1:C:357:MET:HA	1:C:360:GLU:HG3	1.98	0.44
1:D:300:PHE:HB3	1:D:349:VAL:HG11	1.99	0.44
1:E:544:GLN:N	1:E:544:GLN:OE1	2.49	0.44
1:G:538:PRO:HB2	1:H:561:PRO:HD3	1.99	0.44
1:G:357:MET:HA	1:G:360:GLU:HG3	1.99	0.44
1:E:558:VAL:CG2	1:F:535:PHE:CB	2.96	0.44
1:A:376:ARG:HH12	1:A:412:MET:CE	2.30	0.44
1:B:41:PHE:HB2	1:B:403:VAL:HG22	1.99	0.44
1:B:157:VAL:HB	1:B:191:TRP:HB3	1.99	0.44
1:B:510:ARG:HB2	1:B:526:VAL:HG22	1.99	0.44
1:B:544:GLN:N	1:B:544:GLN:OE1	2.47	0.44
1:C:300:PHE:HB3	1:C:349:VAL:HG11	2.00	0.44
1:D:357:MET:HA	1:D:360:GLU:HG3	2.00	0.44
1:G:337:PHE:HB3	1:G:403:VAL:HB	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:99:ILE:HD11	2:N:178:SER:N	2.33	0.44
1:B:300:PHE:HB3	1:B:349:VAL:HG11	1.99	0.44
1:D:544:GLN:N	1:D:544:GLN:OE1	2.47	0.44
1:F:70:ILE:HG21	1:F:78:LEU:HD11	1.99	0.44
2:I:110:PHE:N	2:I:110:PHE:CD1	2.85	0.44
2:J:100:ASP:HA	2:J:112:ARG:HD2	1.99	0.44
2:P:323:GLU:N	2:P:324:GLY:HA2	2.31	0.44
1:D:337:PHE:HB3	1:D:403:VAL:HB	2.00	0.44
1:E:70:ILE:HG21	1:E:78:LEU:HD11	1.98	0.44
2:I:323:GLU:N	2:I:324:GLY:HA2	2.32	0.44
2:M:361:GLN:CB	2:M:372:LEU:HD13	2.45	0.44
1:A:41:PHE:HB2	1:A:403:VAL:HG22	1.98	0.44
1:C:70:ILE:HG21	1:C:78:LEU:HD11	1.99	0.44
1:D:543:LEU:HB2	1:D:563:ILE:HG21	2.00	0.44
1:B:17:HIS:CD2	1:B:99:TYR:CE2	3.04	0.43
1:E:556:GLY:CA	1:F:535:PHE:HD1	2.27	0.43
1:A:510:ARG:HB2	1:A:526:VAL:HG22	1.99	0.43
1:A:337:PHE:HB3	1:A:403:VAL:HB	1.99	0.43
1:A:543:LEU:HB2	1:A:563:ILE:HG21	2.00	0.43
1:C:157:VAL:HB	1:C:191:TRP:HB3	1.99	0.43
1:C:337:PHE:HB3	1:C:403:VAL:HB	1.99	0.43
1:E:357:MET:HA	1:E:360:GLU:HG3	1.99	0.43
1:F:357:MET:HA	1:F:360:GLU:HG3	1.99	0.43
1:F:510:ARG:HB2	1:F:526:VAL:HG22	2.00	0.43
2:I:232:GLU:HG3	2:I:317:TRP:HZ2	1.82	0.43
1:F:41:PHE:HB2	1:F:403:VAL:HG22	1.99	0.43
1:H:503:PRO:HB3	2:O:206:MET:HG3	1.94	0.43
2:I:159:GLU:OE1	2:I:300:ARG:NH2	2.51	0.43
2:K:363:GLY:H	2:K:364:ASP:CB	2.32	0.43
2:M:361:GLN:O	2:M:364:ASP:O	2.36	0.43
2:P:358:LEU:HD11	2:P:376:ALA:HB3	1.94	0.43
2:P:363:GLY:H	2:P:364:ASP:CB	2.32	0.43
1:E:432:PRO:HG3	1:F:454:ALA:HB2	2.01	0.43
1:E:583:ARG:NH1	2:N:360:ASP:HB3	2.34	0.43
2:P:232:GLU:HG3	2:P:317:TRP:HZ2	1.82	0.43
1:E:337:PHE:HB3	1:E:403:VAL:HB	2.01	0.43
1:F:79:TRP:CD1	1:F:79:TRP:C	2.92	0.43
2:L:361:GLN:CB	2:L:372:LEU:HD13	2.44	0.43
1:F:487:HIS:ND1	1:F:524:ASP:OD2	2.50	0.43
1:G:460:SER:CB	1:H:460:SER:HB3	2.49	0.43
1:G:487:HIS:ND1	1:G:524:ASP:OD2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:232:GLU:HG3	2:K:317:TRP:HZ2	1.83	0.43
