Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 05:25 PM EDT

PDB ID	:	3BJL
Title	:	LOC, A LAMBDA 1 TYPE LIGHT-CHAIN DIMER (BENCE-JONES PROTEIN) CRYSTALLIZED IN AMMONIUM SULFATE
Authors	:	Schiffer, M.; Huang, D.B.
Deposited on	:	1995-05-26
Resolution	:	2.30 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 (i) 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 (i)) were used in the production of this report:

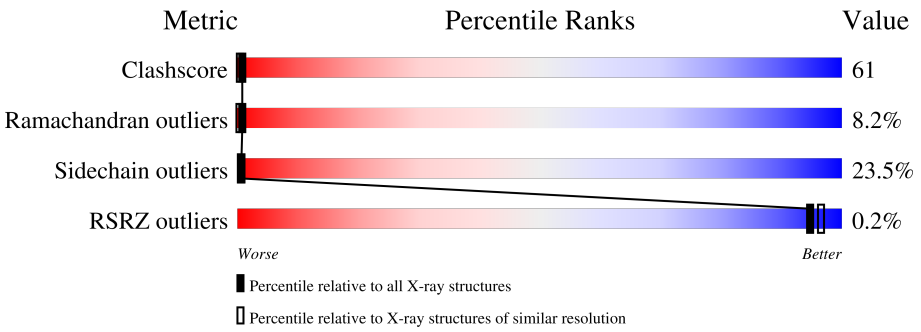
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.30 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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	216	30% 42% 22% 6%
1	B	216	24% 52% 21% •

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 3560 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 LOC - LAMBDA 1 TYPE LIGHT-CHAIN DIMER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	216	1598	992	266	335	5	0	0	0
1	B	216	1598	992	266	335	5	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	THR	ILE	conflict	PIR S25754
A	31	GLU	GLY	conflict	PIR S25754
A	33	SER	THR	conflict	PIR S25754
A	35	THR	ASN	conflict	PIR S25754
A	39	HIS	GLN	conflict	PIR S25754
A	41	SER	PRO	conflict	PIR S25754
A	43	THR	ARG	conflict	PIR S25754
A	50	TYR	HIS	conflict	PIR S25754
A	51	GLU	SER	conflict	PIR S25754
A	52	ASP	ASN	conflict	PIR S25754
A	54	SER	GLN	conflict	PIR S25754
A	56	ALA	PRO	conflict	PIR S25754
A	60	SER	PRO	conflict	PIR S25754
A	65	ALA	GLY	conflict	PIR S25754
A	81	PRO	SER	conflict	PIR S25754
A	85	THR	ALA	conflict	PIR S25754
A	?	-	ASN	deletion	PIR S25754
A	97	ASP	GLY	conflict	PIR S25754
A	98	VAL	ARG	conflict	PIR S25754
A	99	ALA	TYR	conflict	PIR S25754
B	19	THR	ILE	conflict	PIR S25754
B	31	GLU	GLY	conflict	PIR S25754
B	33	SER	THR	conflict	PIR S25754
B	35	THR	ASN	conflict	PIR S25754
B	39	HIS	GLN	conflict	PIR S25754

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	41	SER	PRO	conflict	PIR S25754
B	43	THR	ARG	conflict	PIR S25754
B	50	TYR	HIS	conflict	PIR S25754
B	51	GLU	SER	conflict	PIR S25754
B	52	ASP	ASN	conflict	PIR S25754
B	54	SER	GLN	conflict	PIR S25754
B	56	ALA	PRO	conflict	PIR S25754
B	60	SER	PRO	conflict	PIR S25754
B	65	ALA	GLY	conflict	PIR S25754
B	81	PRO	SER	conflict	PIR S25754
B	85	THR	ALA	conflict	PIR S25754
B	?	-	ASN	deletion	PIR S25754
B	97	ASP	GLY	conflict	PIR S25754
B	98	VAL	ARG	conflict	PIR S25754
B	99	ALA	TYR	conflict	PIR S25754

- Molecule 2 is water.

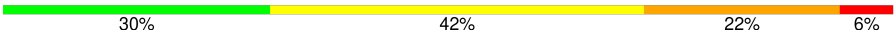
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	175	175	175	0	0
			Total	O		
2	B	189	189	189	0	0

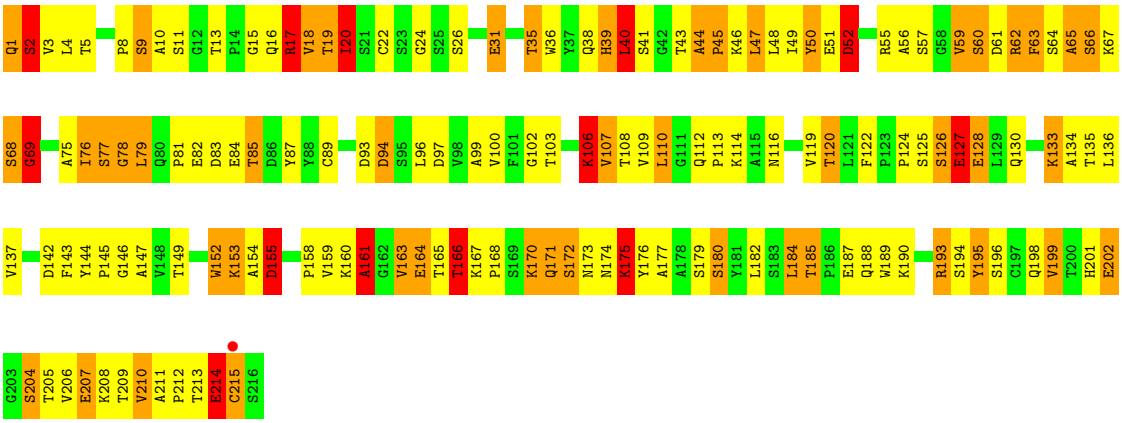
3 Residue-property plots (i)

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: LOC - LAMBDA 1 TYPE LIGHT-CHAIN DIMER

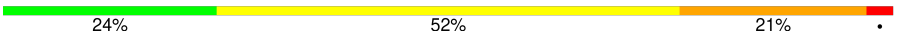
Chain A:

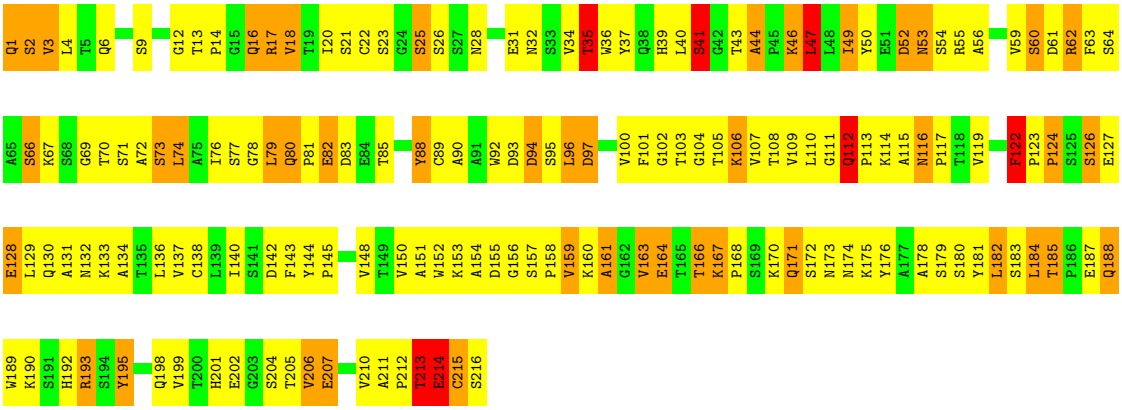




• Molecule 1: LOC - LAMBDA 1 TYPE LIGHT-CHAIN DIMER

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	149.30Å 72.40Å 46.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.30 8.33 – 2.41	Depositor EDS
% Data completeness (in resolution range)	76.6 (10.00-2.30) 74.3 (8.33-2.41)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	0.165 , (Not available) 0.164 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	40.0	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.08 , 93.1	EDS
L-test for twinning[1]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	3560	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.86% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.98	0/1628	1.94	34/2226 (1.5%)
1	B	1.04	0/1628	2.02	40/2226 (1.8%)
All	All	1.01	0/3256	1.98	74/4452 (1.7%)

There are no bond length outliers.

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	17	ARG	CD-NE-CZ	13.91	143.08	123.60
1	B	62	ARG	NE-CZ-NH1	-11.93	114.34	120.30
1	B	17	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	A	176	TYR	CB-CG-CD2	10.21	127.12	121.00
1	B	193	ARG	NE-CZ-NH1	-10.20	115.20	120.30
1	B	62	ARG	NE-CZ-NH2	10.06	125.33	120.30
1	A	176	TYR	CB-CG-CD1	-8.99	115.61	121.00
1	B	47	LEU	CA-CB-CG	8.46	134.76	115.30
1	B	195	TYR	CB-CG-CD2	8.09	125.85	121.00
1	B	62	ARG	CD-NE-CZ	-8.05	112.33	123.60
1	B	97	ASP	CB-CG-OD1	-8.04	111.06	118.30
1	A	50	TYR	CB-CG-CD2	7.70	125.62	121.00
1	B	88	TYR	CB-CG-CD2	7.69	125.61	121.00
1	A	106	LYS	CA-CB-CG	7.63	130.18	113.40
1	B	35	THR	N-CA-CB	-7.62	95.82	110.30
1	A	2	SER	C-N-CA	7.61	140.72	121.70
1	B	178	ALA	N-CA-CB	7.54	120.66	110.10
1	A	69	GLY	C-N-CA	7.24	139.79	121.70
1	A	17	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	B	193	ARG	NE-CZ-NH2	7.08	123.84	120.30
1	B	213	THR	C-N-CA	7.03	139.28	121.70
1	A	62	ARG	NE-CZ-NH2	6.98	123.79	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	133	LYS	CA-CB-CG	6.80	128.35	113.40
1	B	116	ASN	CB-CA-C	6.75	123.89	110.40
1	B	122	PHE	CA-CB-CG	6.72	130.04	113.90
1	A	199	VAL	CB-CA-C	-6.62	98.82	111.40
1	A	142	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	A	20	ILE	O-C-N	6.46	133.04	122.70
1	A	215	CYS	CA-CB-SG	6.41	125.53	114.00
1	A	142	ASP	CB-CG-OD1	-6.34	112.59	118.30
1	B	115	ALA	CB-CA-C	6.24	119.46	110.10
1	B	214	GLU	N-CA-CB	6.17	121.71	110.60
1	B	195	TYR	CB-CG-CD1	-6.09	117.34	121.00
1	B	60	SER	O-C-N	6.04	132.37	122.70
1	A	215	CYS	N-CA-CB	6.04	121.46	110.60
1	B	94	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	A	152	TRP	CA-CB-CG	6.00	125.10	113.70
1	A	161	ALA	O-C-N	5.96	133.33	123.20
1	A	142	ASP	OD1-CG-OD2	5.95	134.61	123.30
1	B	207	GLU	CG-CD-OE1	-5.94	106.41	118.30
1	B	88	TYR	CB-CG-CD1	-5.94	117.44	121.00
1	A	161	ALA	CB-CA-C	-5.93	101.21	110.10
1	B	207	GLU	CA-CB-CG	5.86	126.29	113.40
1	B	207	GLU	CG-CD-OE2	5.83	129.96	118.30
1	B	82	GLU	CA-CB-CG	5.78	126.12	113.40
1	A	163	VAL	CA-CB-CG1	5.74	119.52	110.90
1	A	195	TYR	CB-CG-CD1	-5.71	117.57	121.00
1	A	52	ASP	C-N-CA	5.64	135.81	121.70
1	A	163	VAL	CB-CA-C	5.50	121.85	111.40
1	B	214	GLU	C-N-CA	5.50	135.44	121.70
1	A	59	VAL	O-C-N	5.49	131.48	122.70
1	B	97	ASP	CB-CG-OD2	5.45	123.20	118.30
1	B	206	VAL	CA-CB-CG1	5.45	119.07	110.90
1	A	142	ASP	CA-CB-CG	-5.42	101.48	113.40
1	A	20	ILE	CB-CA-C	-5.39	100.82	111.60
1	A	166	THR	CA-CB-CG2	5.38	119.94	112.40
1	B	112	GLN	CA-CB-CG	5.38	125.25	113.40
1	B	167	LYS	N-CA-CB	5.33	120.20	110.60
1	B	207	GLU	N-CA-CB	5.32	120.18	110.60
1	B	182	LEU	O-C-N	5.29	131.17	122.70
1	A	62	ARG	CD-NE-CZ	5.27	130.97	123.60
1	B	61	ASP	O-C-N	5.27	131.12	122.70
1	A	68	SER	N-CA-CB	5.26	118.39	110.50
1	B	128	GLU	N-CA-CB	5.23	120.01	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	132	ASN	CA-CB-CG	5.22	124.89	113.40
1	A	94	ASP	CA-CB-CG	5.22	124.89	113.40
1	B	73	SER	O-C-N	5.21	131.04	122.70
1	A	39	HIS	N-CA-CB	5.20	119.95	110.60
1	B	34	VAL	C-N-CA	5.17	134.63	121.70
1	A	175	LYS	CA-CB-CG	5.17	124.77	113.40
1	A	24	GLY	O-C-N	5.15	130.94	122.70
1	B	25	SER	O-C-N	-5.11	114.53	122.70
1	B	23	SER	N-CA-CB	-5.06	102.91	110.50
1	A	65	ALA	CB-CA-C	5.06	117.68	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	1598	0	1535	185	1
1	B	1598	0	1535	216	2
2	A	175	0	0	33	1
2	B	189	0	0	25	0
All	All	3560	0	3070	383	2

