Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:39 PM GMT

PDB ID	:	1LBH
Title	:	INTACT LACTOSE OPERON REPRESSOR WITH GRATUITOUS INDUCER IPTG
Authors	:	Lewis, M.; Chang, G.; Horton, N.C.; Kercher, M.A.; Pace, H.C.; Lu, P.
Deposited on	:	1996-02-17
Resolution	:	3.20 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 ⓘ symbol.

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

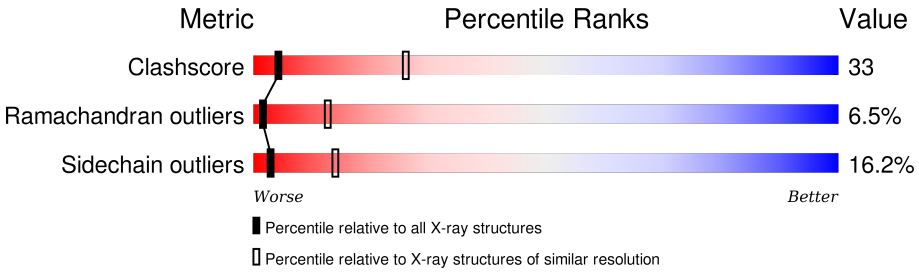
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 3.20 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	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)

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	360	38% 33% 11% • 18%
1	B	360	33% 40% 8% • 18%
1	C	360	36% 38% 8% • 18%
1	D	360	35% 35% 10% • 18%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8932 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.

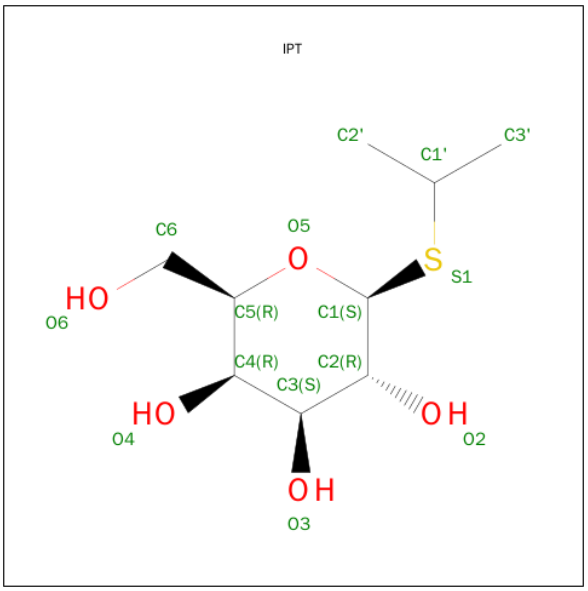
- Molecule 1 is a protein called INTACT LACTOSE OPERON REPRESSOR WITH GRATUITOUS INDUCER IPTG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2218	1383	396	428	11			
1	B	296	Total	C	N	O	S	0	0	0
			2218	1383	396	428	11			
1	C	296	Total	C	N	O	S	0	0	0
			2218	1383	396	428	11			
1	D	296	Total	C	N	O	S	0	0	0
			2218	1383	396	428	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	109	THR	ALA	CONFLICT	UNP P03023
A	286	LEU	SER	CONFLICT	UNP P03023
B	109	THR	ALA	CONFLICT	UNP P03023
B	286	LEU	SER	CONFLICT	UNP P03023
C	109	THR	ALA	CONFLICT	UNP P03023
C	286	LEU	SER	CONFLICT	UNP P03023
D	109	THR	ALA	CONFLICT	UNP P03023
D	286	LEU	SER	CONFLICT	UNP P03023

- Molecule 2 is ISOPROPYL-1-BETA-D-THIOGALACTOSIDE (three-letter code: IPT) (formula: $C_9H_{18}O_5S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O S 15 9 5 1	0	0
2	B	1	Total C O S 15 9 5 1	0	0
2	C	1	Total C O S 15 9 5 1	0	0
2	D	1	Total C O S 15 9 5 1	0	0

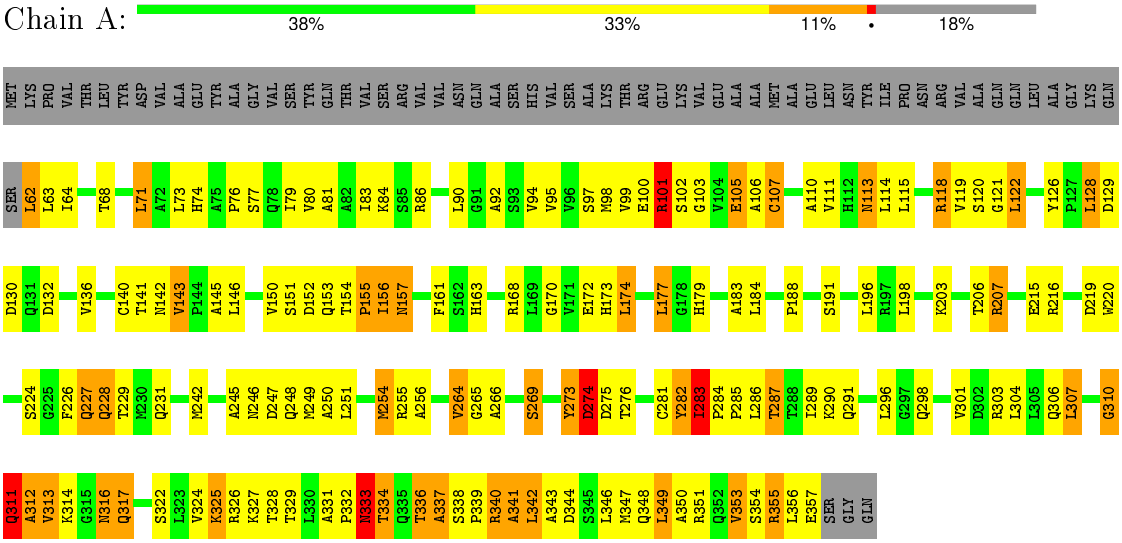
3 Residue-property plots (i)

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.

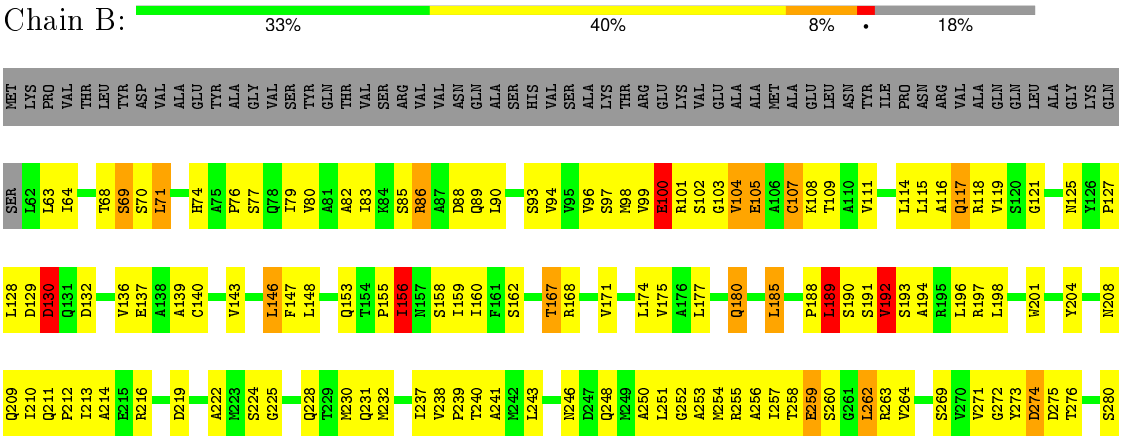
• Molecule 1: INTACT LACTOSE OPERON REPRESSOR WITH GRATUITOUS INDUCER IPTG

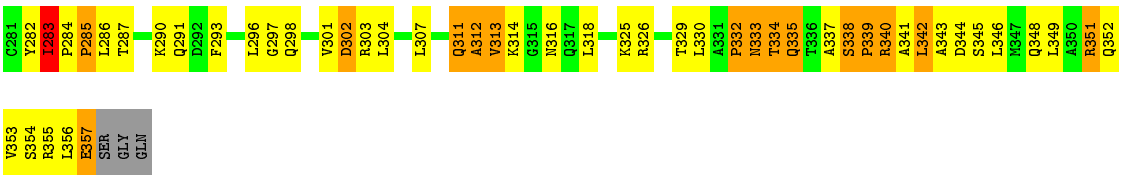
Chain A:



• Molecule 1: INTACT LACTOSE OPERON REPRESSOR WITH GRATUITOUS INDUCER IPTG

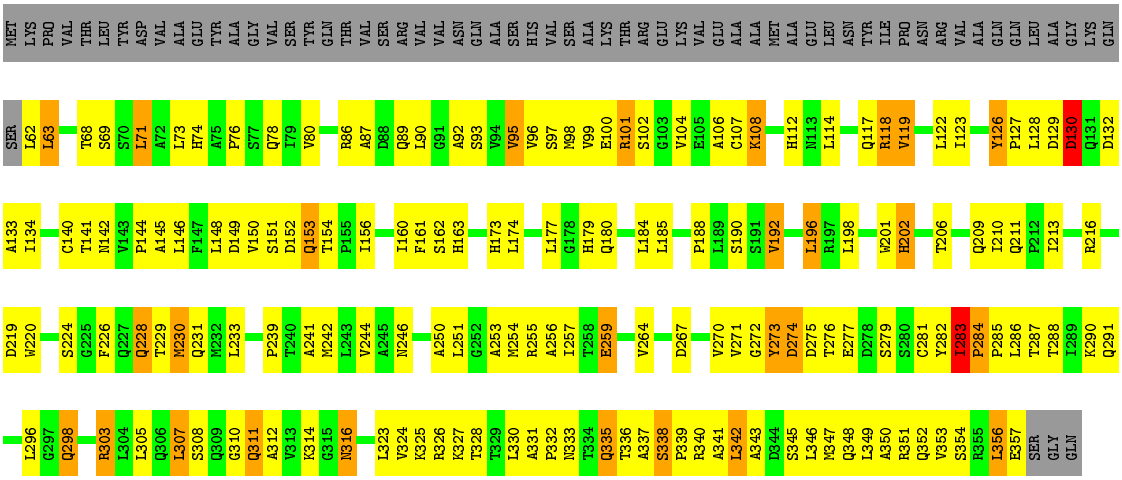
Chain B:





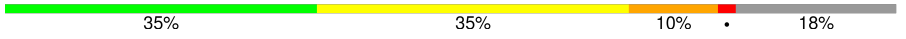
• Molecule 1: INTACT LACTOSE OPERON REPRESSOR WITH GRATUITOUS INDUCER IPTG

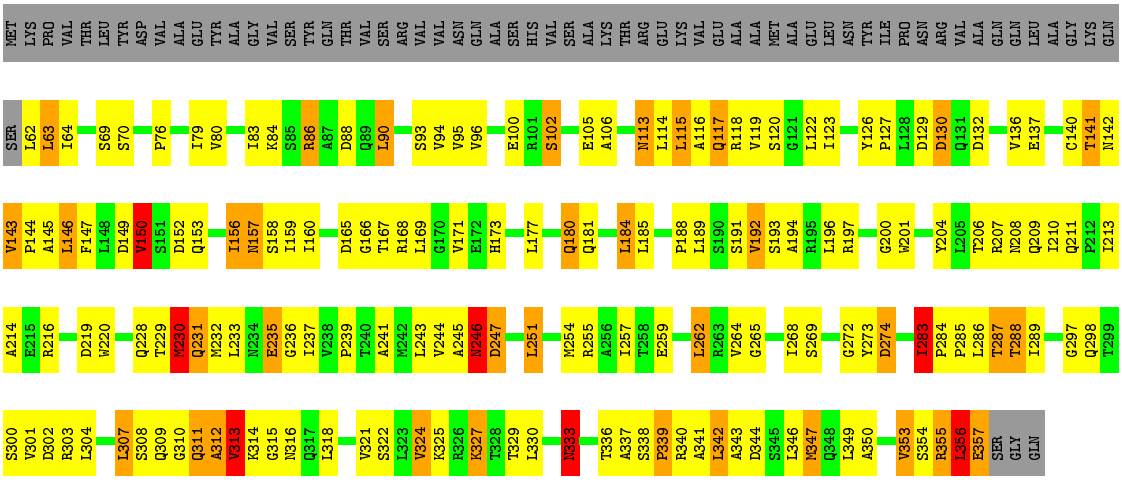
Chain C:



• Molecule 1: INTACT LACTOSE OPERON REPRESSOR WITH GRATUITOUS INDUCER IPTG

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 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	141.20Å 75.10Å 149.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.20	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.20)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.230 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8932	wwPDB-VP
Average B, all atoms (Å^2)	9.0	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: 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	0.72	1/2247 (0.0%)	0.92	4/3055 (0.1%)
1	B	0.72	1/2247 (0.0%)	0.94	1/3055 (0.0%)
1	C	0.73	0/2247	0.93	2/3055 (0.1%)
1	D	0.78	1/2247 (0.0%)	0.96	7/3055 (0.2%)
All	All	0.74	3/8988 (0.0%)	0.94	14/12220 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	230	MET	SD-CE	-9.74	1.23	1.77
1	A	281	CYS	CB-SG	-6.41	1.71	1.82
1	B	107	CYS	CB-SG	-5.40	1.73	1.81

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	283	ILE	C-N-CD	7.56	144.28	128.40
1	D	283	ILE	C-N-CD	6.49	142.04	128.40
1	D	236	GLY	N-CA-C	6.37	129.03	113.10
1	D	356	LEU	CA-CB-CG	6.25	129.67	115.30
1	D	287	THR	N-CA-C	-6.17	94.35	111.00
1	A	283	ILE	C-N-CD	5.98	140.96	128.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	283	ILE	C-N-CD	5.95	140.88	128.40
1	A	287	THR	N-CA-C	-5.46	96.25	111.00
1	D	184	LEU	CA-CB-CG	5.45	127.82	115.30
1	C	284	PRO	N-CA-C	-5.42	98.00	112.10
1	A	313	VAL	N-CA-C	-5.22	96.89	111.00
1	D	327	LYS	N-CA-C	5.19	125.00	111.00
1	D	333	ASN	N-CA-C	5.18	124.99	111.00
1	A	291	GLN	N-CA-C	-5.08	97.29	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	126	TYR	Sidechain

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	2218	0	2269	157	1
1	B	2218	0	2269	177	0
1	C	2218	0	2269	178	0
1	D	2218	0	2269	147	0
2	A	15	0	17	0	0
2	B	15	0	14	3	0
2	C	15	0	16	1	0
2	D	15	0	17	0	0
All	All	8932	0	9140	602	1

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 33.

All (602) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:ILE:HD11	1:B:239:PRO:HB3	1.23	1.17