2:M:101:GLU:N	2:M:102:SER:HA	2.33	0.43
2:O:232:GLU:HG3	2:O:317:TRP:HZ2	1.82	0.43
1:H:337:PHE:HB3	1:H:403:VAL:HB	1.99	0.43
2:L:232:GLU:HG3	2:L:317:TRP:HZ2	1.83	0.43
2:M:363:GLY:H	2:M:364:ASP:CB	2.32	0.43
2:N:365:ASP:HB3	2:N:366:ASP:CA	2.48	0.43
2:O:365:ASP:HB3	2:O:366:ASP:CA	2.49	0.43
2:J:363:GLY:H	2:J:364:ASP:CB	2.31	0.43
2:O:358:LEU:HD11	2:O:376:ALA:HB3	1.93	0.43
2:O:361:GLN:O	2:O:364:ASP:O	2.37	0.43
1:A:70:ILE:HD13	1:A:78:LEU:HD11	2.01	0.43
1:E:556:GLY:HA3	1:F:535:PHE:HB3	2.01	0.43
1:F:300:PHE:HB3	1:F:349:VAL:HG11	1.99	0.43
2:N:232:GLU:HG3	2:N:317:TRP:HZ2	1.83	0.43
1:A:303:MET:HB3	1:A:304:PRO:HD3	2.01	0.42
1:A:453:ASP:HA	1:D:452:GLN:NE2	2.31	0.42
1:E:79:TRP:CD1	1:E:79:TRP:C	2.92	0.42
1:E:543:LEU:HB2	1:E:563:ILE:HG21	2.00	0.42
1:H:357:MET:HA	1:H:360:GLU:HG3	2.00	0.42
2:L:78:ASP:HA	2:L:79:GLY:HA2	1.75	0.42
2:N:363:GLY:H	2:N:364:ASP:CB	2.32	0.42
2:J:175:LEU:HD23	2:J:176:LEU:N	2.33	0.42
2:L:164:LEU:HD21	2:L:243:VAL:HG23	1.99	0.42
1:G:70:ILE:HG23	1:G:75:VAL:CG2	2.50	0.42
2:K:358:LEU:HD11	2:K:376:ALA:HB3	1.94	0.42
1:A:16:GLU:O	1:A:17:HIS:ND1	2.52	0.42
1:A:417:TRP:CG	1:D:449:PRO:HD3	2.54	0.42
1:D:303:MET:HB3	1:D:304:PRO:HD3	2.01	0.42
1:D:515:GLN:O	1:D:515:GLN:HG2	2.20	0.42
1:E:181:THR:HG1	1:E:192:HIS:CD2	2.35	0.42
1:G:543:LEU:HB2	1:G:563:ILE:HG21	2.00	0.42
2:K:258:PHE:HA	2:K:259:PRO:HD3	1.95	0.42
2:M:365:ASP:HB3	2:M:366:ASP:CA	2.49	0.42
2:P:365:ASP:HB3	2:P:366:ASP:CA	2.49	0.42
1:A:232:VAL:N	1:A:233:PRO:CD	2.83	0.42
1:E:558:VAL:HG21	1:F:535:PHE:HB2	2.01	0.42
1:F:70:ILE:HG23	1:F:75:VAL:CG2	2.50	0.42
1:F:303:MET:HB3	1:F:304:PRO:HD3	2.01	0.42
1:H:79:TRP:CD1	1:H:79:TRP:C	2.93	0.42
1:H:232:VAL:N	1:H:233:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:543:LEU:HB2	1:H:563:ILE:HG21	2.00	0.42
2:I:358:LEU:HD11	2:I:376:ALA:HB3	1.94	0.42
2:K:126:VAL:CG2	2:K:137:VAL:HG23	2.50	0.42
2:N:361:GLN:O	2:N:364:ASP:O	2.37	0.42
2:O:243:VAL:O	2:O:247:LEU:HB2	2.19	0.42
2:K:365:ASP:HB3	2:K:366:ASP:CA	2.50	0.42
1:G:569:LEU:HD13	1:H:561:PRO:HG2	2.01	0.42
1:B:70:ILE:HD13	1:B:78:LEU:HD11	2.02	0.42
1:E:102:LEU:HA	1:E:103:PRO:HD2	1.87	0.42
2:I:63:GLY:N	2:I:64:PRO:HD3	2.35	0.42
2:J:361:GLN:HA	2:J:364:ASP:CB	2.50	0.42
1:D:79:TRP:CD1	1:D:79:TRP:C	2.92	0.42
1:F:543:LEU:HB2	1:F:563:ILE:HG21	2.00	0.42
1:H:311:ARG:O	2:O:226:GLY:C	2.58	0.42
2:J:133:ASN:HD22	2:J:145:LYS:HG3	1.85	0.42
2:J:173:ALA:O	2:J:174:ARG:C	2.58	0.42
2:K:243:VAL:O	2:K:247:LEU:HB2	2.19	0.42
2:M:365:ASP:HB3	2:M:366:ASP:HA	2.02	0.42
