



Full wwPDB X-ray Structure Validation Report i

Mar 1, 2014 – 03:19 AM GMT

PDB ID : 1FG9
Title : 3:1 COMPLEX OF INTERFERON-GAMMA RECEPTOR WITH
INTERFERON-GAMMA DIMER
Authors : Thiel, D.J.; le Du, M.-H.; Walter, R.L.; D'Arcy, A.; Chene, C.; Fountoulakis,
M.; Garotta, G.; Winkler, F.K.; Ealick, S.E.
Deposited on : 2000-07-28
Resolution : 2.90 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

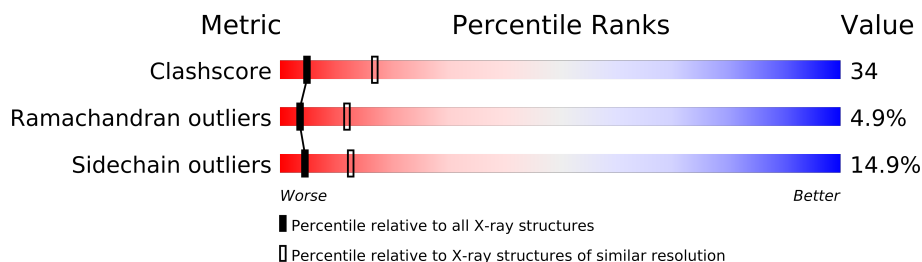
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.90 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))
Clashscore	79885	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	134	
1	B	134	
2	C	245	
2	D	245	
2	E	245	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6905 atoms, of which 0 are hydrogen and 0 are deuterium.

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 INTERFERON GAMMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	127	Total	C	N	O	S	0	0	0
			1046	666	176	200	4			
1	B	127	Total	C	N	O	S	0	0	0
			1044	665	176	199	4			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	INITIATING MET	UNP P01579
B	0	MET	-	INITIATING MET	UNP P01579

- Molecule 2 is a protein called INTERFERON-GAMMA RECEPTOR ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	210	Total	C	N	O	S	0	0	0
			1661	1053	276	320	12			
2	D	205	Total	C	N	O	S	0	0	0
			1617	1025	269	311	12			
2	E	193	Total	C	N	O	S	0	0	0
			1537	972	256	297	12			

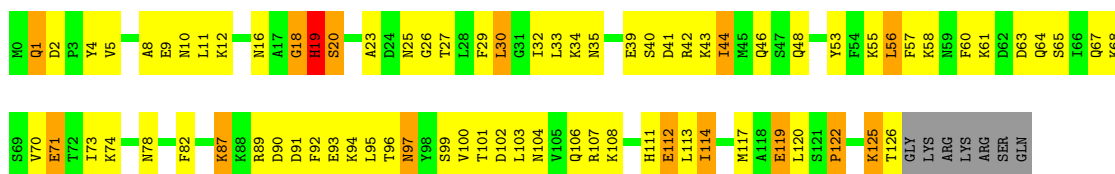
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

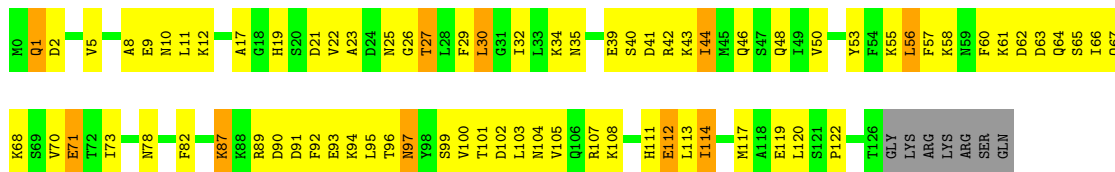
• Molecule 1: INTERFERON GAMMA

Chain A: 



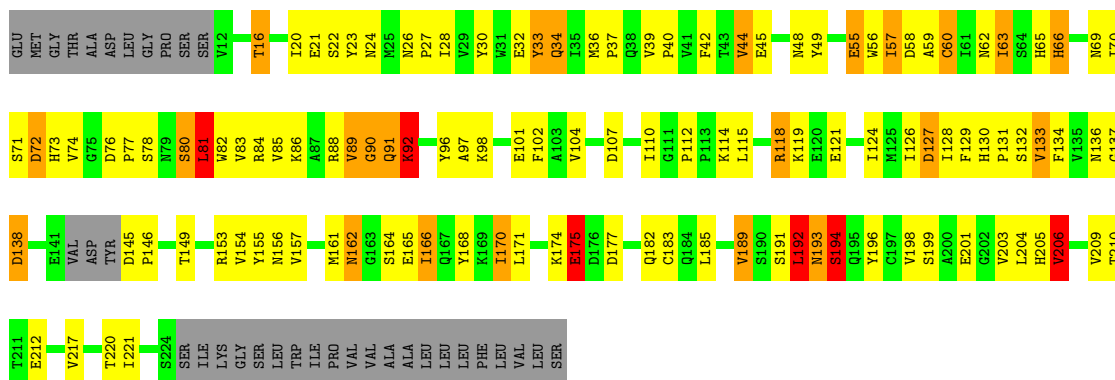
• Molecule 1: INTERFERON GAMMA

Chain B: 



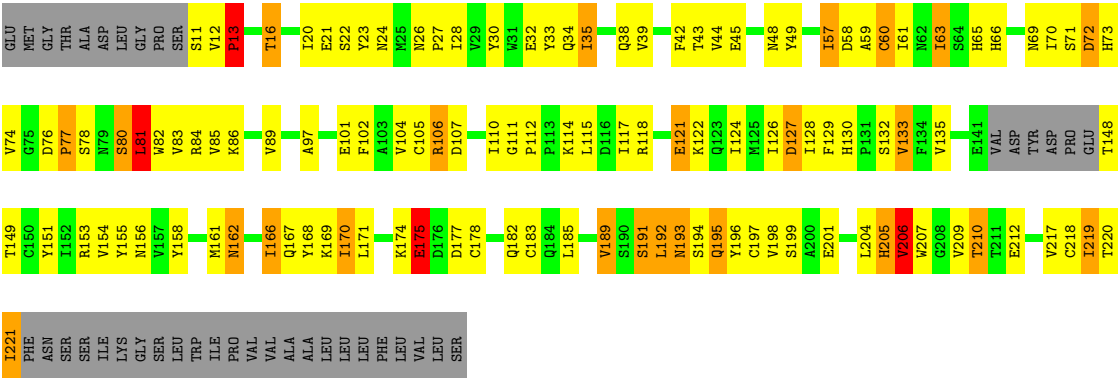
• Molecule 2: INTERFERON-GAMMA RECEPTOR ALPHA CHAIN

Chain C: 



