Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2023 – 03:23 PM EDT

PDB ID	:	2QMH
Title	:	structure of V267F mutant HprK/P
Authors	:	Chaptal, V.; Vincent, F.; Gueguen-Chaignon, V.; Poncet, S.; Deutscher, J.; Nessler, S.; Morera, S.
Deposited on	:	2007-07-16
Resolution	:	2.60 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:

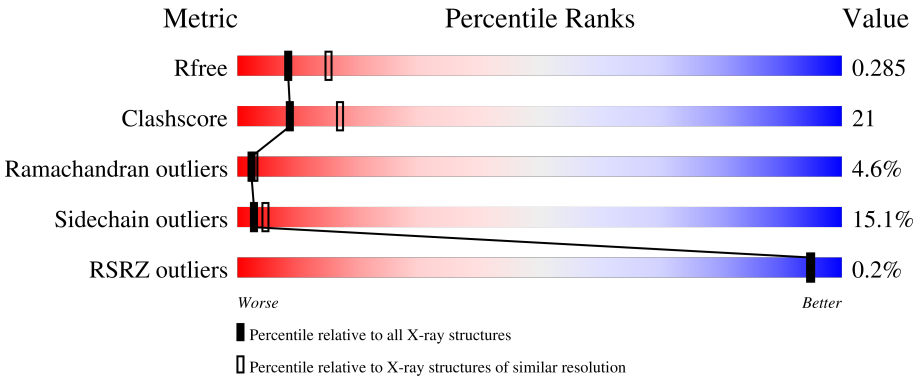
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	205	46% 24% 7% 21%
1	B	205	55% 27% 5% 12%
1	C	205	50% 24% 6% 20%
1	D	205	54% 25% 8% 12%
1	E	205	41% 33% 6% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	205	38% 33% 6% 22%
1	G	205	42% 26% 9% 22%
1	H	205	55% 22% 10% 13%
1	I	205	43% 27% 6% 22%
1	J	205	54% 23% 9% 13%
1	K	205	40% 30% 8% 21%
1	L	205	% 47% 22% 8% 21%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15591 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 HPr kinase/phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	161	Total	C	N	O	S	0	0	0
			1242	787	218	233	4			
1	B	181	Total	C	N	O	S	0	0	0
			1405	887	245	269	4			
1	C	164	Total	C	N	O	S	0	0	0
			1269	806	223	236	4			
1	D	181	Total	C	N	O	S	0	0	0
			1405	887	245	269	4			
1	E	164	Total	C	N	O	S	0	0	0
			1265	799	222	240	4			
1	F	160	Total	C	N	O	S	0	0	0
			1235	783	215	233	4			
1	G	160	Total	C	N	O	S	0	0	0
			1238	785	217	232	4			
1	H	178	Total	C	N	O	S	0	0	0
			1380	872	241	263	4			
1	I	160	Total	C	N	O	S	0	0	0
			1238	785	217	232	4			
1	J	178	Total	C	N	O	S	0	0	0
			1383	873	241	265	4			
1	K	162	Total	C	N	O	S	0	0	0
			1250	791	220	235	4			
1	L	161	Total	C	N	O	S	0	0	0
			1246	789	219	234	4			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	115	MET	-	expression tag	UNP Q9RE09
A	116	ARG	-	expression tag	UNP Q9RE09
A	117	GLY	-	expression tag	UNP Q9RE09
A	118	SER	-	expression tag	UNP Q9RE09
A	119	HIS	-	expression tag	UNP Q9RE09

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	120	HIS	-	expression tag	UNP Q9RE09
A	121	HIS	-	expression tag	UNP Q9RE09
A	122	HIS	-	expression tag	UNP Q9RE09
A	123	HIS	-	expression tag	UNP Q9RE09
A	124	HIS	-	expression tag	UNP Q9RE09
A	125	GLY	-	expression tag	UNP Q9RE09
A	126	SER	-	expression tag	UNP Q9RE09
A	127	MET	-	expression tag	UNP Q9RE09
A	267	PHE	VAL	engineered mutation	UNP Q9RE09
B	115	MET	-	expression tag	UNP Q9RE09
B	116	ARG	-	expression tag	UNP Q9RE09
B	117	GLY	-	expression tag	UNP Q9RE09
B	118	SER	-	expression tag	UNP Q9RE09
B	119	HIS	-	expression tag	UNP Q9RE09
B	120	HIS	-	expression tag	UNP Q9RE09
B	121	HIS	-	expression tag	UNP Q9RE09
B	122	HIS	-	expression tag	UNP Q9RE09
B	123	HIS	-	expression tag	UNP Q9RE09
B	124	HIS	-	expression tag	UNP Q9RE09
B	125	GLY	-	expression tag	UNP Q9RE09
B	126	SER	-	expression tag	UNP Q9RE09
B	127	MET	-	expression tag	UNP Q9RE09
B	267	PHE	VAL	engineered mutation	UNP Q9RE09
C	115	MET	-	expression tag	UNP Q9RE09
C	116	ARG	-	expression tag	UNP Q9RE09
C	117	GLY	-	expression tag	UNP Q9RE09
C	118	SER	-	expression tag	UNP Q9RE09
C	119	HIS	-	expression tag	UNP Q9RE09
C	120	HIS	-	expression tag	UNP Q9RE09
C	121	HIS	-	expression tag	UNP Q9RE09
C	122	HIS	-	expression tag	UNP Q9RE09
C	123	HIS	-	expression tag	UNP Q9RE09
C	124	HIS	-	expression tag	UNP Q9RE09
C	125	GLY	-	expression tag	UNP Q9RE09
C	126	SER	-	expression tag	UNP Q9RE09
C	127	MET	-	expression tag	UNP Q9RE09
C	267	PHE	VAL	engineered mutation	UNP Q9RE09
D	115	MET	-	expression tag	UNP Q9RE09
D	116	ARG	-	expression tag	UNP Q9RE09
D	117	GLY	-	expression tag	UNP Q9RE09
D	118	SER	-	expression tag	UNP Q9RE09
D	119	HIS	-	expression tag	UNP Q9RE09

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	120	HIS	-	expression tag	UNP Q9RE09
D	121	HIS	-	expression tag	UNP Q9RE09
D	122	HIS	-	expression tag	UNP Q9RE09
D	123	HIS	-	expression tag	UNP Q9RE09
D	124	HIS	-	expression tag	UNP Q9RE09
D	125	GLY	-	expression tag	UNP Q9RE09
D	126	SER	-	expression tag	UNP Q9RE09
D	127	MET	-	expression tag	UNP Q9RE09
D	267	PHE	VAL	engineered mutation	UNP Q9RE09
E	115	MET	-	expression tag	UNP Q9RE09
E	116	ARG	-	expression tag	UNP Q9RE09
E	117	GLY	-	expression tag	UNP Q9RE09
E	118	SER	-	expression tag	UNP Q9RE09
E	119	HIS	-	expression tag	UNP Q9RE09
E	120	HIS	-	expression tag	UNP Q9RE09
E	121	HIS	-	expression tag	UNP Q9RE09
E	122	HIS	-	expression tag	UNP Q9RE09
E	123	HIS	-	expression tag	UNP Q9RE09
E	124	HIS	-	expression tag	UNP Q9RE09
E	125	GLY	-	expression tag	UNP Q9RE09
E	126	SER	-	expression tag	UNP Q9RE09
E	127	MET	-	expression tag	UNP Q9RE09
E	267	PHE	VAL	engineered mutation	UNP Q9RE09
F	115	MET	-	expression tag	UNP Q9RE09
F	116	ARG	-	expression tag	UNP Q9RE09
F	117	GLY	-	expression tag	UNP Q9RE09
F	118	SER	-	expression tag	UNP Q9RE09
F	119	HIS	-	expression tag	UNP Q9RE09
F	120	HIS	-	expression tag	UNP Q9RE09
F	121	HIS	-	expression tag	UNP Q9RE09
F	122	HIS	-	expression tag	UNP Q9RE09
F	123	HIS	-	expression tag	UNP Q9RE09
F	124	HIS	-	expression tag	UNP Q9RE09
F	125	GLY	-	expression tag	UNP Q9RE09
F	126	SER	-	expression tag	UNP Q9RE09
F	127	MET	-	expression tag	UNP Q9RE09
F	267	PHE	VAL	engineered mutation	UNP Q9RE09
G	115	MET	-	expression tag	UNP Q9RE09
G	116	ARG	-	expression tag	UNP Q9RE09
G	117	GLY	-	expression tag	UNP Q9RE09
G	118	SER	-	expression tag	UNP Q9RE09
G	119	HIS	-	expression tag	UNP Q9RE09

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
G	120	HIS	-	expression tag	UNP Q9RE09
G	121	HIS	-	expression tag	UNP Q9RE09
G	122	HIS	-	expression tag	UNP Q9RE09
G	123	HIS	-	expression tag	UNP Q9RE09
G	124	HIS	-	expression tag	UNP Q9RE09
G	125	GLY	-	expression tag	UNP Q9RE09
G	126	SER	-	expression tag	UNP Q9RE09
G	127	MET	-	expression tag	UNP Q9RE09
G	267	PHE	VAL	engineered mutation	UNP Q9RE09
H	115	MET	-	expression tag	UNP Q9RE09
H	116	ARG	-	expression tag	UNP Q9RE09
H	117	GLY	-	expression tag	UNP Q9RE09
H	118	SER	-	expression tag	UNP Q9RE09
H	119	HIS	-	expression tag	UNP Q9RE09
H	120	HIS	-	expression tag	UNP Q9RE09
H	121	HIS	-	expression tag	UNP Q9RE09
H	122	HIS	-	expression tag	UNP Q9RE09
H	123	HIS	-	expression tag	UNP Q9RE09
H	124	HIS	-	expression tag	UNP Q9RE09
H	125	GLY	-	expression tag	UNP Q9RE09
H	126	SER	-	expression tag	UNP Q9RE09
H	127	MET	-	expression tag	UNP Q9RE09
H	267	PHE	VAL	engineered mutation	UNP Q9RE09
I	115	MET	-	expression tag	UNP Q9RE09
I	116	ARG	-	expression tag	UNP Q9RE09
I	117	GLY	-	expression tag	UNP Q9RE09
I	118	SER	-	expression tag	UNP Q9RE09
I	119	HIS	-	expression tag	UNP Q9RE09
I	120	HIS	-	expression tag	UNP Q9RE09
I	121	HIS	-	expression tag	UNP Q9RE09
I	122	HIS	-	expression tag	UNP Q9RE09
I	123	HIS	-	expression tag	UNP Q9RE09
I	124	HIS	-	expression tag	UNP Q9RE09
I	125	GLY	-	expression tag	UNP Q9RE09
I	126	SER	-	expression tag	UNP Q9RE09
I	127	MET	-	expression tag	UNP Q9RE09
I	267	PHE	VAL	engineered mutation	UNP Q9RE09
J	115	MET	-	expression tag	UNP Q9RE09
J	116	ARG	-	expression tag	UNP Q9RE09
J	117	GLY	-	expression tag	UNP Q9RE09
J	118	SER	-	expression tag	UNP Q9RE09
J	119	HIS	-	expression tag	UNP Q9RE09

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
J	120	HIS	-	expression tag	UNP Q9RE09
J	121	HIS	-	expression tag	UNP Q9RE09
J	122	HIS	-	expression tag	UNP Q9RE09
J	123	HIS	-	expression tag	UNP Q9RE09
J	124	HIS	-	expression tag	UNP Q9RE09
J	125	GLY	-	expression tag	UNP Q9RE09
J	126	SER	-	expression tag	UNP Q9RE09
J	127	MET	-	expression tag	UNP Q9RE09
J	267	PHE	VAL	engineered mutation	UNP Q9RE09
K	115	MET	-	expression tag	UNP Q9RE09
K	116	ARG	-	expression tag	UNP Q9RE09
K	117	GLY	-	expression tag	UNP Q9RE09
K	118	SER	-	expression tag	UNP Q9RE09
K	119	HIS	-	expression tag	UNP Q9RE09
K	120	HIS	-	expression tag	UNP Q9RE09
K	121	HIS	-	expression tag	UNP Q9RE09
K	122	HIS	-	expression tag	UNP Q9RE09
K	123	HIS	-	expression tag	UNP Q9RE09
K	124	HIS	-	expression tag	UNP Q9RE09
K	125	GLY	-	expression tag	UNP Q9RE09
K	126	SER	-	expression tag	UNP Q9RE09
K	127	MET	-	expression tag	UNP Q9RE09
K	267	PHE	VAL	engineered mutation	UNP Q9RE09
L	115	MET	-	expression tag	UNP Q9RE09
L	116	ARG	-	expression tag	UNP Q9RE09
L	117	GLY	-	expression tag	UNP Q9RE09
L	118	SER	-	expression tag	UNP Q9RE09
L	119	HIS	-	expression tag	UNP Q9RE09
L	120	HIS	-	expression tag	UNP Q9RE09
L	121	HIS	-	expression tag	UNP Q9RE09
L	122	HIS	-	expression tag	UNP Q9RE09
L	123	HIS	-	expression tag	UNP Q9RE09
L	124	HIS	-	expression tag	UNP Q9RE09
L	125	GLY	-	expression tag	UNP Q9RE09
L	126	SER	-	expression tag	UNP Q9RE09
L	127	MET	-	expression tag	UNP Q9RE09
L	267	PHE	VAL	engineered mutation	UNP Q9RE09

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O 1 1	0	0

Continued on next page...

