Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:25 PM GMT

PDB ID	:	1TLF
Title	:	UNPRECEDENTED QUATERNARY STRUCTURE OF E. COLI LAC REPRESSOR CORE TETRAMER: IMPLICATIONS FOR DNA LOOPING
Authors	:	Friedman, A.M.; Fischmann, T.O.; Steitz, T.A.
Deposited on	:	1995-03-06
Resolution	:	2.60 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

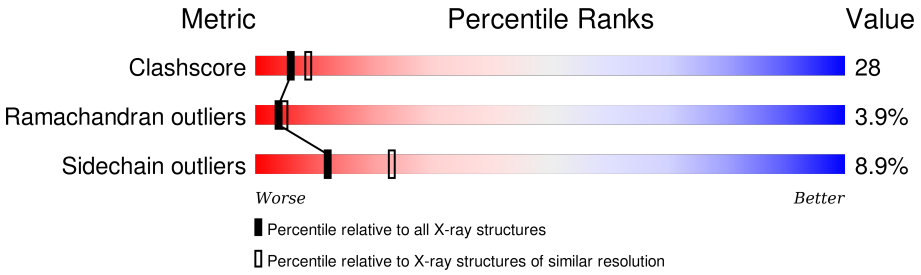
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.60 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	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	301	50% 41% 7% •
1	B	301	48% 41% 9% •
1	C	301	46% 46% 7% • •
1	D	301	50% 42% 6% •

2 Entry composition

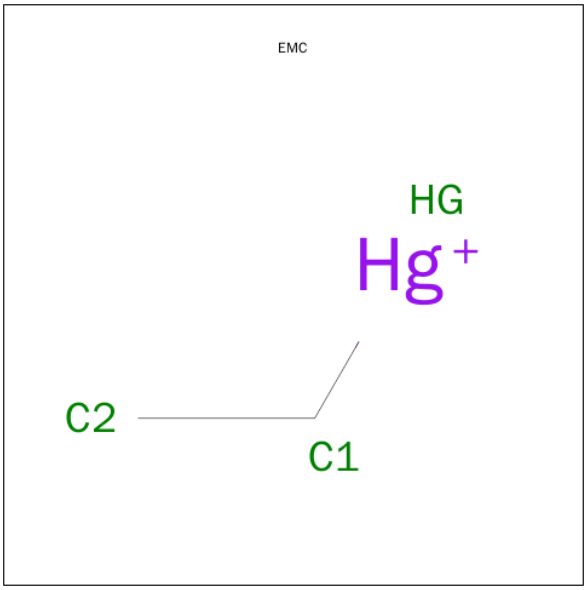
There are 3 unique types of molecules in this entry. The entry contains 10816 atoms, of which 1892 are hydrogens and 0 are deuteriums.

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 LAC REPRESSOR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	296	Total	C	H	N	O	S	0	0	0
			2675	1380	462	396	426	11			
1	B	296	Total	C	H	N	O	S	0	0	0
			2675	1380	462	396	426	11			
1	C	296	Total	C	H	N	O	S	0	0	0
			2675	1380	462	396	426	11			
1	D	296	Total	C	H	N	O	S	0	0	0
			2675	1380	462	396	426	11			

- Molecule 2 is ETHYL MERCURY ION (three-letter code: EMC) (formula: C_2H_5Hg).



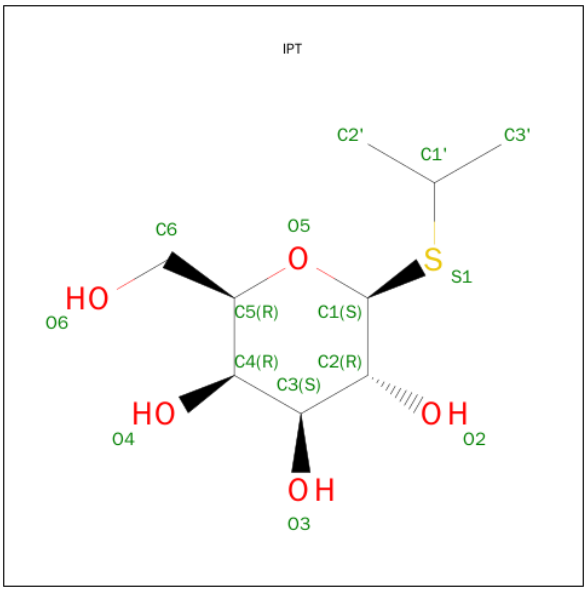
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Hg		0	0
			3	2	1			
2	B	1	Total	C	Hg		0	0
			3	2	1			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	1	Total C Hg 3 2 1	0	0
2	D	1	Total C Hg 3 2 1	0	0

- Molecule 3 is ISOPROPYL-1-BETA-D-THIOGALACTOSIDE (three-letter code: IPT) (formula: $C_9H_{18}O_5S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C H O S 26 9 11 5 1	0	0
3	B	1	Total C H O S 26 9 11 5 1	0	0
3	C	1	Total C H O S 26 9 11 5 1	0	0
3	D	1	Total C H O S 26 9 11 5 1	0	0

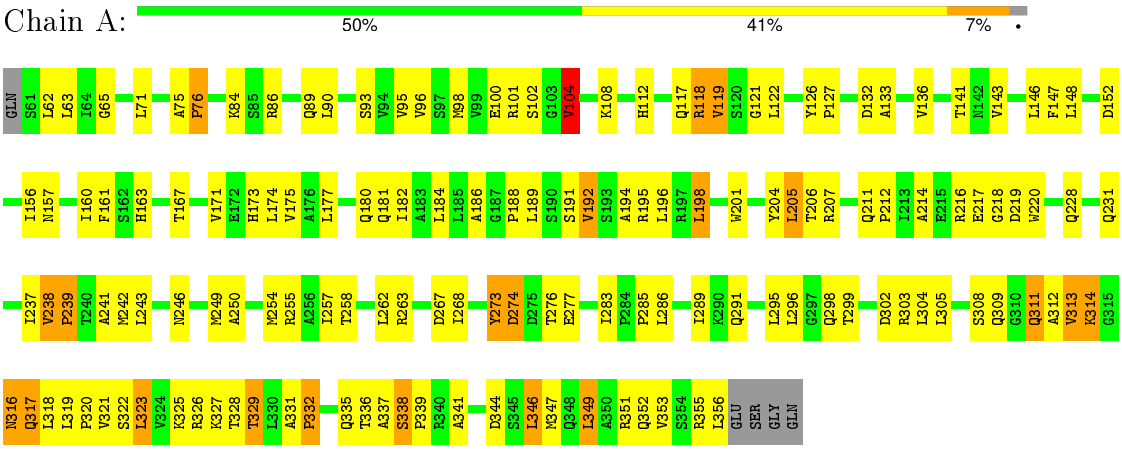
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

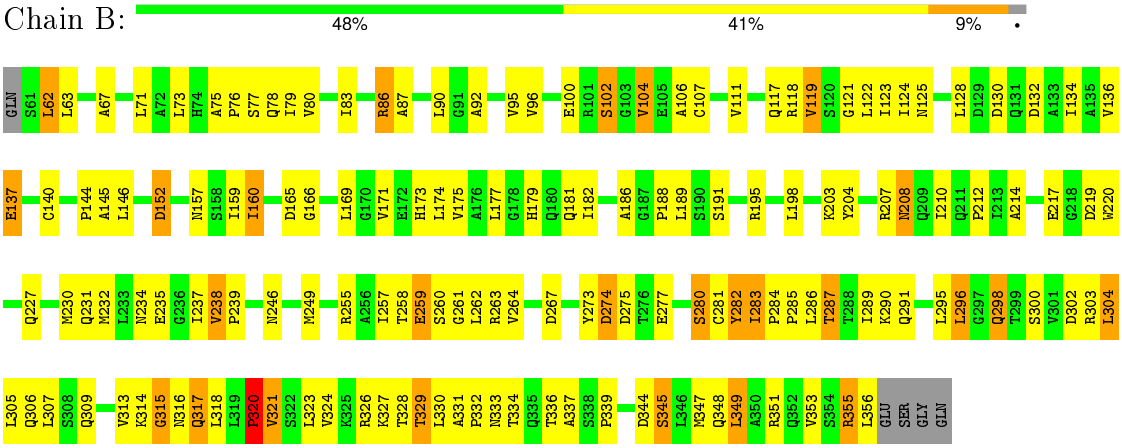
- Molecule 1: LAC REPRESSOR

Chain A:



