



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 2, 2024 – 09:09 pm GMT

PDB ID : 5FT1
Title : Crystal structure of gp37(Dip) from bacteriophage phiKZ bound to RNase E of *Pseudomonas aeruginosa*
Authors : Van den Bossche, A.; Hardwick, S.W.; Ceysens, P.J.; Hendrix, H.; Voet, M.; Dendooven, T.; Bandyra, K.J.; De Maeyer, M.; Aertsen, A.; Noben, J.P.; Luisi, B.F.; Lavigne, R.
Deposited on : 2016-01-08
Resolution : 2.75 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

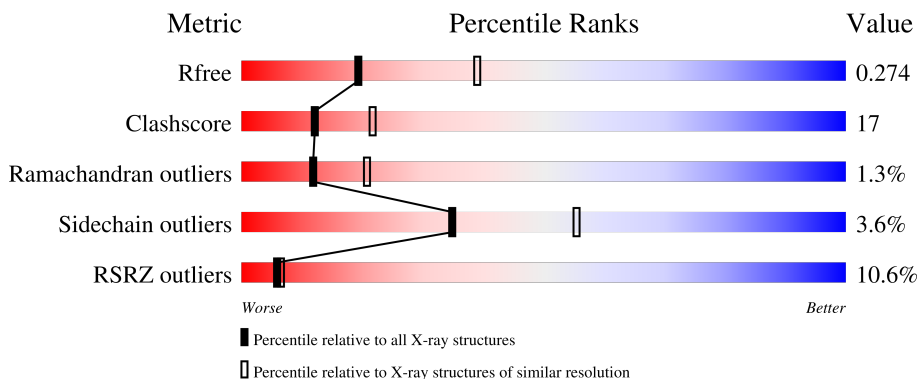
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	281	 11% 56% 30% 1% 1%
1	B	281	 7% 57% 27% 1% 1%
1	E	281	 8% 59% 27% 1% 1%
1	G	281	 13% 65% 23% 1% 1%
1	I	281	 9% 58% 30% 1% 1%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	K	281	
2	C	20	
2	D	20	
2	F	20	
2	H	20	
2	J	20	
2	L	20	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11561 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 GP37.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	250	Total 1891	C 1217	N 306	O 363	S 5	0	0	0
1	B	243	Total 1867	C 1205	N 301	O 354	S 7	0	0	0
1	E	245	Total 1843	C 1191	N 299	O 346	S 7	0	0	0
1	G	249	Total 1892	C 1218	N 306	O 361	S 7	0	0	0
1	I	248	Total 1869	C 1207	N 298	O 358	S 6	0	0	0
1	K	240	Total 1851	C 1195	N 298	O 352	S 6	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	274	LYS	-	expression tag	UNP Q8SDC5
A	275	GLY	-	expression tag	UNP Q8SDC5
A	276	HIS	-	expression tag	UNP Q8SDC5
A	277	HIS	-	expression tag	UNP Q8SDC5
A	278	HIS	-	expression tag	UNP Q8SDC5
A	279	HIS	-	expression tag	UNP Q8SDC5
A	280	HIS	-	expression tag	UNP Q8SDC5
A	281	HIS	-	expression tag	UNP Q8SDC5
B	274	LYS	-	expression tag	UNP Q8SDC5
B	275	GLY	-	expression tag	UNP Q8SDC5
B	276	HIS	-	expression tag	UNP Q8SDC5
B	277	HIS	-	expression tag	UNP Q8SDC5
B	278	HIS	-	expression tag	UNP Q8SDC5
B	279	HIS	-	expression tag	UNP Q8SDC5
B	280	HIS	-	expression tag	UNP Q8SDC5
B	281	HIS	-	expression tag	UNP Q8SDC5
E	274	LYS	-	expression tag	UNP Q8SDC5

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	275	GLY	-	expression tag	UNP Q8SDC5
E	276	HIS	-	expression tag	UNP Q8SDC5
E	277	HIS	-	expression tag	UNP Q8SDC5
E	278	HIS	-	expression tag	UNP Q8SDC5
E	279	HIS	-	expression tag	UNP Q8SDC5
E	280	HIS	-	expression tag	UNP Q8SDC5
E	281	HIS	-	expression tag	UNP Q8SDC5
G	274	LYS	-	expression tag	UNP Q8SDC5
G	275	GLY	-	expression tag	UNP Q8SDC5
G	276	HIS	-	expression tag	UNP Q8SDC5
G	277	HIS	-	expression tag	UNP Q8SDC5
G	278	HIS	-	expression tag	UNP Q8SDC5
G	279	HIS	-	expression tag	UNP Q8SDC5
G	280	HIS	-	expression tag	UNP Q8SDC5
G	281	HIS	-	expression tag	UNP Q8SDC5
I	274	LYS	-	expression tag	UNP Q8SDC5
I	275	GLY	-	expression tag	UNP Q8SDC5
I	276	HIS	-	expression tag	UNP Q8SDC5
I	277	HIS	-	expression tag	UNP Q8SDC5
I	278	HIS	-	expression tag	UNP Q8SDC5
I	279	HIS	-	expression tag	UNP Q8SDC5
I	280	HIS	-	expression tag	UNP Q8SDC5
I	281	HIS	-	expression tag	UNP Q8SDC5
K	274	LYS	-	expression tag	UNP Q8SDC5
K	275	GLY	-	expression tag	UNP Q8SDC5
K	276	HIS	-	expression tag	UNP Q8SDC5
K	277	HIS	-	expression tag	UNP Q8SDC5
K	278	HIS	-	expression tag	UNP Q8SDC5
K	279	HIS	-	expression tag	UNP Q8SDC5
K	280	HIS	-	expression tag	UNP Q8SDC5
K	281	HIS	-	expression tag	UNP Q8SDC5

- Molecule 2 is a protein called RIBONUCLEASE E.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	0	0	0
			61	34	16	11			
2	D	9	Total	C	N	O	0	0	0
			62	35	18	9			
2	F	6	Total	C	N	O	0	0	0
			43	24	12	7			
2	H	8	Total	C	N	O	0	0	0
			63	35	18	10			

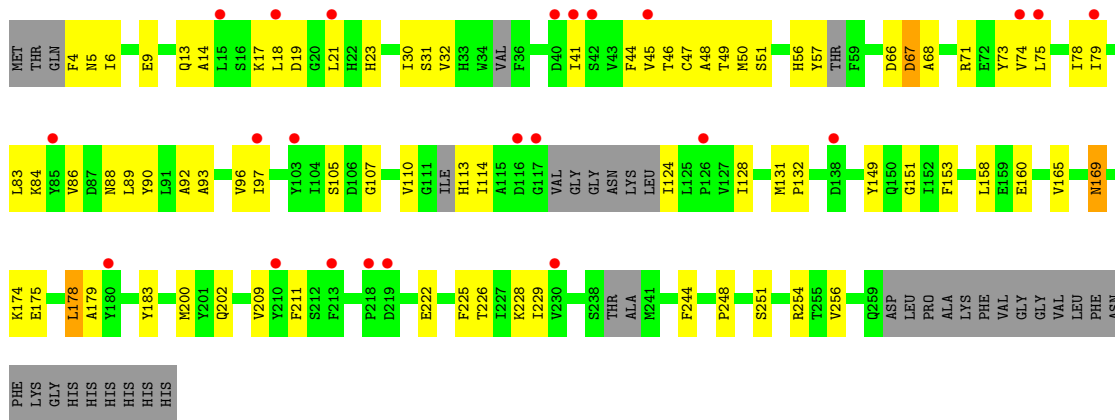
Continued on next page...