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 61.

All (383) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:632:HOH:O	1:B:166:THR:HG21	1.40	1.20
1:B:79:LEU:HD21	1:B:109:VAL:HG22	1.20	1.15
1:A:31:GLU:HG3	2:A:530:HOH:O	1.45	1.12
1:B:114:LYS:HE3	1:B:202:GLU:HG3	1.23	1.11
1:B:128:GLU:HG3	1:B:133:LYS:HD3	1.31	1.10
1:A:214:GLU:HG2	2:A:690:HOH:O	1.55	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:THR:CG2	1:B:90:ALA:HB3	1.87	1.03
1:A:187:GLU:HG3	2:A:646:HOH:O	1.59	1.02
1:B:17:ARG:HD3	2:B:711:HOH:O	1.64	0.98
1:B:35:THR:HG23	1:B:37:TYR:CE1	2.00	0.96
1:B:35:THR:HG22	1:B:90:ALA:HB3	1.45	0.94
1:B:81:PRO:HB3	1:B:112:GLN:HG3	1.49	0.94
1:A:47:LEU:HD12	1:A:48:LEU:N	1.83	0.92
1:B:20:ILE:HD13	1:B:74:LEU:HD23	1.53	0.90
1:A:173:ASN:O	1:A:174:ASN:HB2	1.74	0.87
1:B:2:SER:HA	1:B:103:THR:HG22	1.55	0.86
1:A:172:SER:HB3	1:B:164:GLU:OE2	1.75	0.86
2:A:632:HOH:O	1:B:166:THR:CG2	2.09	0.86
1:A:114:LYS:HE3	2:A:526:HOH:O	1.74	0.86
1:B:128:GLU:CG	1:B:133:LYS:HD3	2.07	0.85
1:A:116:ASN:OD1	1:A:204:SER:HB2	1.79	0.83
1:A:38:GLN:HG2	1:A:85:THR:HG21	1.60	0.83
1:B:55:ARG:HD2	2:B:725:HOH:O	1.79	0.83
1:B:112:GLN:HB2	1:B:144:TYR:CE2	2.14	0.83
1:B:39:HIS:O	1:B:85:THR:HB	1.80	0.82
1:B:124:PRO:HD3	1:B:136:LEU:CD2	2.10	0.81
1:A:3:VAL:O	2:A:522:HOH:O	1.99	0.80
1:B:14:PRO:HA	1:B:79:LEU:O	1.81	0.80
1:B:62:ARG:HH11	1:B:62:ARG:HG3	1.47	0.80
1:B:35:THR:HG21	1:B:90:ALA:HB3	1.64	0.80
1:B:171:GLN:HG3	1:B:175:LYS:O	1.80	0.79
1:B:79:LEU:HD23	1:B:79:LEU:C	2.03	0.79
1:B:123:PRO:HA	1:B:136:LEU:CD2	2.13	0.79
1:A:137:VAL:CG2	1:B:122:PHE:CZ	2.66	0.78
1:A:198:GLN:NE2	2:A:654:HOH:O	2.16	0.78
1:A:154:ALA:O	1:A:155:ASP:HB2	1.82	0.78
1:B:12:GLY:O	1:B:110:LEU:HB2	1.82	0.78
1:B:13:THR:HG23	2:B:801:HOH:O	1.82	0.78
1:A:119:VAL:HG22	1:A:199:VAL:HG21	1.64	0.78
1:A:35:THR:HG21	2:A:567:HOH:O	1.85	0.77
1:B:110:LEU:HD12	2:B:750:HOH:O	1.83	0.77
1:A:127:GLU:OE1	1:A:127:GLU:N	2.18	0.76
1:A:49:ILE:HD12	1:A:55:ARG:HA	1.68	0.76
1:A:184:LEU:HD23	1:A:189:TRP:HB2	1.65	0.76
1:B:79:LEU:HD21	1:B:109:VAL:CG2	2.09	0.76
1:B:128:GLU:HG2	1:B:133:LYS:O	1.87	0.75
1:B:158:PRO:O	1:B:160:LYS:N	2.19	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:CYS:HA	2:B:864:HOH:O	1.87	0.74
1:B:62:ARG:HG3	1:B:62:ARG:NH1	2.03	0.74
1:B:127:GLU:O	1:B:127:GLU:HG3	1.86	0.74
1:A:17:ARG:HG2	1:A:77:SER:HA	1.70	0.74
1:A:153:LYS:HA	1:A:158:PRO:HA	1.70	0.73
1:A:49:ILE:HG22	1:A:49:ILE:O	1.89	0.73
1:B:124:PRO:HD3	1:B:136:LEU:HD21	1.71	0.73
1:B:114:LYS:HE3	1:B:202:GLU:CG	2.12	0.73
1:A:2:SER:O	2:A:521:HOH:O	2.05	0.73
1:A:44:ALA:H	1:A:45:PRO:HD3	1.52	0.72
1:B:81:PRO:HB3	1:B:112:GLN:CG	2.20	0.72
1:B:119:VAL:HG22	1:B:199:VAL:HG21	1.71	0.72
1:A:126:SER:O	1:A:130:GLN:N	2.22	0.72
1:A:137:VAL:HG21	1:B:122:PHE:CE1	2.25	0.72
1:A:62:ARG:NH2	1:A:83:ASP:OD1	2.23	0.71
1:A:50:TYR:HD1	1:A:51:GLU:HG3	1.55	0.71
1:B:40:LEU:CD2	1:B:85:THR:HG21	2.20	0.71
1:A:119:VAL:O	1:A:208:LYS:HE3	1.90	0.71
1:B:213:THR:HG22	1:B:214:GLU:H	1.54	0.71
1:A:93:ASP:O	1:A:97:ASP:CA	2.39	0.71
1:A:49:ILE:HG21	1:A:52:ASP:O	1.91	0.70
1:A:93:ASP:O	1:A:97:ASP:HA	1.90	0.70
1:B:62:ARG:HH21	1:B:83:ASP:CG	1.95	0.70
1:B:119:VAL:CG2	1:B:199:VAL:HG21	2.20	0.70
1:A:8:PRO:HG3	1:A:149:THR:OG1	1.92	0.70
1:A:116:ASN:OD1	1:A:204:SER:CB	2.39	0.70
1:B:35:THR:CG2	1:B:37:TYR:CE1	2.74	0.70