Continued from previous page...

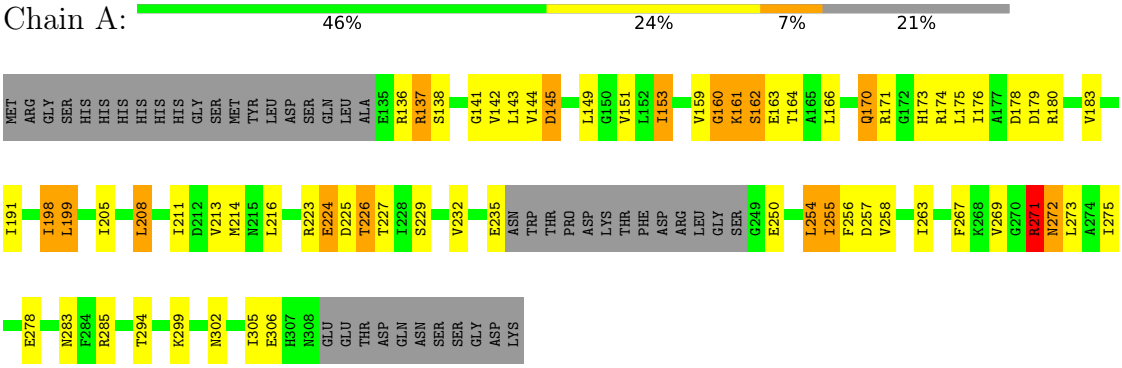
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total O 2 2	0	0
2	C	3	Total O 3 3	0	0
2	D	2	Total O 2 2	0	0
2	F	3	Total O 3 3	0	0
2	G	10	Total O 10 10	0	0
2	H	6	Total O 6 6	0	0
2	I	4	Total O 4 4	0	0
2	K	1	Total O 1 1	0	0
2	L	3	Total O 3 3	0	0

3 Residue-property plots (i)

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

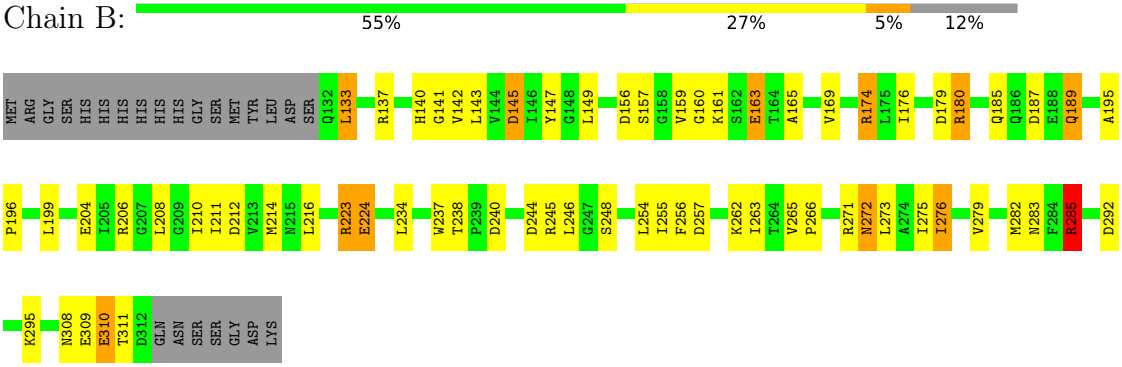
- Molecule 1: HPr kinase/phosphorylase

Chain A:



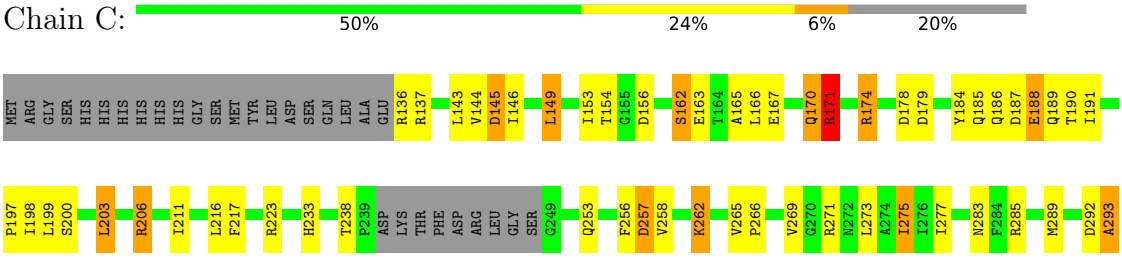
- Molecule 1: HPr kinase/phosphorylase

Chain B:



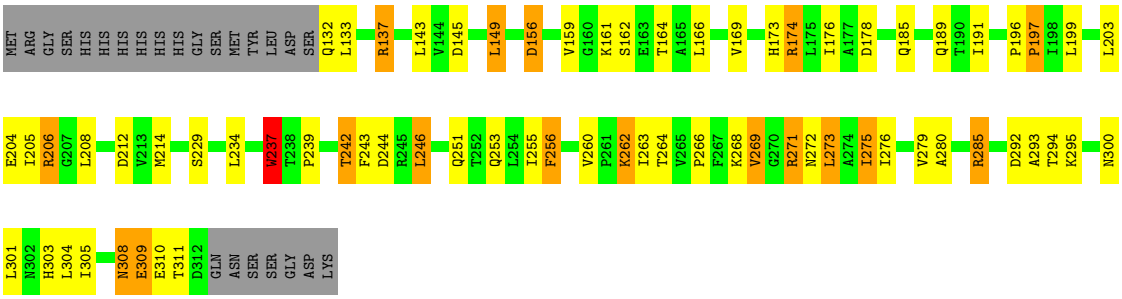
- Molecule 1: HPr kinase/phosphorylase

Chain C:



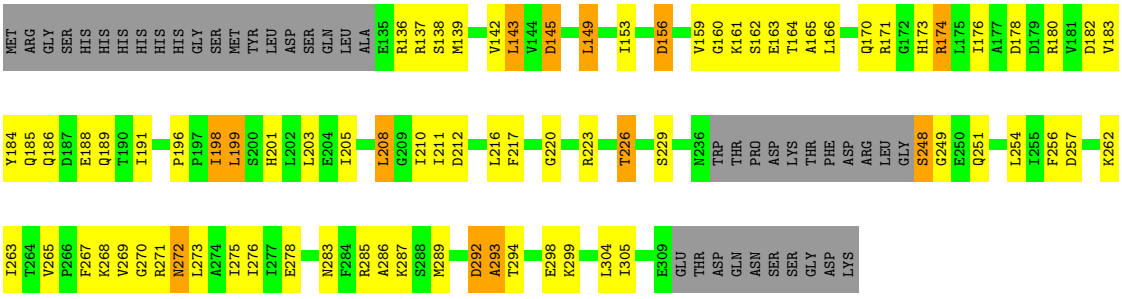
• Molecule 1: HPr kinase/phosphorylase

Chain D:



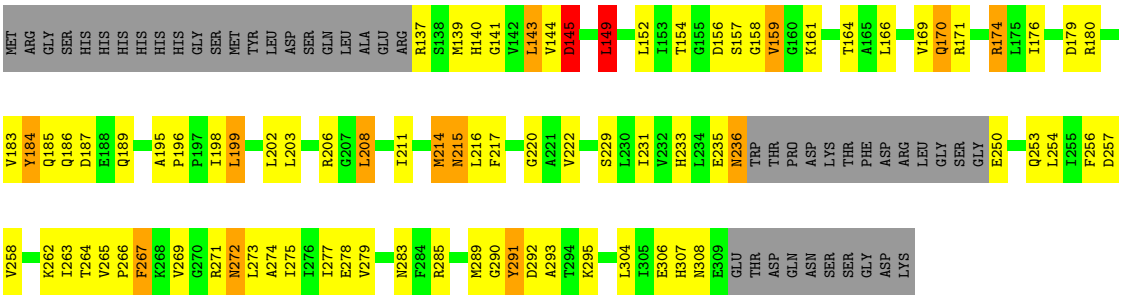
• Molecule 1: HPr kinase/phosphorylase

Chain E:



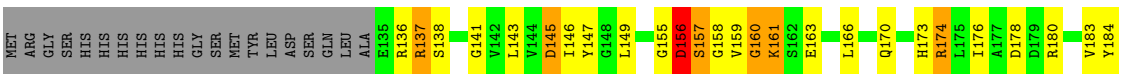
• Molecule 1: HPr kinase/phosphorylase

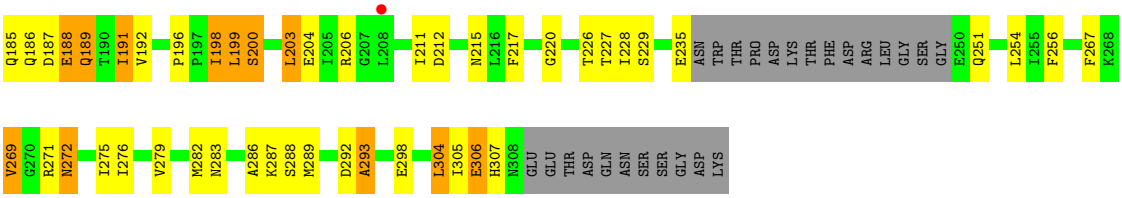
Chain F:



• Molecule 1: HPr kinase/phosphorylase

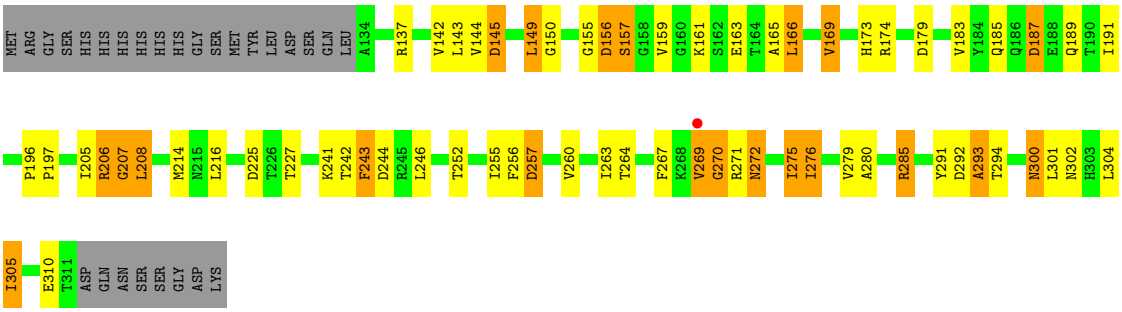
Chain G:





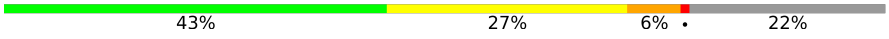
• Molecule 1: HPr kinase/phosphorylase

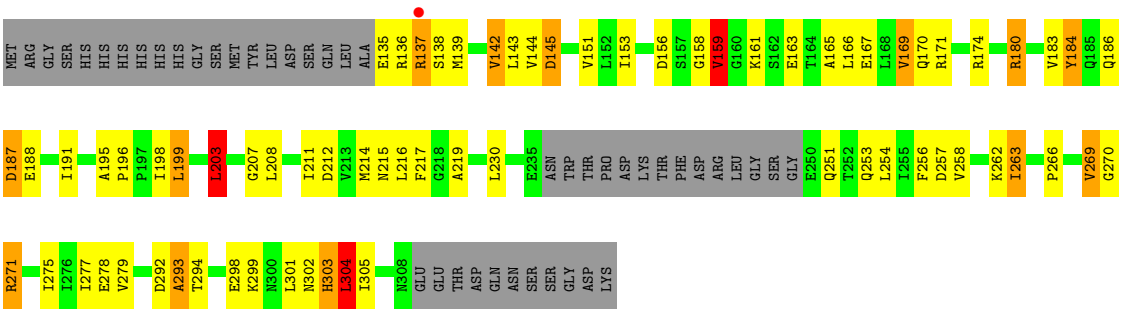
Chain H:



• Molecule 1: HPr kinase/phosphorylase

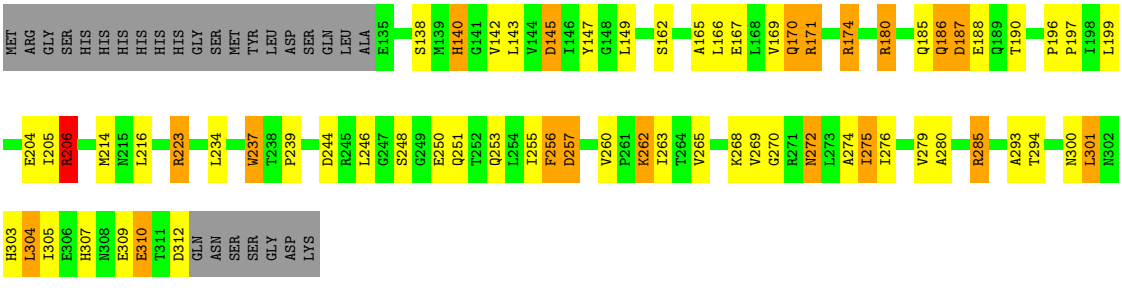
Chain I:





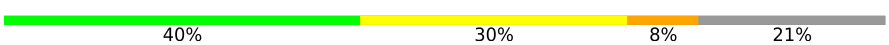
• Molecule 1: HPr kinase/phosphorylase

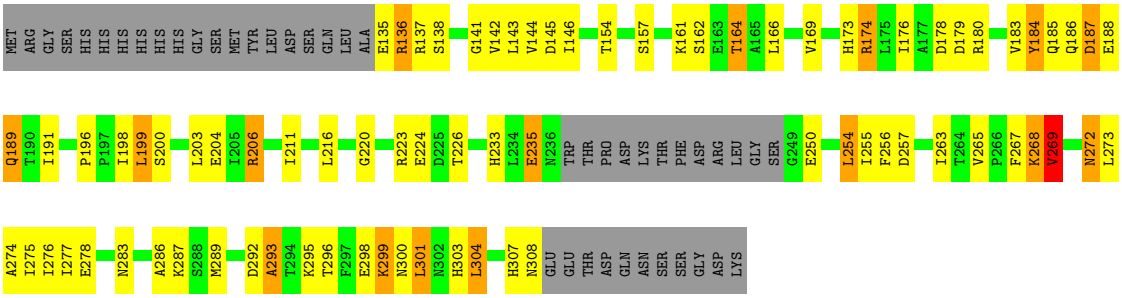
Chain J:



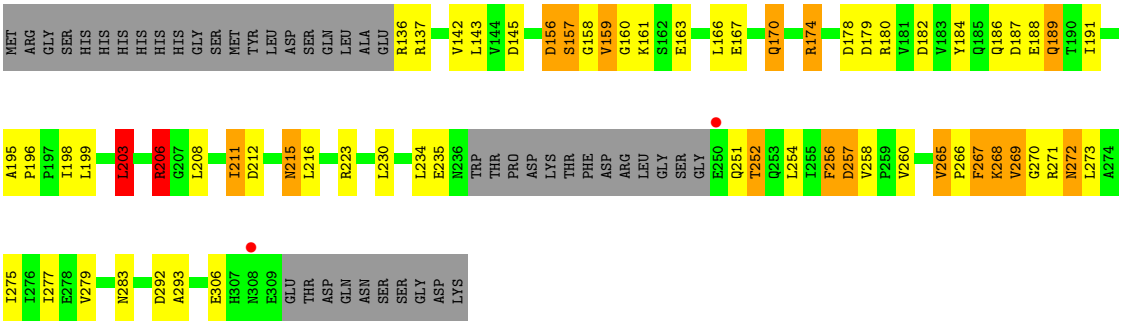
• Molecule 1: HPr kinase/phosphorylase

Chain K:





- Molecule 1: HPr kinase/phosphorylase



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	69.06Å 106.37Å 106.49Å 119.50° 90.02° 89.96°	Depositor
Resolution (Å)	19.43 – 2.60 19.43 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.43-2.60) 99.0 (19.43-2.60)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.221 , 0.298 0.212 , 0.285	Depositor DCC
R_{free} test set	4029 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	55.7	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 13.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-l,k+l 0.019 for h,k+l,-k 0.019 for h,-k-l,k 0.019 for h,l,-k-l 0.469 for h,-k,-l 0.020 for -h,k,-k-l 0.019 for -h,-k-l,l 0.469 for -h,-l,-k 0.467 for -h,l,k 0.019 for -h,-k,k+l 0.019 for -h,k+l,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15591	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.84% 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

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	0.85	0/1259	0.96	1/1703 (0.1%)
1	B	0.93	2/1427 (0.1%)	0.97	5/1934 (0.3%)
1	C	0.85	0/1289	0.95	4/1747 (0.2%)
1	D	0.94	0/1427	1.01	6/1934 (0.3%)
1	E	0.83	0/1282	0.97	3/1734 (0.2%)
1	F	0.85	0/1252	0.91	2/1695 (0.1%)
1	G	0.86	0/1255	0.94	2/1698 (0.1%)
1	H	0.94	0/1402	0.99	4/1900 (0.2%)
1	I	0.79	1/1255 (0.1%)	0.88	2/1698 (0.1%)
1	J	0.91	0/1405	1.03	6/1904 (0.3%)
1	K	0.84	0/1267	0.92	0/1714
1	L	0.84	1/1263 (0.1%)	0.95	1/1709 (0.1%)
All	All	0.87	4/15783 (0.0%)	0.96	36/21370 (0.2%)

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
1	K	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	L	206	ARG	CB-CG	5.35	1.67	1.52
1	B	163	GLU	CG-CD	5.10	1.59	1.51
1	I	217	PHE	CE1-CZ	5.08	1.47	1.37
1	B	224	GLU	CB-CG	5.04	1.61	1.52

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	149	LEU	CA-CB-CG	10.25	138.87	115.30
1	C	171	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	D	285	ARG	NE-CZ-NH2	-8.24	116.18	120.30
1	J	285	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	E	285	ARG	NE-CZ-NH2	-7.59	116.51	120.30
1	J	166	LEU	CB-CG-CD2	-7.57	98.13	111.00
1	I	203	LEU	CA-CB-CG	7.54	132.65	115.30
1	F	149	LEU	CA-CB-CG	7.14	131.72	115.30
1	D	285	ARG	NE-CZ-NH1	7.07	123.84	120.30
1	H	285	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	L	203	LEU	CA-CB-CG	6.83	131.00	115.30
1	H	285	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	I	145	ASP	CB-CG-OD2	6.17	123.85	118.30
1	F	145	ASP	CB-CG-OD2	6.09	123.78	118.30
1	J	285	ARG	NE-CZ-NH1	6.07	123.34	120.30
1	D	149	LEU	CA-CB-CG	6.00	129.11	115.30
1	B	285	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	H	166	LEU	CB-CG-CD2	-5.69	101.32	111.00
1	C	171	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	199	LEU	CA-CB-CG	5.64	128.27	115.30
1	C	149	LEU	CA-CB-CG	5.61	128.21	115.30
1	E	292	ASP	CB-CG-OD2	5.58	123.32	118.30
1	D	246	LEU	CB-CG-CD1	-5.55	101.57	111.00
1	G	203	LEU	CA-CB-CG	5.47	127.89	115.30
1	B	223	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	D	246	LEU	CA-CB-CG	5.24	127.34	115.30
1	J	275	ILE	CG1-CB-CG2	-5.23	99.89	111.40
1	B	149	LEU	CB-CG-CD1	-5.23	102.12	111.00
1	H	149	LEU	CA-CB-CG	5.21	127.29	115.30
1	E	212	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	285	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	D	208	LEU	CA-CB-CG	5.14	127.11	115.30
1	J	223	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	G	254	LEU	CA-CB-CG	5.11	127.05	115.30
1	C	145	ASP	CB-CG-OD2	5.07	122.86	118.30
1	J	171	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	K	300	ASN	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	1242	0	1268	60	0
1	B	1405	0	1415	54	0
1	C	1269	0	1292	49	0
1	D	1405	0	1415	58	0
1	E	1265	0	1285	64	0
1	F	1235	0	1258	69	0
1	G	1238	0	1265	56	0
1	H	1380	0	1392	53	0
1	I	1238	0	1265	53	0
1	J	1383	0	1391	49	0
1	K	1250	0	1274	70	0
1	L	1246	0	1271	59	0
2	A	1	0	0	0	0
2	B	2	0	0	0	0
2	C	3	0	0	0	0
2	D	2	0	0	0	0
2	F	3	0	0	0	0
2	G	10	0	0	1	0
2	H	6	0	0	3	0
2	I	4	0	0	1	0
2	K	1	0	0	0	0
2	L	3	0	0	0	0
All	All	15591	0	15791	646	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 21.

All (646) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:137:ARG:HG2	1:E:138:SER:H	1.10	1.13
1:L:206:ARG:H	1:L:206:ARG:HD2	0.97	1.11
1:D:253:GLN:HB2	1:D:262:LYS:NZ	1.69	1.06
1:H:302:ASN:HA	1:H:305:ILE:HG22	1.41	1.02
1:G:198:ILE:HG13	1:G:199:LEU:H	1.25	0.99

