



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:23 PM UTC

PDB ID : 1O7L / pdb_00001o7l
Title : Molybdate-activated form of ModE from Escherichia coli
Authors : Schuttelkopf, A.W.; Hunter, W.N.
Deposited on : 2002-11-08
Resolution : 2.75 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 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

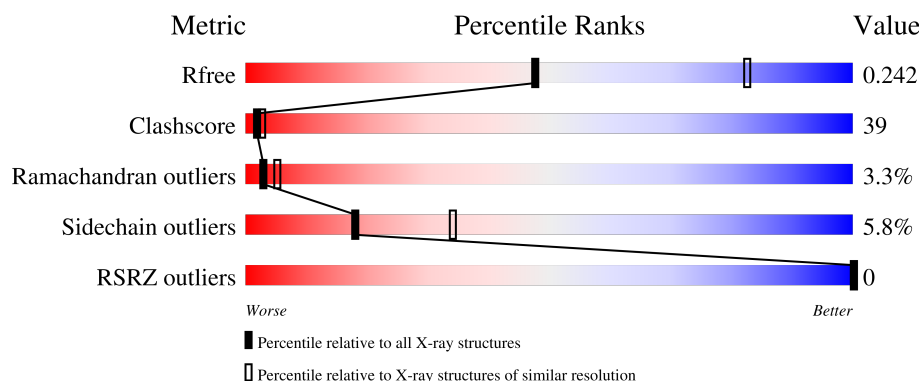
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	262	
1	B	262	
1	C	262	
1	D	262	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	MOO	D	1264	-	-	X	-

2 Entry composition [i](#)

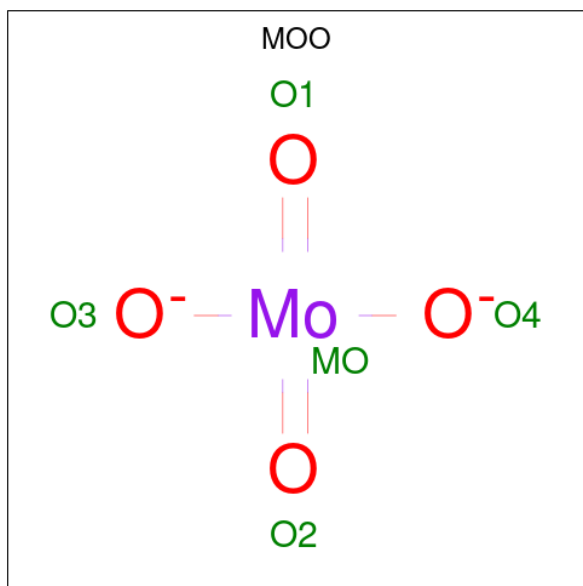
There are 5 unique types of molecules in this entry. The entry contains 7852 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TRANSCRIPTIONAL REGULATOR MODE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	255	Total	C	N	O	S	33	0	0
			1951	1223	343	379	6			
1	B	256	Total	C	N	O	S	30	0	0
			1959	1228	344	381	6			
1	C	255	Total	C	N	O	S	23	0	0
			1944	1219	343	378	4			
1	D	254	Total	C	N	O	S	30	0	0
			1944	1219	342	378	5			

- Molecule 2 is MOLYBDATE ION (CCD ID: MOO) (formula: MoO_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Mo	O	0	0
			5	1	4		
2	B	1	Total	Mo	O	0	0
			5	1	4		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	Mo	O	0	0
			5	1	4		
2	D	1	Total	Mo	O	0	0
			5	1	4		
2	D	1	Total	Mo	O	0	0
			5	1	4		

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	Ca	0	0
			1	1		

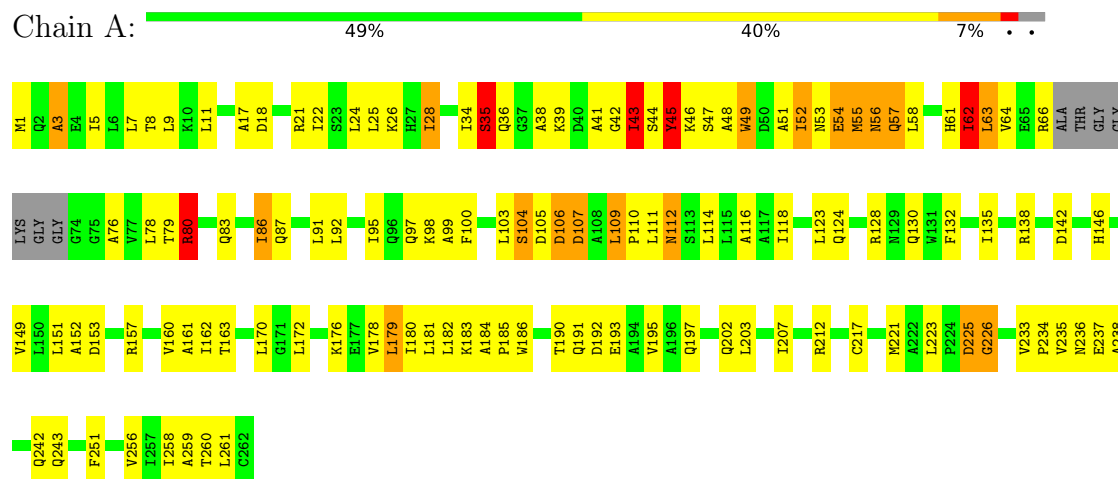
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	O	0	0
			5	5		
5	B	6	Total	O	0	0
			6	6		
5	C	10	Total	O	0	0
			10	10		
5	D	6	Total	O	0	0
			6	6		

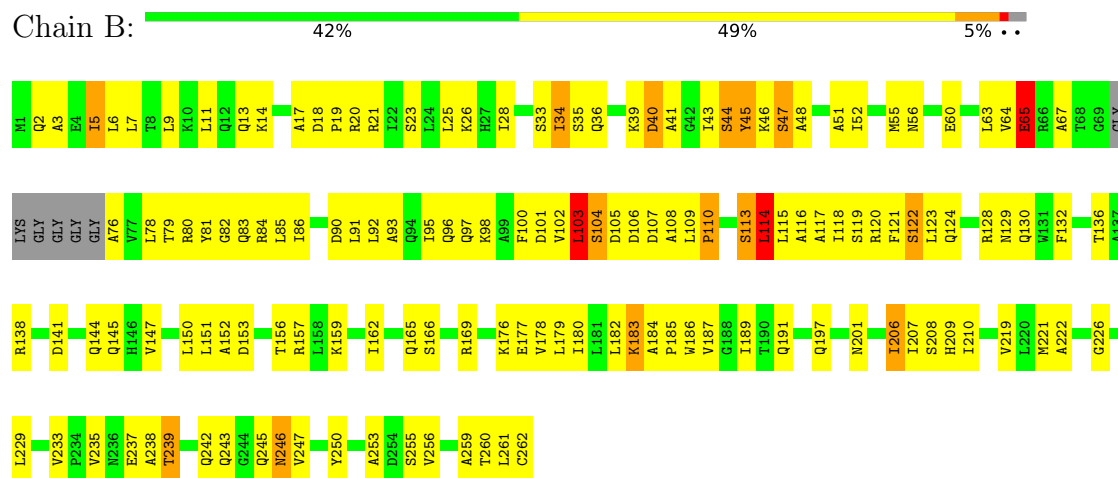
3 Residue-property plots [i](#)

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.

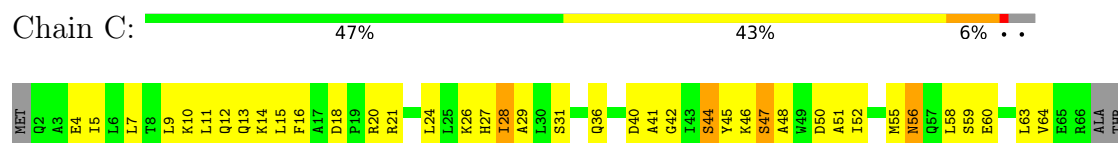
• Molecule 1: TRANSCRIPTIONAL REGULATOR MODE