1:C:17:HIS:HD2	1:C:99:TYR:CE2	2.35	0.42
1:C:70:ILE:HD13	1:C:78:LEU:HD11	2.01	0.42
1:D:232:VAL:N	1:D:233:PRO:CD	2.83	0.42
1:G:560:PHE:CE2	1:H:571:THR:HB	2.55	0.42
2:I:96:LEU:O	2:I:99:ILE:HG22	2.20	0.42
2:N:243:VAL:O	2:N:247:LEU:HB2	2.20	0.42
1:A:276:TRP:CD2	1:A:277:PRO:HD2	2.55	0.41
1:A:487:HIS:ND1	1:A:524:ASP:OD2	2.52	0.41
1:B:70:ILE:HG23	1:B:75:VAL:CG2	2.50	0.41
1:B:486:ARG:HD3	2:J:365:ASP:O	2.20	0.41
1:C:303:MET:HB3	1:C:304:PRO:HD3	2.01	0.41
1:G:305:ARG:HH12	1:G:320:GLU:HB3	1.85	0.41
1:H:503:PRO:HB2	2:O:206:MET:HG3	1.98	0.41
2:I:5:PHE:O	2:I:7:ASP:N	2.53	0.41
2:I:99:ILE:O	2:I:112:ARG:HB3	2.20	0.41
2:K:143:ILE:HG23	2:K:194:THR:HG23	2.02	0.41
2:L:243:VAL:O	2:L:247:LEU:HB2	2.20	0.41
1:B:145:ARG:HG3	1:B:146:HIS:HD2	1.85	0.41
1:B:303:MET:HB3	1:B:304:PRO:HD3	2.01	0.41
1:F:514:ARG:NE	1:F:523:THR:OG1	2.52	0.41
2:J:363:GLY:CA	2:J:364:ASP:CB	2.98	0.41
2:K:361:GLN:O	2:K:364:ASP:O	2.38	0.41
2:L:126:VAL:HG23	2:L:137:VAL:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:ILE:HG23	1:A:75:VAL:CG2	2.50	0.41
1:D:276:TRP:CD2	1:D:277:PRO:HD2	2.55	0.41
1:D:387:GLN:HG2	1:D:575:HIS:ND1	2.36	0.41
1:E:305:ARG:HH12	1:E:320:GLU:HB3	1.85	0.41
1:H:303:MET:HB3	1:H:304:PRO:HD3	2.02	0.41
1:B:519:GLY:CA	1:B:522:LYS:HB2	2.50	0.41
1:C:70:ILE:HG23	1:C:75:VAL:CG2	2.50	0.41
1:H:387:GLN:HG2	1:H:575:HIS:ND1	2.36	0.41
1:B:232:VAL:N	1:B:233:PRO:CD	2.83	0.41
1:D:70:ILE:HD13	1:D:78:LEU:HD11	2.03	0.41
1:F:232:VAL:N	1:F:233:PRO:CD	2.84	0.41
2:J:78:ASP:HA	2:J:79:GLY:HA2	1.71	0.41
1:D:305:ARG:HH12	1:D:320:GLU:HB3	1.86	0.41
2:I:164:LEU:HD13	2:I:247:LEU:CD1	2.51	0.41
1:A:102:LEU:HA	1:A:103:PRO:HD2	1.87	0.41
1:C:487:HIS:ND1	1:C:524:ASP:OD2	2.52	0.41
1:D:70:ILE:HG23	1:D:75:VAL:CG2	2.51	0.41
2:I:223:GLU:HA	2:I:382:ARG:NH1	2.36	0.41
2:M:258:PHE:HA	2:M:259:PRO:HD3	1.94	0.41
1:C:232:VAL:N	1:C:233:PRO:CD	2.84	0.41
1:E:70:ILE:HG23	1:E:75:VAL:CG2	2.50	0.41
1:E:494:THR:O	1:E:510:ARG:HA	2.21	0.41
1:A:316:PHE:CZ	2:J:201:ALA:HB3	2.56	0.41
1:B:276:TRP:CD2	1:B:277:PRO:HD2	2.56	0.41
1:C:79:TRP:CD1	1:C:79:TRP:C	2.95	0.41
1:E:232:VAL:N	1:E:233:PRO:CD	2.83	0.41
1:E:558:VAL:HG23	1:F:535:PHE:HB3	2.03	0.41
1:G:232:VAL:N	1:G:233:PRO:CD	2.83	0.41
1:G:515:GLN:O	1:G:516:GLN:CB	2.69	0.41
2:I:363:GLY:H	2:I:364:ASP:CB	2.34	0.41
2:J:10:THR:HA	2:J:15:TYR:CD2	2.56	0.41
2:J:63:GLY:N	2:J:64:PRO:CD	2.84	0.41
2:K:127:PHE:O	2:K:129:ALA:N	2.54	0.41
2:K:164:LEU:HD21	2:K:243:VAL:CG2	2.48	0.41
2:L:363:GLY:H	2:L:364:ASP:CB	2.34	0.41