1:B:171:GLN:NE2	1:B:173:ASN:OD1	2.22	0.70
1:B:213:THR:HG22	1:B:214:GLU:N	2.06	0.69
1:B:40:LEU:HG	1:B:85:THR:HG21	1.74	0.69
1:A:20:ILE:HD12	1:A:20:ILE:N	2.07	0.69
1:A:85:THR:HG22	1:A:87:TYR:CE1	2.26	0.69
1:B:20:ILE:CD1	1:B:74:LEU:HD23	2.23	0.69
1:B:20:ILE:HG23	1:B:105:THR:HG21	1.74	0.68
1:A:57:SER:HB2	2:A:581:HOH:O	1.93	0.68
1:B:184:LEU:HB2	1:B:188:GLN:HG2	1.74	0.68
1:A:93:ASP:O	1:A:97:ASP:N	2.26	0.68
1:A:206:VAL:HG12	1:A:207:GLU:H	1.57	0.68
1:A:44:ALA:O	1:A:46:LYS:N	2.27	0.68
1:B:47:LEU:HD13	1:B:56:ALA:HB2	1.75	0.68
1:B:79:LEU:HD23	1:B:80:GLN:N	2.09	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:THR:HG23	1:B:37:TYR:HE1	1.56	0.68
1:A:103:THR:OG1	2:A:591:HOH:O	2.11	0.67
1:B:63:PHE:CE1	1:B:76:ILE:HG12	2.29	0.67
1:B:136:LEU:O	1:B:181:TYR:HA	1.95	0.67
1:A:136:LEU:HD23	1:A:152:TRP:HZ3	1.60	0.67
1:A:207:GLU:OE2	2:A:658:HOH:O	2.12	0.67
1:A:116:ASN:HD22	1:A:201:HIS:HD2	1.42	0.67
1:B:62:ARG:HH11	1:B:62:ARG:CG	2.02	0.67
1:A:13:THR:OG1	1:A:16:GLN:NE2	2.28	0.66
1:A:126:SER:C	1:A:128:GLU:H	1.98	0.66
1:B:80:GLN:O	1:B:83:ASP:HB2	1.93	0.66
1:B:35:THR:CG2	1:B:37:TYR:HE1	2.07	0.66
1:A:4:LEU:HG	1:A:100:VAL:HG12	1.75	0.66
1:A:160:LYS:O	1:A:161:ALA:HB2	1.95	0.65
1:B:114:LYS:CE	1:B:202:GLU:HG3	2.13	0.65
1:A:190:LYS:O	2:A:651:HOH:O	2.14	0.65
1:B:159:VAL:HG11	1:B:195:TYR:HE1	1.62	0.65
1:B:79:LEU:CD2	1:B:109:VAL:HG22	2.12	0.65
1:B:163:VAL:HG23	1:B:182:LEU:CD1	2.27	0.65
1:A:185:THR:H	1:A:188:GLN:HB2	1.61	0.64
1:B:96:LEU:HD23	1:B:96:LEU:H	1.63	0.64
1:A:116:ASN:ND2	1:A:201:HIS:HD2	1.95	0.64
1:B:81:PRO:O	1:B:174:ASN:HB2	1.98	0.64
1:A:66:SER:OG	1:A:67:LYS:N	2.29	0.64
1:A:171:GLN:NE2	1:A:173:ASN:OD1	2.26	0.64
1:B:170:LYS:HD3	1:B:174:ASN:OD1	1.97	0.64
1:A:50:TYR:CD1	1:A:51:GLU:HG3	2.33	0.64
1:B:213:THR:CG2	1:B:214:GLU:H	2.10	0.63
1:B:153:LYS:HA	1:B:157:SER:O	1.98	0.63
1:A:99:ALA:CB	1:B:101:PHE:HZ	2.11	0.63
1:B:31:GLU:OE1	1:B:94:ASP:OD2	2.17	0.63
1:A:160:LYS:O	1:A:161:ALA:CB	2.46	0.63
1:A:201:HIS:O	1:A:202:GLU:C	2.38	0.63
1:B:97:ASP:OD1	2:B:742:HOH:O	2.16	0.62
1:A:96:LEU:O	1:A:97:ASP:HB3	2.00	0.62
1:A:84:GLU:HA	1:A:107:VAL:O	2.00	0.61
1:B:176:TYR:HE2	2:B:849:HOH:O	1.83	0.61
1:A:18:VAL:HG11	1:A:79:LEU:HD22	1.82	0.61
1:B:79:LEU:C	1:B:79:LEU:CD2	2.69	0.61
1:A:137:VAL:HG21	1:B:122:PHE:CZ	2.34	0.61
1:A:10:ALA:O	1:A:11:SER:HB3	2.00	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:VAL:HG12	1:A:208:LYS:CG	2.31	0.60
1:B:123:PRO:HA	1:B:136:LEU:HD23	1.82	0.60
1:B:117:PRO:HB3	1:B:143:PHE:HB3	1.84	0.60
1:B:119:VAL:HG13	1:B:138:CYS:SG	2.42	0.60
1:B:124:PRO:HD3	1:B:136:LEU:HD23	1.84	0.60
1:A:202:GLU:HA	2:A:525:HOH:O	2.01	0.60
1:A:114:LYS:CE	2:A:526:HOH:O	2.43	0.59
1:A:173:ASN:OD1	1:A:175:LYS:HB2	2.02	0.59
1:B:22:CYS:O	1:B:71:SER:HA	2.03	0.59
1:A:40:LEU:HD13	2:A:595:HOH:O	2.02	0.59
1:A:9:SER:OG	1:A:202:GLU:HG3	2.01	0.59
1:B:40:LEU:O	1:B:41:SER:C	2.40	0.59
1:A:208:LYS:NZ	2:A:659:HOH:O	2.35	0.59
1:A:11:SER:HB2	1:A:108:THR:O	2.03	0.58
1:A:136:LEU:HD23	1:A:152:TRP:CZ3	2.39	0.58
1:A:195:TYR:HB2	1:A:210:VAL:HG12	1.85	0.58
1:B:214:GLU:CD	1:B:215:CYS:H	2.06	0.58
1:A:39:HIS:CG	1:A:40:LEU:H	2.22	0.58
1:A:44:ALA:N	1:A:45:PRO:CD	2.66	0.57
1:A:47:LEU:HD12	1:A:47:LEU:C	2.24	0.57
1:B:20:ILE:N	1:B:74:LEU:O	2.35	0.57
1:B:184:LEU:HB2	1:B:188:GLN:CG	2.34	0.57
1:B:46:LYS:HD3	2:B:721:HOH:O	2.05	0.57
