



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 16, 2018 – 06:01 pm GMT

PDB ID : 1PV2
Title : Native Form 2 E.coli Chaperone Hsp31
Authors : Quigley, P.M.; Korotkov, K.; Baneyx, F.; Hol, W.G.J.
Deposited on : 2003-06-26
Resolution : 2.71 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

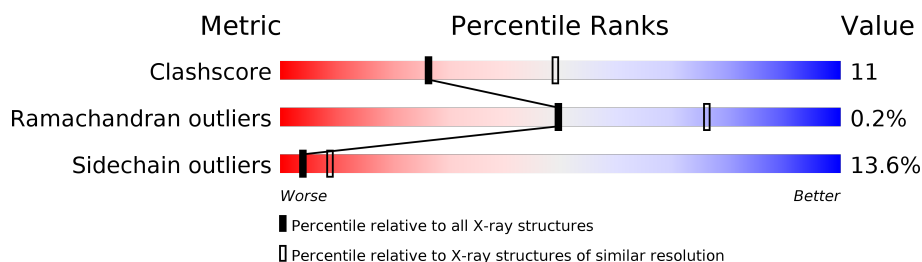
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	122078	3204 (2.74-2.70)
Ramachandran outliers	120005	3156 (2.74-2.70)
Sidechain outliers	119972	3157 (2.74-2.70)


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. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	283	
1	B	283	
1	C	283	
1	D	283	
1	E	283	
1	F	283	
1	G	283	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	H	283	 A horizontal bar chart showing the quality of chain H. The bar is divided into three segments: green (65%), yellow (26%), and red (6%). The red segment is followed by two small black dots. The percentages 65%, 26%, and 6% are written below their respective segments.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16233 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 Chaperone protein hchA.

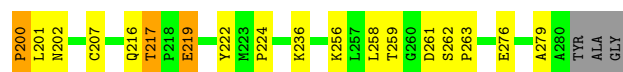
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1864	1203	309	344	8			
1	B	257	Total	C	N	O	S	0	0	0
			2008	1297	337	365	9			
1	C	249	Total	C	N	O	S	0	0	0
			1940	1252	323	356	9			
1	D	264	Total	C	N	O	S	0	0	0
			2048	1319	342	378	9			
1	E	270	Total	C	N	O	S	0	0	0
			2091	1341	352	389	9			
1	F	261	Total	C	N	O	S	0	0	0
			2031	1310	339	373	9			
1	G	260	Total	C	N	O	S	0	0	0
			2023	1305	338	371	9			
1	H	277	Total	C	N	O	S	0	0	0
			2156	1386	359	402	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING MET	UNP P31658
B	1	MET	-	INITIATING MET	UNP P31658
C	1	MET	-	INITIATING MET	UNP P31658
D	1	MET	-	INITIATING MET	UNP P31658
E	1	MET	-	INITIATING MET	UNP P31658
F	1	MET	-	INITIATING MET	UNP P31658
G	1	MET	-	INITIATING MET	UNP P31658
H	1	MET	-	INITIATING MET	UNP P31658

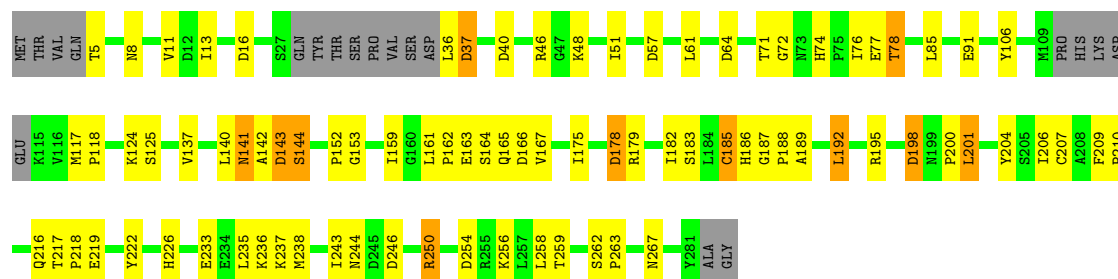
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	7	Total 7	O 7	0	0
2	B	7	Total 7	O 7	0	0
2	C	13	Total 13	O 13	0	0
2	D	7	Total 7	O 7	0	0
2	E	6	Total 6	O 6	0	0
2	F	8	Total 8	O 8	0	0
2	G	11	Total 11	O 11	0	0
2	H	13	Total 13	O 13	0	0



