



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 10:26 PM UTC

PDB ID : 4XM0 / pdb_00004xm0
Title : N,N'-diacetylchitobiose deacetylase (SeMet derivative) from *Pyrococcus furiosus* in the absence of cadmium
Authors : Nakamura, T.; Niiyama, M.; Hashimoto, W.; Ida, K.; Uegaki, K.
Deposited on : 2015-01-14
Resolution : 2.80 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

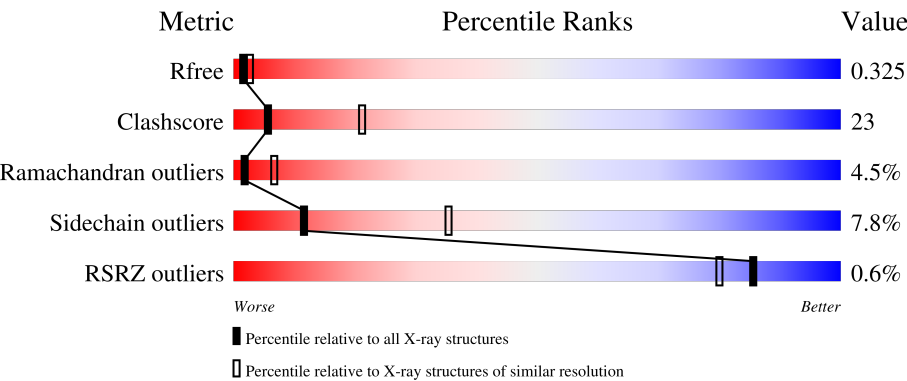
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	267	% 59%36% . .
1	B	267	% 52%36%5% . .
1	C	267	% 45%43%9% . .
1	D	267	53%39%6% .
1	E	267	43%45%9% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	267	57% 38% . .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12890 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	Se	0	0	0
			2162	1397	357	399	3	6			
1	B	255	Total	C	N	O	S	Se	0	0	0
			2089	1350	347	383	3	6			
1	C	262	Total	C	N	O	S	Se	0	0	0
			2147	1388	354	396	3	6			
1	D	262	Total	C	N	O	S	Se	0	0	0
			2147	1388	354	396	3	6			
1	E	262	Total	C	N	O	S	Se	0	0	0
			2147	1388	354	396	3	6			
1	F	264	Total	C	N	O	S	Se	0	0	0
			2162	1397	357	399	3	6			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		
2	E	1	Total	Zn	0	0
			1	1		
2	F	1	Total	Zn	0	0
			1	1		

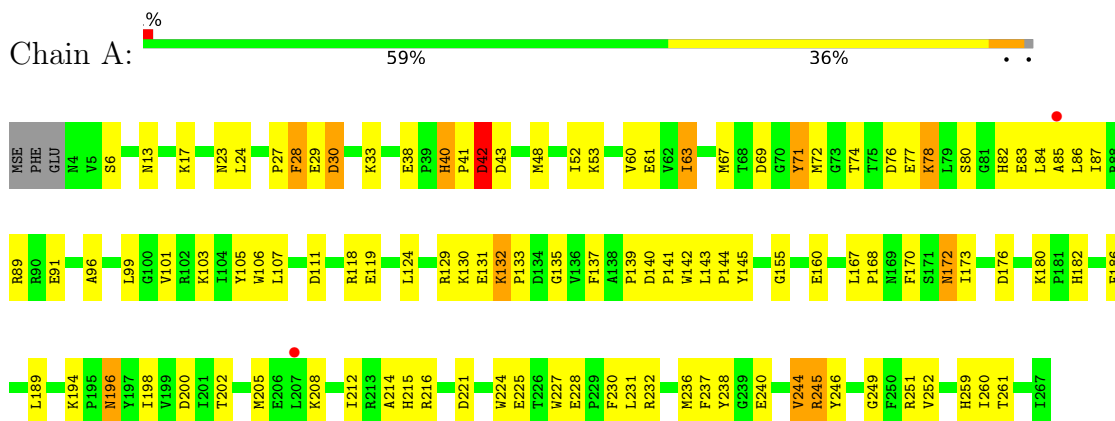
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total 4	O 4	0	0
3	B	5	Total 5	O 5	0	0
3	C	4	Total 4	O 4	0	0
3	D	4	Total 4	O 4	0	0
3	E	3	Total 3	O 3	0	0
3	F	10	Total 10	O 10	0	0

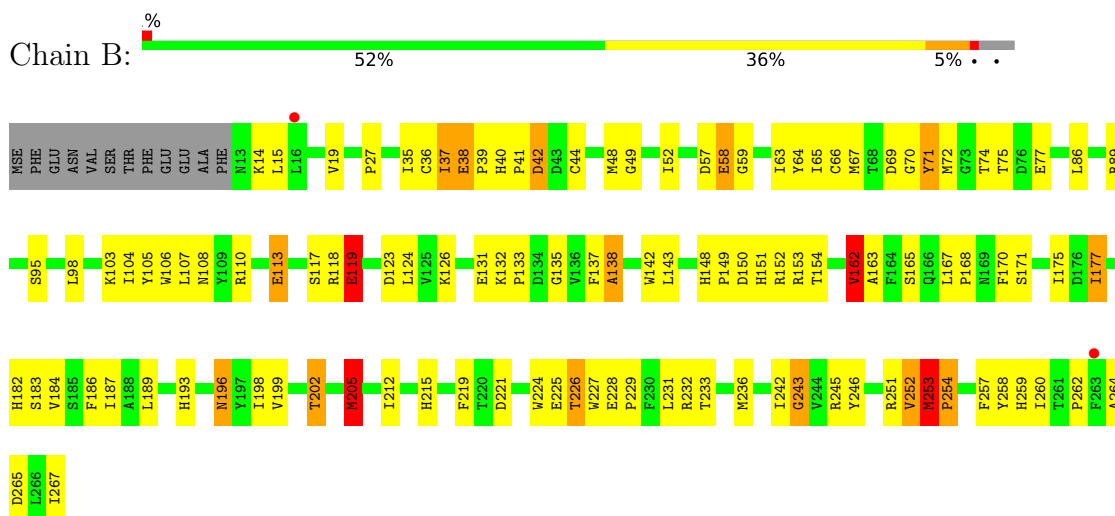
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