1:A:44:ALA:H	1:A:45:PRO:CD	2.17	0.57
1:A:19:THR:O	1:A:19:THR:OG1	2.23	0.57
1:A:4:LEU:O	1:A:102:GLY:HA2	2.04	0.57
1:A:116:ASN:HD22	1:A:201:HIS:CD2	2.22	0.57
1:A:153:LYS:HE3	2:A:658:HOH:O	2.05	0.56
1:A:214:GLU:HA	1:A:214:GLU:OE1	2.04	0.56
1:A:76:ILE:HG21	1:A:79:LEU:HD12	1.87	0.56
1:B:20:ILE:HD13	1:B:74:LEU:CD2	2.31	0.56
1:B:3:VAL:CG1	1:B:100:VAL:CG1	2.84	0.56
1:B:3:VAL:HG11	1:B:100:VAL:HG13	1.86	0.56
1:A:136:LEU:HD22	1:A:182:LEU:HD23	1.88	0.56
1:A:128:GLU:HB2	2:A:609:HOH:O	2.05	0.56
1:B:40:LEU:CG	1:B:85:THR:HG21	2.36	0.55
1:A:36:TRP:HB2	1:A:49:ILE:HB	1.87	0.55
1:A:124:PRO:CG	1:A:134:ALA:HB1	2.37	0.55
1:A:49:ILE:CG2	1:A:52:ASP:O	2.54	0.55
1:A:48:LEU:O	1:A:49:ILE:HD13	2.07	0.55
1:A:190:LYS:HD3	2:A:683:HOH:O	2.06	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:VAL:HG21	1:B:199:VAL:CG2	2.37	0.54
1:A:153:LYS:HD3	2:A:658:HOH:O	2.08	0.54
1:B:163:VAL:HG23	1:B:182:LEU:HD12	1.89	0.54
1:A:205:THR:HG22	1:A:205:THR:O	2.08	0.54
1:B:124:PRO:HG3	1:B:134:ALA:HB1	1.90	0.54
1:B:62:ARG:NH2	1:B:83:ASP:OD2	2.34	0.54
1:B:185:THR:OG1	1:B:188:GLN:HB3	2.07	0.54
1:A:126:SER:C	1:A:128:GLU:N	2.61	0.54
1:B:53:ASN:C	1:B:53:ASN:HD22	2.11	0.54
1:A:68:SER:OG	1:A:69:GLY:N	2.41	0.54
1:A:38:GLN:CG	1:A:85:THR:HG21	2.37	0.53
1:A:119:VAL:HG12	1:A:208:LYS:HG2	1.89	0.53
1:B:4:LEU:HB3	1:B:102:GLY:HA2	1.91	0.53
1:B:35:THR:HG22	1:B:90:ALA:CB	2.31	0.53
1:B:142:ASP:OD2	2:B:827:HOH:O	2.19	0.53
1:B:78:GLY:O	1:B:80:GLN:OE1	2.27	0.53
1:B:140:ILE:CD1	1:B:150:VAL:HG21	2.38	0.53
1:B:185:THR:OG1	1:B:188:GLN:CB	2.56	0.53
1:A:136:LEU:HD13	1:A:184:LEU:HD22	1.90	0.53
1:B:40:LEU:HD23	1:B:85:THR:CG2	2.39	0.53
1:B:128:GLU:O	1:B:133:LYS:HB3	2.09	0.53
1:A:13:THR:O	1:A:16:GLN:HB3	2.08	0.53
1:B:17:ARG:HD2	2:B:764:HOH:O	2.08	0.53
1:B:159:VAL:HG11	1:B:195:TYR:CE1	2.43	0.53
1:B:166:THR:HG23	1:B:167:LYS:O	2.09	0.53
1:A:119:VAL:CG2	1:A:199:VAL:HG21	2.37	0.53
1:A:119:VAL:HG12	1:A:208:LYS:HG3	1.90	0.53
1:A:137:VAL:HG23	1:B:122:PHE:CZ	2.44	0.53
1:A:212:PRO:O	1:A:213:THR:HG23	2.08	0.53
1:B:53:ASN:HD22	1:B:54:SER:N	2.07	0.53
1:B:145:PRO:O	1:B:201:HIS:HE1	1.91	0.53
1:B:168:PRO:HD3	2:B:841:HOH:O	2.08	0.53
1:A:119:VAL:CG1	1:A:208:LYS:HG2	2.39	0.52
1:A:124:PRO:HB3	1:A:134:ALA:HA	1.91	0.52
1:B:144:TYR:CD1	1:B:145:PRO:HA	2.45	0.52
1:B:12:GLY:O	1:B:110:LEU:CB	2.55	0.52
1:B:124:PRO:CG	1:B:134:ALA:HB1	2.40	0.52
1:A:116:ASN:ND2	1:A:201:HIS:CD2	2.77	0.52
1:A:120:THR:HG23	1:B:133:LYS:HZ3	1.75	0.52
1:B:43:THR:O	1:B:44:ALA:CB	2.58	0.52
1:A:2:SER:CA	2:A:521:HOH:O	2.58	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:PRO:O	1:B:1:PCA:HG3	2.10	0.51
1:A:96:LEU:O	1:A:97:ASP:CB	2.59	0.51
1:A:125:SER:OG	2:A:609:HOH:O	2.19	0.51
1:B:82:GLU:CD	2:B:738:HOH:O	2.48	0.51
1:A:52:ASP:O	1:A:65:ALA:HB3	2.10	0.51
1:B:93:ASP:HB2	1:B:100:VAL:HG21	1.93	0.51
1:A:15:GLY:O	1:A:78:GLY:HA2	2.11	0.51
1:A:153:LYS:CD	2:A:658:HOH:O	2.59	0.50
1:B:32:ASN:ND2	1:B:92:TRP:O	2.39	0.50
1:B:80:GLN:O	1:B:109:VAL:HG21	2.11	0.50
1:A:39:HIS:CD2	1:A:40:LEU:H	2.29	0.50
1:B:22:CYS:HB2	1:B:36:TRP:CH2	2.46	0.50
1:B:28:ASN:HA	1:B:92:TRP:O	2.11	0.50
1:A:214:GLU:OE2	1:B:215:CYS:O	2.29	0.50
1:B:96:LEU:N	1:B:96:LEU:CD2	2.75	0.50
1:A:20:ILE:N	1:A:20:ILE:CD1	2.73	0.50
1:B:112:GLN:HB2	1:B:144:TYR:HE2	1.70	0.50
1:A:144:TYR:CD1	1:A:145:PRO:HA	2.47	0.49
1:B:211:ALA:HB3	2:B:862:HOH:O	2.12	0.49