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ARG:HD3	1:C:206:ARG:H	1.24	0.99
1:G:267:PHE:CE2	1:G:271:ARG:HB3	2.00	0.96
1:I:137:ARG:HG2	1:I:138:SER:H	1.30	0.96
1:G:198:ILE:HG13	1:G:199:LEU:N	1.83	0.94
1:L:206:ARG:HD2	1:L:206:ARG:N	1.83	0.93
1:B:156:ASP:O	1:B:159:VAL:HG22	1.70	0.92
1:H:263:ILE:HD11	1:I:207:GLY:O	1.72	0.90
1:H:137:ARG:HG3	1:H:256:PHE:CZ	2.06	0.90
1:J:256:PHE:O	1:J:257:ASP:HB2	1.72	0.90
1:G:267:PHE:HE2	1:G:271:ARG:HB3	1.35	0.89
1:D:292:ASP:O	1:D:294:THR:N	2.06	0.88
1:K:303:HIS:HD2	1:K:308:ASN:HA	1.37	0.87
1:A:223:ARG:O	1:A:224:GLU:CB	2.23	0.87
1:L:235:GLU:O	1:L:267:PHE:HB3	1.74	0.87
1:L:206:ARG:H	1:L:206:ARG:CD	1.85	0.86
1:E:137:ARG:HG2	1:E:138:SER:N	1.90	0.86
1:H:271:ARG:NH1	2:H:324:HOH:O	2.08	0.85
1:H:271:ARG:CZ	2:H:324:HOH:O	2.24	0.85
1:J:268:LYS:HZ1	1:L:159:VAL:HB	1.40	0.83
1:A:223:ARG:O	1:A:224:GLU:HB2	1.79	0.83
1:I:203:LEU:HD22	1:I:211:ILE:HD11	1.60	0.83
1:J:309:GLU:O	1:J:310:GLU:HB2	1.77	0.82
1:F:272:ASN:HD21	1:F:274:ALA:HB3	1.43	0.82
1:D:253:GLN:HB2	1:D:262:LYS:HZ3	1.46	0.81
1:F:272:ASN:ND2	1:F:275:ILE:H	1.78	0.81
1:B:140:HIS:CE1	1:B:180:ARG:NH1	2.48	0.81
1:A:205:ILE:HB	1:A:208:LEU:HD11	1.60	0.81
1:L:272:ASN:OD1	1:L:275:ILE:HG12	1.81	0.81
1:K:211:ILE:HD12	1:K:216:LEU:HD12	1.63	0.79
1:H:291:TYR:HB3	1:I:215:ASN:HD21	1.47	0.79
1:E:198:ILE:HG13	1:E:199:LEU:N	1.97	0.79
1:H:292:ASP:O	1:H:294:THR:N	2.15	0.79
1:H:256:PHE:O	1:H:257:ASP:HB2	1.80	0.78
1:A:198:ILE:HG13	1:C:304:LEU:HD12	1.65	0.78
1:L:156:ASP:HA	1:L:161:LYS:NZ	1.97	0.78
1:I:142:VAL:HG21	1:I:161:LYS:HB3	1.65	0.78
1:K:206:ARG:HG2	1:K:206:ARG:HH21	1.49	0.78
1:L:211:ILE:HD13	1:L:216:LEU:HD12	1.66	0.77
1:F:272:ASN:HD22	1:F:272:ASN:C	1.88	0.77
1:C:206:ARG:H	1:C:206:ARG:CD	1.92	0.77
1:K:211:ILE:HG22	1:L:283:ASN:ND2	2.00	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:137:ARG:CG	1:E:138:SER:H	1.96	0.76
1:G:136:ARG:O	1:G:137:ARG:HB2	1.86	0.76
1:B:254:LEU:HD21	1:B:257:ASP:H	1.51	0.75
1:K:191:ILE:CD1	1:K:255:ILE:HB	2.16	0.75
1:F:292:ASP:O	1:F:293:ALA:HB3	1.86	0.75
1:K:136:ARG:HH11	1:K:136:ARG:CG	1.99	0.75
1:I:303:HIS:C	1:I:305:ILE:H	1.90	0.75
1:A:223:ARG:NH1	1:A:226:THR:HG23	2.01	0.75
1:C:191:ILE:HD11	1:C:258:VAL:HB	1.68	0.75
1:G:198:ILE:CG1	1:G:199:LEU:N	2.49	0.74
1:A:198:ILE:HG23	1:A:199:LEU:H	1.51	0.74
1:E:292:ASP:O	1:E:293:ALA:CB	2.33	0.74
1:E:305:ILE:CG2	1:J:180:ARG:HG2	2.16	0.74
1:A:176:ILE:CD1	1:A:226:THR:OG1	2.35	0.74
1:B:137:ARG:HH12	1:B:255:ILE:HA	1.52	0.74
1:L:156:ASP:HA	1:L:161:LYS:HZ1	1.52	0.74
1:K:189:GLN:O	1:K:189:GLN:HG2	1.87	0.74
1:A:136:ARG:O	1:A:137:ARG:HB2	1.87	0.74
1:I:292:ASP:O	1:I:293:ALA:HB3	1.87	0.73
1:G:176:ILE:HG12	1:G:226:THR:HG22	1.69	0.73
1:I:191:ILE:HD11	1:I:258:VAL:HB	1.70	0.73
1:G:170:GLN:OE1	2:G:325:HOH:O	2.05	0.72
1:G:180:ARG:HH21	1:G:199:LEU:CD1	2.01	0.72
1:A:235:GLU:HB3	1:A:267:PHE:HB3	1.69	0.72
1:J:216:LEU:HD21	1:K:283:ASN:HD22	1.53	0.72
1:K:254:LEU:CD2	1:K:257:ASP:HA	2.20	0.72
1:B:211:ILE:HD12	1:B:216:LEU:HD12	1.69	0.72
1:D:255:ILE:HD12	1:D:260:VAL:HG21	1.72	0.72
1:J:301:LEU:O	1:J:305:ILE:HG12	1.91	0.71
1:D:137:ARG:HB3	1:D:256:PHE:CE1	2.26	0.71
1:B:271:ARG:HD2	1:C:163:GLU:OE1	1.90	0.71
1:D:253:GLN:HB2	1:D:262:LYS:HZ1	1.54	0.71
1:B:140:HIS:CE1	1:B:180:ARG:HH12	2.07	0.70
1:C:162:SER:O	1:C:165:ALA:HB3	1.90	0.70
1:I:299:LYS:NZ	2:I:323:HOH:O	2.24	0.70
1:E:292:ASP:O	1:E:293:ALA:HB3	1.89	0.70
1:K:254:LEU:HD23	1:K:257:ASP:HA	1.74	0.70
1:B:147:TYR:O	1:B:285:ARG:NH2	2.24	0.69
1:C:266:PRO:O	1:C:271:ARG:NH1	2.26	0.69
1:E:185:GLN:OE1	1:E:256:PHE:HB3	1.93	0.69
1:H:291:TYR:HB3	1:I:215:ASN:ND2	2.08	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:211:ILE:HG22	1:L:283:ASN:HD21	1.57	0.69
1:J:142:VAL:HG11	1:J:165:ALA:HB2	1.75	0.68
1:A:180:ARG:HH21	1:A:199:LEU:CD2	2.07	0.68
1:A:171:ARG:NH2	1:A:278:GLU:OE1	2.26	0.67
1:A:272:ASN:C	1:A:272:ASN:HD22	1.97	0.67
1:E:205:ILE:HB	1:E:208:LEU:HD11	1.77	0.67
1:F:137:ARG:HB2	1:F:256:PHE:HE1	1.57	0.67
1:B:271:ARG:HG3	1:B:272:ASN:H	1.60	0.67
1:H:256:PHE:O	1:H:257:ASP:CB	2.42	0.66
1:K:303:HIS:CD2	1:K:308:ASN:HA	2.25	0.66
1:L:275:ILE:O	1:L:279:VAL:HG23	1.95	0.66
1:B:246:LEU:HD12	1:B:248:SER:OG	1.95	0.66
1:L:256:PHE:O	1:L:257:ASP:HB2	1.94	0.66
1:E:171:ARG:NH2	1:E:278:GLU:OE2	2.28	0.66
1:E:198:ILE:CG1	1:E:199:LEU:N	2.59	0.66
1:I:203:LEU:HD22	1:I:211:ILE:CD1	2.26	0.66
1:K:180:ARG:NH2	1:K:199:LEU:CD1	2.59	0.66
1:C:292:ASP:O	1:C:293:ALA:HB3	1.96	0.66
1:H:302:ASN:CA	1:H:305:ILE:HG22	2.24	0.66
1:J:300:ASN:HD22	1:J:303:HIS:HD2	1.42	0.65
1:F:235:GLU:O	1:F:267:PHE:HB3	1.96	0.65
1:B:246:LEU:CD1	1:B:248:SER:OG	2.45	0.65
1:G:292:ASP:O	1:G:293:ALA:CB	2.43	0.65
1:K:183:VAL:O	1:K:184:TYR:HB3	1.95	0.65
1:K:191:ILE:HD11	1:K:255:ILE:HB	1.76	0.65
1:D:304:LEU:HD13	1:F:199:LEU:HD23	1.79	0.65
1:C:154:THR:O	1:C:233:HIS:HA	1.97	0.65
1:I:137:ARG:HG2	1:I:138:SER:N	2.09	0.65
1:I:292:ASP:O	1:I:293:ALA:CB	2.45	0.65
1:D:263:ILE:HG22	1:D:264:THR:N	2.12	0.65
1:E:156:ASP:HB3	1:E:161:LYS:NZ	2.11	0.65
1:B:266:PRO:HG2	1:B:271:ARG:NH2	2.12	0.64
1:K:268:LYS:O	1:K:269:VAL:HG13	1.97	0.64
1:E:185:GLN:HA	1:E:191:ILE:HD13	1.79	0.64
1:A:176:ILE:HD13	1:A:226:THR:OG1	1.96	0.64
1:K:142:VAL:HG12	1:K:144:VAL:HG13	1.80	0.64
1:B:196:PRO:HG2	1:B:199:LEU:HD12	1.79	0.64
1:B:271:ARG:HG3	1:B:272:ASN:N	2.12	0.64
1:H:302:ASN:HA	1:H:305:ILE:CG2	2.24	0.64
1:K:154:THR:O	1:K:233:HIS:HA	1.97	0.63
1:G:286:ALA:HA	1:G:289:MET:HE2	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:LEU:HD22	1:D:229:SER:HB2	1.79	0.63
1:I:142:VAL:CG2	1:I:161:LYS:HB3	2.28	0.63
1:K:180:ARG:HH21	1:K:199:LEU:CD1	2.12	0.63
1:C:136:ARG:HA	1:C:256:PHE:HZ	1.64	0.63
1:C:153:ILE:HD12	1:C:277:ILE:HD13	1.80	0.63
1:B:254:LEU:CD2	1:B:257:ASP:H	2.12	0.63
1:D:266:PRO:HG2	1:D:271:ARG:NH2	2.14	0.62
1:A:305:ILE:HG22	1:A:306:GLU:HG3	1.80	0.62
1:B:256:PHE:O	1:B:257:ASP:HB2	1.98	0.62
1:E:170:GLN:HG2	1:E:217:PHE:CE2	2.34	0.62
1:A:198:ILE:HG13	1:C:304:LEU:CD1	2.30	0.62
1:K:180:ARG:HH21	1:K:199:LEU:HD11	1.63	0.62
1:L:191:ILE:HD11	1:L:258:VAL:HB	1.82	0.62
1:L:292:ASP:O	1:L:293:ALA:HB3	2.00	0.62
1:A:180:ARG:HH21	1:A:199:LEU:HD21	1.64	0.61
1:I:294:THR:O	1:I:298:GLU:HG3	2.00	0.61
1:K:185:GLN:HE21	1:K:188:GLU:HA	1.65	0.61
1:H:272:ASN:C	1:H:272:ASN:HD22	2.02	0.61
1:E:188:GLU:O	1:E:189:GLN:HG2	2.01	0.61
1:H:191:ILE:CD1	1:H:255:ILE:HB	2.31	0.61
1:F:137:ARG:HB2	1:F:256:PHE:CE1	2.36	0.61
1:K:166:LEU:HD21	1:L:279:VAL:HG21	1.83	0.61
1:K:180:ARG:NH2	1:K:199:LEU:HD13	2.15	0.61
1:C:136:ARG:HA	1:C:256:PHE:CZ	2.35	0.61
1:D:309:GLU:C	1:D:311:THR:H	2.04	0.61
1:A:141:GLY:HA2	1:A:161:LYS:HE3	1.82	0.61
1:G:170:GLN:HG3	1:I:275:ILE:HD12	1.83	0.61
1:B:234:LEU:HD23	1:B:265:VAL:HG23	1.83	0.60
1:H:144:VAL:HG22	1:H:145:ASP:N	2.15	0.60
1:D:237:TRP:HZ3	1:D:239:PRO:HB3	1.66	0.60
1:G:180:ARG:HH21	1:G:199:LEU:HD13	1.66	0.60
1:F:214:MET:HG3	1:F:222:VAL:HG21	1.82	0.60
1:D:301:LEU:O	1:D:305:ILE:HG13	2.02	0.60
1:G:292:ASP:O	1:G:293:ALA:HB3	2.01	0.60
1:G:157:SER:O	1:G:160:GLY:HA3	2.01	0.60
1:I:303:HIS:C	1:I:305:ILE:N	2.54	0.60
1:J:246:LEU:HD13	1:J:248:SER:OG	2.02	0.60
1:K:161:LYS:O	1:K:164:THR:HG22	2.02	0.60
1:E:176:ILE:HG12	1:E:226:THR:HG22	1.84	0.60
1:K:189:GLN:O	1:K:189:GLN:CG	2.48	0.60
1:H:159:VAL:HG12	1:H:267:PHE:CD2	2.37	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:266:PRO:O	1:I:271:ARG:NH2	2.35	0.59
1:D:237:TRP:HZ2	1:F:206:ARG:NH1	2.01	0.59
1:F:156:ASP:CG	1:F:157:SER:H	2.05	0.58
1:J:272:ASN:OD1	1:J:275:ILE:HG12	2.02	0.58
1:K:185:GLN:NE2	1:K:188:GLU:HA	2.18	0.58
1:A:283:ASN:HD22	1:B:216:LEU:HD21	1.68	0.58
1:E:142:VAL:HG11	1:E:165:ALA:HB2	1.85	0.58
1:I:165:ALA:O	1:I:169:VAL:HG13	2.03	0.58
1:B:141:GLY:HA2	1:B:161:LYS:HE3	1.86	0.58
1:K:136:ARG:HH11	1:K:136:ARG:HG3	1.68	0.58
1:K:198:ILE:HG22	1:K:199:LEU:N	2.19	0.58
1:A:136:ARG:HG2	1:A:137:ARG:H	1.68	0.58
1:D:244:ASP:OD2	1:D:246:LEU:O	2.21	0.58
1:G:272:ASN:O	1:G:276:ILE:HG12	2.03	0.58
1:K:206:ARG:HG2	1:K:206:ARG:NH2	2.15	0.58
1:E:272:ASN:O	1:E:276:ILE:HG12	2.03	0.58
1:H:263:ILE:CD1	1:I:207:GLY:O	2.51	0.58
1:J:256:PHE:O	1:J:257:ASP:CB	2.46	0.58
1:L:269:VAL:O	1:L:271:ARG:N	2.37	0.58
1:F:266:PRO:O	1:F:267:PHE:O	2.22	0.58
1:E:272:ASN:C	1:E:272:ASN:HD22	2.08	0.57
1:H:300:ASN:HB2	1:I:199:LEU:HD21	1.86	0.57
1:B:145:ASP:CG	1:B:174:ARG:HH21	2.08	0.57
1:A:216:LEU:HD21	1:C:283:ASN:HD22	1.69	0.57
1:D:242:THR:HG23	1:D:243:PHE:N	2.18	0.57
1:A:205:ILE:HB	1:A:208:LEU:CD1	2.34	0.57
1:B:244:ASP:OD1	1:B:246:LEU:O	2.23	0.57
1:H:144:VAL:CG2	1:H:145:ASP:N	2.67	0.57
1:F:140:HIS:HD2	1:F:141:GLY:H	1.51	0.57
1:C:256:PHE:O	1:C:257:ASP:HB2	2.05	0.57
1:I:211:ILE:C	1:I:211:ILE:HD12	2.25	0.57
1:J:204:GLU:OE1	1:J:206:ARG:HG3	2.04	0.57
1:B:271:ARG:CD	1:C:163:GLU:OE1	2.52	0.57
1:K:292:ASP:O	1:K:293:ALA:CB	2.52	0.57
1:D:262:LYS:HG2	1:D:263:ILE:N	2.20	0.56
1:K:136:ARG:CG	1:K:136:ARG:NH1	2.66	0.56
1:L:267:PHE:HD1	1:L:267:PHE:C	2.09	0.56
1:K:184:TYR:HA	1:K:256:PHE:CE1	2.41	0.56
1:D:280:ALA:HB2	1:F:208:LEU:HD11	1.88	0.56
1:A:178:ASP:OD2	1:A:179:ASP:N	2.39	0.56
1:E:143:LEU:HD13	1:E:176:ILE:HB	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:272:ASN:CG	1:L:275:ILE:HG12	2.26	0.56
1:B:187:ASP:C	1:B:187:ASP:OD2	2.45	0.56
1:C:206:ARG:HD3	1:C:206:ARG:N	2.08	0.56
1:G:185:GLN:OE1	1:G:256:PHE:HB3	2.06	0.56
1:D:149:LEU:HD22	1:D:229:SER:CB	2.36	0.55
1:K:307:HIS:O	1:K:307:HIS:ND1	2.38	0.55
1:F:159:VAL:O	1:F:159:VAL:HG13	2.06	0.55
1:B:309:GLU:C	1:B:311:THR:H	2.08	0.55
1:B:279:VAL:HG21	1:C:166:LEU:HD21	1.88	0.55
1:B:204:GLU:OE1	1:B:206:ARG:HG3	2.06	0.55
1:D:237:TRP:HZ3	1:D:239:PRO:CB	2.20	0.55
1:G:166:LEU:HD21	1:I:279:VAL:HG21	1.89	0.55
1:A:176:ILE:HD11	1:A:226:THR:OG1	2.06	0.55
1:B:137:ARG:NH1	1:B:255:ILE:HA	2.19	0.55
1:L:160:GLY:HA3	1:L:206:ARG:HH22	1.70	0.55
1:L:273:LEU:O	1:L:277:ILE:HG13	2.07	0.55
1:A:163:GLU:O	1:A:166:LEU:HB3	2.06	0.55
1:E:139:MET:CE	1:E:183:VAL:HG21	2.36	0.55
1:I:186:GLN:HG2	1:I:187:ASP:H	1.70	0.55
1:J:276:ILE:HD11	1:L:163:GLU:HG3	1.88	0.55
1:C:211:ILE:HD13	1:C:216:LEU:HD12	1.89	0.55
1:H:207:GLY:O	1:H:208:LEU:HB2	2.07	0.55
1:C:256:PHE:O	1:C:257:ASP:CB	2.55	0.54
1:D:185:GLN:OE1	1:D:256:PHE:O	2.24	0.54
1:K:199:LEU:HD12	1:K:199:LEU:H	1.73	0.54
1:A:211:ILE:HD12	1:A:216:LEU:HD12	1.89	0.54
1:D:237:TRP:CZ3	1:D:239:PRO:HB3	2.42	0.54
1:I:163:GLU:OE2	1:I:163:GLU:N	2.38	0.54
1:L:174:ARG:HG2	1:L:223:ARG:HB2	1.90	0.54
1:J:268:LYS:NZ	1:L:159:VAL:HB	2.19	0.54
1:J:304:LEU:HD12	1:L:199:LEU:HD12	1.90	0.54
1:J:147:TYR:O	1:J:285:ARG:NH2	2.31	0.54
1:J:253:GLN:HB2	1:J:262:LYS:NZ	2.22	0.54
1:D:196:PRO:HG2	1:D:199:LEU:HD12	1.89	0.54
1:E:136:ARG:HG3	1:E:136:ARG:HH11	1.71	0.54
1:G:180:ARG:HH21	1:G:199:LEU:HD11	1.73	0.54
1:H:155:GLY:O	1:H:159:VAL:HG21	2.08	0.54
1:D:263:ILE:CG2	1:D:264:THR:N	2.70	0.54
1:F:235:GLU:O	1:F:236:ASN:HB3	2.08	0.54
1:F:235:GLU:HB3	1:F:266:PRO:HA	1.89	0.54
1:L:256:PHE:O	1:L:257:ASP:CB	2.54	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:191:ILE:HG22	1:G:228:ILE:HB	1.90	0.53
1:J:255:ILE:HD12	1:J:260:VAL:HG21	1.90	0.53
1:K:303:HIS:HD2	1:K:308:ASN:CA	2.15	0.53
1:B:185:GLN:OE1	1:B:256:PHE:O	2.26	0.53
1:G:145:ASP:C	1:G:145:ASP:OD2	2.46	0.53
1:K:268:LYS:HG3	1:K:269:VAL:H	1.72	0.53
1:G:267:PHE:CD2	1:G:271:ARG:HB3	2.41	0.53
1:L:254:LEU:HD21	1:L:257:ASP:HA	1.90	0.53
1:D:308:ASN:HA	1:F:180:ARG:HH21	1.73	0.53
1:F:292:ASP:O	1:F:293:ALA:CB	2.50	0.53
1:G:180:ARG:NH2	1:G:199:LEU:HD13	2.24	0.53
1:K:136:ARG:HH11	1:K:136:ARG:HG2	1.71	0.53
1:L:272:ASN:OD1	1:L:275:ILE:CG1	2.52	0.53
1:L:267:PHE:C	1:L:267:PHE:CD1	2.82	0.53
1:C:189:GLN:HG3	1:C:190:THR:OG1	2.09	0.53
1:F:266:PRO:HG2	1:F:271:ARG:HH12	1.72	0.53
1:D:300:ASN:HD22	1:D:303:HIS:HD2	1.56	0.53
1:H:191:ILE:HD11	1:H:255:ILE:HB	1.90	0.53
1:L:187:ASP:OD2	1:L:189:GLN:HG3	2.08	0.53
1:C:273:LEU:O	1:C:277:ILE:HG13	2.08	0.53
1:I:171:ARG:HE	1:I:278:GLU:CD	2.12	0.53
1:K:184:TYR:HD1	1:K:185:GLN:O	1.92	0.52
1:D:166:LEU:HD13	1:D:203:LEU:HD13	1.91	0.52
1:F:272:ASN:ND2	1:F:272:ASN:C	2.57	0.52
1:G:141:GLY:HA2	1:G:161:LYS:HE3	1.90	0.52
1:A:145:ASP:OD1	1:A:145:ASP:C	2.46	0.52
1:A:254:LEU:HD12	1:A:257:ASP:HA	1.91	0.52
1:D:156:ASP:OD2	1:D:156:ASP:N	2.38	0.52
1:H:272:ASN:C	1:H:272:ASN:ND2	2.63	0.52
1:B:254:LEU:HD21	1:B:257:ASP:N	2.21	0.52
1:C:292:ASP:O	1:C:293:ALA:CB	2.57	0.52
1:D:162:SER:OG	1:D:178:ASP:OD2	2.25	0.52
1:A:254:LEU:HA	1:A:258:VAL:O	2.09	0.52
1:E:198:ILE:HG13	1:E:199:LEU:H	1.74	0.52
1:E:145:ASP:OD2	1:E:145:ASP:C	2.47	0.52
1:J:244:ASP:OD1	1:J:246:LEU:O	2.26	0.52
1:K:145:ASP:OD2	1:K:145:ASP:C	2.48	0.52
1:A:143:LEU:HG	1:A:176:ILE:HD12	1.91	0.52
1:G:188:GLU:O	1:G:189:GLN:HB3	2.09	0.52
1:L:268:LYS:O	1:L:269:VAL:O	2.28	0.52
1:D:161:LYS:O	1:D:164:THR:HB	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:273:LEU:O	1:F:277:ILE:HG13	2.10	0.52
1:G:272:ASN:C	1:G:272:ASN:HD22	2.13	0.52
1:H:275:ILE:CG2	1:H:276:ILE:HD13	2.39	0.52
1:J:171:ARG:HH22	1:J:275:ILE:CD1	2.23	0.52
1:J:301:LEU:CD2	1:J:305:ILE:HD11	2.40	0.52
1:K:180:ARG:NH2	1:K:199:LEU:HD11	2.23	0.52
1:A:183:VAL:HG23	1:A:191:ILE:HG23	1.91	0.51
1:F:149:LEU:HD22	1:F:229:SER:HB2	1.93	0.51
1:J:279:VAL:HG21	1:L:166:LEU:HD21	1.92	0.51
1:G:163:GLU:O	1:G:166:LEU:HB3	2.10	0.51
1:K:187:ASP:OD2	1:K:188:GLU:N	2.43	0.51
1:E:149:LEU:HD21	1:E:229:SER:HB2	1.91	0.51
1:J:275:ILE:HD11	1:L:167:GLU:OE2	2.11	0.51
1:F:272:ASN:ND2	1:F:275:ILE:HG12	2.26	0.51
1:K:176:ILE:HG12	1:K:226:THR:HG22	1.91	0.51
1:E:305:ILE:HG22	1:J:180:ARG:HG2	1.93	0.51
1:A:214:MET:HE3	1:F:215:ASN:HD22	1.76	0.51
1:A:272:ASN:C	1:A:272:ASN:ND2	2.64	0.51
1:I:153:ILE:HD13	1:I:277:ILE:HD13	1.93	0.51
1:B:145:ASP:OD2	1:B:174:ARG:NH2	2.44	0.51
1:G:170:GLN:OE1	1:G:170:GLN:HA	2.11	0.51
1:E:268:LYS:O	1:E:270:GLY:N	2.43	0.51
1:D:234:LEU:HD21	1:D:273:LEU:HD21	1.93	0.50
1:H:269:VAL:HG23	1:H:270:GLY:N	2.26	0.50
1:A:142:VAL:HG12	1:A:144:VAL:HG13	1.93	0.50
1:H:155:GLY:O	1:H:159:VAL:CG2	2.59	0.50
1:A:159:VAL:O	1:A:159:VAL:HG13	2.11	0.50
1:B:189:GLN:HE21	1:B:189:GLN:N	2.09	0.50
1:E:216:LEU:HD21	1:F:283:ASN:HD22	1.77	0.50
1:C:188:GLU:OE1	1:C:188:GLU:N	2.44	0.50
1:J:246:LEU:CD1	1:J:248:SER:OG	2.60	0.50
1:K:292:ASP:O	1:K:293:ALA:HB3	2.11	0.50
1:L:156:ASP:HA	1:L:161:LYS:HZ2	1.74	0.50
1:F:254:LEU:HD22	1:F:257:ASP:O	2.11	0.50
1:G:155:GLY:O	1:G:156:ASP:HB3	2.12	0.50
1:I:302:ASN:C	1:I:304:LEU:H	2.15	0.50
1:I:302:ASN:C	1:I:304:LEU:N	2.65	0.50
1:J:246:LEU:HD22	1:J:294:THR:HG23	1.94	0.50
1:H:157:SER:C	1:H:159:VAL:H	2.15	0.50
1:K:204:GLU:O	1:K:206:ARG:NH2	2.45	0.50