2:M:151:THR:CB	2:M:330:LEU:HD11	2.51	0.41
2:O:363:GLY:CA	2:O:364:ASP:CB	2.99	0.41
1:A:452:GLN:NE2	1:D:453:ASP:HA	2.35	0.41
1:B:376:ARG:HH12	1:B:412:MET:HE1	1.86	0.41
1:C:17:HIS:NE2	1:C:99:TYR:CE2	2.89	0.41
1:F:305:ARG:HH12	1:F:320:GLU:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:494:THR:O	1:F:510:ARG:HA	2.20	0.41
1:G:303:MET:HB3	1:G:304:PRO:HD3	2.03	0.41
1:G:494:THR:O	1:G:510:ARG:HA	2.21	0.41
1:G:535:PHE:CG	1:H:556:GLY:O	2.74	0.41
1:H:70:ILE:HG23	1:H:75:VAL:CG2	2.52	0.41
2:M:361:GLN:HA	2:M:364:ASP:CB	2.51	0.41
1:B:387:GLN:HG2	1:B:575:HIS:ND1	2.36	0.40
2:K:152:PRO:O	2:K:330:LEU:HD13	2.20	0.40
1:A:79:TRP:CD1	1:A:79:TRP:C	2.94	0.40
1:B:452:GLN:HE22	1:C:453:ASP:HA	1.86	0.40
1:C:305:ARG:HH12	1:C:320:GLU:HB3	1.87	0.40
1:F:276:TRP:CD2	1:F:277:PRO:HD2	2.55	0.40
1:G:70:ILE:HD13	1:G:78:LEU:HD11	2.03	0.40
1:B:286:ASP:HA	1:B:287:PRO:HD3	1.93	0.40
2:I:64:PRO:HA	2:I:65:ILE:O	2.21	0.40
2:K:223:GLU:HA	2:K:382:ARG:NH1	2.37	0.40
2:P:361:GLN:O	2:P:364:ASP:O	2.39	0.40
1:C:573:PRO:HD3	1:D:573:PRO:HD3	2.03	0.40
1:E:387:GLN:HG2	1:E:575:HIS:ND1	2.37	0.40
1:H:70:ILE:HD13	1:H:78:LEU:HD11	2.03	0.40
2:I:160:LEU:HD13	2:I:160:LEU:HA	1.94	0.40
2:J:223:GLU:HA	2:J:382:ARG:NH1	2.35	0.40
2:L:361:GLN:O	2:L:364:ASP:O	2.39	0.40
1:C:387:GLN:HG2	1:C:575:HIS:ND1	2.37	0.40
1:E:410:ILE:HG22	1:E:474:LEU:HB2	2.03	0.40
1:E:558:VAL:HA	2:N:212:ARG:NE	2.35	0.40
1:G:17:HIS:CD2	1:G:99:TYR:CD1	3.09	0.40
2:J:243:VAL:O	2:J:247:LEU:HB2	2.22	0.40
2:M:243:VAL:O	2:M:247:LEU:HB2	2.21	0.40
2:P:243:VAL:O	2:P:247:LEU:HB2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	561/593 (95%)	546 (97%)	13 (2%)	2 (0%)	34	71
1	B	569/593 (96%)	551 (97%)	16 (3%)	2 (0%)	34	71
1	C	565/593 (95%)	549 (97%)	14 (2%)	2 (0%)	34	71
1	D	569/593 (96%)	550 (97%)	16 (3%)	3 (0%)	29	68
1	E	545/593 (92%)	533 (98%)	12 (2%)	0	100	100
1	F	569/593 (96%)	553 (97%)	14 (2%)	2 (0%)	34	71
1	G	569/593 (96%)	548 (96%)	20 (4%)	1 (0%)	47	79
1	H	538/593 (91%)	528 (98%)	10 (2%)	0	100	100
2	I	431/441 (98%)	382 (89%)	43 (10%)	6 (1%)	11	48
2	J	431/441 (98%)	382 (89%)	41 (10%)	8 (2%)	8	42
2	K	349/441 (79%)	318 (91%)	25 (7%)	6 (2%)	9	45
2	L	432/441 (98%)	388 (90%)	35 (8%)	9 (2%)	7	40
2	M	425/441 (96%)	381 (90%)	35 (8%)	9 (2%)	7	40
2	N	345/441 (78%)	318 (92%)	24 (7%)	3 (1%)	17	57
2	O	235/441 (53%)	221 (94%)	13 (6%)	1 (0%)	34	71
2	P	235/441 (53%)	220 (94%)	14 (6%)	1 (0%)	34	71
All	All	7368/8272 (89%)	6968 (95%)	345 (5%)	55 (1%)	22	61

