Full wwPDB X-ray Structure Validation Report ⓘ

Feb 18, 2024 – 11:55 AM EST

PDB ID	:	4E2L
Title	:	Crystal Structure of the periplasmic domain of mutant FepE LPS O-antigen chain length regulator protein
Authors	:	Kalynych, S.; Yao, D.; Magee, J.D.; Cygler, M.
Deposited on	:	2012-03-08
Resolution	:	2.80 Å(reported)

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

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

The 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:

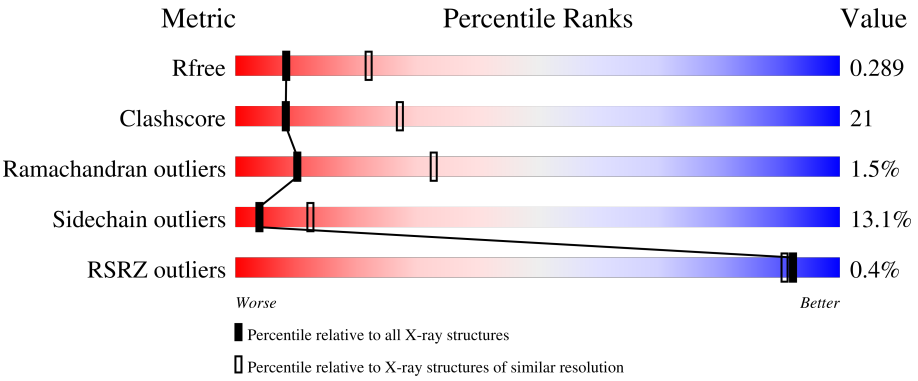
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	271	49% 30% 9% 11%
1	B	271	56% 27% 6% 11%
1	C	271	49% 34% 7% • 9%
1	D	271	% 53% 31% 5% 11%
1	E	271	54% 30% • 11%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	271	53% 32% 5% 10%
1	G	271	60% 23% 6% 11%
1	H	271	59% 25% 5% 11%
1	I	271	% 55% 28% 6% 11%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 16883 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 Ferric enterobactin (Enterochelin) transport.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	240	Total	C	N	O	S	0	0	0
			1881	1204	306	368	3			
1	B	240	Total	C	N	O	S	0	0	0
			1903	1213	317	370	3			
1	C	246	Total	C	N	O	S	0	0	0
			1893	1209	314	367	3			
1	D	240	Total	C	N	O	S	0	0	0
			1869	1195	309	362	3			
1	E	241	Total	C	N	O	S	0	0	0
			1848	1178	301	366	3			
1	F	244	Total	C	N	O	S	0	0	0
			1898	1214	314	367	3			
1	G	240	Total	C	N	O	S	0	0	0
			1859	1193	303	360	3			
1	H	242	Total	C	N	O	S	0	0	0
			1858	1190	306	359	3			
1	I	242	Total	C	N	O	S	0	0	0
			1874	1198	314	359	3			

There are 99 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	57	HIS	-	expression tag	UNP Q8XBV8
A	58	HIS	-	expression tag	UNP Q8XBV8
A	59	HIS	-	expression tag	UNP Q8XBV8
A	60	HIS	-	expression tag	UNP Q8XBV8
A	61	HIS	-	expression tag	UNP Q8XBV8
A	62	HIS	-	expression tag	UNP Q8XBV8
A	63	GLY	-	expression tag	UNP Q8XBV8
A	64	SER	-	expression tag	UNP Q8XBV8
A	262	GLY	-	linker	UNP Q8XBV8
A	263	SER	-	linker	UNP Q8XBV8
A	264	GLY	-	linker	UNP Q8XBV8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	57	HIS	-	expression tag	UNP Q8XBV8
B	58	HIS	-	expression tag	UNP Q8XBV8
B	59	HIS	-	expression tag	UNP Q8XBV8
B	60	HIS	-	expression tag	UNP Q8XBV8
B	61	HIS	-	expression tag	UNP Q8XBV8
B	62	HIS	-	expression tag	UNP Q8XBV8
B	63	GLY	-	expression tag	UNP Q8XBV8
B	64	SER	-	expression tag	UNP Q8XBV8
B	262	GLY	-	linker	UNP Q8XBV8
B	263	SER	-	linker	UNP Q8XBV8
B	264	GLY	-	linker	UNP Q8XBV8
C	57	HIS	-	expression tag	UNP Q8XBV8
C	58	HIS	-	expression tag	UNP Q8XBV8
C	59	HIS	-	expression tag	UNP Q8XBV8
C	60	HIS	-	expression tag	UNP Q8XBV8
C	61	HIS	-	expression tag	UNP Q8XBV8
C	62	HIS	-	expression tag	UNP Q8XBV8
C	63	GLY	-	expression tag	UNP Q8XBV8
C	64	SER	-	expression tag	UNP Q8XBV8
C	262	GLY	-	linker	UNP Q8XBV8
C	263	SER	-	linker	UNP Q8XBV8
C	264	GLY	-	linker	UNP Q8XBV8
D	57	HIS	-	expression tag	UNP Q8XBV8
D	58	HIS	-	expression tag	UNP Q8XBV8
D	59	HIS	-	expression tag	UNP Q8XBV8
D	60	HIS	-	expression tag	UNP Q8XBV8
D	61	HIS	-	expression tag	UNP Q8XBV8
D	62	HIS	-	expression tag	UNP Q8XBV8
D	63	GLY	-	expression tag	UNP Q8XBV8
D	64	SER	-	expression tag	UNP Q8XBV8
D	262	GLY	-	linker	UNP Q8XBV8
D	263	SER	-	linker	UNP Q8XBV8
D	264	GLY	-	linker	UNP Q8XBV8
E	57	HIS	-	expression tag	UNP Q8XBV8
E	58	HIS	-	expression tag	UNP Q8XBV8
E	59	HIS	-	expression tag	UNP Q8XBV8
E	60	HIS	-	expression tag	UNP Q8XBV8
E	61	HIS	-	expression tag	UNP Q8XBV8
E	62	HIS	-	expression tag	UNP Q8XBV8
E	63	GLY	-	expression tag	UNP Q8XBV8
E	64	SER	-	expression tag	UNP Q8XBV8
E	262	GLY	-	linker	UNP Q8XBV8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	263	SER	-	linker	UNP Q8XBV8
E	264	GLY	-	linker	UNP Q8XBV8
F	57	HIS	-	expression tag	UNP Q8XBV8
F	58	HIS	-	expression tag	UNP Q8XBV8
F	59	HIS	-	expression tag	UNP Q8XBV8
F	60	HIS	-	expression tag	UNP Q8XBV8
F	61	HIS	-	expression tag	UNP Q8XBV8
F	62	HIS	-	expression tag	UNP Q8XBV8
F	63	GLY	-	expression tag	UNP Q8XBV8
F	64	SER	-	expression tag	UNP Q8XBV8
F	262	GLY	-	linker	UNP Q8XBV8
F	263	SER	-	linker	UNP Q8XBV8
F	264	GLY	-	linker	UNP Q8XBV8
G	57	HIS	-	expression tag	UNP Q8XBV8
G	58	HIS	-	expression tag	UNP Q8XBV8
G	59	HIS	-	expression tag	UNP Q8XBV8
G	60	HIS	-	expression tag	UNP Q8XBV8
G	61	HIS	-	expression tag	UNP Q8XBV8
G	62	HIS	-	expression tag	UNP Q8XBV8
G	63	GLY	-	expression tag	UNP Q8XBV8
G	64	SER	-	expression tag	UNP Q8XBV8
G	262	GLY	-	linker	UNP Q8XBV8
G	263	SER	-	linker	UNP Q8XBV8
G	264	GLY	-	linker	UNP Q8XBV8
H	57	HIS	-	expression tag	UNP Q8XBV8
H	58	HIS	-	expression tag	UNP Q8XBV8
H	59	HIS	-	expression tag	UNP Q8XBV8
H	60	HIS	-	expression tag	UNP Q8XBV8
H	61	HIS	-	expression tag	UNP Q8XBV8
H	62	HIS	-	expression tag	UNP Q8XBV8
H	63	GLY	-	expression tag	UNP Q8XBV8
H	64	SER	-	expression tag	UNP Q8XBV8
H	262	GLY	-	linker	UNP Q8XBV8
H	263	SER	-	linker	UNP Q8XBV8
H	264	GLY	-	linker	UNP Q8XBV8
I	57	HIS	-	expression tag	UNP Q8XBV8
I	58	HIS	-	expression tag	UNP Q8XBV8
I	59	HIS	-	expression tag	UNP Q8XBV8
I	60	HIS	-	expression tag	UNP Q8XBV8
I	61	HIS	-	expression tag	UNP Q8XBV8
I	62	HIS	-	expression tag	UNP Q8XBV8
I	63	GLY	-	expression tag	UNP Q8XBV8

Continued on next page...

Continued from previous page...

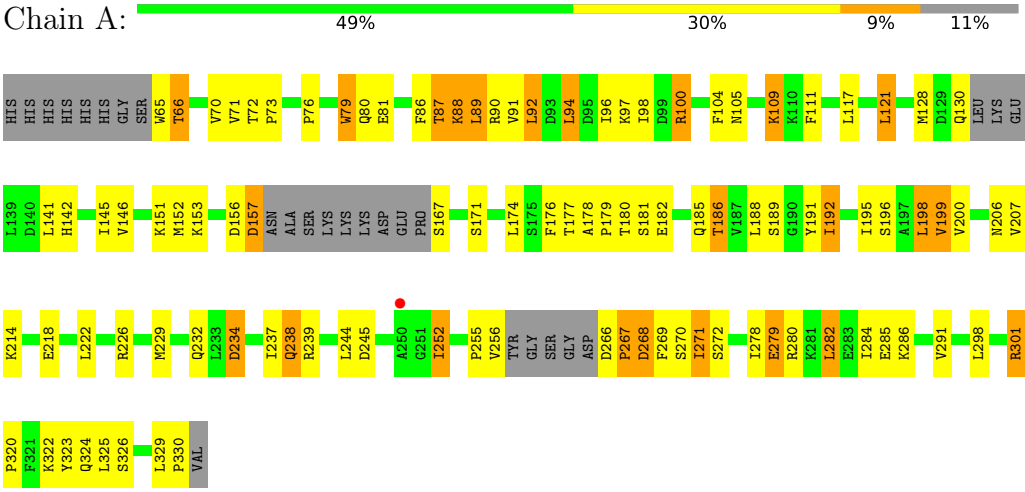
Chain	Residue	Modelled	Actual	Comment	Reference
I	64	SER	-	expression tag	UNP Q8XBV8
I	262	GLY	-	linker	UNP Q8XBV8
I	263	SER	-	linker	UNP Q8XBV8
I	264	GLY	-	linker	UNP Q8XBV8

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.