1:L:159:VAL:HG12	1:L:267:PHE:CZ	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:142:VAL:HG21	1:L:161:LYS:HB3	1.94	0.49
1:A:198:ILE:HD13	1:A:199:LEU:N	2.25	0.49
1:G:159:VAL:O	1:G:160:GLY:O	2.29	0.49
1:H:191:ILE:HD13	1:H:255:ILE:HB	1.94	0.49
1:I:212:ASP:OD1	1:I:215:ASN:HB2	2.12	0.49
1:A:223:ARG:NH1	1:A:226:THR:CG2	2.74	0.49
1:E:198:ILE:C	1:E:198:ILE:HD12	2.32	0.49
1:I:151:VAL:HG22	1:I:230:LEU:HD23	1.93	0.49
1:B:282:MET:HB3	1:C:216:LEU:HD22	1.95	0.49
1:K:286:ALA:HA	1:K:289:MET:HE2	1.94	0.49
1:A:153:ILE:HA	1:A:232:VAL:O	2.10	0.49
1:C:174:ARG:HG2	1:C:223:ARG:HB2	1.95	0.49
1:D:242:THR:CG2	1:D:243:PHE:N	2.75	0.49
1:J:205:ILE:O	1:J:205:ILE:HG22	2.13	0.49
1:D:237:TRP:HZ2	1:F:206:ARG:HH12	1.60	0.49
1:G:286:ALA:HA	1:G:289:MET:CE	2.41	0.49
1:I:180:ARG:HD2	1:I:196:PRO:HG3	1.94	0.49
1:J:167:GLU:O	1:J:171:ARG:HG3	2.12	0.49
1:K:145:ASP:O	1:K:173:HIS:HB3	2.13	0.49
1:B:308:ASN:O	1:B:311:THR:OG1	2.20	0.49
1:E:170:GLN:HG2	1:E:217:PHE:HE2	1.77	0.49
1:D:156:ASP:O	1:D:159:VAL:HG22	2.13	0.49
1:D:292:ASP:O	1:D:292:ASP:OD2	2.31	0.48
1:H:242:THR:O	1:H:243:PHE:O	2.31	0.48
1:L:158:GLY:O	1:L:159:VAL:C	2.52	0.48
1:H:275:ILE:HG22	1:H:276:ILE:HD13	1.94	0.48
1:J:185:GLN:OE1	1:J:256:PHE:O	2.30	0.48
1:E:156:ASP:HB3	1:E:161:LYS:HZ3	1.77	0.48
1:I:167:GLU:O	1:I:171:ARG:HG3	2.13	0.48
1:E:286:ALA:HA	1:E:289:MET:HE2	1.95	0.48
1:G:176:ILE:HG12	1:G:226:THR:CG2	2.42	0.48
1:A:211:ILE:CD1	1:A:216:LEU:HD12	2.43	0.48
1:F:174:ARG:HD3	1:F:220:GLY:O	2.14	0.48
1:L:137:ARG:NH2	1:L:256:PHE:H	2.11	0.48
1:B:275:ILE:HG23	1:B:276:ILE:N	2.28	0.48
1:B:275:ILE:O	1:B:279:VAL:HG23	2.14	0.48
1:E:163:GLU:O	1:E:166:LEU:HB3	2.13	0.48
1:G:211:ILE:C	1:G:211:ILE:HD12	2.33	0.48
1:K:136:ARG:NH1	1:K:136:ARG:HG2	2.28	0.48
1:J:268:LYS:O	1:J:268:LYS:HG2	2.14	0.48
1:D:263:ILE:CG2	1:D:264:THR:H	2.27	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:140:HIS:HD2	1:F:141:GLY:N	2.12	0.48
1:I:214:MET:O	1:I:214:MET:HG2	2.12	0.48
1:A:198:ILE:HG23	1:A:199:LEU:N	2.26	0.48
1:F:211:ILE:HD13	1:F:216:LEU:HD12	1.96	0.48
1:C:170:GLN:HG2	1:C:217:PHE:CE2	2.49	0.47
1:D:145:ASP:CG	1:D:174:ARG:HH21	2.16	0.47
1:F:171:ARG:HE	1:F:278:GLU:CD	2.17	0.47
1:L:195:ALA:HA	1:L:196:PRO:HD2	1.65	0.47
1:G:304:LEU:HA	1:G:304:LEU:HD22	1.67	0.47
1:K:272:ASN:O	1:K:276:ILE:HG12	2.15	0.47
1:C:203:LEU:HD23	1:C:211:ILE:HG13	1.95	0.47
1:H:150:GLY:HA3	1:H:227:THR:O	2.15	0.47
1:I:195:ALA:HA	1:I:196:PRO:HD2	1.63	0.47
1:E:166:LEU:HD21	1:F:279:VAL:HG21	1.95	0.47
1:E:174:ARG:HD3	1:E:220:GLY:O	2.15	0.47
1:D:279:VAL:O	1:D:280:ALA:C	2.50	0.47
1:E:211:ILE:C	1:E:211:ILE:HD12	2.35	0.47
1:F:272:ASN:HD21	1:F:275:ILE:H	1.57	0.47
1:H:244:ASP:OD1	1:H:246:LEU:O	2.32	0.47
1:I:203:LEU:CD2	1:I:211:ILE:HD11	2.39	0.47
1:L:292:ASP:O	1:L:293:ALA:CB	2.63	0.47
1:A:170:GLN:HB2	1:C:275:ILE:HD11	1.96	0.47
1:C:185:GLN:HG3	1:C:186:GLN:H	1.80	0.47
1:E:254:LEU:HD23	1:E:257:ASP:HA	1.97	0.47
1:F:166:LEU:O	1:F:169:VAL:HG22	2.15	0.47
1:A:160:GLY:O	1:A:162:SER:N	2.48	0.46
1:L:166:LEU:HD13	1:L:203:LEU:HD21	1.97	0.46
1:L:235:GLU:O	1:L:267:PHE:CB	2.54	0.46
1:A:214:MET:CE	1:F:215:ASN:HD22	2.28	0.46
1:A:214:MET:CE	1:F:215:ASN:ND2	2.79	0.46
1:B:176:ILE:O	1:B:195:ALA:HB2	2.16	0.46
1:B:262:LYS:HG2	1:B:263:ILE:N	2.29	0.46
1:C:184:TYR:HD1	1:C:185:GLN:O	1.98	0.46
1:G:192:VAL:HA	1:G:227:THR:HA	1.98	0.46
1:K:272:ASN:HD22	1:K:272:ASN:C	2.17	0.46
1:A:255:ILE:O	1:A:256:PHE:HB2	2.16	0.46
1:B:142:VAL:HG11	1:B:165:ALA:HB2	1.98	0.46
1:G:146:ILE:HG22	1:G:147:TYR:CD1	2.51	0.46
1:D:237:TRP:HZ3	1:D:239:PRO:CA	2.29	0.46
1:F:307:HIS:ND1	1:F:308:ASN:N	2.64	0.46
1:G:283:ASN:HD22	1:H:216:LEU:HD21	1.80	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:255:ILE:HD12	1:H:260:VAL:HG21	1.97	0.46
1:I:253:GLN:CB	1:I:262:LYS:HD2	2.46	0.46
1:L:234:LEU:HD22	1:L:273:LEU:HD13	1.97	0.46
1:H:269:VAL:C	1:H:271:ARG:H	2.19	0.46
1:A:163:GLU:OE1	1:C:271:ARG:HB2	2.16	0.46
1:D:145:ASP:O	1:D:173:HIS:HB3	2.16	0.46
1:D:191:ILE:CD1	1:D:260:VAL:CG2	2.93	0.46
1:F:275:ILE:O	1:F:279:VAL:HG23	2.15	0.46
1:H:285:ARG:NH1	2:H:325:HOH:O	2.47	0.46
1:K:178:ASP:CG	1:K:203:LEU:HD23	2.36	0.46
1:E:248:SER:HB2	1:E:249:GLY:H	1.60	0.46
1:I:269:VAL:O	1:I:271:ARG:N	2.48	0.46
1:K:198:ILE:HG22	1:K:199:LEU:H	1.80	0.46
1:D:137:ARG:NH2	1:D:256:PHE:H	2.14	0.46
1:F:157:SER:O	1:F:158:GLY:C	2.54	0.46
1:C:162:SER:HB3	1:C:178:ASP:OD1	2.16	0.46
1:F:145:ASP:CG	1:F:174:ARG:HH21	2.20	0.45
1:G:196:PRO:O	1:G:200:SER:HB2	2.16	0.45
1:K:301:LEU:HD23	1:K:301:LEU:HA	1.69	0.45
1:H:205:ILE:O	1:H:206:ARG:C	2.55	0.45
1:A:183:VAL:HG23	1:A:191:ILE:CG2	2.46	0.45
1:B:212:ASP:OD2	1:B:212:ASP:C	2.55	0.45
1:G:170:GLN:OE1	1:G:217:PHE:HE2	1.98	0.45
1:K:183:VAL:HG23	1:K:256:PHE:HE1	1.82	0.45
1:A:198:ILE:HD13	1:A:198:ILE:C	2.37	0.45
1:G:212:ASP:HB3	1:G:215:ASN:HB3	1.99	0.45
1:G:279:VAL:HA	1:G:282:MET:CE	2.47	0.45
1:H:137:ARG:HG3	1:H:256:PHE:HZ	1.75	0.45
1:H:142:VAL:HG11	1:H:165:ALA:HB2	1.98	0.45
1:L:142:VAL:CG2	1:L:161:LYS:HB3	2.46	0.45
1:E:184:TYR:HA	1:E:256:PHE:HE1	1.80	0.45
1:H:187:ASP:OD2	1:H:187:ASP:C	2.55	0.45
1:J:145:ASP:OD2	1:J:145:ASP:C	2.55	0.45
1:L:203:LEU:HD22	1:L:211:ILE:HG13	1.99	0.45
1:L:251:GLN:HB3	1:L:252:THR:H	1.54	0.45
1:B:279:VAL:HG13	1:C:216:LEU:HD13	1.99	0.45
1:E:156:ASP:HB3	1:E:161:LYS:HZ2	1.81	0.45
1:E:251:GLN:HE21	1:E:262:LYS:HD3	1.82	0.45
1:G:159:VAL:HG11	1:G:206:ARG:HG3	1.98	0.45
1:H:185:GLN:OE1	1:H:256:PHE:O	2.35	0.45
1:H:292:ASP:O	1:H:293:ALA:C	2.55	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:VAL:HG23	1:C:146:ILE:HG13	1.99	0.45
1:E:174:ARG:CD	1:E:220:GLY:O	2.64	0.45
1:E:211:ILE:HD13	1:E:216:LEU:HD12	1.98	0.45
1:H:225:ASP:OD2	1:H:225:ASP:C	2.55	0.45
1:A:149:LEU:HD11	1:A:229:SER:CB	2.47	0.45
1:I:263:ILE:O	1:I:263:ILE:HG13	2.17	0.45
1:E:149:LEU:CD2	1:E:229:SER:HB2	2.47	0.45
1:G:145:ASP:O	1:G:173:HIS:HB3	2.16	0.45
1:J:279:VAL:O	1:J:280:ALA:C	2.54	0.45
1:C:171:ARG:HG2	1:C:171:ARG:HH11	1.82	0.44
1:K:180:ARG:HH22	1:K:199:LEU:HD13	1.82	0.44
1:L:191:ILE:HD12	1:L:260:VAL:CG2	2.47	0.44
1:E:136:ARG:HG3	1:E:136:ARG:NH1	2.32	0.44
1:F:154:THR:O	1:F:233:HIS:HA	2.17	0.44
1:I:216:LEU:HD23	1:I:216:LEU:HA	1.74	0.44
1:J:145:ASP:CG	1:J:174:ARG:HH21	2.20	0.44
1:J:196:PRO:O	1:J:197:PRO:C	2.55	0.44
1:J:234:LEU:HD23	1:J:265:VAL:HG22	2.00	0.44
1:L:170:GLN:OE1	1:L:170:GLN:HA	2.17	0.44
1:A:267:PHE:HE1	1:A:271:ARG:HB3	1.82	0.44
1:F:272:ASN:CG	1:F:275:ILE:HG12	2.38	0.44
1:H:145:ASP:OD2	1:H:145:ASP:C	2.55	0.44
1:F:235:GLU:O	1:F:236:ASN:CB	2.65	0.44
1:G:287:LYS:HB2	1:G:287:LYS:HE3	1.89	0.44
1:G:157:SER:O	1:G:160:GLY:N	2.50	0.44
1:G:157:SER:O	1:G:160:GLY:CA	2.64	0.44
1:G:204:GLU:O	1:G:206:ARG:NH1	2.51	0.44
1:J:140:HIS:CD2	1:J:180:ARG:HH11	2.36	0.44
1:J:196:PRO:HG2	1:J:199:LEU:HD12	1.99	0.44
1:K:274:ALA:O	1:K:278:GLU:HG3	2.17	0.44
1:F:290:GLY:O	1:F:291:TYR:C	2.56	0.44
1:G:279:VAL:HA	1:G:282:MET:HE3	2.00	0.44
1:I:180:ARG:HD2	1:I:196:PRO:HB3	1.98	0.44
1:J:162:SER:O	1:J:165:ALA:HB3	2.17	0.44
1:F:254:LEU:HA	1:F:258:VAL:O	2.18	0.44
1:I:211:ILE:HD12	1:I:211:ILE:O	2.16	0.44
1:A:226:THR:HB	1:A:227:THR:O	2.17	0.44
1:I:137:ARG:H	1:I:256:PHE:HZ	1.65	0.44
1:K:235:GLU:O	1:K:267:PHE:HB3	2.18	0.44
1:A:225:ASP:O	1:A:226:THR:O	2.36	0.44
1:B:137:ARG:HB2	1:B:256:PHE:CZ	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:185:GLN:HG2	1:F:186:GLN:H	1.83	0.44
1:A:175:LEU:HD23	1:A:213:VAL:HG21	2.00	0.43
1:B:160:GLY:O	1:B:163:GLU:HG2	2.18	0.43
1:C:285:ARG:O	1:C:289:MET:HG3	2.18	0.43
1:E:184:TYR:HD1	1:E:185:GLN:O	2.01	0.43
1:G:184:TYR:HA	1:G:256:PHE:HE1	1.83	0.43
1:H:270:GLY:O	1:I:159:VAL:HG11	2.18	0.43
1:F:139:MET:HE3	1:F:183:VAL:HG21	2.00	0.43
1:F:253:GLN:HB2	1:F:262:LYS:HD2	1.99	0.43
1:J:272:ASN:HD21	1:J:274:ALA:HB3	1.83	0.43
1:A:175:LEU:CD2	1:A:213:VAL:HG21	2.48	0.43
1:A:223:ARG:O	1:A:224:GLU:HB3	2.14	0.43
1:E:138:SER:HB2	1:E:182:ASP:OD1	2.19	0.43
1:F:179:ASP:O	1:F:180:ARG:C	2.56	0.43
1:J:301:LEU:HD23	1:J:305:ILE:HD11	2.00	0.43
1:K:304:LEU:HD22	1:K:304:LEU:O	2.18	0.43
1:B:309:GLU:C	1:B:311:THR:N	2.70	0.43
1:F:156:ASP:O	1:F:161:LYS:NZ	2.51	0.43
1:H:145:ASP:O	1:H:173:HIS:HB3	2.17	0.43
1:H:280:ALA:HB2	1:I:208:LEU:HD21	2.00	0.43
1:D:234:LEU:CD2	1:D:273:LEU:HD21	2.48	0.43
1:E:201:HIS:HE1	1:E:223:ARG:O	2.02	0.43
1:I:203:LEU:C	1:I:203:LEU:HD23	2.39	0.43
1:J:187:ASP:OD2	1:J:187:ASP:C	2.57	0.43
1:K:146:ILE:CD1	1:K:277:ILE:HG22	2.49	0.43
1:D:237:TRP:CZ2	1:F:206:ARG:NH1	2.85	0.43
1:F:184:TYR:HD1	1:F:184:TYR:O	2.02	0.43
1:K:295:LYS:O	1:K:299:LYS:HB2	2.18	0.43
1:C:170:GLN:HG2	1:C:217:PHE:HE2	1.84	0.43
1:C:203:LEU:HD23	1:C:203:LEU:C	2.39	0.43
1:H:165:ALA:O	1:H:169:VAL:HG13	2.19	0.43
1:B:279:VAL:HG21	1:C:166:LEU:CD2	2.49	0.43
1:D:269:VAL:HG23	1:D:269:VAL:O	2.19	0.43
1:F:143:LEU:HD13	1:F:176:ILE:HB	2.01	0.43
1:D:275:ILE:O	1:D:279:VAL:HG23	2.18	0.43
1:F:292:ASP:HB3	1:F:295:LYS:HB2	2.01	0.43
1:D:242:THR:HG23	1:D:243:PHE:H	1.81	0.42
1:J:171:ARG:HH22	1:J:275:ILE:HD11	1.83	0.42
1:B:246:LEU:HD13	1:B:248:SER:OG	2.19	0.42
1:H:263:ILE:HG13	1:H:264:THR:N	2.34	0.42
1:I:136:ARG:HG3	1:I:184:TYR:HB3	2.02	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:145:ASP:OD1	1:J:223:ARG:NH1	2.50	0.42
1:L:136:ARG:HG3	1:L:184:TYR:HB3	2.01	0.42
1:E:145:ASP:O	1:E:173:HIS:HB3	2.20	0.42
1:F:161:LYS:O	1:F:164:THR:HB	2.19	0.42
1:G:178:ASP:CG	1:G:203:LEU:HD12	2.39	0.42
1:K:196:PRO:HG3	1:K:199:LEU:HB2	2.00	0.42
1:K:296:THR:O	1:K:299:LYS:HB3	2.19	0.42
1:E:149:LEU:HD23	1:E:149:LEU:HA	1.85	0.42
1:E:196:PRO:CG	1:E:199:LEU:HB2	2.49	0.42
1:F:263:ILE:CG2	1:F:264:THR:N	2.82	0.42
1:L:178:ASP:O	1:L:179:ASP:C	2.58	0.42
1:C:153:ILE:CD1	1:C:277:ILE:HD13	2.48	0.42
1:E:156:ASP:N	1:E:161:LYS:HZ2	2.16	0.42
1:F:265:VAL:HA	1:F:266:PRO:HD2	1.86	0.42
1:H:196:PRO:O	1:H:197:PRO:C	2.58	0.42
1:K:141:GLY:HA2	1:K:161:LYS:HE3	2.02	0.42
1:K:283:ASN:O	1:K:287:LYS:HB2	2.19	0.42
1:K:268:LYS:HG3	1:K:269:VAL:N	2.34	0.42
1:B:275:ILE:HD12	1:C:167:GLU:HA	2.02	0.42
1:G:183:VAL:HG12	1:G:184:TYR:N	2.34	0.42
1:D:205:ILE:O	1:D:206:ARG:C	2.58	0.42
1:D:262:LYS:HG2	1:D:263:ILE:H	1.85	0.42
1:E:160:GLY:O	1:E:163:GLU:N	2.46	0.42
1:F:140:HIS:CD2	1:F:141:GLY:N	2.88	0.42
1:L:137:ARG:HB2	1:L:256:PHE:CE1	2.55	0.42
1:A:183:VAL:CG2	1:A:191:ILE:HG23	2.49	0.41
1:B:310:GLU:O	1:B:310:GLU:HG3	2.20	0.41
1:F:185:GLN:OE1	1:F:256:PHE:HB3	2.20	0.41
1:F:272:ASN:HD21	1:F:274:ALA:CB	2.23	0.41
1:I:156:ASP:HA	1:I:161:LYS:NZ	2.36	0.41
1:L:178:ASP:O	1:L:180:ARG:N	2.53	0.41
1:D:212:ASP:C	1:D:212:ASP:OD2	2.59	0.41
1:F:156:ASP:CG	1:F:157:SER:N	2.73	0.41
1:G:174:ARG:CD	1:G:220:GLY:O	2.68	0.41
1:A:205:ILE:CB	1:A:208:LEU:HD11	2.41	0.41
1:A:267:PHE:CE1	1:A:271:ARG:HB3	2.54	0.41
1:D:309:GLU:O	1:D:311:THR:N	2.53	0.41
1:E:272:ASN:HD22	1:E:273:LEU:N	2.18	0.41
1:E:286:ALA:HA	1:E:289:MET:CE	2.50	0.41
1:K:250:GLU:H	1:K:250:GLU:HG2	1.56	0.41
1:E:180:ARG:HH21	1:E:199:LEU:HD12	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:304:LEU:HD12	1:E:304:LEU:O	2.20	0.41
1:F:152:LEU:HB3	1:F:231:ILE:HG12	2.01	0.41
1:G:198:ILE:HG23	1:G:199:LEU:HD12	2.02	0.41
1:K:187:ASP:CG	1:K:189:GLN:H	2.24	0.41
1:C:253:GLN:HB2	1:C:262:LYS:HZ2	1.86	0.41
1:D:292:ASP:CG	1:D:295:LYS:HG3	2.40	0.41
1:G:158:GLY:C	1:G:160:GLY:H	2.24	0.41
1:A:145:ASP:O	1:A:173:HIS:HB3	2.21	0.41
1:A:153:ILE:H	1:A:153:ILE:HG12	1.76	0.41
1:D:203:LEU:C	1:D:203:LEU:HD23	2.41	0.41
1:E:174:ARG:HD3	1:E:174:ARG:HH11	1.69	0.41
1:E:267:PHE:CE2	1:E:271:ARG:HB2	2.55	0.41
1:F:139:MET:CE	1:F:183:VAL:HG21	2.50	0.41
1:F:179:ASP:CG	1:F:180:ARG:HG2	2.41	0.41
1:K:174:ARG:CD	1:K:220:GLY:O	2.68	0.41
1:K:176:ILE:N	1:K:176:ILE:HD12	2.35	0.41
1:L:191:ILE:HD12	1:L:260:VAL:HG21	2.03	0.41
1:D:196:PRO:O	1:D:197:PRO:C	2.57	0.41
1:D:309:GLU:C	1:D:311:THR:N	2.72	0.41
1:G:186:GLN:O	1:G:187:ASP:HB3	2.21	0.41
1:H:161:LYS:H	1:H:161:LYS:HE3	1.85	0.41
1:I:139:MET:SD	1:I:183:VAL:HG21	2.61	0.41
1:L:184:TYR:C	1:L:184:TYR:CD1	2.94	0.41
1:B:254:LEU:HD23	1:B:255:ILE:N	2.35	0.41
1:B:275:ILE:CG2	1:B:276:ILE:N	2.83	0.41
1:C:171:ARG:HG2	1:C:171:ARG:NH1	2.36	0.41
1:C:303:HIS:O	1:C:303:HIS:ND1	2.54	0.41
1:D:268:LYS:O	1:D:269:VAL:C	2.59	0.41
1:E:191:ILE:HD13	1:E:191:ILE:HA	1.94	0.41
1:H:166:LEU:HD12	1:H:166:LEU:HA	1.71	0.41
1:I:186:GLN:O	1:I:187:ASP:C	2.59	0.41
1:J:145:ASP:OD2	1:J:174:ARG:NH2	2.54	0.41
1:J:149:LEU:HD23	1:J:149:LEU:C	2.41	0.41
1:J:171:ARG:NH2	1:J:275:ILE:CD1	2.84	0.41
1:K:224:GLU:OE2	1:K:224:GLU:HA	2.20	0.41
1:K:272:ASN:HD22	1:K:273:LEU:N	2.19	0.41
1:L:216:LEU:HD23	1:L:216:LEU:HA	1.84	0.41
1:L:265:VAL:HA	1:L:266:PRO:HD2	1.93	0.41
1:B:273:LEU:HD23	1:B:273:LEU:HA	1.88	0.41
1:E:143:LEU:HD13	1:E:176:ILE:CB	2.51	0.41
1:F:170:GLN:HG2	1:F:217:PHE:HE2	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:199:LEU:HD23	1:L:199:LEU:HA	1.87	0.41
1:A:254:LEU:CD1	1:A:257:ASP:HA	2.51	0.40
1:B:256:PHE:O	1:B:257:ASP:CB	2.64	0.40
1:D:166:LEU:HD12	1:D:166:LEU:HA	1.87	0.40
1:D:206:ARG:O	1:E:271:ARG:NH2	2.49	0.40
1:E:178:ASP:CB	1:E:203:LEU:HD23	2.51	0.40
1:G:235:GLU:O	1:G:267:PHE:HB3	2.21	0.40
1:I:253:GLN:HB3	1:I:262:LYS:HD2	2.03	0.40
1:C:136:ARG:CA	1:C:256:PHE:HZ	2.30	0.40
1:C:171:ARG:NH2	1:C:275:ILE:HG12	2.36	0.40
1:I:214:MET:CE	1:I:219:ALA:HB2	2.51	0.40
1:J:186:GLN:HE21	1:J:190:THR:HG21	1.86	0.40
1:E:162:SER:HB2	1:E:203:LEU:HD22	2.03	0.40
1:F:195:ALA:HA	1:F:196:PRO:HD3	1.99	0.40
1:L:156:ASP:O	1:L:157:SER:O	2.40	0.40
1:B:292:ASP:CG	1:B:295:LYS:HD3	2.41	0.40
1:F:166:LEU:HD13	1:F:203:LEU:HD23	2.04	0.40
1:F:285:ARG:O	1:F:289:MET:HG3	2.22	0.40
1:H:279:VAL:O	1:H:280:ALA:C	2.58	0.40
1:I:166:LEU:HD13	1:I:203:LEU:HD21	2.02	0.40
1:J:268:LYS:O	1:J:270:GLY:N	2.54	0.40
1:B:145:ASP:CG	1:B:174:ARG:NH2	2.74	0.40
1:B:283:ASN:HA	1:C:216:LEU:HD21	2.04	0.40
1:C:171:ARG:HH11	1:C:171:ARG:CG	2.34	0.40
1:J:170:GLN:HA	1:J:170:GLN:HE21	1.86	0.40
1:L:212:ASP:HB3	1:L:215:ASN:HB2	2.03	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	157/205 (77%)	127 (81%)	23 (15%)	7 (4%)	2	3
1	B	179/205 (87%)	161 (90%)	16 (9%)	2 (1%)	14	30
1	C	160/205 (78%)	140 (88%)	12 (8%)	8 (5%)	2	2
1	D	179/205 (87%)	155 (87%)	17 (10%)	7 (4%)	3	4
1	E	160/205 (78%)	132 (82%)	23 (14%)	5 (3%)	4	6
1	F	156/205 (76%)	142 (91%)	10 (6%)	4 (3%)	5	9
1	G	156/205 (76%)	130 (83%)	14 (9%)	12 (8%)	1	1
1	H	176/205 (86%)	149 (85%)	17 (10%)	10 (6%)	1	2
1	I	156/205 (76%)	134 (86%)	11 (7%)	11 (7%)	1	1
1	J	176/205 (86%)	151 (86%)	18 (10%)	7 (4%)	3	3
1	K	158/205 (77%)	129 (82%)	20 (13%)	9 (6%)	1	2
1	L	157/205 (77%)	130 (83%)	19 (12%)	8 (5%)	2	2
All	All	1970/2460 (80%)	1680 (85%)	200 (10%)	90 (5%)	2	3