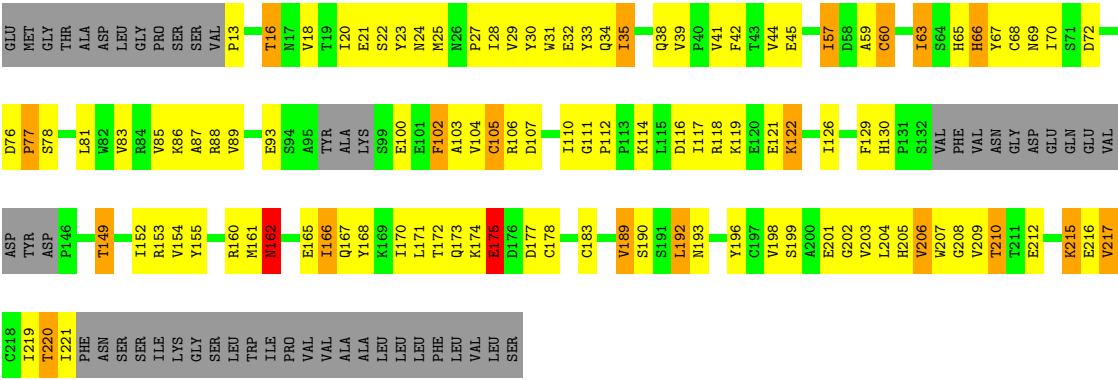
• Molecule 2: INTERFERON-GAMMA RECEPTOR ALPHA CHAIN

Chain D: 



• Molecule 2: INTERFERON-GAMMA RECEPTOR ALPHA CHAIN

Chain E:



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	199.30Å 114.65Å 74.34Å 90.00° 116.27° 90.00°	Depositor
Resolution (Å)	6.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.90)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.237 , 0.302	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6905	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

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	0.71	0/1064	0.96	5/1424 (0.4%)
1	B	0.70	0/1062	0.88	2/1421 (0.1%)
2	C	0.81	1/1699 (0.1%)	1.02	7/2312 (0.3%)
2	D	0.67	0/1653	0.95	4/2249 (0.2%)
2	E	0.64	0/1571	0.86	1/2134 (0.0%)
All	All	0.71	1/7049 (0.0%)	0.94	19/9540 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
2	D	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	89	VAL	CB-CG2	-5.65	1.41	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	LEU	CA-CB-CG	9.44	137.02	115.30
1	B	56	LEU	CA-CB-CG	8.53	134.92	115.30
2	C	90	GLY	N-CA-C	-8.13	92.77	113.10
2	D	121	GLU	N-CA-C	7.66	131.69	111.00
2	D	13	PRO	N-CA-C	6.96	130.21	112.10
2	C	194	SER	N-CA-C	6.94	129.73	111.00
1	A	19	HIS	N-CA-CB	-6.01	99.78	110.60
2	C	137	GLY	N-CA-C	-5.70	98.85	113.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	HIS	C-N-CA	5.59	135.68	121.70
2	D	221	ILE	N-CA-C	5.49	125.83	111.00
1	A	18	GLY	N-CA-C	-5.47	99.42	113.10
2	C	89	VAL	CG1-CB-CG2	-5.45	102.18	110.90
2	C	92	LYS	CA-C-N	-5.42	105.28	117.20
2	E	190	SER	N-CA-C	5.31	125.34	111.00
1	A	11	LEU	CA-CB-CG	5.30	127.48	115.30
2	D	81	LEU	CA-CB-CG	5.21	127.29	115.30
1	B	11	LEU	CA-CB-CG	5.18	127.21	115.30
2	C	193	ASN	N-CA-C	5.11	124.80	111.00
2	C	81	LEU	CA-CB-CG	5.11	127.06	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	96	TYR	Sidechain
2	D	205	HIS	Mainchain

5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1046	0	1048	80	0
1	B	1044	0	1043	89	0
2	C	1661	0	1593	136	0
2	D	1617	0	1557	125	0
2	E	1537	0	1488	90	0
All	All	6905	0	6729	468	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 34.