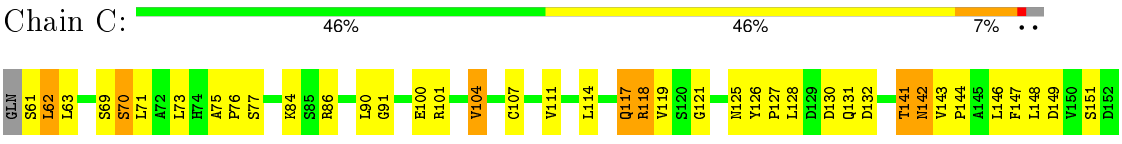
- Molecule 1: LAC REPRESSOR

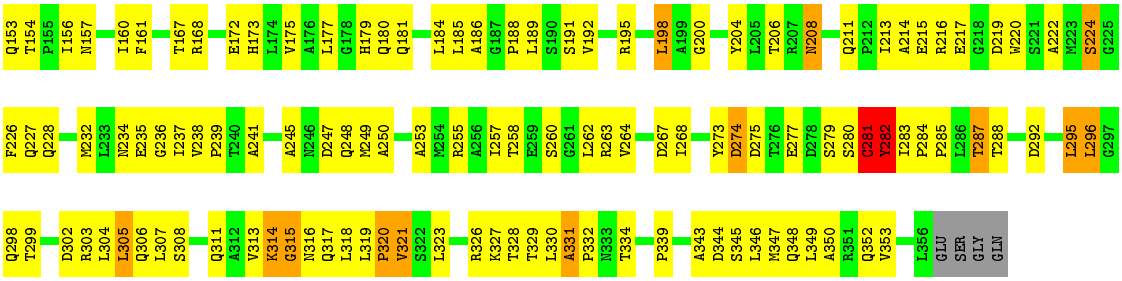
Chain B:



- Molecule 1: LAC REPRESSOR

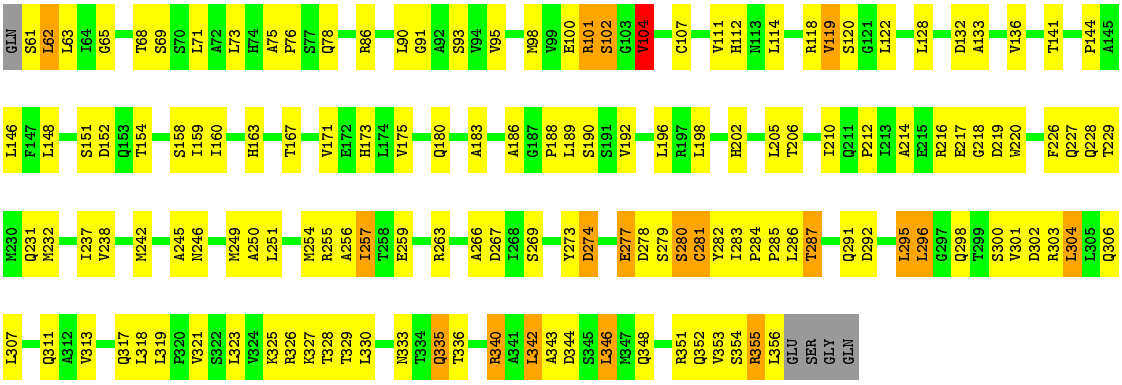
Chain C:





- Molecule 1: LAC REPRESSOR

Chain D:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.16Å 64.73Å 117.94Å 90.00° 91.75° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.222 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10816	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.53	0/2242	0.79	0/3048
1	B	0.52	0/2242	0.83	4/3048 (0.1%)
1	C	0.57	0/2242	0.88	6/3048 (0.2%)
1	D	0.54	0/2242	0.82	2/3048 (0.1%)
All	All	0.54	0/8968	0.83	12/12192 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	331	ALA	C-N-CD	-7.81	103.42	120.60
1	C	281	CYS	CA-CB-SG	-6.86	101.65	114.00
1	C	331	ALA	N-CA-C	6.23	127.83	111.00
1	B	315	GLY	N-CA-C	6.12	128.40	113.10
1	D	280	SER	N-CA-C	-5.99	94.83	111.00
1	C	282	TYR	N-CA-C	-5.60	95.87	111.00
1	C	315	GLY	N-CA-C	5.49	126.82	113.10
1	D	287	THR	N-CA-C	-5.33	96.61	111.00
1	B	282	TYR	N-CA-C	-5.32	96.65	111.00
1	C	296	LEU	CA-CB-CG	5.29	127.45	115.30
1	B	67	ALA	N-CA-C	-5.20	96.95	111.00
1	B	280	SER	N-CA-C	-5.00	97.49	111.00

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	2213	462	2265	137	0
1	B	2213	462	2265	129	0
1	C	2213	462	2266	163	0
1	D	2213	462	2265	133	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	1	0
2	D	3	0	0	0	0
3	A	15	11	18	0	0
3	B	15	11	18	0	0
3	C	15	11	18	0	0
3	D	15	11	18	1	0
All	All	8924	1892	9133	514	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 28.