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	137	ARG
1	A	226	THR
1	B	133	LEU
1	D	269	VAL
1	D	293	ALA
1	E	156	ASP
1	E	159	VAL
1	F	159	VAL
1	F	267	PHE
1	F	269	VAL
1	F	291	TYR
1	G	137	ARG
1	G	189	GLN
1	G	251	GLN
1	G	293	ALA
1	H	157	SER
1	H	243	PHE
1	H	269	VAL
1	H	293	ALA
1	I	159	VAL
1	I	269	VAL
1	I	303	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	269	VAL
1	J	293	ALA
1	J	310	GLU
1	K	199	LEU
1	K	269	VAL
1	K	293	ALA
1	K	301	LEU
1	L	156	ASP
1	L	157	SER
1	L	269	VAL
1	L	270	GLY
1	A	160	GLY
1	A	161	LYS
1	A	224	GLU
1	A	271	ARG
1	B	310	GLU
1	C	200	SER
1	C	257	ASP
1	D	308	ASN
1	D	310	GLU
1	E	269	VAL
1	E	293	ALA
1	G	160	GLY
1	G	199	LEU
1	G	200	SER
1	G	269	VAL
1	H	156	ASP
1	H	208	LEU
1	I	270	GLY
1	I	293	ALA
1	I	304	LEU
1	J	206	ARG
1	J	237	TRP
1	K	137	ARG
1	L	257	ASP
1	C	156	ASP
1	C	293	ALA
1	D	237	TRP
1	D	256	PHE
1	G	306	GLU
1	I	187	ASP
1	J	239	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	157	SER
1	K	184	TYR
1	L	268	LYS
1	C	179	ASP
1	C	302	ASN
1	G	156	ASP
1	G	161	LYS
1	H	257	ASP
1	K	200	SER
1	C	137	ARG
1	D	309	GLU
1	E	199	LEU
1	G	188	GLU
1	H	241	LYS
1	I	137	ARG
1	I	188	GLU
1	I	251	GLN
1	J	257	ASP
1	K	138	SER
1	L	252	THR
1	L	306	GLU
1	C	197	PRO
1	H	207	GLY
1	H	270	GLY
1	I	158	GLY
1	A	269	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	135/174 (78%)	113 (84%)	22 (16%)	2 3
1	B	153/174 (88%)	132 (86%)	21 (14%)	3 6
1	C	138/174 (79%)	118 (86%)	20 (14%)	3 5
1	D	153/174 (88%)	130 (85%)	23 (15%)	3 5

