



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 4, 2017 – 09:43 AM EDT

PDB ID : 5JY7
Title : Complex of Mycobacterium smegmatis trehalose synthase with maltokinase
Authors : Futterer, K.; Kermani, A.A.; Besra, G.S.
Deposited on : unknown
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20029824

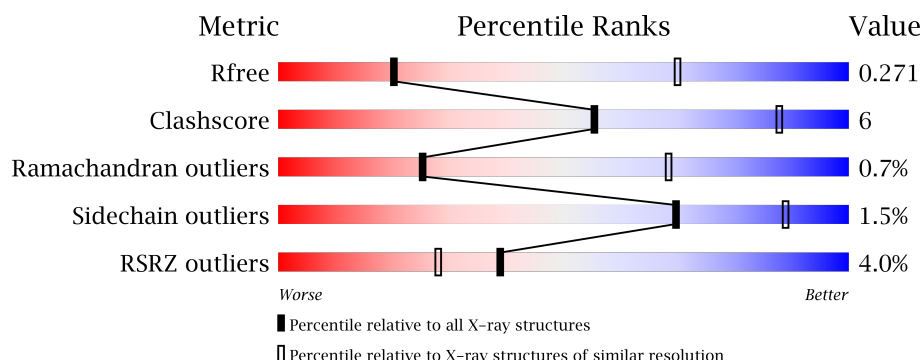
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	100719	1026 (3.74-3.46)
Clashscore	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)
RSRZ outliers	101464	1051 (3.74-3.46)

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

Mol	Chain	Length	Quality of chain
1	A	593	
1	B	593	
1	C	593	
1	D	593	
1	E	593	

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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

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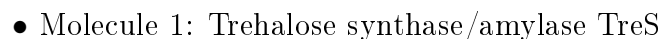
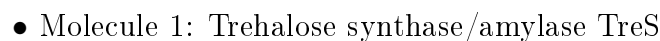
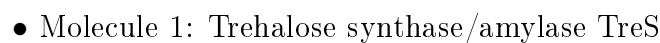
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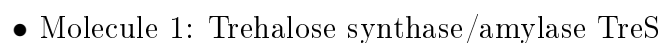
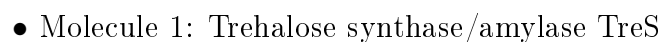
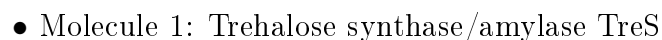
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	239	Total	C	N	O	S	0	0	0
			1584	974	291	315	4			
2	P	239	Total	C	N	O	S	0	0	0
			1584	974	291	315	4			

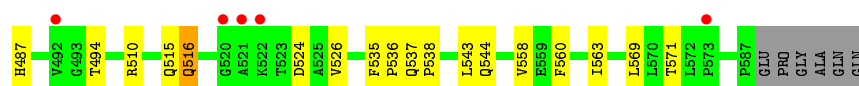
- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	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	H	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	A	1	Total	Ca	0	0
			1	1		
3	F	1	Total	Ca	0	0
			1	1		

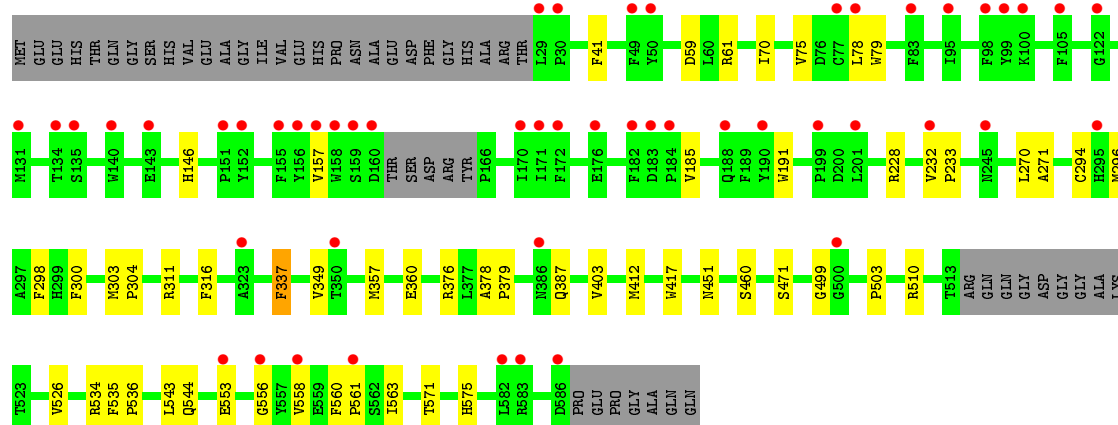
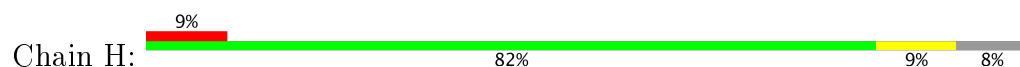
- Molecule 1: Trehalose synthase/amylase TreS