Continued from previous page...

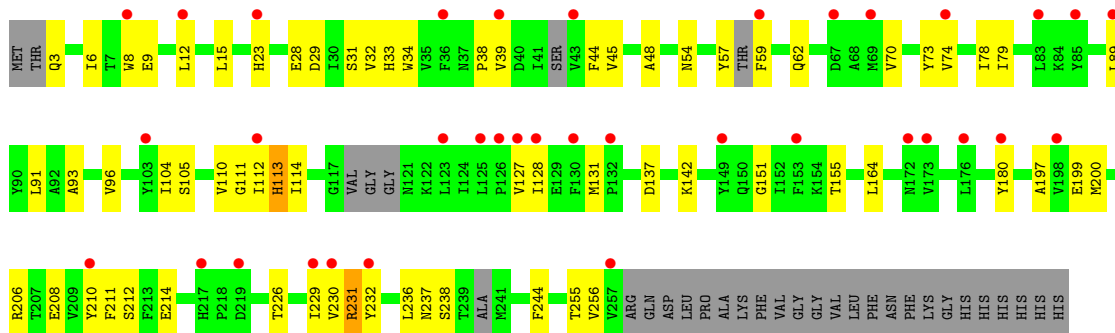
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	J	10	Total	C	N	O	0	0	0
			72	40	20	12			
2	L	6	Total	C	N	O	0	0	0
			46	25	13	8			

- Molecule 3 is water.

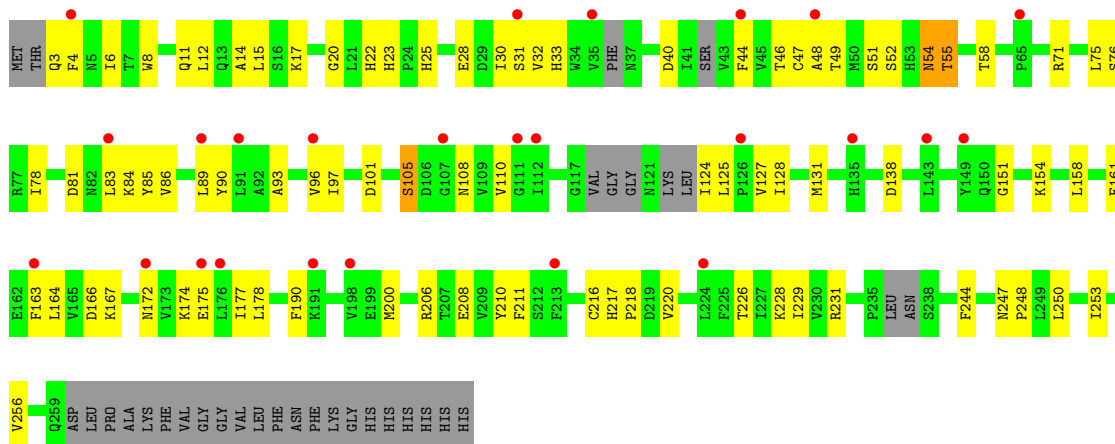
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	O	0	0
			1	1		



• Molecule 1: GP37

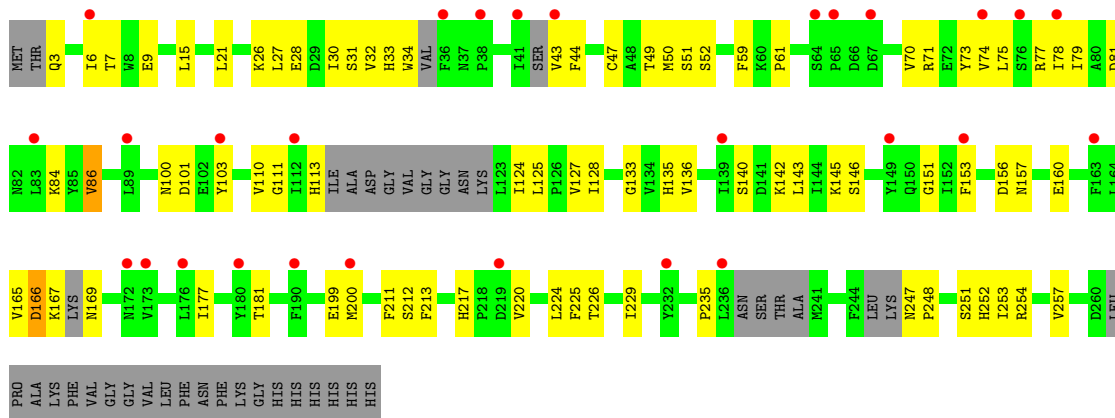


• Molecule 1: GP37

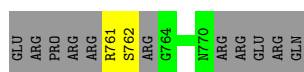
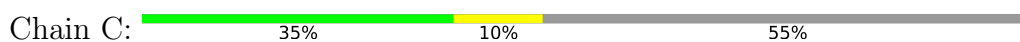


• Molecule 1: GP37

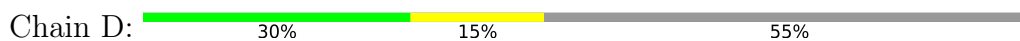




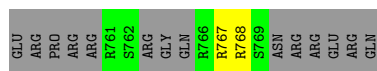
- Molecule 2: RIBONUCLEASE E



- Molecule 2: RIBONUCLEASE E



- Molecule 2: RIBONUCLEASE E



- Molecule 2: RIBONUCLEASE E



- Molecule 2: RIBONUCLEASE E



- Molecule 2: RIBONUCLEASE E



GLU	ARG	PRD	ARG	ARG	SER	ARG	G764	R768	S769	ASN	ARG	ARG	GLU	ARG	GLN
-----	-----	-----	-----	-----	-----	-----	------	------	------	-----	-----	-----	-----	-----	-----

4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.61Å 84.65Å 84.60Å 107.86° 107.88° 107.90°	Depositor
Resolution (Å)	72.19 – 2.75 72.19 – 2.75	Depositor EDS
% Data completeness (in resolution range)	79.8 (72.19-2.75) 77.5 (72.19-2.75)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.40 (at 2.73Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.263 , 0.293 0.238 , 0.274	Depositor DCC
R_{free} test set	2050 reflections (5.18%)	wwPDB-VP
Wilson B-factor (Å ²)	83.6	Xtriage
Anisotropy	0.034	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 69.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.467 for k,l,h 0.467 for l,h,k 0.476 for -l,-k,-h 0.466 for -h,-l,-k 0.467 for -k,-h,-l	Xtriage
Reported twinning fraction	0.500 for -L,-K,-H	Depositor
Outliers	0 of 39555 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11561	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.28	0/1935	0.48	0/2643
1	B	0.31	0/1913	0.46	0/2614
1	E	0.28	0/1887	0.49	0/2576
1	G	0.30	0/1936	0.49	1/2641 (0.0%)
1	I	0.29	0/1911	0.48	0/2608
1	K	0.28	0/1894	0.47	0/2579
2	C	0.20	0/59	0.43	0/75
2	D	0.19	0/60	0.36	0/76
2	F	0.19	0/41	0.27	0/51
2	H	0.24	0/61	0.49	0/77
2	J	0.24	0/71	0.43	0/92
2	L	0.19	0/45	0.36	0/57
All	All	0.29	0/11813	0.48	1/16089 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	91	LEU	CA-CB-CG	5.79	128.63	115.30

There are no chirality outliers.