• Molecule 1: TRANSCRIPTIONAL REGULATOR MODE



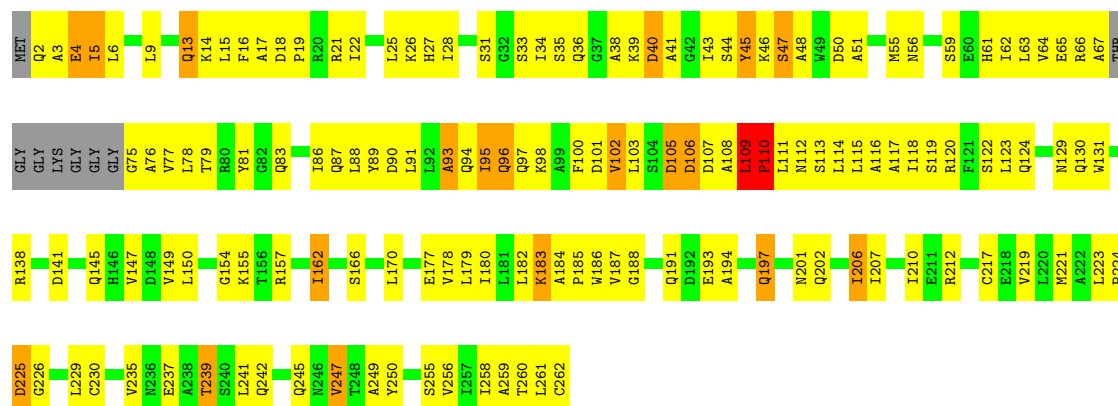
• Molecule 1: TRANSCRIPTIONAL REGULATOR MODE





● Molecule 1: TRANSCRIPTIONAL REGULATOR MODE

Chain D: 40% 49% 7% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 43	Depositor
Cell constants a, b, c, α , β , γ	78.83Å 78.83Å 195.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.75 25.00 – 2.75	Depositor EDS
% Data completeness (in resolution range)	95.3 (25.00-2.75) 95.3 (25.00-2.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.71 (at 2.76Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.207 , 0.254 0.203 , 0.242	Depositor DCC
R_{free} test set	1005 reflections (3.39%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.397	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 21.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.308 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7852	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 14.89% 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: MOO, CA, CL

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	0.34	0/1975	0.99	15/2677 (0.6%)
1	B	0.34	0/1983	1.06	16/2689 (0.6%)
1	C	0.32	0/1968	1.03	13/2669 (0.5%)
1	D	0.32	0/1968	0.95	9/2669 (0.3%)
All	All	0.33	0/7894	1.01	53/10704 (0.5%)

There are no bond length outliers.

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	47	SER	N-CA-C	-12.88	98.20	114.56
1	B	109	LEU	CA-C-N	10.70	133.22	119.84
1	B	109	LEU	C-N-CA	10.70	133.22	119.84
1	B	109	LEU	N-CA-C	10.49	133.00	109.81
1	D	4	GLU	N-CA-C	9.93	121.34	108.34
1	A	109	LEU	N-CA-C	8.64	120.65	109.93
1	B	105	ASP	N-CA-C	8.39	119.71	107.88
1	B	103	LEU	N-CA-C	-8.16	103.84	113.38
1	D	13	GLN	N-CA-C	8.14	122.56	112.47
1	B	106	ASP	N-CA-C	8.13	128.13	110.80
1	A	56	ASN	N-CA-C	-8.01	103.49	113.18
1	C	114	LEU	N-CA-C	7.88	127.59	110.80
1	B	113	SER	N-CA-C	7.56	122.65	109.80
1	C	117	ALA	N-CA-C	-7.52	102.09	111.11
1	B	191	GLN	N-CA-C	-7.41	104.09	113.72
1	C	48	ALA	N-CA-C	-6.97	103.77	112.90
1	A	54	GLU	N-CA-C	-6.94	103.48	112.23
1	A	3	ALA	N-CA-C	6.67	120.40	109.72
1	D	109	LEU	CA-C-N	6.55	128.03	119.84
1	D	109	LEU	C-N-CA	6.55	128.03	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	108	ALA	N-CA-C	6.50	118.05	110.97
1	A	107	ASP	N-CA-C	6.38	124.40	110.80
1	B	47	SER	N-CA-C	-6.28	105.33	112.87
1	B	110	PRO	N-CA-C	6.19	125.21	112.47
1	C	115	LEU	N-CA-C	-6.18	97.64	110.80
1	A	142	ASP	N-CA-C	6.13	117.63	111.07
1	B	109	LEU	CA-CB-CG	-6.13	94.86	116.30
1	A	226	GLY	N-CA-C	-6.08	106.38	114.95
1	A	55	MET	N-CA-C	-5.97	104.71	112.23
1	C	109	LEU	N-CA-C	5.84	122.71	109.81
1	C	226	GLY	N-CA-C	-5.80	107.74	115.40
1	C	199	ALA	N-CA-C	5.73	119.30	110.42
1	D	19	PRO	N-CA-C	-5.70	105.96	113.65
1	A	233	VAL	N-CA-C	5.65	114.05	107.89
1	C	56	ASN	N-CA-C	-5.57	105.22	112.23
1	A	28	ILE	N-CA-C	-5.55	104.78	112.50
1	C	106	ASP	N-CA-C	5.51	122.55	110.80
1	A	80	ARG	N-CA-C	-5.50	105.43	111.82
1	C	44	SER	N-CA-C	5.50	122.52	110.80
1	A	225	ASP	N-CA-C	-5.44	105.25	111.07
1	D	225	ASP	N-CA-C	-5.38	104.97	112.45
1	B	67	ALA	CA-C-N	5.34	131.46	122.87
1	B	67	ALA	C-N-CA	5.34	131.46	122.87
1	D	93	ALA	N-CA-C	-5.25	105.64	111.36
1	A	106	ASP	N-CA-C	-5.21	98.90	108.02
1	D	47	SER	N-CA-C	-5.20	106.19	112.54
1	C	191	GLN	N-CA-C	-5.17	106.89	114.39
1	B	226	GLY	N-CA-C	-5.17	100.93	113.18
1	B	67	ALA	N-CA-C	-5.14	99.84	110.80
1	C	28	ILE	N-CA-C	-5.07	104.58	111.89
1	D	102	VAL	N-CA-C	-5.07	102.40	109.45
1	A	43	ILE	N-CA-C	5.05	119.85	109.34
1	A	49	TRP	N-CA-C	5.01	116.43	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	1951	0	1978	161	0
1	B	1959	0	1987	163	0
1	C	1944	0	1967	151	0
1	D	1944	0	1968	189	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	10	0	0	2	0
3	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	5	0	0	0	0
5	B	6	0	0	0	0
5	C	10	0	0	0	0
5	D	6	0	0	0	0
All	All	7852	0	7900	604	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 39.