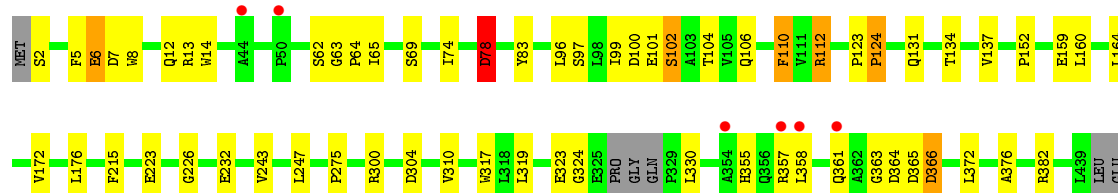
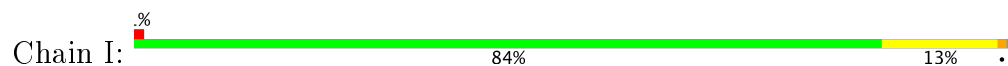




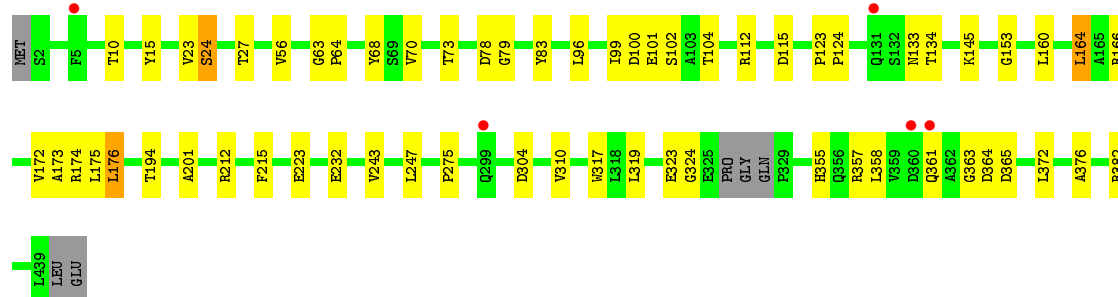
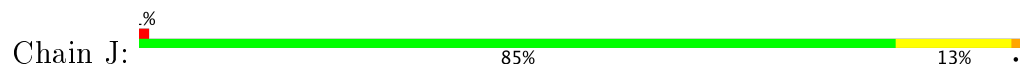
• Molecule 1: Trehalose synthase/amilase TreS