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	ILE
1	B	25	HIS
1	C	10	VAL
2	I	275	PRO
2	J	275	PRO
2	K	275	PRO
2	L	275	PRO
2	M	106	GLN
2	M	275	PRO
2	N	275	PRO
2	O	275	PRO
2	P	275	PRO
1	A	17	HIS
1	B	22	ASP

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Mol	Chain	Res	Type
1	D	516	GLN
1	F	516	GLN
1	G	516	GLN
2	I	6	GLU
2	I	78	ASP
2	J	70	VAL
2	J	124	PRO
2	K	128	GLY
2	L	13	ARG
2	L	106	GLN
2	L	365	ASP
2	M	21	GLU
2	N	123	PRO
1	D	522	LYS
1	F	22	ASP
2	J	24	SER
2	J	73	THR
2	K	106	GLN
2	K	124	PRO
2	M	6	GLU
1	D	24	GLY
2	I	123	PRO
2	J	56	VAL
2	K	123	PRO
2	K	184	GLU
2	L	123	PRO
2	M	13	ARG
2	M	123	PRO
2	M	142	ALA
2	M	184	GLU
2	N	184	GLU
1	C	13	GLY
2	I	106	GLN
2	L	3	VAL
2	I	124	PRO
2	L	124	PRO
2	L	56	VAL
2	L	71	VAL
2	J	123	PRO
2	J	153	GLY
2	M	56	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	489/512 (96%)	486 (99%)	3 (1%)	86	94
1	B	495/512 (97%)	488 (99%)	7 (1%)	67	85
1	C	489/512 (96%)	484 (99%)	5 (1%)	76	88
1	D	495/512 (97%)	491 (99%)	4 (1%)	81	91
1	E	480/512 (94%)	477 (99%)	3 (1%)	86	94
1	F	495/512 (97%)	491 (99%)	4 (1%)	81	91
1	G	495/512 (97%)	491 (99%)	4 (1%)	81	91
1	H	475/512 (93%)	472 (99%)	3 (1%)	86	94
2	I	211/351 (60%)	198 (94%)	13 (6%)	18	53
2	J	208/351 (59%)	198 (95%)	10 (5%)	25	60
2	K	178/351 (51%)	175 (98%)	3 (2%)	60	82
2	L	210/351 (60%)	202 (96%)	8 (4%)	33	66
2	M	210/351 (60%)	202 (96%)	8 (4%)	33	66
2	N	175/351 (50%)	172 (98%)	3 (2%)	60	82
2	O	110/351 (31%)	108 (98%)	2 (2%)	59	81
2	P	110/351 (31%)	108 (98%)	2 (2%)	59	81
All	All	5325/6904 (77%)	5243 (98%)	82 (2%)	65	84

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	ASP
1	A	337	PHE
1	A	451	ASN
1	B	27	ARG
1	B	28	THR
1	B	59	ASP
1	B	61	ARG
1	B	165	TYR

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Mol	Chain	Res	Type
1	B	337	PHE
1	B	451	ASN
1	C	17	HIS
1	C	59	ASP
1	C	61	ARG
1	C	337	PHE
1	C	451	ASN
1	D	22	ASP
1	D	59	ASP
1	D	337	PHE
1	D	451	ASN
1	E	59	ASP
1	E	337	PHE
1	E	451	ASN
1	F	59	ASP
1	F	61	ARG
1	F	337	PHE
1	F	451	ASN
1	G	28	THR
1	G	59	ASP
1	G	337	PHE
1	G	451	ASN
1	H	59	ASP
1	H	337	PHE
1	H	451	ASN
2	I	2	SER
2	I	69	SER
2	I	78	ASP
2	I	97	SER
2	I	100	ASP
2	I	102	SER
2	I	104	THR
2	I	110	PHE
2	I	112	ARG
2	I	134	THR
2	I	176	LEU
2	I	310	VAL
2	I	366	ASP
2	J	27	THR
2	J	68	TYR
2	J	104	THR
2	J	134	THR

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Mol	Chain	Res	Type
2	J	164	LEU
2	J	166	ARG
2	J	172	VAL
2	J	176	LEU
2	J	194	THR
2	J	310	VAL
2	K	194	THR
2	K	310	VAL
2	K	366	ASP
2	L	5	PHE
2	L	104	THR