All (604) 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:D:4:GLU:HG2	1:D:97:GLN:HE22	1.01	1.15
1:B:206:ILE:HG23	1:B:246:ASN:HD22	1.18	1.08
1:A:43:ILE:HG13	1:A:44:SER:H	1.17	1.05
1:D:118:ILE:HG21	1:D:261:LEU:HD21	1.07	1.05
1:A:53:ASN:HD22	1:A:56:ASN:HB2	1.22	1.04
1:C:11:LEU:HD12	1:D:3:ALA:HB3	1.40	1.03
1:B:187:VAL:HG11	1:B:229:LEU:HD21	1.43	0.99
1:C:7:LEU:HD21	1:C:92:LEU:HD23	1.45	0.99
1:A:9:LEU:HB3	1:A:17:ALA:HB3	1.46	0.98
1:C:108:ALA:C	1:C:110:PRO:HD3	1.92	0.95
1:B:206:ILE:HG23	1:B:246:ASN:ND2	1.81	0.94
1:D:2:GLN:HG2	1:D:3:ALA:H	1.32	0.94
1:D:118:ILE:CG2	1:D:261:LEU:HD21	1.98	0.94
1:C:5:ILE:HG13	1:C:96:GLN:HE21	1.30	0.93
1:C:108:ALA:O	1:C:110:PRO:HD3	1.69	0.93
1:C:102:VAL:HG11	1:C:121:PHE:HB3	1.51	0.92
1:D:4:GLU:HG2	1:D:97:GLN:NE2	1.86	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:LEU:HB3	1:C:259:ALA:HB3	1.53	0.90
1:B:118:ILE:HG21	1:B:261:LEU:HD21	1.56	0.88
1:A:112:ASN:C	1:A:112:ASN:HD22	1.81	0.86
1:D:118:ILE:HG21	1:D:261:LEU:CD2	2.01	0.85
1:B:117:ALA:HA	1:B:120:ARG:HE	1.40	0.85
1:C:223:LEU:HD12	1:C:227:GLN:HG3	1.57	0.85
1:A:45:TYR:C	1:A:45:TYR:HD1	1.85	0.85
1:A:45:TYR:C	1:A:45:TYR:CD1	2.55	0.85
1:D:27:HIS:ND1	1:D:41:ALA:HB2	1.93	0.83
1:D:221:MET:HE2	1:D:247:VAL:HG23	1.60	0.83
1:A:114:LEU:O	1:A:118:ILE:HG12	1.79	0.83
1:A:52:ILE:HD11	1:A:64:VAL:HB	1.61	0.82
1:B:5:ILE:HD13	1:B:96:GLN:HB3	1.61	0.82
1:C:135:ILE:HD12	1:C:176:LYS:HB3	1.61	0.81
1:C:99:ALA:O	1:C:103:LEU:HB2	1.81	0.80
1:A:44:SER:O	1:A:46:LYS:N	2.14	0.80
1:A:135:ILE:HD12	1:A:176:LYS:HB3	1.64	0.80
1:A:35:SER:HA	1:A:45:TYR:CE2	2.16	0.79
1:C:115:LEU:HG	1:C:115:LEU:O	1.81	0.79
1:D:67:ALA:HB2	1:D:75:GLY:N	1.98	0.78
1:B:33:SER:HB3	1:B:36:GLN:HB3	1.66	0.78
1:C:13:GLN:HE21	1:C:13:GLN:HA	1.48	0.78
1:A:44:SER:C	1:A:46:LYS:N	2.40	0.78
1:B:235:VAL:O	1:B:239:THR:HG22	1.84	0.78
1:C:12:GLN:H	1:D:3:ALA:HB2	1.47	0.78
1:D:34:ILE:HG22	1:D:76:ALA:HB2	1.66	0.78
1:D:235:VAL:O	1:D:239:THR:HG22	1.83	0.78
1:C:5:ILE:HG22	1:D:9:LEU:HD22	1.64	0.78
1:C:111:LEU:HG	1:D:91:LEU:HD22	1.65	0.78
1:B:117:ALA:HA	1:B:120:ARG:NE	1.99	0.77
1:A:192:ASP:HB3	1:A:195:VAL:HG23	1.67	0.76
1:A:45:TYR:HD1	1:A:45:TYR:O	1.67	0.76
1:B:118:ILE:HD13	1:B:261:LEU:CD2	2.16	0.76
1:C:182:LEU:HD13	1:C:256:VAL:HG22	1.68	0.75
1:B:18:ASP:H	1:B:21:ARG:HB2	1.51	0.75
1:B:207:ILE:HD13	1:B:210:ILE:HD11	1.69	0.75
1:C:84:ARG:HG3	1:D:111:LEU:HD13	1.69	0.75
1:C:12:GLN:H	1:D:3:ALA:CB	2.00	0.75
1:A:35:SER:HA	1:A:45:TYR:CD2	2.22	0.74
1:A:79:THR:HG22	1:A:80:ARG:N	2.02	0.74
1:D:221:MET:CE	1:D:247:VAL:HG23	2.16	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:ASN:O	1:C:113:SER:C	2.31	0.74
1:D:207:ILE:HD13	1:D:210:ILE:HD11	1.69	0.74
1:A:45:TYR:CD1	1:A:45:TYR:O	2.41	0.74
1:A:182:LEU:HD13	1:A:256:VAL:HG22	1.68	0.74
1:B:118:ILE:HD13	1:B:261:LEU:HD21	1.70	0.74
1:B:189:ILE:HD12	1:B:221:MET:HE3	1.70	0.73
1:C:7:LEU:HD13	1:C:96:GLN:OE1	1.88	0.73
1:D:18:ASP:HB2	1:D:21:ARG:HG3	1.70	0.73
1:A:110:PRO:O	1:A:116:ALA:HB3	1.89	0.73
1:A:52:ILE:CD1	1:A:64:VAL:HB	2.17	0.73
1:A:79:THR:HG22	1:A:80:ARG:H	1.53	0.73
1:B:101:ASP:O	1:B:104:SER:HB2	1.89	0.72
1:C:7:LEU:HD11	1:D:5:ILE:HG21	1.69	0.72
1:A:43:ILE:CG1	1:A:44:SER:H	1.92	0.72
1:A:5:ILE:HG13	1:A:5:ILE:O	1.89	0.72
1:B:64:VAL:HG22	1:B:78:LEU:HD23	1.71	0.72
1:B:114:LEU:HD23	1:B:115:LEU:H	1.55	0.72
1:C:213:GLY:HA3	2:D:1264:MOO:O4	1.90	0.72
1:A:44:SER:C	1:A:46:LYS:H	1.98	0.71
1:D:35:SER:O	1:D:39:LYS:HG3	1.91	0.71
1:D:5:ILE:HG22	1:D:6:LEU:H	1.55	0.71
1:A:3:ALA:HB2	1:B:11:LEU:HD12	1.73	0.71
1:B:206:ILE:CG2	1:B:246:ASN:HD22	2.01	0.70
1:A:44:SER:O	1:A:45:TYR:C	2.34	0.70
1:A:53:ASN:HA	1:A:56:ASN:ND2	2.06	0.70
1:A:105:ASP:O	1:B:84:ARG:NH1	2.24	0.70
1:C:83:GLN:O	1:C:87:GLN:HG3	1.91	0.70
1:A:130:GLN:HA	1:A:180:ILE:O	1.91	0.70
1:C:26:LYS:HG2	1:C:86:ILE:HD11	1.74	0.70
1:C:5:ILE:HG22	1:D:9:LEU:CD2	2.21	0.69
1:A:53:ASN:ND2	1:A:56:ASN:HB2	2.02	0.69
1:D:13:GLN:O	1:D:14:LYS:HD2	1.91	0.69
1:A:44:SER:O	1:A:47:SER:N	2.24	0.69
1:B:34:ILE:HD13	1:B:34:ILE:H	1.58	0.69
1:D:65:GLU:HG2	1:D:66:ARG:H	1.58	0.69
1:D:162:ILE:HD13	1:D:162:ILE:H	1.58	0.69
1:A:43:ILE:HG13	1:A:44:SER:N	2.01	0.69
1:B:51:ALA:O	1:B:55:MET:HB2	1.93	0.69
1:A:193:GLU:HB3	1:A:197:GLN:NE2	2.08	0.68
1:C:130:GLN:HA	1:C:180:ILE:O	1.94	0.68
1:A:49:TRP:HA	1:A:52:ILE:HG22	1.74	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:TRP:HA	1:A:52:ILE:CG2	2.23	0.68
1:A:91:LEU:HD22	1:A:95:ILE:HD11	1.75	0.68
1:B:28:ILE:HD11	1:B:76:ALA:HB1	1.74	0.68
1:A:7:LEU:HD11	1:B:5:ILE:HD11	1.75	0.68
1:D:91:LEU:O	1:D:95:ILE:HG12	1.93	0.67
1:D:178:VAL:HG12	1:D:260:THR:CG2	2.24	0.67
1:A:3:ALA:HB2	1:B:11:LEU:CD1	2.25	0.67
1:A:54:GLU:O	1:A:57:GLN:HB3	1.95	0.67
1:B:178:VAL:HG12	1:B:260:THR:CG2	2.24	0.67
1:C:225:ASP:HB2	1:C:227:GLN:HG2	1.74	0.67
1:A:87:GLN:O	1:A:91:LEU:HB2	1.95	0.67
1:B:43:ILE:HG23	1:B:47:SER:HB2	1.76	0.67
1:B:81:TYR:HA	1:B:84:ARG:HG2	1.77	0.67
1:C:5:ILE:HG13	1:C:96:GLN:NE2	2.08	0.67
1:D:36:GLN:HG3	1:D:40:ASP:OD2	1.95	0.66
1:C:13:GLN:HA	1:C:13:GLN:NE2	2.11	0.66
1:C:64:VAL:HG13	1:C:77:VAL:O	1.95	0.66
1:C:111:LEU:O	1:C:117:ALA:HB2	1.95	0.66
1:A:62:ILE:HD13	1:A:62:ILE:N	2.10	0.66
1:C:11:LEU:HA	1:D:3:ALA:HB1	1.78	0.66
1:A:183:LYS:HG2	1:A:185:PRO:HD2	1.78	0.66
1:C:183:LYS:HG2	1:C:185:PRO:HD2	1.78	0.65
1:B:151:LEU:HD12	1:B:156:THR:HB	1.79	0.65
1:B:102:VAL:C	1:B:104:SER:H	2.03	0.65
1:A:26:LYS:HG2	1:A:86:ILE:HD11	1.79	0.64
1:C:84:ARG:HG3	1:D:111:LEU:CD1	2.27	0.64
1:C:138:ARG:HD2	1:C:172:LEU:O	1.97	0.64
1:A:183:LYS:HB3	1:A:186:TRP:CE3	2.33	0.64
1:A:5:ILE:HG22	1:B:9:LEU:HD12	1.78	0.64
1:C:207:ILE:HD11	1:C:241:LEU:HD22	1.79	0.64
1:A:190:THR:HG21	1:A:195:VAL:HB	1.79	0.64
1:C:183:LYS:HB3	1:C:186:TRP:CE3	2.33	0.64
1:C:102:VAL:HG11	1:C:121:PHE:CB	2.26	0.64
1:A:53:ASN:HA	1:A:56:ASN:HD22	1.62	0.63
1:B:7:LEU:HB2	1:B:96:GLN:OE1	1.97	0.63
1:D:187:VAL:HG11	1:D:229:LEU:HD21	1.80	0.63
1:D:120:ARG:HG3	1:D:120:ARG:HH11	1.64	0.63
1:A:138:ARG:HD2	1:A:172:LEU:O	1.98	0.62
1:C:18:ASP:OD1	1:C:21:ARG:HG2	1.99	0.62
1:A:1:MET:HB3	1:B:11:LEU:HD11	1.81	0.62
1:B:65:GLU:OE2	1:B:79:THR:HG22	2.00	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:120:ARG:HG3	1:C:120:ARG:HH11	1.63	0.62
1:A:83:GLN:O	1:A:86:ILE:HG22	1.99	0.62
1:B:64:VAL:HG22	1:B:78:LEU:CD2	2.30	0.62
1:C:51:ALA:O	1:C:55:MET:HG3	2.00	0.61
1:B:102:VAL:C	1:B:104:SER:N	2.53	0.61
1:D:191:GLN:HE22	1:D:241:LEU:HD23	1.65	0.61
1:C:123:LEU:HD12	1:D:118:ILE:HG23	1.83	0.61
1:B:141:ASP:H	1:B:145:GLN:HG2	1.65	0.61
1:B:115:LEU:CD1	1:B:261:LEU:HG	2.31	0.61
1:D:150:LEU:HD13	1:D:157:ARG:HG2	1.83	0.61