• Molecule 2: Maltokinase

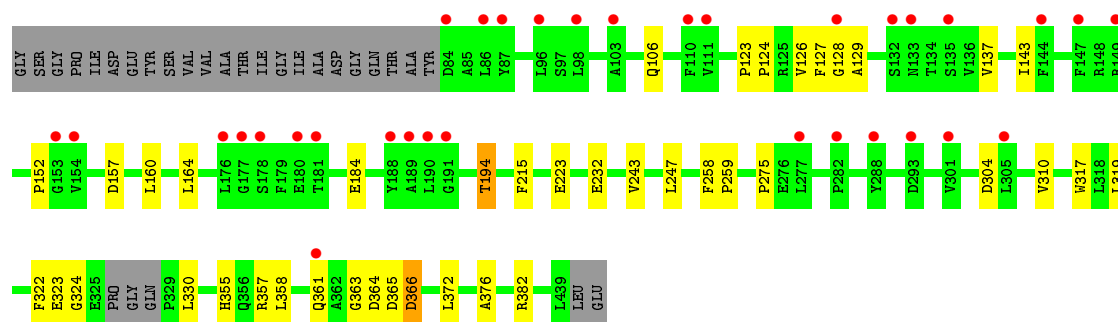


• Molecule 2: Maltokinase

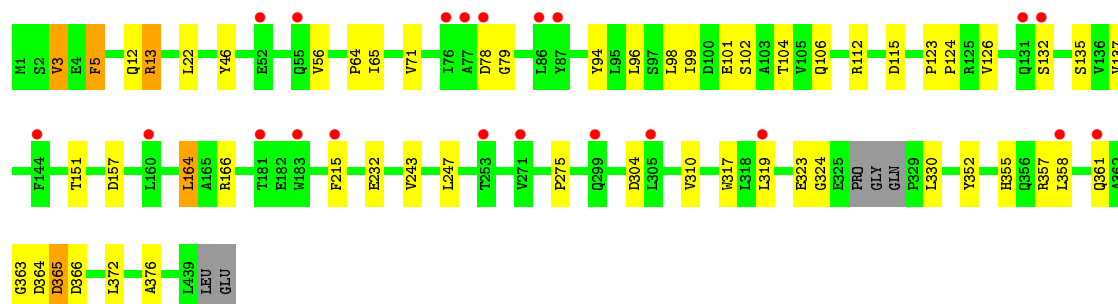
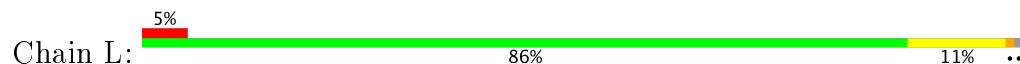


• Molecule 2: Maltokinase

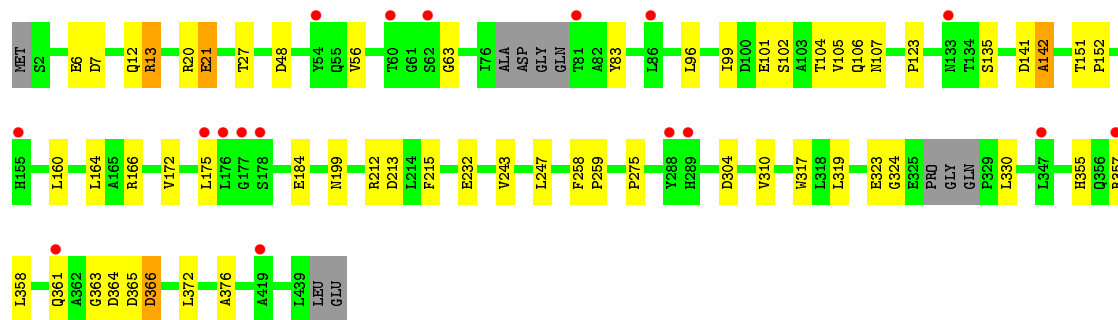
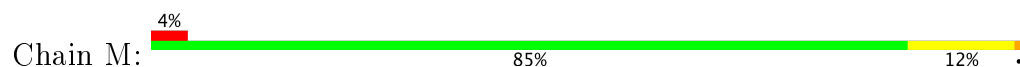




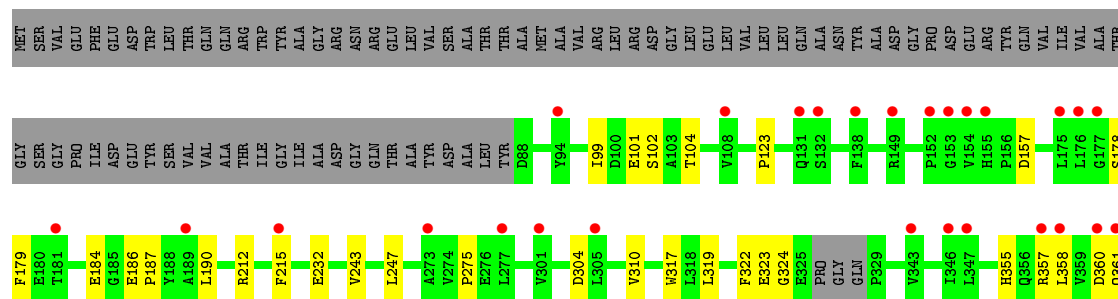
• Molecule 2: Maltokinase



• Molecule 2: Maltokinase



• Molecule 2: Maltokinase



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 (5.26%)	DCC
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 , 76.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	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.*