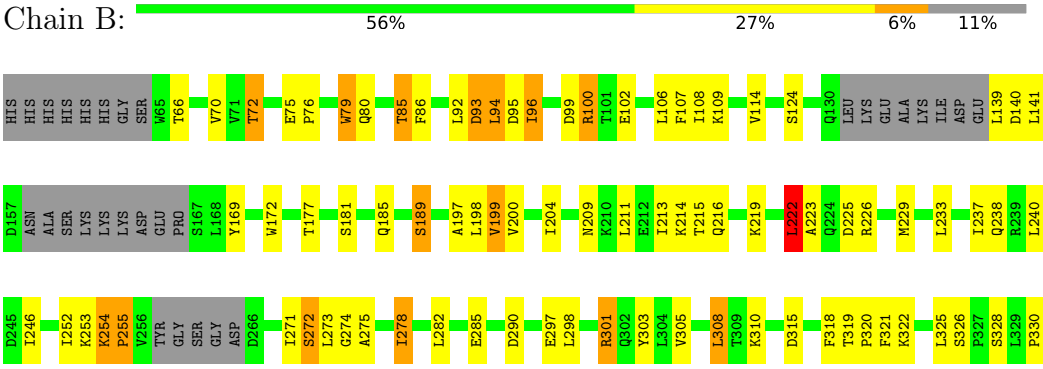
• Molecule 1: Ferric enterobactin (Enterochelin) transport

Chain A:



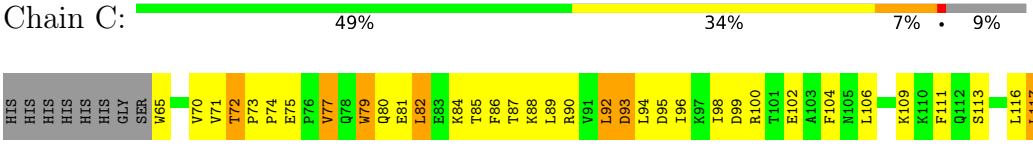
• Molecule 1: Ferric enterobactin (Enterochelin) transport

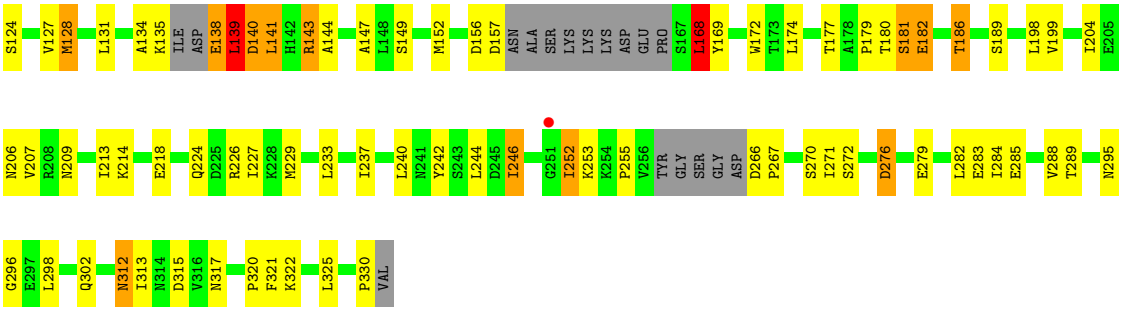
Chain B:



• Molecule 1: Ferric enterobactin (Enterochelin) transport

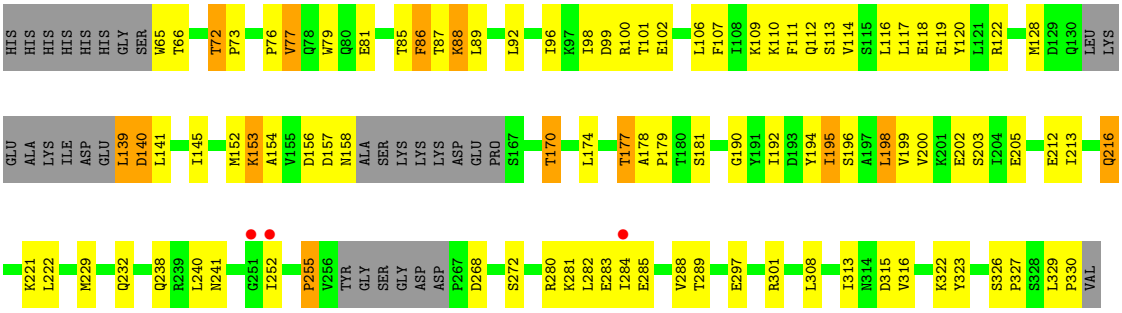
Chain C:





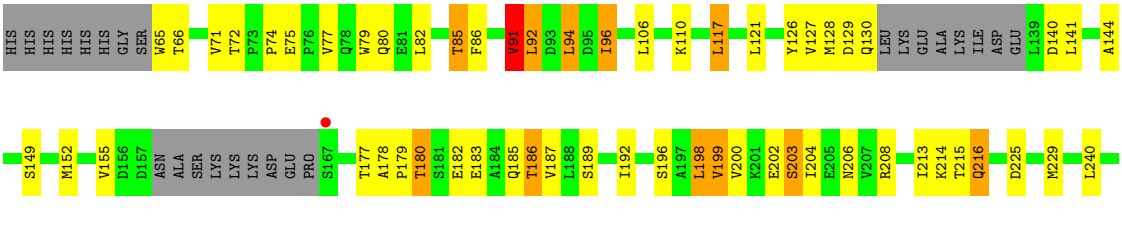
• Molecule 1: Ferric enterobactin (Enterochelin) transport

Chain D:



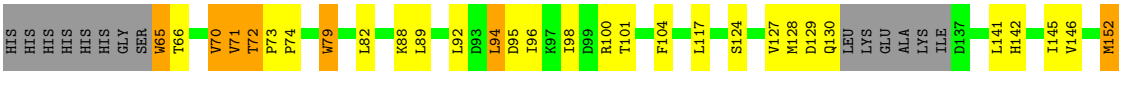
• Molecule 1: Ferric enterobactin (Enterochelin) transport

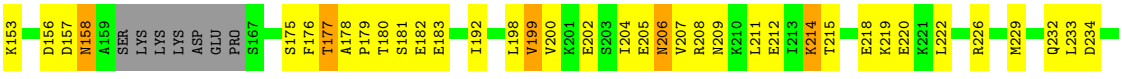
Chain E:



• Molecule 1: Ferric enterobactin (Enterochelin) transport

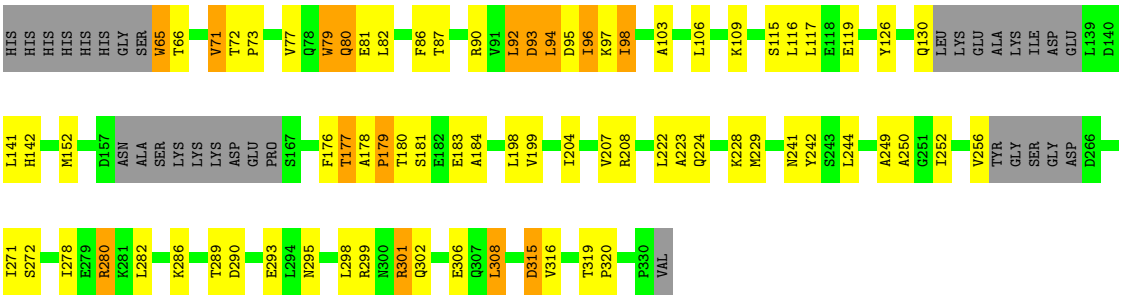
Chain F:





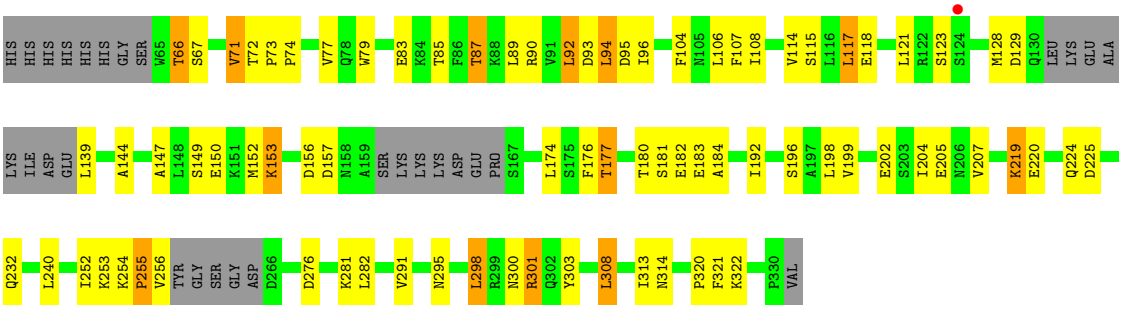
• Molecule 1: Ferric enterobactin (Enterochelin) transport

Chain G:



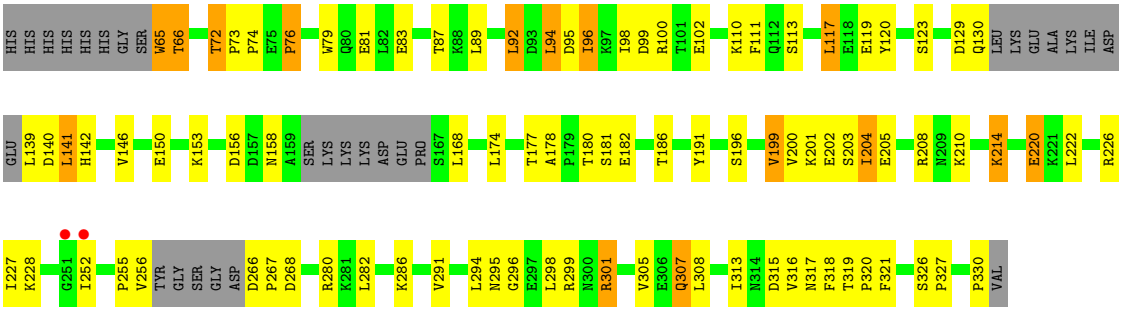
• Molecule 1: Ferric enterobactin (Enterochelin) transport

Chain H:



• Molecule 1: Ferric enterobactin (Enterochelin) transport

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	208.31Å 141.26Å 136.89Å 90.00° 107.03° 90.00°	Depositor
Resolution (Å)	49.72 – 2.80 49.71 – 2.79	Depositor EDS
% Data completeness (in resolution range)	86.8 (49.72-2.80) 98.0 (49.71-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	11.30	Depositor
$< I/\sigma(I) >$ [1]	6.15 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.6.4_486	Depositor
R, R_{free}	0.242 , 0.289 0.242 , 0.289	Depositor DCC
R_{free} test set	4652 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	49.6	Xtriage
Anisotropy	0.341	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	16883	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.88% 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	0.50	0/1911	0.63	0/2594
1	B	0.43	0/1932	0.60	1/2617 (0.0%)
1	C	0.44	0/1923	0.63	1/2617 (0.0%)
1	D	0.44	0/1899	0.57	0/2577
1	E	0.47	0/1877	0.60	0/2557
1	F	0.47	0/1928	0.59	0/2618
1	G	0.46	0/1889	0.58	0/2566
1	H	0.43	0/1887	0.59	0/2565
1	I	0.44	0/1903	0.60	0/2585
All	All	0.45	0/17149	0.60	2/23296 (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
1	A	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	168	LEU	CA-CB-CG	6.11	129.35	115.30
1	B	222	LEU	CA-CB-CG	5.41	127.75	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	87	THR	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	1881	0	1854	113	0
1	B	1903	0	1909	86	0
1	C	1893	0	1832	101	0
1	D	1869	0	1830	80	0
1	E	1848	0	1780	83	0
1	F	1898	0	1862	101	0
1	G	1859	0	1827	73	0
1	H	1858	0	1823	64	0
1	I	1874	0	1856	79	0
All	All	16883	0	16573	702	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 (702) 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:G:79:TRP:CZ2	1:G:98:ILE:HD11	1.80	1.16
1:A:222:LEU:HD13	1:A:301:ARG:HG2	1.27	1.15
1:I:301:ARG:HG2	1:I:301:ARG:HH21	1.06	1.11
1:G:280:ARG:HG3	1:G:280:ARG:HH11	1.08	1.11
1:B:301:ARG:HH11	1:B:301:ARG:HG2	1.10	1.08
1:G:79:TRP:HZ2	1:G:98:ILE:HD11	1.10	1.06
1:A:94:LEU:HG	1:A:214:LYS:HD2	1.31	1.06
1:F:94:LEU:HG	1:F:214:LYS:HG3	1.37	1.06
1:A:284:ILE:HG12	1:B:242:TYR:HD1	1.16	1.04
1:G:106:LEU:HD23	1:G:199:VAL:HG23	1.43	1.00
1:H:301:ARG:HG2	1:H:301:ARG:HH11	1.21	1.00
1:B:255:PRO:HG2	1:C:252:ILE:HD11	1.44	0.98
1:D:153:LYS:HD2	1:D:154:ALA:H	1.26	0.95
1:E:66:THR:HG22	1:E:177:THR:OG1	1.66	0.94
1:G:94:LEU:HD22	1:G:96:ILE:HG12	1.46	0.94
1:E:255:PRO:HG2	1:F:252:ILE:HD11	1.49	0.94
1:A:284:ILE:HG12	1:B:242:TYR:CD1	2.03	0.93
1:C:86:PHE:HZ	1:C:98:ILE:HG13	1.33	0.93