1:A:176:LYS:HE2	1:A:260:THR:OG1	2.00	0.60
1:D:61:HIS:HB3	1:D:81:TYR:CD1	2.36	0.60
1:A:112:ASN:C	1:A:112:ASN:ND2	2.54	0.60
1:C:111:LEU:CD2	1:D:87:GLN:HG2	2.32	0.60
1:A:111:LEU:O	1:A:112:ASN:ND2	2.35	0.60
1:C:183:LYS:CB	1:C:186:TRP:CZ3	2.84	0.60
1:D:34:ILE:CG2	1:D:76:ALA:HB2	2.31	0.59
1:D:22:ILE:HG22	1:D:26:LYS:HD2	1.85	0.59
1:A:186:TRP:HZ2	1:B:255:SER:HA	1.67	0.59
1:D:9:LEU:HB2	1:D:17:ALA:HB3	1.84	0.59
1:A:183:LYS:CB	1:A:186:TRP:CZ3	2.85	0.59
1:C:223:LEU:HB3	1:C:224:PRO:HD2	1.84	0.59
1:D:119:SER:O	1:D:124:GLN:NE2	2.35	0.59
1:D:182:LEU:HD21	1:D:187:VAL:HG22	1.83	0.59
1:B:44:SER:O	1:B:44:SER:OG	2.20	0.59
1:D:223:LEU:C	1:D:225:ASP:H	2.11	0.59
1:C:186:TRP:HZ2	1:D:255:SER:HA	1.67	0.58
1:A:51:ALA:O	1:A:55:MET:HG3	2.02	0.58
1:A:106:ASP:OD1	1:B:81:TYR:HE2	1.86	0.58
1:A:112:ASN:ND2	1:A:112:ASN:O	2.36	0.58
1:D:38:ALA:HB2	1:D:48:ALA:HB1	1.84	0.58
1:B:182:LEU:HD21	1:B:187:VAL:HG22	1.84	0.58
1:D:183:LYS:HD3	1:D:185:PRO:HD2	1.86	0.58
1:A:64:VAL:HG22	1:A:78:LEU:CD2	2.34	0.58
1:B:233:VAL:CG1	1:B:238:ALA:HB2	2.34	0.58
1:D:5:ILE:HD11	1:D:100:PHE:HB2	1.85	0.58
1:C:135:ILE:HD11	1:C:172:LEU:HD22	1.86	0.58
1:A:24:LEU:O	1:A:28:ILE:HG13	2.03	0.58
1:C:7:LEU:CD2	1:C:92:LEU:HD23	2.27	0.58
1:B:221:MET:HE2	1:B:247:VAL:HG23	1.86	0.57
1:A:49:TRP:O	1:A:52:ILE:HG23	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:VAL:O	1:A:157:ARG:HA	2.05	0.57
1:B:183:LYS:HD3	1:B:185:PRO:HD2	1.85	0.57
1:D:34:ILE:HD12	1:D:45:TYR:OH	2.03	0.57
1:D:65:GLU:HB3	1:D:77:VAL:CG1	2.35	0.57
1:C:11:LEU:HD23	1:C:58:LEU:HB3	1.87	0.57
1:D:39:LYS:C	1:D:41:ALA:H	2.12	0.57
1:C:123:LEU:HD23	1:D:259:ALA:HB1	1.87	0.57
1:B:183:LYS:HB3	1:B:186:TRP:CD1	2.40	0.57
1:C:27:HIS:ND1	1:C:41:ALA:HB2	2.20	0.57
1:D:5:ILE:HG22	1:D:6:LEU:N	2.20	0.57
1:D:38:ALA:CB	1:D:48:ALA:CB	2.83	0.57
1:C:183:LYS:HB2	1:C:186:TRP:CZ3	2.40	0.56
1:D:38:ALA:HB2	1:D:48:ALA:CB	2.34	0.56
1:C:83:GLN:O	1:C:86:ILE:HG22	2.06	0.56
1:A:11:LEU:HD13	1:B:3:ALA:HB2	1.87	0.56
1:C:194:ALA:O	1:C:198:ASN:HB2	2.06	0.56
1:D:102:VAL:O	1:D:103:LEU:HB2	2.03	0.56
1:D:194:ALA:O	1:D:197:GLN:HG2	2.05	0.56
1:A:130:GLN:HG2	1:A:181:LEU:HD23	1.87	0.56
1:A:135:ILE:HD11	1:A:172:LEU:HD22	1.86	0.56
1:A:79:THR:CG2	1:A:80:ARG:H	2.19	0.56
1:D:162:ILE:HD13	1:D:162:ILE:N	2.20	0.56
1:A:183:LYS:HB2	1:A:186:TRP:CZ3	2.41	0.56
1:C:132:PHE:CE1	1:C:179:LEU:HG	2.41	0.56
1:C:183:LYS:HB3	1:C:186:TRP:CZ3	2.40	0.56
1:C:18:ASP:H	1:C:21:ARG:HB2	1.70	0.56
1:C:198:ASN:OD1	1:C:198:ASN:C	2.49	0.56
1:A:183:LYS:HB3	1:A:186:TRP:CZ3	2.41	0.56
1:B:201:ASN:O	1:B:250:TYR:HA	2.06	0.56
1:C:223:LEU:HB2	1:C:227:GLN:O	2.06	0.56
1:D:149:VAL:O	1:D:157:ARG:HA	2.06	0.56
1:C:102:VAL:CG1	1:C:121:PHE:HB3	2.28	0.55
1:D:44:SER:O	1:D:46:LYS:N	2.39	0.55
1:D:79:THR:O	1:D:83:GLN:HG3	2.06	0.55
1:A:123:LEU:HD11	1:B:119:SER:HB3	1.87	0.55
1:D:2:GLN:HG2	1:D:3:ALA:N	2.13	0.55
1:A:43:ILE:HG23	1:A:44:SER:N	2.21	0.55
1:C:213:GLY:O	1:C:235:VAL:HG11	2.07	0.55
1:D:207:ILE:HG21	1:D:210:ILE:HG13	1.89	0.55
1:B:113:SER:O	1:B:117:ALA:N	2.38	0.55
1:C:217:CYS:HB3	1:C:233:VAL:O	2.06	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:SER:C	1:D:46:LYS:H	2.15	0.55
1:A:135:ILE:HD13	1:A:172:LEU:HB3	1.89	0.55
1:B:183:LYS:HB3	1:B:186:TRP:HD1	1.71	0.55
1:A:132:PHE:CE1	1:A:179:LEU:HG	2.41	0.55
1:D:105:ASP:OD1	1:D:106:ASP:N	2.39	0.55
1:A:64:VAL:HG22	1:A:78:LEU:HD23	1.89	0.55
1:C:29:ALA:HB2	1:C:78:LEU:HD11	1.89	0.55
1:A:79:THR:CG2	1:A:80:ARG:N	2.70	0.55
1:B:138:ARG:CB	1:B:147:VAL:HG12	2.37	0.55
1:B:141:ASP:HB3	1:B:144:GLN:O	2.07	0.55
1:B:150:LEU:HD13	1:B:157:ARG:HD3	1.89	0.55
1:C:124:GLN:O	1:D:259:ALA:HA	2.07	0.55
1:D:31:SER:HB2	1:D:36:GLN:HB3	1.89	0.54
1:C:98:LYS:O	1:C:102:VAL:HG12	2.08	0.54
1:D:207:ILE:CG2	1:D:210:ILE:HG13	2.37	0.54
1:A:234:PRO:C	1:A:236:ASN:N	2.63	0.54
1:B:207:ILE:CG2	1:B:210:ILE:HG13	2.37	0.54
1:B:207:ILE:HG21	1:B:210:ILE:HG13	1.88	0.54
1:B:18:ASP:CB	1:B:21:ARG:HG3	2.37	0.54
1:C:117:ALA:HB1	1:D:91:LEU:HD21	1.88	0.54
1:A:26:LYS:HG2	1:A:86:ILE:CD1	2.38	0.54
1:A:66:ARG:HA	1:A:76:ALA:HA	1.90	0.54
1:B:9:LEU:HB3	1:B:17:ALA:HB3	1.88	0.54
1:D:66:ARG:O	1:D:77:VAL:HG12	2.07	0.54
1:A:18:ASP:O	1:A:22:ILE:HG12	2.08	0.54
1:A:186:TRP:CZ2	1:B:255:SER:HA	2.43	0.54
1:B:151:LEU:HB2	1:B:153:ASP:OD1	2.08	0.54
1:C:200:ASP:HB2	1:C:252:ASN:HA	1.90	0.54
1:A:162:ILE:CD1	1:A:172:LEU:HD12	2.38	0.54
1:D:45:TYR:HA	1:D:48:ALA:HB3	1.89	0.54
1:A:54:GLU:O	1:A:58:LEU:HG	2.07	0.53
1:D:138:ARG:CB	1:D:147:VAL:HG12	2.37	0.53
1:C:63:LEU:HD22	1:C:82:GLY:HA2	1.90	0.53
1:C:236:ASN:OD1	1:C:237:GLU:HG3	2.08	0.53
1:D:114:LEU:O	1:D:118:ILE:HB	2.07	0.53
1:B:118:ILE:HD13	1:B:261:LEU:HD22	1.90	0.53
1:D:51:ALA:O	1:D:55:MET:HG3	2.07	0.53
1:D:63:LEU:N	1:D:63:LEU:HD12	2.22	0.53
1:B:21:ARG:HD3	1:B:55:MET:HE2	1.90	0.53
1:B:118:ILE:HG13	1:B:121:PHE:CE2	2.43	0.53
1:C:135:ILE:HD13	1:C:172:LEU:HB3	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:GLN:HB3	1:D:96:GLN:NE2	2.24	0.53
1:D:25:LEU:O	1:D:28:ILE:HG22	2.08	0.53
1:C:186:TRP:CZ2	1:D:255:SER:HA	2.43	0.52
1:D:112:ASN:OD1	1:D:113:SER:N	2.33	0.52
1:C:5:ILE:HD11	1:C:97:GLN:N	2.24	0.52
1:D:16:PHE:CE1	1:D:59:SER:HB2	2.45	0.52
1:A:111:LEU:O	1:A:111:LEU:HG	2.10	0.52
1:D:183:LYS:HB2	1:D:186:TRP:CZ2	2.43	0.52
1:D:242:GLN:O	1:D:245:GLN:HG3	2.09	0.52
1:C:5:ILE:HD11	1:C:97:GLN:CA	2.39	0.52
1:B:34:ILE:HD13	1:B:34:ILE:N	2.23	0.52
1:A:92:LEU:HA	1:A:95:ILE:HD12	1.92	0.52
1:B:44:SER:C	1:B:46:LYS:N	2.67	0.52
1:C:18:ASP:OD2	1:C:20:ARG:HB3	2.09	0.52
1:C:5:ILE:CG1	1:C:96:GLN:HE21	2.15	0.52
1:D:43:ILE:HG23	1:D:47:SER:HB2	1.92	0.52
1:D:118:ILE:HD13	1:D:261:LEU:HD22	1.92	0.52
1:B:43:ILE:CG2	1:B:47:SER:HB2	2.39	0.52
1:A:151:LEU:C	1:A:153:ASP:H	2.18	0.52
1:B:197:GLN:HG3	1:D:154:GLY:O	2.10	0.52
1:C:108:ALA:C	1:C:110:PRO:CD	2.77	0.52
1:B:46:LYS:C	1:B:48:ALA:N	2.67	0.52
1:C:5:ILE:HD11	1:C:97:GLN:HA	1.92	0.52
1:B:90:ASP:O	1:B:93:ALA:HB3	2.10	0.51
1:B:115:LEU:O	1:B:118:ILE:HG22	2.11	0.51
1:C:9:LEU:HD13	1:D:5:ILE:HG12	1.92	0.51
1:B:63:LEU:HD22	1:B:82:GLY:HA2	1.91	0.51
1:B:119:SER:HA	1:B:122:SER:OG	2.10	0.51
1:B:189:ILE:HD12	1:B:221:MET:CE	2.38	0.51
1:D:44:SER:C	1:D:46:LYS:N	2.68	0.51
1:A:170:LEU:HB3	1:A:260:THR:HG21	1.91	0.51
1:B:115:LEU:HD12	1:B:261:LEU:HG	1.91	0.51
1:C:13:GLN:O	1:C:13:GLN:HG3	2.11	0.51
1:C:15:LEU:HD11	1:C:18:ASP:HB3	1.93	0.51
1:D:59:SER:CB	1:D:63:LEU:HD11	2.40	0.51
1:A:118:ILE:CD1	1:B:95:ILE:HD12	2.41	0.51
1:A:217:CYS:SG	1:A:235:VAL:HG12	2.51	0.51
1:C:21:ARG:HD2	1:C:55:MET:HE2	1.93	0.51
1:C:45:TYR:CD1	1:C:46:LYS:N	2.74	0.51
1:D:43:ILE:HG22	1:D:44:SER:N	2.25	0.51
