



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:25 AM UTC

PDB ID : 1FG9 / pdb_00001fg9
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 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 : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

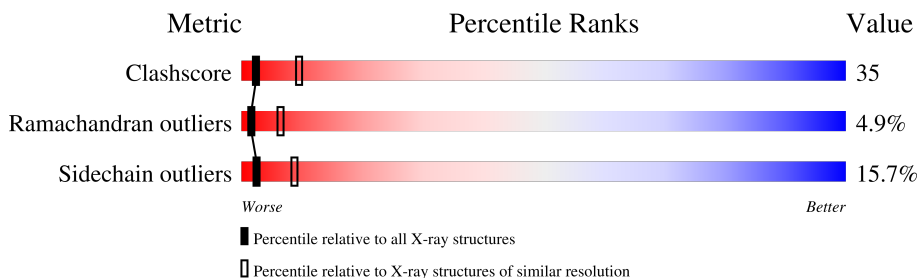
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (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 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 $\leq 5\%$.

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 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 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 methionine	UNP P01579
B	0	MET	-	initiating methionine	UNP P01579

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

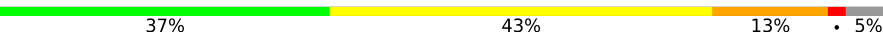
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	210	Total	C	N	O	S	0	0	0
			1661	1053	276	320	12			
2	D	205	Total	C	N	O	S	0	0	0
			1617	1025	269	311	12			
2	E	193	Total	C	N	O	S	0	0	0
			1537	972	256	297	12			

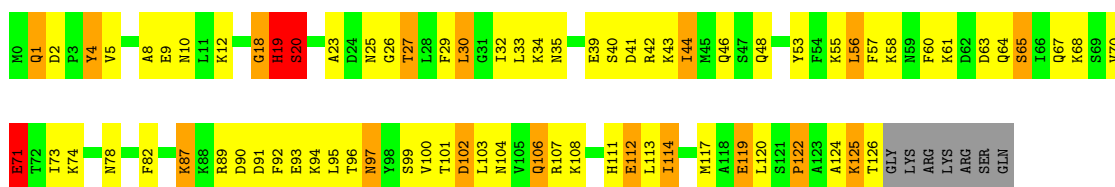
3 Residue-property plots

These plots are drawn for all protein, RNA, 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. 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. 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.

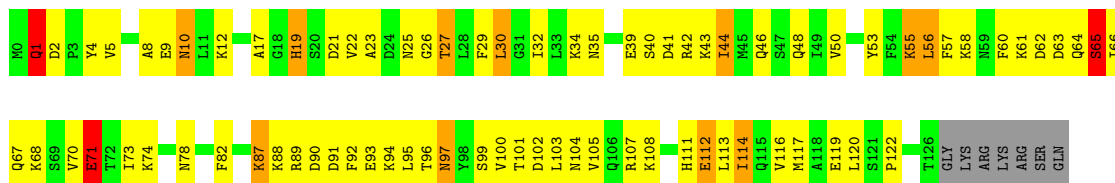
• Molecule 1: INTERFERON GAMMA

Chain A: 

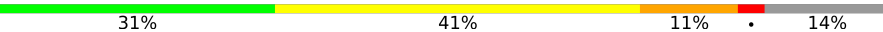


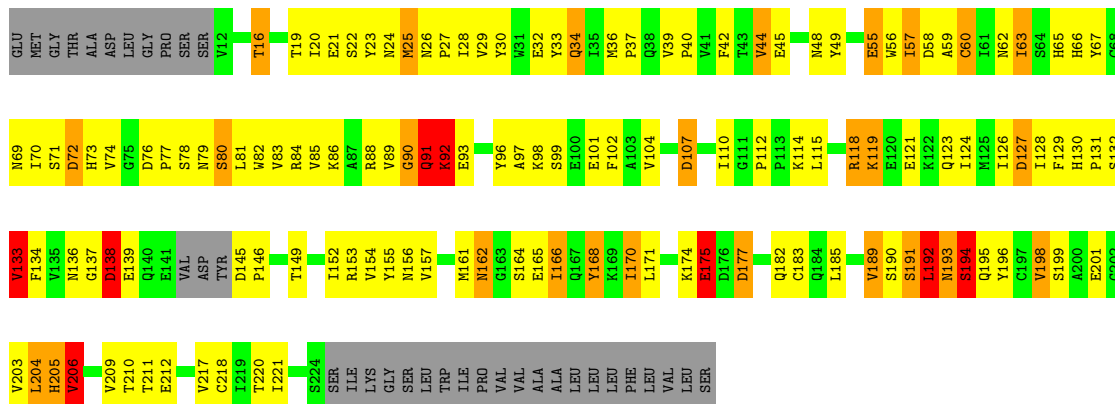
• Molecule 1: INTERFERON GAMMA

Chain B: 