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:ILE:HG22	1:D:284:PRO:HD3	1.23	1.17
1:A:283:ILE:HG12	1:B:283:ILE:HD12	1.29	1.09
1:C:144:PRO:HG2	1:C:308:SER:HA	1.50	0.93
1:D:283:ILE:HG22	1:D:284:PRO:CD	1.98	0.93
1:B:168:ARG:HG2	1:B:168:ARG:HH11	1.33	0.93
1:C:283:ILE:HG12	1:C:284:PRO:HD3	1.51	0.91
1:D:140:CYS:SG	1:D:145:ALA:HB2	2.09	0.91
1:C:62:LEU:HG	1:C:63:LEU:H	1.35	0.91
1:B:216:ARG:HB3	1:B:228:GLN:HE21	1.36	0.90
1:D:213:ILE:HD11	1:D:239:PRO:HB3	1.50	0.90
1:A:188:PRO:HG3	1:A:219:ASP:HA	1.54	0.90
1:D:86:ARG:HG3	1:D:298:GLN:HA	1.54	0.89
1:B:97:SER:HB2	1:B:114:LEU:HD21	1.53	0.89
1:A:62:LEU:HD21	1:A:64:ILE:HG13	1.54	0.87
1:B:283:ILE:HB	1:B:284:PRO:HD3	1.54	0.87
1:A:63:LEU:HG	1:A:119:VAL:HG23	1.58	0.84
1:B:168:ARG:HG3	1:B:204:TYR:CE1	2.12	0.84
1:A:283:ILE:HG22	1:A:284:PRO:HD3	1.60	0.84
1:C:188:PRO:HG3	1:C:219:ASP:HA	1.59	0.84
1:B:104:VAL:O	1:B:108:LYS:HG3	1.78	0.83
1:B:174:LEU:HD12	1:B:243:LEU:HD21	1.61	0.82
1:B:107:CYS:O	1:B:111:VAL:HG23	1.79	0.81
1:A:349:LEU:HD21	1:B:342:LEU:HB2	1.62	0.81
1:B:340:ARG:HB2	1:B:340:ARG:HH11	1.45	0.80
1:C:356:LEU:H	1:C:356:LEU:HD12	1.47	0.80
1:B:357:GLU:OE2	1:D:340:ARG:HA	1.82	0.79
1:C:213:ILE:HD11	1:C:239:PRO:HB3	1.64	0.79
1:C:130:ASP:O	1:C:134:ILE:HG12	1.83	0.79
1:C:348:GLN:HA	1:C:351:ARG:HD2	1.64	0.79
1:B:352:GLN:O	1:B:355:ARG:HB3	1.82	0.78
1:C:62:LEU:HG	1:C:63:LEU:N	1.96	0.78
1:A:226:PHE:HD1	1:A:256:ALA:HB2	1.50	0.77
1:C:283:ILE:CG1	1:C:284:PRO:HD3	2.16	0.76
1:A:343:ALA:CB	1:C:354:SER:HB3	2.15	0.76
1:A:343:ALA:HB1	1:C:350:ALA:O	1.85	0.76
1:C:154:THR:HG22	1:C:156:ILE:HG12	1.68	0.76
1:D:214:ALA:HB2	1:D:237:ILE:HD13	1.68	0.75
1:A:354:SER:HB3	1:C:343:ALA:CB	2.17	0.75
1:C:340:ARG:HD2	1:C:343:ALA:HB3	1.67	0.74
1:A:350:ALA:HA	1:C:346:LEU:HD12	1.69	0.74
1:A:266:ALA:O	1:A:333:ASN:HB3	1.87	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:THR:HG23	1:C:325:LYS:HA	1.68	0.74
1:D:353:VAL:O	1:D:356:LEU:HD13	1.87	0.73
1:B:86:ARG:HH11	1:B:86:ARG:HG2	1.52	0.73
1:B:168:ARG:NH1	1:B:168:ARG:HG2	2.03	0.73
1:D:86:ARG:CG	1:D:298:GLN:HA	2.18	0.73
1:A:354:SER:HB3	1:C:343:ALA:HB1	1.71	0.72
1:C:287:THR:HG22	1:C:323:LEU:HD11	1.71	0.72
1:A:283:ILE:HD13	1:B:283:ILE:HG23	1.70	0.72
1:A:68:THR:O	1:A:99:VAL:HG22	1.91	0.71
1:C:86:ARG:HH21	1:C:90:LEU:HD21	1.56	0.71
1:D:156:ILE:O	1:D:315:GLY:HA2	1.90	0.70
1:D:137:GLU:O	1:D:140:CYS:HB3	1.91	0.70
1:B:354:SER:OG	1:D:343:ALA:HB3	1.89	0.70
1:B:349:LEU:H	1:B:349:LEU:HD12	1.57	0.70
1:D:255:ARG:O	1:D:259:GLU:HG3	1.92	0.70
1:B:339:PRO:HD2	1:B:341:ALA:HB2	1.73	0.70
1:B:349:LEU:O	1:B:353:VAL:HG23	1.91	0.70
1:B:216:ARG:HB3	1:B:228:GLN:NE2	2.07	0.70
1:A:81:ALA:O	1:A:84:LYS:HB3	1.92	0.70
1:A:118:ARG:HH11	1:A:118:ARG:HB2	1.57	0.70
1:B:85:SER:O	1:B:88:ASP:HB2	1.92	0.69
1:C:101:ARG:HA	1:C:126:TYR:OH	1.92	0.69
1:D:152:ASP:HB3	1:D:160:ILE:HD11	1.74	0.69
1:C:76:PRO:O	1:C:80:VAL:HG23	1.93	0.69
1:C:206:THR:HG22	1:C:211:GLN:OE1	1.93	0.69
1:C:230:MET:SD	1:C:230:MET:C	2.71	0.69
1:B:283:ILE:HD13	1:B:283:ILE:H	1.57	0.68
1:D:336:THR:HG23	1:D:339:PRO:HG3	1.74	0.68
1:C:312:ALA:HB1	1:C:314:LYS:HE3	1.76	0.68
1:D:171:VAL:HG21	1:D:204:TYR:HB2	1.76	0.68
1:B:304:LEU:HA	1:B:307:LEU:HD12	1.74	0.68
1:B:86:ARG:HH12	1:B:302:ASP:CG	1.96	0.68
1:C:345:SER:HA	1:C:348:GLN:NE2	2.09	0.67
1:C:338:SER:N	1:C:339:PRO:HD2	2.08	0.67
1:D:235:GLU:HG2	1:D:235:GLU:O	1.95	0.67
1:C:185:LEU:HD23	1:C:244:VAL:HG13	1.76	0.67
1:C:283:ILE:CD1	1:C:284:PRO:HD3	2.24	0.66
1:B:283:ILE:HB	1:B:284:PRO:CD	2.25	0.66
1:A:285:PRO:HD2	1:A:327:LYS:HD2	1.77	0.66
1:C:148:LEU:CD1	1:C:296:LEU:HD11	2.26	0.66
1:A:273:TYR:O	1:A:274:ASP:HB2	1.96	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:ASP:HB3	1:B:290:LYS:HG3	1.77	0.66
1:D:213:ILE:HD11	1:D:239:PRO:CB	2.24	0.66
1:C:226:PHE:HD1	1:C:256:ALA:HB2	1.61	0.66
1:A:62:LEU:HD21	1:A:64:ILE:CG1	2.26	0.66
1:A:357:GLU:OE2	1:C:340:ARG:HA	1.96	0.65
1:D:325:LYS:NZ	1:D:325:LYS:HB2	2.11	0.65
1:D:353:VAL:O	1:D:355:ARG:N	2.30	0.65
1:C:345:SER:CB	1:D:349:LEU:HD21	2.27	0.65
1:C:273:TYR:O	1:C:274:ASP:HB2	1.96	0.64
1:D:297:GLY:O	1:D:300:SER:HB2	1.97	0.64
2:B:400:IPT:H3'2	2:B:400:IPT:O5	1.96	0.64
1:A:121:GLY:HA3	1:A:304:LEU:HD21	1.79	0.64
1:A:203:LYS:O	1:A:207:ARG:HG2	1.97	0.64
1:B:127:PRO:O	1:B:128:LEU:HD13	1.97	0.64
1:B:116:ALA:O	1:B:118:ARG:HG3	1.98	0.63
1:D:102:SER:HB2	1:D:106:ALA:HB2	1.80	0.63
1:C:290:LYS:HB2	1:C:324:VAL:HG23	1.79	0.63
1:C:114:LEU:O	1:C:119:VAL:HG22	1.98	0.63
1:A:163:HIS:CD2	1:A:163:HIS:H	2.16	0.63
1:A:283:ILE:CG1	1:B:283:ILE:HD12	2.19	0.63
1:B:189:LEU:HD21	1:B:198:LEU:HD22	1.79	0.63
1:A:226:PHE:CD1	1:A:256:ALA:HB2	2.32	0.63
1:B:168:ARG:HG3	1:B:204:TYR:CD1	2.33	0.63
1:B:188:PRO:O	1:B:190:SER:N	2.32	0.63
1:D:254:MET:CE	1:D:284:PRO:HD2	2.28	0.63
1:B:333:ASN:C	1:B:335:GLN:H	2.02	0.63
1:C:86:ARG:HG2	1:C:298:GLN:HA	1.81	0.62
1:D:216:ARG:HD3	1:D:232:MET:HB2	1.81	0.62
1:C:216:ARG:HB3	1:C:228:GLN:HG3	1.81	0.62
1:D:173:HIS:O	1:D:177:LEU:HB2	2.00	0.62
1:D:247:ASP:OD2	1:D:286:LEU:HD13	2.00	0.62
1:D:208:ASN:O	1:D:209:GLN:HB2	2.00	0.62
1:D:141:THR:HG22	1:D:142:ASN:H	1.65	0.62
1:C:69:SER:OG	2:C:400:IPT:H3'1	1.99	0.62
1:B:69:SER:HB2	1:B:76:PRO:HB3	1.82	0.61
1:B:185:LEU:HD11	1:B:225:GLY:HA2	1.82	0.61
1:A:353:VAL:O	1:A:356:LEU:HG	1.99	0.61