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:255:PRO:HG2	1:G:252:ILE:HD11	1.48	0.92
1:G:66:THR:OG1	1:G:177:THR:HB	1.71	0.89
1:E:208:ARG:HG2	1:E:313:ILE:CG2	2.03	0.88
1:I:301:ARG:HG2	1:I:301:ARG:NH2	1.87	0.87
1:B:301:ARG:HG2	1:B:301:ARG:NH1	1.90	0.86
1:H:301:ARG:HG2	1:H:301:ARG:NH1	1.87	0.86
1:G:280:ARG:HH11	1:G:280:ARG:CG	1.87	0.86
1:D:86:PHE:CD1	1:D:96:ILE:HG22	2.11	0.86
1:F:180:THR:HG23	1:F:183:GLU:HB3	1.55	0.86
1:I:141:LEU:H	1:I:141:LEU:HD23	1.41	0.86
1:C:72:THR:HG22	1:C:322:LYS:HB3	1.55	0.85
1:F:208:ARG:O	1:F:212:GLU:HG2	1.77	0.84
1:H:301:ARG:HH11	1:H:301:ARG:CG	1.90	0.84
1:D:222:LEU:HD13	1:D:301:ARG:HB3	1.60	0.84
1:E:85:THR:CG2	1:E:313:ILE:HD11	2.07	0.83
1:F:65:TRP:HE3	1:F:65:TRP:N	1.76	0.83
1:H:152:MET:HG2	1:H:176:PHE:HD1	1.44	0.83
1:B:100:ARG:HG3	1:B:100:ARG:HH11	1.42	0.82
1:D:72:THR:HG22	1:D:322:LYS:HB3	1.61	0.82
1:G:79:TRP:HZ2	1:G:98:ILE:CD1	1.90	0.82
1:F:82:LEU:HD13	1:F:98:ILE:HD11	1.60	0.81
1:I:81:GLU:HG2	1:I:316:VAL:HG23	1.61	0.81
1:A:88:LYS:HA	1:A:90:ARG:N	1.96	0.81
1:I:65:TRP:HB2	1:I:178:ALA:O	1.80	0.81
1:A:72:THR:HG21	1:B:109:LYS:NZ	1.96	0.80
1:C:94:LEU:HD13	1:C:214:LYS:HG3	1.63	0.80
1:H:66:THR:OG1	1:H:177:THR:HB	1.80	0.80
1:I:181:SER:OG	1:I:330:PRO:HD2	1.81	0.80
1:D:181:SER:OG	1:D:330:PRO:HD2	1.82	0.79
1:C:135:LYS:CB	1:C:138:GLU:HB3	2.14	0.78
1:G:80:GLN:HA	1:G:80:GLN:HE21	1.49	0.77
1:C:124:SER:HB3	1:C:127:VAL:HG12	1.67	0.77
1:E:208:ARG:HG2	1:E:313:ILE:HG21	1.67	0.77
1:D:65:TRP:HD1	1:D:179:PRO:O	1.66	0.76
1:B:238:GLN:O	1:B:242:TYR:HD2	1.69	0.76
1:A:237:ILE:HD11	1:A:285:GLU:HB3	1.68	0.76
1:F:226:ARG:HG2	1:F:298:LEU:HD21	1.66	0.76
1:B:330:PRO:C	1:C:143:ARG:HH22	1.89	0.75
1:A:213:ILE:HG23	1:I:87:THR:HG21	1.65	0.75
1:C:138:GLU:O	1:C:140:ASP:N	2.19	0.75
1:I:111:PHE:CZ	1:I:174:LEU:HD23	2.22	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:65:TRP:N	1:F:65:TRP:CE3	2.54	0.75
1:B:219:LYS:HG2	1:B:305:VAL:CG1	2.17	0.74
1:B:222:LEU:HD12	1:B:223:ALA:N	2.02	0.74
1:A:109:LYS:NZ	1:I:72:THR:HG21	2.02	0.74
1:F:180:THR:HG23	1:F:183:GLU:CB	2.17	0.74
1:C:96:ILE:HD12	1:C:207:VAL:HG13	1.70	0.73
1:E:182:GLU:O	1:E:186:THR:HG23	1.86	0.73
1:A:72:THR:HG21	1:B:109:LYS:HZ1	1.50	0.73
1:I:111:PHE:CE1	1:I:174:LEU:HD23	2.23	0.73
1:E:85:THR:HG23	1:E:313:ILE:HD11	1.70	0.73
1:F:98:ILE:HD12	1:F:98:ILE:O	1.86	0.73
1:B:181:SER:HB2	1:B:330:PRO:HG2	1.69	0.73
1:D:99:ASP:HB3	1:D:102:GLU:HB2	1.71	0.73
1:F:284:ILE:HD12	1:G:242:TYR:CD1	2.24	0.73
1:B:106:LEU:HD23	1:B:199:VAL:HG22	1.70	0.73
1:B:169:TYR:CD2	1:C:109:LYS:HD2	2.24	0.73
1:H:139:LEU:HD23	1:H:139:LEU:O	1.88	0.73
1:E:92:LEU:HD23	1:E:308:LEU:HD12	1.71	0.72
1:E:200:VAL:HB	1:E:318:PHE:CE2	2.24	0.71
1:C:86:PHE:CZ	1:C:98:ILE:HG13	2.20	0.71
1:G:77:VAL:HG11	1:H:202:GLU:HG3	1.71	0.71
1:A:232:GLN:NE2	1:I:296:GLY:HA3	2.06	0.70
1:G:280:ARG:HG3	1:G:280:ARG:NH1	1.90	0.70
1:F:92:LEU:HD23	1:F:308:LEU:HD23	1.70	0.70
1:H:94:LEU:HD22	1:H:96:ILE:CG2	2.21	0.70
1:H:106:LEU:HD23	1:H:199:VAL:HG23	1.72	0.70
1:C:233:LEU:HD11	1:C:288:VAL:HG11	1.74	0.70
1:F:284:ILE:HD12	1:G:242:TYR:CE1	2.26	0.70
1:B:330:PRO:C	1:C:143:ARG:NH2	2.45	0.70
1:B:301:ARG:HH11	1:B:301:ARG:CG	1.95	0.69
1:A:72:THR:HG23	1:A:322:LYS:HB3	1.74	0.69
1:B:100:ARG:HH11	1:B:100:ARG:CG	2.05	0.69
1:D:153:LYS:HD2	1:D:154:ALA:N	2.04	0.69
1:A:109:LYS:HZ1	1:I:72:THR:HG21	1.56	0.69
1:C:85:THR:HG21	1:C:313:ILE:HG23	1.74	0.68
1:F:300:ASN:O	1:F:303:TYR:HB3	1.93	0.68
1:G:229:MET:CE	1:G:298:LEU:HD11	2.23	0.68
1:G:244:LEU:HD13	1:G:278:ILE:HG22	1.74	0.68
1:C:237:ILE:HD11	1:C:285:GLU:O	1.94	0.68
1:C:117:LEU:HD13	1:C:149:SER:HB2	1.74	0.68
1:E:208:ARG:HG2	1:E:313:ILE:HG22	1.75	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:98:ILE:C	1:G:98:ILE:HD12	2.14	0.68
1:G:79:TRP:CE2	1:G:98:ILE:HD11	2.28	0.68
1:A:325:LEU:HD13	1:B:114:VAL:HB	1.74	0.68
1:C:89:LEU:HD11	1:C:313:ILE:HD11	1.76	0.67
1:D:281:LYS:HG3	1:E:246:ILE:HD13	1.76	0.67
1:A:80:GLN:OE1	1:B:209:ASN:HB3	1.95	0.67
1:A:88:LYS:HA	1:A:89:LEU:C	2.15	0.67
1:B:252:ILE:HD12	1:B:271:ILE:HG21	1.77	0.67
1:A:88:LYS:CA	1:A:90:ARG:N	2.57	0.67
1:H:199:VAL:CG1	1:H:320:PRO:HG3	2.24	0.67
1:C:121:LEU:HD22	1:C:127:VAL:HG21	1.75	0.67
1:I:307:GLN:HA	1:I:307:GLN:NE2	2.10	0.67
1:A:192:ILE:HD11	1:A:323:TYR:OH	1.95	0.66
1:E:117:LEU:HD11	1:E:152:MET:HB2	1.77	0.66
1:D:178:ALA:HB1	1:D:179:PRO:HD2	1.78	0.66
1:C:72:THR:CG2	1:C:322:LYS:HB3	2.24	0.66
1:D:240:LEU:HB3	1:D:282:LEU:HD13	1.77	0.66
1:C:87:THR:HG22	1:C:90:ARG:HH12	1.60	0.66
1:H:225:ASP:OD2	1:H:301:ARG:NH2	2.29	0.66
1:A:70:VAL:H	1:A:325:LEU:HB3	1.61	0.66
1:D:329:LEU:HD12	1:D:330:PRO:HD2	1.76	0.66
1:C:255:PRO:HG3	1:D:252:ILE:HD11	1.78	0.66
1:I:139:LEU:HA	1:I:141:LEU:HD21	1.78	0.65
1:I:208:ARG:NH2	1:I:313:ILE:O	2.29	0.65
1:A:66:THR:OG1	1:A:177:THR:HB	1.96	0.65
1:A:234:ASP:OD2	1:I:299:ARG:CZ	2.44	0.65
1:C:240:LEU:HD23	1:C:282:LEU:HA	1.78	0.65
1:A:182:GLU:O	1:A:186:THR:HG23	1.96	0.65
1:E:183:GLU:O	1:E:187:VAL:HG23	1.96	0.65
1:D:65:TRP:CD1	1:D:179:PRO:O	2.50	0.65
1:C:296:GLY:HA3	1:D:232:GLN:OE1	1.95	0.65
1:F:95:ASP:O	1:F:96:ILE:HD13	1.97	0.64
1:I:83:GLU:O	1:I:87:THR:HG23	1.96	0.64
1:A:244:LEU:HD13	1:A:278:ILE:HG22	1.79	0.64
1:E:85:THR:HG21	1:E:313:ILE:HD11	1.79	0.64
1:B:100:ARG:HG3	1:B:100:ARG:NH1	2.04	0.64
1:B:72:THR:HG22	1:B:322:LYS:HB3	1.78	0.64
1:G:65:TRP:HB2	1:G:179:PRO:O	1.98	0.64
1:H:96:ILE:O	1:H:96:ILE:HG13	1.98	0.64
1:F:182:GLU:N	1:F:182:GLU:OE1	2.31	0.64
1:F:218:GLU:HA	1:F:218:GLU:OE1	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:285:GLU:O	1:D:288:VAL:HG12	1.98	0.64
1:G:86:PHE:HZ	1:G:98:ILE:HG23	1.61	0.64
1:H:152:MET:HG2	1:H:176:PHE:CD1	2.31	0.64
1:B:219:LYS:HG2	1:B:305:VAL:HG13	1.79	0.63
1:D:157:ASP:O	1:D:158:ASN:CB	2.45	0.63
1:G:280:ARG:CG	1:G:280:ARG:NH1	2.54	0.63
1:C:139:LEU:C	1:C:139:LEU:HD12	2.18	0.63
1:I:282:LEU:O	1:I:286:LYS:HG3	1.99	0.63
1:A:87:THR:O	1:A:87:THR:HG23	1.98	0.63
1:E:329:LEU:HB3	1:F:142:HIS:HE2	1.64	0.63
1:F:307:GLN:HE22	1:G:224:GLN:HG3	1.63	0.63
1:D:76:PRO:HG3	1:D:100:ARG:HH12	1.63	0.63
1:D:107:PHE:CD1	1:D:195:ILE:HG22	2.34	0.63
1:E:280:ARG:HD2	1:E:283:GLU:OE2	1.99	0.63
1:F:180:THR:CG2	1:F:183:GLU:HB3	2.29	0.62
1:D:73:PRO:HD3	1:D:170:THR:HG22	1.81	0.62
1:C:135:LYS:CB	1:C:138:GLU:OE1	2.47	0.62
1:F:199:VAL:HG21	1:F:320:PRO:HG3	1.81	0.62
1:C:124:SER:CB	1:C:127:VAL:HG12	2.29	0.62
1:C:233:LEU:HD11	1:C:288:VAL:CG1	2.29	0.62
1:F:204:ILE:HD12	1:F:205:GLU:N	2.14	0.62
1:I:117:LEU:HD23	1:I:191:TYR:CE1	2.34	0.62
1:C:87:THR:HG22	1:C:90:ARG:NH1	2.14	0.62
1:E:178:ALA:HB1	1:E:179:PRO:HD2	1.81	0.62
1:F:284:ILE:HG23	1:G:242:TYR:CD1	2.35	0.62
1:G:86:PHE:CE2	1:G:96:ILE:HG22	2.36	0.61
1:A:180:THR:HG22	1:A:181:SER:H	1.65	0.61
1:F:325:LEU:HA	1:G:115:SER:OG	2.00	0.61
1:C:182:GLU:O	1:C:186:THR:HG23	2.00	0.61
1:E:296:GLY:HA3	1:F:232:GLN:OE1	2.01	0.61
1:B:94:LEU:HD22	1:B:96:ILE:HG12	1.82	0.61
1:D:240:LEU:HD21	1:D:281:LYS:HB3	1.82	0.61
1:I:99:ASP:HB3	1:I:102:GLU:HG3	1.83	0.61
1:B:219:LYS:HG2	1:B:305:VAL:HG11	1.83	0.61
1:C:168:LEU:CD1	1:C:169:TYR:HD2	2.13	0.60
1:F:158:ASN:OD1	1:F:158:ASN:C	2.39	0.60
1:A:94:LEU:CG	1:A:214:LYS:HD2	2.21	0.60
1:C:124:SER:HB3	1:C:127:VAL:CG1	2.30	0.60
1:H:282:LEU:O	1:H:282:LEU:HD23	2.01	0.60
1:G:229:MET:HE3	1:G:298:LEU:HD11	1.83	0.60
1:H:67:SER:HB2	1:H:184:ALA:HB1	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:281:LYS:HG3	1:E:246:ILE:CD1	2.31	0.60
1:F:200:VAL:HG22	1:F:318:PHE:CE2	2.35	0.60
1:G:229:MET:HE1	1:G:298:LEU:HD21	1.82	0.60
1:A:79:TRP:HZ2	1:A:98:ILE:HG22	1.65	0.60
1:C:240:LEU:HB3	1:C:282:LEU:HD13	1.84	0.60
1:C:156:ASP:HB2	1:C:172:TRP:CE2	2.36	0.59
1:E:240:LEU:HD23	1:E:282:LEU:HA	1.83	0.59
1:C:144:ALA:O	1:C:147:ALA:HB3	2.02	0.59
