



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:13 PM UTC

PDB ID : 1A2O / pdb_00001a2o
Title : STRUCTURAL BASIS FOR METHYLESTERASE CHEB REGULATION
BY A PHOSPHORYLATION-ACTIVATED DOMAIN
Authors : Djordjevic, S.; Goudreau, P.N.; Xu, Q.; Stock, A.M.; West, A.H.
Deposited on : 1998-01-06
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	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

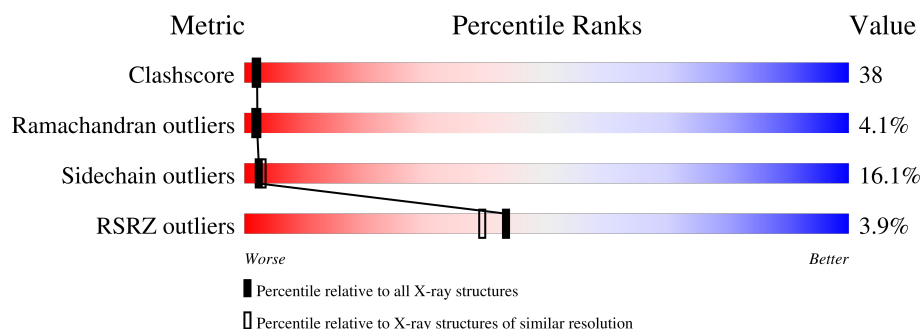
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	349	
1	B	349	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5615 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 CHEB METHYLESTERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	347	Total	C	N	O	S	0	0	0
			2602	1633	465	481	23			
1	B	347	Total	C	N	O	S	0	0	0
			2602	1633	465	481	23			

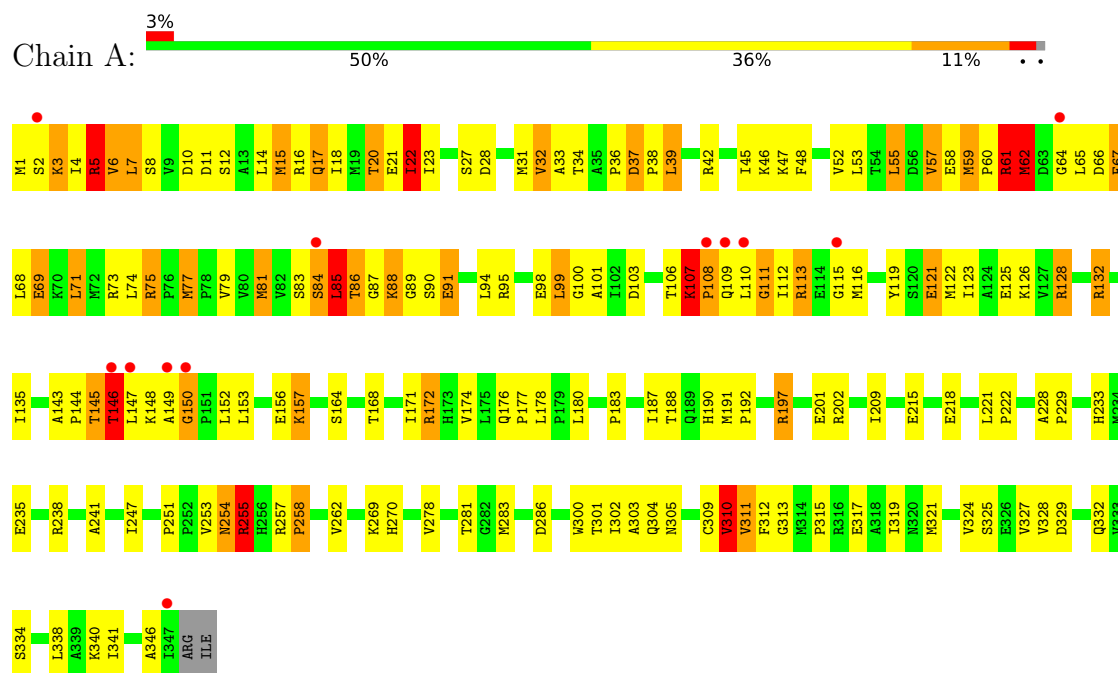
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	221	Total	O	0	0
			221	221		
2	B	190	Total	O	0	0
			190	190		

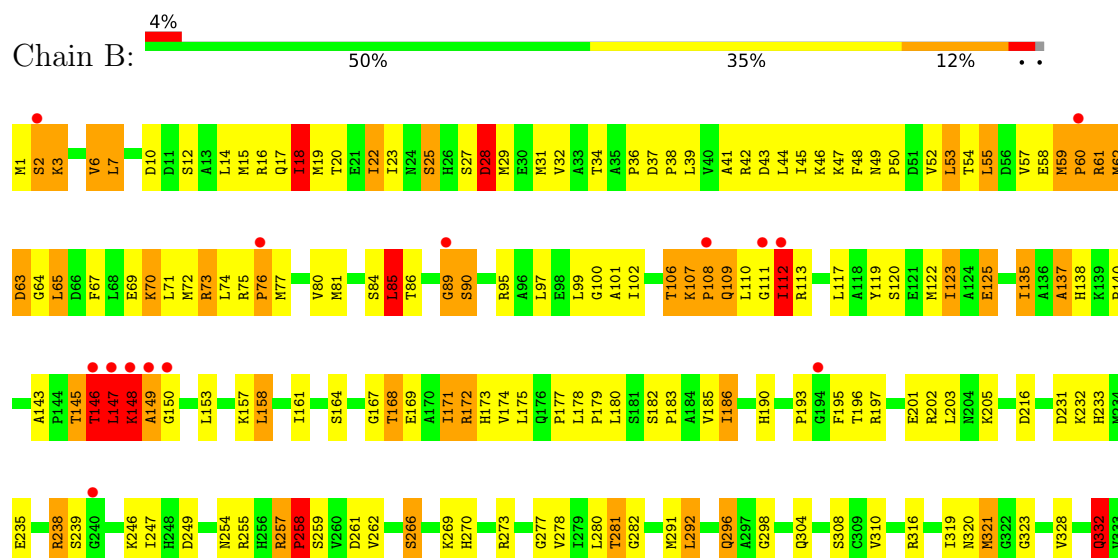
3 Residue-property plots

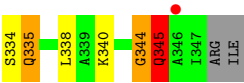
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: CHEB METHYLESTERASE



• Molecule 1: CHEB METHYLESTERASE





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.83Å 100.46Å 53.12Å 90.00° 98.63° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40 10.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	96.9 (10.00-2.40) 96.1 (10.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.93 (at 2.20Å)	Xtriage
Refinement program	REFMAC, X-PLOR	Depositor
R, R_{free}	0.222 , (Not available) 0.231 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	30.2	Xtriage
Anisotropy	0.495	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 99.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5615	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.22% 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

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	0.70	0/2645	1.72	40/3577 (1.1%)
1	B	0.69	0/2645	1.67	30/3577 (0.8%)
All	All	0.70	0/5290	1.69	70/7154 (1.0%)

There are no bond length outliers.