1:C:331:ALA:HB1	1:C:335:GLN:NE2	2.14	0.61
1:B:99:VAL:HG21	1:B:107:CYS:HA	1.81	0.61
1:B:64:ILE:HD13	1:B:301:VAL:HG13	1.83	0.61
1:C:331:ALA:HB3	1:C:339:PRO:HB3	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ALA:HB3	1:C:354:SER:HB3	1.82	0.61
1:A:113:ASN:HD22	1:A:113:ASN:N	1.97	0.61
1:B:357:GLU:HG2	1:D:340:ARG:N	2.16	0.61
1:A:350:ALA:CB	1:C:347:MET:HG3	2.31	0.60
1:A:346:LEU:HD22	1:D:346:LEU:HD22	1.80	0.60
1:A:118:ARG:HH11	1:A:118:ARG:CB	2.14	0.60
1:C:210:ILE:HG22	1:C:211:GLN:N	2.17	0.60
1:B:108:LYS:O	1:B:111:VAL:HB	2.01	0.60
1:C:250:ALA:O	1:C:254:MET:HG3	2.00	0.60
1:D:350:ALA:O	1:D:353:VAL:HB	2.01	0.60
1:C:285:PRO:CB	1:C:326:ARG:HD3	2.31	0.60
1:A:349:LEU:HD11	1:B:345:SER:HB2	1.84	0.60
1:C:345:SER:HB3	1:D:349:LEU:HD21	1.82	0.60
1:B:339:PRO:O	1:D:357:GLU:HG2	2.02	0.60
1:C:310:GLY:O	1:C:312:ALA:N	2.34	0.60
1:C:312:ALA:HB1	1:C:314:LYS:CE	2.31	0.60
1:B:222:ALA:O	1:B:252:GLY:HA3	2.02	0.60
1:B:283:ILE:HD13	1:B:283:ILE:N	2.15	0.59
1:B:316:ASN:HD21	1:B:318:LEU:HD21	1.65	0.59
1:C:352:GLN:O	1:D:338:SER:HB3	2.03	0.59
1:D:349:LEU:O	1:D:353:VAL:HG23	2.02	0.59
1:D:168:ARG:HG2	1:D:168:ARG:HH11	1.67	0.59
1:A:219:ASP:O	1:A:220:TRP:HB2	2.03	0.59
1:A:342:LEU:HD11	1:B:352:GLN:HB3	1.83	0.59
1:B:338:SER:OG	1:B:341:ALA:HB3	2.02	0.59
1:B:175:VAL:HG22	1:B:210:ILE:HD12	1.84	0.59
1:A:64:ILE:HG12	1:A:304:LEU:HD23	1.84	0.59
1:A:141:THR:O	1:A:143:VAL:HG22	2.03	0.59
1:B:86:ARG:HH11	1:B:86:ARG:CG	2.16	0.59
1:D:283:ILE:CG2	1:D:284:PRO:HD3	2.16	0.58
1:B:167:THR:HG22	1:B:201:TRP:CD1	2.38	0.58
1:D:237:ILE:HG22	1:D:239:PRO:HD3	1.84	0.58
1:A:99:VAL:HG21	1:A:126:TYR:CD1	2.37	0.58
1:D:141:THR:HG22	1:D:142:ASN:N	2.18	0.58
1:A:101:ARG:HA	1:A:126:TYR:OH	2.03	0.58
1:A:86:ARG:HG2	1:A:298:GLN:HA	1.84	0.58
1:C:148:LEU:HD12	1:C:296:LEU:HD11	1.85	0.58
1:C:273:TYR:HE1	1:C:291:GLN:OE1	1.86	0.58
1:B:254:MET:CE	1:B:284:PRO:HD2	2.34	0.58
1:C:86:ARG:NH2	1:C:90:LEU:HD21	2.19	0.58
1:D:167:THR:O	1:D:171:VAL:HG23	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ASP:OD1	1:B:224:SER:HB2	2.04	0.57
1:C:202:HIS:O	1:C:206:THR:HG23	2.03	0.57
1:A:285:PRO:HD2	1:A:327:LYS:HB2	1.87	0.57
1:A:350:ALA:HB3	1:C:347:MET:HG3	1.86	0.57
1:C:184:LEU:HD13	1:C:201:TRP:HE3	1.69	0.57
1:C:342:LEU:HD13	1:D:353:VAL:HA	1.87	0.57
1:B:285:PRO:O	1:B:326:ARG:HB3	2.05	0.57
1:A:216:ARG:HB3	1:A:228:GLN:HG3	1.86	0.57
1:C:140:CYS:SG	1:C:145:ALA:HB2	2.44	0.57
1:B:351:ARG:HG3	1:B:351:ARG:HH11	1.69	0.57
1:A:245:ALA:HB3	1:A:249:MET:CE	2.35	0.57
1:D:90:LEU:N	1:D:90:LEU:HD13	2.19	0.57
1:C:188:PRO:CG	1:C:219:ASP:HA	2.32	0.57
1:D:288:THR:HG23	1:D:324:VAL:HG22	1.85	0.57
1:B:174:LEU:CD1	1:B:243:LEU:HD21	2.34	0.56
1:B:132:ASP:O	1:B:136:VAL:HG23	2.05	0.56
1:A:247:ASP:O	1:A:250:ALA:HB3	2.05	0.56
1:C:219:ASP:O	1:C:220:TRP:HB2	2.04	0.56
1:D:312:ALA:HB1	1:D:314:LYS:HG2	1.87	0.56
1:D:356:LEU:HD22	1:D:357:GLU:OE1	2.05	0.56
1:D:63:LEU:HD23	1:D:93:SER:O	2.05	0.56
1:B:121:GLY:HA3	1:B:304:LEU:HD11	1.88	0.56
1:D:239:PRO:O	1:D:268:ILE:HD12	2.06	0.55
1:D:289:ILE:HG23	1:D:321:VAL:HG13	1.87	0.55
1:A:86:ARG:HB3	1:A:301:VAL:HG21	1.88	0.55
1:B:148:LEU:HD22	1:B:296:LEU:HD11	1.88	0.55
1:A:188:PRO:CG	1:A:219:ASP:HA	2.34	0.55
1:D:283:ILE:O	1:D:285:PRO:HD3	2.06	0.55
1:B:342:LEU:HD12	1:B:343:ALA:N	2.21	0.55
1:A:177:LEU:O	1:A:332:PRO:HD3	2.07	0.55
1:A:73:LEU:O	1:A:248:GLN:NE2	2.39	0.55
1:A:151:SER:OG	1:A:153:GLN:NE2	2.40	0.55
1:B:241:ALA:HA	1:B:269:SER:O	2.07	0.55
1:C:345:SER:O	1:C:348:GLN:NE2	2.40	0.55
1:A:343:ALA:O	1:C:350:ALA:HB1	2.06	0.55
1:C:174:LEU:HD13	1:C:241:ALA:HB1	1.89	0.55
1:B:246:ASN:HA	1:B:273:TYR:O	2.06	0.54
1:C:177:LEU:O	1:C:332:PRO:HD3	2.08	0.54
1:A:283:ILE:CG2	1:A:284:PRO:HD3	2.36	0.54
1:C:283:ILE:O	1:C:285:PRO:HD3	2.07	0.54
1:C:286:LEU:O	1:C:326:ARG:HD2	2.08	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:GLU:O	1:A:102:SER:N	2.41	0.54
1:A:341:ALA:O	1:A:344:ASP:N	2.40	0.54
1:D:339:PRO:O	1:D:342:LEU:HG	2.08	0.54
1:A:340:ARG:HA	1:C:357:GLU:HG3	1.89	0.54
1:A:285:PRO:HB3	1:A:326:ARG:HD3	1.90	0.54
1:D:313:VAL:O	1:D:313:VAL:HG13	2.08	0.54
1:A:283:ILE:O	1:A:284:PRO:C	2.45	0.54
1:C:68:THR:O	1:C:99:VAL:HB	2.07	0.54
1:D:129:ASP:O	1:D:132:ASP:N	2.41	0.53
1:C:71:LEU:HD23	1:C:98:MET:SD	2.48	0.53
1:C:342:LEU:HD22	1:D:349:LEU:HD12	1.90	0.53
1:C:285:PRO:HB2	1:C:326:ARG:HD3	1.89	0.53
1:D:144:PRO:HG3	1:D:308:SER:HA	1.91	0.53
1:B:287:THR:HG23	1:B:325:LYS:HA	1.89	0.53
1:A:163:HIS:ND1	1:A:196:LEU:HD22	2.23	0.53
1:C:71:LEU:HB2	1:C:98:MET:SD	2.49	0.53
1:C:126:TYR:CD1	1:C:127:PRO:HD2	2.43	0.53
1:C:337:ALA:C	1:C:339:PRO:HD2	2.27	0.53
1:B:293:PHE:HA	1:B:296:LEU:HB3	1.90	0.53
1:B:282:TYR:O	1:B:283:ILE:O	2.27	0.53
1:B:329:THR:O	1:B:330:LEU:HD12	2.08	0.53
1:B:171:VAL:HG11	1:B:204:TYR:C	2.28	0.53
1:C:331:ALA:HB3	1:C:339:PRO:HG3	1.91	0.53
1:A:355:ARG:NH2	1:B:334:THR:HG22	2.24	0.53
1:C:107:CYS:O	1:C:108:LYS:HB2	2.09	0.53
1:B:147:PHE:CD1	1:B:156:ILE:HG13	2.43	0.53
1:C:144:PRO:HB3	1:C:307:LEU:HD22	1.91	0.53
1:A:339:PRO:O	1:A:341:ALA:N	2.42	0.52
1:B:257:ILE:O	1:B:262:LEU:HB2	2.09	0.52
1:D:232:MET:HG2	1:D:237:ILE:HD12	1.91	0.52
1:C:340:ARG:O	1:C:342:LEU:N	2.42	0.52
1:B:339:PRO:HD2	1:B:341:ALA:CB	2.39	0.52
1:D:115:LEU:CD1	1:D:122:LEU:HD11	2.39	0.52
1:B:192:VAL:O	1:B:196:LEU:HG	2.09	0.52