2	L	132	SER
2	L	135	SER
2	L	157	ASP
2	L	164	LEU
2	L	166	ARG
2	L	310	VAL
2	M	7	ASP
2	M	27	THR
2	M	104	THR
2	M	135	SER
2	M	166	ARG
2	M	175	LEU
2	M	310	VAL
2	M	366	ASP
2	N	104	THR
2	N	310	VAL
2	N	366	ASP
2	O	310	VAL
2	O	366	ASP
2	P	310	VAL
2	P	366	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	146	HIS
1	A	197	HIS
1	A	452	GLN
1	B	17	HIS
1	B	146	HIS
1	B	197	HIS

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Mol	Chain	Res	Type
1	B	452	GLN
1	B	515	GLN
1	C	17	HIS
1	C	146	HIS
1	C	197	HIS
1	C	452	GLN
1	D	146	HIS
1	D	197	HIS
1	D	452	GLN
1	E	146	HIS
1	E	197	HIS
1	F	146	HIS
1	F	197	HIS
1	G	146	HIS
1	G	197	HIS
1	H	146	HIS
1	H	197	HIS
2	J	11	GLN
2	L	11	GLN
2	L	155	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	565/593 (95%)	-0.21	0 100 100	34, 53, 96, 118	0
1	B	571/593 (96%)	-0.25	5 (0%) 84 73	28, 43, 64, 79	0
1	C	569/593 (95%)	-0.21	0 100 100	35, 51, 79, 106	0
1	D	571/593 (96%)	-0.13	5 (0%) 84 73	44, 77, 111, 129	0
1	E	549/593 (92%)	0.06	9 (1%) 72 57	67, 102, 176, 208	0
1	F	571/593 (96%)	0.16	16 (2%) 53 37	68, 119, 249, 314	0
1	G	571/593 (96%)	0.24	21 (3%) 41 27	80, 142, 218, 251	0
1	H	544/593 (91%)	0.60	51 (9%) 8 4	89, 159, 248, 316	0
2	I	435/441 (98%)	-0.32	6 (1%) 75 61	38, 62, 111, 129	0
2	J	435/441 (98%)	-0.09	5 (1%) 80 68	55, 92, 152, 171	0
2	K	353/441 (80%)	0.30	34 (9%) 8 4	106, 160, 228, 246	0
2	L	436/441 (98%)	0.10	21 (4%) 30 19	88, 119, 163, 181	0
2	M	431/441 (97%)	0.09	16 (3%) 41 27	99, 131, 188, 228	0
2	N	349/441 (79%)	0.37	30 (8%) 10 6	116, 177, 233, 254	0
2	O	239/441 (54%)	0.38	26 (10%) 5 3	168, 210, 253, 266	0
2	P	239/441 (54%)	1.04	50 (20%) 1 0	150, 195, 247, 256	0
All	All	7428/8272 (89%)	0.08	295 (3%) 38 25	28, 106, 220, 316	0

All (295) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	301	VAL	6.8
2	L	361	GLN	6.6
2	M	177	GLY	6.3
2	K	132	SER	6.2
2	P	342	ASP	6.1

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Mol	Chain	Res	Type	RSRZ
1	H	134	THR	5.9
1	H	160	ASP	5.8
1	H	131	MET	5.7
2	L	132	SER	5.6
2	N	175	LEU	5.6
2	K	177	GLY	5.6
2	N	176	LEU	5.5
2	P	325	GLU	5.5
1	H	159	SER	5.4
2	P	275	PRO	5.3
2	K	189	ALA	5.3
2	L	358	LEU	5.0
1	H	558	VAL	4.9
2	P	305	LEU	4.9
2	K	128	GLY	4.8
2	P	320	ILE	4.8
2	N	177	GLY	4.8
1	H	586	ASP	4.7
1	D	520	GLY	4.7
2	P	276	GLU	4.6
2	P	419	ALA	4.6
2	N	181	THR	4.5
2	P	302	HIS	4.4
2	L	78	ASP	4.4
1	H	140	TRP	4.3
1	F	518	ASP	4.3
2	P	277	LEU	4.3
2	O	319	LEU	4.2
1	H	171	ILE	4.2
1	H	182	PHE	4.2
2	P	321	ASP	4.2
1	F	203	TYR	4.1