1:A:214:GLU:CD	1:B:215:CYS:O	2.49	0.49
1:B:82:GLU:HA	1:B:174:ASN:HD22	1.76	0.49
1:B:55:ARG:NH2	2:B:726:HOH:O	2.43	0.49
1:B:153:LYS:HG2	1:B:157:SER:C	2.32	0.49
1:A:60:SER:C	1:A:62:ARG:H	2.14	0.49
1:A:110:LEU:HD11	1:A:114:LYS:HG2	1.93	0.49
1:B:3:VAL:HG12	1:B:100:VAL:CG1	2.43	0.49
1:A:206:VAL:HG12	1:A:207:GLU:N	2.28	0.49
1:B:52:ASP:OD1	1:B:67:LYS:HE3	2.13	0.49
1:B:104:GLY:O	2:B:746:HOH:O	2.19	0.49
1:B:9:SER:HB2	1:B:106:LYS:NZ	2.28	0.49
1:A:49:ILE:CD1	1:A:55:ARG:HA	2.42	0.48
1:B:13:THR:O	1:B:14:PRO:C	2.51	0.48
1:B:96:LEU:HD23	1:B:96:LEU:N	2.27	0.48
1:B:161:ALA:HB3	2:B:836:HOH:O	2.12	0.48
1:A:60:SER:C	1:A:62:ARG:N	2.67	0.48
1:A:19:THR:HA	1:A:75:ALA:HA	1.95	0.48
1:A:10:ALA:O	1:A:107:VAL:HA	2.14	0.48
1:A:128:GLU:O	1:A:133:LYS:O	2.32	0.48
1:B:93:ASP:HB2	1:B:100:VAL:CG2	2.42	0.48
1:B:192:HIS:HE1	2:B:889:HOH:O	1.97	0.48
1:B:6:GLN:NE2	1:B:105:THR:OG1	2.47	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:PCA:HG3	1:B:46:LYS:HG2	1.95	0.48
1:A:16:GLN:O	1:A:79:LEU:HB2	2.14	0.48
1:A:152:TRP:HE1	1:A:180:SER:HG	1.61	0.48
1:A:18:VAL:CG1	1:A:79:LEU:HD22	2.44	0.47
1:B:142:ASP:CG	2:B:827:HOH:O	2.52	0.47
1:B:163:VAL:HG23	1:B:182:LEU:HD13	1.96	0.47
1:A:119:VAL:HG22	1:A:199:VAL:CG2	2.38	0.47
1:A:194:SER:HB2	1:A:209:THR:HG23	1.96	0.47
1:A:112:GLN:NE2	1:A:175:LYS:NZ	2.62	0.47
1:A:126:SER:O	1:A:128:GLU:N	2.48	0.47
1:B:199:VAL:O	1:B:205:THR:HA	2.14	0.47
1:A:164:GLU:OE1	1:B:172:SER:OG	2.32	0.47
1:A:2:SER:CB	2:A:521:HOH:O	2.62	0.47
1:A:9:SER:HB3	1:A:147:ALA:HB3	1.96	0.47
1:A:124:PRO:HG2	1:A:134:ALA:HB1	1.97	0.47
1:B:36:TRP:HA	1:B:88:TYR:O	2.15	0.46
1:B:49:ILE:HA	1:B:54:SER:O	2.15	0.46
1:B:107:VAL:HG12	1:B:108:THR:N	2.29	0.46
1:B:53:ASN:ND2	1:B:54:SER:OG	2.48	0.46
1:B:152:TRP:O	1:B:158:PRO:HA	2.15	0.46
1:A:112:GLN:HG3	1:A:113:PRO:HD2	1.98	0.46
1:A:63:PHE:CD1	1:A:63:PHE:N	2.82	0.46
1:A:182:LEU:HG	1:A:184:LEU:HD13	1.98	0.46
1:A:207:GLU:HG3	1:A:208:LYS:N	2.29	0.46
1:B:4:LEU:O	1:B:102:GLY:HA2	2.15	0.46
1:A:20:ILE:HD12	1:A:20:ILE:H	1.78	0.46
1:A:20:ILE:CD1	1:A:20:ILE:H	2.29	0.46
1:A:106:LYS:HG2	1:A:147:ALA:HB2	1.97	0.46
1:A:133:LYS:HB2	1:A:133:LYS:HE3	1.52	0.46
1:A:167:LYS:HD3	1:A:168:PRO:O	2.16	0.46
1:A:39:HIS:CG	1:A:40:LEU:N	2.83	0.46
1:B:18:VAL:HG22	2:B:786:HOH:O	2.16	0.46
1:B:40:LEU:CD2	1:B:85:THR:CG2	2.91	0.46
1:A:164:GLU:O	1:A:180:SER:HA	2.15	0.46
1:A:119:VAL:CG2	1:A:199:VAL:CG2	2.93	0.46
1:A:193:ARG:O	1:A:211:ALA:HB2	2.16	0.46
1:B:2:SER:O	1:B:3:VAL:HG22	2.15	0.46
1:A:171:GLN:HG2	1:A:177:ALA:HB2	1.97	0.45
1:A:114:LYS:NZ	2:A:602:HOH:O	2.49	0.45
1:B:50:TYR:N	1:B:54:SER:O	2.41	0.45
1:A:170:LYS:HB3	1:A:170:LYS:HE3	1.60	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:196:SER:HA	1:A:208:LYS:O	2.17	0.45
1:B:62:ARG:NH1	1:B:62:ARG:CG	2.62	0.45
1:A:108:THR:HG21	1:A:145:PRO:HB3	1.98	0.45
1:A:198:GLN:CD	2:A:654:HOH:O	2.54	0.45
1:B:117:PRO:HD3	1:B:201:HIS:CG	2.51	0.45
1:A:109:VAL:HG12	1:A:109:VAL:O	2.15	0.45
1:B:40:LEU:HD23	1:B:85:THR:HG21	1.98	0.45
1:B:154:ALA:O	1:B:155:ASP:C	2.55	0.45
1:B:117:PRO:HD3	1:B:201:HIS:CD2	2.52	0.45
1:B:161:ALA:CB	2:B:836:HOH:O	2.65	0.45
1:A:1:PCA:HG3	1:B:46:LYS:CG	2.47	0.44
1:A:64:SER:HB2	2:A:542:HOH:O	2.16	0.44
1:A:35:THR:HA	1:A:49:ILE:O	2.17	0.44
1:A:154:ALA:O	1:A:155:ASP:CB	2.58	0.44
1:B:157:SER:HA	1:B:158:PRO:HD3	1.74	0.44