1:C:356:LEU:HD23	1:D:338:SER:O	2.09	0.52
1:B:351:ARG:HA	1:B:351:ARG:NH1	2.25	0.52
1:A:86:ARG:HH12	1:A:90:LEU:HD21	1.75	0.52
1:C:286:LEU:H	1:C:286:LEU:HD23	1.75	0.52
1:B:283:ILE:O	1:B:285:PRO:HD3	2.10	0.52
1:C:345:SER:HB2	1:D:349:LEU:HD21	1.91	0.51
1:B:303:ARG:HH21	1:B:313:VAL:HB	1.74	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ARG:NH2	2:B:400:IPT:O4	2.41	0.51
1:D:168:ARG:HG3	1:D:204:TYR:CE2	2.45	0.51
1:D:219:ASP:O	1:D:220:TRP:HB2	2.10	0.51
1:A:343:ALA:HB2	1:C:353:VAL:C	2.30	0.51
1:B:167:THR:HG21	1:B:197:ARG:O	2.10	0.51
1:A:310:GLY:O	1:A:312:ALA:N	2.43	0.51
1:D:157:ASN:ND2	1:D:157:ASN:H	2.09	0.51
1:A:284:PRO:O	1:A:328:THR:HG23	2.09	0.51
1:D:140:CYS:O	1:D:143:VAL:HG23	2.10	0.51
1:D:301:VAL:O	1:D:304:LEU:HB3	2.10	0.51
1:D:216:ARG:HB3	1:D:228:GLN:HE21	1.76	0.51
1:B:64:ILE:CD1	1:B:301:VAL:HG13	2.40	0.51
1:B:254:MET:HE2	1:B:284:PRO:HD2	1.91	0.51
1:D:246:ASN:HA	1:D:273:TYR:O	2.11	0.51
1:A:183:ALA:HB3	1:A:242:MET:HG2	1.93	0.51
1:A:285:PRO:CB	1:A:326:ARG:HD3	2.41	0.51
1:C:154:THR:CG2	1:C:156:ILE:HG12	2.39	0.51
1:B:177:LEU:O	1:B:332:PRO:HD3	2.11	0.51
1:B:159:ILE:O	1:B:160:ILE:HD13	2.11	0.51
1:C:117:GLN:OE1	1:D:117:GLN:HB3	2.10	0.51
1:D:122:LEU:HD12	1:D:140:CYS:SG	2.51	0.50
1:D:272:GLY:H	1:D:286:LEU:HD22	1.76	0.50
1:A:76:PRO:O	1:A:80:VAL:HG23	2.10	0.50
1:A:303:ARG:O	1:A:307:LEU:HD23	2.10	0.50
1:D:201:TRP:CD1	1:D:243:LEU:HD13	2.45	0.50
1:C:144:PRO:HG2	1:C:308:SER:CA	2.31	0.50
1:A:64:ILE:HB	1:A:94:VAL:HG22	1.93	0.50
1:D:344:ASP:O	1:D:347:MET:HB2	2.12	0.50
1:D:229:THR:O	1:D:233:LEU:HB2	2.11	0.50
1:D:216:ARG:NH2	1:D:231:GLN:HE21	2.09	0.50
1:C:255:ARG:O	1:C:259:GLU:HB2	2.12	0.50
1:A:71:LEU:HD23	1:A:98:MET:HG2	1.94	0.50
1:A:255:ARG:NH1	1:B:280:SER:O	2.45	0.50
1:B:271:VAL:HG22	1:B:329:THR:CG2	2.41	0.50
1:D:273:TYR:O	1:D:274:ASP:HB2	2.12	0.50
1:D:149:ASP:O	1:D:150:VAL:HG13	2.11	0.50
1:A:86:ARG:NH1	1:A:90:LEU:HD21	2.27	0.49
1:B:100:GLU:CD	1:B:100:GLU:H	2.14	0.49
1:B:283:ILE:H	1:B:283:ILE:CD1	2.23	0.49
1:B:297:GLY:O	1:B:301:VAL:HG23	2.12	0.49
1:B:146:LEU:HD22	1:B:147:PHE:N	2.28	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:329:THR:O	1:D:330:LEU:HD23	2.11	0.49
1:A:282:TYR:O	1:A:283:ILE:O	2.30	0.49
1:B:272:GLY:O	1:B:273:TYR:HB2	2.11	0.49
1:C:279:SER:HB3	1:C:286:LEU:HD21	1.93	0.49
1:D:168:ARG:HG3	1:D:204:TYR:CD2	2.47	0.49
1:A:71:LEU:HD23	1:A:98:MET:CG	2.41	0.49
1:A:163:HIS:CE1	1:A:196:LEU:HD22	2.47	0.49
1:A:168:ARG:O	1:A:172:GLU:HG3	2.13	0.49
1:D:230:MET:HG2	1:D:231:GLN:N	2.28	0.49
1:A:347:MET:HG2	1:C:350:ALA:CB	2.42	0.49
1:C:338:SER:O	1:C:339:PRO:C	2.51	0.49
1:B:222:ALA:HA	1:B:248:GLN:O	2.13	0.49
1:D:303:ARG:O	1:D:307:LEU:HD23	2.13	0.49
1:D:338:SER:HA	1:D:342:LEU:HD11	1.94	0.49
1:C:133:ALA:HB1	1:C:156:ILE:HD13	1.94	0.49
1:D:200:GLY:O	1:D:204:TYR:HD1	1.96	0.48
1:A:273:TYR:O	1:A:274:ASP:CB	2.61	0.48
1:C:119:VAL:HG21	1:C:122:LEU:HD21	1.94	0.48
1:A:316:ASN:OD1	1:A:317:GLN:N	2.46	0.48
1:A:336:THR:HG23	1:A:337:ALA:N	2.28	0.48
1:C:338:SER:N	1:C:339:PRO:CD	2.75	0.48
1:C:273:TYR:O	1:C:274:ASP:CB	2.61	0.48
1:A:161:PHE:HE2	1:A:296:LEU:HD22	1.78	0.48
1:B:282:TYR:O	1:B:283:ILE:C	2.52	0.48
1:D:257:ILE:O	1:D:262:LEU:HB2	2.14	0.48
1:C:342:LEU:CD1	1:D:356:LEU:HD11	2.44	0.48
1:C:173:HIS:ND1	1:C:323:LEU:HD21	2.28	0.48
1:A:99:VAL:CG2	1:A:126:TYR:CD1	2.96	0.48
1:A:73:LEU:HB2	1:A:76:PRO:HG3	1.94	0.48
1:A:303:ARG:HG2	1:A:307:LEU:HD23	1.95	0.48
1:D:289:ILE:HG23	1:D:321:VAL:CG1	2.43	0.48
1:B:271:VAL:HA	1:B:287:THR:O	2.14	0.48
1:C:148:LEU:HD11	1:C:296:LEU:HD11	1.95	0.48
1:C:198:LEU:HD13	1:C:198:LEU:O	2.14	0.48
1:D:146:LEU:HD11	1:D:159:ILE:HG13	1.95	0.48
1:D:122:LEU:CD1	1:D:140:CYS:SG	3.02	0.48
1:B:160:ILE:HB	1:B:318:LEU:CD1	2.44	0.48
1:A:62:LEU:HD23	1:A:92:ALA:HB1	1.96	0.48
1:C:219:ASP:OD1	1:C:224:SER:HB3	2.14	0.48
1:A:62:LEU:HG	1:A:63:LEU:N	2.29	0.48
1:C:345:SER:HA	1:C:348:GLN:HE21	1.79	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:LEU:HD23	1:C:90:LEU:N	2.28	0.47
1:B:180:GLN:O	1:B:210:ILE:HG23	2.14	0.47
1:D:273:TYR:O	1:D:274:ASP:CB	2.62	0.47
1:B:103:GLY:O	1:B:105:GLU:N	2.47	0.47
1:C:342:LEU:O	1:C:346:LEU:HG	2.14	0.47
1:A:341:ALA:O	1:A:343:ALA:N	2.47	0.47
1:D:95:VAL:O	1:D:95:VAL:HG13	2.14	0.47
1:D:157:ASN:HB3	1:D:303:ARG:NH2	2.29	0.47
1:A:224:SER:O	1:A:228:GLN:HB2	2.13	0.47
1:D:83:ILE:HD12	1:D:123:ILE:HD12	1.96	0.47
1:A:107:CYS:O	1:A:111:VAL:HG23	2.15	0.47
1:C:129:ASP:H	1:C:132:ASP:HB2	1.79	0.47
1:B:167:THR:O	1:B:171:VAL:HG23	2.15	0.47
1:C:86:ARG:HA	1:C:86:ARG:HD2	1.57	0.47
1:A:265:GLY:HA2	1:A:328:THR:O	2.14	0.47
1:A:346:LEU:HB2	1:C:350:ALA:HB2	1.97	0.47
1:B:301:VAL:O	1:B:304:LEU:HB3	2.14	0.47
1:C:174:LEU:HD13	1:C:241:ALA:CB	2.44	0.47
1:B:211:GLN:HG3	1:B:212:PRO:HD2	1.95	0.47
1:C:283:ILE:CD1	1:D:283:ILE:HG13	2.45	0.47
1:C:283:ILE:HD13	1:C:284:PRO:CD	2.45	0.47
1:D:349:LEU:HA	1:D:349:LEU:HD12	1.69	0.47
1:B:333:ASN:C	1:B:335:GLN:N	2.68	0.47
1:B:114:LEU:O	1:B:119:VAL:HG13	2.15	0.47
1:A:287:THR:HG23	1:A:325:LYS:HA	1.95	0.47
1:C:342:LEU:N	1:C:342:LEU:HD23	2.30	0.47
1:C:185:LEU:HD23	1:C:244:VAL:CG1	2.44	0.47
1:C:100:GLU:C	1:C:102:SER:H	2.18	0.47
1:D:216:ARG:HE	1:D:228:GLN:NE2	2.13	0.46
1:D:245:ALA:O	1:D:246:ASN:CB	2.63	0.46
1:D:113:ASN:O	1:D:116:ALA:HB3	2.15	0.46