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	257	ARG	CA-C-O	-14.97	104.91	120.63
1	B	145	THR	CA-C-N	14.02	148.31	121.54
1	B	145	THR	C-N-CA	14.02	148.31	121.54
1	A	67	PHE	CA-CB-CG	13.01	126.81	113.80
1	A	257	ARG	O-C-N	9.30	126.85	121.27
1	A	145	THR	N-CA-C	-9.30	98.64	112.04
1	B	58	GLU	N-CA-C	-8.83	99.58	110.88
1	A	128	ARG	CD-NE-CZ	7.88	135.43	124.40
1	A	310	VAL	N-CA-C	-7.79	102.51	111.00
1	A	150	GLY	CA-C-N	7.51	129.22	119.84
1	A	150	GLY	C-N-CA	7.51	129.22	119.84
1	B	146	THR	N-CA-C	7.51	126.79	110.80
1	B	148	LYS	CA-C-N	7.47	135.81	121.54
1	B	148	LYS	C-N-CA	7.47	135.81	121.54
1	B	112	ILE	N-CA-C	7.38	124.70	109.34
1	A	254	ASN	N-CA-C	-7.32	103.65	112.58
1	B	137	ALA	N-CA-C	-6.84	104.94	113.28
1	A	251	PRO	O-C-N	6.82	124.45	121.31
1	B	172	ARG	NE-CZ-NH2	6.78	125.30	119.20
1	A	67	PHE	N-CA-CB	6.69	120.03	110.13
1	A	34	THR	CA-C-O	-6.66	113.64	121.44
1	B	150	GLY	O-C-N	-6.56	115.21	121.77
1	A	128	ARG	NE-CZ-NH1	6.55	128.05	121.50
1	B	89	GLY	N-CA-C	-6.54	100.76	110.97
1	A	83	SER	N-CA-C	6.31	119.81	109.85

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137	ALA	CA-C-O	6.30	126.67	119.18
1	A	152	LEU	N-CA-C	6.16	119.28	110.10
1	B	258	PRO	N-CA-C	-6.14	99.81	112.47
1	B	34	THR	CA-C-O	-6.07	114.77	121.33
1	A	172	ARG	CD-NE-CZ	6.06	132.89	124.40
1	B	150	GLY	N-CA-C	6.03	124.64	112.34
1	A	150	GLY	N-CA-C	6.02	124.63	112.34
1	A	116	MET	N-CA-C	5.97	118.28	111.11
1	A	52	VAL	CA-C-O	5.93	126.89	120.43
1	A	305	ASN	OD1-CG-ND2	-5.92	116.68	122.60
1	A	107	LYS	CA-C-N	5.87	127.18	119.84
1	A	107	LYS	C-N-CA	5.87	127.18	119.84
1	A	172	ARG	NE-CZ-NH2	-5.85	113.94	119.20
1	A	258	PRO	N-CD-CG	5.78	110.74	103.80
1	A	5	ARG	CD-NE-CZ	5.76	132.47	124.40
1	A	115	GLY	N-CA-C	5.76	121.56	111.25
1	A	111	GLY	N-CA-C	-5.73	99.61	113.18
1	B	28	ASP	CA-CB-CG	5.66	118.26	112.60
1	B	62	MET	N-CA-C	-5.62	104.39	111.92
1	A	37	ASP	N-CA-C	5.56	113.02	108.07
1	B	147	LEU	N-CA-CB	-5.54	99.45	110.64
1	A	309	CYS	O-C-N	5.46	129.50	123.16
1	B	148	LYS	CA-C-O	5.41	126.82	120.43
1	A	258	PRO	N-CA-CB	5.35	108.49	102.60
1	B	76	PRO	N-CA-C	5.35	120.46	111.32
1	B	277	GLY	O-C-N	5.34	129.36	123.49
1	B	18	ILE	N-CA-C	-5.32	105.53	110.53
1	A	149	ALA	N-CA-C	5.29	117.72	109.52
1	A	145	THR	CA-C-N	5.28	131.62	121.54
1	A	145	THR	C-N-CA	5.28	131.62	121.54
1	A	209	ILE	CA-C-O	-5.18	116.38	122.13
1	B	332	GLN	OE1-CD-NE2	5.16	127.76	122.60
1	B	112	ILE	CA-C-N	5.15	131.00	121.52
1	B	112	ILE	C-N-CA	5.15	131.00	121.52
1	B	175	LEU	N-CA-C	5.11	117.98	111.69
1	B	292	LEU	N-CA-C	-5.11	105.61	111.07
1	A	22	ILE	N-CA-CB	5.10	117.47	110.54
1	B	320	ASN	CB-CG-ND2	5.08	124.02	116.40
1	A	247	ILE	CA-C-O	-5.05	115.12	120.48
1	A	67	PHE	N-CA-C	-5.05	105.24	111.40
1	A	150	GLY	O-C-N	-5.03	116.74	121.77
1	A	255	ARG	NH1-CZ-NH2	5.03	125.83	119.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	266	SER	CA-CB-OG	5.02	121.13	111.10
1	A	187	ILE	N-CA-C	5.01	115.93	108.46
1	B	270	HIS	N-CA-C	5.01	118.55	112.23

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	2602	0	2686	189	0
1	B	2602	0	2686	208	0
2	A	221	0	0	20	0
2	B	190	0	0	11	0
All	All	5615	0	5372	397	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 38.