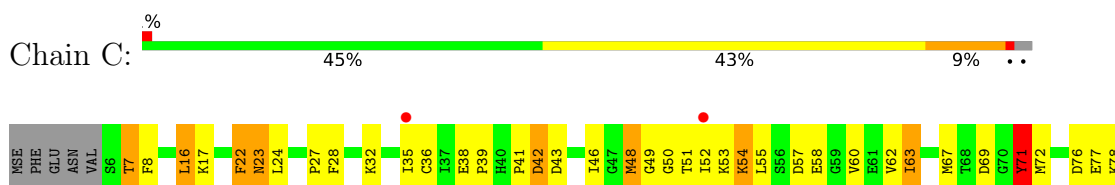
• Molecule 1: Uncharacterized protein

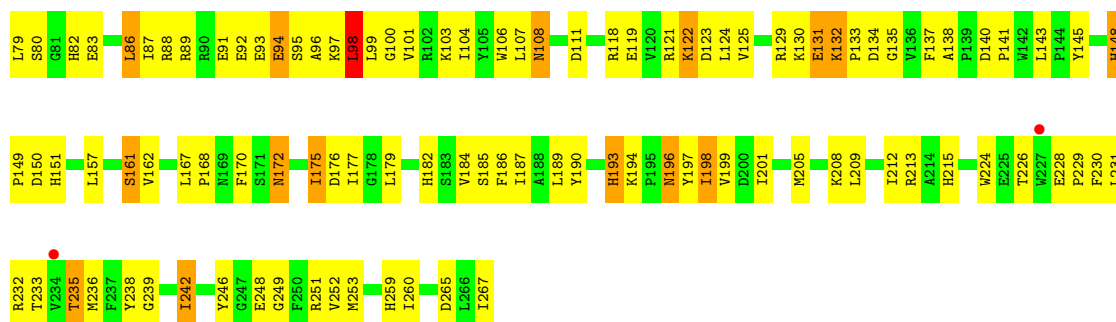


• Molecule 1: Uncharacterized protein



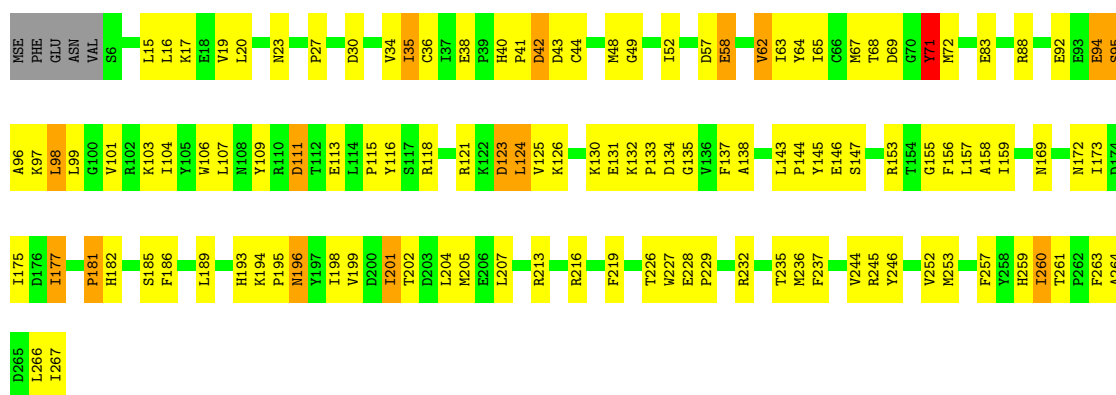
• Molecule 1: Uncharacterized protein





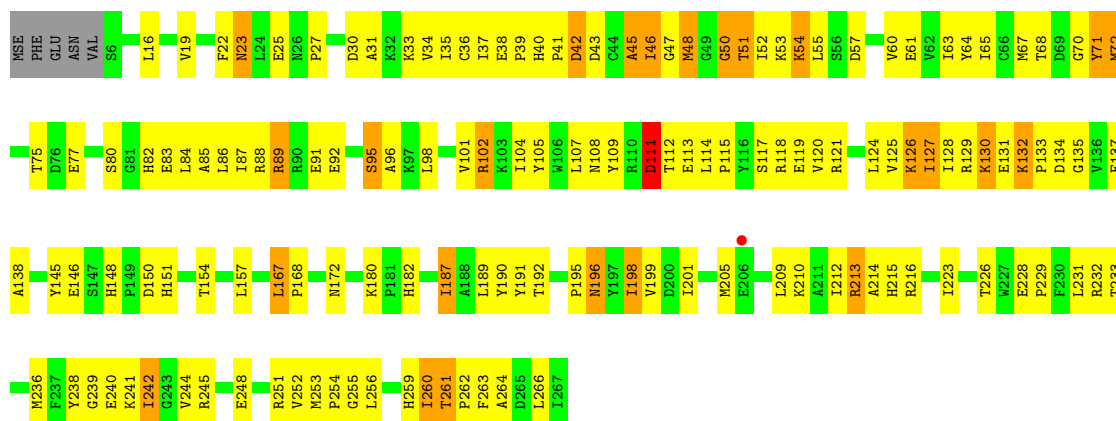
• Molecule 1: Uncharacterized protein

Chain D: 53% 39% 6%



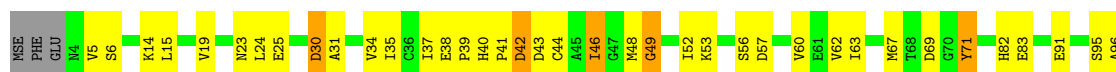
• Molecule 1: Uncharacterized protein

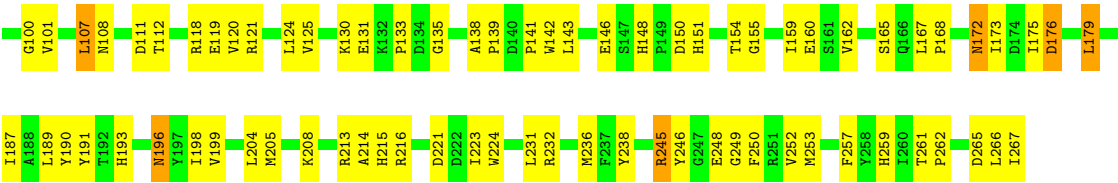
Chain E: 43% 45% 9%



• Molecule 1: Uncharacterized protein

Chain F: 57% 38% 5%





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.01Å 121.93Å 92.27Å 90.00° 114.21° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.5 (50.00-2.80) 99.5 (50.00-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.22 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.262 , 0.346 0.247 , 0.325	Depositor DCC
R_{free} test set	2034 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	70.2	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 33.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	12890	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
ZN

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	0.72	0/2213	0.99	2/2985 (0.1%)
1	B	0.71	0/2138	1.06	10/2883 (0.3%)
1	C	0.71	0/2198	1.01	2/2964 (0.1%)
1	D	0.73	0/2198	0.98	1/2964 (0.0%)
1	E	0.72	0/2198	1.03	7/2964 (0.2%)
1	F	0.74	0/2213	0.99	0/2985
All	All	0.72	0/13158	1.01	22/17745 (0.1%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	114	LEU	CA-C-N	-9.01	110.84	120.66
1	E	114	LEU	C-N-CA	-9.01	110.84	120.66
1	B	119	GLU	N-CA-C	-9.00	100.31	111.11
1	B	38	GLU	CA-C-N	8.03	127.32	118.97
1	B	38	GLU	C-N-CA	8.03	127.32	118.97
1	B	138	ALA	N-CA-C	7.80	115.02	108.07
1	C	148	HIS	CA-C-N	6.48	127.94	119.84
1	C	148	HIS	C-N-CA	6.48	127.94	119.84
1	E	261	THR	CA-C-N	6.28	125.97	119.82
1	E	261	THR	C-N-CA	6.28	125.97	119.82
1	E	167	LEU	CA-C-N	6.10	125.82	119.05
1	E	167	LEU	C-N-CA	6.10	125.82	119.05
1	B	253	MSE	CA-C-N	5.97	127.30	119.84
1	B	253	MSE	C-N-CA	5.97	127.30	119.84
1	A	261	THR	CA-C-N	5.72	125.34	119.56
1	A	261	THR	C-N-CA	5.72	125.34	119.56
1	E	117	SER	N-CA-C	5.39	116.99	108.96
1	B	74	THR	N-CA-C	5.33	116.95	108.79

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	71	TYR	N-CA-C	5.28	118.81	112.38
1	B	117	SER	N-CA-C	5.22	115.94	108.74
1	B	219	PHE	N-CA-C	5.12	115.75	108.54
1	B	205	MSE	N-CA-C	5.11	116.54	110.97

There are no chirality outliers.

There are no planarity outliers.

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	2162	0	2134	97	0
1	B	2089	0	2072	118	0
1	C	2147	0	2119	127	0
1	D	2147	0	2119	96	0
1	E	2147	0	2119	124	0
1	F	2162	0	2134	96	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	4	0	0	1	0
3	B	5	0	0	0	0
3	C	4	0	0	1	0
3	D	4	0	0	0	0
3	E	3	0	0	2	0
3	F	10	0	0	0	0
All	All	12890	0	12697	597	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 23.