There are no planarity outliers.

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	1891	0	1705	86	0
1	B	1867	0	1722	56	0
1	E	1843	0	1650	62	0
1	G	1892	0	1711	56	0
1	I	1869	0	1691	70	0
1	K	1851	0	1694	61	0
2	C	61	0	48	3	0
2	D	62	0	50	1	0
2	F	43	0	35	1	0
2	H	63	0	56	6	0
2	J	72	0	62	3	0
2	L	46	0	43	1	0
3	A	1	0	0	0	0
All	All	11561	0	10467	376	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 17.

All (376) 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:A:55:THR:O	1:A:56:HIS:ND1	1.80	1.14
1:A:51:SER:CB	1:A:52:SER:HA	2.05	0.87
1:A:102:GLU:OE1	1:A:113:HIS:NE2	2.09	0.85
1:B:168:LYS:O	1:B:171:ASN:ND2	2.09	0.85
1:A:30:ILE:HG23	1:A:47:CYS:HB3	1.58	0.85
1:A:111:GLY:O	1:A:112:ILE:HG13	1.76	0.84
1:A:49:THR:O	1:A:53:HIS:N	2.10	0.84
2:C:761:ARG:CB	2:C:762:SER:HA	2.08	0.84
1:B:135:HIS:HB2	1:B:224:LEU:HD22	1.62	0.81
1:E:4:PHE:N	1:E:32:VAL:O	2.15	0.80
1:E:49:THR:HG22	1:E:50:MET:H	1.45	0.80
1:G:34:TRP:HB2	1:G:45:VAL:HG12	1.62	0.80
1:A:102:GLU:CD	1:A:113:HIS:HE2	1.87	0.79
1:B:126:PRO:O	1:B:232:TYR:OH	2.03	0.77
1:E:46:THR:OG1	1:E:56:HIS:ND1	2.15	0.77
1:G:113:HIS:O	1:G:113:HIS:ND1	2.18	0.76
1:I:175:GLU:HA	1:I:178:LEU:HB2	1.67	0.75
1:A:158:LEU:O	1:A:161:PHE:N	2.20	0.74
1:K:127:VAL:HG23	1:K:128:ILE:HG13	1.67	0.74
1:A:158:LEU:HA	1:A:161:PHE:HD2	1.53	0.74
1:A:162:GLU:HG2	1:A:167:LYS:HG2	1.69	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:THR:HG22	1:E:50:MET:N	2.02	0.74
1:B:17:LYS:HD3	1:B:218:PRO:HG2	1.70	0.74
1:A:30:ILE:HD12	1:A:78:ILE:HD11	1.70	0.73
1:K:6:ILE:HG21	1:K:71:ARG:HD3	1.71	0.73
1:E:4:PHE:N	1:E:32:VAL:HG13	2.05	0.72
1:E:49:THR:CG2	1:E:50:MET:H	2.02	0.72
1:A:54:ASN:HD22	1:A:55:THR:N	1.88	0.71
1:A:30:ILE:CG2	1:A:47:CYS:HB3	2.21	0.70
1:B:33:HIS:O	1:B:46:THR:HG22	1.90	0.70
1:I:110:VAL:HG22	1:I:128:ILE:HB	1.75	0.69
1:A:111:GLY:C	1:A:112:ILE:HG13	2.12	0.69
1:K:151:GLY:O	1:K:200:MET:HB3	1.93	0.69
1:K:7:THR:OG1	1:K:9:GLU:OE1	2.08	0.68
1:I:3:GLN:N	1:I:32:VAL:O	2.27	0.68
1:A:30:ILE:CD1	1:A:78:ILE:HD11	2.24	0.67
1:E:49:THR:HG22	1:E:51:SER:H	1.58	0.67
1:G:105:SER:HB2	1:G:110:VAL:HG22	1.76	0.67
1:A:93:ALA:O	1:A:96:VAL:N	2.28	0.67
1:G:137:ASP:HB2	2:H:767:ARG:HD3	1.75	0.66
1:G:3:GLN:N	1:G:32:VAL:O	2.28	0.66
1:G:128:ILE:HG12	1:G:229:ILE:HG13	1.77	0.66
1:A:254:ARG:O	1:E:124:ILE:N	2.29	0.66
1:A:72:GLU:HG2	1:A:220:VAL:HG12	1.77	0.66
1:A:102:GLU:CD	1:A:113:HIS:NE2	2.48	0.65
1:G:8:TRP:O	1:G:12:LEU:HB3	1.96	0.65
1:I:49:THR:OG1	1:I:52:SER:O	2.15	0.64
1:I:174:LYS:O	1:I:177:ILE:HG13	1.97	0.64
1:K:110:VAL:HG22	1:K:128:ILE:HB	1.80	0.64
1:G:15:LEU:HD23	1:G:79:ILE:HG22	1.79	0.64
1:A:124:ILE:N	1:E:254:ARG:O	2.31	0.64
1:A:135:HIS:HD2	1:A:137:ASP:H	1.44	0.64
1:G:231:ARG:NH1	1:G:232:TYR:O	2.30	0.64
1:B:8:TRP:HB2	1:B:27:LEU:HD13	1.79	0.63
1:E:30:ILE:HG13	1:E:47:CYS:HB2	1.79	0.63
1:K:127:VAL:O	1:K:229:ILE:HA	1.98	0.63
1:A:109:VAL:HG12	1:A:129:GLU:HG3	1.80	0.63
1:B:81:ASP:O	1:B:84:LYS:NZ	2.30	0.63
1:I:247:ASN:OD1	1:I:250:LEU:N	2.17	0.63
1:K:77:ARG:NH1	1:K:133:GLY:O	2.31	0.63
1:G:208:GLU:HG2	1:G:230:VAL:HG13	1.81	0.63
1:I:30:ILE:HG22	1:I:49:THR:HG22	1.79	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:34:TRP:CB	1:G:45:VAL:HG12	2.28	0.63
1:G:112:ILE:C	1:G:112:ILE:HD12	2.19	0.62
1:I:8:TRP:O	1:I:12:LEU:HB2	1.99	0.62
1:A:134:VAL:O	1:A:224:LEU:HD13	1.99	0.62
1:I:84:LYS:NZ	1:I:108:ASN:OD1	2.32	0.62
1:A:34:TRP:HB3	1:A:45:VAL:HG13	1.82	0.62
1:B:81:ASP:OD1	1:B:84:LYS:NZ	2.31	0.62
1:B:97:ILE:HG12	1:B:105:SER:HB2	1.80	0.61
1:I:158:LEU:HD23	1:I:174:LYS:HD3	1.83	0.61
1:A:33:HIS:HB2	1:A:46:THR:OG1	2.01	0.61
1:E:32:VAL:HA	1:E:47:CYS:HB3	1.83	0.61
1:E:68:ALA:HA	1:E:71:ARG:HE	1.65	0.61
1:B:8:TRP:HE1	1:I:22:HIS:HA	1.65	0.61
1:E:49:THR:CG2	1:E:50:MET:N	2.63	0.61
1:B:171:ASN:OD1	1:B:172:ASN:N	2.34	0.60
1:A:18:LEU:HD11	1:A:79:ILE:HG23	1.82	0.60
1:I:78:ILE:O	1:I:81:ASP:N	2.35	0.60
1:G:57:TYR:HB3	1:G:73:TYR:OH	2.01	0.60
1:E:66:ASP:OD1	1:E:67:ASP:N	2.35	0.60
1:A:208:GLU:OE1	1:A:210:TYR:OH	2.20	0.59
1:I:250:LEU:HA	1:I:253:ILE:CD1	2.32	0.59
1:B:13:GLN:O	1:B:17:LYS:NZ	2.33	0.59
1:A:127:VAL:O	1:A:229:ILE:HA	2.01	0.59
1:E:175:GLU:HG3	1:E:178:LEU:HG	1.82	0.59
1:G:142:LYS:HE2	1:K:142:LYS:HE2	1.83	0.59
1:K:49:THR:OG1	1:K:52:SER:O	2.20	0.59
1:A:55:THR:C	1:A:56:HIS:ND1	2.55	0.59
1:B:110:VAL:HG22	1:B:128:ILE:HB	1.85	0.59
1:A:150:GLN:HG3	1:A:201:TYR:CD1	2.38	0.58
1:B:22:HIS:ND1	1:B:87:ASP:OD2	2.36	0.58
1:G:34:TRP:HB2	1:G:45:VAL:CG1	2.30	0.58
1:I:97:ILE:HD13	1:I:105:SER:OG	2.03	0.58
1:K:166:ASP:HB3	1:K:235:PRO:HB2	1.86	0.58
1:K:111:GLY:HA3	1:K:125:LEU:O	2.02	0.58
1:E:153:PHE:CE2	1:E:160:GLU:HB3	2.39	0.58
1:B:109:VAL:HG12	1:B:129:GLU:HG3	1.85	0.57
1:I:163:PHE:CD2	1:I:164:LEU:HD12	2.38	0.57
1:A:14:ALA:HB1	1:A:79:ILE:HD11	1.85	0.57
1:I:47:CYS:HB2	1:I:55:THR:HG23	1.85	0.57
1:K:217:HIS:HB3	1:K:220:VAL:HG22	1.86	0.57
1:B:124:ILE:HG22	1:G:255:THR:HA	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:59:PHE:HB3	1:G:73:TYR:CE2	2.39	0.57
1:G:62:GLN:OE1	2:H:765:GLN:NE2	2.28	0.57
1:K:156:ASP:OD1	1:K:157:ASN:N	2.37	0.57
1:A:199:GLU:OE1	1:A:201:TYR:OH	2.21	0.57
1:B:175:GLU:O	1:B:179:ALA:HB2	2.05	0.57
1:B:166:ASP:OD1	1:B:167:LYS:N	2.35	0.57
1:I:20:GLY:C	1:I:86:VAL:HG23	2.24	0.57
1:G:38:PRO:HB2	1:I:248:PRO:HB3	1.86	0.56
1:G:236:LEU:O	1:G:237:ASN:ND2	2.39	0.56
1:E:13:GLN:O	1:E:17:LYS:NZ	2.37	0.56
1:I:151:GLY:O	1:I:200:MET:HB3	2.04	0.56
1:K:160:GLU:CD	1:K:160:GLU:N	2.58	0.56
1:E:30:ILE:HD12	1:E:49:THR:N	2.21	0.56
1:K:165:VAL:HG11	1:K:169:ASN:HB2	1.86	0.56
1:E:175:GLU:O	1:E:179:ALA:HB2	2.06	0.56
1:K:213:PHE:O	1:K:224:LEU:HA	2.06	0.56
1:K:153:PHE:HE1	1:K:160:GLU:HB2	1.70	0.56
1:E:19:ASP:O	1:E:183:TYR:OH	2.17	0.55
1:E:158:LEU:HD23	1:E:174:LYS:HD3	1.88	0.55
1:E:6:ILE:HG13	1:E:30:ILE:HG22	1.89	0.55