• Molecule 1: Chaperone protein hchA

Chain D: 63% 26% 7%



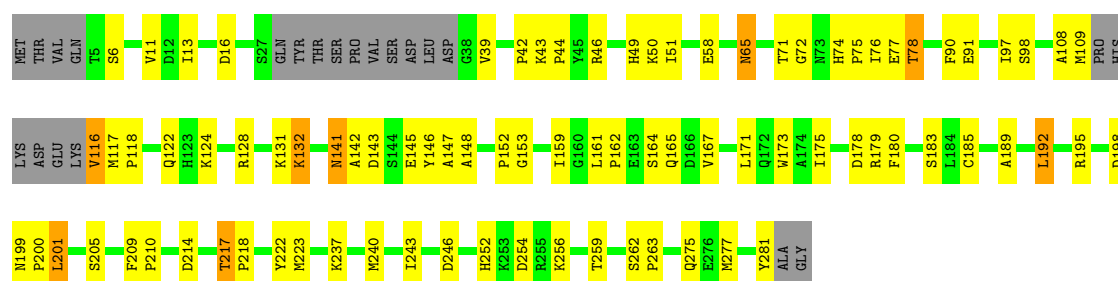
• Molecule 1: Chaperone protein hchA

Chain E: 64% 25% 5% 5%



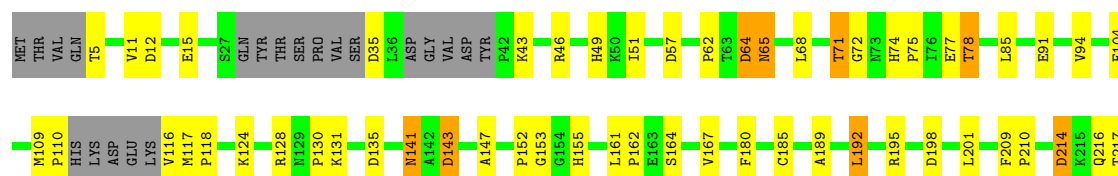
• Molecule 1: Chaperone protein hchA

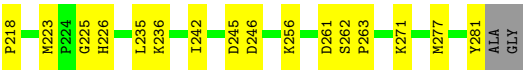
Chain F: 62% 28% 8%



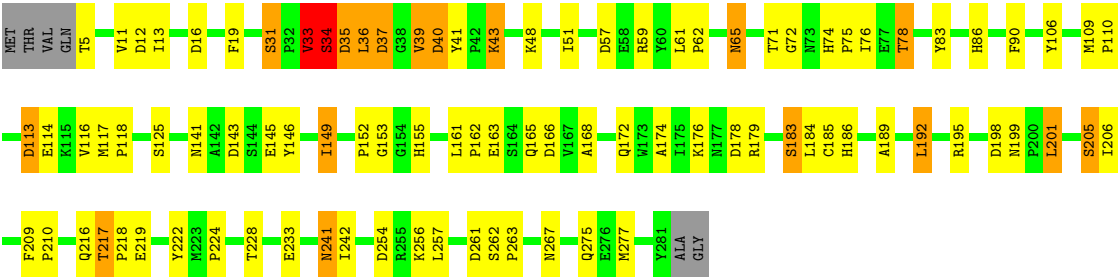
• Molecule 1: Chaperone protein hchA

Chain G: 66% 23% 8%





● Molecule 1: Chaperone protein hchA



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.49Å 99.02Å 116.80Å 102.95° 101.52° 94.19°	Depositor
Resolution (Å)	48.80 – 2.71	Depositor
% Data completeness (in resolution range)	94.0 (48.80-2.71)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.221 , 0.286	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	16233	wwPDB-VP
Average B, all atoms (Å ²)	45.0	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	0.42	0/1912	0.98	24/2591 (0.9%)
1	B	0.26	0/2062	0.60	8/2792 (0.3%)
1	C	0.39	2/1991 (0.1%)	0.61	6/2698 (0.2%)
1	D	0.26	0/2104	0.62	10/2853 (0.4%)
1	E	0.32	0/2147	0.68	16/2912 (0.5%)
1	F	0.26	0/2087	0.61	6/2831 (0.2%)
1	G	0.26	0/2078	0.61	11/2817 (0.4%)
1	H	0.30	1/2218 (0.0%)	0.65	12/3014 (0.4%)
All	All	0.31	3/16599 (0.0%)	0.68	93/22508 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	C	0	1
1	E	0	2
1	H	0	1
All	All	0	8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	7	LYS	C-N	-10.12	1.10	1.34
1	C	200	PRO	C-N	8.60	1.53	1.34
1	H	34	SER	C-N	-6.46	1.19	1.34

All (93) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	146	TYR	CB-CG-CD2	18.61	132.17	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	ALA	C-N-CA	12.80	153.70	121.70
1	A	146	TYR	CB-CG-CD1	-12.66	113.40	121.00
1	A	87	ALA	N-CA-CB	8.19	121.56	110.10
1	A	146	TYR	CZ-CE2-CD2	-7.67	112.89	119.80
1	A	89	GLY	O-C-N	7.61	134.88	122.70
1	E	280	ALA	C-N-CA	7.49	140.42	121.70
1	A	88	ALA	N-CA-CB	7.09	120.02	110.10
1	A	87	ALA	CA-C-N	-6.76	102.32	117.20
1	A	149	ILE	O-C-N	-6.70	111.98	122.70
1	A	148	ALA	CB-CA-C	-6.54	100.28	110.10
1	A	148	ALA	N-CA-CB	-6.22	101.40	110.10
1	E	279	ALA	CB-CA-C	6.11	119.27	110.10
1	A	57	ASP	CB-CG-OD2	5.67	123.41	118.30
1	E	12	ASP	CB-CG-OD2	5.55	123.30	118.30
1	H	166	ASP	CB-CG-OD2	5.54	123.29	118.30
1	D	37	ASP	CB-CG-OD2	5.51	123.26	118.30
1	H	37	ASP	CB-CG-OD2	5.51	123.26	118.30
1	D	178	ASP	CB-CG-OD2	5.42	123.18	118.30
1	H	198	ASP	CB-CG-OD2	5.42	123.18	118.30
1	E	113	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	85	LEU	N-CA-C	5.41	125.59	111.00
1	A	146	TYR	CG-CD2-CE2	5.40	125.62	121.30
1	C	57	ASP	CB-CG-OD2	5.39	123.15	118.30
1	C	261	ASP	CB-CG-OD2	5.39	123.15	118.30
1	E	198	ASP	CB-CG-OD2	5.37	123.13	118.30
1	D	166	ASP	CB-CG-OD2	5.34	123.10	118.30
1	H	178	ASP	CB-CG-OD2	5.33	123.10	118.30
1	H	16	ASP	CB-CG-OD2	5.33	123.10	118.30
1	C	198	ASP	CB-CG-OD2	5.32	123.09	118.30
1	A	146	TYR	CD1-CE1-CZ	5.31	124.58	119.80
1	A	135	ASP	CB-CG-OD2	5.30	123.07	118.30