2	O	320	ILE	4.1
1	H	50	TYR	4.1
1	H	156	TYR	4.1
2	I	361	GLN	4.1
2	P	322	PHE	4.1
1	H	183	ASP	4.1
2	O	372	LEU	4.0
1	G	386	ASN	4.0
2	N	132	SER	4.0
1	B	520	GLY	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	521	ALA	4.0
2	N	360	ASP	3.9
2	P	273	ALA	3.9
2	K	149	ARG	3.9
2	K	191	GLY	3.9
2	K	144	PHE	3.8
2	N	155	HIS	3.8
2	K	86	LEU	3.7
2	K	176	LEU	3.7
1	H	582	LEU	3.7
1	H	172	PHE	3.6
1	B	521	ALA	3.6
2	O	357	ARG	3.6
2	P	331	ASP	3.6
2	P	289	HIS	3.6
2	N	108	VAL	3.6
1	H	184	PRO	3.6
1	G	522	LYS	3.5
2	P	198	ALA	3.5
2	P	274	VAL	3.5
2	N	149	ARG	3.5
2	O	222	ALA	3.5
1	H	151	PRO	3.5
2	P	353	ALA	3.5
2	N	361	GLN	3.5
1	H	155	PHE	3.5
2	P	346	ILE	3.5
2	K	301	VAL	3.5
2	O	361	GLN	3.4
1	H	143	GLU	3.4
2	M	176	LEU	3.4
1	G	24	GLY	3.4
2	O	323	GLU	3.4
2	O	338	THR	3.4
2	K	293	ASP	3.3
2	N	301	VAL	3.3
2	P	355	HIS	3.3
2	P	343	VAL	3.3
1	H	386	ASN	3.3
1	H	135	SER	3.3
1	F	157	VAL	3.3
1	D	521	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	F	168	ALA	3.3
2	P	285	GLU	3.3
2	P	262	VAL	3.3
1	H	201	LEU	3.2
2	P	265	GLN	3.2
1	H	98	PHE	3.2
2	M	288	TYR	3.2
1	H	83	PHE	3.2
1	G	215	VAL	3.2
2	O	404	ASP	3.1
2	L	55	GLN	3.1
2	N	365	ASP	3.1
2	K	87	TYR	3.1
1	E	99	TYR	3.1
1	G	67	LEU	3.1
2	O	358	LEU	3.1
2	M	81	THR	3.1
2	N	358	LEU	3.1
2	P	384	CYS	3.0
2	N	347	LEU	3.0
2	P	301	VAL	3.0
2	O	322	PHE	3.0
2	P	432	PRO	3.0
2	L	131	GLN	3.0
1	H	157	VAL	3.0
2	O	343	VAL	3.0
1	H	295	HIS	3.0
1	H	556	GLY	2.9
2	P	319	LEU	2.9
2	O	310	VAL	2.9
1	G	219	TRP	2.9
1	H	323	ALA	2.9
2	P	426	PRO	2.9
2	N	277	LEU	2.9
1	H	188	GLN	2.9
1	F	24	GLY	2.9
2	L	253	THR	2.9
2	J	361	GLN	2.9
1	F	386	ASN	2.9
2	M	133	ASN	2.9
2	O	341	ARG	2.9
1	G	520	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
2	L	144	PHE	2.8
2	K	135	SER	2.8
2	O	337	ASP	2.8
1	H	561	PRO	2.8
2	K	96	LEU	2.8
2	L	52	GLU	2.8
2	P	341	ARG	2.8
2	I	44	ALA	2.8
1	G	128	ASP	2.8
2	I	358	LEU	2.8
1	F	187	ARG	2.8
2	P	284	ILE	2.8
2	M	361	GLN	2.8
1	H	100	LYS	2.7
2	M	155	HIS	2.7
1	H	29	LEU	2.7
1	H	77	CYS	2.7
2	O	331	ASP	2.7
1	E	84	TYR	2.7
2	N	343	VAL	2.7
2	N	138	PHE	2.7
2	O	215	PHE	2.7
2	M	62	SER	2.7
1	F	522	LYS	2.7
1	H	190	TYR	2.7
2	L	77	ALA	2.7
2	L	183	TRP	2.7
1	G	77	CYS	2.7
2	L	319	LEU	2.7
2	O	308	GLY	2.7
2	L	215	PHE	2.7
1	E	156	TYR	2.6
2	O	221	TYR	2.6
1	F	184	PRO	2.6
2	I	50	PRO	2.6
2	P	263	MET	2.6
2	L	305	LEU	2.6
2	J	131	GLN	2.6
2	N	357	ARG	2.6
1	D	185	VAL	2.6
2	K	154	VAL	2.6
2	P	261	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
2	N	152	PRO	2.6
2	K	110	PHE	2.6
2	K	181	THR	2.6