1:G:9:GLU:N	1:G:9:GLU:OE1	2.39	0.55
1:G:197:ALA:HB3	1:G:212:SER:HB2	1.89	0.54
1:I:211:PHE:O	1:I:226:THR:HA	2.07	0.54
1:K:111:GLY:CA	1:K:125:LEU:O	2.56	0.54
1:K:212:SER:HA	1:K:225:PHE:O	2.08	0.54
1:B:231:ARG:NH1	1:B:232:TYR:O	2.41	0.54
1:I:97:ILE:HD11	1:I:110:VAL:HG11	1.89	0.54
1:E:93:ALA:O	1:E:97:ILE:HG13	2.08	0.54
1:K:135:HIS:CD2	1:K:212:SER:HB3	2.42	0.54
1:G:111:GLY:HA2	1:G:127:VAL:HG12	1.90	0.54
1:K:160:GLU:N	1:K:160:GLU:OE1	2.34	0.54
1:K:43:VAL:HG23	1:K:61:PRO:HG3	1.89	0.53
1:E:14:ALA:HB1	1:E:79:ILE:HD11	1.90	0.53
1:A:77:ARG:NH1	1:A:133:GLY:O	2.42	0.53
1:I:174:LYS:HG2	1:I:175:GLU:HG2	1.89	0.53
1:E:128:ILE:HG22	1:E:229:ILE:HG13	1.90	0.53
1:B:7:THR:OG1	1:B:9:GLU:OE1	2.18	0.53
1:E:88:ASN:O	1:E:92:ALA:HB2	2.09	0.53
1:B:129:GLU:HG2	1:B:131:MET:HG2	1.89	0.53
1:G:211:PHE:O	1:G:226:THR:HA	2.08	0.53
1:A:7:THR:OG1	1:A:9:GLU:OE1	2.22	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:165:VAL:O	1:K:167:LYS:N	2.37	0.53
1:B:37:ASN:ND2	1:B:40:ASP:O	2.42	0.53
1:A:6:ILE:HG12	1:A:71:ARG:NH2	2.23	0.52
1:E:18:LEU:HD11	1:E:79:ILE:HG23	1.91	0.52
1:K:140:SER:HA	1:K:143:LEU:HD13	1.89	0.52
1:E:9:GLU:OE1	1:E:9:GLU:N	2.41	0.52
1:E:45:VAL:HG22	1:E:57:TYR:HB2	1.90	0.52
1:E:149:TYR:CZ	1:E:202:GLN:HG3	2.44	0.52
1:A:100:ASN:HB2	1:A:169:ASN:HD21	1.73	0.52
1:B:127:VAL:HG13	1:B:128:ILE:HG13	1.91	0.52
1:K:135:HIS:HB2	1:K:224:LEU:HD22	1.91	0.52
1:I:127:VAL:O	1:I:229:ILE:HA	2.09	0.52
1:K:28:GLU:OE1	1:K:51:SER:OG	2.26	0.52
1:A:100:ASN:HB3	1:A:103:TYR:HB2	1.92	0.52
1:A:211:PHE:O	1:A:226:THR:HA	2.10	0.52
1:B:140:SER:O	1:B:143:LEU:N	2.29	0.52
1:K:34:TRP:CE2	1:K:70:VAL:HG11	2.44	0.52
1:K:211:PHE:O	1:K:226:THR:HA	2.09	0.52
1:E:131:MET:HB2	1:E:226:THR:HG23	1.92	0.52
1:I:131:MET:HB2	1:I:226:THR:HG23	1.92	0.52
1:K:101:ASP:OD1	1:K:101:ASP:N	2.43	0.52
1:B:42:SER:HA	1:B:61:PRO:HD2	1.92	0.51
1:G:34:TRP:CB	1:G:45:VAL:CG1	2.88	0.51
1:I:210:TYR:CE2	1:I:228:LYS:HG3	2.45	0.51
1:A:135:HIS:CD2	1:A:137:ASP:H	2.26	0.51
1:B:8:TRP:HZ3	1:I:12:LEU:HD21	1.75	0.51
1:B:104:ILE:O	1:B:110:VAL:HA	2.09	0.51
2:C:761:ARG:CB	2:C:762:SER:CA	2.85	0.51
2:C:761:ARG:N	2:C:762:SER:CB	2.73	0.51
1:I:110:VAL:CG2	1:I:128:ILE:HB	2.40	0.51
1:A:110:VAL:HG22	1:A:128:ILE:HB	1.92	0.51
1:E:30:ILE:CG1	1:E:47:CYS:HB2	2.40	0.51
1:I:253:ILE:HG13	1:K:125:LEU:HD13	1.92	0.51
1:A:88:ASN:HA	1:A:91:LEU:CD2	2.41	0.51
1:G:208:GLU:OE1	1:G:210:TYR:OH	2.24	0.51
1:B:225:PHE:HE1	1:B:227:ILE:HG12	1.75	0.51
1:E:71:ARG:O	1:E:74:VAL:HG22	2.11	0.51
1:B:38:PRO:HG3	1:E:248:PRO:HB3	1.93	0.51
1:G:9:GLU:HA	1:G:12:LEU:HD23	1.91	0.51
1:I:138:ASP:OD1	2:J:767:ARG:NH1	2.44	0.51
1:G:131:MET:HB2	1:G:226:THR:HG23	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:4:PHE:H	1:I:32:VAL:HG22	1.76	0.50
1:A:17:LYS:HD3	1:A:218:PRO:HG2	1.93	0.50
1:A:93:ALA:O	1:A:96:VAL:HG22	2.11	0.50
1:I:125:LEU:HD11	1:K:252:HIS:HB2	1.93	0.50
1:K:143:LEU:HA	1:K:146:SER:OG	2.11	0.50
1:A:116:ASP:O	1:A:118:VAL:N	2.43	0.50
1:I:164:LEU:HD22	1:I:229:ILE:HD11	1.94	0.50
2:H:765:GLN:N	2:H:765:GLN:OE1	2.44	0.50
1:E:23:HIS:ND1	1:G:28:GLU:OE2	2.45	0.50
1:A:49:THR:O	1:A:49:THR:HG23	2.12	0.49
1:I:11:GLN:O	1:I:15:LEU:HD12	2.12	0.49
1:G:199:GLU:OE2	2:H:768:ARG:NH2	2.44	0.49
1:K:21:LEU:HA	1:K:86:VAL:HA	1.94	0.49
1:E:75:LEU:O	1:E:79:ILE:HB	2.13	0.49
1:K:74:VAL:O	1:K:78:ILE:HG12	2.12	0.49
1:K:199:GLU:OE2	2:L:768:ARG:NH2	2.45	0.49
1:A:41:ILE:O	1:A:61:PRO:HG3	2.12	0.49
1:A:52:SER:O	1:A:53:HIS:HB2	2.12	0.49
1:A:88:ASN:HA	1:A:91:LEU:HD22	1.94	0.49
1:B:30:ILE:HD11	1:B:47:CYS:HB2	1.95	0.49
1:E:165:VAL:HG11	1:E:169:ASN:HB2	1.94	0.49
1:A:47:CYS:HB2	1:A:55:THR:HG23	1.95	0.48
1:B:32:VAL:HA	1:B:47:CYS:HA	1.95	0.48
1:A:8:TRP:CZ3	1:A:9:GLU:HG3	2.48	0.48
1:A:102:GLU:OE1	1:A:113:HIS:CD2	2.66	0.48
1:B:8:TRP:CZ3	1:B:9:GLU:HG3	2.48	0.48
1:B:208:GLU:HG2	1:B:230:VAL:HG13	1.95	0.48
1:G:6:ILE:O	1:G:29:ASP:HA	2.14	0.48
1:G:112:ILE:HD11	1:G:114:ILE:HD11	1.94	0.48
1:E:200:MET:HG3	1:E:209:VAL:HG22	1.95	0.48
1:B:102:GLU:O	1:B:112:ILE:HA	2.14	0.48
1:G:112:ILE:C	1:G:112:ILE:CD1	2.82	0.48
1:E:86:VAL:HB	1:E:89:LEU:HD12	1.96	0.48
1:A:39:VAL:O	1:A:40:ASP:CB	2.63	0.47
1:E:83:LEU:HD22	1:E:183:TYR:HE2	1.79	0.47
1:I:17:LYS:HD3	1:I:218:PRO:HG2	1.95	0.47
1:K:3:GLN:N	1:K:33:HIS:HA	2.29	0.47
1:I:33:HIS:HB2	1:I:46:THR:HG23	1.95	0.47
1:E:89:LEU:HD21	1:E:183:TYR:HB2	1.97	0.47
1:E:211:PHE:O	1:E:226:THR:HA	2.13	0.47
1:G:237:ASN:HA	1:G:238:SER:HA	1.69	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:4:PHE:HE1	1:I:6:ILE:HG12	1.78	0.47
1:B:75:LEU:O	1:B:79:ILE:HG12	2.14	0.47
1:A:10:GLU:OE1	1:A:71:ARG:NH2	2.45	0.47
1:I:208:GLU:OE1	1:I:210:TYR:OH	2.32	0.47
1:A:3:GLN:OE1	1:A:34:TRP:NE1	2.47	0.47
1:G:15:LEU:CD2	1:G:79:ILE:HG22	2.42	0.47
1:I:97:ILE:CD1	1:I:110:VAL:HG11	2.44	0.47
1:K:28:GLU:OE2	1:K:50:MET:N	2.48	0.47
1:E:21:LEU:HB2	1:E:86:VAL:HG22	1.96	0.47
1:I:124:ILE:N	1:K:254:ARG:O	2.48	0.47
1:A:50:MET:HA	1:A:51:SER:HA	1.65	0.47
1:A:134:VAL:C	1:A:224:LEU:HD13	2.35	0.47
1:K:212:SER:OG	1:K:226:THR:OG1	2.28	0.47
1:A:8:TRP:O	1:A:12:LEU:HD12	2.15	0.46
1:I:31:SER:OG	1:I:48:ALA:HB3	2.15	0.46
1:E:57:TYR:HB3	1:E:73:TYR:HE1	1.80	0.46
1:I:75:LEU:HD22	1:I:78:ILE:HD11	1.97	0.46
1:A:150:GLN:HG3	1:A:201:TYR:HD1	1.80	0.46
1:G:31:SER:HG	1:G:48:ALA:HB3	1.80	0.46
1:A:87:ASP:O	1:A:91:LEU:HD22	2.15	0.46
1:B:46:THR:HG1	1:B:56:HIS:CE1	2.34	0.46
1:I:6:ILE:HG21	1:I:75:LEU:HD21	1.97	0.46
1:A:158:LEU:HA	1:A:161:PHE:CD2	2.42	0.46
1:I:76:SER:CB	1:I:220:VAL:HG21	2.46	0.46
1:K:32:VAL:HG23	1:K:47:CYS:SG	2.56	0.46
1:G:164:LEU:HA	1:G:231:ARG:HD2	1.98	0.46
1:I:54:ASN:OD1	1:I:55:THR:N	2.50	0.45
1:I:93:ALA:O	1:I:96:VAL:HG22	2.17	0.45
1:K:113:HIS:O	1:K:113:HIS:ND1	2.45	0.45
1:K:181:THR:HG22	1:K:213:PHE:CE1	2.51	0.45
1:G:137:ASP:CB	2:H:767:ARG:HD3	2.46	0.45