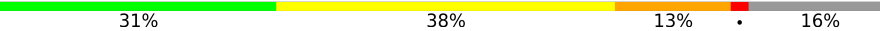


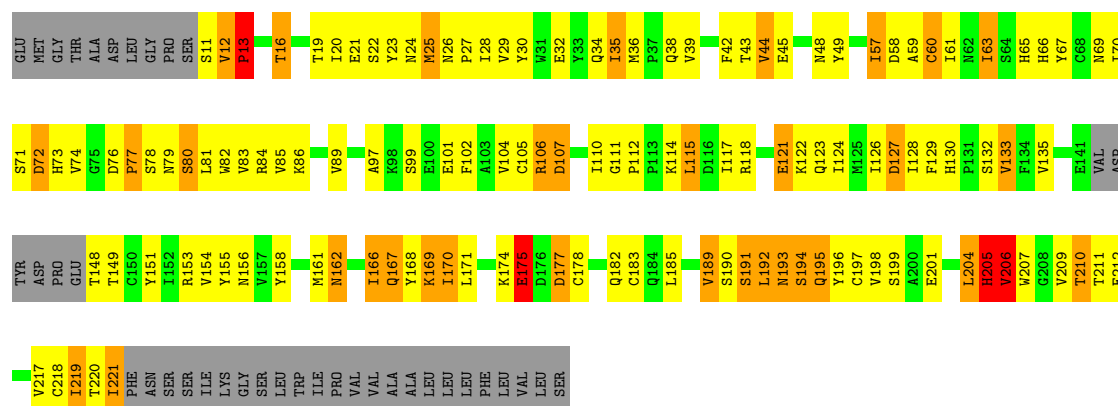
• Molecule 2: INTERFERON-GAMMA RECEPTOR ALPHA CHAIN

Chain C: 

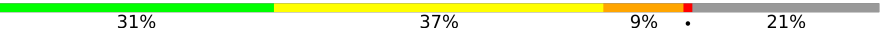


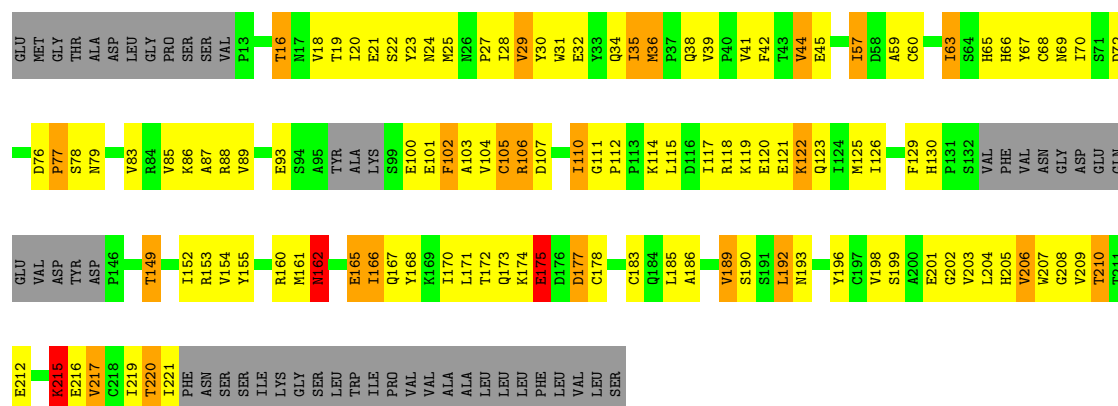
• Molecule 2: INTERFERON-GAMMA RECEPTOR ALPHA CHAIN

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 is therefore 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 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	0.89	2/1064 (0.2%)	1.28	9/1424 (0.6%)
1	B	0.81	0/1062	1.18	7/1421 (0.5%)
2	C	1.03	3/1699 (0.2%)	1.42	31/2312 (1.3%)
2	D	0.87	3/1653 (0.2%)	1.34	19/2249 (0.8%)
2	E	0.79	0/1571	1.22	11/2134 (0.5%)
All	All	0.89	8/7049 (0.1%)	1.31	77/9540 (0.8%)

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 (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	206	VAL	CA-CB	-6.89	1.45	1.54
2	D	167	GLN	CA-C	-6.40	1.44	1.53
2	C	205	HIS	CA-CB	6.20	1.61	1.53
2	D	106	ARG	CA-C	-5.33	1.46	1.52
1	A	19	HIS	CA-C	5.33	1.59	1.52
1	A	20	SER	CA-C	-5.26	1.45	1.52
2	D	12	VAL	CA-C	5.15	1.58	1.52
2	C	93	GLU	N-CA	-5.11	1.38	1.45