1:A:40:LEU:CD1	2:A:595:HOH:O	2.65	0.44
1:B:193:ARG:HA	2:B:856:HOH:O	2.16	0.44
1:B:198:GLN:NE2	1:B:207:GLU:OE1	2.51	0.44
1:B:3:VAL:HG11	1:B:100:VAL:CG1	2.47	0.44
1:B:145:PRO:O	1:B:201:HIS:CE1	2.71	0.44
1:A:59:VAL:O	1:A:59:VAL:HG12	2.18	0.44
1:B:81:PRO:CB	1:B:112:GLN:HG3	2.34	0.44
1:A:164:GLU:CD	1:B:172:SER:HG	2.22	0.44
1:B:112:GLN:HB3	1:B:113:PRO:HD2	2.00	0.44
1:A:214:GLU:HG3	1:B:215:CYS:SG	2.58	0.43
1:B:184:LEU:CD1	1:B:189:TRP:HB2	2.48	0.43
1:B:189:TRP:CZ2	1:B:212:PRO:HA	2.53	0.43
1:B:43:THR:O	1:B:44:ALA:HB2	2.17	0.43
1:B:136:LEU:HD12	1:B:182:LEU:HD23	1.99	0.43
1:A:31:GLU:CG	2:A:530:HOH:O	2.27	0.43
1:B:150:VAL:HA	1:B:198:GLN:O	2.19	0.43
1:A:120:THR:CG2	1:B:133:LYS:HZ3	2.31	0.43
1:B:151:ALA:HA	1:B:160:LYS:HE3	2.01	0.43
1:B:214:GLU:CG	1:B:215:CYS:N	2.81	0.43
1:B:90:ALA:HA	1:B:100:VAL:O	2.18	0.43
1:B:142:ASP:CA	1:B:175:LYS:HD2	2.48	0.43
1:B:49:ILE:CG2	1:B:50:TYR:N	2.78	0.43
1:A:143:PHE:CE1	1:A:146:GLY:HA2	2.54	0.43
1:B:126:SER:O	1:B:130:GLN:N	2.51	0.43
1:B:127:GLU:O	1:B:127:GLU:CG	2.64	0.43
1:B:187:GLU:C	1:B:189:TRP:N	2.71	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LEU:C	1:A:49:ILE:HD13	2.39	0.43
1:A:116:ASN:HA	1:A:201:HIS:HD2	1.84	0.43
1:A:137:VAL:HG11	1:B:137:VAL:HG11	2.01	0.42
1:B:40:LEU:HB2	1:B:43:THR:OG1	2.19	0.42
1:B:55:ARG:HB3	1:B:59:VAL:HB	2.01	0.42
1:B:116:ASN:N	1:B:116:ASN:HD22	2.17	0.42
1:A:55:ARG:HB3	1:A:59:VAL:HG11	2.01	0.42
1:B:96:LEU:H	1:B:96:LEU:CD2	2.30	0.42
1:B:22:CYS:N	1:B:72:ALA:O	2.53	0.42
1:B:170:LYS:HE3	1:B:170:LYS:HB2	1.70	0.42
1:B:82:GLU:CG	2:B:738:HOH:O	2.67	0.42
1:B:152:TRP:H	1:B:160:LYS:HE3	1.83	0.42
1:A:47:LEU:HD12	1:A:48:LEU:H	1.73	0.42
1:B:142:ASP:HA	1:B:175:LYS:HD2	2.01	0.42
1:A:120:THR:HG23	1:B:133:LYS:NZ	2.34	0.42
1:B:95:SER:O	1:B:96:LEU:C	2.58	0.42
1:B:171:GLN:HB3	2:B:844:HOH:O	2.19	0.42
1:A:116:ASN:HA	1:A:201:HIS:CD2	2.55	0.42
1:A:133:LYS:CD	2:A:617:HOH:O	2.67	0.42
1:B:166:THR:HG23	1:B:167:LYS:N	2.33	0.42
1:A:165:THR:HG23	1:A:180:SER:HB2	2.01	0.41
1:B:1:PCA:O	1:B:2:SER:OG	2.35	0.41
1:B:204:SER:C	1:B:205:THR:OG1	2.59	0.41
1:B:18:VAL:HG12	1:B:76:ILE:HD12	2.02	0.41
1:B:123:PRO:HA	1:B:136:LEU:HD21	1.95	0.41
1:B:127:GLU:HA	1:B:130:GLN:HB2	2.02	0.41
1:A:40:LEU:HD23	1:A:40:LEU:HA	1.83	0.41
1:B:119:VAL:HG21	1:B:199:VAL:HG21	1.93	0.41
1:A:196:SER:CA	1:A:208:LYS:O	2.68	0.41
1:B:175:LYS:HZ3	1:B:175:LYS:HG3	1.55	0.41
1:B:185:THR:OG1	1:B:188:GLN:HB2	2.20	0.41
1:A:81:PRO:C	1:A:83:ASP:H	2.23	0.41
1:A:126:SER:O	1:A:130:GLN:HB2	2.20	0.41
1:A:153:LYS:CE	2:A:658:HOH:O	2.65	0.41
1:B:187:GLU:O	1:B:189:TRP:N	2.54	0.41
1:B:187:GLU:O	1:B:190:LYS:N	2.52	0.41
1:B:16:GLN:HB3	1:B:17:ARG:H	1.43	0.41
1:B:49:ILE:HG23	1:B:50:TYR:N	2.36	0.41
1:B:66:SER:O	1:B:72:ALA:HA	2.20	0.41
1:B:124:PRO:HB2	1:B:129:LEU:HD11	2.03	0.41
1:B:159:VAL:HG13	1:B:159:VAL:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:GLU:HA	1:A:130:GLN:HB2	2.03	0.41
1:A:166:THR:CG2	1:A:167:LYS:N	2.84	0.41
1:B:21:SER:HB2	2:B:714:HOH:O	2.21	0.41
1:B:171:GLN:HA	2:B:844:HOH:O	2.21	0.40
1:A:36:TRP:CZ3	1:A:89:CYS:HB3	2.56	0.40
1:B:129:LEU:C	1:B:131:ALA:H	2.25	0.40
1:A:16:GLN:HE21	1:A:16:GLN:HB2	1.45	0.40
1:B:9:SER:HB2	1:B:106:LYS:HZ1	1.85	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:VAL:CG1	2:A:704:HOH:O[2_664]	1.75	0.45
1:A:51:GLU:OE1	1:B:54:SER:OG[2_664]	2.18	0.02