All (514) 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:189:LEU:HD11	1:A:217:GLU:OE2	1.26	1.34
1:D:189:LEU:HD11	1:D:217:GLU:OE2	1.17	1.32
1:C:189:LEU:CD2	1:C:217:GLU:OE2	1.79	1.30
1:C:189:LEU:HD21	1:C:217:GLU:OE2	1.09	1.24
1:A:189:LEU:HG	1:A:217:GLU:OE1	1.41	1.19
1:B:186:ALA:HB3	1:B:217:GLU:HG2	1.25	1.17
1:C:186:ALA:HB3	1:C:217:GLU:HG2	1.21	1.16
1:D:189:LEU:CD1	1:D:217:GLU:OE2	1.95	1.14
1:C:189:LEU:HG	1:C:217:GLU:OE1	1.51	1.07
1:A:189:LEU:CD1	1:A:217:GLU:OE2	2.03	1.06
1:D:189:LEU:HG	1:D:217:GLU:OE1	1.54	1.06
1:D:86:ARG:HG2	1:D:301:VAL:HB	1.39	1.05
1:C:281:CYS:SG	1:C:282:TYR:N	2.29	1.02
1:D:295:LEU:HD13	1:D:319:LEU:HD22	1.46	0.96
1:C:71:LEU:HD13	1:D:71:LEU:HD13	1.47	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:ARG:HD3	1:B:281:CYS:HA	1.47	0.95
1:B:146:LEU:HD11	1:B:159:ILE:HG13	1.48	0.91
1:C:104:VAL:HG13	1:C:132:ASP:HB3	1.53	0.91
1:C:189:LEU:CD2	1:C:217:GLU:CD	2.38	0.91
1:A:189:LEU:HG	1:A:217:GLU:CD	1.91	0.91
1:B:104:VAL:HG13	1:B:132:ASP:HB3	1.52	0.90
1:C:255:ARG:HG2	1:D:281:CYS:HA	1.52	0.89
1:C:189:LEU:HG	1:C:217:GLU:CD	1.93	0.89
1:C:177:LEU:HB3	1:C:331:ALA:CB	2.03	0.89
1:C:62:LEU:HD13	1:C:305:LEU:HD21	1.53	0.88
1:C:189:LEU:CG	1:C:217:GLU:OE1	2.20	0.88
1:B:177:LEU:HD11	1:B:329:THR:HG23	1.56	0.87
1:B:86:ARG:HG3	1:B:298:GLN:HA	1.56	0.86
1:C:177:LEU:HB3	1:C:331:ALA:HB3	1.56	0.85
1:D:189:LEU:CG	1:D:217:GLU:OE1	2.24	0.85
1:A:71:LEU:O	1:B:77:SER:HB3	1.77	0.84
1:A:255:ARG:HG2	1:B:281:CYS:HB2	1.59	0.84
1:D:351:ARG:HH11	1:D:351:ARG:HB3	1.42	0.84
1:B:173:HIS:CE1	1:B:329:THR:HG21	2.14	0.83
1:C:189:LEU:CG	1:C:217:GLU:OE2	2.27	0.82
1:D:189:LEU:HG	1:D:217:GLU:CD	1.99	0.82
1:C:186:ALA:HB3	1:C:217:GLU:CG	2.07	0.81
1:D:254:MET:HA	1:D:257:ILE:HD12	1.62	0.81
1:A:84:LYS:HE3	1:B:100:GLU:HG3	1.62	0.80
1:A:285:PRO:HG3	1:B:255:ARG:NH1	1.96	0.80
1:A:216:ARG:HB3	1:A:228:GLN:HE21	1.47	0.80
1:A:189:LEU:CG	1:A:217:GLU:OE1	2.28	0.79
1:C:148:LEU:HD13	1:C:296:LEU:HD11	1.61	0.79
1:D:189:LEU:CD1	1:D:217:GLU:CD	2.53	0.77
1:B:203:LYS:O	1:B:207:ARG:HG2	1.86	0.76
1:A:218:GLY:HA3	1:A:249:MET:HE3	1.67	0.76
1:A:189:LEU:CG	1:A:217:GLU:CD	2.55	0.75
1:A:201:TRP:O	1:A:205:LEU:HB2	1.87	0.75
1:A:119:VAL:HG11	1:A:122:LEU:HD23	1.67	0.75
1:B:75:ALA:HB3	1:B:76:PRO:HD3	1.68	0.75
1:A:148:LEU:HD13	1:A:296:LEU:HD11	1.67	0.75
1:C:189:LEU:CG	1:C:217:GLU:CD	2.56	0.74
1:A:75:ALA:HB3	1:A:76:PRO:HD3	1.68	0.74
1:A:205:LEU:HD13	1:A:212:PRO:HD3	1.68	0.73
1:B:347:MET:SD	1:C:347:MET:SD	2.87	0.72
1:D:188:PRO:HD3	1:D:219:ASP:HA	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:SER:HA	1:C:227:GLN:HG2	1.70	0.72
1:C:306:GLN:HB3	1:C:311:GLN:HB3	1.72	0.72
1:A:160:ILE:HD12	1:A:161:PHE:O	1.90	0.72
1:D:189:LEU:CG	1:D:217:GLU:CD	2.59	0.71
1:B:320:PRO:O	1:B:321:VAL:HB	1.89	0.71
1:D:351:ARG:NH1	1:D:351:ARG:HB3	2.06	0.70
1:D:266:ALA:HA	1:D:330:LEU:HD23	1.74	0.70
1:C:69:SER:HB2	1:C:101:ARG:CZ	2.21	0.70
1:B:349:LEU:O	1:B:353:VAL:HG23	1.92	0.70
1:A:117:GLN:O	1:A:118:ARG:HB3	1.91	0.69
1:A:214:ALA:HB2	1:A:237:ILE:HG21	1.73	0.69
1:B:165:ASP:O	1:B:169:LEU:HG	1.91	0.69
1:D:186:ALA:HB3	1:D:217:GLU:HG2	1.74	0.69
1:A:218:GLY:HA3	1:A:249:MET:CE	2.22	0.68
1:C:186:ALA:CB	1:C:217:GLU:HG2	2.12	0.68
1:A:274:ASP:HB3	1:A:276:THR:HG23	1.76	0.68
1:A:303:ARG:NH1	1:A:317:GLN:HG2	2.09	0.68
1:B:351:ARG:HD2	1:B:355:ARG:HH22	1.59	0.68
1:D:173:HIS:HE1	1:D:329:THR:OG1	1.77	0.67
1:B:152:ASP:HA	1:B:316:ASN:HD21	1.60	0.67
1:D:86:ARG:HG2	1:D:301:VAL:CB	2.22	0.67
1:B:144:PRO:HB3	1:B:307:LEU:HG	1.76	0.67
1:A:152:ASP:HB2	1:A:318:LEU:HD21	1.75	0.67
1:D:205:LEU:HD13	1:D:212:PRO:HG3	1.77	0.67
1:A:346:LEU:HD23	1:D:346:LEU:HD12	1.75	0.66
1:C:86:ARG:NH2	1:C:90:LEU:HD21	2.09	0.66
1:D:175:VAL:HG12	1:D:210:ILE:HD12	1.75	0.66
1:A:173:HIS:CE1	1:A:329:THR:HG21	2.30	0.66
1:D:189:LEU:CD1	1:D:217:GLU:OE1	2.44	0.66
1:C:189:LEU:CD2	1:C:217:GLU:OE1	2.42	0.66
1:C:179:HIS:NE2	1:C:331:ALA:HB2	2.10	0.66
1:A:346:LEU:HD21	1:C:346:LEU:HD21	1.78	0.65
1:C:285:PRO:HD2	1:C:327:LYS:HB2	1.78	0.65
1:A:152:ASP:HB3	1:A:160:ILE:HD11	1.77	0.65
1:B:152:ASP:HA	1:B:316:ASN:ND2	2.12	0.65
1:C:191:SER:O	1:C:195:ARG:HG3	1.96	0.65
1:A:189:LEU:CG	1:A:217:GLU:OE2	2.44	0.64
1:D:218:GLY:HA3	1:D:249:MET:CE	2.27	0.64
1:A:285:PRO:O	1:A:328:THR:HG23	1.97	0.64
1:B:232:MET:HG2	1:B:237:ILE:HB	1.80	0.64
1:A:132:ASP:O	1:A:136:VAL:HG23	1.99	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ALA:O	1:A:254:MET:HG3	1.96	0.63
1:B:307:LEU:HD13	1:B:313:VAL:HG22	1.80	0.63
1:B:264:VAL:HG11	1:B:328:THR:HG22	1.80	0.63
1:D:189:LEU:CG	1:D:217:GLU:OE2	2.47	0.63
1:A:262:LEU:HD13	1:A:268:ILE:HD11	1.80	0.62
1:C:281:CYS:O	1:C:282:TYR:HB2	1.99	0.62
1:A:355:ARG:CD	1:B:334:THR:HB	2.29	0.62
1:B:90:LEU:HD11	1:B:302:ASP:OD1	1.99	0.62
1:A:96:VAL:HB	1:B:96:VAL:HB	1.82	0.62
1:B:273:TYR:HE1	1:B:291:GLN:NE2	1.97	0.62
1:B:246:ASN:HA	1:B:273:TYR:O	1.98	0.62
1:C:329:THR:O	1:C:330:LEU:HD12	2.00	0.62
1:D:353:VAL:O	1:D:356:LEU:HB3	1.99	0.62
1:A:285:PRO:HD2	1:A:327:LYS:HB2	1.82	0.62
1:B:171:VAL:O	1:B:175:VAL:HG13	2.00	0.62
1:A:188:PRO:HG3	1:A:219:ASP:HA	1.82	0.61
1:C:214:ALA:HB2	1:C:237:ILE:HG21	1.81	0.61
1:A:242:MET:CE	1:A:257:ILE:HD11	2.30	0.61
1:A:255:ARG:HH11	1:B:281:CYS:HA	1.64	0.61
1:B:189:LEU:HD13	1:B:195:ARG:HG2	1.81	0.61
1:C:295:LEU:HD13	1:C:319:LEU:HD22	1.81	0.61
1:D:111:VAL:HG13	1:D:122:LEU:HD22	1.81	0.61
1:B:246:ASN:OD1	1:B:249:MET:HG3	2.01	0.61
1:A:117:GLN:NE2	1:B:117:GLN:HG3	2.16	0.60
1:D:306:GLN:HB3	1:D:311:GLN:O	2.02	0.60
1:D:227:GLN:O	1:D:231:GLN:HG2	2.02	0.60
1:A:171:VAL:O	1:A:175:VAL:HG13	2.02	0.60
1:B:104:VAL:HG13	1:B:132:ASP:CB	2.29	0.60
1:A:255:ARG:HG2	1:B:281:CYS:CB	2.31	0.59
1:D:148:LEU:HD21	1:D:300:SER:OG	2.01	0.59
1:C:348:GLN:O	1:C:352:GLN:HG3	2.01	0.59
1:D:68:THR:HG21	1:D:71:LEU:HD21	1.83	0.59
1:B:173:HIS:HE1	1:B:329:THR:HG21	1.68	0.59
1:C:179:HIS:HE2	1:C:331:ALA:HB2	1.68	0.59
1:D:148:LEU:HD22	1:D:296:LEU:HD21	1.85	0.59
1:B:111:VAL:HG21	1:B:136:VAL:HG13	1.85	0.59
1:D:214:ALA:HB2	1:D:237:ILE:HG21	1.85	0.59
1:A:255:ARG:CG	1:B:281:CYS:HB2	2.31	0.59
1:B:177:LEU:HD11	1:B:329:THR:CG2	2.31	0.58
1:A:323:LEU:HD21	1:A:325:LYS:HG3	1.85	0.58
1:A:283:ILE:HB	1:B:283:ILE:HG13	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:VAL:HG23	1:A:314:LYS:H	1.68	0.58
1:B:121:GLY:HA3	1:B:304:LEU:HD11	1.84	0.58
1:C:160:ILE:HG13	1:C:318:LEU:HD23	1.85	0.58
1:D:340:ARG:NH1	1:D:343:ALA:HB3	2.18	0.58
1:A:285:PRO:HB2	1:A:326:ARG:HB3	1.85	0.58
1:B:79:ILE:O	1:B:83:ILE:HG13	2.03	0.58
1:A:352:GLN:HG2	1:A:355:ARG:HH22	1.69	0.58
1:C:273:TYR:O	1:C:274:ASP:HB2	2.03	0.58
1:D:86:ARG:HD3	1:D:302:ASP:OD1	2.04	0.58
1:C:234:ASN:ND2	1:D:351:ARG:NH2	2.51	0.58
1:C:303:ARG:NH1	1:C:317:GLN:HG3	2.19	0.57
1:A:86:ARG:HG2	1:A:298:GLN:HA	1.86	0.57
1:B:290:LYS:O	1:B:321:VAL:HA	2.05	0.57
1:C:126:TYR:CD1	1:C:127:PRO:HD2	2.39	0.57
1:B:289:ILE:HD13	1:B:323:LEU:HD13	1.85	0.57
1:D:173:HIS:CD2	1:D:323:LEU:HD21	2.40	0.57
1:C:238:VAL:HG23	1:C:268:ILE:HD11	1.85	0.57
1:A:186:ALA:HB2	1:A:198:LEU:HG	1.87	0.57
1:A:216:ARG:NH1	1:A:231:GLN:HB3	2.19	0.57
1:D:107:CYS:O	1:D:111:VAL:HG23	2.05	0.57
1:B:107:CYS:SG	1:B:128:LEU:HD11	2.44	0.57
1:A:295:LEU:HD13	1:A:299:THR:HG21	1.87	0.57
1:C:121:GLY:HA3	1:C:304:LEU:HD11	1.86	0.57
1:A:313:VAL:HG23	1:A:314:LYS:N	2.20	0.57
1:A:317:GLN:HE21	1:A:317:GLN:HA	1.69	0.57
1:A:349:LEU:HD11	1:B:345:SER:HB2	1.87	0.57
1:B:351:ARG:HD2	1:B:355:ARG:NH2	2.19	0.57
1:D:73:LEU:O	1:D:76:PRO:HD2	2.05	0.57
1:C:117:GLN:O	1:C:118:ARG:HB3	2.05	0.57
1:B:102:SER:HB2	1:B:106:ALA:HB2	1.86	0.57
1:D:152:ASP:HB3	1:D:160:ILE:HD11	1.87	0.56
1:C:100:GLU:CD	1:C:100:GLU:H	2.08	0.56
1:C:172:GLU:HA	1:C:175:VAL:HG22	1.85	0.56