1:G:164:LEU:CD2	1:G:231:ARG:HD2	2.47	0.45
1:I:40:ASP:OD1	1:I:40:ASP:N	2.36	0.45
1:K:136:VAL:HG11	1:K:199:GLU:HG3	1.98	0.45
1:I:4:PHE:CE2	1:I:32:VAL:HG21	2.51	0.45
1:I:84:LYS:HG3	1:I:85:TYR:CE1	2.52	0.45
1:I:166:ASP:OD1	1:I:167:LYS:HD2	2.17	0.45
1:I:253:ILE:HG23	1:K:124:ILE:O	2.16	0.45
1:I:250:LEU:HA	1:I:253:ILE:HD11	1.99	0.45
1:K:30:ILE:CG1	1:K:47:CYS:HB3	2.47	0.45
1:A:55:THR:OG1	1:A:56:HIS:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ILE:HG22	1:A:113:HIS:N	2.32	0.45
1:B:198:VAL:HA	1:B:210:TYR:O	2.17	0.45
1:A:141:ASP:OD1	1:A:141:ASP:N	2.50	0.44
1:B:213:PHE:O	1:B:224:LEU:HA	2.16	0.44
1:A:158:LEU:O	1:A:160:GLU:N	2.50	0.44
1:I:158:LEU:CD2	1:I:174:LYS:HD3	2.46	0.44
1:A:54:ASN:ND2	1:A:55:THR:N	2.60	0.44
1:E:4:PHE:HD1	1:E:5:ASN:H	1.65	0.44
1:G:31:SER:OG	1:G:48:ALA:HB3	2.17	0.44
1:A:156:ASP:HA	1:A:178:LEU:HD11	2.00	0.44
1:B:158:LEU:HD12	1:B:161:PHE:HB2	1.98	0.44
1:G:74:VAL:O	1:G:78:ILE:HG12	2.18	0.44
1:G:93:ALA:O	1:G:96:VAL:HG22	2.17	0.44
1:G:9:GLU:O	1:G:12:LEU:HG	2.18	0.44
1:A:97:ILE:HG12	1:A:105:SER:HB2	1.98	0.44
1:B:144:ILE:HG23	1:B:150:GLN:OE1	2.18	0.44
1:E:151:GLY:O	1:E:200:MET:HB3	2.17	0.44
1:A:41:ILE:O	1:A:61:PRO:HD3	2.17	0.43
1:E:97:ILE:HD13	1:E:105:SER:OG	2.17	0.43
1:G:151:GLY:O	1:G:200:MET:HB3	2.18	0.43
1:K:177:ILE:O	1:K:181:THR:HG23	2.17	0.43
1:B:250:LEU:HD21	1:G:244:PHE:HZ	1.83	0.43
1:G:104:ILE:O	1:G:110:VAL:HA	2.18	0.43
1:I:44:PHE:HD1	1:I:58:THR:HG22	1.83	0.43
1:K:81:ASP:OD1	1:K:84:LYS:HE2	2.18	0.43
1:B:38:PRO:CG	1:E:248:PRO:HB3	2.49	0.43
1:E:74:VAL:O	1:E:78:ILE:HG12	2.17	0.43
1:G:89:LEU:HB3	1:G:180:TYR:CE1	2.53	0.43
1:I:127:VAL:HG23	1:I:128:ILE:HG13	2.01	0.43
1:B:50:MET:SD	1:B:50:MET:N	2.91	0.43
1:K:100:ASN:HB3	1:K:103:TYR:HB2	2.00	0.43
1:A:6:ILE:HG23	1:A:10:GLU:OE1	2.19	0.43
1:B:158:LEU:HD11	1:B:170:ALA:HB1	2.00	0.43
1:E:113:HIS:O	1:E:124:ILE:HA	2.19	0.43
1:A:3:GLN:NE2	1:A:34:TRP:O	2.52	0.43
1:A:11:GLN:NE2	1:A:28:GLU:O	2.51	0.43
1:B:8:TRP:HZ3	1:I:12:LEU:CD2	2.31	0.43
1:E:93:ALA:O	1:E:96:VAL:HG22	2.18	0.43
1:E:132:PRO:HB3	1:E:225:PHE:CE2	2.54	0.43
1:G:44:PHE:CE1	1:G:59:PHE:N	2.87	0.43
1:E:84:LYS:NZ	1:E:107:GLY:O	2.44	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:113:HIS:HA	1:E:114:ILE:HA	1.56	0.43
1:I:28:GLU:OE2	1:I:51:SER:OG	2.36	0.43
1:G:206:ARG:NE	1:G:208:GLU:OE2	2.45	0.43
1:K:32:VAL:HA	1:K:47:CYS:HA	2.00	0.43
1:K:136:VAL:HG23	1:K:212:SER:OG	2.18	0.43
1:A:160:GLU:O	1:A:163:PHE:HB3	2.19	0.43
1:A:4:PHE:CD2	1:A:32:VAL:HG11	2.53	0.42
1:A:93:ALA:O	1:A:97:ILE:HD12	2.18	0.42
1:E:4:PHE:CE1	1:E:32:VAL:HG11	2.54	0.42
1:E:50:MET:CB	1:G:23:HIS:HE2	2.32	0.42
1:G:70:VAL:O	1:G:74:VAL:HG13	2.19	0.42
1:A:12:LEU:HA	1:A:15:LEU:HB2	2.01	0.42
1:I:97:ILE:HG21	1:I:105:SER:OG	2.19	0.42
1:E:31:SER:O	1:E:47:CYS:HA	2.19	0.42
1:I:190:PHE:CG	2:J:766:ARG:NH2	2.88	0.42
1:K:15:LEU:HD23	1:K:79:ILE:HG12	2.02	0.42
1:K:151:GLY:C	1:K:200:MET:HB3	2.40	0.42
1:A:4:PHE:HE1	1:A:6:ILE:HG13	1.84	0.42
1:A:8:TRP:CE3	1:A:9:GLU:HG3	2.55	0.42
1:I:83:LEU:O	1:I:89:LEU:HD12	2.19	0.42
1:B:49:THR:OG1	1:B:53:HIS:N	2.49	0.42
1:I:161:PHE:CE1	1:I:174:LYS:HA	2.55	0.42
1:K:143:LEU:HA	1:K:146:SER:HG	1.84	0.42
1:B:151:GLY:HA3	1:B:200:MET:HE3	2.01	0.42
1:K:153:PHE:HE1	1:K:160:GLU:CB	2.33	0.42
1:A:4:PHE:CE2	1:A:32:VAL:HG11	2.55	0.42
1:I:96:VAL:HG23	1:I:97:ILE:HG13	2.02	0.42
1:G:33:HIS:ND1	1:I:101:ASP:OD2	2.53	0.42
1:I:71:ARG:O	1:I:75:LEU:HG	2.19	0.42
1:A:135:HIS:HB2	1:A:224:LEU:HD22	2.01	0.42
1:B:30:ILE:HD13	1:B:49:THR:CG2	2.49	0.42
2:D:764:GLY:O	2:D:766:ARG:NH1	2.37	0.42
1:E:30:ILE:HD12	1:E:48:ALA:C	2.40	0.42
1:A:54:ASN:ND2	1:A:54:ASN:C	2.73	0.41
1:E:222:GLU:OE2	2:F:767:ARG:NH2	2.52	0.41
1:I:125:LEU:HD13	1:K:253:ILE:HD13	2.01	0.41
2:J:761:ARG:HA	2:J:762:SER:HA	1.49	0.41
1:B:53:HIS:O	1:B:53:HIS:ND1	2.53	0.41
1:E:110:VAL:HG22	1:E:128:ILE:CG1	2.50	0.41
1:I:190:PHE:CD1	1:I:216:CYS:HB2	2.55	0.41
1:B:28:GLU:HB3	1:I:23:HIS:CD2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:127:VAL:O	1:G:229:ILE:HA	2.20	0.41
1:A:43:VAL:HG23	1:A:61:PRO:HB3	2.02	0.41
1:G:112:ILE:CD1	1:G:113:HIS:N	2.83	0.41
1:I:164:LEU:O	1:I:231:ARG:HG3	2.20	0.41
1:A:177:ILE:HD12	1:A:178:LEU:N	2.36	0.41
1:I:14:ALA:O	1:I:217:HIS:NE2	2.53	0.41
1:A:55:THR:O	1:A:56:HIS:CE1	2.65	0.41
1:I:125:LEU:HD12	1:I:125:LEU:HA	1.93	0.41
1:K:74:VAL:HG23	1:K:75:LEU:HD12	2.03	0.41
1:E:151:GLY:C	1:E:200:MET:HB3	2.41	0.41
1:B:11:GLN:O	1:B:15:LEU:HG	2.21	0.41
1:B:123:LEU:HA	1:G:255:THR:HB	2.03	0.41
1:E:128:ILE:HA	1:E:228:LYS:O	2.21	0.41
1:K:3:GLN:N	1:K:32:VAL:O	2.53	0.41
1:A:206:ARG:HD2	1:A:230:VAL:HG21	2.03	0.40
1:B:37:ASN:O	1:B:41:ILE:HA	2.21	0.40
1:B:6:ILE:HG22	1:B:71:ARG:HD3	2.02	0.40
1:K:103:TYR:HA	1:K:111:GLY:O	2.21	0.40
1:A:171:ASN:OD1	1:A:171:ASN:N	2.53	0.40
1:A:209:VAL:HG22	1:A:229:ILE:O	2.22	0.40
1:B:190:PHE:CD2	1:B:216:CYS:HB2	2.57	0.40
1:G:214:GLU:OE1	2:H:766:ARG:HG3	2.21	0.40
1:K:143:LEU:HD12	1:K:143:LEU:H	1.87	0.40
1:B:164:LEU:O	1:B:231:ARG:HG3	2.21	0.40
1:K:248:PRO:O	1:K:251:SER:OG	2.32	0.40
1:I:96:VAL:HG12	1:I:172:ASN:HB3	2.03	0.40
1:K:59:PHE:HB3	1:K:73:TYR:CZ	2.57	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	238/281 (85%)	218 (92%)	17 (7%)	3 (1%)	12	21
1	B	237/281 (84%)	222 (94%)	13 (6%)	2 (1%)	19	34
1	E	233/281 (83%)	220 (94%)	10 (4%)	3 (1%)	12	21
1	G	239/281 (85%)	224 (94%)	13 (5%)	2 (1%)	19	34
1	I	237/281 (84%)	221 (93%)	12 (5%)	4 (2%)	9	16
1	K	226/281 (80%)	211 (93%)	13 (6%)	2 (1%)	17	31
2	C	5/20 (25%)	2 (40%)	3 (60%)	0	100	100
2	D	5/20 (25%)	2 (40%)	2 (40%)	1 (20%)	0	0
2	F	2/20 (10%)	0	1 (50%)	1 (50%)	0	0
2	H	4/20 (20%)	3 (75%)	1 (25%)	0	100	100
2	J	8/20 (40%)	5 (62%)	3 (38%)	0	100	100
2	L	4/20 (20%)	3 (75%)	1 (25%)	0	100	100
All	All	1438/1806 (80%)	1331 (93%)	89 (6%)	18 (1%)	12	21