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	139	GLU	N-CA-C	-10.55	102.60	114.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	190	SER	N-CA-C	10.04	125.34	110.48
2	D	121	GLU	N-CA-C	9.81	131.69	110.80
2	C	193	ASN	N-CA-C	9.76	124.80	108.90
2	C	194	SER	N-CA-C	8.89	129.73	110.80
2	D	190	SER	N-CA-C	8.64	121.94	110.53
2	C	90	GLY	N-CA-C	-8.61	92.77	113.18
2	D	13	PRO	N-CA-C	8.61	130.21	112.47
2	D	12	VAL	CA-C-N	8.21	130.10	119.84
2	D	12	VAL	C-N-CA	8.21	130.10	119.84
2	E	101	GLU	N-CA-C	-8.11	99.07	110.50
2	C	190	SER	N-CA-C	8.03	120.89	110.53
2	C	25	MET	N-CA-C	7.77	120.00	110.91
2	C	92	LYS	N-CA-C	7.66	121.22	108.73
2	E	165	GLU	N-CA-C	-7.65	98.11	110.20
2	E	177	ASP	N-CA-C	-7.52	104.08	113.55
2	D	25	MET	N-CA-C	7.43	119.61	110.91
1	A	19	HIS	CA-C-N	7.40	135.68	121.54
1	A	19	HIS	C-N-CA	7.40	135.68	121.54
2	C	107	ASP	N-CA-C	7.40	122.30	113.28
2	D	107	ASP	N-CA-C	7.38	122.29	113.28
1	B	4	TYR	N-CA-C	7.08	120.03	111.82
2	D	115	LEU	N-CA-C	6.94	121.62	109.96
2	D	123	GLN	N-CA-C	6.90	120.90	108.69
2	E	115	LEU	N-CA-C	6.84	120.61	110.48
2	C	177	ASP	N-CA-C	-6.78	105.14	113.41
1	B	71	GLU	N-CA-C	-6.74	103.17	111.40
2	D	204	LEU	N-CA-C	6.72	120.98	110.17
2	D	177	ASP	N-CA-C	-6.68	105.26	113.41
1	A	4	TYR	N-CA-C	6.62	119.49	111.82
2	E	110	ILE	N-CA-C	-6.50	99.10	108.53
2	C	218	CYS	N-CA-C	6.50	119.54	109.60
1	A	19	HIS	N-CA-CB	-6.33	99.78	110.49
2	D	194	SER	N-CA-C	-6.21	101.02	110.14
2	D	79	ASN	N-CA-C	6.20	118.90	107.99
2	C	168	TYR	CB-CA-C	-6.20	103.30	111.42
2	D	169	LYS	N-CA-C	-6.15	100.19	109.79
2	E	120	GLU	N-CA-C	-6.08	98.36	108.75
2	C	79	ASN	N-CA-C	6.05	119.35	107.98
2	C	137	GLY	N-CA-C	-6.05	98.85	113.18
2	C	119	LYS	N-CA-C	6.04	118.48	108.99
2	C	206	VAL	N-CA-C	5.98	121.78	109.34
2	C	192	LEU	N-CA-C	5.95	123.46	110.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	LEU	CA-CB-CG	5.92	137.02	116.30
2	C	123	GLN	N-CA-C	5.91	119.15	108.69
2	E	123	GLN	N-CA-C	5.90	119.14	108.69
1	A	18	GLY	N-CA-C	-5.81	99.42	113.18
2	C	195	GLN	N-CA-C	-5.80	98.44	110.80
2	D	211	THR	N-CA-C	-5.80	101.37	110.36
1	A	71	GLU	N-CA-C	-5.79	104.88	111.14
2	D	99	SER	N-CA-C	-5.79	102.73	110.55
2	E	79	ASN	N-CA-C	5.78	118.16	107.99
2	D	205	HIS	CA-C-N	5.60	132.05	121.97
2	D	205	HIS	C-N-CA	5.60	132.05	121.97
2	C	99	SER	N-CA-C	-5.56	103.05	110.55
2	C	92	LYS	CA-C-O	5.53	126.28	120.36
2	C	138	ASP	N-CA-C	5.47	122.44	110.80
2	C	192	LEU	CA-C-N	-5.45	115.30	122.99
2	C	192	LEU	C-N-CA	-5.45	115.30	122.99
1	B	10	ASN	N-CA-C	-5.43	105.26	111.07
1	B	56	LEU	CA-CB-CG	5.32	134.92	116.30
2	C	204	LEU	N-CA-C	5.31	118.37	110.52
2	D	221	ILE	N-CA-C	5.29	125.83	111.00
2	C	205	HIS	N-CA-C	-5.24	101.58	109.60
2	E	106	ARG	N-CA-C	5.24	116.80	111.14
2	C	211	THR	N-CA-C	-5.23	101.63	109.79
1	B	65	SER	N-CA-C	5.19	118.39	111.75
2	C	198	VAL	N-CA-C	5.18	116.43	108.71
2	C	91	GLN	N-CA-C	-5.14	99.86	110.80
1	B	1	GLN	N-CA-C	5.13	117.66	110.23
2	C	133	VAL	N-CA-C	5.09	115.52	110.23
1	A	124	ALA	N-CA-C	5.05	116.12	107.28
1	B	55	LYS	N-CA-C	-5.03	105.49	110.97
2	C	193	ASN	CA-C-N	5.02	131.12	121.54
2	C	193	ASN	C-N-CA	5.02	131.12	121.54
1	A	102	ASP	N-CA-C	-5.01	100.13	110.80
2	E	215	LYS	N-CA-C	-5.00	103.45	110.50

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 Too-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 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	1046	0	1048	82	0
1	B	1044	0	1043	91	0
2	C	1661	0	1593	139	0
2	D	1617	0	1557	128	0
2	E	1537	0	1488	95	0
All	All	6905	0	6729	483	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 35.