1:B:134:ILE:O	1:B:137:GLU:HB3	2.05	0.56
1:B:286:LEU:O	1:B:326:ARG:HD2	2.06	0.56
1:A:62:LEU:HD21	1:A:305:LEU:HD22	1.87	0.56
1:B:63:LEU:HD12	1:B:119:VAL:HA	1.87	0.56
1:C:69:SER:HB3	1:C:126:TYR:CD1	2.39	0.56
1:C:147:PHE:CD1	1:C:156:ILE:HD12	2.41	0.56
1:A:163:HIS:CD2	1:A:163:HIS:H	2.22	0.56
1:B:182:ILE:O	1:B:212:PRO:HA	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:PRO:HG2	1:B:327:LYS:HB2	1.87	0.55
1:D:348:GLN:O	1:D:352:GLN:HG3	2.06	0.55
1:A:206:THR:HG22	1:A:211:GLN:OE1	2.06	0.55
1:D:86:ARG:HD2	1:D:298:GLN:HB2	1.88	0.55
1:A:63:LEU:HD23	1:A:93:SER:HB2	1.87	0.55
1:C:216:ARG:HD3	1:C:228:GLN:HE21	1.71	0.55
1:A:173:HIS:O	1:A:177:LEU:HG	2.07	0.55
1:A:104:VAL:HG22	1:A:132:ASP:CG	2.27	0.55
1:C:86:ARG:HG2	1:C:298:GLN:HA	1.89	0.55
1:A:121:GLY:HA3	1:A:304:LEU:HD11	1.87	0.55
1:C:295:LEU:HD22	1:C:299:THR:HG23	1.87	0.55
1:D:273:TYR:O	1:D:274:ASP:HB2	2.07	0.55
1:A:191:SER:HB3	1:A:194:ALA:HB3	1.89	0.55
1:C:287:THR:HG21	1:C:329:THR:HB	1.89	0.54
1:D:335:GLN:O	1:D:336:THR:HB	2.05	0.54
1:C:234:ASN:HD21	1:D:351:ARG:NH2	2.05	0.54
1:A:152:ASP:CB	1:A:318:LEU:HD21	2.37	0.54
1:A:263:ARG:O	1:A:267:ASP:HB2	2.07	0.54
1:B:287:THR:HA	1:B:324:VAL:O	2.07	0.54
1:A:312:ALA:O	1:A:313:VAL:HG13	2.07	0.54
1:A:86:ARG:HH11	1:A:89:GLN:NE2	2.05	0.54
1:D:101:ARG:HH22	3:D:998:IPT:C6	2.20	0.54
1:C:281:CYS:SG	1:D:251:LEU:HG	2.48	0.54
1:C:329:THR:HG23	1:C:329:THR:O	2.07	0.54
1:D:218:GLY:HA3	1:D:249:MET:HE3	1.90	0.54
1:A:347:MET:O	1:A:351:ARG:HG2	2.08	0.54
1:C:234:ASN:HD21	1:D:351:ARG:HH21	1.57	0.53
1:B:238:VAL:O	1:B:238:VAL:HG22	2.08	0.53
1:D:279:SER:C	1:D:280:SER:O	2.43	0.53
1:A:71:LEU:HD13	1:B:71:LEU:HD13	1.90	0.53
1:A:118:ARG:HG2	1:A:119:VAL:N	2.23	0.53
1:C:303:ARG:HD2	1:C:317:GLN:OE1	2.09	0.53
1:A:104:VAL:HG22	1:A:132:ASP:OD2	2.08	0.53
1:C:349:LEU:HD12	1:D:342:LEU:HD12	1.90	0.53
1:D:280:SER:O	1:D:282:TYR:N	2.42	0.53
1:C:111:VAL:HA	1:C:114:LEU:HD12	1.90	0.53
1:C:219:ASP:O	1:C:220:TRP:HB2	2.09	0.53
1:C:141:THR:O	1:C:143:VAL:HG23	2.09	0.52
1:A:192:VAL:O	1:A:196:LEU:HG	2.10	0.52
1:A:204:TYR:HA	1:A:207:ARG:HB2	1.91	0.52
1:A:189:LEU:CD1	1:A:217:GLU:CD	2.74	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:SER:O	1:C:227:GLN:HG2	2.10	0.52
1:A:86:ARG:HH11	1:A:89:GLN:HE22	1.57	0.52
1:A:191:SER:HB3	1:A:194:ALA:CB	2.38	0.52
1:D:132:ASP:O	1:D:136:VAL:HG23	2.09	0.52
1:C:101:ARG:HA	1:C:126:TYR:OH	2.09	0.52
1:C:161:PHE:HB3	1:C:321:VAL:HG23	1.91	0.52
1:B:204:TYR:O	1:B:207:ARG:HB2	2.10	0.52
1:B:264:VAL:CG1	1:B:328:THR:HG22	2.39	0.52
1:C:295:LEU:HD22	1:C:299:THR:CG2	2.38	0.52
1:A:323:LEU:HD21	1:A:325:LYS:HE3	1.92	0.52
1:B:287:THR:HB	1:B:326:ARG:H	1.74	0.52
1:A:104:VAL:O	1:A:108:LYS:HG3	2.10	0.52
1:C:126:TYR:CG	1:C:127:PRO:HD2	2.45	0.52
1:D:173:HIS:CE1	1:D:329:THR:OG1	2.60	0.52
1:C:227:GLN:HG3	1:C:228:GLN:N	2.24	0.52
1:A:295:LEU:O	1:A:299:THR:HG23	2.09	0.52
1:C:151:SER:C	1:C:153:GLN:H	2.13	0.52
1:A:273:TYR:O	1:A:274:ASP:HB2	2.10	0.52
1:C:255:ARG:CG	1:D:281:CYS:HA	2.33	0.52
1:C:86:ARG:CZ	1:C:90:LEU:HD21	2.39	0.52
1:C:179:HIS:NE2	1:C:331:ALA:CB	2.73	0.51
1:B:307:LEU:HD13	1:B:313:VAL:CG2	2.40	0.51
1:D:205:LEU:CD1	1:D:212:PRO:HG3	2.41	0.51
1:A:157:ASN:ND2	1:A:314:LYS:HA	2.25	0.51
1:C:260:SER:O	1:D:355:ARG:NH2	2.43	0.51
1:B:336:THR:O	1:B:337:ALA:HB3	2.10	0.51
1:A:238:VAL:HG22	1:A:238:VAL:O	2.09	0.51
1:D:273:TYR:HE1	1:D:291:GLN:NE2	2.09	0.51
1:C:189:LEU:HD23	1:C:217:GLU:OE1	2.10	0.51
1:B:303:ARG:NH2	1:B:314:LYS:O	2.43	0.51
1:D:286:LEU:O	1:D:326:ARG:HD2	2.10	0.51
1:D:61:SER:N	1:D:91:GLY:O	2.42	0.51
1:C:71:LEU:CD1	1:D:71:LEU:HD13	2.29	0.51
1:C:239:PRO:HB2	1:C:241:ALA:O	2.11	0.51
1:B:124:ILE:N	1:B:124:ILE:HD12	2.25	0.51
1:C:296:LEU:O	1:C:296:LEU:HD13	2.11	0.51
1:C:343:ALA:O	1:C:347:MET:HG2	2.11	0.51
1:C:118:ARG:HG2	1:C:118:ARG:O	2.10	0.51
1:A:355:ARG:HH21	1:B:336:THR:HA	1.76	0.50
1:B:351:ARG:HB3	1:B:355:ARG:NH1	2.27	0.50
1:C:61:SER:N	1:C:91:GLY:O	2.43	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:VAL:O	1:B:356:LEU:HG	2.11	0.50
1:C:281:CYS:O	1:C:282:TYR:CB	2.59	0.50
1:C:247:ASP:O	1:C:250:ALA:HB3	2.11	0.50
1:D:280:SER:C	1:D:282:TYR:H	2.15	0.50
1:B:235:GLU:HG3	1:B:237:ILE:HG12	1.94	0.50
1:A:355:ARG:O	1:A:355:ARG:HG2	2.12	0.50
1:D:256:ALA:HA	1:D:259:GLU:HB2	1.93	0.50
1:D:285:PRO:HD2	1:D:327:LYS:HB2	1.93	0.50
1:A:184:LEU:CD2	1:A:243:LEU:HD12	2.42	0.50
1:D:167:THR:O	1:D:171:VAL:HG23	2.11	0.50
1:C:161:PHE:CZ	1:C:296:LEU:HB2	2.47	0.50
1:D:202:HIS:O	1:D:206:THR:HG23	2.12	0.50
1:D:188:PRO:C	1:D:190:SER:H	2.15	0.49
1:C:264:VAL:HG11	1:C:328:THR:HG22	1.93	0.49
1:B:140:CYS:SG	1:B:145:ALA:HB2	2.52	0.49
1:A:174:LEU:HD22	1:A:241:ALA:HB1	1.95	0.49
1:C:189:LEU:HD23	1:C:217:GLU:CD	2.29	0.49
1:B:86:ARG:CG	1:B:298:GLN:HA	2.36	0.49
1:C:344:ASP:O	1:C:347:MET:HB2	2.13	0.49
1:C:146:LEU:HD11	1:C:303:ARG:HD3	1.93	0.49
1:B:208:ASN:HD22	1:B:208:ASN:H	1.61	0.49
1:C:222:ALA:HA	1:C:248:GLN:O	2.12	0.49
1:C:188:PRO:HD3	1:C:219:ASP:HA	1.95	0.49
1:D:263:ARG:HD3	1:D:267:ASP:OD2	2.13	0.49
1:A:352:GLN:HG2	1:A:355:ARG:NH2	2.26	0.49
1:C:349:LEU:O	1:C:353:VAL:HG23	2.12	0.49
1:C:90:LEU:HD11	1:C:302:ASP:OD1	2.13	0.48
1:A:295:LEU:HD13	1:A:299:THR:CG2	2.43	0.48
1:D:280:SER:O	1:D:281:CYS:HB2	2.13	0.48
1:A:167:THR:HG22	1:A:201:TRP:CD1	2.48	0.48
1:B:273:TYR:O	1:B:274:ASP:CB	2.61	0.48
1:D:295:LEU:CD1	1:D:319:LEU:HD22	2.31	0.48
1:B:177:LEU:CD1	1:B:329:THR:HG23	2.34	0.48
1:A:285:PRO:HB3	1:A:326:ARG:HD3	1.95	0.48
1:A:148:LEU:HD13	1:A:296:LEU:CD1	2.41	0.48
1:C:279:SER:O	1:C:281:CYS:O	2.31	0.48
1:C:232:MET:HG2	1:C:237:ILE:HB	1.95	0.48
1:D:63:LEU:HD23	1:D:93:SER:HB2	1.95	0.48
1:C:245:ALA:O	1:C:273:TYR:HB3	2.14	0.48
1:D:303:ARG:O	1:D:307:LEU:HD13	2.13	0.48
1:B:230:MET:HA	1:B:230:MET:CE	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:VAL:HG11	1:B:122:LEU:CD2	2.44	0.48
1:D:188:PRO:HD2	1:D:220:TRP:CE2	2.49	0.48
1:C:125:ASN:HB2	1:C:148:LEU:HD12	1.96	0.48
1:B:273:TYR:O	1:B:274:ASP:HB2	2.14	0.48
1:A:192:VAL:HG13	1:A:195:ARG:NH2	2.28	0.48
1:C:69:SER:HB3	1:C:126:TYR:HD1	1.77	0.47
1:A:346:LEU:CD2	1:C:346:LEU:HD21	2.43	0.47
1:C:173:HIS:HE1	1:C:329:THR:HG21	1.80	0.47
1:C:181:GLN:HB3	1:C:213:ILE:HD13	1.95	0.47
1:B:146:LEU:HD21	1:B:300:SER:HA	1.97	0.47
1:C:73:LEU:HD12	1:C:101:ARG:NH2	2.30	0.47
1:D:75:ALA:HB3	1:D:76:PRO:HD3	1.96	0.47
1:A:356:LEU:HA	1:B:336:THR:OG1	2.15	0.47
1:D:354:SER:C	1:D:356:LEU:H	2.17	0.47
1:C:107:CYS:SG	1:C:128:LEU:HD11	2.54	0.47
1:B:284:PRO:HG2	1:B:328:THR:HG22	1.97	0.47
1:B:336:THR:HG23	1:B:337:ALA:O	2.15	0.47
1:D:284:PRO:HG2	1:D:328:THR:HG22	1.95	0.47
1:C:206:THR:HG22	1:C:211:GLN:NE2	2.29	0.47
1:D:100:GLU:O	1:D:102:SER:N	2.48	0.47
1:B:260:SER:HB2	1:B:262:LEU:HD12	1.97	0.47
1:A:263:ARG:H	1:A:267:ASP:HB2	1.80	0.47
1:B:208:ASN:O	1:B:210:ILE:HG13	2.14	0.47
1:B:119:VAL:HG13	1:B:121:GLY:O	2.15	0.47
1:B:234:ASN:HB3	1:C:226:PHE:HE1	1.80	0.47
1:A:317:GLN:HE21	1:A:317:GLN:CA	2.29	0.46
1:C:281:CYS:SG	1:D:255:ARG:HB2	2.55	0.46
1:A:316:ASN:OD1	1:A:318:LEU:HD22	2.14	0.46
1:D:175:VAL:CG1	1:D:210:ILE:HD12	2.44	0.46
1:C:173:HIS:CE1	1:C:329:THR:HG21	2.51	0.46
1:A:289:ILE:HA	1:A:322:SER:O	2.15	0.46
1:C:255:ARG:HH11	1:D:281:CYS:H	1.63	0.46
1:C:303:ARG:HH12	1:C:317:GLN:HG3	1.79	0.46
1:D:344:ASP:O	1:D:348:GLN:HG3	2.16	0.46
1:A:173:HIS:HE1	1:A:329:THR:HG21	1.78	0.46
1:B:214:ALA:HB2	1:B:237:ILE:HG21	1.97	0.46
1:C:303:ARG:HE	1:C:313:VAL:HG21	1.80	0.46
1:D:104:VAL:HG13	1:D:132:ASP:HB3	1.96	0.46
1:B:339:PRO:HB3	1:C:353:VAL:O	2.15	0.46
1:B:179:HIS:ND1	1:B:332:PRO:HG3	2.31	0.46
1:C:263:ARG:HD3	1:C:267:ASP:OD1	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:PRO:HB2	1:C:307:LEU:HD23	1.98	0.46
1:A:65:GLY:O	1:A:122:LEU:HA	2.16	0.46