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: 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(°)	Ideal(°)
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	Mainchain,Peptide

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: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:B:17:HIS:HD2	1:B:99:TYR:CE2	2.24	0.56
2:I:358:LEU:CD2	2:I:372:LEU:HB3	2.35	0.56
1:G:558:VAL:HG22	2:O:212:ARG:HD3	1.88	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
2:K:358:LEU:HA	2:K:361:GLN:HB2	1.88	0.56
1:E:534:ARG:HH22	2:M:213:ASP:CG	2.09	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:357:ARG:O	2:I:361:GLN:N	2.39	0.56
2:I:63:GLY:HA2	2:I:83:TYR:CZ	2.40	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:C:378:ALA:HB3	1:C:379:PRO:HD3	1.89	0.53
1:A:449:PRO:HD3	1:D:417:TRP:CG	2.44	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
2:L:22:LEU:HA	2:L:46:TYR:HA	1.92	0.52
1:E:558:VAL:HA	2:N:212:ARG:HE	1.74	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:243:VAL:HG11	2:I:319:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:62:SER:C	2:I:64:PRO:HD3	2.35	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:N:215:PHE:CD2	2:N:361:GLN:CD	2.88	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
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:N	1:F:544:GLN:OE1	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:G:544:GLN:N	1:G:544:GLN:OE1	2.48	0.46
1:H:376:ARG:HH12	1:H:412:MET:CE	2.28	0.46
1:F:445:ARG:HG2	1:H:417:TRP:CE2	2.50	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:569:LEU:CD1	1:H:561:PRO:HG2	2.44	0.46
1:G:70:ILE:HG21	1:G:78:LEU:HD11	1.98	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: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:F:558:VAL:HG22	2:M:212:ARG:HD3	1.98	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:112:ARG:NH2	2:L:115:ASP:O	2.48	0.45
2:L:64:PRO:CB	2:L:65:ILE:HA	2.46	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:510:ARG:HB2	1:H:526:VAL:HG22	1.99	0.45
1:H:70:ILE:HG21	1:H:78:LEU:HD11	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
2:J:232:GLU:HG3	2:J:317:TRP:HZ2	1.81	0.45
1:F:521:ALA:HB3	2:M:364:ASP:H	1.82	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:157:VAL:HB	1:B:191:TRP:HB3	1.99	0.44
1:B:41:PHE:HB2	1:B:403:VAL:HG22	1.99	0.44
1:B:510:ARG:HB2	1:B:526:VAL:HG22	1.99	0.44
1:B:544:GLN:OE1	1:B:544:GLN:N	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:CD1	2:I:110:PHE:N	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
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
1:H:503:PRO:HB3	2:O:206:MET:HG3	1.94	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:583:ARG:NH1	2:N:360:ASP:HB3	2.34	0.43
1:E:432:PRO:HG3	1:F:454:ALA:HB2	2.01	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:C	1:F:79:TRP:CD1	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:487:HIS:ND1	1:G:524:ASP:OD2	2.52	0.43
1:G:460:SER:CB	1:H:460:SER:HB3	2.49	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:543:LEU:HB2	1:E:563:ILE:HG21	2.00	0.42
1:E:79:TRP:CD1	1:E:79:TRP:C	2.92	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:HG2	1:D:515:GLN:O	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:F:303:MET:HB3	1:F:304:PRO:HD3	2.01	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:H:232:VAL:N	1:H:233:PRO:CD	2.83	0.42
1:H:543:LEU:HB2	1:H:563:ILE:HG21	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:79:TRP:CD1	1:H:79:TRP:C	2.93	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:C	1:D:79:TRP:CD1	2.92	0.42
1:F:543:LEU:HB2	1:F:563:ILE:HG21	2.00	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:H:311:ARG:O	2:O:226:GLY:C	2.58	0.42
1:C:70:ILE:HD13	1:C:78:LEU:HD11	2.01	0.42
1:C:17:HIS:HD2	1:C:99:TYR:CE2	2.35	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: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
2:I:99:ILE:O	2:I:112:ARG:HB3	2.20	0.41
2:I:5:PHE:O	2:I:7:ASP:N	2.53	0.41
1:B:486:ARG:HD3	2:J:365:ASP:O	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:H:503:PRO:HB2	2:O:206:MET:HG3	1.98	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:494:THR:O	1:E:510:ARG:HA	2.21	0.41
1:E:70:ILE:HG23	1:E:75:VAL:CG2	2.50	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: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:B:276:TRP:CD2	1:B:277:PRO:HD2	2.56	0.41
1:C:79:TRP:C	1:C:79:TRP:CD1	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
2:J:10:THR:HA	2:J:15:TYR:CD2	2.56	0.41
1:A:316:PHE:CZ	2:J:201:ALA:HB3	2.56	0.41
2:J:63:GLY:N	2:J:64:PRO:CD	2.84	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:A:452:GLN:NE2	1:D:453:ASP:HA	2.35	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:C	1:A:79:TRP:CD1	2.94	0.40
1:C:305:ARG:HH12	1:C:320:GLU:HB3	1.87	0.40
1:B:452:GLN:HE22	1:C:453:ASP:HA	1.86	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%)	38	77
1	B	569/593 (96%)	551 (97%)	16 (3%)	2 (0%)	38	77
1	C	565/593 (95%)	549 (97%)	14 (2%)	2 (0%)	38	77
1	D	569/593 (96%)	550 (97%)	16 (3%)	3 (0%)	32	73
1	E	545/593 (92%)	533 (98%)	12 (2%)	0	100	100
1	F	569/593 (96%)	553 (97%)	14 (2%)	2 (0%)	38	77
1	G	569/593 (96%)	548 (96%)	20 (4%)	1 (0%)	51	85
1	H	538/593 (91%)	528 (98%)	10 (2%)	0	100	100
2	I	431/441 (98%)	382 (89%)	43 (10%)	6 (1%)	13	56
2	J	431/441 (98%)	382 (89%)	41 (10%)	8 (2%)	9	50
2	K	349/441 (79%)	318 (91%)	25 (7%)	6 (2%)	11	52
2	L	432/441 (98%)	388 (90%)	35 (8%)	9 (2%)	8	48
2	M	425/441 (96%)	381 (90%)	35 (8%)	9 (2%)	8	48
2	N	345/441 (78%)	318 (92%)	24 (7%)	3 (1%)	20	64
2	O	235/441 (53%)	221 (94%)	13 (6%)	1 (0%)	38	77
2	P	235/441 (53%)	220 (94%)	14 (6%)	1 (0%)	38	77
All	All	7368/8272 (89%)	6968 (95%)	345 (5%)	55 (1%)	25	68