All (483) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2: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:D:161:MET:HE1	2:D:191:SER:HB2	1.53	0.88
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:C:194:SER:OG	2:C:221:ILE:HB	1.84	0.77
2:E:78:SER:HA	2:E:103:ALA:CB	2.14	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:12:LYS:HZ1	1:B:111:HIS:CD2	2.03	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:C:168:TYR:CD1	2:C:185:LEU:HD11	2.23	0.73
2:E:204:LEU:O	2:E:208:GLY:HA2	1.88	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:161:MET:HE1	2:C:191:SER:HB2	1.70	0.72
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
1:A:18:GLY:O	1:A:19:HIS:HB2	1.88	0.72
2:E:171:LEU:O	2:E:175:GLU:HB3	1.89	0.72
2:C:119:LYS:HZ1	2:C:221:ILE:CG1	2.02	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:91:GLN:C	2:C:92:LYS:HD3	2.15	0.71
2:C:189:VAL:HG13	2:C:221:ILE:HD12	1.72	0.70
2:C:205:HIS:CD2	2:C:206:VAL:HG22	2.21	0.70
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
1:B:99:SER:HB3	1:B:102:ASP:HB2	1.73	0.70
2:D:23:TYR:CE2	2:D:24:ASN:ND2	2.60	0.70
1:A:20:SER:OG	2:C:98:LYS:HD2	1.92	0.69
2:D:161:MET:HG2	2:D:193:ASN:ND2	2.07	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
1:B:57:PHE:O	1:B:61:LYS:HD3	1.94	0.68
2:E:35:ILE:HD13	2:E:35:ILE:H	1.57	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:C:171:LEU:HD23	2:C:174:LYS:HE3	1.74	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:81:LEU:HD12	2:D:102:PHE:HB3	1.75	0.67
2:D:44:VAL:HG12	2:D:59:ALA:HB3	1.76	0.67
2:E:114:LYS:O	2:E:129:PHE:HD1	1.78	0.67
2:C:40:PRO:HA	2:C:89:VAL:CG2	2.25	0.67
2:C:44:VAL:HG12	2:C:59:ALA:HB3	1.77	0.67
2:D:195:GLN:HA	2:D:195:GLN:HE21	1.58	0.67
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
2:D:195:GLN:HA	2:D:195:GLN:NE2	2.10	0.66
1:A:99:SER:HB3	1:A:102:ASP:HB2	1.77	0.66
1:B:27:THR:HG22	2:D:49:TYR:CE2	2.31	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
2:C:119:LYS:HZ1	2:C:221:ILE:HG12	1.59	0.64
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
2:C:119:LYS:HZ1	2:C:221:ILE:HG23	1.62	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:C:28:ILE:HD13	2:C:69:ASN:HA	1.80	0.62
2:D:21:GLU:O	2:D:27:PRO:HA	2.00	0.62
1:A:57:PHE:HB3	1:A:70:VAL:HG11	1.80	0.62
2:C:171:LEU:CD2	2:C:174:LYS:HE3	2.29	0.62
2:D:110:ILE:HD13	2:D:133:VAL:HG21	1.81	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:166:ILE:HG12	2:E:166:ILE:O	2.01	0.60
2:C:136:ASN:ND2	2:C:138:ASP:HA	2.16	0.60
1:A:82:PHE:HZ	1:A:92:PHE:CD1	2.19	0.60
1:B:57:PHE:HB3	1:B:70:VAL:CG1	2.31	0.60
2:C:119:LYS:CE	2:C:221:ILE:HG12	2.31	0.60
2:D:28:ILE:HD13	2:D:69:ASN:HA	1.83	0.60
1:B:82:PHE:HZ	1:B:92:PHE:CD1	2.20	0.60
2:D:23:TYR:HE2	2:D:24:ASN:HD22	1.48	0.60
2:C:119:LYS:HZ1	2:C:221:ILE:CB	2.15	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:C:168:TYR:HD1	2:C:185:LEU:HD11	1.64	0.59
2:E:103:ALA:HB3	2:E:106:ARG:CB	2.31	0.59
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
2:C:89:VAL:C	2:C:91:GLN:H	2.11	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:20:ILE:HD11	2:C:83:VAL:HG12	1.85	0.58
2:C:40:PRO:HB3	2:C:89:VAL:HG21	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
1:A:30:LEU:HG	1:B:112:GLU:HB3	1.87	0.57
2:E:112:PRO:CD	2:E:212:GLU:HB2	2.35	0.57
2:C:91:GLN:O	2:C:92:LYS:HD3	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:35:ILE:HD13	2:D:35:ILE:H	1.70	0.56
2:D:112:PRO:HD3	2:D:212:GLU:HB2	1.87	0.56
2:D:117:ILE:CD1	2:D:219:ILE:HB	2.35	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:D:161:MET:HE3	2:D:193:ASN:HB3	1.87	0.56
2:E:38:GLN:HG2	2:E:89:VAL:HG13	1.87	0.56
2:C:119:LYS:HZ1	2:C:221:ILE:CG2	2.18	0.56
2:D:191:SER:O	2:D:193:ASN:N	2.39	0.56
2:E:205:HIS:O	2:E:207:TRP:N	2.38	0.56