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	E	138/174 (79%)	117 (85%)	21 (15%)	3 4
1	F	135/174 (78%)	115 (85%)	20 (15%)	3 5
1	G	135/174 (78%)	116 (86%)	19 (14%)	3 6
1	H	150/174 (86%)	128 (85%)	22 (15%)	3 5
1	I	135/174 (78%)	115 (85%)	20 (15%)	3 5
1	J	151/174 (87%)	127 (84%)	24 (16%)	2 4
1	K	136/174 (78%)	112 (82%)	24 (18%)	2 3
1	L	136/174 (78%)	116 (85%)	20 (15%)	3 5
All	All	1695/2088 (81%)	1439 (85%)	256 (15%)	3 4

All (256) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	SER
1	A	145	ASP
1	A	151	VAL
1	A	153	ILE
1	A	162	SER
1	A	164	THR
1	A	170	GLN
1	A	174	ARG
1	A	198	ILE
1	A	208	LEU
1	A	250	GLU
1	A	254	LEU
1	A	255	ILE
1	A	263	ILE
1	A	271	ARG
1	A	272	ASN
1	A	273	LEU
1	A	275	ILE
1	A	285	ARG
1	A	294	THR
1	A	299	LYS
1	A	302	ASN
1	B	133	LEU
1	B	143	LEU
1	B	145	ASP
1	B	157	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	169	VAL
1	B	174	ARG
1	B	179	ASP
1	B	180	ARG
1	B	189	GLN
1	B	208	LEU
1	B	210	ILE
1	B	214	MET
1	B	223	ARG
1	B	224	GLU
1	B	237	TRP
1	B	238	THR
1	B	240	ASP
1	B	245	ARG
1	B	272	ASN
1	B	276	ILE
1	B	285	ARG
1	C	143	LEU
1	C	145	ASP
1	C	149	LEU
1	C	162	SER
1	C	170	GLN
1	C	171	ARG
1	C	174	ARG
1	C	187	ASP
1	C	188	GLU
1	C	198	ILE
1	C	199	LEU
1	C	203	LEU
1	C	206	ARG
1	C	238	THR
1	C	262	LYS
1	C	265	VAL
1	C	269	VAL
1	C	275	ILE
1	C	306	GLU
1	C	308	ASN
1	D	132	GLN
1	D	133	LEU
1	D	137	ARG
1	D	143	LEU
1	D	156	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	169	VAL
1	D	174	ARG
1	D	176	ILE
1	D	189	GLN
1	D	197	PRO
1	D	204	GLU
1	D	206	ARG
1	D	214	MET
1	D	237	TRP
1	D	242	THR
1	D	251	GLN
1	D	262	LYS
1	D	271	ARG
1	D	272	ASN
1	D	273	LEU
1	D	275	ILE
1	D	276	ILE
1	D	285	ARG
1	E	143	LEU
1	E	145	ASP
1	E	149	LEU
1	E	153	ILE
1	E	164	THR
1	E	174	ARG
1	E	186	GLN
1	E	198	ILE
1	E	208	LEU
1	E	210	ILE
1	E	226	THR
1	E	248	SER
1	E	263	ILE
1	E	265	VAL
1	E	272	ASN
1	E	275	ILE
1	E	283	ASN
1	E	287	LYS
1	E	294	THR
1	E	298	GLU
1	E	299	LYS
1	F	143	LEU
1	F	144	VAL
1	F	145	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	149	LEU
1	F	170	GLN
1	F	174	ARG
1	F	184	TYR
1	F	187	ASP
1	F	189	GLN
1	F	198	ILE
1	F	199	LEU
1	F	202	LEU
1	F	208	LEU
1	F	214	MET
1	F	215	ASN
1	F	236	ASN
1	F	250	GLU
1	F	272	ASN
1	F	304	LEU
1	F	306	GLU
1	G	138	SER
1	G	143	LEU
1	G	145	ASP
1	G	149	LEU
1	G	156	ASP
1	G	157	SER
1	G	174	ARG
1	G	191	ILE
1	G	198	ILE
1	G	229	SER
1	G	269	VAL
1	G	272	ASN
1	G	275	ILE
1	G	288	SER
1	G	298	GLU
1	G	304	LEU
1	G	305	ILE
1	G	306	GLU
1	G	307	HIS
1	H	143	LEU
1	H	145	ASP
1	H	149	LEU
1	H	156	ASP
1	H	163	GLU
1	H	169	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	174	ARG
1	H	179	ASP
1	H	183	VAL
1	H	187	ASP
1	H	189	GLN
1	H	206	ARG
1	H	214	MET
1	H	252	THR
1	H	272	ASN
1	H	275	ILE
1	H	276	ILE
1	H	300	ASN
1	H	301	LEU
1	H	304	LEU
1	H	305	ILE
1	H	310	GLU
1	I	135	GLU
1	I	142	VAL
1	I	143	LEU
1	I	144	VAL
1	I	145	ASP
1	I	159	VAL
1	I	169	VAL
1	I	170	GLN
1	I	174	ARG
1	I	180	ARG
1	I	184	TYR
1	I	198	ILE
1	I	199	LEU
1	I	203	LEU
1	I	254	LEU
1	I	257	ASP
1	I	263	ILE
1	I	271	ARG
1	I	301	LEU
1	I	304	LEU
1	J	138	SER
1	J	140	HIS
1	J	143	LEU
1	J	145	ASP
1	J	169	VAL
1	J	170	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	J	174	ARG
1	J	180	ARG
1	J	186	GLN
1	J	187	ASP
1	J	188	GLU
1	J	206	ARG
1	J	214	MET
1	J	237	TRP
1	J	250	GLU
1	J	251	GLN
1	J	256	PHE
1	J	262	LYS
1	J	263	ILE
1	J	272	ASN
1	J	301	LEU
1	J	304	LEU
1	J	307	HIS
1	J	312	ASP
1	K	135	GLU
1	K	136	ARG
1	K	143	LEU
1	K	162	SER
1	K	164	THR
1	K	169	VAL
1	K	174	ARG
1	K	179	ASP
1	K	186	GLN
1	K	187	ASP
1	K	189	GLN
1	K	206	ARG
1	K	223	ARG
1	K	235	GLU
1	K	254	LEU
1	K	263	ILE
1	K	265	VAL
1	K	268	LYS
1	K	269	VAL
1	K	272	ASN
1	K	275	ILE
1	K	298	GLU
1	K	299	LYS
1	K	304	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	L	143	LEU
1	L	145	ASP
1	L	159	VAL
1	L	170	GLN
1	L	174	ARG
1	L	182	ASP
1	L	186	GLN
1	L	188	GLU
1	L	189	GLN
1	L	198	ILE
1	L	203	LEU
1	L	206	ARG
1	L	208	LEU
1	L	211	ILE
1	L	215	ASN
1	L	230	LEU
1	L	256	PHE
1	L	265	VAL
1	L	267	PHE
1	L	272	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	189	GLN
1	A	215	ASN
1	A	233	HIS
1	A	272	ASN
1	A	283	ASN
1	B	140	HIS
1	B	189	GLN
1	B	272	ASN
1	B	283	ASN
1	C	283	ASN
1	D	201	HIS
1	D	272	ASN
1	D	283	ASN
1	D	300	ASN
1	D	303	HIS
1	E	201	HIS
1	E	251	GLN
1	E	272	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	283	ASN
1	E	300	ASN
1	F	140	HIS
1	F	215	ASN
1	F	251	GLN
1	F	272	ASN
1	F	283	ASN
1	G	140	HIS
1	G	283	ASN
1	G	300	ASN
1	H	189	GLN
1	H	272	ASN
1	H	283	ASN
1	I	140	HIS
1	I	186	GLN
1	I	215	ASN
1	I	233	HIS
1	I	251	GLN
1	I	300	ASN
1	J	140	HIS
1	J	170	GLN
1	J	186	GLN
1	J	272	ASN
1	J	283	ASN
1	J	303	HIS
1	K	272	ASN
1	K	283	ASN
1	K	300	ASN
1	K	303	HIS
1	L	186	GLN
1	L	272	ASN
1	L	283	ASN
1	L	300	ASN