All (597) 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:B:162:VAL:HG11	1:B:187:ILE:HD11	1.27	1.14
1:A:170:PHE:HB2	1:B:72:MSE:HE1	1.12	1.11
1:D:253:MSE:HE2	1:D:257:PHE:HB3	1.35	1.09
1:B:187:ILE:H	1:B:254:PRO:HG3	1.12	1.08
1:B:37:ILE:CG2	1:B:67:MSE:HE1	1.84	1.07
1:B:170:PHE:HB2	1:C:72:MSE:HE1	1.47	0.97
1:A:170:PHE:HB2	1:B:72:MSE:CE	1.95	0.96
1:B:70:GLY:O	1:B:72:MSE:N	2.02	0.93
1:B:253:MSE:H	1:B:254:PRO:CD	1.80	0.93
1:F:48:MSE:HE3	1:F:250:PHE:CE1	2.03	0.93
1:B:37:ILE:HG22	1:B:67:MSE:HE1	1.47	0.92
1:F:67:MSE:HE1	1:F:124:LEU:HD11	1.51	0.92
1:A:170:PHE:CB	1:B:72:MSE:HE1	1.98	0.91
1:B:253:MSE:N	1:B:254:PRO:HD2	1.87	0.89
1:C:130:LYS:HG3	1:C:131:GLU:OE1	1.71	0.88
1:E:64:TYR:HB2	1:E:104:ILE:HG12	1.55	0.88
1:D:62:VAL:HG12	1:D:101:VAL:HG13	1.57	0.87
1:B:37:ILE:HG21	1:B:67:MSE:HE1	1.56	0.86
1:F:196:ASN:HD21	1:F:252:VAL:H	1.19	0.86
1:A:172:ASN:HD22	1:A:172:ASN:H	1.21	0.84
1:B:67:MSE:HE3	1:B:154:THR:HG23	1.59	0.84
1:B:253:MSE:N	1:B:254:PRO:CD	2.40	0.83
1:B:253:MSE:HE2	1:B:257:PHE:HB3	1.59	0.82
1:B:196:ASN:HD21	1:B:252:VAL:H	1.28	0.82
1:F:111:ASP:OD1	1:F:112:THR:HG23	1.81	0.81
1:E:35:ILE:HD12	1:E:133:PRO:HG3	1.59	0.81
1:D:44:CYS:O	1:D:48:MSE:HB3	1.79	0.81
1:E:196:ASN:HD21	1:E:252:VAL:H	1.27	0.80
1:F:143:LEU:HD23	1:F:146:GLU:HB2	1.64	0.78
1:E:213:ARG:HH22	1:E:216:ARG:HG2	1.47	0.78
1:B:253:MSE:HE1	1:B:264:ALA:HB1	1.64	0.78
1:E:151:HIS:NE2	3:E:402:HOH:O	2.07	0.78
1:C:96:ALA:HB2	1:C:104:ILE:HD11	1.67	0.77
1:D:253:MSE:CE	1:D:257:PHE:HB3	2.14	0.76
1:A:40:HIS:CD2	1:A:111:ASP:OD2	2.38	0.76
1:E:31:ALA:O	1:E:60:VAL:HG22	1.86	0.75
1:E:48:MSE:SE	1:E:137:PHE:CD1	2.89	0.75
1:B:253:MSE:H	1:B:254:PRO:HD2	1.49	0.75
1:A:40:HIS:HD2	1:A:111:ASP:OD2	1.70	0.74
1:E:150:ASP:O	1:E:154:THR:OG1	2.05	0.74
1:A:196:ASN:HD21	1:A:252:VAL:H	1.34	0.74
1:B:37:ILE:HG22	1:B:67:MSE:CE	2.17	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:GLU:O	1:C:98:LEU:HD21	1.88	0.74
1:E:48:MSE:SE	1:E:137:PHE:HD1	2.20	0.74
1:E:95:SER:HA	1:E:98:LEU:HD12	1.69	0.74
1:A:63:ILE:HG23	1:A:103:LYS:HB3	1.70	0.73
1:A:13:ASN:O	1:A:17:LYS:HG2	1.88	0.73
1:E:253:MSE:HE1	1:E:264:ALA:HB1	1.70	0.72
1:C:172:ASN:HD22	1:C:172:ASN:H	1.35	0.72
1:F:48:MSE:HE3	1:F:250:PHE:HE1	1.55	0.71
1:B:41:PRO:HD3	1:B:66:CYS:SG	2.29	0.71
1:B:162:VAL:CG1	1:B:187:ILE:HD11	2.13	0.71
1:D:196:ASN:HD21	1:D:252:VAL:H	1.36	0.71
1:E:87:ILE:O	1:E:91:GLU:HG3	1.91	0.71
1:F:96:ALA:HB1	1:F:101:VAL:HB	1.72	0.71
1:C:72:MSE:HB2	1:C:111:ASP:OD2	1.89	0.71
1:E:132:LYS:HG3	1:E:182:HIS:ND1	2.05	0.70
1:F:53:LYS:HG2	1:F:204:LEU:HD21	1.73	0.70
1:D:253:MSE:HE1	1:D:264:ALA:HB1	1.74	0.70
1:F:232:ARG:O	1:F:236:MSE:HG3	1.93	0.69
1:C:86:LEU:HD21	1:F:83:GLU:HG3	1.72	0.69
1:C:259:HIS:NE2	3:C:403:HOH:O	2.25	0.69
1:B:133:PRO:O	1:B:182:HIS:NE2	2.25	0.69
1:A:91:GLU:OE1	1:A:215:HIS:HA	1.92	0.69
1:C:209:LEU:O	1:C:213:ARG:HG3	1.93	0.69
1:F:39:PRO:HG2	1:F:151:HIS:CD2	2.28	0.69
1:C:92:GLU:HA	1:C:215:HIS:CE1	2.27	0.68
1:F:71:TYR:O	1:F:71:TYR:CD2	2.46	0.68
1:D:253:MSE:HG2	1:D:267:ILE:HD11	1.73	0.68
1:A:119:GLU:OE1	1:D:118:ARG:NH2	2.24	0.68
1:C:251:ARG:HH21	1:C:253:MSE:HE3	1.58	0.68
1:A:135:GLY:HA3	1:A:186:PHE:CE2	2.29	0.68
1:D:205:MSE:HG3	1:D:246:TYR:CD2	2.28	0.68
1:A:96:ALA:HB1	1:A:101:VAL:HB	1.75	0.68
1:B:196:ASN:H	1:B:196:ASN:HD22	1.43	0.68
1:C:251:ARG:HH21	1:C:253:MSE:CE	2.07	0.67
1:C:28:PHE:CE2	1:C:197:TYR:HE2	2.12	0.67
1:B:251:ARG:HE	1:B:253:MSE:SE	2.27	0.67
1:E:51:THR:OG1	1:E:248:GLU:OE1	2.09	0.67
1:E:48:MSE:HE3	1:E:52:ILE:HD11	1.76	0.67
1:B:221:ASP:O	1:B:225:GLU:HB2	1.95	0.67
1:C:48:MSE:O	1:C:52:ILE:HG13	1.95	0.67
1:D:147:SER:OG	1:F:159:ILE:HG21	1.95	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:ASN:HD22	1:A:172:ASN:N	1.92	0.66
1:C:93:GLU:C	1:C:95:SER:H	2.04	0.66
1:A:72:MSE:HE1	1:C:170:PHE:HB2	1.77	0.66
1:B:162:VAL:HG12	1:B:163:ALA:N	2.11	0.66
1:E:133:PRO:O	1:E:182:HIS:NE2	2.20	0.66
1:F:53:LYS:HG2	1:F:204:LEU:CD2	2.25	0.65
1:F:216:ARG:NH2	1:F:216:ARG:HB2	2.11	0.65
1:B:187:ILE:N	1:B:254:PRO:HG3	1.98	0.65
1:B:198:ILE:HG22	1:B:199:VAL:N	2.12	0.65
1:F:141:PRO:HG3	1:F:155:GLY:HA3	1.79	0.64
1:F:143:LEU:HD13	1:F:191:TYR:O	1.96	0.64
1:E:83:GLU:O	1:E:86:LEU:N	2.32	0.63
1:A:76:ASP:C	1:A:78:LYS:H	2.06	0.63
1:D:260:ILE:HB	1:E:191:TYR:CE1	2.34	0.63
1:A:87:ILE:O	1:A:91:GLU:HG3	1.98	0.63
1:A:173:ILE:HG22	1:D:126:LYS:NZ	2.14	0.63
1:D:261:THR:HB	1:D:264:ALA:HB2	1.81	0.63
1:C:107:LEU:O	1:C:108:ASN:HB2	1.98	0.62
1:B:48:MSE:HE2	1:B:52:ILE:HG12	1.81	0.62
1:F:49:GLY:HA3	1:F:208:LYS:HG3	1.82	0.62
1:A:72:MSE:HE1	1:C:170:PHE:CB	2.30	0.62
1:C:79:LEU:CD1	1:C:83:GLU:HG2	2.29	0.62
1:F:216:ARG:HB2	1:F:216:ARG:HH21	1.62	0.62
1:D:97:LYS:C	1:D:99:LEU:H	2.07	0.62
1:A:74:THR:HG22	1:A:84:LEU:HD22	1.82	0.62
1:E:40:HIS:CE1	1:E:148:HIS:NE2	2.67	0.62
1:D:193:HIS:C	1:D:195:PRO:HD3	2.25	0.62
1:E:40:HIS:HE1	1:E:148:HIS:NE2	1.98	0.62
1:F:141:PRO:HD2	1:F:142:TRP:CE3	2.34	0.61
1:B:48:MSE:O	1:B:52:ILE:HG13	2.00	0.61
1:D:68:THR:HA	1:D:109:TYR:O	2.00	0.61
1:A:76:ASP:O	1:A:78:LYS:N	2.32	0.61
1:A:83:GLU:HB2	1:E:86:LEU:HD22	1.81	0.61
1:D:259:HIS:HE1	1:E:151:HIS:CD2	2.18	0.61
1:D:143:LEU:HD12	1:D:144:PRO:HD2	1.83	0.61
1:E:40:HIS:HE1	1:E:148:HIS:CD2	2.19	0.61
1:B:35:ILE:HD12	1:B:133:PRO:HG3	1.83	0.60
1:C:212:ILE:HG22	1:C:212:ILE:O	2.02	0.60
1:E:226:THR:O	1:E:229:PRO:HD2	2.02	0.60
1:B:107:LEU:HD11	1:B:123:ASP:HB3	1.83	0.60
1:B:162:VAL:HG11	1:B:187:ILE:CD1	2.18	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:LYS:O	1:C:99:LEU:N	2.35	0.60
1:B:67:MSE:CE	1:B:154:THR:HG23	2.31	0.60
1:D:38:GLU:HB2	1:D:43:ASP:HB2	1.83	0.60
1:E:259:HIS:HE1	1:F:151:HIS:CE1	2.20	0.60
1:C:97:LYS:C	1:C:99:LEU:H	2.09	0.59
1:C:118:ARG:NH2	1:E:119:GLU:OE1	2.34	0.59
1:E:35:ILE:CD1	1:E:133:PRO:HG3	2.30	0.59
1:A:33:LYS:HD3	1:A:63:ILE:HD11	1.84	0.59
1:E:67:MSE:SE	1:E:124:LEU:HD21	2.52	0.59
1:A:143:LEU:HD12	1:A:144:PRO:HD2	1.84	0.59
1:B:63:ILE:HG23	1:B:103:LYS:O	2.03	0.59
1:B:205:MSE:HG3	1:B:246:TYR:CD2	2.38	0.59
1:A:48:MSE:SE	1:A:137:PHE:HB3	2.53	0.59
1:C:92:GLU:HA	1:C:215:HIS:HE1	1.66	0.59
1:F:107:LEU:O	1:F:108:ASN:HB2	2.03	0.59
1:D:113:GLU:O	1:D:115:PRO:HD3	2.02	0.59
1:B:170:PHE:CB	1:C:72:MSE:HE1	2.30	0.59
1:A:208:LYS:HE2	1:A:212:ILE:HD11	1.85	0.58
1:C:87:ILE:O	1:C:91:GLU:HG3	2.02	0.58
1:C:172:ASN:H	1:C:172:ASN:ND2	2.01	0.58
1:A:198:ILE:HD13	1:A:249:GLY:HA2	1.85	0.58
1:B:148:HIS:HD2	1:B:149:PRO:HD2	1.68	0.58
1:E:61:GLU:OE2	1:E:102:ARG:NH2	2.37	0.58
1:D:228:GLU:O	1:D:232:ARG:HG3	2.03	0.58
1:E:151:HIS:CE1	3:E:402:HOH:O	2.53	0.58