All (397) 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:319:ILE:HG13	2:A:547:HOH:O	1.40	1.20
1:A:85:LEU:HD11	1:A:108:PRO:HD3	1.21	1.19
1:A:85:LEU:N	1:A:85:LEU:HD22	1.55	1.17
1:B:147:LEU:HD22	1:B:338:LEU:HD23	1.26	1.16
1:B:157:LYS:HZ1	1:B:345:GLN:HG2	0.99	1.12
1:B:109:GLN:NE2	1:B:112:ILE:HG13	1.66	1.11
1:B:147:LEU:HD11	1:B:178:LEU:HD23	1.32	1.07
1:B:147:LEU:HD22	1:B:338:LEU:CD2	1.85	1.06
1:B:110:LEU:HD12	1:B:110:LEU:O	1.55	1.06
1:B:42:ARG:HD3	2:B:506:HOH:O	1.56	1.05
1:A:144:PRO:HB2	1:A:146:THR:OG1	1.56	1.05
1:A:55:LEU:HD12	1:A:81:MET:HE1	1.36	1.03
1:A:109:GLN:HE22	1:A:110:LEU:HB2	1.24	1.01

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:ILE:HG13	1:A:23:ILE:N	1.74	1.00
1:A:147:LEU:HD12	1:A:338:LEU:HD22	1.40	1.00
1:B:157:LYS:NZ	1:B:345:GLN:HG2	1.77	0.99
1:A:88:LYS:HA	1:A:88:LYS:HE3	1.41	0.99
1:B:147:LEU:CD2	1:B:338:LEU:CD2	2.40	0.98
1:B:147:LEU:HD21	1:B:338:LEU:HB2	1.46	0.97
1:B:109:GLN:HE21	1:B:112:ILE:HG13	1.26	0.97
1:B:147:LEU:CD1	1:B:178:LEU:HA	1.95	0.96
1:B:147:LEU:HD13	1:B:147:LEU:O	1.67	0.95
1:A:109:GLN:NE2	1:A:110:LEU:HB2	1.80	0.95
1:A:10:ASP:OD2	1:A:15:MET:HG2	1.66	0.94
1:B:149:ALA:HA	2:B:509:HOH:O	1.67	0.94
1:B:110:LEU:O	1:B:110:LEU:CD1	2.15	0.94
1:B:65:LEU:HD12	1:B:99:LEU:HD23	1.51	0.92
1:B:257:ARG:HB3	1:B:258:PRO:HD3	1.50	0.92
1:A:147:LEU:HD11	1:A:178:LEU:HD23	1.53	0.91
1:B:167:GLY:O	1:B:171:ILE:HG23	1.70	0.91
1:B:108:PRO:HG3	1:B:122:MET:CE	2.00	0.91
1:B:147:LEU:O	1:B:177:PRO:O	1.90	0.90
1:A:94:LEU:O	1:A:98:GLU:HG2	1.71	0.89
1:B:111:GLY:C	1:B:112:ILE:HG12	1.97	0.88
1:A:5:ARG:HB3	1:A:32:VAL:HG21	1.56	0.88
1:A:22:ILE:HD11	1:A:123:ILE:HG21	1.55	0.87
1:B:119:TYR:CE1	1:B:123:ILE:HD11	2.10	0.87
1:B:22:ILE:HD13	1:B:23:ILE:N	1.89	0.87
1:A:4:ILE:HD11	1:A:132:ARG:NH2	1.90	0.86
1:A:85:LEU:HD22	1:A:85:LEU:H	1.42	0.85
1:A:300:TRP:CD1	1:A:340:LYS:HG3	2.11	0.85
1:A:65:LEU:O	1:A:69:GLU:HB2	1.75	0.85
1:A:7:LEU:HB3	2:A:535:HOH:O	1.76	0.85
1:B:147:LEU:HD21	1:B:338:LEU:CB	2.07	0.84
1:A:147:LEU:HD21	1:A:334:SER:OG	1.79	0.82
1:A:238:ARG:HD3	2:A:549:HOH:O	1.80	0.82
1:B:147:LEU:CD1	1:B:178:LEU:HD23	2.08	0.81
1:A:107:LYS:HD2	1:A:107:LYS:O	1.79	0.81
1:B:112:ILE:HG22	1:B:113:ARG:H	1.45	0.81
1:B:147:LEU:CD2	1:B:338:LEU:HD22	2.10	0.81
1:A:85:LEU:N	1:A:85:LEU:CD2	2.32	0.80
1:A:85:LEU:HD21	1:A:108:PRO:HA	1.60	0.80
1:A:84:SER:C	1:A:85:LEU:HD22	2.05	0.80
1:B:145:THR:O	1:B:148:LYS:CE	2.29	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:147:LEU:CD2	1:B:338:LEU:HD23	2.07	0.80
1:A:108:PRO:O	1:A:109:GLN:HB3	1.82	0.80
1:B:55:LEU:HD13	1:B:57:VAL:CG2	2.11	0.80
1:A:147:LEU:HD12	1:A:338:LEU:CD2	2.12	0.79
1:B:158:LEU:HD11	1:B:186:ILE:HD13	1.63	0.78
1:B:106:THR:O	1:B:108:PRO:HD3	1.84	0.77
1:A:55:LEU:CD1	1:A:81:MET:HE1	2.12	0.77
1:B:61:ARG:HA	1:B:61:ARG:NE	2.00	0.77
1:A:61:ARG:O	1:A:62:MET:C	2.28	0.77
1:B:147:LEU:CD2	1:B:338:LEU:CB	2.62	0.76
1:B:158:LEU:HD11	1:B:186:ILE:CD1	2.16	0.76
1:B:147:LEU:HD11	1:B:178:LEU:HA	1.67	0.76
1:A:22:ILE:HD11	1:A:123:ILE:CG2	2.16	0.75
1:B:45:ILE:HD13	1:B:77:MET:HE1	1.66	0.75
1:A:45:ILE:CG2	1:A:77:MET:HE1	2.16	0.75
1:A:192:PRO:HG3	2:A:417:HOH:O	1.86	0.75
1:A:53:LEU:HD12	1:A:79:VAL:HG13	1.68	0.74
1:B:147:LEU:CD1	1:B:147:LEU:O	2.35	0.74
1:A:85:LEU:HD21	1:A:108:PRO:CA	2.16	0.74
1:A:91:GLU:HB2	2:A:502:HOH:O	1.86	0.74
1:A:17:GLN:OE1	2:A:437:HOH:O	2.06	0.73
1:B:108:PRO:HG3	1:B:122:MET:HE1	1.70	0.73
1:B:171:ILE:HD11	1:B:203:LEU:CD1	2.18	0.73