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	41	ILE
1	A	114	ILE
1	I	55	THR
1	I	54	ASN
1	A	113	HIS
1	E	251	SER
1	K	166	ASP
1	G	39	VAL
1	I	154	LYS
2	D	767	ARG
2	F	768	ARG
1	G	256	VAL
1	E	41	ILE
1	B	127	VAL
1	I	256	VAL
1	K	257	VAL
1	B	38	PRO
1	E	256	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	190/251 (76%)	181 (95%)	9 (5%)	26	45
1	B	194/251 (77%)	185 (95%)	9 (5%)	27	46
1	E	182/251 (72%)	176 (97%)	6 (3%)	38	58
1	G	191/251 (76%)	187 (98%)	4 (2%)	53	71
1	I	187/251 (74%)	182 (97%)	5 (3%)	44	65
1	K	192/251 (76%)	185 (96%)	7 (4%)	35	55
2	C	4/19 (21%)	4 (100%)	0	100	100
2	D	3/19 (16%)	3 (100%)	0	100	100
2	F	3/19 (16%)	3 (100%)	0	100	100
2	H	5/19 (26%)	5 (100%)	0	100	100
2	J	5/19 (26%)	3 (60%)	2 (40%)	0	0
2	L	4/19 (21%)	4 (100%)	0	100	100
All	All	1160/1620 (72%)	1118 (96%)	42 (4%)	35	55