1:C:26:LYS:CG	1:C:86:ILE:HD11	2.39	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:ILE:HG13	1:D:89:TYR:CD2	2.46	0.50
1:D:25:LEU:HA	1:D:28:ILE:HG22	1.92	0.50
1:D:25:LEU:HD11	1:D:55:MET:HE1	1.93	0.50
1:A:1:MET:HE2	1:B:60:GLU:HB3	1.93	0.50
1:A:49:TRP:O	1:A:52:ILE:CG2	2.58	0.50
1:D:191:GLN:NE2	1:D:241:LEU:HD23	2.26	0.50
1:B:235:VAL:C	1:B:237:GLU:H	2.19	0.50
1:C:21:ARG:HD2	1:C:55:MET:CE	2.41	0.50
1:C:79:THR:HG22	1:C:80:ARG:N	2.26	0.50
1:D:39:LYS:O	1:D:41:ALA:N	2.44	0.50
1:D:130:GLN:HA	1:D:180:ILE:O	2.11	0.50
1:A:34:ILE:HG13	1:A:76:ALA:CB	2.41	0.50
1:D:115:LEU:O	1:D:118:ILE:HG22	2.11	0.50
1:D:223:LEU:C	1:D:225:ASP:N	2.69	0.50
1:B:44:SER:C	1:B:46:LYS:H	2.18	0.50
1:C:225:ASP:C	1:C:227:GLN:H	2.19	0.50
1:B:81:TYR:O	1:B:84:ARG:HG3	2.12	0.50
1:B:39:LYS:C	1:B:41:ALA:H	2.19	0.50
1:B:130:GLN:HA	1:B:180:ILE:O	2.12	0.50
1:B:18:ASP:HB2	1:B:21:ARG:HG3	1.94	0.50
1:D:262:CYS:OXT	1:D:262:CYS:SG	2.70	0.50
1:B:117:ALA:HB2	1:B:120:ARG:NH2	2.27	0.49
1:A:21:ARG:O	1:A:25:LEU:HG	2.11	0.49
1:C:111:LEU:HD22	1:D:87:GLN:HG2	1.94	0.49
1:D:103:LEU:HD11	1:D:117:ALA:O	2.12	0.49
1:A:39:LYS:C	1:A:41:ALA:H	2.21	0.49
1:A:61:HIS:C	1:A:62:ILE:HD13	2.37	0.49
1:C:162:ILE:CD1	1:C:172:LEU:HD12	2.42	0.49
1:B:91:LEU:O	1:B:95:ILE:HG12	2.13	0.49
1:B:207:ILE:HG21	1:B:210:ILE:CD1	2.42	0.49
1:C:170:LEU:HB3	1:C:260:THR:HG21	1.93	0.49
1:D:207:ILE:HG21	1:D:210:ILE:CD1	2.42	0.49
1:D:261:LEU:O	1:D:262:CYS:C	2.54	0.49
1:B:261:LEU:O	1:B:262:CYS:C	2.56	0.49
1:B:84:ARG:HG3	1:B:85:LEU:N	2.27	0.49
1:A:53:ASN:HA	1:A:56:ASN:HB2	1.93	0.49
1:C:9:LEU:CD1	1:D:5:ILE:HG12	2.42	0.49
1:C:83:GLN:C	1:C:86:ILE:HG22	2.38	0.49
1:A:123:LEU:HD21	1:B:115:LEU:HD11	1.94	0.49
1:B:206:ILE:HG22	1:B:245:GLN:O	2.12	0.49
1:D:33:SER:OG	1:D:36:GLN:N	2.40	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:VAL:HG12	1:D:260:THR:HG23	1.95	0.48
1:D:207:ILE:HG21	1:D:210:ILE:HD11	1.94	0.48
1:B:46:LYS:C	1:B:48:ALA:H	2.21	0.48
1:B:138:ARG:HB2	1:B:147:VAL:HG12	1.96	0.48
1:D:206:ILE:HG22	1:D:245:GLN:O	2.13	0.48
1:B:102:VAL:O	1:B:103:LEU:HB2	2.12	0.48
1:B:206:ILE:CG2	1:B:246:ASN:ND2	2.65	0.48
1:D:33:SER:OG	1:D:36:GLN:CB	2.62	0.48
1:A:186:TRP:CD1	1:B:186:TRP:CH2	3.02	0.48
1:A:242:GLN:HG2	1:A:243:GLN:H	1.78	0.48
1:B:44:SER:O	1:B:46:LYS:N	2.47	0.48
1:B:123:LEU:HD12	1:B:123:LEU:H	1.78	0.48
1:C:11:LEU:HA	1:D:3:ALA:CB	2.43	0.48
1:C:178:VAL:HB	1:C:258:ILE:HG23	1.94	0.48
1:D:15:LEU:HD11	1:D:18:ASP:OD1	2.13	0.48
1:A:44:SER:OG	1:A:47:SER:HB2	2.13	0.48
1:A:242:GLN:HG2	1:A:243:GLN:N	2.29	0.48
1:B:34:ILE:H	1:B:34:ILE:CD1	2.26	0.48
1:C:5:ILE:HG12	1:C:97:GLN:OE1	2.13	0.48
1:C:56:ASN:N	1:C:56:ASN:HD22	2.10	0.48
1:D:62:ILE:HD11	1:D:64:VAL:O	2.14	0.48
1:B:26:LYS:HG2	1:B:86:ILE:HD13	1.96	0.47
1:B:103:LEU:HD11	1:B:117:ALA:O	2.14	0.47
1:C:36:GLN:O	1:C:40:ASP:CG	2.56	0.47
1:C:123:LEU:CD1	1:D:118:ILE:HG23	2.43	0.47
1:A:49:TRP:CA	1:A:52:ILE:HG22	2.44	0.47
1:C:103:LEU:HD23	1:D:91:LEU:HD23	1.96	0.47
1:B:207:ILE:HG21	1:B:210:ILE:HD11	1.94	0.47
1:C:24:LEU:O	1:C:28:ILE:HG13	2.15	0.47
1:A:48:ALA:O	1:A:52:ILE:HG22	2.14	0.47
1:C:224:PRO:C	1:C:226:GLY:H	2.21	0.47
1:A:190:THR:OG1	1:A:191:GLN:N	2.47	0.47
1:D:118:ILE:HD13	1:D:261:LEU:CD2	2.43	0.47
1:D:177:GLU:O	1:D:260:THR:HG22	2.14	0.47
1:B:136:THR:HG21	1:B:157:ARG:HH12	1.79	0.47
1:C:102:VAL:HG13	1:C:103:LEU:HD13	1.97	0.47
1:A:52:ILE:HA	1:A:55:MET:HE3	1.96	0.47
1:A:103:LEU:O	1:A:105:ASP:N	2.48	0.47
1:A:183:LYS:HG2	1:A:185:PRO:CD	2.44	0.47
1:B:151:LEU:C	1:B:153:ASP:H	2.23	0.47
1:B:207:ILE:HG21	1:B:210:ILE:CG1	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:LEU:CB	1:C:259:ALA:HB3	2.36	0.47
1:D:39:LYS:C	1:D:41:ALA:N	2.73	0.47
1:C:13:GLN:NE2	1:C:13:GLN:CA	2.76	0.47
1:C:127:ALA:O	1:C:130:GLN:NE2	2.45	0.47
1:C:109:LEU:O	1:C:111:LEU:N	2.45	0.47
1:C:207:ILE:O	1:C:244:GLY:N	2.39	0.47
1:B:21:ARG:HD3	1:B:55:MET:CE	2.45	0.47
1:B:182:LEU:HD13	1:B:256:VAL:HG22	1.96	0.47
1:C:112:ASN:O	1:C:114:LEU:N	2.47	0.47
1:D:65:GLU:HB3	1:D:77:VAL:HG13	1.97	0.47
1:B:18:ASP:OD1	1:B:19:PRO:HD2	2.15	0.46
1:B:159:LYS:HG2	1:B:253:ALA:HB2	1.96	0.46
1:D:207:ILE:HG21	1:D:210:ILE:CG1	2.45	0.46
1:D:138:ARG:HB2	1:D:147:VAL:HG12	1.95	0.46
1:B:177:GLU:O	1:B:260:THR:HG22	2.16	0.46
1:C:128:ARG:HD3	1:D:166:SER:OG	2.15	0.46
1:C:44:SER:HB3	1:C:47:SER:OG	2.15	0.46
1:A:128:ARG:HD3	1:B:166:SER:OG	2.15	0.46
1:A:192:ASP:HB3	1:A:195:VAL:CG2	2.43	0.46
1:A:5:ILE:HG22	1:B:9:LEU:CD1	2.42	0.46
1:A:21:ARG:HG2	1:A:21:ARG:HH11	1.81	0.46
1:C:183:LYS:HG2	1:C:185:PRO:CD	2.44	0.46
1:A:123:LEU:HD21	1:B:115:LEU:CD1	2.45	0.46
1:A:202:GLN:O	1:A:203:LEU:HD23	2.15	0.46
1:C:10:LYS:HA	1:C:16:PHE:H	1.80	0.46
1:A:47:SER:O	1:A:48:ALA:C	2.59	0.46
1:B:178:VAL:HG12	1:B:260:THR:HG23	1.96	0.46
1:B:221:MET:HE2	1:B:247:VAL:CG2	2.46	0.46
1:D:61:HIS:HB3	1:D:81:TYR:CG	2.51	0.46
1:D:77:VAL:HG22	1:D:78:LEU:N	2.30	0.46
1:D:184:ALA:HB3	1:D:185:PRO:HD3	1.98	0.46
1:A:223:LEU:O	1:A:226:GLY:N	2.47	0.46
1:D:170:LEU:HD23	1:D:262:CYS:SG	2.56	0.46
1:A:98:LYS:O	1:A:99:ALA:C	2.59	0.45
1:A:110:PRO:O	1:A:116:ALA:CB	2.63	0.45
1:D:202:GLN:CD	1:D:202:GLN:N	2.74	0.45
1:C:50:ASP:C	1:C:52:ILE:N	2.73	0.45
1:C:150:LEU:HD13	1:C:157:ARG:NH1	2.30	0.45
1:D:43:ILE:CG2	1:D:47:SER:HB2	2.46	0.45
1:A:100:PHE:O	1:A:104:SER:N	2.46	0.45
1:A:21:ARG:O	1:A:24:LEU:HB3	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ARG:HH11	1:A:80:ARG:HG2	1.82	0.45
1:A:109:LEU:HA	1:A:110:PRO:HD3	1.67	0.45
1:C:28:ILE:HD11	1:C:52:ILE:HD11	1.99	0.45
1:C:114:LEU:O	1:C:114:LEU:HG	2.16	0.45
1:D:91:LEU:O	1:D:94:GLN:HB2	2.17	0.45
1:A:44:SER:HB2	1:A:47:SER:OG	2.17	0.45
1:B:25:LEU:O	1:B:28:ILE:HG22	2.16	0.45
1:B:102:VAL:HG12	1:B:103:LEU:N	2.31	0.45
1:D:26:LYS:HG2	1:D:86:ILE:HG21	1.98	0.45
1:D:109:LEU:CG	1:D:110:PRO:HD3	2.47	0.45
1:A:170:LEU:HD22	1:A:260:THR:HG22	1.97	0.45
1:B:180:ILE:HG23	1:B:256:VAL:HG11	1.98	0.45
1:B:184:ALA:HB3	1:B:185:PRO:HD3	1.98	0.45
1:C:13:GLN:O	1:C:13:GLN:CG	2.65	0.45
1:D:180:ILE:HG23	1:D:256:VAL:HG11	1.98	0.45
1:A:114:LEU:HD23	1:B:98:LYS:HE3	1.99	0.45
1:B:123:LEU:HD12	1:B:123:LEU:N	2.32	0.45
1:B:209:HIS:HA	1:B:243:GLN:OE1	2.16	0.45
1:C:111:LEU:CG	1:D:91:LEU:HD22	2.40	0.45
1:C:112:ASN:C	1:C:114:LEU:N	2.73	0.45
1:C:139:ASP:OD1	1:C:139:ASP:C	2.60	0.45
1:C:160:VAL:HG12	1:C:161:ALA:N	2.32	0.45
1:A:42:GLY:O	1:A:43:ILE:HG22	2.16	0.45
1:A:160:VAL:HG12	1:A:161:ALA:N	2.32	0.45
1:B:18:ASP:N	1:B:21:ARG:HB2	2.28	0.45
1:B:52:ILE:CG2	1:B:56:ASN:HD21	2.30	0.45
1:D:223:LEU:O	1:D:226:GLY:N	2.49	0.45
1:B:18:ASP:HB3	1:B:21:ARG:HG3	1.98	0.45
1:B:102:VAL:HG11	1:B:120:ARG:C	2.41	0.44
1:C:115:LEU:HD22	1:C:177:GLU:O	2.18	0.44