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	214/216 (99%)	172 (80%)	21 (10%)	21 (10%)	0 0
1	B	214/216 (99%)	179 (84%)	21 (10%)	14 (6%)	1 0
All	All	428/432 (99%)	351 (82%)	42 (10%)	35 (8%)	1 0

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	THR
1	A	110	LEU
1	A	161	ALA
1	A	202	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	2	SER
1	B	16	GLN
1	B	44	ALA
1	B	213	THR
1	B	214	GLU
1	A	31	GLU
1	A	44	ALA
1	A	45	PRO
1	A	56	ALA
1	A	69	GLY
1	A	171	GLN
1	B	3	VAL
1	B	111	GLY
1	B	156	GLY
1	B	159	VAL
1	B	215	CYS
1	A	40	LEU
1	A	79	LEU
1	A	127	GLU
1	A	155	ASP
1	A	214	GLU
1	B	41	SER
1	B	188	GLN
1	A	41	SER
1	A	82	GLU
1	A	166	THR
1	A	215	CYS
1	B	161	ALA
1	A	52	ASP
1	B	69	GLY
1	A	78	GLY

5.3.2 Protein sidechains (i)

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	181/181 (100%)	135 (75%)	46 (25%)	0 0
1	B	181/181 (100%)	142 (78%)	39 (22%)	1 1
All	All	362/362 (100%)	277 (76%)	85 (24%)	1 0

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	5	THR
1	A	9	SER
1	A	17	ARG
1	A	18	VAL
1	A	19	THR
1	A	20	ILE
1	A	22	CYS
1	A	26	SER
1	A	35	THR
1	A	40	LEU
1	A	47	LEU
1	A	60	SER
1	A	61	ASP
1	A	63	PHE
1	A	66	SER
1	A	76	ILE
1	A	77	SER
1	A	85	THR
1	A	94	ASP
1	A	106	LYS
1	A	107	VAL
1	A	120	THR
1	A	122	PHE
1	A	126	SER
1	A	127	GLU
1	A	128	GLU
1	A	135	THR
1	A	153	LYS
1	A	155	ASP
1	A	159	VAL
1	A	163	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	164	GLU
1	A	166	THR
1	A	170	LYS
1	A	172	SER
1	A	175	LYS
1	A	179	SER
1	A	180	SER
1	A	184	LEU
1	A	185	THR
1	A	193	ARG
1	A	204	SER
1	A	207	GLU
1	A	210	VAL
1	A	214	GLU
1	B	18	VAL
1	B	25	SER
1	B	26	SER
1	B	35	THR
1	B	41	SER
1	B	46	LYS
1	B	47	LEU
1	B	49	ILE
1	B	52	ASP
1	B	53	ASN
1	B	60	SER
1	B	64	SER
1	B	66	SER
1	B	70	THR
1	B	73	SER
1	B	74	LEU
1	B	77	SER
1	B	79	LEU
1	B	80	GLN
1	B	89	CYS
1	B	96	LEU
1	B	106	LYS
1	B	112	GLN
1	B	122	PHE
1	B	124	PRO
1	B	126	SER
1	B	148	VAL
1	B	163	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	164	GLU
1	B	166	THR
1	B	171	GLN
1	B	179	SER
1	B	180	SER
1	B	183	SER
1	B	184	LEU
1	B	185	THR
1	B	206	VAL
1	B	210	VAL
1	B	216	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	39	HIS
1	A	80	GLN
1	A	112	GLN
1	A	174	ASN
1	A	201	HIS
1	B	39	HIS
1	B	53	ASN
1	B	116	ASN
1	B	130	GLN
1	B	192	HIS
1	B	201	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	PCA	B	1	1	6,7,9	0.64	0	7,8,12	1.49	3 (42%)
1	PCA	A	1	1	6,7,9	0.97	1 (16%)	7,8,12	1.59	2 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PCA	B	1	1	-	0/0/9/13	0/1/1/1
1	PCA	A	1	1	-	0/0/9/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	PCA	O-C	2.30	1.28	1.20

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1	PCA	O-C-CA	-3.20	116.55	124.77
1	B	1	PCA	CG-CD-N	-2.24	99.43	105.72
1	B	1	PCA	O-C-CA	-2.23	119.04	124.77
1	A	1	PCA	CD-N-CA	2.16	112.71	107.21
1	B	1	PCA	CB-CA-C	2.14	115.59	112.66

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	1	PCA	2	0
1	A	1	PCA	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (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	215/216 (99%)	-0.75	1 (0%) 91 94	16, 32, 50, 69	0
1	B	215/216 (99%)	-0.71	0 100 100	14, 31, 49, 72	0
All	All	430/432 (99%)	-0.73	1 (0%) 95 96	14, 32, 50, 72	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	215	CYS	2.2

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	PCA	A	1	7/9	0.91	0.15	46,46,46,47	0
1	PCA	B	1	7/9	0.91	0.12	47,48,48,49	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.