1:A:122:LEU:O	1:A:145:ALA:HA	2.14	0.46
1:A:156:ILE:HG12	1:A:156:ILE:H	1.56	0.46
1:A:350:ALA:CB	1:C:346:LEU:HB2	2.45	0.46
1:C:126:TYR:O	1:C:149:ASP:HB3	2.15	0.46
1:A:157:ASN:N	1:A:157:ASN:OD1	2.48	0.46
1:C:303:ARG:HD2	1:C:307:LEU:HD12	1.98	0.46
1:C:342:LEU:H	1:C:342:LEU:CD2	2.28	0.46
1:A:332:PRO:O	1:A:334:THR:N	2.48	0.46
1:D:283:ILE:O	1:D:285:PRO:CD	2.63	0.46
1:C:342:LEU:H	1:C:342:LEU:HD23	1.78	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:ALA:HB3	1:C:339:PRO:CB	2.45	0.46
1:C:96:VAL:HB	1:D:96:VAL:HB	1.97	0.46
1:D:287:THR:HG23	1:D:325:LYS:HA	1.96	0.46
1:D:76:PRO:O	1:D:80:VAL:HG23	2.15	0.46
1:C:192:VAL:O	1:C:196:LEU:N	2.45	0.46
1:C:347:MET:O	1:C:350:ALA:HB3	2.16	0.46
1:B:191:SER:O	1:B:194:ALA:N	2.49	0.46
1:D:168:ARG:HG2	1:D:168:ARG:NH1	2.31	0.46
1:A:71:LEU:O	1:A:77:SER:OG	2.31	0.46
1:D:241:ALA:HA	1:D:269:SER:O	2.16	0.46
1:A:342:LEU:HD23	1:B:349:LEU:HD23	1.97	0.46
1:A:354:SER:HB3	1:C:343:ALA:HB2	1.97	0.46
1:D:180:GLN:O	1:D:210:ILE:HG21	2.16	0.46
1:C:286:LEU:HA	1:C:328:THR:OG1	2.16	0.46
1:A:332:PRO:C	1:A:334:THR:H	2.18	0.46
1:D:79:ILE:O	1:D:83:ILE:HG12	2.15	0.46
1:C:87:ALA:HB1	1:C:92:ALA:O	2.16	0.46
1:D:115:LEU:HD11	1:D:122:LEU:HD11	1.98	0.45
1:C:106:ALA:O	1:C:108:LYS:N	2.49	0.45
1:C:117:GLN:O	1:C:118:ARG:HB2	2.15	0.45
1:D:185:LEU:HD23	1:D:244:VAL:HG13	1.98	0.45
1:C:219:ASP:O	1:C:220:TRP:CB	2.64	0.45
1:B:86:ARG:HB3	1:B:301:VAL:HG21	1.98	0.45
1:C:209:GLN:N	1:C:209:GLN:OE1	2.50	0.45
1:B:63:LEU:HD12	1:B:93:SER:HB3	1.99	0.45
1:C:340:ARG:O	1:C:342:LEU:HG	2.16	0.45
1:B:116:ALA:C	1:B:118:ARG:H	2.18	0.45
1:D:356:LEU:HD13	1:D:356:LEU:H	1.81	0.45
1:A:73:LEU:O	1:A:74:HIS:HB2	2.16	0.45
1:C:177:LEU:HD22	1:C:330:LEU:C	2.36	0.45
1:D:283:ILE:HD13	1:D:283:ILE:HA	1.61	0.45
1:A:273:TYR:HA	1:A:289:ILE:HB	1.98	0.45
1:D:325:LYS:CB	1:D:325:LYS:NZ	2.79	0.45
1:B:79:ILE:HD12	1:B:125:ASN:HD21	1.82	0.45
1:D:192:VAL:O	1:D:196:LEU:HG	2.17	0.45
1:A:283:ILE:O	1:A:285:PRO:N	2.50	0.45
1:D:338:SER:N	1:D:339:PRO:HD3	2.31	0.45
1:A:338:SER:N	1:A:339:PRO:CD	2.79	0.45
1:A:350:ALA:HB2	1:C:346:LEU:CB	2.46	0.45
1:C:90:LEU:HD12	1:C:305:LEU:HD11	1.98	0.45
1:B:283:ILE:O	1:B:285:PRO:N	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:LEU:O	1:B:352:GLN:HB2	2.16	0.45
1:B:86:ARG:NH1	1:B:86:ARG:CG	2.77	0.45
1:B:136:VAL:O	1:B:139:ALA:HB3	2.17	0.45
1:B:232:MET:HG2	1:B:237:ILE:HB	1.97	0.45
1:B:283:ILE:O	1:B:285:PRO:CD	2.65	0.45
2:B:400:IPT:C3'	2:B:400:IPT:O5	2.64	0.45
1:A:188:PRO:HD2	1:A:220:TRP:CE2	2.52	0.45
1:B:96:VAL:CG1	1:B:97:SER:N	2.80	0.45
1:C:336:THR:C	1:C:338:SER:H	2.19	0.45
1:A:163:HIS:H	1:A:163:HIS:HD2	1.64	0.45
1:C:184:LEU:HD13	1:C:201:TRP:CE3	2.50	0.45
1:C:100:GLU:O	1:C:102:SER:N	2.50	0.45
1:B:216:ARG:HE	1:B:228:GLN:NE2	2.15	0.44
1:B:313:VAL:O	1:B:314:LYS:HB2	2.17	0.44
1:A:342:LEU:HD21	1:B:349:LEU:HB3	1.99	0.44
1:D:102:SER:CB	1:D:106:ALA:HB2	2.45	0.44
1:D:243:LEU:HA	1:D:243:LEU:HD23	1.73	0.44
1:A:77:SER:HB3	1:B:71:LEU:O	2.17	0.44
1:B:115:LEU:HD11	1:B:140:CYS:HA	1.99	0.44
1:C:287:THR:HA	1:C:324:VAL:O	2.18	0.44
1:B:70:SER:HA	1:B:98:MET:HE1	1.98	0.44
1:C:282:TYR:O	1:C:283:ILE:C	2.56	0.44
1:B:283:ILE:N	1:B:283:ILE:CD1	2.81	0.44
1:B:216:ARG:HH21	1:B:231:GLN:HE21	1.66	0.44
1:A:63:LEU:O	1:A:120:SER:N	2.50	0.44
1:B:332:PRO:O	1:B:333:ASN:C	2.56	0.44
1:C:71:LEU:H	1:C:98:MET:HE1	1.82	0.44
1:A:336:THR:CG2	1:A:337:ALA:N	2.80	0.44
1:C:152:ASP:HB2	1:C:316:ASN:ND2	2.33	0.44
1:C:163:HIS:H	1:C:163:HIS:CD2	2.35	0.44
1:D:191:SER:O	1:D:194:ALA:N	2.50	0.44
1:B:198:LEU:HA	1:B:201:TRP:CE3	2.53	0.44
1:A:343:ALA:CB	1:C:354:SER:CB	2.92	0.44
1:C:331:ALA:HB3	1:C:339:PRO:CG	2.47	0.44
1:B:351:ARG:HA	1:B:351:ARG:CZ	2.48	0.44
1:B:240:THR:HG22	1:B:334:THR:HG23	2.00	0.44
1:B:346:LEU:HD11	1:C:346:LEU:HD11	2.00	0.44
1:B:346:LEU:HA	1:B:349:LEU:HD13	1.99	0.44
1:A:118:ARG:NH1	1:A:118:ARG:CB	2.80	0.44
1:C:210:ILE:CG2	1:C:211:GLN:N	2.80	0.44
1:C:148:LEU:O	1:C:160:ILE:HG22	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ARG:HE	1:A:298:GLN:HB2	1.83	0.44
1:B:129:ASP:O	1:B:130:ASP:C	2.56	0.44
1:B:271:VAL:HG22	1:B:329:THR:HG21	1.98	0.44
1:B:140:CYS:HB3	1:B:143:VAL:CG2	2.48	0.44
1:B:284:PRO:O	1:B:286:LEU:N	2.51	0.44
1:B:198:LEU:O	1:B:201:TRP:HB2	2.18	0.44
1:D:298:GLN:HG2	1:D:302:ASP:OD2	2.18	0.44
1:C:174:LEU:HD21	1:C:271:VAL:CG2	2.48	0.44
1:A:184:LEU:O	1:A:215:GLU:HA	2.17	0.44
1:A:152:ASP:OD1	1:A:152:ASP:N	2.51	0.44
1:B:211:GLN:OE1	1:B:211:GLN:HA	2.17	0.44
1:D:257:ILE:HG21	1:D:268:ILE:HB	1.99	0.43
1:A:339:PRO:HA	1:C:357:GLU:OE1	2.17	0.43
1:A:129:ASP:HB2	1:A:132:ASP:OD2	2.18	0.43
1:A:303:ARG:HG3	1:A:313:VAL:HG11	2.00	0.43
1:A:170:GLY:O	1:A:174:LEU:HD23	2.18	0.43
1:A:177:LEU:HD22	1:A:331:ALA:N	2.33	0.43
1:B:284:PRO:O	1:B:285:PRO:C	2.54	0.43
1:A:113:ASN:ND2	1:A:113:ASN:N	2.65	0.43
1:B:180:GLN:HA	1:B:210:ILE:HD13	2.01	0.43
1:A:105:GLU:O	1:A:106:ALA:C	2.57	0.43
1:D:213:ILE:CD1	1:D:239:PRO:HB3	2.35	0.43
1:A:340:ARG:N	1:C:357:GLU:CD	2.71	0.43
1:C:123:ILE:HG23	1:C:148:LEU:HD23	2.01	0.43
1:A:246:ASN:HA	1:A:273:TYR:O	2.18	0.43
1:D:208:ASN:O	1:D:209:GLN:CB	2.66	0.43
1:B:191:SER:O	1:B:194:ALA:HB3	2.19	0.43
1:A:254:MET:HG3	1:A:264:VAL:HG21	2.00	0.43
1:C:73:LEU:HA	1:C:73:LEU:HD23	1.74	0.43
1:B:148:LEU:HD13	1:B:296:LEU:HD21	1.99	0.43