1	F	214	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	178	ASP	CB-CG-OD2	5.30	123.07	118.30
1	D	16	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	214	ASP	CB-CG-OD2	5.28	123.05	118.30
1	G	261	ASP	CB-CG-OD2	5.28	123.05	118.30
1	H	254	ASP	CB-CG-OD2	5.27	123.04	118.30
1	B	57	ASP	CB-CG-OD2	5.26	123.04	118.30
1	E	261	ASP	CB-CG-OD2	5.26	123.03	118.30
1	A	12	ASP	CB-CG-OD2	5.23	123.00	118.30
1	G	198	ASP	CB-CG-OD2	5.23	123.00	118.30
1	G	35	ASP	CB-CG-OD2	5.23	123.00	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	16	ASP	CB-CG-OD2	5.22	123.00	118.30
1	F	178	ASP	CB-CG-OD2	5.21	122.99	118.30
1	E	35	ASP	CB-CG-OD2	5.20	122.98	118.30
1	G	57	ASP	CB-CG-OD2	5.20	122.98	118.30
1	D	40	ASP	CB-CG-OD2	5.19	122.97	118.30
1	E	178	ASP	CB-CG-OD2	5.19	122.97	118.30
1	F	198	ASP	CB-CG-OD2	5.19	122.97	118.30
1	F	254	ASP	CB-CG-OD2	5.19	122.97	118.30
1	G	143	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	178	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	16	ASP	CB-CG-OD2	5.17	122.95	118.30
1	E	254	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	214	ASP	CB-CG-OD2	5.17	122.95	118.30
1	H	12	ASP	CB-CG-OD2	5.17	122.95	118.30
1	B	166	ASP	CB-CG-OD2	5.16	122.94	118.30
1	C	178	ASP	CB-CG-OD2	5.15	122.94	118.30
1	B	246	ASP	CB-CG-OD2	5.14	122.93	118.30
1	F	16	ASP	CB-CG-OD2	5.14	122.93	118.30
1	A	146	TYR	CA-CB-CG	5.14	123.16	113.40
1	B	254	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	261	ASP	CB-CG-OD2	5.12	122.90	118.30
1	E	166	ASP	CB-CG-OD2	5.11	122.90	118.30
1	G	214	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	166	ASP	CB-CG-OD2	5.11	122.90	118.30
1	D	198	ASP	CB-CG-OD2	5.11	122.89	118.30
1	G	12	ASP	CB-CG-OD2	5.11	122.89	118.30
1	G	245	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	261	ASP	CB-CG-OD2	5.10	122.89	118.30
1	E	143	ASP	CB-CG-OD2	5.10	122.89	118.30
1	H	261	ASP	CB-CG-OD2	5.10	122.89	118.30
1	C	166	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	246	ASP	CB-CG-OD2	5.09	122.88	118.30
1	G	246	ASP	CB-CG-OD2	5.09	122.88	118.30
1	C	113	ASP	CB-CG-OD2	5.09	122.88	118.30
1	H	40	ASP	CB-CG-OD2	5.09	122.88	118.30
1	D	254	ASP	CB-CG-OD2	5.08	122.88	118.30
1	E	57	ASP	CB-CG-OD2	5.08	122.87	118.30
1	D	143	ASP	CB-CG-OD2	5.07	122.86	118.30
1	H	143	ASP	CB-CG-OD2	5.07	122.86	118.30
1	G	64	ASP	CB-CG-OD2	5.07	122.86	118.30
1	E	16	ASP	CB-CG-OD2	5.06	122.85	118.30
1	E	246	ASP	CB-CG-OD2	5.05	122.85	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	214	ASP	CB-CG-OD2	5.05	122.84	118.30
1	G	135	ASP	CB-CG-OD2	5.04	122.83	118.30
1	E	281	TYR	CA-C-O	5.03	130.67	120.10
1	H	113	ASP	CB-CG-OD2	5.03	122.83	118.30
1	D	246	ASP	CB-CG-OD2	5.03	122.83	118.30
1	D	57	ASP	CB-CG-OD2	5.01	122.81	118.30
1	H	57	ASP	CB-CG-OD2	5.01	122.81	118.30
1	F	246	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	146	TYR	Sidechain
1	A	148	ALA	Mainchain,Peptide
1	A	85	LEU	Peptide
1	C	7	LYS	Mainchain
1	E	280	ALA	Mainchain,Peptide
1	H	33	VAL	Peptide