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 ⓘ

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%)	89	96
1	B	495/512 (97%)	488 (99%)	7 (1%)	71	89
1	C	489/512 (96%)	484 (99%)	5 (1%)	80	91
1	D	495/512 (97%)	491 (99%)	4 (1%)	85	94
1	E	480/512 (94%)	477 (99%)	3 (1%)	89	96
1	F	495/512 (97%)	491 (99%)	4 (1%)	85	94
1	G	495/512 (97%)	491 (99%)	4 (1%)	85	94
1	H	475/512 (93%)	472 (99%)	3 (1%)	89	96
2	I	211/351 (60%)	198 (94%)	13 (6%)	21	61
2	J	208/351 (59%)	198 (95%)	10 (5%)	30	68
2	K	178/351 (51%)	175 (98%)	3 (2%)	66	88
2	L	210/351 (60%)	202 (96%)	8 (4%)	38	74
2	M	210/351 (60%)	202 (96%)	8 (4%)	38	74
2	N	175/351 (50%)	172 (98%)	3 (2%)	66	88
2	O	110/351 (31%)	108 (98%)	2 (2%)	64	87
2	P	110/351 (31%)	108 (98%)	2 (2%)	64	87
All	All	5325/6904 (77%)	5243 (98%)	82 (2%)	70	89