1:I:307:GLN:HA	1:I:307:GLN:HE21	1.65	0.59
1:D:329:LEU:HD12	1:D:330:PRO:CD	2.32	0.59
1:E:65:TRP:HD1	1:E:179:PRO:O	1.85	0.59
1:E:85:THR:HG22	1:E:86:PHE:N	2.16	0.59
1:F:72:THR:HG21	1:G:109:LYS:NZ	2.16	0.59
1:B:225:ASP:OD2	1:B:301:ARG:NH2	2.36	0.59
1:G:98:ILE:HD12	1:G:98:ILE:O	2.02	0.59
1:H:174:LEU:HD11	1:H:192:ILE:HD11	1.85	0.59
1:A:244:LEU:HD21	1:A:279:GLU:HG3	1.84	0.59
1:D:76:PRO:HG3	1:D:100:ARG:NH1	2.16	0.59
1:F:284:ILE:CG2	1:G:242:TYR:HD1	2.16	0.59
1:I:301:ARG:HH21	1:I:301:ARG:CG	1.96	0.59
1:B:252:ILE:HD12	1:B:271:ILE:CG2	2.33	0.59
1:B:226:ARG:HH22	1:B:290:ASP:HB2	1.67	0.59
1:D:212:GLU:OE1	1:D:212:GLU:HA	2.03	0.59
1:D:222:LEU:HD13	1:D:301:ARG:CB	2.32	0.58
1:I:98:ILE:HD13	1:I:203:SER:HB3	1.85	0.58
1:D:77:VAL:HG21	1:E:202:GLU:OE1	2.04	0.58
1:I:72:THR:HG22	1:I:73:PRO:O	2.03	0.58
1:G:302:GLN:O	1:G:306:GLU:HG3	2.03	0.58
1:I:74:PRO:HD3	1:I:320:PRO:O	2.03	0.58
1:E:82:LEU:CD2	1:E:316:VAL:HG11	2.33	0.58
1:I:298:LEU:O	1:I:298:LEU:HD23	2.04	0.58
1:D:120:TYR:OH	1:D:190:GLY:HA3	2.04	0.58
1:C:96:ILE:CD1	1:C:207:VAL:HG13	2.34	0.58
1:D:140:ASP:OD1	1:D:140:ASP:N	2.35	0.58
1:G:96:ILE:HG21	1:G:207:VAL:HG13	1.85	0.58
1:H:199:VAL:HG13	1:H:320:PRO:HG3	1.86	0.58
1:D:216:GLN:O	1:D:216:GLN:HG2	2.04	0.58
1:H:199:VAL:HG11	1:H:320:PRO:HG3	1.86	0.58
1:A:94:LEU:HD22	1:A:96:ILE:HG23	1.87	0.57
1:B:200:VAL:HG23	1:B:318:PHE:CE2	2.39	0.57
1:A:180:THR:HG22	1:A:181:SER:N	2.19	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:TRP:CZ2	1:G:98:ILE:CD1	2.71	0.57
1:E:243:SER:OG	1:E:269:PHE:HB3	2.04	0.57
1:F:226:ARG:CG	1:F:298:LEU:HD21	2.34	0.57
1:G:86:PHE:CZ	1:G:98:ILE:HG23	2.39	0.57
1:H:240:LEU:HD21	1:H:281:LYS:HG2	1.87	0.57
1:C:77:VAL:HG11	1:D:202:GLU:OE2	2.05	0.57
1:D:139:LEU:O	1:D:139:LEU:HD12	2.04	0.57
1:F:204:ILE:HD13	1:F:208:ARG:HH21	1.69	0.57
1:F:152:MET:HE1	1:F:176:PHE:HB2	1.87	0.57
1:D:86:PHE:N	1:D:86:PHE:CD2	2.72	0.57
1:F:89:LEU:HD11	1:F:313:ILE:HD11	1.86	0.57
1:H:96:ILE:CD1	1:H:207:VAL:HG13	2.34	0.57
1:H:254:LYS:O	1:H:255:PRO:O	2.23	0.57
1:A:111:PHE:CZ	1:A:174:LEU:HD22	2.40	0.57
1:B:303:TYR:OH	1:C:227:ILE:HD12	2.05	0.57
1:A:79:TRP:CZ2	1:A:98:ILE:HG22	2.39	0.56
1:A:252:ILE:HD11	1:A:256:VAL:HG23	1.87	0.56
1:B:185:GLN:HB2	1:B:328:SER:O	2.04	0.56
1:C:139:LEU:O	1:C:141:LEU:N	2.38	0.56
1:F:72:THR:HG22	1:F:322:LYS:HB3	1.87	0.56
1:H:67:SER:HB2	1:H:184:ALA:CB	2.36	0.56
1:H:74:PRO:HG3	1:H:321:PHE:N	2.19	0.56
1:I:142:HIS:O	1:I:146:VAL:HG23	2.05	0.56
1:D:86:PHE:N	1:D:86:PHE:HD2	2.02	0.56
1:A:111:PHE:CE2	1:A:174:LEU:HD22	2.41	0.56
1:C:168:LEU:C	1:C:168:LEU:HD12	2.26	0.56
1:D:86:PHE:CZ	1:D:98:ILE:HG13	2.40	0.56
1:G:282:LEU:HD11	1:G:286:LYS:HE2	1.87	0.56
1:I:307:GLN:HE21	1:I:307:GLN:CA	2.19	0.56
1:B:240:LEU:HD23	1:B:282:LEU:HA	1.86	0.56
1:C:79:TRP:CE2	1:C:100:ARG:HG2	2.41	0.56
1:F:192:ILE:HG21	1:F:323:TYR:OH	2.06	0.56
1:A:76:PRO:HG3	1:A:100:ARG:HH12	1.71	0.56
1:E:96:ILE:C	1:E:96:ILE:HD12	2.26	0.56
1:F:181:SER:HB3	1:F:182:GLU:OE1	2.06	0.56
1:H:77:VAL:HG21	1:I:202:GLU:HG3	1.87	0.56
1:D:280:ARG:HH11	1:D:283:GLU:HG3	1.71	0.55
1:A:268:ASP:OD2	1:A:268:ASP:N	2.39	0.55
1:B:106:LEU:HD23	1:B:199:VAL:CG2	2.36	0.55
1:D:156:ASP:C	1:D:156:ASP:OD1	2.42	0.55
1:E:117:LEU:HD13	1:E:149:SER:HA	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:199:VAL:HG11	1:I:320:PRO:HG2	1.87	0.55
1:B:238:GLN:O	1:B:242:TYR:CD2	2.55	0.55
1:I:180:THR:HG22	1:I:181:SER:H	1.72	0.55
1:B:156:ASP:HB2	1:B:172:TRP:CE2	2.42	0.55
1:F:199:VAL:CG2	1:F:320:PRO:HG3	2.37	0.55
1:I:120:TYR:CE2	1:I:191:TYR:HB2	2.42	0.55
1:A:329:LEU:HD12	1:A:330:PRO:HD2	1.88	0.55
1:G:86:PHE:CD2	1:G:96:ILE:HG22	2.42	0.55
1:E:85:THR:CG2	1:E:86:PHE:N	2.70	0.55
1:F:124:SER:O	1:F:128:MET:HG2	2.07	0.55
1:I:119:GLU:O	1:I:123:SER:HB3	2.06	0.55
1:A:70:VAL:HG12	1:A:324:GLN:HB2	1.88	0.55
1:D:114:VAL:O	1:D:118:GLU:HG3	2.07	0.55
1:F:65:TRP:HB3	1:F:178:ALA:O	2.06	0.55
1:C:279:GLU:O	1:C:283:GLU:HG2	2.07	0.54
1:F:207:VAL:HG12	1:F:313:ILE:HG13	1.88	0.54
1:B:169:TYR:CG	1:C:109:LYS:HD2	2.42	0.54
1:E:117:LEU:HD11	1:E:152:MET:CB	2.35	0.54
1:F:256:VAL:O	1:F:256:VAL:HG23	2.07	0.54
1:E:247:ALA:N	1:E:271:ILE:HD11	2.23	0.54
1:C:253:LYS:O	1:C:276:ASP:OD2	2.26	0.54
1:F:309:THR:O	1:F:309:THR:HG22	2.07	0.54
1:A:88:LYS:CA	1:A:90:ARG:H	2.21	0.54
1:A:157:ASP:OD2	1:A:157:ASP:N	2.41	0.54
1:F:153:LYS:HG3	1:F:175:SER:OG	2.08	0.54
1:D:255:PRO:HG2	1:E:252:ILE:HD11	1.90	0.54
1:B:229:MET:HG3	1:B:298:LEU:HD11	1.89	0.54
1:C:71:VAL:HG13	1:C:104:PHE:HE1	1.72	0.54
1:C:168:LEU:HD12	1:C:169:TYR:HD2	1.72	0.54
1:H:253:LYS:NZ	1:H:276:ASP:CB	2.70	0.54
1:A:196:SER:HA	1:A:199:VAL:CG1	2.38	0.54
1:C:266:ASP:HB3	1:C:270:SER:HA	1.89	0.53
1:A:244:LEU:HD13	1:A:278:ILE:CG2	2.37	0.53
1:G:126:TYR:OH	1:G:183:GLU:HG2	2.07	0.53
1:H:174:LEU:HD12	1:H:174:LEU:O	2.08	0.53
1:B:94:LEU:HG	1:B:214:LYS:HG2	1.89	0.53
1:D:86:PHE:CE1	1:D:98:ILE:HG13	2.44	0.53
1:H:89:LEU:HD21	1:H:313:ILE:HD11	1.90	0.53
1:A:199:VAL:HG11	1:A:320:PRO:HG3	1.91	0.53
1:B:76:PRO:HA	1:B:100:ARG:HE	1.72	0.53
1:D:117:LEU:HD21	1:D:152:MET:HG3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:293:GLU:HA	1:G:299:ARG:HH21	1.73	0.53
1:I:140:ASP:OD1	1:I:140:ASP:C	2.46	0.53
1:A:239:ARG:HH12	1:I:294:LEU:HB3	1.73	0.53
1:A:88:LYS:CB	1:A:91:VAL:HB	2.39	0.53
1:A:284:ILE:HG23	1:B:242:TYR:CD1	2.43	0.53
1:E:74:PRO:HD3	1:E:321:PHE:HA	1.90	0.53
1:H:96:ILE:HD11	1:H:207:VAL:HG13	1.90	0.53
1:E:282:LEU:HD13	1:E:282:LEU:C	2.29	0.53
1:A:239:ARG:NH1	1:I:294:LEU:HB3	2.23	0.53
1:A:156:ASP:C	1:A:157:ASP:OD2	2.47	0.52
1:F:66:THR:OG1	1:F:177:THR:HB	2.09	0.52
1:A:80:GLN:HE22	1:B:213:ILE:HD11	1.75	0.52
1:A:256:VAL:HG12	1:A:256:VAL:O	2.09	0.52
1:C:255:PRO:CG	1:D:252:ILE:HD11	2.39	0.52
1:B:197:ALA:HA	1:B:200:VAL:HG12	1.92	0.52
1:H:196:SER:OG	1:H:320:PRO:HD2	2.09	0.52
1:I:96:ILE:HD11	1:I:210:LYS:HD3	1.92	0.52
1:C:168:LEU:HD12	1:C:169:TYR:CD2	2.45	0.52
1:D:89:LEU:HD11	1:D:313:ILE:HD11	1.91	0.52
1:F:284:ILE:CG2	1:G:242:TYR:CD1	2.93	0.52
1:I:81:GLU:HG2	1:I:316:VAL:CG2	2.37	0.52
1:A:71:VAL:HG13	1:A:104:PHE:HE1	1.74	0.52
1:E:214:LYS:HG3	1:E:308:LEU:HD21	1.92	0.52
1:H:204:ILE:HD12	1:H:205:GLU:N	2.24	0.52
1:I:66:THR:O	1:I:66:THR:HG22	2.09	0.52
1:A:252:ILE:HG12	1:A:252:ILE:O	2.08	0.52
1:I:301:ARG:O	1:I:305:VAL:HG23	2.10	0.52
1:A:255:PRO:HG3	1:B:252:ILE:HD11	1.92	0.52
1:B:237:ILE:HD11	1:B:285:GLU:O	2.09	0.52
1:C:74:PRO:HG3	1:C:320:PRO:C	2.30	0.52
1:C:181:SER:HB2	1:C:330:PRO:HD2	1.91	0.52
1:G:71:VAL:HG12	1:G:71:VAL:O	2.09	0.52
1:D:106:LEU:HD21	1:D:110:LYS:NZ	2.24	0.52
1:E:299:ARG:NH1	1:F:234:ASP:HB3	2.24	0.52
1:G:106:LEU:HD23	1:G:199:VAL:CG2	2.29	0.52
1:I:72:THR:HG23	1:I:73:PRO:HD2	1.92	0.52
1:D:107:PHE:CE1	1:D:195:ILE:HG22	2.45	0.51
1:E:229:MET:HG3	1:E:298:LEU:HD11	1.92	0.51
1:A:76:PRO:HG3	1:A:100:ARG:NH1	2.26	0.51
1:C:131:LEU:CB	1:C:141:LEU:HD21	2.40	0.51
1:E:75:GLU:CG	1:E:322:LYS:HD2	2.40	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:94:LEU:HD22	1:E:96:ILE:CG2	2.40	0.51
1:E:117:LEU:HD11	1:E:152:MET:HG3	1.91	0.51
1:F:117:LEU:HD21	1:F:152:MET:HB2	1.93	0.51
1:F:74:PRO:O	1:F:100:ARG:HD2	2.11	0.51
1:G:117:LEU:HD21	1:G:152:MET:HB2	1.92	0.51
1:H:72:THR:HB	1:H:73:PRO:CD	2.40	0.51
1:D:323:TYR:CE2	1:D:327:PRO:HD3	2.46	0.51
1:G:82:LEU:HB3	1:G:86:PHE:CE1	2.45	0.51
1:H:156:ASP:OD1	1:H:157:ASP:N	2.44	0.51
1:D:65:TRP:HB2	1:D:178:ALA:O	2.11	0.51
1:E:75:GLU:HG2	1:E:322:LYS:HD2	1.93	0.51
1:E:130:GLN:N	1:E:130:GLN:OE1	2.44	0.51
1:A:284:ILE:CG2	1:B:242:TYR:CD1	2.94	0.51
1:E:106:LEU:O	1:E:110:LYS:HG2	2.11	0.51
1:F:204:ILE:HD12	1:F:205:GLU:HG2	1.93	0.51
1:I:139:LEU:HA	1:I:141:LEU:CD2	2.40	0.51
1:A:199:VAL:CG1	1:A:320:PRO:HG3	2.41	0.51
1:D:86:PHE:HD2	1:D:86:PHE:H	1.59	0.51