All (468) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:12:VAL:HB	2:D:13:PRO:HD2	1.37	1.07
1:B:1:GLN:HB2	1:B:5:VAL:HG21	1.45	0.98
2:C:205:HIS:HD2	2:C:206:VAL:HG22	1.32	0.92
2:D:149:THR:O	2:D:205:HIS:HB3	1.69	0.91
2:D:169:LYS:O	2:D:170:ILE:HG13	1.73	0.89
2:E:103:ALA:HB3	2:E:106:ARG:HB3	1.56	0.88
2:D:220:THR:HG22	2:D:221:ILE:H	1.40	0.87
2:E:78:SER:HA	2:E:103:ALA:HB1	1.58	0.85
2:E:16:THR:HG23	2:E:32:GLU:HB2	1.58	0.85
1:A:113:LEU:HD21	1:B:73:ILE:HD13	1.60	0.84
2:E:130:HIS:HE1	2:E:183:CYS:SG	2.01	0.83
1:A:91:ASP:O	1:A:95:LEU:HD12	1.80	0.82
2:E:44:VAL:HB	2:E:60:CYS:SG	2.21	0.81
2:C:149:THR:O	2:C:205:HIS:HB3	1.81	0.80
2:C:88:ARG:O	2:C:89:VAL:HG23	1.81	0.80
2:E:44:VAL:HG12	2:E:59:ALA:HB3	1.62	0.79
1:A:73:ILE:HD13	1:B:113:LEU:HD21	1.65	0.79
2:E:106:ARG:HD2	2:E:207:TRP:CE2	2.19	0.78
1:B:1:GLN:HB2	1:B:5:VAL:CG2	2.14	0.78
2:E:78:SER:HA	2:E:103:ALA:CB	2.14	0.77
2:C:194:SER:OG	2:C:221:ILE:HB	1.84	0.77
2:D:12:VAL:CB	2:D:13:PRO:HD2	2.10	0.77
1:B:91:ASP:O	1:B:95:LEU:HD12	1.85	0.76
1:B:27:THR:HG22	2:D:49:TYR:HE2	1.51	0.75
2:D:130:HIS:HE1	2:D:183:CYS:SG	2.10	0.75
1:A:12:LYS:NZ	1:B:111:HIS:CD2	2.55	0.75
1:A:111:HIS:CD2	1:B:12:LYS:NZ	2.56	0.74
2:D:170:ILE:HD11	2:D:185:LEU:HD12	1.70	0.74
2:E:25:MET:HG2	2:E:104:VAL:HG12	1.69	0.74
2:E:204:LEU:HD12	2:E:209:VAL:HB	1.69	0.74
1:A:39:GLU:OE2	1:B:122:PRO:HB3	1.88	0.74
2:E:204:LEU:O	2:E:208:GLY:HA2	1.88	0.73
2:C:168:TYR:CD1	2:C:185:LEU:HD11	2.23	0.73
2:E:162:ASN:HB3	2:E:193:ASN:ND2	2.03	0.73
2:C:194:SER:CB	2:C:221:ILE:H	2.01	0.73
2:C:170:ILE:HD11	2:C:185:LEU:HD12	1.71	0.72
2:E:112:PRO:HD3	2:E:212:GLU:HB2	1.72	0.72
2:E:171:LEU:O	2:E:175:GLU:HB3	1.89	0.72
1:A:18:GLY:O	1:A:19:HIS:HB2	1.88	0.72
2:C:130:HIS:HE1	2:C:183:CYS:SG	2.13	0.71
2:D:195:GLN:HA	2:D:219:ILE:O	1.89	0.71
2:C:205:HIS:CD2	2:C:206:VAL:HG22	2.21	0.70
2:C:189:VAL:HG13	2:C:221:ILE:HD12	1.72	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:117:ILE:HG12	2:D:219:ILE:HD12	1.72	0.70
2:C:55:GLU:HG3	2:C:56:TRP:O	1.92	0.70
2:D:23:TYR:CE2	2:D:24:ASN:ND2	2.60	0.70
1:B:99:SER:HB3	1:B:102:ASP:HB2	1.73	0.70
2:D:161:MET:HG2	2:D:193:ASN:ND2	2.07	0.69
1:A:20:SER:OG	2:C:98:LYS:HD2	1.92	0.69
2:D:117:ILE:HD13	2:D:219:ILE:HB	1.75	0.69
2:D:220:THR:HG22	2:D:221:ILE:N	2.08	0.68
1:A:122:PRO:HA	1:B:39:GLU:OE2	1.94	0.68
2:E:35:ILE:H	2:E:35:ILE:HD13	1.57	0.68
1:B:57:PHE:O	1:B:61:LYS:HD3	1.94	0.68
2:C:112:PRO:HD3	2:C:212:GLU:HB2	1.76	0.68
2:C:161:MET:HG2	2:C:162:ASN:H	1.59	0.68
2:D:110:ILE:O	2:D:212:GLU:HG3	1.93	0.67
2:D:81:LEU:HD12	2:D:102:PHE:HB3	1.75	0.67
2:C:171:LEU:HD23	2:C:174:LYS:HE3	1.74	0.67
2:E:114:LYS:O	2:E:129:PHE:HD1	1.78	0.67
2:D:44:VAL:HG12	2:D:59:ALA:HB3	1.76	0.67
2:C:40:PRO:HA	2:C:89:VAL:CG2	2.25	0.67
2:C:91:GLN:C	2:C:92:LYS:HD3	2.15	0.67
2:C:44:VAL:HG12	2:C:59:ALA:HB3	1.77	0.67
2:D:195:GLN:HE21	2:D:195:GLN:HA	1.58	0.67
2:D:195:GLN:NE2	2:D:195:GLN:HA	2.10	0.66
2:C:16:THR:HG23	2:C:32:GLU:HB2	1.76	0.66
2:C:23:TYR:CE2	2:C:24:ASN:ND2	2.63	0.66
1:B:27:THR:HG22	2:D:49:TYR:CE2	2.31	0.66
1:A:99:SER:HB3	1:A:102:ASP:HB2	1.77	0.66
2:C:171:LEU:O	2:C:175:GLU:HB3	1.95	0.66
1:A:114:ILE:HD11	1:B:8:ALA:HB3	1.78	0.66
2:D:16:THR:HG23	2:D:32:GLU:HB2	1.76	0.65
2:C:119:LYS:NZ	2:C:221:ILE:HG23	2.11	0.65
2:E:106:ARG:O	2:E:209:VAL:HG21	1.96	0.65
2:C:81:LEU:HD12	2:C:102:PHE:HB3	1.77	0.65
1:B:57:PHE:HB3	1:B:70:VAL:HG11	1.79	0.64
2:E:130:HIS:CE1	2:E:183:CYS:SG	2.88	0.64
2:D:161:MET:CG	2:D:193:ASN:ND2	2.61	0.64
2:E:20:ILE:HD11	2:E:83:VAL:HG12	1.78	0.64
2:C:115:LEU:HD13	2:C:198:VAL:HG12	1.79	0.64
2:C:21:GLU:O	2:C:27:PRO:HA	1.98	0.63
2:D:106:ARG:HD3	2:D:207:TRP:NE1	2.14	0.63
1:A:57:PHE:O	1:A:61:LYS:HD3	1.99	0.63
2:D:114:LYS:O	2:D:129:PHE:HD1	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:12:LYS:HZ1	1:B:111:HIS:CD2	2.16	0.63
2:D:171:LEU:O	2:D:175:GLU:HB3	1.99	0.63
2:D:115:LEU:HD21	2:D:128:ILE:HG12	1.81	0.62
2:D:21:GLU:O	2:D:27:PRO:HA	2.00	0.62
2:C:28:ILE:HD13	2:C:69:ASN:HA	1.80	0.62
2:C:161:MET:HE3	2:C:162:ASN:HB2	1.81	0.62
2:D:110:ILE:HD13	2:D:133:VAL:HG21	1.81	0.62
2:C:171:LEU:CD2	2:C:174:LYS:HE3	2.29	0.62
1:A:57:PHE:HB3	1:A:70:VAL:HG11	1.80	0.62
1:A:12:LYS:NZ	1:B:111:HIS:HD2	1.96	0.62
2:C:205:HIS:HD2	2:C:206:VAL:CG2	2.08	0.62
2:C:119:LYS:HZ1	2:C:221:ILE:HG12	1.65	0.62
2:D:20:ILE:HD11	2:D:83:VAL:HG12	1.80	0.62
2:D:23:TYR:HE2	2:D:24:ASN:ND2	1.98	0.62
2:C:44:VAL:HG23	2:C:85:VAL:HB	1.81	0.61
1:A:23:ALA:HB2	2:C:82:TRP:CZ3	2.35	0.61
2:C:23:TYR:HE2	2:C:24:ASN:ND2	1.98	0.61
1:A:111:HIS:CD2	1:B:12:LYS:HZ1	2.18	0.61
2:E:21:GLU:O	2:E:27:PRO:HA	2.01	0.61
1:A:111:HIS:HD2	1:B:12:LYS:NZ	1.98	0.61
2:E:154:VAL:HG23	2:E:203:VAL:HB	1.81	0.61
2:D:161:MET:SD	2:D:196:TYR:CE2	2.94	0.61
2:C:119:LYS:HZ3	2:C:221:ILE:HG23	1.65	0.60
2:E:166:ILE:HG12	2:E:166:ILE:O	2.01	0.60
2:E:13:PRO:N	2:E:33:TYR:HH	1.98	0.60
2:C:136:ASN:ND2	2:C:138:ASP:HA	2.16	0.60
2:C:119:LYS:CE	2:C:221:ILE:HG12	2.31	0.60
1:B:57:PHE:HB3	1:B:70:VAL:CG1	2.31	0.60
2:D:28:ILE:HD13	2:D:69:ASN:HA	1.83	0.60
1:A:82:PHE:HZ	1:A:92:PHE:CD1	2.19	0.60
2:D:23:TYR:HE2	2:D:24:ASN:HD22	1.48	0.60
1:B:82:PHE:HZ	1:B:92:PHE:CD1	2.20	0.60
2:E:112:PRO:HB3	2:E:212:GLU:O	2.02	0.60