1:F:31:ALA:O	1:F:60:VAL:HG22	2.04	0.58
1:F:138:ALA:O	1:F:189:LEU:HA	2.03	0.58
1:C:41:PRO:HG2	1:C:88:ARG:HE	1.68	0.58
1:E:187:ILE:HD12	1:E:187:ILE:H	1.69	0.58
1:E:209:LEU:O	1:E:213:ARG:CG	2.52	0.58
1:A:33:LYS:HG3	1:A:61:GLU:HG2	1.86	0.58
1:F:91:GLU:HB3	1:F:215:HIS:HA	1.86	0.58
1:F:265:ASP:OD1	1:F:266:LEU:HG	2.02	0.58
1:A:168:PRO:HB3	1:B:77:GLU:HG2	1.86	0.58
1:E:71:TYR:HD2	1:E:72:MSE:HG2	1.69	0.58
1:E:233:THR:HA	1:E:236:MSE:HE3	1.85	0.58
1:E:38:GLU:HB2	1:E:43:ASP:HB2	1.86	0.57
1:B:253:MSE:H	1:B:254:PRO:HD3	1.66	0.57
1:D:138:ALA:O	1:D:189:LEU:HA	2.04	0.57
1:E:37:ILE:O	1:E:190:TYR:OH	2.22	0.57
1:E:130:LYS:O	1:E:132:LYS:N	2.38	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ARG:O	1:B:119:GLU:C	2.46	0.57
1:B:232:ARG:O	1:B:236:MSE:HG3	2.03	0.57
1:D:123:ASP:O	1:D:124:LEU:C	2.48	0.57
1:F:253:MSE:HG2	1:F:267:ILE:HD11	1.86	0.57
1:C:7:THR:HG22	1:C:8:PHE:H	1.70	0.57
1:F:139:PRO:HA	1:F:190:TYR:O	2.05	0.57
1:B:123:ASP:O	1:B:124:LEU:C	2.47	0.57
1:A:133:PRO:HD2	1:A:182:HIS:CD2	2.39	0.56
1:C:67:MSE:SE	1:C:107:LEU:HD12	2.55	0.56
1:F:34:VAL:HG12	1:F:135:GLY:HA3	1.86	0.56
1:A:214:ALA:O	1:A:216:ARG:NH2	2.39	0.56
1:B:48:MSE:SE	1:B:137:PHE:CD1	3.08	0.56
1:C:122:LYS:HE3	1:E:119:GLU:OE2	2.05	0.56
1:D:237:PHE:CE2	1:F:262:PRO:HB2	2.41	0.56
1:A:38:GLU:HB2	1:A:43:ASP:HB2	1.88	0.56
1:C:201:ILE:HG12	1:C:248:GLU:HG3	1.88	0.56
1:D:15:LEU:HA	1:D:19:VAL:HG23	1.87	0.56
1:D:64:TYR:HB2	1:D:104:ILE:HG12	1.88	0.56
1:A:198:ILE:HD12	1:A:238:TYR:HB3	1.86	0.56
1:A:74:THR:O	1:C:168:PRO:HD2	2.04	0.56
1:D:219:PHE:HE1	1:D:227:TRP:CE3	2.24	0.56
1:A:129:ARG:NH2	1:A:167:LEU:O	2.38	0.56
1:D:123:ASP:O	1:D:126:LYS:N	2.38	0.56
1:E:40:HIS:CD2	1:E:111:ASP:OD2	2.59	0.56
1:E:196:ASN:HD22	1:E:196:ASN:H	1.54	0.56
1:D:48:MSE:HE1	1:D:137:PHE:CE1	2.41	0.56
1:D:97:LYS:O	1:D:99:LEU:N	2.38	0.56
1:D:158:ALA:O	1:D:159:ILE:C	2.49	0.56
1:C:62:VAL:O	1:C:101:VAL:HG13	2.05	0.55
1:C:98:LEU:H	1:C:98:LEU:HD23	1.70	0.55
1:D:58:GLU:N	1:D:58:GLU:CD	2.64	0.55
1:C:94:GLU:C	1:C:98:LEU:HD21	2.30	0.55
1:A:118:ARG:NH1	1:B:113:GLU:OE2	2.30	0.55
1:C:198:ILE:HA	1:C:249:GLY:HA2	1.89	0.55
1:A:194:LYS:HB3	1:A:251:ARG:NH1	2.21	0.55
1:C:131:GLU:HB2	1:C:133:PRO:HD3	1.89	0.55
1:D:198:ILE:HG22	1:D:199:VAL:N	2.22	0.55
1:C:135:GLY:HA3	1:C:186:PHE:CE2	2.42	0.55
1:D:132:LYS:HA	1:D:182:HIS:CD2	2.41	0.55
1:D:196:ASN:N	1:D:196:ASN:HD22	2.03	0.55
1:E:259:HIS:CE1	1:F:151:HIS:CE1	2.94	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:ASN:HD22	1:A:196:ASN:H	1.53	0.55
1:C:79:LEU:HD11	1:C:83:GLU:HG2	1.89	0.55
1:E:38:GLU:HB2	1:E:43:ASP:CB	2.37	0.55
1:A:82:HIS:O	1:E:82:HIS:HB3	2.07	0.55
1:A:130:LYS:HG2	1:D:177:ILE:HG22	1.89	0.55
1:B:196:ASN:H	1:B:196:ASN:ND2	2.05	0.54
1:E:198:ILE:HG22	1:E:199:VAL:N	2.22	0.54
1:A:41:PRO:O	1:A:42:ASP:HB3	2.06	0.54
1:A:237:PHE:HB2	1:C:8:PHE:CE1	2.42	0.54
1:E:40:HIS:HB3	1:E:41:PRO:HD2	1.88	0.54
1:D:16:LEU:HA	1:D:20:LEU:HD12	1.90	0.54
1:A:145:TYR:HE2	1:C:265:ASP:HB3	1.73	0.54
1:F:198:ILE:HD13	1:F:249:GLY:HA2	1.88	0.54
1:C:51:THR:O	1:C:55:LEU:HG	2.08	0.54
1:C:91:GLU:O	1:C:94:GLU:HB2	2.08	0.54
1:D:253:MSE:CE	1:D:264:ALA:HB1	2.38	0.54
1:E:138:ALA:O	1:E:189:LEU:HA	2.08	0.54
1:F:213:ARG:NH2	1:F:221:ASP:OD2	2.41	0.54
1:C:194:LYS:HB3	1:C:251:ARG:NH1	2.23	0.54
1:F:175:ILE:HA	1:F:179:LEU:O	2.07	0.54
1:B:64:TYR:HB2	1:B:104:ILE:HG23	1.89	0.54
1:C:232:ARG:O	1:C:236:MSE:HG3	2.07	0.54
1:D:36:CYS:HB3	1:D:44:CYS:SG	2.48	0.54
1:E:115:PRO:HD2	1:E:120:VAL:HG21	1.88	0.54
1:B:182:HIS:CG	1:B:183:SER:N	2.76	0.53
1:F:52:ILE:HG23	1:F:62:VAL:HG11	1.90	0.53
1:B:40:HIS:CE1	1:B:148:HIS:CE1	2.96	0.53
1:B:228:GLU:HB3	1:B:229:PRO:HD3	1.91	0.53
1:A:232:ARG:O	1:A:236:MSE:HG3	2.08	0.53
1:D:196:ASN:HD22	1:D:196:ASN:H	1.57	0.53
1:E:125:VAL:HG12	1:E:129:ARG:HD2	1.90	0.53
1:A:131:GLU:O	1:A:132:LYS:C	2.50	0.53
1:B:123:ASP:O	1:B:126:LYS:N	2.38	0.53
1:E:41:PRO:O	1:E:42:ASP:HB3	2.07	0.53
1:D:38:GLU:OE1	1:D:44:CYS:HB2	2.09	0.53
1:E:82:HIS:O	1:E:85:ALA:HB3	2.08	0.53
1:A:224:TRP:CE2	1:A:228:GLU:HB2	2.44	0.53
1:B:37:ILE:CG2	1:B:67:MSE:CE	2.73	0.53
1:B:226:THR:O	1:B:229:PRO:HD2	2.09	0.53
1:A:83:GLU:C	1:A:85:ALA:N	2.62	0.53
1:C:235:THR:HB	1:C:246:TYR:HD1	1.74	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:ILE:HG13	1:B:243:GLY:H	1.74	0.52
1:C:32:LYS:O	1:C:60:VAL:HA	2.09	0.52
1:D:123:ASP:O	1:D:125:VAL:N	2.42	0.52
1:A:72:MSE:HE1	1:C:170:PHE:CA	2.39	0.52
1:A:259:HIS:NE2	3:A:402:HOH:O	2.34	0.52
1:F:69:ASP:C	1:F:69:ASP:OD1	2.53	0.52
1:B:41:PRO:O	1:B:42:ASP:CG	2.51	0.52
1:C:175:ILE:HA	1:C:179:LEU:O	2.10	0.52
1:C:198:ILE:HD13	1:C:249:GLY:HA3	1.91	0.52
1:F:30:ASP:OD1	1:F:30:ASP:N	2.42	0.52
1:C:16:LEU:HD12	1:C:17:LYS:HG3	1.92	0.52
1:D:65:ILE:HG21	1:D:124:LEU:CD2	2.40	0.52
1:F:40:HIS:HB3	1:F:41:PRO:HD2	1.91	0.52
1:D:259:HIS:CE1	1:E:151:HIS:CD2	2.98	0.52
1:E:50:GLY:O	1:E:52:ILE:N	2.43	0.52
1:E:259:HIS:CE1	1:E:260:ILE:HG23	2.44	0.52
1:A:135:GLY:HA3	1:A:186:PHE:CZ	2.45	0.52
1:F:38:GLU:HB3	1:F:44:CYS:SG	2.50	0.52
1:C:123:ASP:O	1:C:124:LEU:C	2.53	0.52
1:C:251:ARG:NH2	1:C:253:MSE:HE3	2.24	0.52
1:E:228:GLU:HB3	1:E:229:PRO:HD3	1.92	0.52
1:C:23:ASN:OD1	1:C:23:ASN:N	2.42	0.51
1:D:145:TYR:HA	1:F:142:TRP:CZ2	2.45	0.51
1:C:198:ILE:HB	1:C:242:ILE:HG12	1.92	0.51
1:D:204:LEU:O	1:D:207:LEU:HB3	2.10	0.51
1:E:205:MSE:HE1	1:E:232:ARG:HG2	1.93	0.51
1:B:138:ALA:O	1:B:189:LEU:HA	2.11	0.51
1:B:148:HIS:CD2	1:B:149:PRO:HD2	2.46	0.51
1:E:40:HIS:CE1	1:E:148:HIS:CD2	2.99	0.51
1:B:253:MSE:HG2	1:B:267:ILE:HD11	1.93	0.51
1:E:50:GLY:HA3	1:E:201:ILE:HG21	1.91	0.51
1:E:130:LYS:C	1:E:132:LYS:H	2.18	0.51
1:D:34:VAL:HG23	1:D:62:VAL:HG22	1.93	0.51
1:E:213:ARG:NH2	1:E:216:ARG:HG2	2.21	0.50
1:E:213:ARG:HH12	1:E:216:ARG:HG2	1.77	0.50
1:D:44:CYS:O	1:D:48:MSE:CB	2.57	0.50
1:D:69:ASP:OD1	1:D:71:TYR:CB	2.60	0.50
1:C:53:LYS:C	1:C:55:LEU:H	2.19	0.50
1:D:38:GLU:HB3	1:D:44:CYS:SG	2.52	0.50
1:F:56:SER:OG	1:F:100:GLY:HA3	2.11	0.50
1:A:118:ARG:O	1:A:119:GLU:C	2.55	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:ILE:HG22	1:B:199:VAL:H	1.77	0.50
1:E:68:THR:HA	1:E:109:TYR:O	2.12	0.50
1:A:173:ILE:HG22	1:D:126:LYS:HZ2	1.76	0.49
1:E:45:ALA:O	1:E:47:GLY:N	2.45	0.49
1:F:44:CYS:O	1:F:48:MSE:HB2	2.12	0.49
1:C:134:ASP:O	1:C:185:SER:HB2	2.11	0.49
1:F:67:MSE:HE1	1:F:124:LEU:HD21	1.93	0.49
1:C:208:LYS:HE3	1:C:248:GLU:OE2	2.11	0.49
1:E:33:LYS:HG2	1:E:133:PRO:HB3	1.93	0.49
1:A:72:MSE:CE	1:C:170:PHE:HB2	2.41	0.49
1:B:205:MSE:HG3	1:B:246:TYR:CG	2.48	0.49
1:E:50:GLY:O	1:E:51:THR:C	2.55	0.49