1:B:69:GLU:O	1:B:73:ARG:HB2	1.89	0.72
1:B:153:LEU:HD12	1:B:183:PRO:HG3	1.70	0.72
1:B:147:LEU:HD21	1:B:338:LEU:CD2	2.17	0.72
1:B:257:ARG:HB3	1:B:258:PRO:CD	2.19	0.72
1:A:88:LYS:HA	1:A:88:LYS:CE	2.16	0.72
1:A:37:ASP:HB2	1:A:38:PRO:HD2	1.70	0.72
1:B:135:ILE:N	1:B:135:ILE:HD13	2.04	0.72
1:B:147:LEU:HD21	1:B:338:LEU:HD22	1.70	0.71
1:B:7:LEU:O	1:B:53:LEU:HD22	1.90	0.71
1:B:110:LEU:HD12	1:B:110:LEU:C	2.15	0.71
1:A:85:LEU:CD1	1:A:108:PRO:HD3	2.11	0.71
1:A:221:LEU:HB3	1:A:222:PRO:HD2	1.73	0.71
1:A:69:GLU:O	1:A:73:ARG:HG3	1.89	0.70
1:A:88:LYS:HE2	1:A:91:GLU:HB3	1.73	0.70
1:B:85:LEU:H	1:B:85:LEU:HD22	1.57	0.70
1:B:147:LEU:HD11	1:B:178:LEU:CD2	2.16	0.70
1:A:147:LEU:HD23	1:A:147:LEU:H	1.56	0.70
1:A:5:ARG:HB3	1:A:32:VAL:CG2	2.22	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:MET:HG2	2:A:512:HOH:O	1.92	0.69
1:B:20:THR:HG22	1:B:31:MET:HG2	1.74	0.69
1:B:95:ARG:HD3	1:B:202:ARG:HH22	1.58	0.69
1:B:158:LEU:CD1	1:B:186:ILE:HD13	2.22	0.69
1:A:110:LEU:C	1:A:112:ILE:H	2.00	0.69
1:A:45:ILE:HG21	1:A:77:MET:CE	2.22	0.69
1:B:147:LEU:HD13	1:B:147:LEU:C	2.17	0.68
1:A:11:ASP:HB2	1:A:59:MET:HG2	1.75	0.68
1:B:235:GLU:HB2	1:B:266:SER:OG	1.92	0.67
1:B:41:ALA:O	1:B:45:ILE:HG13	1.95	0.67
1:B:257:ARG:O	1:B:259:SER:N	2.28	0.67
1:B:292:LEU:O	1:B:296:GLN:HG2	1.95	0.67
1:A:147:LEU:CD1	1:A:178:LEU:HD23	2.25	0.67
1:B:157:LYS:HZ1	1:B:345:GLN:CG	1.92	0.67
1:A:310:VAL:HG22	1:A:311:VAL:HG23	1.77	0.66
1:B:32:VAL:HG22	1:B:48:PHE:CD2	2.31	0.66
1:B:161:ILE:HG12	1:B:278:VAL:HB	1.76	0.66
1:A:281:THR:H	1:A:304:GLN:NE2	1.93	0.66
1:A:147:LEU:CD2	1:A:177:PRO:HB2	2.26	0.66
1:A:2:SER:HA	1:A:28:ASP:C	2.21	0.66
1:A:45:ILE:HG21	1:A:77:MET:HE1	1.79	0.65
1:A:147:LEU:C	1:A:148:LYS:HG2	2.22	0.65
1:B:22:ILE:HD13	1:B:23:ILE:H	1.56	0.65
1:B:153:LEU:HD22	1:B:345:GLN:HG3	1.78	0.65
1:A:10:ASP:OD2	1:A:15:MET:CG	2.43	0.64
1:A:77:MET:HE2	2:A:524:HOH:O	1.96	0.64
1:B:62:MET:HB3	2:B:507:HOH:O	1.97	0.64
1:A:39:LEU:CD1	1:A:42:ARG:HH21	2.12	0.63
1:A:110:LEU:HG	1:A:111:GLY:H	1.64	0.62
1:B:57:VAL:HG23	1:B:81:MET:HE1	1.81	0.62
1:B:7:LEU:HD21	1:B:44:LEU:HB2	1.82	0.62
1:B:135:ILE:H	1:B:135:ILE:CD1	2.12	0.62
1:B:147:LEU:HD23	1:B:335:GLN:HA	1.79	0.62
1:B:108:PRO:O	1:B:109:GLN:O	2.18	0.62
1:A:128:ARG:O	1:A:132:ARG:HD2	2.00	0.62
1:B:147:LEU:CD2	1:B:338:LEU:HB2	2.22	0.62
1:B:147:LEU:HD12	1:B:177:PRO:C	2.24	0.61
1:A:10:ASP:CG	1:A:15:MET:HG2	2.25	0.61
1:B:171:ILE:HD11	1:B:203:LEU:HD11	1.81	0.61
1:A:45:ILE:HG23	1:A:77:MET:HE1	1.82	0.61
1:B:171:ILE:HD11	1:B:203:LEU:HD13	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ARG:O	1:B:20:THR:HG23	2.01	0.61
1:A:84:SER:O	1:A:85:LEU:C	2.43	0.61
1:B:73:ARG:HH22	1:B:140:PRO:HG2	1.67	0.60
1:B:135:ILE:N	1:B:135:ILE:CD1	2.64	0.60
1:A:321:MET:HG3	2:A:369:HOH:O	2.01	0.60
1:A:147:LEU:HD21	1:A:177:PRO:HB2	1.82	0.60
1:B:61:ARG:NH1	1:B:62:MET:HG2	2.16	0.60
1:A:53:LEU:CD1	1:A:79:VAL:HG13	2.32	0.60
1:B:147:LEU:HD12	1:B:178:LEU:HA	1.83	0.60
1:B:216:ASP:HB2	1:B:247:ILE:HB	1.84	0.60
1:A:301:THR:OG1	1:A:324:VAL:HA	2.02	0.59
1:B:112:ILE:CG2	1:B:113:ARG:H	2.07	0.59
1:A:3:LYS:NZ	1:A:28:ASP:HB2	2.17	0.59
1:A:39:LEU:HD13	1:A:42:ARG:HH21	1.67	0.59
1:B:205:LYS:HD3	2:B:459:HOH:O	2.01	0.59
1:A:283:MET:HE2	2:A:553:HOH:O	2.01	0.59
1:A:328:VAL:HG12	1:A:329:ASP:O	2.03	0.59
1:B:147:LEU:C	1:B:148:LYS:CG	2.76	0.59
1:B:119:TYR:CZ	1:B:123:ILE:HD11	2.38	0.59
1:A:55:LEU:HD12	1:A:81:MET:CE	2.24	0.59
1:B:292:LEU:HD22	1:B:321:MET:HE2	1.85	0.59
1:A:88:LYS:CE	1:A:91:GLU:HB3	2.33	0.58