2:C:91:GLN:CB	2:C:92:LYS:HE3	2.32	0.59
2:E:23:TYR:CE2	2:E:24:ASN:ND2	2.70	0.59
2:E:219:ILE:HG12	2:E:220:THR:H	1.66	0.59
2:E:154:VAL:HA	2:E:170:ILE:O	2.01	0.59
2:D:130:HIS:HB2	2:D:135:VAL:HG23	1.85	0.59
2:D:115:LEU:CD2	2:D:128:ILE:HG12	2.32	0.59
2:E:153:ARG:HG3	2:E:154:VAL:HG22	1.85	0.59
2:E:103:ALA:HB3	2:E:106:ARG:CB	2.31	0.59
2:C:168:TYR:HD1	2:C:185:LEU:HD11	1.64	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:27:THR:HG22	2:C:49:TYR:CE2	2.38	0.59
1:A:27:THR:HG22	2:C:49:TYR:HE2	1.66	0.59
1:A:114:ILE:HD13	1:B:5:VAL:HA	1.83	0.59
2:C:194:SER:HB3	2:C:221:ILE:H	1.66	0.59
1:A:42:ARG:HB3	1:A:46:GLN:NE2	2.18	0.58
2:C:23:TYR:HE2	2:C:24:ASN:HD22	1.50	0.58
2:C:40:PRO:HB3	2:C:89:VAL:HG21	1.85	0.58
2:C:20:ILE:HD11	2:C:83:VAL:HG12	1.85	0.58
1:B:68:LYS:O	1:B:71:GLU:HG3	2.03	0.58
2:C:165:GLU:H	2:E:215:LYS:HE3	1.67	0.58
2:C:45:GLU:HA	2:C:57:ILE:O	2.03	0.57
2:E:161:MET:SD	2:E:196:TYR:HE2	2.28	0.57
2:E:112:PRO:CD	2:E:212:GLU:HB2	2.35	0.57
1:A:30:LEU:HG	1:B:112:GLU:HB3	1.87	0.57
2:C:91:GLN:O	2:C:92:LYS:HD3	2.04	0.57
2:C:82:TRP:NE1	2:C:101:GLU:HB2	2.20	0.57
1:A:57:PHE:HB3	1:A:70:VAL:CG1	2.34	0.57
2:D:117:ILE:CD1	2:D:219:ILE:HB	2.35	0.56
2:D:112:PRO:HD3	2:D:212:GLU:HB2	1.87	0.56
2:D:35:ILE:HD13	2:D:35:ILE:H	1.70	0.56
2:D:151:TYR:HH	2:D:205:HIS:CE1	2.24	0.56
1:B:23:ALA:HB2	2:D:82:TRP:CZ3	2.40	0.56
2:D:130:HIS:CE1	2:D:183:CYS:SG	2.96	0.56
2:E:38:GLN:HG2	2:E:89:VAL:HG13	1.87	0.56
2:E:205:HIS:O	2:E:207:TRP:N	2.38	0.56
2:D:191:SER:O	2:D:193:ASN:N	2.39	0.56
2:D:82:TRP:NE1	2:D:101:GLU:HB2	2.20	0.56
1:B:41:ASP:HA	1:B:44:ILE:HG23	1.86	0.56
2:D:166:ILE:HG12	2:D:168:TYR:HE2	1.70	0.56
2:D:45:GLU:HA	2:D:57:ILE:O	2.06	0.56
2:C:80:SER:HA	2:C:102:PHE:O	2.06	0.56
2:C:27:PRO:HG2	2:C:70:ILE:HG13	1.87	0.56
2:C:28:ILE:CG2	2:C:30:TYR:HE1	2.19	0.56
1:A:114:ILE:CD1	1:B:8:ALA:HB3	2.36	0.55
2:D:170:ILE:HD11	2:D:185:LEU:CD1	2.34	0.55
2:C:119:LYS:NZ	2:C:221:ILE:HG12	2.21	0.55
2:D:195:GLN:NE2	2:D:219:ILE:O	2.39	0.55
2:C:115:LEU:CD1	2:C:198:VAL:HG12	2.36	0.55
2:C:119:LYS:HZ1	2:C:221:ILE:HA	1.72	0.55
1:B:42:ARG:HB3	1:B:46:GLN:NE2	2.21	0.55
1:A:25:ASN:O	1:B:108:LYS:HE2	2.07	0.55
2:D:166:ILE:HD11	2:D:168:TYR:OH	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:113:LEU:HG	1:A:117:MET:HE3	1.89	0.55
2:C:130:HIS:CE1	2:C:183:CYS:SG	2.99	0.54
1:B:82:PHE:CZ	1:B:92:PHE:CD1	2.95	0.54
2:E:117:ILE:HG12	2:E:219:ILE:HD12	1.89	0.54
2:E:25:MET:HG2	2:E:104:VAL:CG1	2.35	0.54
2:E:23:TYR:HE2	2:E:24:ASN:ND2	2.04	0.54
2:C:217:VAL:HG13	2:C:217:VAL:O	2.06	0.54
2:D:126:ILE:HD13	2:D:198:VAL:HG11	1.88	0.54
1:A:82:PHE:CZ	1:A:92:PHE:CD1	2.96	0.54
2:E:45:GLU:HA	2:E:57:ILE:O	2.08	0.54
2:C:89:VAL:C	2:C:91:GLN:H	2.11	0.54
2:C:118:ARG:HG3	2:C:119:LYS:N	2.22	0.54
2:D:161:MET:CE	2:D:193:ASN:HB3	2.38	0.54
2:D:44:VAL:HG23	2:D:85:VAL:HB	1.89	0.54
2:C:153:ARG:HG3	2:C:154:VAL:HG22	1.89	0.54
1:A:113:LEU:CD2	1:B:73:ILE:HD13	2.35	0.54
2:C:126:ILE:HD13	2:C:198:VAL:HG11	1.89	0.54
1:B:89:ARG:NH1	1:B:93:GLU:HG2	2.23	0.54
2:C:63:ILE:HD12	2:C:65:HIS:NE2	2.22	0.53
2:D:124:ILE:HD11	2:D:196:TYR:CD1	2.43	0.53
2:E:27:PRO:HG2	2:E:70:ILE:HG13	1.91	0.53
1:B:23:ALA:CB	2:D:49:TYR:HA	2.39	0.53
2:C:166:ILE:HG13	2:C:168:TYR:CE2	2.44	0.53
1:B:23:ALA:HB1	2:D:49:TYR:HA	1.91	0.53
2:C:166:ILE:HD11	2:C:168:TYR:HE2	1.73	0.53
2:D:63:ILE:HD12	2:D:65:HIS:NE2	2.23	0.53
1:A:68:LYS:O	1:A:71:GLU:HG3	2.09	0.53
2:D:185:LEU:O	2:D:185:LEU:HD23	2.09	0.53
2:C:89:VAL:HG12	2:C:90:GLY:N	2.24	0.53
1:A:89:ARG:NH1	1:A:93:GLU:HG2	2.23	0.53
2:C:110:ILE:O	2:C:212:GLU:HG3	2.09	0.53
1:A:48:GLN:OE1	1:B:96:THR:HG22	2.08	0.53
2:C:40:PRO:HB3	2:C:89:VAL:CG2	2.39	0.52
2:D:80:SER:HA	2:D:102:PHE:O	2.10	0.52
1:A:111:HIS:CD2	1:B:12:LYS:HZ3	2.25	0.52
1:B:61:LYS:NZ	1:B:67:GLN:HE22	2.07	0.52
2:E:25:MET:HE2	2:E:105:CYS:HA	1.92	0.52
2:D:130:HIS:HB2	2:D:135:VAL:CG2	2.39	0.52
1:B:2:ASP:O	1:B:5:VAL:HG22	2.10	0.52
2:D:153:ARG:HG3	2:D:154:VAL:HG22	1.92	0.52
2:D:166:ILE:HG12	2:D:168:TYR:CE2	2.45	0.52
2:D:48:ASN:HB3	2:D:81:LEU:HB3	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:161:MET:HE1	2:D:191:SER:HB2	1.91	0.52
1:A:42:ARG:NH1	1:B:119:GLU:O	2.42	0.52
2:C:204:LEU:HD12	2:C:209:VAL:HB	1.90	0.52
2:C:40:PRO:CA	2:C:89:VAL:CG2	2.88	0.51
1:A:9:GLU:O	1:A:12:LYS:HB3	2.10	0.51
2:C:119:LYS:HZ1	2:C:221:ILE:CG1	2.23	0.51
2:C:166:ILE:HD11	2:C:168:TYR:CE2	2.45	0.51
2:C:48:ASN:HB3	2:C:81:LEU:HB3	1.92	0.51
2:C:74:VAL:HG13	2:C:104:VAL:HG21	1.91	0.51
2:D:80:SER:HB3	2:D:101:GLU:HG3	1.92	0.51
2:C:28:ILE:HB	2:C:30:TYR:CE1	2.45	0.51
1:A:61:LYS:NZ	1:A:67:GLN:HE22	2.09	0.51
2:E:102:PHE:HA	2:E:107:ASP:OD2	2.11	0.51
2:C:34:GLN:HE22	2:C:36:MET:HG2	1.74	0.51
1:A:99:SER:C	1:A:101:THR:H	2.14	0.51
1:A:30:LEU:HG	1:B:112:GLU:OE1	2.11	0.51
2:E:28:ILE:HD13	2:E:69:ASN:HA	1.93	0.51
1:B:39:GLU:O	1:B:43:LYS:HG2	2.10	0.50
1:A:112:GLU:HB3	1:B:30:LEU:HG	1.92	0.50
1:A:97:ASN:OD1	1:A:97:ASN:N	2.44	0.50
2:E:122:LYS:O	2:E:189:VAL:HG23	2.10	0.50
2:E:126:ILE:HD13	2:E:198:VAL:HG11	1.93	0.50
1:A:41:ASP:HA	1:A:44:ILE:HG23	1.92	0.50
2:D:27:PRO:HG2	2:D:70:ILE:HG13	1.93	0.50
2:E:102:PHE:C	2:E:102:PHE:CD2	2.85	0.50