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

Some 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 carbohydrates 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, 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	565/593 (95%)	-0.21	0 100 100	34, 53, 96, 118	0
1	B	571/593 (96%)	-0.25	5 (0%) 84 72	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 72	44, 77, 111, 129	0
1	E	549/593 (92%)	0.06	9 (1%) 72 59	67, 102, 176, 208	0
1	F	571/593 (96%)	0.16	16 (2%) 53 40	68, 119, 249, 314	0
1	G	571/593 (96%)	0.24	22 (3%) 40 29	80, 142, 218, 251	0
1	H	544/593 (91%)	0.60	51 (9%) 9 7	89, 159, 248, 316	0
2	I	435/441 (98%)	-0.32	6 (1%) 75 62	38, 62, 111, 129	0
2	J	435/441 (98%)	-0.09	5 (1%) 80 67	55, 92, 152, 171	0
2	K	353/441 (80%)	0.31	33 (9%) 9 7	106, 160, 228, 246	0
2	L	436/441 (98%)	0.10	21 (4%) 31 22	88, 119, 163, 181	0
2	M	431/441 (97%)	0.10	17 (3%) 40 29	99, 131, 188, 228	0
2	N	349/441 (79%)	0.37	30 (8%) 11 9	116, 177, 233, 254	0
2	O	239/441 (54%)	0.39	28 (11%) 5 5	168, 210, 253, 266	0
2	P	239/441 (54%)	1.05	52 (21%) 1 1	150, 195, 247, 256	0
All	All	7428/8272 (89%)	0.08	300 (4%) 39 28	28, 106, 220, 316	0

All (300) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	O	301	VAL	6.9
2	L	361	GLN	6.5
2	P	342	ASP	6.3
2	M	177	GLY	6.2
2	K	132	SER	6.2

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Mol	Chain	Res	Type	RSRZ
1	H	134	THR	6.1
1	H	131	MET	5.8
1	H	160	ASP	5.7
2	K	177	GLY	5.7
2	L	132	SER	5.6
2	P	275	PRO	5.6
2	N	175	LEU	5.6
2	N	176	LEU	5.6
2	P	325	GLU	5.5
1	H	159	SER	5.3
2	K	189	ALA	5.2
2	N	177	GLY	5.1
2	P	305	LEU	5.0
1	H	558	VAL	4.8
2	L	358	LEU	4.8
2	K	128	GLY	4.8
1	H	586	ASP	4.7
1	D	520	GLY	4.7
2	P	276	GLU	4.7
2	P	320	ILE	4.7
1	F	518	ASP	4.5
2	P	419	ALA	4.5
2	P	302	HIS	4.4
2	P	277	LEU	4.4
2	L	78	ASP	4.4
1	H	140	TRP	4.4
2	N	181	THR	4.3
2	P	321	ASP	4.2
1	H	50	TYR	4.2
2	O	320	ILE	4.2
2	O	319	LEU	4.2
2	N	132	SER	4.1
1	H	183	ASP	4.1
2	P	322	PHE	4.1
1	H	171	ILE	4.1
1	H	156	TYR	4.1
1	F	203	TYR	4.1
2	I	361	GLN	4.1
2	O	372	LEU	4.0
1	H	182	PHE	4.0
1	G	386	ASN	4.0
2	P	273	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	G	521	ALA	4.0
2	K	144	PHE	3.9
2	K	191	GLY	3.9
2	N	155	HIS	3.9
1	B	520	GLY	3.9
2	N	360	ASP	3.8
2	K	86	LEU	3.8
2	P	289	HIS	3.8
2	K	149	ARG	3.8
1	H	582	LEU	3.7
2	K	176	LEU	3.7
2	O	357	ARG	3.7
2	P	331	ASP	3.6
2	P	274	VAL	3.6
1	G	522	LYS	3.6
2	P	198	ALA	3.6
2	N	108	VAL	3.6
2	N	149	ARG	3.6
2	P	343	VAL	3.6
2	O	222	ALA	3.6
1	H	172	PHE	3.6
1	H	184	PRO	3.5
2	P	346	ILE	3.5
1	H	151	PRO	3.5
2	K	301	VAL	3.5
1	H	143	GLU	3.5
2	P	353	ALA	3.5
1	D	521	ALA	3.5
2	M	176	LEU	3.5
2	N	361	GLN	3.5
1	H	155	PHE	3.5
2	O	361	GLN	3.4
2	P	262	VAL	3.4
2	O	323	GLU	3.4
1	B	521	ALA	3.4
1	G	24	GLY	3.4
1	H	201	LEU	3.3
1	F	157	VAL	3.3
2	O	338	THR	3.3
2	K	293	ASP	3.3
2	P	355	HIS	3.3
1	H	135	SER	3.3