1:G:289:THR:HG22	1:G:290:ASP:N	2.25	0.51
1:A:282:LEU:HD22	1:A:286:LYS:HE3	1.91	0.50
1:I:200:VAL:HG22	1:I:318:PHE:CE2	2.47	0.50
1:I:220:GLU:OE1	1:I:220:GLU:HA	2.10	0.50
1:A:98:ILE:HG22	1:A:98:ILE:O	2.10	0.50
1:H:94:LEU:HD22	1:H:96:ILE:HG23	1.93	0.50
1:H:180:THR:HB	1:H:183:GLU:HB2	1.92	0.50
1:H:300:ASN:O	1:H:303:TYR:HB3	2.11	0.50
1:I:307:GLN:NE2	1:I:307:GLN:CA	2.73	0.50
1:I:150:GLU:O	1:I:153:LYS:HE2	2.11	0.50
1:C:122:ARG:HD2	1:C:128:MET:CE	2.42	0.50
1:E:180:THR:OG1	1:E:183:GLU:HB2	2.12	0.50
1:F:280:ARG:NH1	1:G:249:ALA:HB2	2.27	0.50
1:A:117:LEU:HD13	1:A:191:TYR:CZ	2.47	0.50
1:C:218:GLU:OE1	1:C:218:GLU:HA	2.12	0.50
1:E:117:LEU:HD11	1:E:152:MET:CG	2.41	0.50
1:F:88:LYS:O	1:F:92:LEU:HD13	2.11	0.50
1:C:87:THR:HG21	1:D:213:ILE:HG23	1.94	0.50
1:C:122:ARG:HD2	1:C:128:MET:HE3	1.93	0.50
1:E:299:ARG:HH12	1:F:234:ASP:HB3	1.77	0.50
1:F:127:VAL:HG12	1:F:128:MET:CE	2.42	0.50
1:H:174:LEU:CD1	1:H:192:ILE:HD11	2.41	0.50
1:H:219:LYS:HG3	1:H:220:GLU:N	2.20	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:ASP:HB3	1:B:102:GLU:HB2	1.95	0.49
1:C:135:LYS:HA	1:C:138:GLU:HB3	1.94	0.49
1:D:110:LYS:O	1:D:113:SER:HB3	2.12	0.49
1:D:111:PHE:C	1:D:113:SER:H	2.15	0.49
1:C:156:ASP:HB2	1:C:172:TRP:CZ2	2.47	0.49
1:I:182:GLU:O	1:I:186:THR:HG23	2.12	0.49
1:A:270:SER:O	1:A:271:ILE:HD12	2.12	0.49
1:A:96:ILE:HD11	1:A:207:VAL:HG13	1.94	0.49
1:A:200:VAL:HG12	1:A:318:PHE:CE2	2.47	0.49
1:A:232:GLN:CD	1:I:296:GLY:HA3	2.33	0.49
1:B:70:VAL:HG23	1:B:325:LEU:HB3	1.95	0.49
1:A:195:ILE:O	1:A:199:VAL:HG12	2.12	0.49
1:B:80:GLN:OE1	1:C:209:ASN:HB3	2.12	0.49
1:B:215:THR:OG1	1:B:308:LEU:HB3	2.13	0.49
1:F:73:PRO:HA	1:F:104:PHE:CD1	2.48	0.49
1:B:240:LEU:HB3	1:B:282:LEU:HD23	1.94	0.49
1:D:117:LEU:CD2	1:D:152:MET:HG3	2.43	0.49
1:D:85:THR:HA	1:D:88:LYS:HZ3	1.77	0.48
1:F:237:ILE:HD13	1:F:286:LYS:HG2	1.95	0.48
1:D:280:ARG:NH1	1:D:283:GLU:HG3	2.28	0.48
1:E:225:ASP:CB	1:E:301:ARG:HH12	2.25	0.48
1:C:75:GLU:OE2	1:D:109:LYS:NZ	2.46	0.48
1:F:129:ASP:OD1	1:F:130:GLN:N	2.45	0.48
1:F:275:ALA:HA	1:F:278:ILE:HB	1.95	0.48
1:I:319:THR:HG22	1:I:321:PHE:H	1.79	0.48
1:H:74:PRO:HG3	1:H:320:PRO:C	2.33	0.48
1:A:80:GLN:OE1	1:B:209:ASN:CB	2.61	0.48
1:C:80:GLN:O	1:C:84:LYS:HG3	2.13	0.48
1:E:66:THR:HG22	1:E:177:THR:HG1	1.75	0.48
1:H:96:ILE:O	1:H:96:ILE:CG1	2.61	0.48
1:A:111:PHE:HE1	1:A:192:ILE:HG22	1.77	0.48
1:A:280:ARG:O	1:A:284:ILE:HD12	2.13	0.48
1:C:113:SER:HB3	1:C:116:LEU:HB2	1.96	0.48
1:G:295:ASN:O	1:G:299:ARG:HG3	2.14	0.48
1:E:91:VAL:HG21	1:F:220:GLU:HB3	1.96	0.48
1:F:142:HIS:O	1:F:146:VAL:HG23	2.14	0.48
1:F:329:LEU:HB3	1:G:142:HIS:NE2	2.29	0.48
1:I:204:ILE:HG22	1:I:205:GLU:N	2.28	0.48
1:A:268:ASP:HB2	1:A:269:PHE:CD1	2.49	0.48
1:C:134:ALA:O	1:C:135:LYS:CB	2.61	0.48
1:D:323:TYR:CD2	1:D:326:SER:HA	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:284:ILE:HG23	1:G:242:TYR:CE1	2.49	0.48
1:F:289:THR:HG22	1:F:290:ASP:N	2.28	0.48
1:C:74:PRO:HG3	1:C:321:PHE:N	2.29	0.48
1:D:196:SER:O	1:D:200:VAL:HG13	2.13	0.48
1:E:329:LEU:HB3	1:F:142:HIS:NE2	2.28	0.48
1:G:199:VAL:HG13	1:G:320:PRO:HG3	1.96	0.48
1:I:226:ARG:HG2	1:I:298:LEU:HD11	1.96	0.48
1:C:233:LEU:C	1:C:233:LEU:HD23	2.35	0.47
1:C:89:LEU:HD12	1:C:96:ILE:HD11	1.96	0.47
1:C:135:LYS:CA	1:C:138:GLU:HB3	2.44	0.47
1:E:141:LEU:O	1:E:144:ALA:HB3	2.14	0.47
1:E:204:ILE:C	1:E:204:ILE:HD12	2.34	0.47
1:E:216:GLN:HG2	1:E:216:GLN:O	2.14	0.47
1:E:269:PHE:CD1	1:E:269:PHE:N	2.81	0.47
1:F:70:VAL:HG13	1:F:325:LEU:HB3	1.96	0.47
1:F:127:VAL:HG12	1:F:128:MET:HE1	1.97	0.47
1:F:180:THR:CG2	1:F:183:GLU:CB	2.90	0.47
1:H:295:ASN:HB3	1:H:298:LEU:HB2	1.95	0.47
1:A:213:ILE:CG2	1:I:87:THR:HG21	2.39	0.47
1:A:237:ILE:CD1	1:A:285:GLU:HB3	2.39	0.47
1:B:254:LYS:HD3	1:B:254:LYS:N	2.30	0.47
1:E:196:SER:O	1:E:199:VAL:HG13	2.15	0.47
1:F:233:LEU:HD22	1:F:291:VAL:HG12	1.96	0.47
1:I:256:VAL:O	1:I:256:VAL:HG23	2.13	0.47
1:A:222:LEU:O	1:A:226:ARG:HG3	2.14	0.47
1:B:199:VAL:HG11	1:B:320:PRO:HG3	1.96	0.47
1:B:85:THR:HG22	1:B:86:PHE:N	2.29	0.47
1:B:66:THR:O	1:B:330:PRO:HB3	2.15	0.47
1:C:139:LEU:HD12	1:C:139:LEU:O	2.14	0.47
1:E:273:LEU:HG	1:E:277:GLY:HA3	1.95	0.47
1:H:300:ASN:OD1	1:I:228:LYS:HA	2.15	0.47
1:E:279:GLU:O	1:E:279:GLU:HG2	2.15	0.46
1:E:313:ILE:HG23	1:E:313:ILE:O	2.15	0.46
1:G:178:ALA:HB1	1:G:179:PRO:HD2	1.96	0.46
1:G:204:ILE:HD11	1:G:316:VAL:O	2.15	0.46
1:H:94:LEU:HD22	1:H:96:ILE:HG21	1.97	0.46
1:A:267:PRO:HG2	1:A:268:ASP:OD2	2.15	0.46
1:D:72:THR:CG2	1:D:322:LYS:HB3	2.39	0.46
1:E:185:GLN:HB2	1:E:328:SER:O	2.15	0.46
1:A:66:THR:OG1	1:A:177:THR:CB	2.63	0.46
1:E:85:THR:HG23	1:E:313:ILE:CD1	2.42	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:295:ASN:N	1:F:295:ASN:OD1	2.47	0.46
1:I:326:SER:O	1:I:327:PRO:C	2.54	0.46
1:C:85:THR:CG2	1:C:313:ILE:HG23	2.45	0.46
1:E:126:TYR:C	1:E:126:TYR:CD2	2.88	0.46
1:G:72:THR:HB	1:G:73:PRO:HD2	1.96	0.46
1:F:72:THR:HG23	1:F:73:PRO:O	2.16	0.46
1:H:114:VAL:O	1:H:118:GLU:HG3	2.15	0.46
1:C:99:ASP:HB3	1:C:102:GLU:HB2	1.96	0.46
1:F:82:LEU:HD23	1:F:82:LEU:HA	1.71	0.46
1:A:284:ILE:HG23	1:B:242:TYR:CE1	2.50	0.46
1:B:75:GLU:HB3	1:B:76:PRO:HD2	1.98	0.46
1:F:321:PHE:CD1	1:F:321:PHE:C	2.89	0.46
1:B:93:ASP:CG	1:B:93:ASP:O	2.54	0.46
1:B:75:GLU:OE2	1:C:109:LYS:NZ	2.49	0.46
1:C:285:GLU:O	1:C:288:VAL:HG12	2.16	0.46
1:H:71:VAL:HG13	1:H:104:PHE:HE1	1.81	0.46
1:I:117:LEU:HD23	1:I:191:TYR:CD1	2.50	0.46
1:D:195:ILE:O	1:D:199:VAL:HG23	2.16	0.46
1:F:79:TRP:CZ2	1:F:98:ILE:CD1	2.99	0.46
1:I:222:LEU:HD13	1:I:301:ARG:HB3	1.97	0.46
1:C:135:LYS:CB	1:C:138:GLU:CB	2.88	0.45
1:G:65:TRP:C	1:G:65:TRP:CD1	2.90	0.45
1:I:199:VAL:HG11	1:I:320:PRO:CG	2.45	0.45
1:B:204:ILE:HD13	1:B:204:ILE:HA	1.81	0.45
1:B:278:ILE:O	1:B:282:LEU:HB2	2.15	0.45
1:E:127:VAL:HG12	1:E:128:MET:CE	2.47	0.45
1:F:66:THR:HA	1:F:177:THR:HA	1.98	0.45
1:F:70:VAL:CG1	1:F:325:LEU:HB3	2.46	0.45
1:A:66:THR:O	1:A:66:THR:HG22	2.16	0.45
1:A:90:ARG:HA	1:A:94:LEU:O	2.17	0.45
1:F:307:GLN:NE2	1:G:224:GLN:HG3	2.31	0.45
1:C:116:LEU:HD23	1:C:116:LEU:HA	1.69	0.45
1:A:176:PHE:HB3	1:A:188:LEU:HB2	1.98	0.45
1:G:250:ALA:HB3	1:G:252:ILE:HG13	1.98	0.45
1:G:95:ASP:O	1:G:96:ILE:HD13	2.17	0.45
1:H:121:LEU:O	1:H:128:MET:HE2	2.17	0.45
1:I:141:LEU:HD23	1:I:141:LEU:N	2.22	0.45
1:B:272:SER:O	1:B:274:GLY:N	2.49	0.45
1:A:80:GLN:NE2	1:B:213:ILE:HD11	2.32	0.45
1:C:92:LEU:O	1:C:93:ASP:OD1	2.35	0.45
1:C:242:TYR:O	1:C:246:ILE:HD12	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:178:ALA:HB1	1:E:179:PRO:CD	2.46	0.45
1:E:314:ASN:O	1:E:316:VAL:N	2.50	0.45
1:A:245:ASP:HB3	1:I:280:ARG:HE	1.82	0.44
1:A:266:ASP:CG	1:A:267:PRO:HD2	2.38	0.44
1:B:242:TYR:O	1:B:246:ILE:HG13	2.17	0.44
1:F:156:ASP:O	1:F:158:ASN:N	2.44	0.44
1:F:222:LEU:HD13	1:F:301:ARG:HB3	2.00	0.44
1:D:85:THR:HG21	1:D:313:ILE:HG23	1.99	0.44
1:F:329:LEU:HD23	1:G:142:HIS:CD2	2.52	0.44
1:H:66:THR:HG22	1:H:66:THR:O	2.17	0.44
1:I:266:ASP:HA	1:I:267:PRO:HD3	1.85	0.44
1:D:111:PHE:O	1:D:113:SER:N	2.50	0.44
1:D:141:LEU:O	1:D:145:ILE:HG12	2.17	0.44
1:E:80:GLN:OE1	1:F:209:ASN:HB3	2.16	0.44
1:H:83:GLU:O	1:H:87:THR:OG1	2.34	0.44
1:A:128:MET:HA	1:A:128:MET:HE2	2.00	0.44
1:C:111:PHE:CZ	1:C:174:LEU:HD22	2.52	0.44
1:C:181:SER:CB	1:C:330:PRO:HD2	2.48	0.44
1:A:87:THR:CG2	1:B:216:GLN:NE2	2.81	0.44
1:A:282:LEU:O	1:A:286:LYS:HG3	2.18	0.44
1:E:282:LEU:HD13	1:E:282:LEU:O	2.18	0.44
1:F:284:ILE:HG21	1:G:242:TYR:HD1	1.82	0.44
1:H:253:LYS:HZ3	1:H:276:ASP:CB	2.31	0.44
1:I:94:LEU:HG	1:I:214:LYS:HG3	1.99	0.44
1:D:116:LEU:HD23	1:D:116:LEU:HA	1.89	0.44
1:E:280:ARG:HA	1:E:283:GLU:HG2	1.99	0.44
1:F:156:ASP:OD2	1:F:158:ASN:HB3	2.16	0.44
1:A:117:LEU:HD13	1:A:191:TYR:CE2	2.53	0.44
1:D:255:PRO:HA	1:D:272:SER:O	2.17	0.44
1:H:150:GLU:O	1:H:153:LYS:NZ	2.51	0.44