2:E:106:ARG:HD2	2:E:207:TRP:CD2	2.46	0.50
2:E:28:ILE:HA	2:E:68:CYS:O	2.11	0.50
1:A:1:GLN:NE2	1:A:5:VAL:HG21	2.26	0.50
1:A:100:VAL:HG21	1:B:55:LYS:HB2	1.94	0.50
2:E:175:GLU:HG3	2:E:177:ASP:H	1.77	0.50
2:D:191:SER:C	2:D:193:ASN:H	2.15	0.50
2:C:205:HIS:CD2	2:C:206:VAL:CG2	2.90	0.50
2:E:63:ILE:HD12	2:E:65:HIS:NE2	2.27	0.50
1:A:8:ALA:HB3	1:B:114:ILE:HD11	1.94	0.50
2:C:80:SER:HB3	2:C:101:GLU:HG3	1.94	0.49
2:D:171:LEU:HD23	2:D:174:LYS:HE3	1.94	0.49
2:C:89:VAL:C	2:C:91:GLN:N	2.65	0.49
1:B:99:SER:C	1:B:101:THR:H	2.15	0.49
1:B:29:PHE:HE2	1:B:53:TYR:OH	1.94	0.49
2:D:74:VAL:HG13	2:D:104:VAL:HG21	1.94	0.49
2:D:22:SER:HB2	2:D:27:PRO:HB3	1.93	0.49
2:D:117:ILE:HG22	2:D:217:VAL:HG22	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:161:MET:O	2:D:162:ASN:C	2.51	0.49
2:D:175:GLU:HG3	2:D:177:ASP:H	1.77	0.49
1:B:111:HIS:CE1	2:C:49:TYR:CD1	3.01	0.49
1:A:108:LYS:HE2	1:B:25:ASN:O	2.13	0.49
2:C:84:ARG:HA	2:C:97:ALA:O	2.13	0.49
2:E:22:SER:HB2	2:E:27:PRO:HB3	1.95	0.49
1:A:12:LYS:HZ3	1:B:111:HIS:CD2	2.28	0.49
2:D:84:ARG:HA	2:D:97:ALA:O	2.13	0.49
2:D:205:HIS:C	2:D:206:VAL:HG23	2.33	0.49
1:A:29:PHE:HE2	1:A:53:TYR:HH	1.59	0.49
2:E:201:GLU:HB2	2:E:210:THR:HG22	1.95	0.49
2:C:89:VAL:CG1	2:C:90:GLY:N	2.76	0.48
2:C:192:LEU:HD23	2:C:192:LEU:H	1.76	0.48
2:C:34:GLN:HE22	2:C:36:MET:CG	2.25	0.48
2:C:44:VAL:CG2	2:C:85:VAL:HB	2.43	0.48
2:C:175:GLU:HG3	2:C:177:ASP:H	1.77	0.48
2:E:42:PHE:CE2	2:E:66:HIS:CE1	3.01	0.48
2:D:167:GLN:C	2:D:168:TYR:CD2	2.87	0.48
2:C:156:ASN:HB2	2:C:201:GLU:HG2	1.95	0.48
2:D:122:LYS:O	2:D:189:VAL:HG23	2.13	0.48
1:A:39:GLU:O	1:A:43:LYS:HG2	2.14	0.48
2:D:28:ILE:CG2	2:D:30:TYR:HE1	2.26	0.48
1:A:2:ASP:O	1:A:5:VAL:HG22	2.12	0.48
2:E:31:TRP:CZ2	2:E:66:HIS:HA	2.48	0.48
2:E:85:VAL:HG22	2:E:86:LYS:N	2.29	0.48
1:B:97:ASN:N	1:B:97:ASN:OD1	2.43	0.48
1:B:104:ASN:CG	1:B:107:ARG:HH11	2.16	0.48
1:A:73:ILE:HD13	1:B:113:LEU:CD2	2.41	0.48
1:B:63:ASP:OD2	1:B:66:ILE:HG12	2.13	0.48
2:E:152:ILE:HD12	2:E:202:GLY:HA3	1.96	0.48
1:A:104:ASN:CG	1:A:107:ARG:HH11	2.17	0.48
2:C:157:VAL:HB	2:C:168:TYR:HB2	1.95	0.48
1:B:22:VAL:HG22	2:D:49:TYR:HE1	1.79	0.47
2:D:102:PHE:CE1	2:D:107:ASP:HB2	2.48	0.47
2:C:170:ILE:HD11	2:C:185:LEU:CD1	2.41	0.47
1:A:96:THR:HG22	1:B:48:GLN:OE1	2.14	0.47
2:D:153:ARG:HG3	2:D:154:VAL:N	2.28	0.47
2:C:161:MET:O	2:C:162:ASN:C	2.53	0.47
2:C:44:VAL:HB	2:C:60:CYS:SG	2.55	0.47
2:C:26:ASN:HB2	2:C:71:SER:OG	2.14	0.47
2:C:168:TYR:CE1	2:C:185:LEU:HD21	2.50	0.47
1:A:44:ILE:HG22	1:B:43:LYS:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:110:ILE:CG2	2:D:111:GLY:N	2.78	0.47
2:D:28:ILE:HB	2:D:30:TYR:CE1	2.50	0.47
2:D:166:ILE:HD11	2:D:168:TYR:CZ	2.50	0.47
1:B:87:LYS:O	1:B:90:ASP:N	2.48	0.47
2:C:57:ILE:HD13	2:C:58:ASP:H	1.80	0.47
2:D:158:TYR:CD2	2:D:167:GLN:HG2	2.50	0.47
2:E:149:THR:O	2:E:205:HIS:HB3	2.15	0.46
1:A:112:GLU:OE1	1:B:30:LEU:HG	2.15	0.46
2:C:110:ILE:HD12	2:C:134:PHE:HZ	1.80	0.46
2:D:204:LEU:HD12	2:D:209:VAL:HB	1.97	0.46
2:E:44:VAL:HG23	2:E:85:VAL:HB	1.96	0.46
2:C:40:PRO:HA	2:C:89:VAL:HG22	1.97	0.46
1:A:55:LYS:HB2	1:B:100:VAL:HG21	1.98	0.46
1:A:42:ARG:HB3	1:A:46:GLN:HE21	1.80	0.46
2:C:92:LYS:N	2:C:92:LYS:HD3	2.30	0.46
2:C:119:LYS:HZ1	2:C:221:ILE:CA	2.28	0.46
1:A:94:LYS:HB2	1:A:94:LYS:NZ	2.30	0.46
2:E:29:VAL:O	2:E:67:TYR:HA	2.14	0.46
2:D:26:ASN:HB2	2:D:71:SER:OG	2.15	0.46
2:C:205:HIS:CG	2:C:206:VAL:H	2.34	0.46
2:C:42:PHE:O	2:C:62:ASN:HA	2.15	0.46
1:A:114:ILE:HG23	1:B:5:VAL:HG12	1.97	0.46
1:B:46:GLN:O	1:B:50:VAL:HG23	2.16	0.46
2:D:44:VAL:HB	2:D:60:CYS:SG	2.55	0.46
2:E:63:ILE:HA	2:E:63:ILE:HD13	1.74	0.46
1:A:58:LYS:C	1:A:60:PHE:H	2.19	0.46
2:C:119:LYS:HZ1	2:C:221:ILE:CB	2.29	0.45
2:E:161:MET:SD	2:E:196:TYR:CE2	3.07	0.45
1:B:58:LYS:C	1:B:60:PHE:H	2.18	0.45
1:A:125:LYS:O	1:A:126:THR:HB	2.17	0.45
2:E:154:VAL:CG2	2:E:203:VAL:HB	2.47	0.45
2:C:153:ARG:HG3	2:C:154:VAL:N	2.32	0.45
2:E:202:GLY:O	2:E:210:THR:HA	2.17	0.45
1:A:33:LEU:HA	1:A:33:LEU:HD12	1.74	0.45
2:E:172:THR:HA	2:E:178:CYS:SG	2.56	0.45
2:D:205:HIS:O	2:D:206:VAL:HG23	2.17	0.45
2:E:41:VAL:O	2:E:87:ALA:HA	2.17	0.45
1:A:119:GLU:HG2	1:B:42:ARG:HH12	1.81	0.45
1:B:120:LEU:HA	1:B:120:LEU:HD23	1.71	0.45
2:C:85:VAL:HG22	2:C:86:LYS:N	2.31	0.45
2:C:20:ILE:HD12	2:C:102:PHE:HB2	1.98	0.45
2:E:215:LYS:HD3	2:E:215:LYS:HA	1.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:C:149:THR:O	2:C:205:HIS:CB	2.59	0.45
2:D:178:CYS:HA	2:D:183:CYS:HA	1.99	0.45
1:B:9:GLU:O	1:B:12:LYS:HB3	2.17	0.45
1:A:29:PHE:HE2	1:A:53:TYR:OH	2.00	0.45
2:C:112:PRO:CD	2:C:212:GLU:HB2	2.45	0.44
2:D:115:LEU:HD13	2:D:198:VAL:HG12	1.99	0.44
2:D:57:ILE:HD13	2:D:58:ASP:H	1.82	0.44
2:D:80:SER:HB3	2:D:101:GLU:CG	2.47	0.44
2:D:161:MET:CE	2:D:191:SER:HB2	2.47	0.44
2:C:115:LEU:HD21	2:C:128:ILE:HG12	1.99	0.44
1:B:29:PHE:HE2	1:B:53:TYR:CZ	2.35	0.44
2:C:130:HIS:HA	2:C:155:TYR:OH	2.18	0.44
2:E:88:ARG:HA	2:E:93:GLU:HA	1.99	0.44
2:D:130:HIS:HA	2:D:155:TYR:OH	2.16	0.44
1:B:55:LYS:O	1:B:58:LYS:HB3	2.16	0.44
1:B:1:GLN:HE21	1:B:1:GLN:HB3	1.60	0.44
1:A:87:LYS:HE2	1:A:87:LYS:HB3	1.71	0.44
2:C:114:LYS:O	2:C:129:PHE:HD1	2.00	0.44
2:C:80:SER:HB3	2:C:101:GLU:CG	2.48	0.44
2:C:136:ASN:HD21	2:C:138:ASP:HA	1.82	0.44