1:B:41:ASP:HA	1:B:44:ILE:HG23	1.86	0.56
2:D:82:TRP:NE1	2:D:101:GLU:HB2	2.20	0.56
2:D:166:ILE:HG12	2:D:168:TYR:HE2	1.70	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
2:C:80:SER:HA	2:C:102:PHE:O	2.06	0.56
2:D:45:GLU:HA	2:D:57:ILE:O	2.06	0.56
1:A:114:ILE:CD1	1:B:8:ALA:HB3	2.36	0.55
2:C:119:LYS:NZ	2:C:221:ILE:HG12	2.21	0.55
2:D:170:ILE:HD11	2:D:185:LEU:CD1	2.34	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
1:A:99:SER:C	1:A:101:THR:H	2.14	0.55
1:B:99:SER:C	1:B:101:THR:H	2.15	0.55
1:A:25:ASN:O	1:B:108:LYS:HE2	2.07	0.55
1:B:42:ARG:HB3	1:B:46:GLN:NE2	2.21	0.55
2:E:102:PHE:C	2:E:102:PHE:CD2	2.85	0.55
2:D:166:ILE:HD11	2:D:168:TYR:OH	2.07	0.55
2:D:191:SER:C	2:D:193:ASN:H	2.15	0.55
1:B:82:PHE:CZ	1:B:92:PHE:CD1	2.95	0.54
2:C:130:HIS:CE1	2:C:183:CYS:SG	2.99	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
1:A:82:PHE:CZ	1:A:92:PHE:CD1	2.96	0.54
2:D:126:ILE:HD13	2:D:198:VAL:HG11	1.88	0.54
2:E:45:GLU:HA	2:E:57:ILE:O	2.08	0.54
2:C:118:ARG:HG3	2:C:119:LYS:N	2.22	0.54
2:C:217:VAL:HG13	2:C:217:VAL:O	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:161:MET:O	2:D:162:ASN:C	2.51	0.54
2:C:89:VAL:C	2:C:91:GLN:N	2.65	0.54
2:C:153:ARG:HG3	2:C:154:VAL:HG22	1.89	0.54
2:D:44:VAL:HG23	2:D:85:VAL:HB	1.89	0.54
2:D:161:MET:CE	2:D:193:ASN:HB3	2.38	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:D:205:HIS:C	2:D:206:VAL:HG23	2.33	0.54
2:C:63:ILE:HD12	2:C:65:HIS:NE2	2.22	0.53
1:A:104:ASN:CG	1:A:107:ARG:HH11	2.17	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
1:A:89:ARG:NH1	1:A:93:GLU:HG2	2.23	0.53
1:B:104:ASN:CG	1:B:107:ARG:HH11	2.16	0.53
2:C:89:VAL:HG12	2:C:90:GLY:N	2.24	0.53
2:D:185:LEU:O	2:D:185:LEU:HD23	2.09	0.53
1:A:48:GLN:OE1	1:B:96:THR:HG22	2.08	0.53
2:C:110:ILE:O	2:C:212:GLU:HG3	2.09	0.53
2:E:25:MET:HE2	2:E:105:CYS:HA	1.91	0.53
2:C:40:PRO:HB3	2:C:89:VAL:CG2	2.39	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:D:80:SER:HA	2:D:102:PHE:O	2.10	0.52
2:D:130:HIS:HB2	2:D:135:VAL:CG2	2.39	0.52
2:D:167:GLN:C	2:D:168:TYR:CD2	2.87	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:C:161:MET:O	2:C:162:ASN:C	2.53	0.52
1:A:42:ARG:NH1	1:B:119:GLU:O	2.42	0.52
2:D:48:ASN:HB3	2:D:81:LEU:HB3	1.92	0.52
2:C:204:LEU:HD12	2:C:209:VAL:HB	1.90	0.52
1:A:9:GLU:O	1:A:12:LYS:HB3	2.10	0.51
2:C:40:PRO:CA	2:C:89:VAL:CG2	2.88	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:166:ILE:HD11	2:C:168:TYR:CE2	2.45	0.51
2:C:28:ILE:HB	2:C:30:TYR:CE1	2.45	0.51
2:D:80:SER:HB3	2:D:101:GLU:HG3	1.92	0.51
1:A:61:LYS:NZ	1:A:67:GLN:HE22	2.09	0.51
2:E:36:MET:HE1	2:E:89:VAL:HG21	1.93	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: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:A:97:ASN:N	1:A:97:ASN:OD1	2.44	0.50
1:A:112:GLU:HB3	1:B:30:LEU:HG	1.92	0.50
1:B:39:GLU:O	1:B:43:LYS:HG2	2.10	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
1:A:58:LYS:C	1:A:60:PHE:H	2.19	0.50
2:D:27:PRO:HG2	2:D:70:ILE:HG13	1.93	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:28:ILE:HA	2:E:68:CYS:O	2.11	0.50
2:E:106:ARG:HD2	2:E:207:TRP:CD2	2.46	0.50
2:E:175:GLU:HG3	2:E:177:ASP:H	1.77	0.50
1:B:58:LYS:C	1:B:60:PHE:H	2.18	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
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
2:D:175:GLU:HG3	2:D:177:ASP:H	1.77	0.49
1:A:108:LYS:HE2	1:B:25:ASN:O	2.13	0.49
1:B:111:HIS:CE1	2:C:49:TYR:CD1	3.01	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
2:D:84:ARG:HA	2:D:97:ALA:O	2.13	0.49
1:A:29:PHE:HE2	1:A:53:TYR:HH	1.59	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	2:C:192:LEU:HD23	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: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:2:ASP:O	1:A:5:VAL:HG22	2.12	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