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Mol	Chain	Res	Type	RSRZ
2	P	285	GLU	3.3
1	H	386	ASN	3.3
1	F	168	ALA	3.3
2	O	404	ASP	3.3
2	N	301	VAL	3.2
1	H	98	PHE	3.2
1	H	83	PHE	3.2
2	M	288	TYR	3.2
2	K	87	TYR	3.1
1	G	215	VAL	3.1
1	F	24	GLY	3.1
1	H	295	HIS	3.1
2	P	265	GLN	3.1
2	N	365	ASP	3.1
2	O	343	VAL	3.1
2	O	358	LEU	3.1
2	P	384	CYS	3.1
2	L	55	GLN	3.0
1	E	99	TYR	3.0
2	N	358	LEU	3.0
2	N	347	LEU	3.0
1	G	67	LEU	3.0
2	O	310	VAL	3.0
1	H	157	VAL	3.0
2	P	301	VAL	3.0
2	P	426	PRO	3.0
2	P	432	PRO	3.0
2	M	81	THR	3.0
2	M	155	HIS	3.0
2	O	322	PHE	3.0
1	H	323	ALA	2.9
1	H	556	GLY	2.9
2	L	253	THR	2.9
1	G	219	TRP	2.9
1	H	188	GLN	2.9
2	L	131	GLN	2.9
1	F	386	ASN	2.9
2	K	96	LEU	2.9
2	O	337	ASP	2.9
2	K	135	SER	2.8
2	N	277	LEU	2.8
1	H	29	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
2	M	361	GLN	2.8
1	H	561	PRO	2.8
2	P	319	LEU	2.8
2	P	284	ILE	2.8
1	G	520	GLY	2.8
2	L	144	PHE	2.8
2	J	361	GLN	2.8
2	O	341	ARG	2.8
2	N	343	VAL	2.8
2	M	62	SER	2.8
2	I	358	LEU	2.8
2	P	263	MET	2.8
1	F	522	LYS	2.8
2	M	133	ASN	2.8
1	F	187	ARG	2.7
2	I	44	ALA	2.7
2	P	341	ARG	2.7
2	L	52	GLU	2.7
1	D	185	VAL	2.7
1	E	84	TYR	2.7
2	L	77	ALA	2.7
1	G	77	CYS	2.7
1	H	100	LYS	2.7
2	N	138	PHE	2.7
1	F	184	PRO	2.7
2	J	131	GLN	2.7
2	O	215	PHE	2.7
1	H	77	CYS	2.7
2	P	259	PRO	2.6
2	P	261	ASP	2.6
2	P	280	HIS	2.6
1	G	128	ASP	2.6
2	L	183	TRP	2.6
2	L	215	PHE	2.6
2	O	305	LEU	2.6
2	O	308	GLY	2.6
2	K	190	LEU	2.6
2	L	319	LEU	2.6
1	D	522	LYS	2.6
2	K	181	THR	2.6
1	E	156	TYR	2.6
2	I	50	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	191	TRP	2.6
1	F	171	ILE	2.6
2	M	419	ALA	2.6
2	K	361	GLN	2.6
2	O	221	TYR	2.6
2	P	286	GLU	2.6
1	H	158	TRP	2.6
2	N	346	ILE	2.5
2	O	331	ASP	2.5
2	N	152	PRO	2.5
1	H	190	TYR	2.5
2	L	305	LEU	2.5
1	E	155	PHE	2.5
1	G	203	TYR	2.5
2	K	110	PHE	2.5
1	H	350	THR	2.5
1	H	583	ARG	2.5
2	P	366	ASP	2.5
2	K	180	GLU	2.5
2	K	188	TYR	2.5
2	N	357	ARG	2.5
1	G	131	MET	2.5
2	P	347	LEU	2.5
2	O	309	GLN	2.5
2	P	215	PHE	2.5
2	L	87	TYR	2.4
2	M	175	LEU	2.4
2	P	323	GLU	2.4
2	K	154	VAL	2.4
1	H	95	ILE	2.4
2	P	199	ASN	2.4
2	P	357	ARG	2.4
2	O	318	LEU	2.4
1	E	154	ASP	2.4
2	K	98	LEU	2.4
1	F	185	VAL	2.4