1:A:1:GLN:HE21	1:A:1:GLN:HA	1.82	0.44
2:C:192:LEU:HD22	2:C:192:LEU:HA	1.84	0.44
2:E:44:VAL:CG2	2:E:85:VAL:HB	2.48	0.43
2:D:127:ASP:OD1	2:D:182:GLN:NE2	2.51	0.43
1:B:94:LYS:NZ	1:B:94:LYS:HB2	2.33	0.43
2:C:166:ILE:CD1	2:C:168:TYR:HE2	2.30	0.43
1:A:5:VAL:HA	1:B:114:ILE:HD13	2.00	0.43
2:D:197:CYS:HA	2:D:218:CYS:HA	1.99	0.43
2:C:168:TYR:CD1	2:C:185:LEU:HD21	2.52	0.43
2:D:112:PRO:CD	2:D:212:GLU:HB2	2.49	0.43
2:E:28:ILE:HG22	2:E:68:CYS:H	1.84	0.43
1:B:19:HIS:CE1	1:B:21:ASP:OD2	2.71	0.43
2:C:40:PRO:CB	2:C:89:VAL:CG2	2.96	0.43
1:B:87:LYS:HB3	1:B:87:LYS:HE2	1.71	0.43
1:B:19:HIS:HE1	1:B:21:ASP:OD2	2.02	0.43
2:E:77:PRO:O	2:E:103:ALA:HB1	2.18	0.43
2:C:161:MET:SD	2:C:196:TYR:CE2	3.11	0.43
2:E:153:ARG:HG3	2:E:154:VAL:N	2.33	0.43
2:C:65:HIS:HB2	2:C:66:HIS:H	1.74	0.43
2:E:205:HIS:HD2	2:E:206:VAL:HG23	1.83	0.43
1:B:17:ALA:O	1:B:22:VAL:HG11	2.18	0.43
1:B:64:GLN:HG3	1:B:65:SER:N	2.32	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:76:ASP:O	2:D:78:SER:N	2.51	0.43
2:E:160:ARG:NH2	2:E:216:GLU:OE2	2.51	0.43
1:B:44:ILE:HG21	1:B:44:ILE:HD13	1.73	0.43
2:C:166:ILE:CG1	2:C:168:TYR:HE2	2.31	0.43
2:D:44:VAL:CG2	2:D:85:VAL:HB	2.48	0.43
2:D:167:GLN:C	2:D:168:TYR:HD2	2.22	0.43
2:E:167:GLN:O	2:E:168:TYR:CD2	2.72	0.43
1:A:32:ILE:HA	1:A:35:ASN:ND2	2.34	0.43
2:C:82:TRP:HE1	2:C:101:GLU:HB2	1.84	0.43
1:B:41:ASP:O	1:B:42:ARG:C	2.58	0.42
2:D:126:ILE:HD11	2:D:198:VAL:HG21	2.01	0.42
2:E:23:TYR:HE2	2:E:24:ASN:HD22	1.66	0.42
2:E:42:PHE:N	2:E:63:ILE:O	2.51	0.42
2:E:76:ASP:C	2:E:78:SER:H	2.23	0.42
1:A:64:GLN:HG3	1:A:65:SER:N	2.34	0.42
2:E:217:VAL:O	2:E:217:VAL:HG13	2.19	0.42
2:E:171:LEU:HD23	2:E:174:LYS:HG3	2.00	0.42
1:B:99:SER:C	1:B:101:THR:N	2.72	0.42
1:B:39:GLU:CD	1:B:43:LYS:HE2	2.40	0.42
1:A:99:SER:C	1:A:101:THR:N	2.72	0.42
2:E:77:PRO:O	2:E:104:VAL:N	2.52	0.42
1:B:102:ASP:HB3	1:B:105:VAL:HB	2.01	0.42
2:D:193:ASN:C	2:D:193:ASN:ND2	2.73	0.42
2:D:171:LEU:CD2	2:D:174:LYS:HE3	2.49	0.42
2:C:165:GLU:O	2:E:215:LYS:HG3	2.18	0.42
2:C:42:PHE:N	2:C:63:ILE:O	2.52	0.42
2:C:145:ASP:N	2:C:146:PRO:HD3	2.34	0.42
2:D:20:ILE:HD12	2:D:102:PHE:HB2	2.00	0.42
2:D:45:GLU:O	2:D:83:VAL:HG23	2.19	0.42
1:B:42:ARG:HB3	1:B:46:GLN:HE21	1.84	0.42
2:E:220:THR:HG23	2:E:220:THR:O	2.19	0.42
2:C:154:VAL:HG23	2:C:203:VAL:HB	2.01	0.42
2:E:18:VAL:HA	2:E:30:TYR:O	2.19	0.42
1:B:32:ILE:HA	1:B:35:ASN:ND2	2.35	0.42
2:D:151:TYR:OH	2:D:205:HIS:CE1	2.72	0.42
2:E:102:PHE:HD2	2:E:102:PHE:C	2.22	0.42
1:A:55:LYS:O	1:A:58:LYS:HB3	2.20	0.42
2:D:156:ASN:HB2	2:D:201:GLU:HG2	2.02	0.42
2:E:130:HIS:HA	2:E:155:TYR:OH	2.20	0.42
2:C:166:ILE:CD1	2:C:168:TYR:CE2	3.03	0.42
2:C:166:ILE:CG1	2:C:168:TYR:CE2	3.03	0.42
2:E:28:ILE:HB	2:E:30:TYR:CE1	2.55	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:149:THR:HB	2:D:205:HIS:HD2	1.85	0.42
2:D:85:VAL:HG22	2:D:86:LYS:N	2.35	0.42
1:B:63:ASP:O	1:B:67:GLN:HG2	2.20	0.42
1:A:8:ALA:HB3	1:B:114:ILE:CD1	2.50	0.41
2:C:45:GLU:O	2:C:83:VAL:HG23	2.20	0.41
2:D:72:ASP:O	2:D:73:HIS:ND1	2.53	0.41
2:D:38:GLN:HG2	2:D:89:VAL:HG13	2.01	0.41
2:C:22:SER:HB2	2:C:27:PRO:HB3	2.02	0.41
2:E:173:GLN:O	2:E:175:GLU:N	2.54	0.41
2:C:161:MET:HG3	2:C:196:TYR:CE2	2.55	0.41
1:A:43:LYS:HB3	1:B:44:ILE:HG22	2.02	0.41
2:C:110:ILE:HD13	2:C:133:VAL:HG21	2.02	0.41
2:D:161:MET:SD	2:D:193:ASN:HB3	2.61	0.41
2:C:171:LEU:HD23	2:C:174:LYS:HG3	2.03	0.41
2:D:126:ILE:CD1	2:D:198:VAL:HG21	2.51	0.41
2:D:63:ILE:HD13	2:D:63:ILE:HA	1.78	0.41
2:C:33:TYR:HD1	2:C:33:TYR:HA	1.73	0.41
1:B:61:LYS:HA	1:B:67:GLN:OE1	2.21	0.41
2:C:171:LEU:HD12	2:C:171:LEU:N	2.36	0.41
2:E:219:ILE:HG12	2:E:220:THR:N	2.35	0.41
2:D:201:GLU:HB2	2:D:210:THR:HG22	2.03	0.41
1:A:4:TYR:CD1	1:B:117:MET:CE	3.04	0.41
2:D:77:PRO:O	2:D:105:CYS:HB2	2.21	0.41
1:A:106:GLN:HG2	1:A:106:GLN:H	1.70	0.41
2:C:72:ASP:O	2:C:73:HIS:ND1	2.54	0.41
2:D:82:TRP:HE1	2:D:101:GLU:HB2	1.84	0.41
2:D:102:PHE:CE1	2:D:107:ASP:CB	3.04	0.41
2:D:182:GLN:HB2	2:D:183:CYS:H	1.70	0.41
2:C:110:ILE:CD1	2:C:134:PHE:CZ	3.04	0.41
2:C:127:ASP:OD1	2:C:182:GLN:NE2	2.54	0.41
2:D:154:VAL:HA	2:D:170:ILE:O	2.21	0.40
2:D:185:LEU:C	2:D:185:LEU:HD23	2.41	0.40
2:E:78:SER:HA	2:E:103:ALA:HB2	2.00	0.40
2:D:20:ILE:HG22	2:D:21:GLU:N	2.36	0.40
2:C:102:PHE:CE1	2:C:107:ASP:HB2	2.57	0.40
2:C:124:ILE:HD13	2:C:124:ILE:HG21	1.91	0.40
2:C:76:ASP:O	2:C:78:SER:N	2.54	0.40
2:D:43:THR:OG1	2:D:61:ILE:HG13	2.21	0.40
1:A:119:GLU:HG2	1:B:42:ARG:NH1	2.35	0.40
1:A:114:ILE:HG22	2:D:206:VAL:HG11	2.02	0.40
1:A:108:LYS:O	1:A:111:HIS:HB3	2.21	0.40
2:D:114:LYS:HB2	2:D:129:PHE:HB2	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:42:PHE:N	2:D:63:ILE:O	2.55	0.40
2:E:65:HIS:H	2:E:65:HIS:CD2	2.38	0.40
1:A:87:LYS:O	1:A:90:ASP:N	2.54	0.40
1:A:87:LYS:NZ	1:B:35:ASN:OD1	2.55	0.40
2:E:119:LYS:NZ	2:E:221:ILE:HA	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	125/134 (93%)	99 (79%)	20 (16%)	6 (5%)	4	12
1	B	125/134 (93%)	105 (84%)	18 (14%)	2 (2%)	14	47
2	C	206/245 (84%)	153 (74%)	40 (19%)	13 (6%)	2	6
2	D	201/245 (82%)	154 (77%)	35 (17%)	12 (6%)	2	7
2	E	187/245 (76%)	140 (75%)	39 (21%)	8 (4%)	4	15
All	All	844/1003 (84%)	651 (77%)	152 (18%)	41 (5%)	3	12