2:E:31:TRP:CZ2	2:E:66:HIS:HA	2.48	0.48
1:B:97:ASN:OD1	1:B:97:ASN:N	2.43	0.48
2:E:85:VAL:HG22	2:E:86:LYS:N	2.29	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
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
1:A:99:SER:C	1:A:101:THR:N	2.72	0.47
2:C:170:ILE:HD11	2:C:185:LEU:CD1	2.41	0.47
2:D:102:PHE:CE1	2:D:107:ASP:HB2	2.48	0.47
2:D:167:GLN:C	2:D:168:TYR:HD2	2.22	0.47
1:A:96:THR:HG22	1:B:48:GLN:OE1	2.14	0.47
1:B:41:ASP:O	1:B:42:ARG:C	2.58	0.47
2:D:153:ARG:HG3	2:D:154:VAL:N	2.28	0.47
2:E:36:MET:HE1	2:E:89:VAL:CG2	2.44	0.47
2:E:76:ASP:C	2:E:78:SER:H	2.23	0.47
2:C:26:ASN:HB2	2:C:71:SER:OG	2.14	0.47
2:C:44:VAL:HB	2:C:60:CYS:SG	2.55	0.47
2:E:125:MET:HE1	2:E:186:ALA:HB2	1.96	0.47
1:A:44:ILE:HG22	1:B:43:LYS:HB3	1.97	0.47
2:C:168:TYR:CE1	2:C:185:LEU:HD21	2.50	0.47
2:D:193:ASN:ND2	2:D:193:ASN:C	2.73	0.47
1:B:39:GLU:CD	1:B:43:LYS:HE2	2.40	0.47
1:B:87:LYS:O	1:B:90:ASP:N	2.48	0.47
2:D:28:ILE:HB	2:D:30:TYR:CE1	2.50	0.47
2:D:110:ILE:CG2	2:D:111:GLY:N	2.78	0.47
2:D:166:ILE:HD11	2:D:168:TYR:CZ	2.50	0.47
2:E:102:PHE:C	2:E:102:PHE:HD2	2.22	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:112:GLU:OE1	1:B:30:LEU:HG	2.15	0.46
2:E:149:THR:O	2:E:205:HIS:HB3	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
1:A:55:LYS:HB2	1:B:100:VAL:HG21	1.98	0.46
1:B:99:SER:C	1:B:101:THR:N	2.72	0.46
2:C:40:PRO:HA	2:C:89:VAL:HG22	1.97	0.46
2:E:44:VAL:HG23	2:E:85:VAL:HB	1.96	0.46
1:A:4:TYR:CD1	1:B:117:MET:HE3	2.51	0.46
1:A:42:ARG:HB3	1:A:46:GLN:HE21	1.80	0.46
1:A:94:LYS:NZ	1:A:94:LYS:HB2	2.30	0.46
2:D:26:ASN:HB2	2:D:71:SER:OG	2.15	0.46
2:E:29:VAL:O	2:E:67:TYR:HA	2.14	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:HD13	2:E:63:ILE:HA	1.74	0.46
1:A:125:LYS:O	1:A:126:THR:HB	2.17	0.45
2:C:25:MET:HE3	2:C:110:ILE:HD11	1.97	0.45
2:E:161:MET:SD	2:E:196:TYR:CE2	3.07	0.45
2:C:153:ARG:HG3	2:C:154:VAL:N	2.32	0.45
2:D:185:LEU:HD23	2:D:185:LEU:C	2.41	0.45
2:E:154:VAL:CG2	2:E:203:VAL:HB	2.47	0.45
2:E:202:GLY:O	2:E:210:THR:HA	2.17	0.45
1:A:33:LEU:HD12	1:A:33:LEU:HA	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:HD23	1:B:120:LEU:HA	1.71	0.45
2:D:25:MET:HE3	2:D:110:ILE:HD11	1.99	0.45
2:C:20:ILE:HD12	2:C:102:PHE:HB2	1.98	0.45
2:C:85:VAL:HG22	2:C:86:LYS:N	2.31	0.45
2:E:215:LYS:HD3	2:E:215:LYS:HA	1.51	0.45
2:C:65:HIS:C	2:C:66:HIS:HD1	2.24	0.45
1:A:29:PHE:HE2	1:A:53:TYR:OH	2.00	0.45
1:B:9:GLU:O	1:B:12:LYS:HB3	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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
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
1:B:29:PHE:HE2	1:B:53:TYR:CZ	2.35	0.44
2:C:115:LEU:HD21	2:C:128:ILE:HG12	1.99	0.44
2:D:57:ILE:HD13	2:D:58:ASP:H	1.82	0.44
2:D:67:TYR:CD2	2:D:67:TYR:C	2.95	0.44
2:D:80:SER:HB3	2:D:101:GLU:CG	2.47	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
1:B:55:LYS:O	1:B:58:LYS:HB3	2.16	0.44
2:D:130:HIS:HA	2:D:155:TYR:OH	2.16	0.44
1:A:41:ASP:O	1:A:42:ARG:C	2.56	0.44
1:A:87:LYS:HE2	1:A:87:LYS:HB3	1.71	0.44
1:B:1:GLN:HE21	1:B:1:GLN:HB3	1.60	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
1:A:117:MET:HE3	1:A:117:MET:HB2	1.57	0.44
2:C:192:LEU:HD22	2:C:192:LEU:HA	1.84	0.44
1:B:94:LYS:NZ	1:B:94:LYS:HB2	2.33	0.43
2:D:127:ASP:OD1	2:D:182:GLN:NE2	2.51	0.43
2:E:44:VAL:CG2	2:E:85:VAL:HB	2.48	0.43
1:A:5:VAL:HA	1:B:114:ILE:HD13	2.00	0.43
2:C:166:ILE:CD1	2:C:168:TYR:HE2	2.30	0.43
2:D:197:CYS:HA	2:D:218:CYS:HA	1.99	0.43
1:B:19:HIS:CE1	1:B:21:ASP:OD2	2.71	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:HE1	1:B:21:ASP:OD2	2.02	0.43
1:B:87:LYS:HE2	1:B:87:LYS:HB3	1.71	0.43
2:C:40:PRO:CB	2:C:89:VAL:CG2	2.96	0.43
2:C:161:MET:SD	2:C:196:TYR:CE2	3.11	0.43
2:E:77:PRO:O	2:E:103:ALA:HB1	2.18	0.43
2:C:65:HIS:HB2	2:C:66:HIS:H	1.74	0.43