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	SER
1	A	54	ASN
1	A	55	THR
1	A	72	GLU
1	A	103	TYR
1	A	141	ASP
1	A	159	GLU
1	A	163	PHE
1	A	171	ASN
1	B	27	LEU
1	B	44	PHE
1	B	47	CYS
1	B	101	ASP
1	B	103	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	143	LEU
1	B	146	SER
1	B	224	LEU
1	B	231	ARG
1	E	44	PHE
1	E	67	ASP
1	E	90	TYR
1	E	169	ASN
1	E	178	LEU
1	E	244	PHE
1	G	54	ASN
1	G	113	HIS
1	G	155	THR
1	G	231	ARG
1	I	25	HIS
1	I	90	TYR
1	I	105	SER
1	I	206	ARG
1	I	244	PHE
2	J	767	ARG
2	J	769	SER
1	K	26	LYS
1	K	27	LEU
1	K	31	SER
1	K	44	PHE
1	K	86	VAL
1	K	145	LYS
1	K	247	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	GLN
1	A	54	ASN
1	A	135	HIS
1	A	169	ASN
1	A	172	ASN
1	G	62	GLN
1	G	186	ASN
2	H	765	GLN
1	I	169	ASN
1	I	186	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	K	11	GLN
1	K	247	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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 i