1:A:238:GLN:HB3	1:I:294:LEU:HD23	1.99	0.44
1:D:66:THR:OG1	1:D:177:THR:HB	2.17	0.44
1:D:106:LEU:HD21	1:D:110:LYS:HZ3	1.83	0.44
1:I:92:LEU:HD23	1:I:308:LEU:HD23	2.00	0.44
1:I:117:LEU:HA	1:I:191:TYR:CE1	2.53	0.44
1:A:105:ASN:ND2	1:I:168:LEU:HD11	2.33	0.44
1:C:87:THR:C	1:C:89:LEU:N	2.70	0.44
1:D:194:TYR:HD2	1:D:195:ILE:HD13	1.82	0.44
1:I:156:ASP:C	1:I:158:ASN:H	2.21	0.44
1:A:100:ARG:HE	1:A:100:ARG:HB2	1.37	0.43
1:A:152:MET:O	1:A:153:LYS:HD3	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:ILE:HG22	1:B:271:ILE:HD11	1.98	0.43
1:D:119:GLU:O	1:D:119:GLU:OE2	2.36	0.43
1:H:180:THR:HG22	1:H:181:SER:N	2.34	0.43
1:B:156:ASP:HB2	1:B:172:TRP:CZ2	2.53	0.43
1:C:168:LEU:CD1	1:C:168:LEU:C	2.87	0.43
1:E:268:ASP:HB3	1:E:269:PHE:CD1	2.53	0.43
1:F:117:LEU:CD2	1:F:152:MET:HB2	2.48	0.43
1:H:92:LEU:HG	1:H:308:LEU:HD13	2.00	0.43
1:A:65:TRP:HA	1:A:178:ALA:O	2.18	0.43
1:A:185:GLN:O	1:A:189:SER:HB2	2.18	0.43
1:E:198:LEU:HD12	1:E:198:LEU:HA	1.68	0.43
1:H:298:LEU:HD22	1:H:298:LEU:HA	1.74	0.43
1:C:295:ASN:OD1	1:C:298:LEU:HG	2.18	0.43
1:E:92:LEU:HD21	1:E:307:GLN:HB3	2.00	0.43
1:A:121:LEU:HB3	1:A:145:ILE:HD12	2.00	0.43
1:C:65:TRP:N	1:C:181:SER:HA	2.34	0.43
1:D:65:TRP:HA	1:D:65:TRP:CE3	2.54	0.43
1:E:280:ARG:HE	1:F:245:ASP:HB3	1.84	0.43
1:D:89:LEU:HD11	1:D:313:ILE:CD1	2.48	0.43
1:G:92:LEU:HD12	1:G:92:LEU:HA	1.86	0.43
1:G:98:ILE:CD1	1:G:98:ILE:O	2.66	0.43
1:G:181:SER:O	1:G:184:ALA:HB3	2.19	0.43
1:H:107:PHE:CD2	1:H:108:ILE:HD13	2.53	0.43
1:A:229:MET:HB2	1:A:229:MET:HE2	1.35	0.43
1:D:178:ALA:HB1	1:D:179:PRO:CD	2.47	0.43
1:F:72:THR:OG1	1:F:73:PRO:HD2	2.18	0.43
1:F:256:VAL:O	1:F:256:VAL:CG2	2.66	0.43
1:G:92:LEU:O	1:G:93:ASP:OD1	2.37	0.43
1:I:301:ARG:NH2	1:I:301:ARG:CG	2.66	0.43
1:F:284:ILE:HD13	1:F:284:ILE:HA	1.86	0.42
1:G:92:LEU:HG	1:G:308:LEU:HD13	2.01	0.42
1:A:109:LYS:HZ3	1:I:72:THR:HG21	1.80	0.42
1:A:212:GLU:O	1:A:212:GLU:HG2	2.18	0.42
1:C:88:LYS:HE2	1:C:312:ASN:O	2.19	0.42
1:D:73:PRO:CD	1:D:170:THR:HG22	2.49	0.42
1:E:65:TRP:HA	1:E:65:TRP:CE3	2.53	0.42
1:G:93:ASP:CG	1:G:93:ASP:O	2.57	0.42
1:G:319:THR:HA	1:G:320:PRO:HD3	1.90	0.42
1:C:90:ARG:HG3	1:C:95:ASP:OD1	2.19	0.42
1:H:252:ILE:O	1:H:252:ILE:HG22	2.18	0.42
1:A:92:LEU:HB3	1:A:308:LEU:CD1	2.49	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ALA:O	1:B:200:VAL:HG12	2.18	0.42
1:B:199:VAL:HG11	1:B:320:PRO:HB3	2.02	0.42
1:B:319:THR:C	1:B:321:PHE:H	2.22	0.42
1:F:204:ILE:CD1	1:F:205:GLU:HG2	2.50	0.42
1:G:152:MET:SD	1:G:176:PHE:HB2	2.60	0.42
1:G:208:ARG:NH2	1:G:315:ASP:OD1	2.50	0.42
1:H:255:PRO:HG2	1:I:252:ILE:HD11	2.01	0.42
1:A:87:THR:HG23	1:B:216:GLN:NE2	2.33	0.42
1:A:142:HIS:O	1:A:146:VAL:HG23	2.19	0.42
1:B:308:LEU:HD12	1:B:308:LEU:HA	1.83	0.42
1:A:92:LEU:HD23	1:A:308:LEU:HD12	2.00	0.42
1:A:301:ARG:HE	1:A:301:ARG:HB2	1.67	0.42
1:C:70:VAL:HG23	1:C:325:LEU:HD23	2.01	0.42
1:C:168:LEU:HD11	1:C:169:TYR:HD2	1.82	0.42
1:I:110:LYS:O	1:I:113:SER:HB3	2.20	0.42
1:A:86:PHE:CE2	1:A:97:LYS:HA	2.54	0.42
1:B:255:PRO:CG	1:C:252:ILE:HD11	2.32	0.42
1:B:305:VAL:O	1:B:305:VAL:HG12	2.19	0.42
1:C:72:THR:HG23	1:C:73:PRO:O	2.19	0.42
1:C:213:ILE:HD13	1:C:213:ILE:HA	1.92	0.42
1:D:221:LYS:HB3	1:D:301:ARG:NH2	2.35	0.42
1:I:92:LEU:HB3	1:I:308:LEU:HD21	2.01	0.42
1:C:168:LEU:CD1	1:C:169:TYR:CD2	2.99	0.42
1:D:198:LEU:HD12	1:D:198:LEU:HA	1.73	0.42
1:D:280:ARG:NH1	1:D:284:ILE:HG13	2.35	0.42
1:F:65:TRP:HD1	1:F:179:PRO:O	2.03	0.42
1:G:199:VAL:CG1	1:G:320:PRO:HG3	2.50	0.42
1:A:66:THR:HG1	1:A:177:THR:CB	2.32	0.42
1:B:92:LEU:HD23	1:B:308:LEU:HD12	2.02	0.42
1:E:82:LEU:HD23	1:E:316:VAL:HG11	2.01	0.42
1:E:94:LEU:HD22	1:E:96:ILE:HG23	2.01	0.42
1:I:76:PRO:HD3	1:I:100:ARG:CZ	2.49	0.42
1:A:96:ILE:HD12	1:A:207:VAL:HG22	2.02	0.42
1:A:198:LEU:HD12	1:A:198:LEU:HA	1.77	0.42
1:C:266:ASP:HA	1:C:267:PRO:HD3	1.80	0.42
1:E:192:ILE:HG21	1:E:323:TYR:OH	2.19	0.42
1:H:253:LYS:HZ1	1:H:276:ASP:CB	2.32	0.42
1:A:79:TRP:HZ2	1:A:98:ILE:CG2	2.32	0.41
1:C:81:GLU:H	1:C:81:GLU:HG2	1.39	0.41
1:C:246:ILE:HG22	1:C:271:ILE:HG21	2.02	0.41
1:E:65:TRP:HA	1:E:65:TRP:HE3	1.85	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:117:LEU:O	1:E:121:LEU:HG	2.20	0.41
1:F:282:LEU:O	1:F:286:LYS:HG3	2.20	0.41
1:I:286:LYS:HE2	1:I:286:LYS:HB3	1.80	0.41
1:A:72:THR:HG21	1:B:109:LYS:HZ3	1.79	0.41
1:A:87:THR:O	1:A:87:THR:CG2	2.66	0.41
1:B:271:ILE:O	1:B:272:SER:C	2.57	0.41
1:E:65:TRP:HB2	1:E:178:ALA:O	2.20	0.41
1:F:240:LEU:HD12	1:F:240:LEU:HA	1.90	0.41
1:G:98:ILE:HD13	1:G:103:ALA:HB2	2.02	0.41
1:H:85:THR:HG21	1:H:313:ILE:HG23	2.01	0.41
1:H:117:LEU:HD11	1:H:152:MET:HB2	2.02	0.41
1:C:106:LEU:HD23	1:C:199:VAL:HG13	2.02	0.41
1:C:156:ASP:OD2	1:C:157:ASP:N	2.53	0.41
1:E:215:THR:HA	1:E:308:LEU:HD23	2.01	0.41
1:B:253:LYS:C	1:B:254:LYS:HD3	2.39	0.41
1:F:71:VAL:HG12	1:F:71:VAL:O	2.20	0.41
1:G:77:VAL:HG11	1:H:202:GLU:CG	2.47	0.41
1:G:116:LEU:HD23	1:G:116:LEU:HA	1.87	0.41
1:H:92:LEU:O	1:H:93:ASP:CB	2.69	0.41
1:H:303:TYR:OH	1:I:227:ILE:HD12	2.20	0.41
1:B:185:GLN:O	1:B:189:SER:HB2	2.20	0.41
1:G:86:PHE:O	1:G:90:ARG:HB2	2.21	0.41
1:I:96:ILE:HD12	1:I:96:ILE:HA	1.58	0.41
1:A:73:PRO:HG3	1:A:104:PHE:CG	2.55	0.41
1:D:81:GLU:HG2	1:D:316:VAL:HG13	2.01	0.41
1:G:222:LEU:HD13	1:G:301:ARG:HB2	2.02	0.41
1:A:218:GLU:OE2	1:A:218:GLU:HA	2.21	0.41
1:H:72:THR:HB	1:H:73:PRO:HD2	2.02	0.41
1:B:319:THR:O	1:B:321:PHE:N	2.53	0.41
1:C:94:LEU:HG	1:C:96:ILE:HG23	2.02	0.41
1:D:122:ARG:HA	1:D:128:MET:CE	2.51	0.41
1:B:79:TRP:CG	1:B:100:ARG:HD3	2.56	0.41
1:B:219:LYS:CG	1:B:305:VAL:HG13	2.46	0.41
1:D:174:LEU:HD12	1:D:192:ILE:HD11	2.01	0.41
1:E:127:VAL:HG12	1:E:128:MET:HE2	2.02	0.41
1:E:203:SER:O	1:E:206:ASN:HB2	2.20	0.41
1:F:229:MET:HG3	1:F:298:LEU:CD1	2.50	0.41
1:H:144:ALA:O	1:H:147:ALA:HB3	2.21	0.41
1:B:107:PHE:HD2	1:B:108:ILE:HD13	1.85	0.41
1:F:79:TRP:HE1	1:F:98:ILE:HD12	1.86	0.41
1:F:94:LEU:HA	1:F:94:LEU:HD23	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:145:ILE:HD13	1:F:145:ILE:HA	1.94	0.41
1:I:321:PHE:CD1	1:I:321:PHE:C	2.94	0.41
1:A:153:LYS:HD3	1:A:153:LYS:HA	1.85	0.40
1:C:229:MET:HG3	1:C:298:LEU:HD11	2.01	0.40
1:C:244:LEU:HA	1:C:244:LEU:HD12	1.86	0.40
1:D:76:PRO:CG	1:D:100:ARG:NH1	2.83	0.40
1:H:87:THR:HG23	1:H:90:ARG:NH1	2.35	0.40
1:A:252:ILE:HD13	1:A:271:ILE:HG23	2.02	0.40
1:C:99:ASP:HB3	1:C:102:GLU:CB	2.51	0.40
1:C:143:ARG:HD3	1:C:143:ARG:HA	1.31	0.40
1:F:71:VAL:HG13	1:F:104:PHE:HE1	1.85	0.40
1:F:215:THR:O	1:F:219:LYS:HB3	2.21	0.40
1:A:252:ILE:HD11	1:A:256:VAL:CG2	2.51	0.40
1:B:139:LEU:C	1:B:141:LEU:H	2.24	0.40
1:F:202:GLU:O	1:F:206:ASN:HB2	2.21	0.40
1:F:275:ALA:O	1:F:279:GLU:HB2	2.20	0.40
1:I:140:ASP:OD1	1:I:140:ASP:O	2.39	0.40
1:I:196:SER:HA	1:I:199:VAL:HG12	2.03	0.40
1:A:73:PRO:HG3	1:A:104:PHE:CD2	2.56	0.40
1:A:178:ALA:HB1	1:A:179:PRO:HD2	2.02	0.40
1:B:199:VAL:CG1	1:B:320:PRO:HG3	2.52	0.40
1:C:117:LEU:HD11	1:C:152:MET:HB2	2.02	0.40
1:E:282:LEU:HD11	1:E:286:LYS:NZ	2.36	0.40
1:E:318:PHE:CD2	1:E:318:PHE:N	2.90	0.40
1:C:79:TRP:O	1:C:82:LEU:N	2.53	0.40
1:D:86:PHE:CE1	1:D:96:ILE:HG22	2.56	0.40
1:E:240:LEU:HD21	1:E:281:LYS:HG2	2.03	0.40
1:F:158:ASN:OD1	1:F:158:ASN:O	2.38	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	232/271 (86%)	211 (91%)	17 (7%)	4 (2%)	9 29
1	B	232/271 (86%)	212 (91%)	14 (6%)	6 (3%)	5 18
1	C	238/271 (88%)	214 (90%)	18 (8%)	6 (2%)	5 19
1	D	232/271 (86%)	215 (93%)	14 (6%)	3 (1%)	12 36
1	E	233/271 (86%)	212 (91%)	18 (8%)	3 (1%)	12 36
1	F	236/271 (87%)	212 (90%)	23 (10%)	1 (0%)	34 66
1	G	232/271 (86%)	214 (92%)	15 (6%)	3 (1%)	12 36
1	H	234/271 (86%)	219 (94%)	14 (6%)	1 (0%)	34 66
1	I	234/271 (86%)	214 (92%)	16 (7%)	4 (2%)	9 29
All	All	2103/2439 (86%)	1923 (91%)	149 (7%)	31 (2%)	10 33