1:A:95:ARG:HD2	1:A:202:ARG:HH22	1.68	0.58
1:B:145:THR:O	1:B:148:LYS:HE3	2.03	0.58
1:B:61:ARG:HA	1:B:61:ARG:HE	1.67	0.58
1:A:85:LEU:H	1:A:85:LEU:HD13	1.67	0.58
1:A:110:LEU:C	1:A:112:ILE:N	2.62	0.58
1:B:231:ASP:C	1:B:257:ARG:HG2	2.29	0.58
1:B:57:VAL:HG13	1:B:64:GLY:HA3	1.85	0.57
1:A:183:PRO:HG2	1:A:341:ILE:HG21	1.87	0.57
1:B:233:HIS:CE1	1:B:257:ARG:O	2.58	0.57
1:A:37:ASP:OD1	1:A:39:LEU:HB2	2.05	0.57
1:B:37:ASP:HB2	1:B:38:PRO:CD	2.35	0.57
1:A:319:ILE:CG1	2:A:547:HOH:O	2.20	0.56
1:A:55:LEU:CD1	1:A:81:MET:CE	2.81	0.56
1:A:147:LEU:O	1:A:148:LYS:HG2	2.05	0.56
1:A:303:ALA:HB3	1:A:319:ILE:HD11	1.87	0.56
1:A:22:ILE:HG13	1:A:23:ILE:H	1.70	0.56
1:A:176:GLN:HB3	1:A:177:PRO:HD3	1.87	0.56
1:B:122:MET:O	1:B:125:GLU:HG3	2.06	0.56
1:A:74:LEU:O	1:A:75:ARG:HB2	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:VAL:CG1	1:A:332:GLN:HB2	2.36	0.55
1:A:32:VAL:O	1:A:33:ALA:HB2	2.06	0.55
1:B:57:VAL:HA	1:B:59:MET:HE2	1.88	0.55
1:B:100:GLY:O	1:B:138:HIS:NE2	2.39	0.54
1:B:62:MET:O	1:B:63:ASP:C	2.49	0.54
1:B:10:ASP:O	1:B:36:PRO:HA	2.07	0.54
1:B:97:LEU:HA	1:B:101:ALA:HB3	1.90	0.54
1:A:95:ARG:NH2	2:A:475:HOH:O	2.39	0.54
1:A:192:PRO:CG	2:A:417:HOH:O	2.51	0.54
1:A:312:PHE:O	1:A:315:PRO:HD2	2.08	0.54
1:B:106:THR:O	1:B:108:PRO:CD	2.56	0.54
1:A:71:LEU:O	1:A:71:LEU:HD22	2.08	0.54
1:B:119:TYR:O	1:B:123:ILE:HD12	2.08	0.54
1:B:147:LEU:HG	1:B:334:SER:OG	2.08	0.54
1:B:2:SER:HB3	2:B:424:HOH:O	2.06	0.54
1:A:190:HIS:NE2	1:A:286:ASP:OD2	2.41	0.54
1:B:145:THR:O	1:B:148:LYS:CD	2.55	0.54
1:A:150:GLY:N	2:A:364:HOH:O	2.41	0.53
1:A:3:LYS:HE2	1:A:132:ARG:NH2	2.24	0.53
1:A:147:LEU:HD11	1:A:178:LEU:CD2	2.34	0.53
1:B:89:GLY:O	1:B:90:SER:CB	2.55	0.53
1:A:346:ALA:HB2	2:A:488:HOH:O	2.09	0.53
1:A:16:ARG:O	1:A:20:THR:HG23	2.08	0.53
1:B:112:ILE:HG22	1:B:113:ARG:N	2.20	0.53
1:B:147:LEU:CD2	1:B:338:LEU:HB3	2.38	0.53
1:B:62:MET:O	1:B:63:ASP:O	2.27	0.53
1:B:145:THR:O	1:B:148:LYS:HE2	2.08	0.53
1:A:64:GLY:O	1:A:68:LEU:HB3	2.09	0.52
1:A:4:ILE:HD11	1:A:132:ARG:HH21	1.71	0.52
1:A:145:THR:OG1	1:A:146:THR:N	2.42	0.52
1:B:15:MET:HE3	1:B:19:MET:SD	2.50	0.52
1:B:61:ARG:O	1:B:62:MET:HB2	2.08	0.52
1:B:108:PRO:HG3	1:B:122:MET:HE3	1.89	0.52
1:B:254:ASN:OD1	1:B:261:ASP:OD2	2.25	0.52
1:A:58:GLU:O	1:A:58:GLU:HG2	2.10	0.52
1:B:157:LYS:NZ	1:B:345:GLN:HA	2.25	0.52
1:B:32:VAL:HG22	1:B:48:PHE:HD2	1.72	0.52
1:A:109:GLN:CD	1:A:110:LEU:HB2	2.35	0.52
1:A:147:LEU:O	1:A:177:PRO:O	2.28	0.52
1:B:74:LEU:C	1:B:76:PRO:HD3	2.33	0.52
1:A:3:LYS:HE2	1:A:132:ARG:HH21	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:LEU:N	1:B:44:LEU:HD23	2.25	0.51
1:B:147:LEU:O	1:B:148:LYS:HG2	2.09	0.51
1:A:113:ARG:HE	1:A:113:ARG:HA	1.75	0.51
1:B:95:ARG:O	1:B:99:LEU:HB2	2.11	0.51
1:B:84:SER:O	1:B:86:THR:N	2.44	0.51
1:A:84:SER:O	1:A:86:THR:N	2.43	0.51
1:B:193:PRO:HG3	1:B:231:ASP:HB2	1.93	0.51
1:A:47:LYS:HG2	1:A:48:PHE:CD2	2.46	0.51
1:A:119:TYR:CZ	1:A:123:ILE:HD11	2.45	0.51
1:B:232:LYS:HD3	1:B:249:ASP:OD2	2.10	0.51
1:A:57:VAL:HG22	1:A:81:MET:HE3	1.93	0.51
1:B:19:MET:O	1:B:22:ILE:HD13	2.11	0.51
1:A:215:GLU:HG2	1:A:218:GLU:OE2	2.10	0.51
1:B:17:GLN:O	1:B:20:THR:OG1	2.28	0.51
1:B:107:LYS:O	1:B:108:PRO:C	2.54	0.51
1:B:238:ARG:NH2	2:B:378:HOH:O	2.44	0.50
1:A:32:VAL:HG11	1:A:48:PHE:HB3	1.92	0.50
1:B:18:ILE:N	1:B:18:ILE:HD13	2.27	0.50
1:B:10:ASP:HB3	1:B:16:ARG:HG3	1.92	0.50
1:A:269:LYS:HE2	1:A:270:HIS:CE1	2.47	0.50
1:A:6:VAL:HG22	1:A:31:MET:SD	2.51	0.50
1:A:109:GLN:CD	1:A:109:GLN:C	2.78	0.50