1:C:10:LYS:HB2	1:C:14:LYS:O	2.17	0.44
1:D:88:LEU:O	1:D:89:TYR:C	2.60	0.44
1:D:210:ILE:HG12	1:D:219:VAL:HG13	1.99	0.44
1:B:129:ASN:HB2	1:B:182:LEU:HB3	2.00	0.44
1:D:191:GLN:HG3	1:D:247:VAL:HG12	1.98	0.44
1:A:39:LYS:C	1:A:41:ALA:N	2.75	0.44
1:D:182:LEU:HD13	1:D:256:VAL:HG22	1.98	0.44
1:A:5:ILE:HD11	1:A:97:GLN:N	2.33	0.44
1:B:179:LEU:HB3	1:B:259:ALA:HB3	2.00	0.44
1:C:59:SER:O	1:C:60:GLU:HB3	2.17	0.44
1:C:125:THR:HA	1:D:258:ILE:O	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:31:SER:C	1:D:33:SER:H	2.25	0.44
1:A:203:LEU:O	1:A:221:MET:HE1	2.17	0.44
1:D:145:GLN:O	1:D:162:ILE:HD13	2.17	0.44
1:D:235:VAL:C	1:D:237:GLU:H	2.25	0.44
1:A:170:LEU:O	1:A:176:LYS:NZ	2.50	0.44
1:B:45:TYR:O	1:B:45:TYR:CG	2.69	0.44
1:B:210:ILE:HG12	1:B:219:VAL:HG13	1.99	0.44
1:D:38:ALA:HB1	1:D:48:ALA:CB	2.48	0.44
1:A:223:LEU:C	1:A:225:ASP:N	2.74	0.44
1:B:51:ALA:O	1:B:55:MET:HE3	2.18	0.44
1:D:88:LEU:O	1:D:91:LEU:N	2.50	0.44
1:D:141:ASP:HB3	2:D:1264:MOO:O1	2.17	0.44
1:A:56:ASN:OD1	1:A:63:LEU:N	2.50	0.44
1:B:113:SER:OG	1:B:114:LEU:N	2.49	0.44
1:D:223:LEU:O	1:D:225:ASP:N	2.51	0.44
1:A:146:HIS:CE1	1:A:161:ALA:HB2	2.53	0.43
1:B:97:GLN:O	1:B:101:ASP:N	2.46	0.43
1:A:212:ARG:NH2	1:A:238:ALA:O	2.50	0.43
1:A:234:PRO:C	1:A:236:ASN:H	2.25	0.43
1:B:36:GLN:HE21	1:B:40:ASP:CG	2.26	0.43
1:C:146:HIS:CE1	1:C:161:ALA:HB2	2.53	0.43
1:D:206:ILE:HA	1:D:245:GLN:O	2.18	0.43
1:B:165:GLN:O	1:B:169:ARG:HG2	2.18	0.43
1:B:180:ILE:HG23	1:B:256:VAL:CG1	2.49	0.43
1:D:106:ASP:C	1:D:108:ALA:H	2.25	0.43
1:D:129:ASN:HB2	1:D:182:LEU:HB3	1.99	0.43
1:D:221:MET:HE3	1:D:247:VAL:HG23	1.98	0.43
1:B:18:ASP:O	1:B:19:PRO:C	2.60	0.43
1:B:150:LEU:HD13	1:B:157:ARG:CD	2.47	0.43
1:D:28:ILE:O	1:D:28:ILE:HG12	2.18	0.43
1:D:201:ASN:O	1:D:250:TYR:HA	2.18	0.43
1:A:49:TRP:HZ2	1:A:66:ARG:HH22	1.66	0.43
1:A:163:THR:OG1	1:B:128:ARG:HD3	2.17	0.43
1:A:183:LYS:NZ	1:B:256:VAL:O	2.48	0.43
1:B:176:LYS:HA	1:B:176:LYS:HD2	1.86	0.43
1:C:88:LEU:O	1:C:92:LEU:HB2	2.18	0.43
1:A:57:GLN:HE21	1:A:57:GLN:HB2	1.55	0.43
1:C:183:LYS:HD2	1:C:186:TRP:CH2	2.53	0.43
1:D:98:LYS:HD2	1:D:98:LYS:HA	1.80	0.43
1:D:179:LEU:HB3	1:D:259:ALA:HB3	2.00	0.43
1:C:119:SER:CB	1:D:123:LEU:HD11	2.49	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:109:LEU:HD12	1:D:110:PRO:HD3	2.00	0.43
1:D:183:LYS:HB3	1:D:186:TRP:CE2	2.54	0.43
1:B:150:LEU:HB2	1:B:157:ARG:NH1	2.33	0.43
1:C:92:LEU:HA	1:C:95:ILE:HD12	2.01	0.43
1:D:109:LEU:CB	1:D:110:PRO:CD	2.96	0.43
1:D:43:ILE:HG22	1:D:44:SER:O	2.19	0.43
1:D:212:ARG:HG2	1:D:217:CYS:SG	2.59	0.43
1:A:184:ALA:HB3	1:A:185:PRO:HD3	2.00	0.43
1:D:180:ILE:HG23	1:D:256:VAL:CG1	2.48	0.43
1:B:39:LYS:O	1:B:41:ALA:N	2.50	0.42
1:C:46:LYS:HA	1:C:46:LYS:HD3	1.81	0.42
1:C:27:HIS:C	1:C:29:ALA:N	2.76	0.42
1:C:27:HIS:O	1:C:31:SER:N	2.52	0.42
1:B:116:ALA:HA	1:B:132:PHE:CZ	2.54	0.42
1:C:5:ILE:CD1	1:C:96:GLN:HG3	2.49	0.42
1:C:261:LEU:HD23	1:D:123:LEU:HD23	2.02	0.42
1:A:256:VAL:O	1:B:183:LYS:HE2	2.19	0.42
1:B:92:LEU:O	1:B:96:GLN:HG3	2.19	0.42
1:C:184:ALA:HB3	1:C:185:PRO:HD3	2.00	0.42
1:D:56:ASN:OD1	1:D:62:ILE:HG13	2.20	0.42
1:A:35:SER:CA	1:A:45:TYR:CE2	2.94	0.42
1:A:114:LEU:HB3	1:A:261:LEU:HD11	2.01	0.42
1:B:34:ILE:HG12	1:B:35:SER:N	2.34	0.42
1:B:151:LEU:C	1:B:153:ASP:N	2.75	0.42
1:D:27:HIS:CE1	1:D:40:ASP:O	2.73	0.42
1:A:36:GLN:C	1:A:38:ALA:N	2.75	0.42
1:A:183:LYS:HD2	1:A:186:TRP:CH2	2.54	0.42
1:A:207:ILE:HD12	1:A:242:GLN:O	2.19	0.42
1:B:9:LEU:CB	1:B:17:ALA:HB3	2.49	0.42
1:B:183:LYS:HD3	1:B:185:PRO:CD	2.50	0.42
1:B:207:ILE:HD12	1:B:242:GLN:O	2.19	0.42
1:C:120:ARG:HG3	1:C:120:ARG:NH1	2.33	0.42
1:C:150:LEU:HG	1:C:154:GLY:HA2	2.01	0.42
1:C:196:ALA:C	1:C:198:ASN:N	2.75	0.42
1:C:256:VAL:O	1:D:183:LYS:HE2	2.20	0.42
1:D:5:ILE:HD11	1:D:100:PHE:CB	2.48	0.42
1:D:21:ARG:O	1:D:25:LEU:HG	2.20	0.42
1:D:110:PRO:C	1:D:112:ASN:H	2.28	0.42
1:A:44:SER:HB2	1:A:47:SER:CB	2.50	0.42
1:A:114:LEU:HD12	1:A:114:LEU:HA	1.87	0.42
1:A:25:LEU:HD22	1:A:64:VAL:CG2	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ILE:HG13	1:A:76:ALA:HB3	2.01	0.41
1:B:80:ARG:O	1:B:83:GLN:HB2	2.19	0.41
1:D:109:LEU:HG	1:D:110:PRO:CD	2.50	0.41
1:A:124:GLN:HG3	1:B:262:CYS:SG	2.60	0.41
1:B:206:ILE:HA	1:B:245:GLN:O	2.19	0.41
1:C:50:ASP:O	1:C:51:ALA:C	2.63	0.41
1:A:178:VAL:HB	1:A:258:ILE:HG23	2.01	0.41
1:B:102:VAL:HG12	1:B:103:LEU:H	1.86	0.41
1:C:7:LEU:HD11	1:D:5:ILE:CG2	2.46	0.41
1:D:131:TRP:O	1:D:179:LEU:HD12	2.21	0.41
1:D:229:LEU:HD23	1:D:230:CYS:N	2.34	0.41
1:B:20:ARG:O	1:B:23:SER:HB3	2.21	0.41
1:C:11:LEU:N	1:C:14:LYS:O	2.53	0.41
1:C:98:LYS:HE3	1:C:98:LYS:HB3	1.86	0.41
1:C:233:VAL:O	1:C:234:PRO:C	2.61	0.41
1:D:90:ASP:O	1:D:93:ALA:HB3	2.21	0.41
1:A:35:SER:HB3	1:A:45:TYR:HE2	1.86	0.41
1:C:11:LEU:CD1	1:D:3:ALA:HB3	2.29	0.41
1:C:162:ILE:HD13	1:C:172:LEU:HD12	2.03	0.41
1:D:100:PHE:O	1:D:101:ASP:C	2.64	0.41
1:D:188:GLY:O	1:D:249:ALA:HA	2.20	0.41
1:C:96:GLN:HB3	1:D:96:GLN:CD	2.46	0.41
1:D:119:SER:HA	1:D:122:SER:OG	2.21	0.41
1:D:212:ARG:NH2	1:D:241:LEU:O	2.54	0.41
1:A:106:ASP:OD1	1:B:81:TYR:CE2	2.69	0.41
1:A:251:PHE:CD1	1:A:251:PHE:N	2.89	0.41
1:B:117:ALA:HA	1:B:120:ARG:CZ	2.51	0.41
1:B:233:VAL:HG11	1:B:238:ALA:HB2	2.03	0.41
1:C:130:GLN:HG2	1:C:181:LEU:HD23	2.03	0.41
1:A:197:GLN:HA	1:A:202:GLN:OE1	2.21	0.41
1:D:21:ARG:HD3	1:D:55:MET:SD	2.60	0.41
1:D:100:PHE:O	1:D:102:VAL:O	2.38	0.41
1:D:116:ALA:O	1:D:120:ARG:HG2	2.21	0.41
1:A:51:ALA:O	1:A:55:MET:HE2	2.21	0.41
1:B:3:ALA:HB3	1:B:100:PHE:CZ	2.56	0.41
1:D:120:ARG:HG3	1:D:120:ARG:NH1	2.33	0.41
1:D:162:ILE:N	1:D:162:ILE:CD1	2.83	0.41
1:B:114:LEU:HD23	1:B:115:LEU:N	2.29	0.40
1:D:43:ILE:CG2	1:D:44:SER:N	2.84	0.40
1:A:8:THR:HB	1:B:6:LEU:HB2	2.04	0.40
1:A:234:PRO:O	1:A:237:GLU:N	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ALA:HA	1:B:124:GLN:O	2.21	0.40
1:B:118:ILE:HG23	1:B:119:SER:N	2.36	0.40
1:D:65:GLU:HB3	1:D:77:VAL:HG12	2.02	0.40
1:D:182:LEU:HD12	1:D:186:TRP:HE3	1.86	0.40
1:D:183:LYS:HD3	1:D:185:PRO:CD	2.50	0.40
1:A:22:ILE:O	1:A:26:LYS:HG3	2.21	0.40
1:A:44:SER:CB	1:A:47:SER:HB2	2.52	0.40
1:B:208:SER:HB3	1:B:222:ALA:HB2	2.03	0.40
1:C:5:ILE:HD11	1:C:96:GLN:HG3	2.03	0.40
1:C:27:HIS:ND1	1:C:41:ALA:CA	2.85	0.40
1:D:22:ILE:O	1:D:26:LYS:HG3	2.21	0.40
1:A:62:ILE:O	1:A:63:LEU:C	2.63	0.40
1:D:114:LEU:O	1:D:118:ILE:CB	2.70	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	251/262 (96%)	210 (84%)	35 (14%)	6 (2%)	4	9
1	B	252/262 (96%)	210 (83%)	32 (13%)	10 (4%)	2	3
1	C	251/262 (96%)	220 (88%)	23 (9%)	8 (3%)	3	5
1	D	250/262 (95%)	205 (82%)	36 (14%)	9 (4%)	2	4
All	All	1004/1048 (96%)	845 (84%)	126 (12%)	33 (3%)	3	5