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	255	PRO
1	C	139	LEU
1	C	140	ASP
1	D	112	GLN
1	D	255	PRO
1	D	315	ASP
1	E	255	PRO
1	E	315	ASP
1	G	179	PRO
1	H	255	PRO
1	I	255	PRO
1	A	88	LYS
1	A	272	SER
1	B	273	LEU
1	B	275	ALA
1	I	315	ASP
1	A	89	LEU
1	B	272	SER
1	B	315	ASP
1	C	272	SER
1	I	129	ASP
1	C	141	LEU
1	G	223	ALA
1	B	278	ILE
1	C	179	PRO
1	F	157	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	315	ASP
1	I	76	PRO
1	C	252	ILE
1	E	91	VAL
1	A	267	PRO

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	204/243 (84%)	172 (84%)	32 (16%)	2 8
1	B	210/243 (86%)	184 (88%)	26 (12%)	4 14
1	C	197/243 (81%)	166 (84%)	31 (16%)	2 8
1	D	198/243 (82%)	173 (87%)	25 (13%)	4 14
1	E	196/243 (81%)	170 (87%)	26 (13%)	4 12
1	F	201/243 (83%)	181 (90%)	20 (10%)	7 22
1	G	198/243 (82%)	172 (87%)	26 (13%)	4 12
1	H	196/243 (81%)	170 (87%)	26 (13%)	4 12
1	I	200/243 (82%)	176 (88%)	24 (12%)	5 15
All	All	1800/2187 (82%)	1564 (87%)	236 (13%)	4 12