2:E:153:ARG:HG3	2:E:154:VAL:N	2.33	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	Interatomic distance (Å)	Clash overlap (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
2:E:205:HIS:HD2	2:E:206:VAL:HG23	1.83	0.43
1:B:44:ILE:HD13	1:B:44:ILE:HG21	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
1:A:32:ILE:HA	1:A:35:ASN:ND2	2.34	0.43
2:D:65:HIS:C	2:D:66:HIS:HD1	2.26	0.43
2:E:167:GLN:O	2:E:168:TYR:CD2	2.72	0.43
2:C:82:TRP:HE1	2:C:101:GLU:HB2	1.84	0.43
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
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:102:ASP:HB3	1:B:105:VAL:HB	2.01	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:C:165:GLU:O	2:E:215:LYS:HG3	2.18	0.42
2:D:171:LEU:CD2	2:D:174:LYS:HE3	2.49	0.42
2:E:77:PRO:O	2:E:104:VAL:N	2.52	0.42
1:B:32:ILE:HA	1:B:35:ASN:ND2	2.35	0.42
1:B:42:ARG:HB3	1:B:46:GLN:HE21	1.84	0.42
2:C:154:VAL:HG23	2:C:203:VAL:HB	2.01	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
2:E:18:VAL:HA	2:E:30:TYR:O	2.19	0.42
2:E:185:LEU:HD23	2:E:185:LEU:C	2.45	0.42
2:E:220:THR:O	2:E:220:THR:HG23	2.19	0.42
1:A:55:LYS:O	1:A:58:LYS:HB3	2.20	0.42
2:D:151:TYR:OH	2:D:205:HIS:CE1	2.72	0.42
2:D:156:ASN:HB2	2:D:201:GLU:HG2	2.02	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:HG23	2:E:68:CYS:C	2.44	0.42
2:E:130:HIS:HA	2:E:155:TYR:OH	2.20	0.42
2:E:28:ILE:HB	2:E:30:TYR:CE1	2.55	0.42
1:A:91:ASP:C	1:A:95:LEU:HD12	2.42	0.42
2:D:85:VAL:HG22	2:D:86:LYS:N	2.35	0.42
2:D:149:THR:HB	2:D:205:HIS:HD2	1.85	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:38:GLN:HG2	2:D:89:VAL:HG13	2.01	0.41
2:D:72:ASP:O	2:D:73:HIS:ND1	2.53	0.41
2:D:76:ASP:C	2:D:78:SER:H	2.27	0.41
2:C:67:TYR:CD2	2:C:67:TYR:C	2.98	0.41
2:C:22:SER:HB2	2:C:27:PRO:HB3	2.02	0.41
2:C:161:MET:HG3	2:C:196:TYR:CE2	2.55	0.41
2:E:173:GLN:O	2:E:175:GLU:N	2.54	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:C:33:TYR:HD1	2:C:33:TYR:HA	1.73	0.41
2:C:171:LEU:HD23	2:C:174:LYS:HG3	2.03	0.41
2:D:63:ILE:HA	2:D:63:ILE:HD13	1.78	0.41
2:D:126:ILE:CD1	2:D:198:VAL:HG21	2.51	0.41
2:D:161:MET:SD	2:D:193:ASN:HB3	2.61	0.41
1:A:4:TYR:CD1	1:B:117:MET:CE	3.04	0.41
1:A:106:GLN:H	1:A:106:GLN:HG2	1.70	0.41
1:B:61:LYS:HA	1:B:67:GLN:OE1	2.21	0.41
1:B:87:LYS:O	1:B:88:LYS:C	2.64	0.41
2:C:72:ASP:O	2:C:73:HIS:ND1	2.54	0.41
2:C:161:MET:HE3	2:C:162:ASN:HB2	2.03	0.41
2:C:171:LEU:HD12	2:C:171:LEU:N	2.36	0.41
2:D:77:PRO:O	2:D:105:CYS:HB2	2.21	0.41
2:D:201:GLU:HB2	2:D:210:THR:HG22	2.03	0.41
2:E:219:ILE:HG12	2:E:220:THR:N	2.35	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: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:E:67:TYR:CD2	2:E:67:TYR:C	2.99	0.41
2:D:154:VAL:HA	2:D:170:ILE:O	2.21	0.40
2:C:23:TYR:CD2	2:C:23:TYR:C	2.99	0.40
2:C:76:ASP:O	2:C:78:SER:N	2.54	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:D:20:ILE:HG22	2:D:21:GLU:N	2.36	0.40
2:D:43:THR:OG1	2:D:61:ILE:HG13	2.21	0.40
2:E:78:SER:HA	2:E:103:ALA:HB2	2.00	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLU:HG2	1:B:42:ARG:NH1	2.35	0.40
1:A:108:LYS:O	1:A:111:HIS:HB3	2.21	0.40
1:A:114:ILE:HG22	2:D:206:VAL:HG11	2.02	0.40
1:B:91:ASP:C	1:B:95:LEU:HD12	2.45	0.40
2:D:42:PHE:N	2:D:63:ILE:O	2.55	0.40
2:D:114:LYS:HB2	2:D:129:PHE:HB2	2.02	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:65:HIS:CD2	2:E:65:HIS:H	2.38	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 [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	125/134 (93%)	99 (79%)	20 (16%)	6 (5%)	2	7
1	B	125/134 (93%)	105 (84%)	18 (14%)	2 (2%)	7	27
2	C	206/245 (84%)	153 (74%)	40 (19%)	13 (6%)	1	3
2	D	201/245 (82%)	154 (77%)	35 (17%)	12 (6%)	1	4
2	E	187/245 (76%)	140 (75%)	39 (21%)	8 (4%)	2	8
All	All	844/1003 (84%)	651 (77%)	152 (18%)	41 (5%)	1	6