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	30	LEU
1	B	30	LEU
2	C	91	GLN
2	C	121	GLU
2	C	162	ASN
2	C	192	LEU
2	C	194	SER
2	C	206	VAL
2	D	13	PRO
2	D	121	GLU
2	D	170	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	192	LEU
2	D	195	GLN
2	D	206	VAL
1	A	20	SER
1	A	63	ASP
2	C	191	SER
2	D	162	ASN
2	D	191	SER
2	E	111	GLY
2	E	122	LYS
2	E	162	ASN
1	A	19	HIS
2	C	80	SER
2	D	80	SER
1	A	26	GLY
1	B	26	GLY
2	C	138	ASP
2	C	175	GLU
2	D	77	PRO
2	E	192	LEU
2	E	206	VAL
2	C	77	PRO
2	D	175	GLU
2	E	189	VAL
2	E	77	PRO
2	E	175	GLU
2	D	189	VAL
2	C	170	ILE
1	A	122	PRO
2	C	189	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	117/123 (95%)	99 (85%)	18 (15%)	4	12
1	B	116/123 (94%)	101 (87%)	15 (13%)	6	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	188/223 (84%)	160 (85%)	28 (15%)	4	12
2	D	183/223 (82%)	156 (85%)	27 (15%)	4	13
2	E	177/223 (79%)	149 (84%)	28 (16%)	4	11
All	All	781/915 (85%)	665 (85%)	116 (15%)	4	12