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	ILE
1	A	45	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	14	LYS
1	B	114	LEU
1	C	109	LEU
1	C	112	ASN
1	D	105	ASP
1	D	110	PRO
1	A	104	SER
1	B	40	ASP
1	B	45	TYR
1	B	104	SER
1	C	106	ASP
1	C	200	ASP
1	D	40	ASP
1	D	45	TYR
1	D	95	ILE
1	A	152	ALA
1	B	65	GLU
1	B	110	PRO
1	D	193	GLU
1	A	35	SER
1	B	13	GLN
1	B	122	SER
1	B	152	ALA
1	C	42	GLY
1	C	75	GLY
1	D	107	ASP
1	C	114	LEU
1	C	138	ARG
1	A	62	ILE
1	D	109	LEU
1	D	224	PRO

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	209/211 (99%)	198 (95%)	11 (5%)	20	39
1	B	210/211 (100%)	197 (94%)	13 (6%)	16	31
1	C	207/211 (98%)	196 (95%)	11 (5%)	20	39
1	D	208/211 (99%)	195 (94%)	13 (6%)	16	30
All	All	834/844 (99%)	786 (94%)	48 (6%)	18	34

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	SER
1	A	45	TYR
1	A	52	ILE
1	A	57	GLN
1	A	62	ILE
1	A	63	LEU
1	A	80	ARG
1	A	86	ILE
1	A	107	ASP
1	A	112	ASN
1	A	179	LEU
1	B	2	GLN
1	B	5	ILE
1	B	34	ILE
1	B	44	SER
1	B	65	GLU
1	B	103	LEU
1	B	107	ASP
1	B	114	LEU
1	B	162	ILE
1	B	183	LYS
1	B	206	ILE
1	B	239	THR
1	B	246	ASN
1	C	4	GLU
1	C	103	LEU
1	C	104	SER
1	C	109	LEU
1	C	111	LEU
1	C	115	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	123	LEU
1	C	179	LEU
1	C	193	GLU
1	C	236	ASN
1	C	248	THR
1	D	5	ILE
1	D	50	ASP
1	D	96	GLN
1	D	106	ASP
1	D	109	LEU
1	D	110	PRO
1	D	155	LYS
1	D	162	ILE
1	D	183	LYS
1	D	197	GLN
1	D	206	ILE
1	D	239	THR
1	D	247	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	57	GLN
1	A	112	ASN
1	A	146	HIS
1	A	197	GLN
1	A	209	HIS
1	A	242	GLN
1	A	245	GLN
1	B	36	GLN
1	B	53	ASN
1	B	56	ASN
1	B	144	GLN
1	B	198	ASN
1	B	202	GLN
1	B	216	GLN
1	B	227	GLN
1	B	246	ASN
1	C	13	GLN
1	C	56	ASN
1	C	57	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	96	GLN
1	C	112	ASN
1	C	146	HIS
1	C	191	GLN
1	C	197	GLN
1	C	202	GLN
1	C	245	GLN
1	D	2	GLN
1	D	57	GLN
1	D	97	GLN
1	D	144	GLN
1	D	191	GLN
1	D	197	GLN
1	D	216	GLN
1	D	227	GLN
1	D	242	GLN