1:D:64:ILE:CD1	1:D:301:VAL:HG13	2.48	0.43
1:B:89:GLN:H	1:B:89:GLN:HG2	1.59	0.43
1:A:283:ILE:CD1	1:B:283:ILE:HG23	2.42	0.43
1:B:171:VAL:HG21	1:B:204:TYR:HB2	2.00	0.43
1:B:253:ALA:O	1:B:256:ALA:HB3	2.18	0.43
1:B:258:THR:C	1:B:260:SER:N	2.72	0.43
1:A:102:SER:OG	1:A:103:GLY:N	2.51	0.43
1:A:146:LEU:HD21	1:A:303:ARG:HD3	2.00	0.43
1:B:74:HIS:ND1	1:B:74:HIS:N	2.67	0.43
1:A:311:GLN:O	1:A:313:VAL:HG23	2.19	0.43
1:A:275:ASP:HB3	1:A:290:LYS:HG3	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:GLN:O	1:A:231:GLN:HG3	2.19	0.43
1:C:283:ILE:CD1	1:C:284:PRO:CD	2.95	0.43
1:C:336:THR:C	1:C:338:SER:N	2.71	0.43
1:C:331:ALA:CB	1:C:339:PRO:HB3	2.48	0.43
1:C:246:ASN:HA	1:C:273:TYR:O	2.19	0.43
1:B:116:ALA:C	1:B:118:ARG:N	2.72	0.43
1:C:95:VAL:HG22	1:D:95:VAL:CG2	2.48	0.43
1:C:188:PRO:HD2	1:C:220:TRP:CE2	2.54	0.42
1:D:341:ALA:O	1:D:344:ASP:N	2.52	0.42
1:A:351:ARG:HG2	1:B:262:LEU:HD13	2.01	0.42
1:A:269:SER:HB3	1:A:329:THR:HA	2.01	0.42
1:D:286:LEU:O	1:D:288:THR:HG22	2.19	0.42
1:D:188:PRO:HD3	1:D:219:ASP:HA	2.01	0.42
1:B:258:THR:C	1:B:260:SER:H	2.21	0.42
1:C:352:GLN:NE2	1:D:337:ALA:O	2.53	0.42
1:B:263:ARG:NH2	1:B:335:GLN:HG3	2.33	0.42
1:C:216:ARG:HB3	1:C:228:GLN:CG	2.48	0.42
1:D:288:THR:OG1	1:D:289:ILE:N	2.51	0.42
1:A:355:ARG:NH2	1:B:262:LEU:HD11	2.34	0.42
1:D:116:ALA:HB3	1:D:117:GLN:OE1	2.19	0.42
1:D:147:PHE:HB2	1:D:158:SER:HB3	2.01	0.42
1:D:356:LEU:HD22	1:D:357:GLU:CD	2.40	0.42
1:D:126:TYR:HA	1:D:127:PRO:HD3	1.90	0.42
1:A:79:ILE:O	1:A:83:ILE:HG13	2.19	0.42
1:D:86:ARG:NH1	1:D:302:ASP:OD2	2.52	0.42
1:D:116:ALA:C	1:D:118:ARG:H	2.23	0.42
1:D:210:ILE:HG22	1:D:211:GLN:N	2.34	0.42
1:C:179:HIS:O	1:C:180:GLN:HG3	2.20	0.42
1:C:161:PHE:HE2	1:C:296:LEU:HD22	1.85	0.42
1:B:273:TYR:O	1:B:274:ASP:CB	2.68	0.42
1:B:250:ALA:HA	1:B:253:ALA:HB3	2.01	0.42
1:D:165:ASP:O	1:D:169:LEU:HG	2.19	0.42
1:B:117:GLN:OE1	1:B:117:GLN:N	2.53	0.42
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.83	0.42
1:C:283:ILE:N	1:C:283:ILE:HD13	2.35	0.42
1:B:180:GLN:HA	1:B:210:ILE:CD1	2.50	0.42
1:B:79:ILE:O	1:B:83:ILE:HG12	2.19	0.42
1:C:63:LEU:HA	1:C:93:SER:O	2.20	0.42
1:A:179:HIS:ND1	1:A:332:PRO:HG3	2.34	0.42
1:A:336:THR:HG23	1:A:337:ALA:O	2.20	0.42
1:C:356:LEU:HD12	1:C:356:LEU:N	2.23	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:MET:HG2	1:C:350:ALA:HB1	2.01	0.42
1:A:68:THR:HG22	1:A:97:SER:O	2.19	0.42
1:D:321:VAL:CG1	1:D:322:SER:N	2.83	0.42
1:D:201:TRP:NE1	1:D:243:LEU:HD13	2.35	0.42
1:C:326:ARG:HB3	1:C:327:LYS:H	1.69	0.42
1:D:181:GLN:HB3	1:D:213:ILE:HG21	2.01	0.42
1:A:338:SER:CB	1:A:342:LEU:HD12	2.50	0.42
1:D:325:LYS:HZ2	1:D:325:LYS:HB2	1.81	0.42
1:C:281:CYS:O	1:D:251:LEU:HD22	2.20	0.42
1:B:77:SER:HA	1:B:80:VAL:HG22	2.02	0.42
1:B:129:ASP:O	1:B:132:ASP:N	2.53	0.41
1:B:137:GLU:OE1	1:B:156:ILE:HG22	2.19	0.41
1:A:132:ASP:O	1:A:136:VAL:HG23	2.19	0.41
1:C:272:GLY:H	1:C:288:THR:HA	1.84	0.41
1:B:188:PRO:C	1:B:190:SER:H	2.23	0.41
1:B:351:ARG:NH2	1:D:347:MET:SD	2.88	0.41
1:A:154:THR:HA	1:A:155:PRO:HD2	1.70	0.41
1:C:285:PRO:HB3	1:C:326:ARG:HD3	2.01	0.41
1:A:342:LEU:HD11	1:B:352:GLN:CB	2.50	0.41
1:A:250:ALA:HB3	1:A:286:LEU:HD11	2.03	0.41
1:C:108:LYS:O	1:C:112:HIS:ND1	2.53	0.41
1:B:79:ILE:O	1:B:82:ALA:HB3	2.19	0.41
1:B:70:SER:HA	1:B:98:MET:CE	2.50	0.41
1:C:229:THR:O	1:C:233:LEU:HG	2.20	0.41
1:A:355:ARG:HH22	1:B:262:LEU:HD11	1.84	0.41
1:D:84:LYS:HD3	1:D:94:VAL:HB	2.02	0.41
1:C:90:LEU:HD12	1:C:305:LEU:CD1	2.51	0.41
1:B:127:PRO:C	1:B:128:LEU:HD22	2.40	0.41
1:A:173:HIS:CD2	1:A:329:THR:HG21	2.56	0.41
1:B:255:ARG:O	1:B:259:GLU:HG2	2.19	0.41
1:C:275:ASP:HB3	1:C:290:LYS:HG2	2.03	0.41
1:D:220:TRP:HZ3	1:D:245:ALA:O	2.03	0.41
1:D:70:SER:O	1:D:76:PRO:HG3	2.21	0.41
1:A:115:LEU:CD1	1:A:140:CYS:HA	2.50	0.41
1:C:146:LEU:HA	1:C:146:LEU:HD12	1.81	0.41
1:D:283:ILE:HD12	1:D:283:ILE:HG23	1.81	0.41
1:D:265:GLY:N	1:D:268:ILE:O	2.51	0.41
1:A:349:LEU:HD11	1:B:345:SER:CB	2.50	0.41
1:B:147:PHE:O	1:B:158:SER:HA	2.21	0.41
1:C:242:MET:O	1:C:270:VAL:HA	2.21	0.41
1:B:216:ARG:NH2	1:B:231:GLN:HE21	2.18	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:THR:O	1:B:99:VAL:HG12	2.21	0.41
1:A:250:ALA:CB	1:A:286:LEU:HD11	2.51	0.41
1:B:211:GLN:CG	1:B:212:PRO:HD2	2.51	0.41
1:C:153:GLN:HB2	1:C:153:GLN:HE21	1.71	0.41
1:A:62:LEU:CD2	1:A:64:ILE:HG13	2.38	0.41
1:A:126:TYR:O	1:A:128:LEU:HD22	2.21	0.41
1:B:311:GLN:HB3	1:B:312:ALA:H	1.50	0.41
1:D:283:ILE:O	1:D:285:PRO:N	2.54	0.41
1:A:97:SER:HB3	1:A:110:ALA:HB1	2.03	0.41
1:C:226:PHE:CD1	1:C:256:ALA:HB2	2.48	0.41
1:B:168:ARG:NH1	1:B:168:ARG:CG	2.75	0.40
1:C:345:SER:O	1:C:346:LEU:C	2.59	0.40
1:D:166:GLY:HA3	1:D:273:TYR:OH	2.21	0.40
1:B:338:SER:HG	1:B:341:ALA:HB3	1.84	0.40
1:B:64:ILE:HB	1:B:94:VAL:HG22	2.03	0.40
1:C:253:ALA:O	1:C:257:ILE:HG13	2.21	0.40
1:B:174:LEU:HA	1:B:174:LEU:HD23	1.87	0.40
1:B:86:ARG:CZ	1:B:90:LEU:HD11	2.50	0.40
1:C:73:LEU:O	1:C:76:PRO:HD2	2.20	0.40
1:A:286:LEU:HD23	1:A:286:LEU:HA	1.85	0.40
1:D:193:SER:O	1:D:197:ARG:HB2	2.21	0.40
1:C:290:LYS:HB2	1:C:324:VAL:CG2	2.48	0.40
1:B:214:ALA:HB2	1:B:237:ILE:HG21	2.02	0.40
1:B:283:ILE:CB	1:B:284:PRO:CD	2.96	0.40
1:B:274:ASP:HA	1:B:291:GLN:HG3	2.03	0.40
1:A:312:ALA:HA	1:A:314:LYS:HG3	2.04	0.40
1:D:114:LEU:O	1:D:119:VAL:HG13	2.22	0.40