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	1864	0	1818	76	0
1	B	2008	0	1965	45	0
1	C	1940	0	1898	37	0
1	D	2048	0	1987	41	0
1	E	2091	0	2034	37	0
1	F	2031	0	1979	44	0
1	G	2023	0	1976	32	0
1	H	2156	0	2087	48	0
2	A	7	0	0	1	0
2	B	7	0	0	0	0
2	C	13	0	0	1	0
2	D	7	0	0	0	0
2	E	6	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	8	0	0	0	0
2	G	11	0	0	0	0
2	H	13	0	0	0	0
All	All	16233	0	15744	354	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 11.

All (354) 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:74:HIS:O	1:A:78:THR:HG22	1.59	1.00
1:A:50:LYS:N	1:A:51:ILE:HA	1.72	0.99
1:A:85:LEU:O	1:A:90:PHE:HB2	1.74	0.86
1:B:49:HIS:HB3	1:B:147:ALA:HB2	1.59	0.85
1:A:75:PRO:HG2	1:A:109:MET:HB3	1.59	0.85
1:H:262:SER:HB2	1:H:263:PRO:CD	2.09	0.83
1:H:205:SER:OG	1:H:241:ASN:ND2	2.11	0.83
1:A:50:LYS:HB2	1:A:146:TYR:HA	1.60	0.81
1:A:52:LEU:HD23	1:A:149:ILE:HD13	1.63	0.81
1:B:28:GLN:H	1:B:29:TYR:C	1.83	0.80
1:G:74:HIS:O	1:G:78:THR:HG22	1.79	0.80
1:A:75:PRO:CG	1:A:109:MET:HB3	2.12	0.80
1:A:50:LYS:N	1:A:51:ILE:CA	2.45	0.80
1:B:51:ILE:HD11	1:B:90:PHE:HB3	1.64	0.79
1:E:78:THR:HG21	1:E:104:PHE:HE2	1.47	0.79
1:F:142:ALA:O	1:F:179:ARG:NH2	2.16	0.79
1:B:51:ILE:CD1	1:B:90:PHE:HB3	2.16	0.75
1:G:65:ASN:HD22	1:G:65:ASN:H	1.33	0.75
1:E:71:THR:OG1	1:E:72:GLY:N	2.19	0.74
1:H:19:PHE:HB2	1:H:224:PRO:HG3	1.68	0.74
1:B:28:GLN:HB3	1:B:29:TYR:HB2	1.70	0.72
1:A:217:THR:N	1:A:218:PRO:HD2	2.05	0.71
1:A:262:SER:HB2	1:A:263:PRO:HD2	1.70	0.71
1:G:262:SER:HB2	1:G:263:PRO:HD2	1.71	0.70
1:H:34:SER:CB	1:H:113:ASP:OD2	2.39	0.70
1:H:262:SER:HB2	1:H:263:PRO:HD2	1.74	0.70
1:H:34:SER:OG	1:H:116:VAL:HG21	1.92	0.69
1:B:71:THR:OG1	1:B:72:GLY:N	2.24	0.69
1:B:169:ALA:HA	1:B:172:GLN:HG3	1.75	0.69
1:C:71:THR:OG1	1:C:72:GLY:N	2.24	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ALA:N	1:A:109:MET:HA	2.05	0.68
1:A:74:HIS:O	1:A:78:THR:CG2	2.38	0.68
1:C:262:SER:HB2	1:C:263:PRO:HD2	1.76	0.68
1:B:262:SER:HB2	1:B:263:PRO:HD2	1.77	0.67
1:E:262:SER:HB2	1:E:263:PRO:HD2	1.76	0.67
1:F:74:HIS:O	1:F:78:THR:CG2	2.42	0.67
1:F:74:HIS:O	1:F:78:THR:HG22	1.93	0.67
1:D:217:THR:HB	1:D:222:TYR:HB3	1.77	0.67
1:G:262:SER:HB2	1:G:263:PRO:CD	2.24	0.67
1:C:262:SER:HB2	1:C:263:PRO:CD	2.25	0.66
1:E:75:PRO:HA	1:E:78:THR:CG2	2.25	0.66
1:F:262:SER:HB2	1:F:263:PRO:CD	2.25	0.66
1:F:49:HIS:HB3	1:F:147:ALA:HB2	1.77	0.66
1:B:164:SER:HB3	1:B:167:VAL:HB	1.77	0.66
1:F:116:VAL:HG13	1:F:118:PRO:HD2	1.76	0.66
1:F:164:SER:HB3	1:F:167:VAL:HG23	1.77	0.65
1:C:117:MET:HB2	1:C:118:PRO:HD3	1.78	0.65
1:A:74:HIS:HB3	1:A:77:GLU:HB2	1.79	0.65
1:G:74:HIS:O	1:G:78:THR:CG2	2.45	0.64
1:C:74:HIS:O	1:C:78:THR:HG22	1.96	0.64
1:H:117:MET:HB2	1:H:118:PRO:HD3	1.80	0.64
1:F:262:SER:HB2	1:F:263:PRO:HD2	1.80	0.64
1:C:189:ALA:O	1:C:192:LEU:HB2	1.97	0.64
1:B:74:HIS:O	1:B:78:THR:HG23	1.97	0.63
1:E:49:HIS:HB3	1:E:147:ALA:HB2	1.80	0.63
1:E:74:HIS:O	1:E:78:THR:HG22	1.97	0.63
1:H:74:HIS:O	1:H:78:THR:HG22	1.99	0.63
1:D:78:THR:HB	1:D:152:PRO:HB3	1.81	0.63
1:D:164:SER:HB3	1:D:167:VAL:HB	1.80	0.63
1:F:74:HIS:HB3	1:F:77:GLU:HB2	1.80	0.62
1:H:34:SER:HB3	1:H:113:ASP:OD2	1.97	0.62
1:B:28:GLN:HB3	1:B:29:TYR:CB	2.29	0.62
1:B:74:HIS:O	1:B:78:THR:CG2	2.47	0.62
1:E:207:CYS:SG	1:E:250:ARG:HD3	2.40	0.62
1:E:78:THR:HG21	1:E:104:PHE:CE2	2.31	0.61
1:A:50:LYS:O	1:A:91:GLU:O	2.17	0.61
1:G:164:SER:HB3	1:G:167:VAL:HB	1.82	0.61
1:G:74:HIS:HB3	1:G:77:GLU:HB2	1.82	0.61
1:E:52:LEU:HD23	1:E:149:ILE:HD13	1.82	0.61
1:G:71:THR:OG1	1:G:72:GLY:N	2.30	0.61
1:A:65:ASN:C	1:A:65:ASN:HD22	2.04	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:PHE:HB2	1:C:224:PRO:HG3	1.81	0.60
1:A:194:LEU:HB2	1:A:238:MET:HE3	1.83	0.60
1:B:183:SER:O	1:B:259:THR:HA	2.00	0.60
1:H:217:THR:N	1:H:218:PRO:CD	2.65	0.60
1:B:262:SER:HB2	1:B:263:PRO:CD	2.32	0.60
1:C:171:LEU:O	1:C:175:ILE:HD12	2.01	0.60
1:G:117:MET:N	1:G:118:PRO:HD2	2.15	0.60
1:A:78:THR:O	1:A:82:LEU:HD12	2.02	0.60
1:G:78:THR:HG21	1:G:104:PHE:HE2	1.67	0.60
1:H:216:GLN:O	1:H:219:GLU:HB2	2.02	0.59
1:A:59:ARG:HG3	1:A:71:THR:O	2.03	0.59