1:B:65:LEU:CD1	1:B:99:LEU:HD23	2.32	0.50
1:B:2:SER:HA	1:B:29:MET:N	2.26	0.50
1:A:109:GLN:OE1	1:A:112:ILE:HG21	2.11	0.50
1:A:171:ILE:O	1:A:174:VAL:HG22	2.12	0.49
1:A:255:ARG:HA	1:A:255:ARG:NE	2.26	0.49
1:A:18:ILE:O	1:A:22:ILE:HG23	2.13	0.49
1:A:321:MET:CG	2:A:369:HOH:O	2.60	0.49
1:B:257:ARG:O	1:B:258:PRO:C	2.55	0.49
1:A:53:LEU:HD12	1:A:79:VAL:CG1	2.40	0.49
1:A:95:ARG:HD2	1:A:202:ARG:NH2	2.26	0.49
1:B:110:LEU:CD1	1:B:110:LEU:C	2.82	0.49
1:B:119:TYR:CD1	1:B:123:ILE:HD11	2.48	0.49
1:A:2:SER:HA	1:A:28:ASP:CA	2.43	0.48
1:A:64:GLY:O	1:A:68:LEU:CB	2.61	0.48
1:A:45:ILE:CG2	1:A:77:MET:CE	2.83	0.48
1:B:145:THR:OG1	1:B:146:THR:N	2.45	0.48
1:B:42:ARG:HG3	1:B:43:ASP:N	2.28	0.48
1:A:110:LEU:HG	1:A:111:GLY:N	2.29	0.48
1:B:233:HIS:ND1	1:B:262:VAL:HG21	2.28	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ILE:HD13	1:A:324:VAL:HG11	1.96	0.48
1:B:147:LEU:HD13	1:B:179:PRO:HD3	1.95	0.48
1:A:57:VAL:HG23	2:A:501:HOH:O	2.13	0.47
1:A:84:SER:CA	1:A:85:LEU:HD22	2.44	0.47
1:B:110:LEU:O	1:B:110:LEU:HD13	2.11	0.47
1:B:135:ILE:HD13	1:B:135:ILE:H	1.70	0.47
1:A:153:LEU:HD12	1:A:183:PRO:HG3	1.96	0.47
1:B:55:LEU:HD13	1:B:57:VAL:HG22	1.93	0.47
1:A:188:THR:HG23	1:A:258:PRO:HB2	1.96	0.47
1:B:135:ILE:HA	1:B:138:HIS:HB3	1.96	0.47
1:A:16:ARG:NH1	1:A:36:PRO:HB3	2.29	0.47
1:A:233:HIS:CE1	1:A:262:VAL:HG21	2.49	0.47
1:A:32:VAL:CG1	1:A:48:PHE:HB3	2.44	0.47
1:A:122:MET:HE2	1:A:122:MET:HA	1.96	0.47
1:A:281:THR:H	1:A:304:GLN:HE22	1.63	0.47
1:B:344:GLY:O	1:B:345:GLN:HB2	2.14	0.47
1:A:253:VAL:HG12	1:A:254:ASN:OD1	2.15	0.46
1:B:59:MET:HE3	1:B:59:MET:O	2.15	0.46
1:B:61:ARG:NE	1:B:61:ARG:CA	2.75	0.46
1:B:95:ARG:CD	1:B:202:ARG:HH22	2.28	0.46
1:A:16:ARG:CZ	1:A:36:PRO:HB3	2.45	0.46
1:A:310:VAL:CG2	1:A:311:VAL:HG23	2.43	0.46
1:A:319:ILE:HD12	1:A:327:VAL:HG22	1.98	0.46
1:B:42:ARG:HG3	1:B:43:ASP:OD1	2.16	0.46
1:A:2:SER:HA	1:A:28:ASP:HA	1.97	0.46
1:A:215:GLU:O	1:A:218:GLU:HG2	2.16	0.46
1:A:16:ARG:NH2	1:A:36:PRO:HB3	2.31	0.46
1:A:319:ILE:CD1	1:A:324:VAL:HG11	2.46	0.46
1:B:255:ARG:HA	1:B:255:ARG:HD3	1.80	0.46
1:A:16:ARG:O	1:A:20:THR:CG2	2.64	0.46
1:A:3:LYS:HZ2	1:A:28:ASP:HB2	1.80	0.46
1:A:7:LEU:CD1	1:A:7:LEU:C	2.89	0.46
1:A:103:ASP:OD2	1:A:126:LYS:NZ	2.48	0.46
1:A:269:LYS:HD3	2:A:545:HOH:O	2.16	0.46
1:B:255:ARG:N	1:B:255:ARG:CD	2.79	0.46
1:B:72:MET:HG3	1:B:100:GLY:HA3	1.98	0.46
1:A:107:LYS:O	1:A:107:LYS:CD	2.59	0.45
1:B:32:VAL:CG2	1:B:48:PHE:HD2	2.28	0.45
1:A:85:LEU:H	1:A:85:LEU:CD2	2.10	0.45
1:A:228:ALA:HA	1:A:229:PRO:HD3	1.75	0.45
1:B:1:MET:O	1:B:2:SER:C	2.57	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:PRO:HB3	1:B:67:PHE:HB2	1.98	0.45
1:B:195:PHE:HD2	2:B:521:HOH:O	1.99	0.45
1:A:312:PHE:O	1:A:313:GLY:C	2.59	0.45
1:B:197:ARG:NH1	1:B:201:GLU:OE1	2.49	0.45
1:B:49:ASN:N	1:B:50:PRO:HD3	2.31	0.45
1:B:172:ARG:HG3	1:B:203:LEU:HD23	1.99	0.45
1:B:292:LEU:CD2	1:B:321:MET:HE2	2.46	0.45
1:A:100:GLY:O	1:A:101:ALA:C	2.59	0.45
1:A:317:GLU:O	1:A:321:MET:HG3	2.17	0.45
1:B:90:SER:HA	1:B:195:PHE:CE2	2.51	0.45
1:A:253:VAL:O	1:A:254:ASN:HB2	2.17	0.44
1:B:54:THR:HA	1:B:80:VAL:O	2.17	0.44
1:B:60:PRO:HB2	1:B:61:ARG:H	1.61	0.44
1:B:113:ARG:N	1:B:113:ARG:HD2	2.32	0.44
1:B:257:ARG:CB	1:B:258:PRO:CD	2.91	0.44
1:B:316:ARG:HA	1:B:319:ILE:HD12	1.99	0.44
1:A:135:ILE:HD12	1:A:135:ILE:N	2.33	0.44
1:B:6:VAL:HA	1:B:52:VAL:O	2.17	0.44
1:B:27:SER:O	1:B:28:ASP:HB3	2.17	0.44
1:B:135:ILE:O	1:B:138:HIS:HB3	2.16	0.44
1:A:340:LYS:HA	1:A:340:LYS:HD3	1.78	0.44