1:D:196:ASN:N	1:D:196:ASN:ND2	2.58	0.49
1:A:196:ASN:ND2	1:A:251:ARG:HA	2.27	0.49
1:B:170:PHE:HB2	1:C:72:MSE:CE	2.31	0.49
1:E:45:ALA:O	1:E:46:ILE:C	2.55	0.49
1:E:212:ILE:HD13	1:E:231:LEU:HD22	1.94	0.49
1:F:190:TYR:O	1:F:191:TYR:HB2	2.13	0.49
1:E:34:VAL:HG12	1:E:135:GLY:HA3	1.95	0.49
1:A:118:ARG:HD3	1:B:113:GLU:OE2	2.13	0.49
1:B:119:GLU:CD	1:F:118:ARG:HE	2.21	0.49
1:C:253:MSE:HG2	1:C:267:ILE:HD11	1.94	0.49
1:F:46:ILE:HG23	1:F:231:LEU:HD21	1.95	0.49
1:B:36:CYS:HA	1:B:137:PHE:HB2	1.95	0.48
1:B:105:TYR:OH	1:B:131:GLU:OE2	2.31	0.48
1:A:80:SER:HB3	1:E:89:ARG:HH11	1.78	0.48
1:E:23:ASN:N	1:E:23:ASN:HD22	2.11	0.48
1:C:129:ARG:NH2	1:C:167:LEU:O	2.46	0.48
1:B:107:LEU:O	1:B:108:ASN:HB2	2.13	0.48
1:D:135:GLY:HA3	1:D:186:PHE:CZ	2.47	0.48
1:B:64:TYR:CB	1:B:104:ILE:HG23	2.43	0.48
1:B:131:GLU:O	1:B:132:LYS:C	2.56	0.48
1:E:190:TYR:CD2	1:E:191:TYR:CD2	3.02	0.48
1:A:173:ILE:HD11	1:D:107:LEU:HD23	1.96	0.48
1:A:200:ASP:OD2	1:A:244:VAL:HG11	2.12	0.48
1:B:70:GLY:O	1:B:71:TYR:C	2.57	0.48
1:B:262:PRO:O	1:C:193:HIS:HB2	2.14	0.48
1:E:195:PRO:HG3	1:E:238:TYR:CE1	2.48	0.48
1:F:205:MSE:HE3	1:F:208:LYS:HB3	1.95	0.48
1:A:83:GLU:O	1:A:86:LEU:N	2.47	0.48
1:B:227:TRP:O	1:B:231:LEU:HG	2.12	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:LYS:O	1:C:100:GLY:N	2.40	0.48
1:E:16:LEU:HD22	1:E:22:PHE:HB3	1.96	0.48
1:B:86:LEU:HD21	1:D:83:GLU:HG3	1.96	0.48
1:B:229:PRO:O	1:B:233:THR:OG1	2.27	0.48
1:C:55:LEU:O	1:C:60:VAL:HB	2.13	0.48
1:D:97:LYS:C	1:D:99:LEU:N	2.72	0.48
1:D:236:MSE:HE1	1:F:6:SER:O	2.13	0.48
1:B:48:MSE:HE2	1:B:52:ILE:CG1	2.44	0.48
1:C:95:SER:HA	1:C:98:LEU:HG	1.95	0.48
1:D:69:ASP:OD1	1:D:71:TYR:HB2	2.14	0.48
1:E:91:GLU:CD	1:E:215:HIS:HA	2.39	0.48
1:F:69:ASP:OD1	1:F:71:TYR:HB2	2.14	0.48
1:C:138:ALA:O	1:C:189:LEU:HA	2.14	0.48
1:E:63:ILE:HG21	1:E:105:TYR:HE2	1.77	0.48
1:E:129:ARG:NH2	1:E:167:LEU:O	2.46	0.48
1:F:95:SER:HB2	1:F:214:ALA:HB3	1.95	0.48
1:A:48:MSE:O	1:A:52:ILE:HG13	2.14	0.47
1:C:121:ARG:HB3	1:C:170:PHE:HZ	1.78	0.47
1:E:53:LYS:NZ	1:E:57:ASP:OD1	2.47	0.47
1:F:205:MSE:HG2	1:F:246:TYR:CE2	2.49	0.47
1:C:233:THR:HA	1:C:236:MSE:HE2	1.95	0.47
1:E:92:GLU:HB2	1:E:215:HIS:HE1	1.79	0.47
1:C:49:GLY:O	1:C:99:LEU:HD22	2.13	0.47
1:D:201:ILE:HD12	1:D:205:MSE:HG2	1.96	0.47
1:E:167:LEU:HA	1:E:168:PRO:HD2	1.68	0.47
1:F:120:VAL:O	1:F:121:ARG:C	2.57	0.47
1:F:131:GLU:HB2	1:F:133:PRO:HD3	1.96	0.47
1:A:173:ILE:HG22	1:D:126:LYS:HZ1	1.79	0.47
1:A:173:ILE:CG2	1:D:126:LYS:HZ1	2.26	0.47
1:B:72:MSE:HE3	1:B:72:MSE:HB3	1.75	0.47
1:C:36:CYS:HA	1:C:137:PHE:HB2	1.97	0.47
1:C:39:PRO:HA	1:C:67:MSE:HB2	1.95	0.47
1:C:71:TYR:CD2	1:C:71:TYR:O	2.67	0.47
1:C:228:GLU:N	1:C:229:PRO:CD	2.78	0.47
1:A:96:ALA:CB	1:A:101:VAL:HB	2.44	0.47
1:A:140:ASP:HA	1:A:141:PRO:HD3	1.82	0.47
1:C:54:LYS:O	1:C:54:LYS:HG2	2.15	0.47
1:C:63:ILE:HD12	1:C:131:GLU:HG3	1.97	0.47
1:E:132:LYS:HG3	1:E:182:HIS:CE1	2.49	0.47
1:E:67:MSE:HA	1:E:107:LEU:HD12	1.96	0.47
1:C:41:PRO:O	1:C:42:ASP:OD2	2.32	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:ILE:HG22	1:C:199:VAL:H	1.80	0.47
1:F:198:ILE:HG22	1:F:199:VAL:N	2.30	0.47
1:F:257:PHE:CE2	1:F:267:ILE:HG12	2.49	0.47
1:C:71:TYR:CD2	1:C:71:TYR:C	2.93	0.46
1:F:67:MSE:HE2	1:F:154:THR:HG23	1.97	0.46
1:A:83:GLU:O	1:A:84:LEU:C	2.57	0.46
1:B:162:VAL:HG12	1:B:163:ALA:H	1.80	0.46
1:D:259:HIS:CE1	1:D:260:ILE:HG23	2.50	0.46
1:E:55:LEU:O	1:E:60:VAL:HB	2.15	0.46
1:E:196:ASN:HD22	1:E:196:ASN:N	2.11	0.46
1:F:213:ARG:HD2	1:F:224:TRP:CD2	2.50	0.46
1:B:175:ILE:HD12	1:B:175:ILE:H	1.80	0.46
1:C:205:MSE:O	1:C:209:LEU:HG	2.16	0.46
1:A:24:LEU:HA	1:A:27:PRO:HG3	1.98	0.46
1:E:130:LYS:C	1:E:132:LYS:N	2.74	0.46
1:E:261:THR:HA	1:E:262:PRO:HD2	1.84	0.46
1:B:182:HIS:CG	1:B:183:SER:H	2.34	0.46
1:B:253:MSE:CE	1:B:264:ALA:HB1	2.38	0.46
1:E:96:ALA:HB1	1:E:101:VAL:HB	1.98	0.46
1:F:39:PRO:CG	1:F:151:HIS:CD2	2.98	0.46
1:B:259:HIS:HE1	1:C:151:HIS:CD2	2.33	0.46
1:B:149:PRO:O	1:B:153:ARG:HG3	2.16	0.46
1:A:89:ARG:HG3	1:A:106:TRP:CE2	2.51	0.46
1:C:82:HIS:O	1:C:83:GLU:C	2.59	0.46
1:C:119:GLU:OE1	1:E:118:ARG:NH2	2.41	0.46
1:D:35:ILE:HG13	1:D:133:PRO:HG3	1.98	0.46
1:D:41:PRO:O	1:D:42:ASP:HB3	2.15	0.46
1:C:196:ASN:HD21	1:C:252:VAL:H	1.64	0.46
1:E:263:PHE:HB2	1:E:266:LEU:HD12	1.98	0.46
1:D:92:GLU:HB3	1:D:106:TRP:HH2	1.80	0.45
1:D:260:ILE:HB	1:E:191:TYR:HE1	1.80	0.45
1:A:196:ASN:HD22	1:A:196:ASN:N	2.13	0.45
1:A:227:TRP:HA	1:A:230:PHE:HB3	1.98	0.45
1:E:259:HIS:HE1	1:F:151:HIS:ND1	2.12	0.45
1:F:172:ASN:HD22	1:F:173:ILE:N	2.15	0.45
1:B:198:ILE:CG2	1:B:199:VAL:N	2.78	0.45
1:D:40:HIS:HD2	1:D:68:THR:OG1	1.99	0.45
1:D:144:PRO:HD3	1:D:193:HIS:CE1	2.51	0.45
1:E:41:PRO:O	1:E:42:ASP:CB	2.63	0.45
1:A:240:GLU:OE1	1:C:8:PHE:HB3	2.17	0.45
1:D:253:MSE:HE2	1:D:257:PHE:CB	2.26	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:LYS:C	1:E:55:LEU:H	2.23	0.45
1:F:198:ILE:HD12	1:F:238:TYR:HB3	1.97	0.45
1:B:42:ASP:HB3	1:B:215:HIS:CE1	2.50	0.45
1:C:69:ASP:OD2	1:F:82:HIS:CE1	2.70	0.45
1:C:131:GLU:O	1:C:132:LYS:HB2	2.16	0.45
1:D:96:ALA:HB1	1:D:101:VAL:HB	1.98	0.45
1:C:87:ILE:O	1:C:91:GLU:CG	2.64	0.45
1:A:172:ASN:N	1:A:172:ASN:ND2	2.61	0.45
1:C:48:MSE:SE	1:C:137:PHE:CD1	3.19	0.45
1:F:236:MSE:HE3	1:F:245:ARG:HD3	1.98	0.45
1:A:67:MSE:SE	1:A:124:LEU:HD21	2.67	0.45
1:B:148:HIS:CD2	1:B:150:ASP:HB2	2.52	0.45
1:B:151:HIS:O	1:B:152:ARG:C	2.60	0.45
1:D:175:ILE:HD12	1:D:181:PRO:HD3	1.97	0.45
1:E:157:LEU:HD23	1:E:157:LEU:HA	1.76	0.45
1:F:121:ARG:NH2	1:F:160:GLU:OE1	2.44	0.45
1:B:15:LEU:HD21	1:C:230:PHE:HA	1.98	0.45
1:D:263:PHE:HB2	1:D:266:LEU:HD12	1.98	0.45
1:C:41:PRO:O	1:C:42:ASP:CG	2.60	0.44
1:C:86:LEU:HD12	1:C:89:ARG:HH11	1.81	0.44
1:A:89:ARG:HG3	1:A:106:TRP:CZ2	2.52	0.44
1:B:135:GLY:HA3	1:B:186:PHE:CE2	2.52	0.44
1:D:63:ILE:HG23	1:D:103:LYS:O	2.17	0.44
1:A:72:MSE:HE1	1:C:170:PHE:HA	1.99	0.44
1:A:205:MSE:HG2	1:A:246:TYR:CD2	2.53	0.44
1:D:94:GLU:O	1:D:96:ALA:N	2.51	0.44
1:C:48:MSE:HG3	1:C:190:TYR:CG	2.51	0.44
1:D:169:ASN:HD21	1:E:80:SER:HA	1.81	0.44
1:E:112:THR:C	1:E:113:GLU:HG3	2.42	0.44
1:E:195:PRO:HG3	1:E:238:TYR:HE1	1.82	0.44
1:F:39:PRO:CB	1:F:151:HIS:CD2	3.00	0.44
1:A:83:GLU:C	1:A:85:ALA:H	2.26	0.44
1:B:57:ASP:C	1:B:59:GLY:H	2.26	0.44
1:B:65:ILE:HG23	1:B:107:LEU:HD23	1.99	0.44
1:B:167:LEU:HA	1:B:168:PRO:HD2	1.80	0.44
1:B:170:PHE:O	1:B:171:SER:C	2.60	0.44
1:C:48:MSE:HE2	1:C:52:ILE:CG1	2.46	0.44
1:D:123:ASP:C	1:D:125:VAL:N	2.75	0.44
1:E:187:ILE:HD12	1:E:187:ILE:N	2.31	0.44
1:A:140:ASP:HB2	1:A:189:LEU:HB3	2.00	0.44