1:A:309:GLN:HB3	1:A:311:GLN:OE1	2.16	0.46
1:B:296:LEU:HD23	1:B:296:LEU:HA	1.76	0.46
1:B:78:GLN:HE22	1:B:277:GLU:H	1.64	0.46
1:C:216:ARG:HH11	1:C:228:GLN:NE2	2.14	0.46
1:D:283:ILE:HA	1:D:284:PRO:HA	1.83	0.46
1:C:75:ALA:HB3	1:C:76:PRO:HD3	1.98	0.46
1:A:133:ALA:HB1	1:A:156:ILE:HD13	1.97	0.46
1:B:123:ILE:HA	1:B:146:LEU:O	2.16	0.46
1:B:145:ALA:O	1:B:157:ASN:HB2	2.16	0.46
1:D:186:ALA:O	1:D:217:GLU:HA	2.16	0.45
1:D:226:PHE:CD1	1:D:255:ARG:HG3	2.50	0.45
1:B:263:ARG:O	1:B:267:ASP:HB2	2.16	0.45
1:C:168:ARG:HH11	1:C:168:ARG:HG2	1.81	0.45
1:D:278:ASP:O	1:D:280:SER:O	2.35	0.45
1:D:186:ALA:HA	1:D:245:ALA:HB2	1.99	0.45
1:A:220:TRP:HE3	1:A:246:ASN:ND2	2.14	0.45
1:D:86:ARG:HD2	1:D:298:GLN:CB	2.46	0.45
1:B:280:SER:O	1:B:281:CYS:SG	2.75	0.45
1:C:326:ARG:C	1:C:327:LYS:HD2	2.37	0.45
1:C:258:THR:HG21	1:D:283:ILE:HD13	1.98	0.45
1:A:182:ILE:O	1:A:212:PRO:HA	2.17	0.45
1:A:274:ASP:HA	1:A:291:GLN:HG3	1.98	0.45
1:C:287:THR:HG22	1:C:328:THR:OG1	2.16	0.45
1:D:78:GLN:HE22	1:D:277:GLU:H	1.65	0.45
1:A:95:VAL:HG23	1:B:95:VAL:HG13	1.99	0.45
1:D:151:SER:HA	1:D:196:LEU:HD11	1.99	0.45
1:B:87:ALA:HA	1:B:92:ALA:HB3	1.98	0.45
1:C:283:ILE:HD11	1:D:255:ARG:HA	1.98	0.45
1:A:219:ASP:O	1:A:220:TRP:HB2	2.16	0.45
1:A:254:MET:O	1:A:258:THR:HG23	2.17	0.45
1:C:339:PRO:HG3	1:D:356:LEU:HD21	1.98	0.45
1:D:146:LEU:HD21	1:D:159:ILE:HD12	1.98	0.45
1:B:287:THR:HG21	1:B:329:THR:HB	1.99	0.44
1:C:90:LEU:HD23	1:C:90:LEU:N	2.32	0.44
1:D:273:TYR:O	1:D:274:ASP:CB	2.65	0.44
1:A:186:ALA:HB3	1:A:217:GLU:HG2	1.99	0.44
1:A:323:LEU:CD2	1:A:325:LYS:HE3	2.47	0.44
1:B:255:ARG:O	1:B:259:GLU:HB2	2.18	0.44
1:C:228:GLN:HA	1:C:228:GLN:NE2	2.32	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:163:HIS:CE1	1:D:196:LEU:HD22	2.53	0.44
1:C:281:CYS:SG	1:D:251:LEU:HD11	2.58	0.44
1:C:303:ARG:HE	1:C:313:VAL:CG2	2.31	0.44
1:C:349:LEU:HA	1:C:349:LEU:HD13	1.83	0.44
1:A:147:PHE:CD1	1:A:156:ILE:HD12	2.53	0.44
1:D:128:LEU:O	1:D:192:VAL:HG21	2.18	0.44
1:D:133:ALA:HB3	1:D:154:THR:HG21	2.00	0.44
1:C:347:MET:O	1:C:350:ALA:HB3	2.18	0.44
1:D:246:ASN:OD1	1:D:249:MET:HG3	2.18	0.44
1:D:63:LEU:O	1:D:120:SER:N	2.50	0.44
1:B:219:ASP:O	1:B:220:TRP:HB2	2.17	0.44
1:A:98:MET:SD	1:B:80:VAL:HG12	2.58	0.44
1:C:305:LEU:O	1:C:308:SER:HB3	2.18	0.43
1:C:160:ILE:O	1:C:319:LEU:N	2.48	0.43
1:B:186:ALA:HB3	1:B:217:GLU:CG	2.18	0.43
1:D:250:ALA:O	1:D:254:MET:HG3	2.18	0.43
1:B:166:GLY:HA3	1:B:273:TYR:OH	2.18	0.43
1:C:70:SER:H	1:C:101:ARG:HE	1.66	0.43
1:C:285:PRO:HB2	1:C:326:ARG:HB3	1.98	0.43
1:C:273:TYR:O	1:C:274:ASP:CB	2.64	0.43
1:C:154:THR:HG22	1:C:156:ILE:HG12	2.00	0.43
1:B:160:ILE:O	1:B:318:LEU:HA	2.18	0.43
1:C:167:THR:CB	1:C:200:GLY:HA3	2.47	0.43
1:A:286:LEU:O	1:A:326:ARG:HD2	2.18	0.43
1:C:126:TYR:O	1:C:149:ASP:HB3	2.18	0.43
1:B:306:GLN:HA	1:B:309:GLN:HB3	2.00	0.43
1:A:283:ILE:O	1:B:283:ILE:HG13	2.18	0.43
1:B:227:GLN:O	1:B:231:GLN:HG3	2.18	0.43
1:C:326:ARG:HH21	2:C:999:EMC:C1	2.30	0.43
1:D:160:ILE:O	1:D:318:LEU:HA	2.18	0.43
1:B:177:LEU:HB3	1:B:331:ALA:HA	2.00	0.43
1:C:224:SER:CA	1:C:227:GLN:HG2	2.42	0.43
1:C:253:ALA:O	1:C:257:ILE:HG13	2.19	0.43
1:A:90:LEU:HD11	1:A:302:ASP:OD1	2.18	0.43
1:C:283:ILE:HA	1:C:284:PRO:HA	1.93	0.43
1:C:104:VAL:HG13	1:C:132:ASP:CB	2.36	0.43
1:A:63:LEU:HD12	1:A:119:VAL:HA	2.00	0.43
1:B:258:THR:O	1:B:261:GLY:N	2.52	0.43
1:B:300:SER:O	1:B:304:LEU:HB2	2.17	0.43
1:D:218:GLY:HA3	1:D:249:MET:HE1	1.99	0.43
1:B:344:ASP:O	1:B:348:GLN:HG3	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:319:LEU:HA	1:C:320:PRO:HD3	1.90	0.43
1:A:126:TYR:HA	1:A:127:PRO:HD3	1.77	0.43
1:D:296:LEU:HD22	1:D:296:LEU:O	2.19	0.43
1:C:157:ASN:OD1	1:C:307:LEU:HD21	2.19	0.42
1:B:305:LEU:O	1:B:309:GLN:N	2.51	0.42
1:D:254:MET:HE1	1:D:282:TYR:CD2	2.53	0.42
1:B:208:ASN:ND2	1:B:208:ASN:N	2.67	0.42
1:D:63:LEU:HB3	1:D:119:VAL:HA	2.01	0.42
1:C:198:LEU:HD11	1:C:215:GLU:OE2	2.19	0.42
1:C:281:CYS:HA	1:D:255:ARG:HD3	2.00	0.42
1:C:77:SER:HB2	1:D:71:LEU:O	2.20	0.42
1:C:157:ASN:HA	1:C:314:LYS:O	2.18	0.42
1:C:234:ASN:C	1:C:236:GLY:H	2.23	0.42
1:A:346:LEU:HD21	1:C:346:LEU:CD2	2.48	0.42
1:B:235:GLU:HG3	1:B:237:ILE:CG1	2.49	0.42
1:C:144:PRO:HG3	1:C:308:SER:HA	2.01	0.42
1:A:353:VAL:O	1:A:356:LEU:HB3	2.19	0.42
1:D:114:LEU:HB3	1:D:119:VAL:HG21	2.00	0.42
1:D:63:LEU:HA	1:D:63:LEU:HD23	1.86	0.42
1:C:287:THR:HB	1:C:326:ARG:H	1.83	0.42
1:B:345:SER:HA	1:B:348:GLN:NE2	2.35	0.42
1:C:107:CYS:O	1:C:111:VAL:HG23	2.20	0.42
1:D:65:GLY:O	1:D:122:LEU:HA	2.18	0.42
1:D:189:LEU:HD12	1:D:217:GLU:OE1	2.18	0.42
1:C:69:SER:HB2	1:C:101:ARG:NH2	2.34	0.42
1:C:69:SER:O	1:C:70:SER:C	2.57	0.42
1:B:302:ASP:O	1:B:306:GLN:HG3	2.19	0.42
1:C:279:SER:C	1:C:281:CYS:O	2.58	0.42
1:B:174:LEU:O	1:B:179:HIS:HB2	2.20	0.42
1:B:73:LEU:HD23	1:B:73:LEU:HA	1.74	0.42
1:B:179:HIS:CE1	1:B:332:PRO:HG3	2.55	0.42
1:B:188:PRO:HD2	1:B:220:TRP:CE2	2.55	0.42
1:C:185:LEU:HG	1:C:249:MET:HE2	2.02	0.42
1:A:100:GLU:C	1:A:102:SER:H	2.23	0.42
1:A:346:LEU:HG	1:B:349:LEU:HD23	2.02	0.41
1:B:284:PRO:HG2	1:B:328:THR:CG2	2.49	0.41
1:A:349:LEU:O	1:A:353:VAL:HG23	2.20	0.41
1:D:304:LEU:O	1:D:307:LEU:HB2	2.20	0.41
1:C:184:LEU:HD13	1:C:198:LEU:CD2	2.51	0.41
1:A:246:ASN:OD1	1:A:249:MET:HG3	2.20	0.41
1:D:188:PRO:C	1:D:190:SER:N	2.73	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ASN:OD1	1:B:317:GLN:N	2.52	0.41
1:C:292:ASP:HB3	1:C:295:LEU:HB2	2.02	0.41
1:C:117:GLN:O	1:C:118:ARG:CB	2.67	0.41
1:C:172:GLU:O	1:C:175:VAL:HG22	2.20	0.41
1:D:86:ARG:NH2	1:D:90:LEU:HD21	2.34	0.41
1:A:160:ILE:O	1:A:318:LEU:HA	2.20	0.41
1:C:168:ARG:HD3	1:C:204:TYR:CE2	2.55	0.41
1:A:255:ARG:HD3	1:B:281:CYS:CA	2.35	0.41
1:A:305:LEU:O	1:A:308:SER:HB3	2.20	0.41
1:C:84:LYS:HE2	1:D:98:MET:O	2.20	0.41
1:C:305:LEU:HD22	1:C:305:LEU:HA	1.85	0.41
1:B:62:LEU:HD13	1:B:305:LEU:HD22	2.03	0.41
1:C:273:TYR:N	1:C:288:THR:OG1	2.54	0.41
1:A:238:VAL:HA	1:A:239:PRO:HD2	1.80	0.41
1:D:216:ARG:HB3	1:D:228:GLN:HE21	1.86	0.41
1:D:287:THR:HG23	1:D:325:LYS:HA	2.01	0.41
1:D:69:SER:HB3	1:D:101:ARG:HH21	1.85	0.41
1:D:146:LEU:HD11	1:D:159:ILE:HG13	2.03	0.41
1:D:313:VAL:HG11	1:D:317:GLN:NE2	2.36	0.41
1:A:285:PRO:HG3	1:B:255:ARG:HH12	1.82	0.41
1:A:313:VAL:CG2	1:A:314:LYS:H	2.32	0.41
1:B:257:ILE:O	1:B:262:LEU:HB2	2.20	0.41
1:D:183:ALA:HB1	1:D:232:MET:HE3	2.02	0.41
1:B:289:ILE:CG2	1:B:321:VAL:HG13	2.51	0.41
1:A:167:THR:O	1:A:171:VAL:HG23	2.21	0.41
1:D:219:ASP:O	1:D:220:TRP:HB2	2.21	0.41
1:C:232:MET:O	1:C:235:GLU:HB2	2.20	0.41
1:B:191:SER:O	1:B:195:ARG:HG3	2.21	0.41
1:D:291:GLN:HG2	1:D:321:VAL:HG23	2.03	0.41
1:C:257:ILE:HG23	1:C:262:LEU:HB2	2.03	0.41
1:A:338:SER:O	1:A:341:ALA:HB3	2.21	0.41
1:A:319:LEU:HA	1:A:320:PRO:HD3	1.78	0.41
1:B:181:GLN:O	1:B:239:PRO:HB2	2.20	0.41
1:D:280:SER:C	1:D:282:TYR:N	2.75	0.40
1:B:291:GLN:HG2	1:B:321:VAL:HG22	2.04	0.40
1:A:146:LEU:HD12	1:A:157:ASN:HB2	2.02	0.40
1:D:242:MET:N	1:D:269:SER:O	2.53	0.40
1:D:175:VAL:HG12	1:D:210:ILE:CD1	2.46	0.40
1:D:62:LEU:HB2	1:D:120:SER:OG	2.21	0.40
1:D:229:THR:O	1:D:232:MET:HB3	2.21	0.40
1:A:218:GLY:HA3	1:A:249:MET:HE1	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:GLY:HA2	1:A:143:VAL:HG12	2.03	0.40
1:D:100:GLU:H	1:D:100:GLU:CD	2.25	0.40
1:D:335:GLN:HE21	1:D:335:GLN:HB2	1.73	0.40
1:D:144:PRO:HB2	1:D:307:LEU:HB3	2.03	0.40
1:C:345:SER:O	1:C:349:LEU:HD23	2.22	0.40
1:C:208:ASN:HD22	1:C:208:ASN:N	2.18	0.40
1:A:331:ALA:O	1:A:332:PRO:O	2.39	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	294/301 (98%)	258 (88%)	22 (8%)	14 (5%)	3	3
1	B	294/301 (98%)	259 (88%)	26 (9%)	9 (3%)	5	8
1	C	294/301 (98%)	253 (86%)	29 (10%)	12 (4%)	3	4
1	D	294/301 (98%)	255 (87%)	28 (10%)	11 (4%)	4	5
All	All	1176/1204 (98%)	1025 (87%)	105 (9%)	46 (4%)	4	5