1:B:147:LEU:C	1:B:148:LYS:HG3	2.42	0.44
1:A:85:LEU:CD1	1:A:106:THR:HB	2.47	0.44
1:B:101:ALA:O	1:B:138:HIS:HE1	2.01	0.44
1:A:73:ARG:NH1	1:A:73:ARG:HG2	2.33	0.44
1:B:232:LYS:N	1:B:257:ARG:HG2	2.33	0.44
1:A:8:SER:OG	1:A:31:MET:HE1	2.18	0.44
1:A:147:LEU:HD23	1:A:177:PRO:HB2	2.00	0.44
1:A:176:GLN:N	1:A:177:PRO:CD	2.81	0.43
1:B:61:ARG:HB2	2:B:423:HOH:O	2.18	0.43
1:A:283:MET:CE	2:A:553:HOH:O	2.64	0.43
1:B:71:LEU:CD2	1:B:75:ARG:O	2.66	0.43
1:B:168:THR:HG22	1:B:169:GLU:N	2.33	0.43
1:B:321:MET:HE2	1:B:321:MET:HB3	1.94	0.43
1:A:238:ARG:HH21	1:A:241:ALA:C	2.27	0.43
1:B:112:ILE:CG2	1:B:113:ARG:N	2.79	0.43
1:A:300:TRP:NE1	1:A:340:LYS:HG3	2.33	0.43
1:B:19:MET:O	1:B:22:ILE:CD1	2.65	0.43
1:A:73:ARG:HG2	1:A:73:ARG:HH11	1.83	0.43
1:A:319:ILE:CD1	1:A:327:VAL:HG22	2.48	0.43
1:A:10:ASP:OD2	1:A:15:MET:SD	2.77	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:ARG:HD2	1:A:132:ARG:N	2.33	0.43
1:A:143:ALA:HB2	1:A:172:ARG:NH2	2.34	0.43
1:A:221:LEU:CB	1:A:222:PRO:HD2	2.44	0.43
1:B:344:GLY:O	1:B:345:GLN:CB	2.67	0.43
1:A:121:GLU:O	1:A:125:GLU:HG2	2.18	0.43
1:B:57:VAL:CG2	1:B:81:MET:HE1	2.48	0.43
1:B:3:LYS:HA	2:B:460:HOH:O	2.19	0.42
1:B:108:PRO:HG3	1:B:122:MET:SD	2.59	0.42
1:B:39:LEU:HD12	1:B:39:LEU:HA	1.82	0.42
1:B:273:ARG:HB3	1:B:298:GLY:HA3	2.02	0.42
1:A:191:MET:HG2	1:A:192:PRO:HD2	2.02	0.42
1:B:37:ASP:HB2	1:B:38:PRO:HD2	2.01	0.42
1:B:179:PRO:HD2	1:B:182:SER:OG	2.19	0.42
1:A:157:LYS:N	1:A:157:LYS:HD3	2.35	0.42
1:A:238:ARG:HE	1:A:238:ARG:HB3	1.75	0.42
1:A:156:GLU:OE2	1:A:238:ARG:NH1	2.52	0.42
1:A:278:VAL:HA	1:A:302:ILE:O	2.18	0.42
1:B:258:PRO:HD2	2:B:368:HOH:O	2.19	0.42
1:A:1:MET:HG2	1:A:27:SER:O	2.20	0.42
1:A:90:SER:O	1:A:91:GLU:C	2.62	0.42
1:B:190:HIS:HA	2:B:368:HOH:O	2.20	0.42
1:B:269:LYS:HB2	1:B:269:LYS:HE3	1.89	0.41
1:A:39:LEU:HD13	1:A:39:LEU:HA	1.77	0.41
1:B:15:MET:HE1	1:B:119:TYR:OH	2.21	0.41
1:B:73:ARG:HH22	1:B:140:PRO:CG	2.32	0.41
1:B:147:LEU:HD23	1:B:338:LEU:HB3	2.00	0.41
1:B:143:ALA:HA	1:B:173:HIS:CD2	2.55	0.41
1:B:280:LEU:HB3	1:B:304:GLN:NE2	2.36	0.41
1:A:321:MET:HE2	1:A:321:MET:HB3	1.96	0.41
1:A:197:ARG:NH1	1:A:201:GLU:OE1	2.52	0.41
1:B:328:VAL:CG1	1:B:332:GLN:HB3	2.51	0.41
1:A:85:LEU:HD21	1:A:108:PRO:CB	2.50	0.41
1:B:70:LYS:HD2	1:B:70:LYS:HA	1.46	0.41
1:A:69:GLU:HG2	1:A:99:LEU:HD21	2.01	0.41
1:B:55:LEU:HD23	1:B:55:LEU:HA	1.82	0.41
1:B:147:LEU:HD21	1:B:338:LEU:CG	2.50	0.41
1:B:147:LEU:C	1:B:148:LYS:HG2	2.44	0.41
1:B:280:LEU:O	1:B:281:THR:C	2.63	0.41
1:B:137:ALA:HB1	1:B:308:SER:O	2.20	0.41
1:B:22:ILE:HD13	1:B:22:ILE:C	2.39	0.41
1:A:2:SER:N	1:A:27:SER:O	2.54	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:100:GLY:O	1:B:138:HIS:CE1	2.75	0.40
1:B:233:HIS:ND1	1:B:257:ARG:O	2.54	0.40
1:A:5:ARG:HG3	2:A:433:HOH:O	2.20	0.40
1:A:86:THR:O	1:A:89:GLY:N	2.54	0.40
1:B:7:LEU:C	1:B:7:LEU:HD12	2.46	0.40
1:B:55:LEU:HD13	1:B:57:VAL:HG21	2.00	0.40
1:B:71:LEU:HD22	1:B:75:ARG:O	2.22	0.40
1:B:164:SER:HB3	1:B:282:GLY:CA	2.51	0.40
1:A:85:LEU:O	1:A:86:THR:C	2.65	0.40
1:B:3:LYS:H	1:B:28:ASP:C	2.30	0.40
1:B:43:ASP:O	1:B:47:LYS:HG3	2.22	0.40
1:B:95:ARG:HD3	1:B:202:ARG:NH2	2.33	0.40
1:B:291:MET:HG2	1:B:323:GLY:O	2.21	0.40
1:B:65:LEU:HA	1:B:65:LEU:HD13	1.73	0.40
1:B:158:LEU:HD11	1:B:186:ILE:HD11	1.97	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	345/349 (99%)	320 (93%)	15 (4%)	10 (3%)	3	3
1	B	345/349 (99%)	300 (87%)	27 (8%)	18 (5%)	1	1
All	All	690/698 (99%)	620 (90%)	42 (6%)	28 (4%)	2	2