1:C:119:GLU:CD	1:E:118:ARG:HE	2.26	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:41:PRO:O	1:D:88:ARG:NH2	2.46	0.44
1:F:162:VAL:HG21	1:F:187:ILE:HG12	1.98	0.44
1:A:172:ASN:H	1:A:172:ASN:ND2	1.99	0.44
1:B:89:ARG:NH2	1:B:106:TRP:CD1	2.86	0.44
1:B:196:ASN:HD22	1:B:196:ASN:N	2.06	0.44
1:C:50:GLY:H	1:C:208:LYS:CE	2.30	0.44
1:D:67:MSE:SE	1:D:124:LEU:HD21	2.68	0.44
1:E:63:ILE:HG21	1:E:105:TYR:CE2	2.52	0.44
1:E:71:TYR:HB3	1:E:111:ASP:HB2	2.00	0.44
1:E:118:ARG:O	1:E:121:ARG:HB2	2.18	0.44
1:A:139:PRO:O	1:A:155:GLY:HA3	2.18	0.44
1:D:67:MSE:SE	1:D:124:LEU:HD11	2.68	0.44
1:E:201:ILE:HD12	1:E:205:MSE:HG2	1.99	0.44
1:A:260:ILE:HA	1:B:143:LEU:HD21	1.99	0.44
1:C:52:ILE:HG23	1:C:62:VAL:HG11	1.99	0.44
1:F:38:GLU:HB2	1:F:43:ASP:HB2	1.99	0.44
1:A:41:PRO:O	1:A:42:ASP:CB	2.65	0.43
1:B:162:VAL:CG1	1:B:163:ALA:N	2.81	0.43
1:C:89:ARG:HG2	1:C:106:TRP:CZ2	2.53	0.43
1:C:118:ARG:O	1:C:119:GLU:C	2.59	0.43
1:A:53:LYS:HB2	1:A:99:LEU:CD2	2.48	0.43
1:D:226:THR:C	1:D:229:PRO:HD2	2.43	0.43
1:E:38:GLU:O	1:E:67:MSE:HG2	2.19	0.43
1:E:126:LYS:O	1:E:128:ILE:N	2.51	0.43
1:B:42:ASP:HB3	1:B:215:HIS:CD2	2.53	0.43
1:C:35:ILE:HA	1:C:63:ILE:O	2.18	0.43
1:C:212:ILE:O	1:C:212:ILE:CG2	2.65	0.43
1:D:146:GLU:OE2	1:F:259:HIS:HA	2.18	0.43
1:F:14:LYS:O	1:F:19:VAL:HG23	2.18	0.43
1:B:142:TRP:CE3	1:C:145:TYR:HD1	2.36	0.43
1:C:48:MSE:SE	1:C:137:PHE:CG	3.21	0.43
1:E:65:ILE:HD11	1:E:127:ILE:HG21	2.00	0.43
1:E:107:LEU:O	1:E:108:ASN:HB2	2.18	0.43
1:C:69:ASP:OD2	1:F:82:HIS:HE1	2.01	0.43
1:C:148:HIS:NE2	1:C:150:ASP:OD2	2.35	0.43
1:B:135:GLY:HA3	1:B:186:PHE:CZ	2.53	0.43
1:E:70:GLY:HA3	1:E:88:ARG:HD3	2.00	0.43
1:C:49:GLY:HA2	1:C:52:ILE:HD12	2.00	0.43
1:D:52:ILE:HG23	1:D:62:VAL:HG11	2.00	0.43
1:F:35:ILE:CD1	1:F:133:PRO:HG3	2.48	0.43
1:B:38:GLU:HA	1:B:39:PRO:HD3	1.87	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:ASP:OD1	1:C:141:PRO:HD2	2.19	0.43
1:D:121:ARG:HG3	1:D:157:LEU:HD22	2.01	0.43
1:C:38:GLU:HB2	1:C:43:ASP:HB2	2.01	0.43
1:B:69:ASP:C	1:B:71:TYR:H	2.26	0.42
1:B:212:ILE:HG22	1:B:224:TRP:HZ3	1.83	0.42
1:E:254:PRO:C	1:E:256:LEU:H	2.27	0.42
1:B:71:TYR:CD2	1:B:110:ARG:HD3	2.54	0.42
1:B:177:ILE:HB	1:F:130:LYS:HD3	2.01	0.42
1:C:46:ILE:O	1:C:46:ILE:HG22	2.19	0.42
1:E:38:GLU:HA	1:E:39:PRO:HD2	1.78	0.42
1:A:48:MSE:HE3	1:A:48:MSE:HB2	1.96	0.42
1:B:39:PRO:HG2	1:B:151:HIS:CD2	2.54	0.42
1:C:213:ARG:HG2	1:C:224:TRP:CZ3	2.54	0.42
1:F:125:VAL:HG13	1:F:165:SER:HA	1.99	0.42
1:A:245:ARG:HD2	1:A:246:TYR:CZ	2.54	0.42
1:D:41:PRO:O	1:D:42:ASP:CB	2.67	0.42
1:E:262:PRO:O	1:F:193:HIS:HB2	2.19	0.42
1:F:35:ILE:HD11	1:F:133:PRO:HG3	2.02	0.42
1:C:162:VAL:HG11	1:C:187:ILE:HD11	2.02	0.42
1:D:63:ILE:HG23	1:D:103:LYS:HB3	2.02	0.42
1:E:120:VAL:O	1:E:120:VAL:HG12	2.20	0.42
1:E:70:GLY:O	1:E:72:MSE:N	2.53	0.42
1:C:175:ILE:O	1:C:177:ILE:N	2.52	0.42
1:E:239:GLY:C	1:E:241:LYS:H	2.27	0.42
1:F:35:ILE:HA	1:F:63:ILE:O	2.20	0.42
1:F:38:GLU:HA	1:F:39:PRO:HD3	1.93	0.42
1:F:67:MSE:CE	1:F:124:LEU:HD11	2.36	0.42
1:A:28:PHE:O	1:A:30:ASP:N	2.53	0.42
1:A:167:LEU:HA	1:A:168:PRO:HD2	1.81	0.42
1:B:48:MSE:HE3	1:B:48:MSE:HB2	1.79	0.42
1:B:196:ASN:ND2	1:B:196:ASN:N	2.66	0.42
1:C:133:PRO:O	1:C:182:HIS:NE2	2.47	0.42
1:D:194:LYS:N	1:D:195:PRO:HD3	2.35	0.42
1:F:141:PRO:HD2	1:F:142:TRP:CZ3	2.54	0.42
1:F:232:ARG:HD3	1:F:246:TYR:OH	2.20	0.42
1:F:253:MSE:CG	1:F:267:ILE:HD11	2.50	0.42
1:A:83:GLU:O	1:A:85:ALA:N	2.53	0.41
1:B:118:ARG:HH21	1:F:119:GLU:CD	2.27	0.41
1:C:76:ASP:C	1:C:78:LYS:H	2.28	0.41
1:E:209:LEU:O	1:E:213:ARG:HG2	2.20	0.41
1:F:15:LEU:HA	1:F:19:VAL:HB	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:167:LEU:HA	1:F:168:PRO:HD3	1.86	0.41
1:F:196:ASN:H	1:F:196:ASN:HD22	1.67	0.41
1:A:202:THR:HA	1:A:246:TYR:HB2	2.01	0.41
1:A:245:ARG:HD2	1:A:246:TYR:CE2	2.55	0.41
1:B:14:LYS:O	1:B:19:VAL:HG23	2.20	0.41
1:B:38:GLU:HG2	1:B:44:CYS:SG	2.59	0.41
1:D:36:CYS:HB2	1:D:64:TYR:HD1	1.84	0.41
1:E:36:CYS:HA	1:E:137:PHE:HB2	2.02	0.41
1:E:196:ASN:ND2	1:E:251:ARG:HA	2.35	0.41
1:E:242:ILE:HD13	1:E:244:VAL:HG22	2.02	0.41
1:F:148:HIS:HD2	1:F:150:ASP:H	1.68	0.41
1:D:131:GLU:O	1:D:132:LYS:C	2.64	0.41
1:F:53:LYS:HE3	1:F:57:ASP:OD2	2.20	0.41
1:C:148:HIS:CD2	1:C:150:ASP:HB2	2.55	0.41
1:D:145:TYR:HA	1:F:142:TRP:CE2	2.56	0.41
1:A:74:THR:CG2	1:A:84:LEU:HD22	2.50	0.41
1:B:69:ASP:O	1:B:71:TYR:N	2.46	0.41
1:C:125:VAL:HG21	1:C:170:PHE:CE2	2.55	0.41
1:F:232:ARG:O	1:F:236:MSE:CG	2.66	0.41
1:A:198:ILE:HD13	1:A:249:GLY:CA	2.49	0.41
1:B:107:LEU:HD12	1:B:123:ASP:OD2	2.20	0.41
1:E:145:TYR:O	1:E:146:GLU:C	2.63	0.41
1:E:190:TYR:HD2	1:E:191:TYR:CD2	2.38	0.41
1:F:37:ILE:HG21	1:F:67:MSE:HE2	2.02	0.41
1:F:111:ASP:O	1:F:112:THR:OG1	2.34	0.41
1:C:22:PHE:HZ	1:C:252:VAL:HG12	1.85	0.41
1:D:72:MSE:HG2	1:D:111:ASP:HB3	2.03	0.41
1:D:155:GLY:O	1:D:156:PHE:C	2.64	0.41
1:E:83:GLU:O	1:E:84:LEU:C	2.64	0.41
1:B:48:MSE:SE	1:B:137:PHE:HD1	2.54	0.41
1:B:95:SER:O	1:B:98:LEU:HB2	2.20	0.41
1:B:253:MSE:HB2	1:B:258:TYR:CE2	2.55	0.41
1:C:132:LYS:N	1:C:133:PRO:CD	2.84	0.41
1:C:140:ASP:HA	1:C:189:LEU:HD22	2.03	0.41
1:D:94:GLU:O	1:D:95:SER:C	2.63	0.41
1:E:92:GLU:HB2	1:E:215:HIS:CE1	2.56	0.41
1:E:148:HIS:NE2	1:E:150:ASP:OD2	2.53	0.41
1:A:221:ASP:O	1:A:225:GLU:HG2	2.21	0.41
1:B:202:THR:HA	1:B:246:TYR:HB2	2.02	0.41
1:B:236:MSE:HE3	1:B:245:ARG:HG3	2.03	0.41
1:C:27:PRO:HD2	1:C:197:TYR:CZ	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:53:LYS:HD3	1:C:99:LEU:HA	2.02	0.41
1:C:62:VAL:HB	1:C:101:VAL:HG22	2.03	0.41
1:F:261:THR:HA	1:F:262:PRO:HD3	1.89	0.41
1:A:69:ASP:OD1	1:A:71:TYR:HB2	2.21	0.40
1:A:105:TYR:OH	1:A:131:GLU:CD	2.64	0.40
1:A:205:MSE:O	1:A:205:MSE:HG3	2.20	0.40
1:B:264:ALA:O	1:B:267:ILE:HG12	2.22	0.40
1:C:148:HIS:HA	1:C:149:PRO:HD2	1.69	0.40
1:C:193:HIS:O	1:C:193:HIS:CG	2.75	0.40
1:D:116:TYR:HB2	1:D:153:ARG:HD3	2.02	0.40
1:D:205:MSE:HG3	1:D:246:TYR:HD2	1.84	0.40
1:E:260:ILE:O	1:E:262:PRO:HD3	2.21	0.40
1:A:107:LEU:HD12	1:D:173:ILE:HD11	2.03	0.40
1:B:49:GLY:HA2	1:B:52:ILE:HD12	2.03	0.40
1:C:157:LEU:O	1:C:161:SER:HB2	2.20	0.40
1:E:198:ILE:HB	1:E:242:ILE:HG12	2.03	0.40
1:F:173:ILE:HA	1:F:176:ASP:HB2	2.04	0.40
1:D:72:MSE:O	1:F:167:LEU:HD13	2.22	0.40
1:E:36:CYS:HB3	1:E:48:MSE:HE1	2.02	0.40
1:A:141:PRO:HD2	1:A:142:TRP:CE3	2.56	0.40
1:F:38:GLU:OE1	1:F:43:ASP:N	2.54	0.40
1:F:198:ILE:HA	1:F:248:GLU:O	2.22	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	262/267 (98%)	228 (87%)	29 (11%)	5 (2%)	6	22
1	B	253/267 (95%)	206 (81%)	37 (15%)	10 (4%)	2	8
1	C	260/267 (97%)	200 (77%)	43 (16%)	17 (6%)	1	3