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	10	ASN
1	A	16	ASN
1	A	34	LYS
1	A	40	SER
1	A	44	ILE
1	A	56	LEU
1	A	71	GLU
1	A	74	LYS
1	A	78	ASN
1	A	87	LYS
1	A	97	ASN
1	A	103	LEU
1	A	112	GLU
1	A	114	ILE
1	A	119	GLU
1	A	120	LEU
1	A	125	LYS
1	B	1	GLN
1	B	10	ASN
1	B	27	THR
1	B	34	LYS
1	B	40	SER
1	B	44	ILE
1	B	56	LEU
1	B	62	ASP
1	B	71	GLU
1	B	78	ASN
1	B	87	LYS
1	B	97	ASN
1	B	103	LEU
1	B	112	GLU
1	B	114	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	16	THR
2	C	33	TYR
2	C	34	GLN
2	C	37	PRO
2	C	39	VAL
2	C	44	VAL
2	C	55	GLU
2	C	57	ILE
2	C	60	CYS
2	C	63	ILE
2	C	66	HIS
2	C	72	ASP
2	C	81	LEU
2	C	92	LYS
2	C	118	ARG
2	C	127	ASP
2	C	131	PRO
2	C	132	SER
2	C	133	VAL
2	C	164	SER
2	C	166	ILE
2	C	175	GLU
2	C	192	LEU
2	C	193	ASN
2	C	199	SER
2	C	206	VAL
2	C	210	THR
2	C	220	THR
2	D	11	SER
2	D	16	THR
2	D	33	TYR
2	D	34	GLN
2	D	35	ILE
2	D	39	VAL
2	D	57	ILE
2	D	60	CYS
2	D	63	ILE
2	D	66	HIS
2	D	72	ASP
2	D	81	LEU
2	D	106	ARG
2	D	118	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	127	ASP
2	D	132	SER
2	D	133	VAL
2	D	148	THR
2	D	166	ILE
2	D	175	GLU
2	D	192	LEU
2	D	193	ASN
2	D	194	SER
2	D	199	SER
2	D	206	VAL
2	D	210	THR
2	D	219	ILE
2	E	16	THR
2	E	34	GLN
2	E	35	ILE
2	E	39	VAL
2	E	57	ILE
2	E	60	CYS
2	E	63	ILE
2	E	66	HIS
2	E	72	ASP
2	E	81	LEU
2	E	100	GLU
2	E	102	PHE
2	E	105	CYS
2	E	110	ILE
2	E	116	ASP
2	E	118	ARG
2	E	121	GLU
2	E	149	THR
2	E	162	ASN
2	E	165	GLU
2	E	166	ILE
2	E	175	GLU
2	E	192	LEU
2	E	199	SER
2	E	210	THR
2	E	215	LYS
2	E	217	VAL
2	E	220	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	10	ASN
1	A	16	ASN
1	A	67	GLN
1	A	106	GLN
1	A	111	HIS
1	B	1	GLN
1	B	10	ASN
1	B	67	GLN
1	B	111	HIS
2	C	34	GLN
2	C	167	GLN
2	C	173	GLN
2	C	195	GLN
2	C	205	HIS
2	D	167	GLN
2	D	173	GLN
2	D	182	GLN
2	D	184	GLN
2	D	193	ASN
2	D	195	GLN
2	E	167	GLN
2	E	173	GLN
2	E	193	ASN
2	E	205	HIS

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.