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	85	LEU
1	A	108	PRO
1	B	25	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	63	ASP
1	B	109	GLN
1	B	112	ILE
1	B	146	THR
1	A	60	PRO
1	A	62	MET
1	A	87	GLY
1	A	146	THR
1	B	28	ASP
1	B	60	PRO
1	B	90	SER
1	B	281	THR
1	B	345	GLN
1	A	86	THR
1	B	61	ARG
1	B	85	LEU
1	B	108	PRO
1	B	149	ALA
1	B	2	SER
1	A	61	ARG
1	B	257	ARG
1	A	164	SER
1	B	258	PRO
1	B	344	GLY
1	A	75	ARG

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	280/282 (99%)	236 (84%)	44 (16%)	2	3
1	B	280/282 (99%)	234 (84%)	46 (16%)	2	3
All	All	560/564 (99%)	470 (84%)	90 (16%)	2	3

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	5	ARG
1	A	6	VAL
1	A	7	LEU
1	A	12	SER
1	A	14	LEU
1	A	15	MET
1	A	17	GLN
1	A	20	THR
1	A	21	GLU
1	A	22	ILE
1	A	32	VAL
1	A	39	LEU
1	A	46	LYS
1	A	55	LEU
1	A	57	VAL
1	A	59	MET
1	A	61	ARG
1	A	62	MET
1	A	66	ASP
1	A	67	PHE
1	A	69	GLU
1	A	71	LEU
1	A	77	MET
1	A	81	MET
1	A	84	SER
1	A	85	LEU
1	A	88	LYS
1	A	91	GLU
1	A	99	LEU
1	A	107	LYS
1	A	113	ARG
1	A	121	GLU
1	A	132	ARG
1	A	146	THR
1	A	157	LYS
1	A	168	THR
1	A	180	LEU
1	A	197	ARG
1	A	235	GLU
1	A	255	ARG
1	A	310	VAL
1	A	311	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	325	SER
1	B	3	LYS
1	B	6	VAL
1	B	7	LEU
1	B	12	SER
1	B	14	LEU
1	B	18	ILE
1	B	22	ILE
1	B	25	SER
1	B	46	LYS
1	B	53	LEU
1	B	55	LEU
1	B	59	MET
1	B	65	LEU
1	B	70	LYS
1	B	73	ARG
1	B	85	LEU
1	B	102	ILE
1	B	106	THR
1	B	107	LYS
1	B	112	ILE
1	B	117	LEU
1	B	120	SER
1	B	123	ILE
1	B	125	GLU
1	B	135	ILE
1	B	146	THR
1	B	147	LEU
1	B	148	LYS
1	B	158	LEU
1	B	168	THR
1	B	171	ILE
1	B	174	VAL
1	B	180	LEU
1	B	185	VAL
1	B	186	ILE
1	B	196	THR
1	B	238	ARG
1	B	239	SER
1	B	246	LYS
1	B	296	GLN
1	B	310	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	321	MET
1	B	332	GLN
1	B	335	GLN
1	B	340	LYS
1	B	345	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	242	ASN
1	A	256	HIS
1	A	304	GLN
1	B	109	GLN
1	B	173	HIS
1	B	176	GLN
1	B	204	ASN
1	B	254	ASN
1	B	270	HIS
1	B	296	GLN
1	B	304	GLN
1	B	332	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	347/349 (99%)	-0.05	12 (3%) 47 43	6, 20, 54, 60	0
1	B	347/349 (99%)	0.03	15 (4%) 40 36	6, 23, 50, 60	0
All	All	694/698 (99%)	-0.01	27 (3%) 43 39	6, 22, 52, 60	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	146	THR	4.5
1	B	149	ALA	4.4
1	A	2	SER	4.3
1	B	346	ALA	4.1
1	A	150	GLY	3.9
1	A	84	SER	3.9
1	B	147	LEU	3.5
1	A	108	PRO	3.4
1	B	60	PRO	3.4
1	A	149	ALA	3.2
1	A	64	GLY	3.1
1	B	148	LYS	3.0
1	B	112	ILE	2.8
1	B	111	GLY	2.8
1	A	115	GLY	2.7
1	B	108	PRO	2.6
1	B	76	PRO	2.6
1	B	146	THR	2.5
1	A	110	LEU	2.5
1	B	150	GLY	2.4
1	B	194	GLY	2.4
1	B	240	GLY	2.2
1	A	109	GLN	2.1
1	B	89	GLY	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	347	ILE	2.1
1	B	2	SER	2.0
1	A	147	LEU	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.