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	104	VAL
1	A	274	ASP
1	A	313	VAL
1	A	314	LYS
1	A	332	PRO
1	B	274	ASP
1	C	141	THR
1	C	274	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	282	TYR
1	C	321	VAL
1	D	104	VAL
1	D	141	THR
1	D	274	ASP
1	D	277	GLU
1	A	119	VAL
1	A	141	THR
1	A	277	GLU
1	A	337	ALA
1	B	130	ASP
1	B	259	GLU
1	B	275	ASP
1	B	320	PRO
1	B	333	ASN
1	C	142	ASN
1	C	315	GLY
1	D	101	ARG
1	D	119	VAL
1	D	292	ASP
1	A	118	ARG
1	A	336	THR
1	B	321	VAL
1	C	70	SER
1	C	275	ASP
1	C	314	LYS
1	D	333	ASN
1	D	355	ARG
1	A	338	SER
1	C	277	GLU
1	C	332	PRO
1	D	281	CYS
1	A	101	ARG
1	A	239	PRO
1	B	62	LEU
1	C	118	ARG
1	B	315	GLY
1	D	257	ILE

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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	242/246 (98%)	221 (91%)	21 (9%)	13 24
1	B	242/246 (98%)	216 (89%)	26 (11%)	8 15
1	C	242/246 (98%)	220 (91%)	22 (9%)	12 22
1	D	242/246 (98%)	225 (93%)	17 (7%)	19 37
All	All	968/984 (98%)	882 (91%)	86 (9%)	12 23