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 (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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	161/205 (78%)	-0.30	0 100 100	23, 53, 79, 88	0
1	B	181/205 (88%)	-0.33	0 100 100	22, 44, 85, 98	0
1	C	164/205 (80%)	-0.22	0 100 100	30, 54, 89, 102	0
1	D	181/205 (88%)	-0.29	0 100 100	23, 43, 85, 101	0
1	E	164/205 (80%)	-0.35	0 100 100	27, 51, 78, 91	0
1	F	160/205 (78%)	-0.25	0 100 100	32, 52, 89, 98	0
1	G	160/205 (78%)	-0.26	1 (0%) 89 88	23, 51, 78, 84	0
1	H	178/205 (86%)	-0.34	1 (0%) 89 88	21, 43, 81, 101	0
1	I	160/205 (78%)	-0.26	1 (0%) 89 88	33, 54, 86, 97	0
1	J	178/205 (86%)	-0.28	0 100 100	23, 43, 82, 100	0
1	K	162/205 (79%)	-0.33	0 100 100	21, 52, 78, 82	0
1	L	161/205 (78%)	-0.20	2 (1%) 79 76	30, 54, 87, 106	0
All	All	2010/2460 (81%)	-0.28	5 (0%) 95 95	21, 50, 85, 106	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	250	GLU	3.3
1	G	208	LEU	2.7
1	L	308	ASN	2.6
1	H	269	VAL	2.5
1	I	137	ARG	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.