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	260/267 (97%)	213 (82%)	34 (13%)	13 (5%)	1	5
1	E	260/267 (97%)	206 (79%)	35 (14%)	19 (7%)	1	2
1	F	262/267 (98%)	213 (81%)	43 (16%)	6 (2%)	5	18
All	All	1557/1602 (97%)	1266 (81%)	221 (14%)	70 (4%)	2	7

All (70) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	42	ASP
1	A	77	GLU
1	B	71	TYR
1	B	162	VAL
1	B	254	PRO
1	B	260	ILE
1	C	94	GLU
1	C	98	LEU
1	D	94	GLU
1	D	98	LEU
1	E	42	ASP
1	E	45	ALA
1	E	46	ILE
1	F	42	ASP
1	B	42	ASP
1	C	24	LEU
1	C	58	GLU
1	C	71	TYR
1	C	77	GLU
1	C	176	ASP
1	C	184	VAL
1	D	42	ASP
1	D	49	GLY
1	D	95	SER
1	D	124	LEU
1	E	50	GLY
1	E	51	THR
1	E	71	TYR
1	E	95	SER
1	E	111	ASP
1	E	127	ILE
1	E	131	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	240	GLU
1	F	49	GLY
1	A	28	PHE
1	B	184	VAL
1	B	243	GLY
1	B	253	MSE
1	C	22	PHE
1	C	57	ASP
1	D	111	ASP
1	D	245	ARG
1	E	126	LYS
1	F	71	TYR
1	C	54	LYS
1	C	108	ASN
1	C	239	GLY
1	D	130	LYS
1	D	181	PRO
1	E	25	GLU
1	E	54	LYS
1	E	130	LYS
1	F	179	LEU
1	B	58	GLU
1	C	132	LYS
1	C	238	TYR
1	D	27	PRO
1	D	123	ASP
1	F	176	ASP
1	E	27	PRO
1	E	214	ALA
1	C	175	ILE
1	C	260	ILE
1	E	255	GLY
1	B	27	PRO
1	E	260	ILE
1	F	46	ILE
1	A	132	LYS
1	D	260	ILE