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	PRO
1	A	104	VAL
1	A	112	HIS
1	A	180	GLN
1	A	181	GLN
1	A	192	VAL
1	A	198	LEU
1	A	205	LEU
1	A	238	VAL
1	A	273	TYR
1	A	311	GLN
1	A	316	ASN
1	A	317	GLN
1	A	321	VAL
1	A	323	LEU
1	A	329	THR
1	A	335	GLN
1	A	339	PRO
1	A	344	ASP
1	A	346	LEU
1	A	349	LEU
1	B	86	ARG
1	B	102	SER
1	B	104	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	118	ARG
1	B	119	VAL
1	B	125	ASN
1	B	137	GLU
1	B	152	ASP
1	B	160	ILE
1	B	198	LEU
1	B	208	ASN
1	B	238	VAL
1	B	282	TYR
1	B	283	ILE
1	B	287	THR
1	B	295	LEU
1	B	296	LEU
1	B	298	GLN
1	B	304	LEU
1	B	317	GLN
1	B	320	PRO
1	B	329	THR
1	B	330	LEU
1	B	345	SER
1	B	349	LEU
1	B	355	ARG
1	C	62	LEU
1	C	63	LEU
1	C	104	VAL
1	C	117	GLN
1	C	119	VAL
1	C	130	ASP
1	C	131	GLN
1	C	142	ASN
1	C	180	GLN
1	C	192	VAL
1	C	198	LEU
1	C	208	ASN
1	C	224	SER
1	C	280	SER
1	C	281	CYS
1	C	287	THR
1	C	295	LEU
1	C	305	LEU
1	C	316	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	320	PRO
1	C	323	LEU
1	C	334	THR
1	D	62	LEU
1	D	95	VAL
1	D	102	SER
1	D	104	VAL
1	D	112	HIS
1	D	118	ARG
1	D	158	SER
1	D	180	GLN
1	D	198	LEU
1	D	238	VAL
1	D	295	LEU
1	D	296	LEU
1	D	304	LEU
1	D	335	GLN
1	D	340	ARG
1	D	342	LEU
1	D	346	LEU