All (236) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	THR
1	A	79	TRP
1	A	81	GLU
1	A	92	LEU
1	A	94	LEU
1	A	100	ARG
1	A	109	LYS
1	A	121	LEU
1	A	130	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	141	LEU
1	A	151	LYS
1	A	157	ASP
1	A	167	SER
1	A	171	SER
1	A	186	THR
1	A	192	ILE
1	A	198	LEU
1	A	199	VAL
1	A	206	ASN
1	A	210	LYS
1	A	234	ASP
1	A	238	GLN
1	A	252	ILE
1	A	268	ASP
1	A	271	ILE
1	A	279	GLU
1	A	282	LEU
1	A	291	VAL
1	A	298	LEU
1	A	301	ARG
1	A	308	LEU
1	A	326	SER
1	B	72	THR
1	B	79	TRP
1	B	85	THR
1	B	93	ASP
1	B	94	LEU
1	B	95	ASP
1	B	96	ILE
1	B	100	ARG
1	B	124	SER
1	B	140	ASP
1	B	153	LYS
1	B	177	THR
1	B	189	SER
1	B	198	LEU
1	B	199	VAL
1	B	211	LEU
1	B	222	LEU
1	B	233	LEU
1	B	243	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	244	LEU
1	B	254	LYS
1	B	297	GLU
1	B	301	ARG
1	B	308	LEU
1	B	310	LYS
1	B	326	SER
1	C	72	THR
1	C	77	VAL
1	C	79	TRP
1	C	82	LEU
1	C	92	LEU
1	C	93	ASP
1	C	117	LEU
1	C	128	MET
1	C	138	GLU
1	C	139	LEU
1	C	143	ARG
1	C	168	LEU
1	C	177	THR
1	C	180	THR
1	C	181	SER
1	C	182	GLU
1	C	186	THR
1	C	189	SER
1	C	198	LEU
1	C	204	ILE
1	C	206	ASN
1	C	224	GLN
1	C	226	ARG
1	C	246	ILE
1	C	276	ASP
1	C	284	ILE
1	C	289	THR
1	C	302	GLN
1	C	312	ASN
1	C	315	ASP
1	C	317	ASN
1	D	72	THR
1	D	77	VAL
1	D	79	TRP
1	D	86	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	87	THR
1	D	88	LYS
1	D	92	LEU
1	D	101	THR
1	D	139	LEU
1	D	140	ASP
1	D	153	LYS
1	D	170	THR
1	D	177	THR
1	D	195	ILE
1	D	198	LEU
1	D	203	SER
1	D	205	GLU
1	D	216	GLN
1	D	229	MET
1	D	238	GLN
1	D	241	ASN
1	D	268	ASP
1	D	289	THR
1	D	297	GLU
1	D	308	LEU
1	E	71	VAL
1	E	72	THR
1	E	77	VAL
1	E	79	TRP
1	E	85	THR
1	E	91	VAL
1	E	92	LEU
1	E	94	LEU
1	E	96	ILE
1	E	117	LEU
1	E	129	ASP
1	E	140	ASP
1	E	155	VAL
1	E	180	THR
1	E	186	THR
1	E	189	SER
1	E	198	LEU
1	E	199	VAL
1	E	203	SER
1	E	213	ILE
1	E	216	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	256	VAL
1	E	291	VAL
1	E	309	THR
1	E	312	ASN
1	E	325	LEU
1	F	65	TRP
1	F	70	VAL
1	F	71	VAL
1	F	72	THR
1	F	79	TRP
1	F	94	LEU
1	F	101	THR
1	F	141	LEU
1	F	152	MET
1	F	158	ASN
1	F	177	THR
1	F	198	LEU
1	F	199	VAL
1	F	206	ASN
1	F	211	LEU
1	F	214	LYS
1	F	283	GLU
1	F	289	THR
1	F	294	LEU
1	F	298	LEU
1	G	65	TRP
1	G	71	VAL
1	G	79	TRP
1	G	80	GLN
1	G	81	GLU
1	G	87	THR
1	G	92	LEU
1	G	93	ASP
1	G	94	LEU
1	G	96	ILE
1	G	97	LYS
1	G	98	ILE
1	G	119	GLU
1	G	130	GLN
1	G	141	LEU
1	G	177	THR
1	G	180	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	198	LEU
1	G	228	LYS
1	G	241	ASN
1	G	256	VAL
1	G	271	ILE
1	G	272	SER
1	G	280	ARG
1	G	301	ARG
1	G	308	LEU
1	H	66	THR
1	H	71	VAL
1	H	79	TRP
1	H	87	THR
1	H	92	LEU
1	H	94	LEU
1	H	95	ASP
1	H	115	SER
1	H	117	LEU
1	H	123	SER
1	H	129	ASP
1	H	149	SER
1	H	153	LYS
1	H	177	THR
1	H	182	GLU
1	H	198	LEU
1	H	219	LYS
1	H	224	GLN
1	H	232	GLN
1	H	256	VAL
1	H	291	VAL
1	H	298	LEU
1	H	301	ARG
1	H	308	LEU
1	H	314	ASN
1	H	322	LYS
1	I	65	TRP
1	I	66	THR
1	I	72	THR
1	I	79	TRP
1	I	89	LEU
1	I	92	LEU
1	I	94	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	95	ASP
1	I	96	ILE
1	I	117	LEU
1	I	130	GLN
1	I	141	LEU
1	I	177	THR
1	I	199	VAL
1	I	201	LYS
1	I	204	ILE
1	I	214	LYS
1	I	220	GLU
1	I	268	ASP
1	I	291	VAL
1	I	295	ASN
1	I	301	ARG
1	I	307	GLN
1	I	317	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	216	GLN
1	F	307	GLN
1	G	80	GLN
1	G	224	GLN
1	I	158	ASN
1	I	307	GLN
1	I	314	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	240/271 (88%)	-0.07	1 (0%) 92 91	41, 56, 74, 88	0
1	B	240/271 (88%)	-0.10	0 100 100	44, 60, 77, 89	0
1	C	246/271 (90%)	-0.01	1 (0%) 92 91	44, 64, 80, 89	0
1	D	240/271 (88%)	0.01	3 (1%) 77 72	43, 62, 82, 95	0
1	E	241/271 (88%)	-0.08	1 (0%) 92 91	41, 61, 80, 94	0
1	F	244/271 (90%)	-0.10	0 100 100	38, 58, 78, 89	0
1	G	240/271 (88%)	-0.13	0 100 100	40, 56, 76, 94	0
1	H	242/271 (89%)	-0.09	1 (0%) 92 91	42, 56, 75, 97	0
1	I	242/271 (89%)	-0.06	2 (0%) 86 81	39, 58, 75, 89	0
All	All	2175/2439 (89%)	-0.07	9 (0%) 92 91	38, 59, 79, 97	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	252	ILE	4.6
1	I	251	GLY	3.7
1	D	252	ILE	3.2
1	A	250	ALA	3.0
1	D	251	GLY	2.9
1	C	251	GLY	2.4
1	E	167	SER	2.4
1	H	124	SER	2.0
1	D	284	ILE	2.0

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.