1:D:74:HIS:HB3	1:D:77:GLU:HB2	1.84	0.59
1:E:262:SER:HB2	1:E:263:PRO:CD	2.32	0.59
1:F:141:ASN:HD22	1:F:143:ASP:H	1.50	0.59
1:F:252:HIS:HE1	1:G:216:GLN:OE1	1.86	0.59
1:E:19:PHE:HB2	1:E:224:PRO:HG3	1.85	0.58
1:A:178:ASP:OD1	1:A:256:LYS:HG3	2.02	0.58
1:A:262:SER:HB2	1:A:263:PRO:CD	2.32	0.58
1:A:50:LYS:HB2	1:A:146:TYR:CA	2.34	0.58
1:D:153:GLY:HA3	1:D:185:CYS:HB3	1.86	0.58
1:H:39:VAL:O	1:H:39:VAL:HG22	2.02	0.58
1:D:64:ASP:OD2	1:D:226:HIS:HB2	2.04	0.58
1:E:189:ALA:O	1:E:192:LEU:HB2	2.03	0.57
1:E:149:ILE:HG13	1:E:174:ALA:HB2	1.84	0.57
1:B:217:THR:N	1:B:218:PRO:CD	2.67	0.57
1:C:97:ILE:HD11	1:C:161:LEU:HD23	1.86	0.57
1:F:164:SER:HB3	1:F:167:VAL:CG2	2.34	0.57
1:A:273:ALA:O	1:A:277:MET:HG3	2.04	0.57
1:F:171:LEU:O	1:F:175:ILE:HD12	2.04	0.57
1:F:189:ALA:O	1:F:192:LEU:HB2	2.04	0.57
1:F:97:ILE:HD11	1:F:161:LEU:HD23	1.85	0.57
1:A:176:LYS:HG2	1:A:176:LYS:O	2.05	0.57
1:A:252:HIS:HE1	1:D:216:GLN:OE1	1.88	0.57
1:A:92:PHE:C	1:A:92:PHE:CD1	2.78	0.56
1:D:262:SER:HB2	1:D:263:PRO:HD2	1.87	0.56
1:D:262:SER:HB2	1:D:263:PRO:CD	2.35	0.56
1:A:58:GLU:HB2	1:B:100:LEU:HD13	1.88	0.56
1:B:217:THR:N	1:B:218:PRO:HD2	2.21	0.56
1:E:117:MET:HB2	1:E:118:PRO:HD3	1.86	0.56
1:A:75:PRO:HG2	1:A:109:MET:CB	2.32	0.56
1:C:16:ASP:HB2	1:D:106:TYR:CZ	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:34:SER:HB2	1:H:113:ASP:OD2	2.05	0.55
1:A:217:THR:HB	1:A:222:TYR:HB3	1.88	0.55
1:A:204:TYR:CZ	1:A:255:ARG:HD2	2.41	0.55
1:F:51:ILE:CD1	1:F:90:PHE:HB3	2.36	0.55
1:E:75:PRO:HA	1:E:78:THR:HG22	1.87	0.55
1:A:153:GLY:HA3	1:A:185:CYS:HB3	1.89	0.55
1:B:28:GLN:HB3	1:B:29:TYR:CG	2.41	0.55
1:G:141:ASN:HD22	1:G:143:ASP:H	1.54	0.55
1:A:194:LEU:HB2	1:A:238:MET:CE	2.37	0.54
1:B:101:MET:HG3	1:B:103:LYS:HE3	1.89	0.54
1:D:77:GLU:OE1	1:D:185:CYS:HB2	2.07	0.54
1:D:51:ILE:HD13	1:D:85:LEU:HD13	1.89	0.54
1:B:153:GLY:HA3	1:B:185:CYS:HB3	1.90	0.54
1:A:232:GLY:O	1:A:236:LYS:HG3	2.07	0.53
1:C:217:THR:HB	1:C:222:TYR:HB3	1.90	0.53
1:F:217:THR:N	1:F:218:PRO:CD	2.72	0.53
1:A:149:ILE:HG13	1:A:174:ALA:HB2	1.90	0.53
1:B:28:GLN:N	1:B:29:TYR:C	2.58	0.53
1:C:55:ALA:HB1	1:C:102:THR:HG23	1.91	0.53
1:D:137:VAL:HA	1:D:140:LEU:HD12	1.91	0.53
1:A:51:ILE:HD13	1:A:85:LEU:HD13	1.91	0.53
1:A:80:LEU:HB2	1:A:81:PRO:HD3	1.91	0.53
1:E:183:SER:O	1:E:259:THR:HA	2.09	0.53
1:A:156:GLY:HA2	1:A:159:ILE:HD12	1.90	0.53
1:H:192:LEU:O	1:H:195:ARG:HB2	2.08	0.53
1:C:74:HIS:CE1	1:C:76:ILE:HB	2.44	0.53
1:E:217:THR:N	1:E:218:PRO:CD	2.71	0.52
1:C:200:PRO:C	1:C:202:ASN:H	2.12	0.52
1:H:149:ILE:HD12	1:H:174:ALA:HB2	1.92	0.52
1:B:198:ASP:N	1:B:198:ASP:OD1	2.42	0.52
1:G:217:THR:N	1:G:218:PRO:CD	2.73	0.52
1:A:82:LEU:O	1:A:86:HIS:CB	2.58	0.52
1:G:192:LEU:HD13	1:G:235:LEU:HD23	1.92	0.52
1:A:164:SER:HB3	1:A:167:VAL:HB	1.92	0.52
1:D:74:HIS:CE1	1:D:76:ILE:HB	2.45	0.52
1:H:217:THR:HB	1:H:222:TYR:HB3	1.92	0.52
1:A:75:PRO:HG3	1:A:109:MET:HB3	1.92	0.52
1:A:65:ASN:HD21	1:A:67:LYS:HB2	1.74	0.52
1:H:51:ILE:CD1	1:H:90:PHE:HB3	2.40	0.52
1:H:78:THR:HB	1:H:152:PRO:HB3	1.92	0.52
1:H:161:LEU:N	1:H:162:PRO:CD	2.72	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:TYR:CZ	1:B:16:ASP:HB2	2.45	0.51
1:B:189:ALA:O	1:B:192:LEU:HB2	2.09	0.51
1:C:110:PRO:HB2	1:C:113:ASP:HB2	1.92	0.51
1:A:78:THR:HG21	1:A:104:PHE:HE2	1.76	0.51
1:C:65:ASN:HD22	1:C:65:ASN:C	2.13	0.51
1:B:161:LEU:HB2	1:B:162:PRO:HD3	1.92	0.51
1:A:71:THR:OG1	1:A:72:GLY:N	2.41	0.51
1:A:50:LYS:HD3	1:A:145:GLU:O	2.11	0.50
1:C:119:PHE:CE1	1:C:123:HIS:CE1	2.98	0.50
1:F:108:ALA:O	1:F:109:MET:HB2	2.12	0.50
1:G:189:ALA:O	1:G:192:LEU:HB2	2.11	0.50
1:E:217:THR:HB	1:E:222:TYR:HB3	1.92	0.50
1:G:223:MET:HE2	1:G:225:GLY:O	2.12	0.50
1:F:78:THR:HB	1:F:152:PRO:HB3	1.94	0.50
1:C:183:SER:O	1:C:259:THR:HA	2.11	0.49
1:G:153:GLY:HA3	1:G:185:CYS:HB3	1.92	0.49
1:A:78:THR:HB	1:A:152:PRO:CB	2.42	0.49
1:E:109:MET:SD	1:E:110:PRO:HD2	2.53	0.49
1:G:78:THR:HB	1:G:152:PRO:HB3	1.95	0.49
1:C:119:PHE:HE1	1:C:123:HIS:CE1	2.30	0.49
1:F:74:HIS:CE1	1:F:76:ILE:HB	2.47	0.49
1:F:117:MET:HB2	1:F:118:PRO:HD3	1.93	0.49
1:G:49:HIS:HB3	1:G:147:ALA:HB2	1.94	0.49