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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%)	96 (82%)	21 (18%)	2	6
1	B	116/123 (94%)	97 (84%)	19 (16%)	2	8
2	C	188/223 (84%)	160 (85%)	28 (15%)	3	10
2	D	183/223 (82%)	156 (85%)	27 (15%)	3	10
2	E	177/223 (79%)	149 (84%)	28 (16%)	2	8
All	All	781/915 (85%)	658 (84%)	123 (16%)	2	9

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	10	ASN
1	A	19	HIS
1	A	27	THR
1	A	34	LYS
1	A	40	SER
1	A	44	ILE
1	A	56	LEU
1	A	65	SER
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	106	GLN
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	19	HIS
1	B	27	THR
1	B	34	LYS
1	B	40	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	44	ILE
1	B	56	LEU
1	B	62	ASP
1	B	65	SER
1	B	71	GLU
1	B	74	LYS
1	B	78	ASN
1	B	87	LYS
1	B	97	ASN
1	B	103	LEU
1	B	112	GLU
1	B	114	ILE
1	B	116	VAL
2	C	16	THR
2	C	19	THR
2	C	29	VAL
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	72	ASP
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	152	ILE
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	16	THR
2	D	19	THR
2	D	29	VAL
2	D	34	GLN
2	D	35	ILE
2	D	36	MET
2	D	39	VAL
2	D	44	VAL
2	D	57	ILE
2	D	60	CYS
2	D	63	ILE
2	D	72	ASP
2	D	118	ARG
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	19	THR
2	E	29	VAL
2	E	34	GLN
2	E	35	ILE
2	E	36	MET
2	E	39	VAL
2	E	44	VAL
2	E	57	ILE
2	E	63	ILE
2	E	72	ASP
2	E	100	GLU
2	E	102	PHE
2	E	105	CYS
2	E	110	ILE
2	E	118	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	10	ASN
1	A	16	ASN
1	A	46	GLN
1	A	67	GLN
1	A	106	GLN
1	A	111	HIS
1	B	1	GLN
1	B	10	ASN
1	B	25	ASN
1	B	46	GLN
1	B	67	GLN
1	B	106	GLN
1	B	111	HIS
2	C	34	GLN
2	C	62	ASN
2	C	162	ASN
2	C	167	GLN
2	C	173	GLN
2	C	205	HIS
2	D	167	GLN
2	D	182	GLN
2	D	184	GLN
2	D	193	ASN
2	D	195	GLN
2	D	205	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	167	GLN
2	E	173	GLN
2	E	193	ASN
2	E	205	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.