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

Mol	Chain	Res	Type
1	A	78	GLN
1	A	89	GLN
1	A	125	ASN
1	A	131	GLN
1	A	142	ASN
1	A	173	HIS
1	A	227	GLN
1	A	228	GLN
1	A	234	ASN
1	A	309	GLN
1	A	317	GLN
1	B	78	GLN
1	B	117	GLN
1	B	125	ASN
1	B	173	HIS
1	B	208	ASN
1	B	228	GLN
1	B	234	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	291	GLN
1	B	348	GLN
1	C	78	GLN
1	C	125	ASN
1	C	153	GLN
1	C	173	HIS
1	C	227	GLN
1	C	228	GLN
1	C	234	ASN
1	C	316	ASN
1	D	78	GLN
1	D	153	GLN
1	D	163	HIS
1	D	173	HIS
1	D	228	GLN
1	D	234	ASN
1	D	291	GLN
1	D	335	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 carbohydrates in this entry.

5.6 Ligand geometry

8 ligands 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	$\#\|Z\| > 2$
3	IPT	A	998	-	15,15,15	0.45	0	19,21,21	0.75	0
2	EMC	A	999	-	1,2,2	0.44	0	0,1,1	0.00	-
3	IPT	B	998	-	15,15,15	1.27	1 (6%)	19,21,21	0.52	0
2	EMC	B	999	-	1,2,2	0.75	0	0,1,1	0.00	-
3	IPT	C	998	-	15,15,15	1.11	1 (6%)	19,21,21	0.68	0
2	EMC	C	999	-	1,2,2	0.43	0	0,1,1	0.00	-
3	IPT	D	998	-	15,15,15	1.19	1 (6%)	19,21,21	0.92	1 (5%)
2	EMC	D	999	-	1,2,2	0.37	0	0,1,1	0.00	-

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
3	IPT	A	998	-	-	0/6/26/26	0/1/1/1
2	EMC	A	999	-	-	0/0/0/0	0/0/0/0
3	IPT	B	998	-	-	0/6/26/26	0/1/1/1
2	EMC	B	999	-	-	0/0/0/0	0/0/0/0
3	IPT	C	998	-	-	0/6/26/26	0/1/1/1
2	EMC	C	999	-	-	0/0/0/0	0/0/0/0
3	IPT	D	998	-	-	0/6/26/26	0/1/1/1
2	EMC	D	999	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	998	IPT	C1-S1	-4.22	1.73	1.80
3	B	998	IPT	C1-S1	-4.01	1.73	1.80
3	C	998	IPT	C1-S1	-3.98	1.73	1.80

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	998	IPT	C6-C5-C4	2.03	118.02	113.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	999	EMC	1	0
3	D	998	IPT	1	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

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.