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](#)

Of 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	MOO	A	1263	-	2,4,4	0.66	0	-		
2	MOO	B	1263	-	2,4,4	0.68	0	-		
2	MOO	D	1263	1	2,4,4	0.69	0	-		
2	MOO	C	1262	-	2,4,4	0.76	0	-		
2	MOO	D	1264	4	2,4,4	0.74	0	-		

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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1264	MOO	2	0

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	255/262 (97%)	-1.25	0 100 100	23, 48, 87, 92	8 (3%)
1	B	255/262 (97%)	-1.29	0 100 100	21, 50, 82, 92	5 (1%)
1	C	255/262 (97%)	-1.28	0 100 100	22, 49, 86, 95	5 (1%)
1	D	254/262 (96%)	-1.29	0 100 100	22, 52, 79, 90	7 (2%)
All	All	1019/1048 (97%)	-1.28	0 100 100	21, 51, 85, 95	25 (2%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
2	MOO	A	1263	5/5	1.00	0.02	20,21,22,22	0
2	MOO	B	1263	5/5	1.00	0.01	29,30,32,36	0
2	MOO	C	1262	5/5	1.00	0.02	19,21,27,31	0
2	MOO	D	1263	5/5	1.00	0.02	28,29,30,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	MOO	D	1264	5/5	1.00	0.02	34,37,41,42	0
3	CL	B	1264	1/1	1.00	0.03	19,19,19,19	0
4	CA	D	1265	1/1	1.00	0.03	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.