6.1 Protein, DNA and RNA chains i

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	250/281 (88%)	0.53	30 (12%) 4 4	61, 100, 134, 162	0
1	B	243/281 (86%)	0.42	19 (7%) 13 15	59, 97, 127, 144	0
1	E	245/281 (87%)	0.48	23 (9%) 8 10	61, 93, 132, 161	0
1	G	249/281 (88%)	0.67	36 (14%) 2 2	67, 96, 136, 152	0
1	I	248/281 (88%)	0.47	25 (10%) 7 7	64, 98, 131, 140	0
1	K	240/281 (85%)	0.59	28 (11%) 4 5	62, 94, 127, 150	0
2	C	9/20 (45%)	-0.25	0 100 100	83, 106, 120, 121	0
2	D	9/20 (45%)	-0.18	0 100 100	107, 112, 135, 137	0
2	F	6/20 (30%)	0.26	0 100 100	106, 121, 128, 128	0
2	H	8/20 (40%)	0.11	0 100 100	93, 108, 121, 145	0
2	J	10/20 (50%)	-0.04	0 100 100	91, 104, 142, 145	0
2	L	6/20 (30%)	-0.42	0 100 100	107, 117, 131, 133	0
All	All	1523/1806 (84%)	0.51	161 (10%) 6 6	59, 97, 132, 162	0

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	83	LEU	8.5
1	A	116	ASP	6.8
1	G	89	LEU	6.7
1	A	115	ALA	6.6
1	K	83	LEU	5.9
1	A	104	ILE	5.5
1	A	117	GLY	5.4
1	K	153	PHE	5.4
1	G	180	TYR	5.2
1	I	35	VAL	5.2
1	I	83	LEU	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	125	LEU	5.0
1	K	89	LEU	4.8
1	A	103	TYR	4.8
1	K	36	PHE	4.7
1	K	6	ILE	4.7
1	E	138	ASP	4.7
1	E	40	ASP	4.4
1	K	176	LEU	4.4
1	G	103	TYR	4.3
1	A	97	ILE	4.3
1	B	111	GLY	4.3
1	E	117	GLY	4.2
1	A	173	VAL	4.2
1	A	125	LEU	4.2
1	E	213	PHE	4.2
1	A	149	TYR	4.1
1	K	41	ILE	4.1
1	G	85	TYR	4.1
1	G	69	MET	4.1
1	E	103	TYR	4.0
1	I	224	LEU	4.0
1	G	67	ASP	4.0
1	I	31	SER	4.0
1	K	236	LEU	3.9
1	E	45	VAL	3.9
1	K	180	TYR	3.9
1	I	149	TYR	3.8
1	G	39	VAL	3.8
1	K	64	SER	3.7
1	I	213	PHE	3.7
1	B	112	ILE	3.7
1	G	126	PRO	3.7
1	B	250	LEU	3.6
1	A	138	ASP	3.5
1	G	172	ASN	3.5
1	I	89	LEU	3.5
1	I	44	PHE	3.5
1	K	149	TYR	3.5
1	B	65	PRO	3.4
1	G	59	PHE	3.4
1	K	219	ASP	3.3
1	A	126	PRO	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	91	LEU	3.3
1	I	65	PRO	3.3
1	K	74	VAL	3.3
1	E	126	PRO	3.3
1	A	164	LEU	3.3
1	A	153	PHE	3.2
1	B	110	VAL	3.2
1	E	41	ILE	3.2
1	G	23	HIS	3.2
1	I	191	LYS	3.1
1	B	126	PRO	3.0
1	I	48	ALA	3.0
1	K	76	SER	3.0
1	B	125	LEU	3.0
1	I	163	PHE	3.0
1	I	91	LEU	3.0
1	G	8	TRP	3.0
1	B	194	ALA	3.0
1	E	42	SER	2.9
1	E	18	LEU	2.9
1	B	165	VAL	2.9
1	I	96	VAL	2.9
1	B	197	ALA	2.9
1	A	213	PHE	2.9
1	K	38	PRO	2.8
1	E	15	LEU	2.8
1	E	219	ASP	2.8
1	G	132	PRO	2.8
1	A	105	SER	2.8
1	G	149	TYR	2.8
1	A	96	VAL	2.7
1	I	135	HIS	2.7
1	K	112	ILE	2.7
1	G	217	HIS	2.6
1	G	232	TYR	2.6
1	B	252	HIS	2.6
1	G	219	ASP	2.6
1	G	198	VAL	2.6
1	G	12	LEU	2.6
1	G	112	ILE	2.6
1	G	176	LEU	2.6
1	I	4	PHE	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	K	103	TYR	2.6
1	A	136	VAL	2.6
1	A	156	ASP	2.6
1	K	43	VAL	2.6
1	E	116	ASP	2.5
1	B	75	LEU	2.5
1	G	153	PHE	2.5
1	K	67	ASP	2.5
1	A	180	TYR	2.5
1	K	190	PHE	2.5
1	A	30	ILE	2.5
1	E	79	ILE	2.4
1	A	224	LEU	2.4
1	A	83	LEU	2.4
1	G	43	VAL	2.4
1	K	200	MET	2.4
1	E	97	ILE	2.4
1	A	175	GLU	2.4
1	E	75	LEU	2.4
1	E	210	TYR	2.3
1	K	163	PHE	2.3
1	A	89	LEU	2.3
1	G	230	VAL	2.3
1	I	111	GLY	2.3
1	B	91	LEU	2.3
1	K	139	ILE	2.3
1	G	123	LEU	2.3
1	I	143	LEU	2.3
1	G	210	TYR	2.3
1	A	211	PHE	2.3
1	E	180	TYR	2.3
1	G	74	VAL	2.2
1	E	21	LEU	2.2
1	I	175	GLU	2.2
1	G	257	VAL	2.2
1	K	65	PRO	2.2
1	A	4	PHE	2.2
1	K	172	ASN	2.2
1	E	85	TYR	2.2
1	I	107	GLY	2.2
1	K	232	TYR	2.2
1	G	130	PHE	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	230	VAL	2.1
1	G	229	ILE	2.1
1	I	172	ASN	2.1
1	G	173	VAL	2.1
1	A	113	HIS	2.1
1	B	218	PRO	2.1
1	B	244	PHE	2.1
1	B	113	HIS	2.1
1	G	128	ILE	2.1
1	A	93	ALA	2.1
1	B	191	LYS	2.1
1	B	199	GLU	2.1
1	A	75	LEU	2.1
1	I	176	LEU	2.1
1	K	173	VAL	2.1
1	E	218	PRO	2.1
1	G	36	PHE	2.1
1	E	74	VAL	2.0
1	G	127	VAL	2.0
1	K	78	ILE	2.0
1	I	198	VAL	2.0
1	I	112	ILE	2.0
1	B	35	VAL	2.0
1	I	126	PRO	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.