1:D:201:LEU:HD12	1:D:204:TYR:CD1	2.47	0.49
1:H:51:ILE:HD11	1:H:90:PHE:HB3	1.95	0.49
1:F:77:GLU:OE1	1:F:153:GLY:HA3	2.13	0.48
1:H:31:SER:HB3	1:H:33:VAL:O	2.13	0.48
1:C:216:GLN:O	1:C:219:GLU:HB2	2.14	0.48
1:H:74:HIS:O	1:H:78:THR:CG2	2.61	0.48
1:G:161:LEU:N	1:G:162:PRO:CD	2.76	0.48
1:D:141:ASN:HD22	1:D:143:ASP:H	1.60	0.48
1:E:164:SER:HB3	1:E:167:VAL:HB	1.94	0.48
1:H:153:GLY:HA3	1:H:185:CYS:HB3	1.95	0.48
1:F:262:SER:CB	1:F:263:PRO:CD	2.88	0.48
1:H:168:ALA:O	1:H:172:GLN:HG3	2.14	0.48
1:B:57:ASP:OD1	1:B:57:ASP:N	2.47	0.48
1:E:74:HIS:CE1	1:E:76:ILE:HB	2.49	0.48
1:F:217:THR:HB	1:F:222:TYR:HB3	1.94	0.48
1:G:180:PHE:CD1	1:G:277:MET:HG2	2.49	0.48
1:B:61:LEU:HD12	1:B:62:PRO:HD2	1.95	0.47
1:C:74:HIS:O	1:C:78:THR:CG2	2.62	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ILE:HD13	1:A:200:PRO:HG2	1.97	0.47
1:D:142:ALA:O	1:D:179:ARG:NH2	2.45	0.47
1:E:161:LEU:N	1:E:162:PRO:CD	2.77	0.47
1:C:262:SER:CB	1:C:263:PRO:CD	2.90	0.47
1:C:65:ASN:HD21	1:C:67:LYS:HB2	1.80	0.47
1:H:189:ALA:O	1:H:192:LEU:HB2	2.15	0.47
1:A:189:ALA:O	1:A:192:LEU:HB2	2.15	0.47
1:B:25:SER:O	1:B:29:TYR:HB2	2.15	0.47
1:B:192:LEU:O	1:B:195:ARG:HB2	2.15	0.47
1:F:146:TYR:HB2	1:F:173:TRP:CH2	2.50	0.47
1:B:29:TYR:N	1:B:29:TYR:CD1	2.82	0.47
1:B:43:LYS:HE2	1:B:43:LYS:HB2	1.78	0.47
1:C:164:SER:HB3	1:C:167:VAL:HB	1.97	0.47
1:H:65:ASN:HD22	1:H:65:ASN:C	2.18	0.47
1:A:161:LEU:HB2	1:A:162:PRO:HD3	1.96	0.46
1:F:71:THR:OG1	1:F:72:GLY:N	2.48	0.46
1:H:262:SER:HB2	1:H:263:PRO:HD3	1.95	0.46
1:C:117:MET:CB	1:C:118:PRO:HD3	2.45	0.46
1:C:5:THR:C	1:C:7:LYS:H	2.17	0.46
1:A:217:THR:N	1:A:218:PRO:CD	2.76	0.46
1:C:78:THR:HB	1:C:152:PRO:HB3	1.96	0.46
1:E:62:PRO:HA	1:E:68:LEU:HD23	1.97	0.46
1:F:161:LEU:N	1:F:162:PRO:CD	2.77	0.46
1:H:71:THR:OG1	1:H:72:GLY:N	2.44	0.46
1:D:74:HIS:O	1:D:78:THR:CG2	2.64	0.46
1:H:43:LYS:HD3	1:H:43:LYS:HA	1.55	0.46
1:A:52:LEU:HD23	1:A:149:ILE:CD1	2.41	0.45
1:B:74:HIS:HE1	1:B:76:ILE:HB	1.81	0.45
1:C:161:LEU:N	1:C:162:PRO:CD	2.78	0.45
1:D:185:CYS:HB3	1:D:186:HIS:H	1.60	0.45
1:E:19:PHE:HE1	1:E:67:LYS:HG2	1.80	0.45
1:F:277:MET:O	1:F:281:TYR:HD1	2.00	0.45
1:A:61:LEU:HB2	1:A:159:ILE:HD11	1.96	0.45
1:A:51:ILE:H	1:A:92:PHE:HA	1.81	0.45
1:H:206:ILE:CG2	1:H:257:LEU:HD21	2.47	0.45
1:F:183:SER:O	1:F:259:THR:HA	2.17	0.45
1:G:74:HIS:HA	1:G:75:PRO:HD3	1.86	0.45
1:A:61:LEU:HA	1:A:62:PRO:HD3	1.83	0.45
1:D:71:THR:OG1	1:D:72:GLY:N	2.47	0.45
1:E:217:THR:N	1:E:218:PRO:HD2	2.32	0.45
1:F:153:GLY:HA3	1:F:185:CYS:HB3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:46:ARG:HA	1:E:46:ARG:HD2	1.71	0.45
1:G:64:ASP:OD2	1:G:226:HIS:HB2	2.16	0.45
1:A:201:LEU:HD12	1:A:201:LEU:HA	1.77	0.45
1:G:62:PRO:HA	1:G:68:LEU:HD23	1.99	0.45
1:F:74:HIS:O	1:F:78:THR:HG23	2.15	0.45
1:A:183:SER:O	1:A:259:THR:HA	2.17	0.45
1:A:210:PRO:HA	2:A:421:HOH:O	2.17	0.44
1:A:192:LEU:HD13	1:A:235:LEU:HD23	1.98	0.44
1:B:57:ASP:O	1:B:103:LYS:NZ	2.50	0.44
1:D:183:SER:O	1:D:259:THR:HA	2.17	0.44
1:D:182:ILE:HA	1:D:258:LEU:O	2.17	0.44
1:E:57:ASP:HB3	1:E:96:THR:HB	1.99	0.44
1:H:201:LEU:HA	1:H:201:LEU:HD12	1.80	0.44
1:B:45:TYR:CZ	1:B:47:GLY:HA3	2.52	0.44
1:A:50:LYS:N	1:A:146:TYR:HB3	2.33	0.44
1:A:161:LEU:N	1:A:162:PRO:CD	2.80	0.44
1:C:74:HIS:HE1	1:C:76:ILE:HB	1.83	0.44
1:C:119:PHE:CE1	1:C:123:HIS:ND1	2.86	0.44
1:F:146:TYR:HB2	1:F:173:TRP:HH2	1.82	0.44
1:D:178:ASP:O	1:D:256:LYS:NZ	2.51	0.44
1:F:74:HIS:HA	1:F:75:PRO:HD3	1.87	0.44
1:D:117:MET:N	1:D:118:PRO:CD	2.80	0.43
1:G:109:MET:SD	1:G:110:PRO:HD2	2.58	0.43
1:G:51:ILE:HD13	1:G:85:LEU:HD13	2.00	0.43
1:F:175:ILE:HD13	1:F:200:PRO:HG2	1.99	0.43
1:G:155:HIS:HE1	1:G:214:ASP:OD1	2.02	0.43
1:G:161:LEU:N	1:G:161:LEU:HD23	2.33	0.43
1:G:209:PHE:HA	1:G:210:PRO:HD3	1.87	0.43
1:B:179:ARG:HD3	1:B:179:ARG:HA	1.72	0.43
1:B:187:GLY:N	1:B:188:PRO:CD	2.81	0.43
1:E:12:ASP:OD2	1:E:60:TYR:OH	2.32	0.43
1:H:74:HIS:CE1	1:H:76:ILE:HB	2.53	0.43
1:A:171:LEU:HA	1:A:171:LEU:HD23	1.86	0.43
1:C:258:LEU:HD21	1:C:276:GLU:HG3	2.00	0.43
1:C:65:ASN:ND2	1:C:67:LYS:H	2.16	0.43
1:G:236:LYS:HE2	1:G:242:ILE:HD12	2.01	0.43