1	E	182	PHE	2.4
2	I	354	ALA	2.4
2	K	282	PRO	2.4
1	H	49	PHE	2.4
2	P	376	ALA	2.4
1	F	501	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	K	153	GLY	2.4
2	L	86	LEU	2.4
1	H	152	TYR	2.4
1	E	98	PHE	2.4
2	K	288	TYR	2.4
1	H	199	PRO	2.4
2	M	54	TYR	2.4
2	L	181	THR	2.4
1	H	176	GLU	2.3
1	G	169	ARG	2.3
1	G	267	ARG	2.3
1	B	519	GLY	2.3
2	J	299	GLN	2.3
2	N	364	ASP	2.3
2	M	357	ARG	2.3
2	K	178	SER	2.3
1	H	170	ILE	2.3
2	N	94	TYR	2.3
2	O	302	HIS	2.3
1	H	30	PRO	2.3
2	M	178	SER	2.3
1	D	519	GLY	2.3
1	E	524	ASP	2.3
2	K	111	VAL	2.3
2	M	347	LEU	2.3
2	N	432	PRO	2.2
1	B	522	LYS	2.2
2	J	5	PHE	2.2
2	N	153	GLY	2.2
1	G	573	PRO	2.2
1	H	500	GLY	2.2
2	P	324	GLY	2.2
2	K	305	LEU	2.2
2	K	133	ASN	2.2
1	F	517	GLY	2.2
1	G	163	ASP	2.2
2	K	277	LEU	2.2
2	I	357	ARG	2.2
2	K	147	PHE	2.2
2	N	189	ALA	2.2
2	P	282	PRO	2.2
1	E	525	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
2	L	271	VAL	2.2
2	N	154	VAL	2.2
2	P	287	ARG	2.2
2	N	305	LEU	2.2
2	L	76	ILE	2.2
2	L	299	GLN	2.2
2	N	131	GLN	2.2
1	F	109	ASP	2.2
2	K	84	ASP	2.2
1	H	99	TYR	2.2
2	P	252	GLY	2.2
2	J	360	ASP	2.2
2	K	103	ALA	2.2
1	G	99	TYR	2.1
1	H	232	VAL	2.1
1	G	256	CYS	2.1
2	P	288	TYR	2.1
1	H	245	ASN	2.1
2	L	160	LEU	2.1
2	O	373	ALA	2.1
2	M	86	LEU	2.1
1	F	454	ALA	2.1
1	G	25	HIS	2.1
1	B	587	PRO	2.1
1	H	122	GLY	2.1
1	H	553	GLU	2.1
1	G	23	PHE	2.1
2	P	264	ALA	2.1
1	G	492	VAL	2.1
2	M	289	HIS	2.1
1	F	113	THR	2.1
1	H	105	PHE	2.0
2	P	354	ALA	2.0
2	P	253	THR	2.0
2	P	412	ASP	2.0
2	N	273	ALA	2.0
2	O	250	GLU	2.0
1	H	78	LEU	2.0
2	N	215	PHE	2.0
2	P	350	PHE	2.0
2	O	340	VAL	2.0
2	M	60	THR	2.0

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Mol	Chain	Res	Type	RSRZ
2	O	288	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	CA	F	601	1/1	0.80	0.80	1.56	20,20,20,20	0
3	CA	H	601	1/1	0.53	0.34	-0.49	20,20,20,20	0
3	CA	E	601	1/1	0.93	0.21	-0.87	20,20,20,20	0
3	CA	G	601	1/1	0.99	0.16	-1.38	20,20,20,20	0
3	CA	C	601	1/1	0.99	0.11	-1.65	20,20,20,20	0
3	CA	A	601	1/1	0.98	0.05	-2.02	20,20,20,20	0
3	CA	B	601	1/1	0.97	0.13	-2.19	20,20,20,20	0
3	CA	D	601	1/1	0.93	0.06	-3.36	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.