2	P	280	HIS	2.6
1	H	158	TRP	2.6
2	K	188	TYR	2.5
2	K	190	LEU	2.5
2	P	286	GLU	2.5
2	M	419	ALA	2.5
2	K	98	LEU	2.5
2	O	318	LEU	2.5
2	P	366	ASP	2.5
1	H	350	THR	2.5
2	P	259	PRO	2.5
1	F	171	ILE	2.5
1	D	522	LYS	2.5
1	E	182	PHE	2.5
2	P	357	ARG	2.5
2	O	309	GLN	2.5
2	K	180	GLU	2.4
2	K	361	GLN	2.4
1	H	95	ILE	2.4
1	B	519	GLY	2.4
1	F	501	SER	2.4
1	G	131	MET	2.4
1	E	155	PHE	2.4
2	N	346	ILE	2.4
1	E	98	PHE	2.4
1	G	191	TRP	2.4
1	G	203	TYR	2.4
1	H	583	ARG	2.4
2	M	178	SER	2.4
2	P	347	LEU	2.4
2	K	288	TYR	2.4
1	H	170	ILE	2.4
2	P	376	ALA	2.4
1	F	185	VAL	2.4
2	O	305	LEU	2.4
2	N	154	VAL	2.4
1	H	176	GLU	2.4
2	M	54	TYR	2.4
2	P	323	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	N	153	GLY	2.4
1	H	49	PHE	2.4
1	H	152	TYR	2.4
1	E	524	ASP	2.4
1	B	522	LYS	2.4
1	H	199	PRO	2.4
2	L	87	TYR	2.4
2	P	199	ASN	2.4
2	I	354	ALA	2.4
2	P	215	PHE	2.3
2	L	181	THR	2.3
2	J	299	GLN	2.3
1	G	267	ARG	2.3
2	K	153	GLY	2.3
2	L	86	LEU	2.3
1	G	573	PRO	2.3
2	K	282	PRO	2.3
2	K	111	VAL	2.3
1	H	99	TYR	2.3
1	G	163	ASP	2.3
1	D	519	GLY	2.3
1	H	500	GLY	2.3
2	N	364	ASP	2.3
1	H	30	PRO	2.3
2	K	178	SER	2.3
1	E	154	ASP	2.3
2	J	360	ASP	2.3
2	N	189	ALA	2.3
2	M	347	LEU	2.3
2	N	94	TYR	2.2
1	F	109	ASP	2.2
2	K	103	ALA	2.2
2	N	432	PRO	2.2
2	K	305	LEU	2.2
2	L	299	GLN	2.2
2	I	357	ARG	2.2
2	M	175	LEU	2.2
2	K	147	PHE	2.2
2	O	302	HIS	2.2
2	L	271	VAL	2.2
2	L	76	ILE	2.2
1	H	245	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
2	K	133	ASN	2.2
2	J	5	PHE	2.2
2	M	357	ARG	2.2
2	K	84	ASP	2.2
2	P	287	ARG	2.2
2	L	160	LEU	2.2
1	E	525	ALA	2.2
2	N	131	GLN	2.2
2	P	324	GLY	2.2
2	K	277	LEU	2.2
2	O	250	GLU	2.1
1	H	105	PHE	2.1
1	F	517	GLY	2.1
1	H	232	VAL	2.1
2	N	305	LEU	2.1
2	P	264	ALA	2.1
2	M	60	THR	2.1
1	G	169	ARG	2.1
1	F	113	THR	2.1
1	H	553	GLU	2.1
2	P	282	PRO	2.1
2	K	289	HIS	2.1
2	N	322	PHE	2.1
2	P	412	ASP	2.1
2	P	252	GLY	2.1
1	B	587	PRO	2.0
1	G	492	VAL	2.0
2	M	86	LEU	2.0
2	O	373	ALA	2.0
1	G	99	TYR	2.0
1	F	454	ALA	2.0
2	P	354	ALA	2.0
1	G	114	LEU	2.0
2	P	350	PHE	2.0
1	G	23	PHE	2.0
2	N	215	PHE	2.0
1	H	78	LEU	2.0
1	H	122	GLY	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	H	601	1/1	0.53	0.33	20,20,20,20	0
3	CA	F	601	1/1	0.79	0.81	20,20,20,20	0
3	CA	D	601	1/1	0.93	0.06	20,20,20,20	0
3	CA	E	601	1/1	0.93	0.21	20,20,20,20	0
3	CA	B	601	1/1	0.97	0.13	20,20,20,20	0
3	CA	G	601	1/1	0.98	0.16	20,20,20,20	0
3	CA	A	601	1/1	0.98	0.05	20,20,20,20	0
3	CA	C	601	1/1	0.99	0.11	20,20,20,20	0

6.5 Other polymers (i)

There are no such residues in this entry.