1:D:243:ILE:HD12	1:D:250:ARG:NH2	2.34	0.43
1:H:109:MET:SD	1:H:110:PRO:HD2	2.58	0.43
1:D:61:LEU:HB2	1:D:159:ILE:HD11	1.99	0.43
1:D:161:LEU:N	1:D:162:PRO:CD	2.81	0.43
1:A:7:LYS:H	1:A:7:LYS:HG2	1.47	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:HIS:O	1:D:78:THR:HG22	2.18	0.43
1:E:146:TYR:HB2	1:E:173:TRP:CH2	2.54	0.43
1:E:52:LEU:HD23	1:E:149:ILE:CD1	2.48	0.43
1:H:86:HIS:HA	1:H:90:PHE:O	2.19	0.43
1:E:187:GLY:N	1:E:188:PRO:CD	2.82	0.42
1:E:201:LEU:HA	1:E:201:LEU:HD12	1.86	0.42
1:E:186:HIS:NE2	1:E:214:ASP:OD2	2.35	0.42
1:A:80:LEU:CB	1:A:81:PRO:HD3	2.49	0.42
1:G:15:GLU:OE1	1:H:106:TYR:HE2	2.03	0.42
1:H:36:LEU:HD21	1:H:83:TYR:CE1	2.54	0.42
1:B:74:HIS:HA	1:B:75:PRO:HD3	1.85	0.42
1:F:97:ILE:CD1	1:F:161:LEU:HD23	2.49	0.42
1:E:74:HIS:HE1	1:E:76:ILE:HB	1.84	0.42
1:F:201:LEU:HA	1:F:201:LEU:HD12	1.88	0.42
1:A:192:LEU:O	1:A:195:ARG:HB2	2.19	0.42
1:B:74:HIS:CE1	1:B:76:ILE:HB	2.55	0.42
1:C:161:LEU:HB2	1:C:162:PRO:HD3	2.02	0.42
1:D:175:ILE:HG21	1:D:200:PRO:HB2	2.00	0.42
1:A:78:THR:HB	1:A:152:PRO:HB3	2.00	0.42
1:D:209:PHE:HA	1:D:210:PRO:HD3	1.86	0.42
1:H:146:TYR:O	1:H:179:ARG:HD2	2.19	0.42
1:H:35:ASP:O	1:H:36:LEU:C	2.58	0.42
1:H:36:LEU:HA	1:H:267:ASN:ND2	2.35	0.42
1:A:92:PHE:HD1	1:A:93:GLU:N	2.17	0.42
1:A:94:VAL:HG12	1:A:95:ALA:N	2.34	0.42
1:D:262:SER:CB	1:D:263:PRO:CD	2.94	0.42
1:H:40:ASP:HB3	1:H:41:TYR:H	1.72	0.42
1:H:78:THR:HB	1:H:152:PRO:CB	2.50	0.42
1:A:118:PRO:O	1:A:122:GLN:NE2	2.51	0.42
1:A:211:ASP:OD2	1:A:232:GLY:HA3	2.20	0.42
1:B:74:HIS:O	1:B:78:THR:HG22	2.20	0.42
1:E:65:ASN:HD22	1:E:65:ASN:C	2.23	0.42
1:H:155:HIS:CE1	1:H:186:HIS:CE1	3.07	0.42
1:A:88:ALA:HB1	1:A:278:LEU:HD21	2.02	0.41
1:B:161:LEU:N	1:B:162:PRO:CD	2.82	0.41
1:D:192:LEU:HA	1:D:192:LEU:HD12	1.88	0.41
1:D:217:THR:N	1:D:218:PRO:CD	2.82	0.41
1:H:74:HIS:HA	1:H:75:PRO:HD3	1.85	0.41
1:C:97:ILE:CD1	1:C:161:LEU:HD23	2.49	0.41
1:D:216:GLN:O	1:D:219:GLU:HB2	2.20	0.41
1:F:148:ALA:HB2	1:F:180:PHE:HB2	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:117:MET:CB	1:H:118:PRO:HD3	2.47	0.41
1:B:52:LEU:HB3	1:B:149:ILE:HD13	2.01	0.41
1:C:185:CYS:HB3	1:C:186:HIS:H	1.66	0.41
1:F:42:PRO:O	1:F:44:PRO:HD3	2.21	0.41
1:F:98:SER:C	1:F:132:LYS:HG3	2.40	0.41
1:A:57:ASP:OD1	1:A:57:ASP:N	2.49	0.41
1:C:171:LEU:HA	1:C:171:LEU:HD23	1.90	0.41
1:D:140:LEU:HA	1:D:144:SER:OG	2.21	0.41
1:E:65:ASN:HD21	1:E:67:LYS:HB2	1.85	0.41
1:B:238:MET:O	1:B:238:MET:HG3	2.19	0.41
1:D:187:GLY:N	1:D:188:PRO:CD	2.84	0.41
1:D:192:LEU:HD13	1:D:235:LEU:CD2	2.50	0.41
1:D:36:LEU:HA	1:D:267:ASN:ND2	2.36	0.41
1:F:192:LEU:HA	1:F:192:LEU:HD12	1.92	0.41
1:G:94:VAL:HG12	1:G:130:PRO:HB3	2.02	0.41
1:B:201:LEU:HD12	1:B:201:LEU:HA	1.86	0.41
1:F:58:GLU:HG2	1:F:159:ILE:HG21	2.03	0.41
1:H:209:PHE:HA	1:H:210:PRO:HD3	1.81	0.41
1:A:75:PRO:O	1:A:79:LEU:HG	2.21	0.41
1:A:85:LEU:C	1:A:90:PHE:HB2	2.37	0.41
1:H:61:LEU:HA	1:H:62:PRO:HD3	1.87	0.41
1:A:55:ALA:HB1	1:A:102:THR:HG23	2.03	0.40
1:D:207:CYS:HA	1:D:244:ASN:OD1	2.22	0.40
1:F:209:PHE:HA	1:F:210:PRO:HD3	1.81	0.40
1:H:183:SER:O	1:H:184:LEU:HB3	2.21	0.40
1:H:36:LEU:HD11	1:H:83:TYR:CD1	2.56	0.40
1:A:52:LEU:HB2	1:A:146:TYR:CD1	2.55	0.40
1:A:65:ASN:C	1:A:65:ASN:ND2	2.71	0.40
1:B:71:THR:C	1:B:105:GLU:HG2	2.41	0.40
1:D:189:ALA:O	1:D:192:LEU:HB2	2.22	0.40
1:D:161:LEU:HB2	1:D:162:PRO:HD3	2.03	0.40
1:F:74:HIS:HE1	1:F:76:ILE:HB	1.87	0.40
1:B:192:LEU:HD12	1:B:192:LEU:HA	1.90	0.40
1:C:9:PRO:HB3	2:C:286:HOH:O	2.21	0.40
1:A:137:VAL:HG12	1:A:138:ALA:N	2.37	0.40
1:E:8:ASN:HA	1:E:9:PRO:HD3	1.95	0.40
1:F:65:ASN:C	1:F:65:ASN:HD22	2.24	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	233/283 (82%)	204 (88%)	27 (12%)	2 (1%)	19	43
1	B	249/283 (88%)	232 (93%)	17 (7%)	0	100	100
1	C	241/283 (85%)	226 (94%)	14 (6%)	1 (0%)	36	63
1	D	258/283 (91%)	248 (96%)	10 (4%)	0	100	100
1	E	266/283 (94%)	251 (94%)	14 (5%)	1 (0%)	36	63
1	F	255/283 (90%)	242 (95%)	13 (5%)	0	100	100
1	G	252/283 (89%)	242 (96%)	10 (4%)	0	100	100
1	H	275/283 (97%)	256 (93%)	18 (6%)	1 (0%)	36	63
All	All	2029/2264 (90%)	1901 (94%)	123 (6%)	5 (0%)	49	76