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	236/232 (102%)	219 (93%)	17 (7%)	13	39
1	B	228/232 (98%)	213 (93%)	15 (7%)	15	43
1	C	234/232 (101%)	211 (90%)	23 (10%)	7	25
1	D	234/232 (101%)	214 (92%)	20 (8%)	10	31
1	E	234/232 (101%)	210 (90%)	24 (10%)	7	23
1	F	236/232 (102%)	225 (95%)	11 (5%)	23	57
All	All	1402/1392 (101%)	1292 (92%)	110 (8%)	11	35

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	23	ASN
1	A	30	ASP
1	A	40	HIS
1	A	42	ASP
1	A	60	VAL
1	A	63	ILE
1	A	71	TYR
1	A	78	LYS
1	A	160	GLU
1	A	172	ASN
1	A	176	ASP
1	A	180	LYS
1	A	196	ASN
1	A	231	LEU
1	A	244	VAL
1	A	245	ARG
1	B	37	ILE
1	B	58	GLU
1	B	75	THR
1	B	113	GLU
1	B	119	GLU
1	B	162	VAL
1	B	165	SER
1	B	177	ILE
1	B	193	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	196	ASN
1	B	202	THR
1	B	205	MSE
1	B	226	THR
1	B	252	VAL
1	B	265	ASP
1	C	7	THR
1	C	16	LEU
1	C	23	ASN
1	C	42	ASP
1	C	48	MSE
1	C	63	ILE
1	C	71	TYR
1	C	80	SER
1	C	86	LEU
1	C	98	LEU
1	C	103	LYS
1	C	122	LYS
1	C	131	GLU
1	C	143	LEU
1	C	161	SER
1	C	172	ASN
1	C	193	HIS
1	C	196	ASN
1	C	198	ILE
1	C	226	THR
1	C	231	LEU
1	C	235	THR
1	C	242	ILE
1	D	17	LYS
1	D	23	ASN
1	D	30	ASP
1	D	35	ILE
1	D	57	ASP
1	D	58	GLU
1	D	62	VAL
1	D	71	TYR
1	D	98	LEU
1	D	134	ASP
1	D	172	ASN
1	D	177	ILE
1	D	185	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	196	ASN
1	D	201	ILE
1	D	202	THR
1	D	213	ARG
1	D	216	ARG
1	D	235	THR
1	D	244	VAL
1	E	19	VAL
1	E	23	ASN
1	E	30	ASP
1	E	48	MSE
1	E	54	LYS
1	E	72	MSE
1	E	75	THR
1	E	77	GLU
1	E	89	ARG
1	E	102	ARG
1	E	111	ASP
1	E	132	LYS
1	E	134	ASP
1	E	172	ASN
1	E	180	LYS
1	E	187	ILE
1	E	192	THR
1	E	196	ASN
1	E	198	ILE
1	E	210	LYS
1	E	213	ARG
1	E	223	ILE
1	E	242	ILE
1	E	245	ARG
1	F	5	VAL
1	F	23	ASN
1	F	24	LEU
1	F	25	GLU
1	F	30	ASP
1	F	42	ASP
1	F	107	LEU
1	F	172	ASN
1	F	196	ASN
1	F	223	ILE
1	F	245	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	148	HIS
1	A	166	GLN
1	A	169	ASN
1	A	172	ASN
1	A	196	ASN
1	B	148	HIS
1	B	169	ASN
1	B	172	ASN
1	B	196	ASN
1	B	218	GLN
1	C	13	ASN
1	C	108	ASN
1	C	169	ASN
1	C	172	ASN
1	C	196	ASN
1	C	215	HIS
1	D	13	ASN
1	D	23	ASN
1	D	108	ASN
1	D	169	ASN
1	D	172	ASN
1	D	193	HIS
1	D	196	ASN
1	E	40	HIS
1	E	169	ASN
1	E	196	ASN
1	E	215	HIS
1	F	23	ASN
1	F	26	ASN
1	F	82	HIS
1	F	108	ASN
1	F	172	ASN
1	F	196	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	258/267 (96%)	-0.10	2 (0%) 82 75	26, 64, 94, 97	0
1	B	249/267 (93%)	-0.09	2 (0%) 82 75	18, 63, 99, 110	0
1	C	256/267 (95%)	0.12	4 (1%) 70 61	26, 70, 115, 121	0
1	D	256/267 (95%)	-0.08	0 100 100	27, 62, 100, 110	0
1	E	256/267 (95%)	0.08	1 (0%) 88 84	25, 67, 93, 99	0
1	F	258/267 (96%)	-0.19	0 100 100	18, 58, 84, 88	0
All	All	1533/1602 (95%)	-0.04	9 (0%) 85 80	18, 65, 99, 121	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	234	VAL	5.5
1	C	227	TRP	3.1
1	C	52	ILE	2.9
1	C	35	ILE	2.3
1	E	206	GLU	2.2
1	B	16	LEU	2.2
1	A	207	LEU	2.1
1	B	263	PHE	2.1
1	A	85	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	301	1/1	0.99	0.03	52,52,52,52	0
2	ZN	C	301	1/1	0.99	0.03	49,49,49,49	0
2	ZN	D	301	1/1	0.99	0.04	40,40,40,40	0
2	ZN	E	301	1/1	0.99	0.02	50,50,50,50	0
2	ZN	F	301	1/1	0.99	0.06	54,54,54,54	0
2	ZN	B	301	1/1	1.00	0.02	40,40,40,40	0

6.5 Other polymers [i](#)

There are no such residues in this entry.