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	36	LEU
1	A	86	HIS
1	A	87	ALA
1	E	280	ALA
1	C	279	ALA

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	192/230 (84%)	166 (86%)	26 (14%)	4	9

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	207/230 (90%)	178 (86%)	29 (14%)	4	8
1	C	202/230 (88%)	177 (88%)	25 (12%)	5	11
1	D	211/230 (92%)	185 (88%)	26 (12%)	5	12
1	E	218/230 (95%)	182 (84%)	36 (16%)	2	6
1	F	210/230 (91%)	179 (85%)	31 (15%)	3	7
1	G	210/230 (91%)	191 (91%)	19 (9%)	10	24
1	H	225/230 (98%)	190 (84%)	35 (16%)	3	7
All	All	1675/1840 (91%)	1448 (86%)	227 (14%)	4	9

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	11	VAL
1	A	13	ILE
1	A	65	ASN
1	A	76	ILE
1	A	78	THR
1	A	92	PHE
1	A	121	GLU
1	A	125	SER
1	A	131	LYS
1	A	137	VAL
1	A	139	SER
1	A	149	ILE
1	A	163	GLU
1	A	176	LYS
1	A	192	LEU
1	A	194	LEU
1	A	201	LEU
1	A	202	ASN
1	A	217	THR
1	A	223	MET
1	A	228	THR
1	A	245	ASP
1	A	272	LEU
1	A	275	GLN
1	A	277	MET
1	B	7	LYS
1	B	13	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	26	LEU
1	B	29	TYR
1	B	43	LYS
1	B	46	ARG
1	B	65	ASN
1	B	71	THR
1	B	78	THR
1	B	109	MET
1	B	115	LYS
1	B	128	ARG
1	B	137	VAL
1	B	141	ASN
1	B	144	SER
1	B	165	GLN
1	B	176	LYS
1	B	179	ARG
1	B	183	SER
1	B	192	LEU
1	B	195	ARG
1	B	198	ASP
1	B	201	LEU
1	B	217	THR
1	B	236	LYS
1	B	237	LYS
1	B	238	MET
1	B	240	MET
1	B	250	ARG
1	C	5	THR
1	C	6	SER
1	C	7	LYS
1	C	13	ILE
1	C	23	GLU
1	C	54	ILE
1	C	65	ASN
1	C	71	THR
1	C	76	ILE
1	C	78	THR
1	C	91	GLU
1	C	114	GLU
1	C	122	GLN
1	C	131	LYS
1	C	139	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	144	SER
1	C	179	ARG
1	C	192	LEU
1	C	195	ARG
1	C	201	LEU
1	C	207	CYS
1	C	217	THR
1	C	219	GLU
1	C	236	LYS
1	C	256	LYS
1	D	5	THR
1	D	8	ASN
1	D	11	VAL
1	D	13	ILE
1	D	37	ASP
1	D	46	ARG
1	D	48	LYS
1	D	78	THR
1	D	91	GLU
1	D	124	LYS
1	D	125	SER
1	D	141	ASN
1	D	144	SER
1	D	163	GLU
1	D	165	GLN
1	D	185	CYS
1	D	192	LEU
1	D	195	ARG
1	D	198	ASP
1	D	201	LEU
1	D	206	ILE
1	D	233	GLU
1	D	236	LYS
1	D	237	LYS
1	D	238	MET
1	D	250	ARG
1	E	7	LYS
1	E	8	ASN
1	E	11	VAL
1	E	23	GLU
1	E	27	SER
1	E	31	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	33	VAL
1	E	35	ASP
1	E	36	LEU
1	E	46	ARG
1	E	48	LYS
1	E	65	ASN
1	E	71	THR
1	E	73	ASN
1	E	76	ILE
1	E	78	THR
1	E	112	LYS
1	E	114	GLU
1	E	115	LYS
1	E	122	GLN
1	E	139	SER
1	E	141	ASN
1	E	144	SER
1	E	145	GLU
1	E	159	ILE
1	E	165	GLN
1	E	176	LYS
1	E	183	SER
1	E	192	LEU
1	E	195	ARG
1	E	201	LEU
1	E	217	THR
1	E	219	GLU
1	E	250	ARG
1	E	253	LYS
1	E	275	GLN
1	F	6	SER
1	F	11	VAL
1	F	13	ILE
1	F	39	VAL
1	F	43	LYS
1	F	46	ARG
1	F	50	LYS
1	F	65	ASN
1	F	78	THR
1	F	91	GLU
1	F	116	VAL
1	F	122	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	124	LYS
1	F	128	ARG
1	F	131	LYS
1	F	132	LYS
1	F	141	ASN
1	F	145	GLU
1	F	165	GLN
1	F	192	LEU
1	F	195	ARG
1	F	199	ASN
1	F	201	LEU
1	F	205	SER
1	F	217	THR
1	F	223	MET
1	F	237	LYS
1	F	240	MET
1	F	243	ILE
1	F	256	LYS
1	F	275	GLN
1	G	5	THR
1	G	11	VAL
1	G	43	LYS
1	G	46	ARG
1	G	65	ASN
1	G	71	THR
1	G	78	THR
1	G	91	GLU
1	G	116	VAL
1	G	124	LYS
1	G	128	ARG
1	G	131	LYS
1	G	141	ASN
1	G	192	LEU
1	G	195	ARG
1	G	201	LEU
1	G	256	LYS
1	G	271	LYS
1	G	281	TYR
1	H	5	THR
1	H	11	VAL
1	H	13	ILE
1	H	31	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	33	VAL
1	H	34	SER
1	H	35	ASP
1	H	37	ASP
1	H	39	VAL
1	H	43	LYS
1	H	48	LYS
1	H	59	ARG
1	H	65	ASN
1	H	78	THR
1	H	114	GLU
1	H	125	SER
1	H	141	ASN
1	H	145	GLU
1	H	149	ILE
1	H	163	GLU
1	H	165	GLN
1	H	176	LYS
1	H	183	SER
1	H	192	LEU
1	H	199	ASN
1	H	201	LEU
1	H	205	SER
1	H	217	THR
1	H	228	THR
1	H	233	GLU
1	H	241	ASN
1	H	242	ILE
1	H	256	LYS
1	H	275	GLN
1	H	277	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	65	ASN
1	A	155	HIS
1	A	177	ASN
1	A	199	ASN
1	A	202	ASN
1	A	252	HIS
1	A	267	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	141	ASN
1	B	155	HIS
1	B	199	ASN
1	B	267	ASN
1	C	10	GLN
1	C	65	ASN
1	C	199	ASN
1	C	241	ASN
1	C	267	ASN
1	D	141	ASN
1	D	155	HIS
1	D	199	ASN
1	D	267	ASN
1	E	65	ASN
1	E	122	GLN
1	E	141	ASN
1	E	155	HIS
1	E	196	HIS
1	E	199	ASN
1	E	267	ASN
1	F	49	HIS
1	F	65	ASN
1	F	141	ASN
1	F	155	HIS
1	F	199	ASN
1	F	252	HIS
1	F	267	ASN
1	G	65	ASN
1	G	141	ASN
1	G	155	HIS
1	H	65	ASN
1	H	141	ASN
1	H	155	HIS
1	H	196	HIS
1	H	199	ASN
1	H	241	ASN
1	H	267	ASN

5.3.3 RNA ⓘ

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 carbohydrates 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	H	1
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	34:SER	C	35:ASP	N	1.19
1	C	7:LYS	C	8:ASN	N	1.10

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.