All (1) 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:A:334:THR:O	1:A:334:THR:O[2_555]	2.19	0.01

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	294/360 (82%)	237 (81%)	41 (14%)	16 (5%)	2 19
1	B	294/360 (82%)	231 (79%)	41 (14%)	22 (8%)	1 9
1	C	294/360 (82%)	244 (83%)	33 (11%)	17 (6%)	2 17
1	D	294/360 (82%)	242 (82%)	31 (10%)	21 (7%)	1 10
All	All	1176/1440 (82%)	954 (81%)	146 (12%)	76 (6%)	1 13

All (76) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	ARG
1	A	142	ASN
1	A	274	ASP
1	A	283	ILE
1	A	312	ALA
1	A	337	ALA
1	A	340	ARG
1	A	342	LEU
1	B	100	GLU
1	B	102	SER
1	B	156	ILE
1	B	189	LEU
1	B	283	ILE
1	B	338	SER
1	C	108	LYS
1	C	311	GLN
1	D	274	ASP
1	D	283	ILE
1	D	339	PRO
1	D	354	SER
1	A	333	ASN
1	B	162	SER
1	B	274	ASP
1	B	312	ALA
1	B	333	ASN
1	B	335	GLN
1	B	339	PRO
1	C	118	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	142	ASN
1	C	162	SER
1	C	274	ASP
1	D	141	THR
1	D	189	LEU
1	D	246	ASN
1	D	312	ALA
1	D	316	ASN
1	A	282	TYR
1	A	310	GLY
1	B	69	SER
1	B	104	VAL
1	B	130	ASP
1	B	311	GLN
1	B	332	PRO
1	C	63	LEU
1	C	341	ALA
1	C	342	LEU
1	D	130	ASP
1	D	311	GLN
1	D	342	LEU
1	A	273	TYR
1	A	311	GLN
1	A	341	ALA
1	B	285	PRO
1	B	337	ALA
1	C	74	HIS
1	C	101	ARG
1	C	307	LEU
1	D	69	SER
1	D	100	GLU
1	D	117	GLN
1	D	231	GLN
1	D	310	GLY
1	D	313	VAL
1	D	333	ASN
1	A	155	PRO
1	B	302	ASP
1	B	313	VAL
1	C	130	ASP
1	C	277	GLU
1	D	353	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	150	VAL
1	C	267	ASP
1	D	150	VAL
1	C	150	VAL
1	C	338	SER
1	B	192	VAL

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	243/295 (82%)	199 (82%)	44 (18%)	2	11
1	B	243/295 (82%)	206 (85%)	37 (15%)	3	17
1	C	243/295 (82%)	210 (86%)	33 (14%)	5	22
1	D	243/295 (82%)	200 (82%)	43 (18%)	2	11
All	All	972/1180 (82%)	815 (84%)	157 (16%)	3	14

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	LEU
1	A	71	LEU
1	A	95	VAL
1	A	101	ARG
1	A	105	GLU
1	A	107	CYS
1	A	113	ASN
1	A	118	ARG
1	A	122	LEU
1	A	128	LEU
1	A	130	ASP
1	A	143	VAL
1	A	156	ILE
1	A	157	ASN
1	A	174	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	177	LEU
1	A	191	SER
1	A	198	LEU
1	A	206	THR
1	A	207	ARG
1	A	227	GLN
1	A	228	GLN
1	A	229	THR
1	A	251	LEU
1	A	254	MET
1	A	264	VAL
1	A	269	SER
1	A	274	ASP
1	A	276	THR
1	A	306	GLN
1	A	307	LEU
1	A	311	GLN
1	A	316	ASN
1	A	317	GLN
1	A	322	SER
1	A	324	VAL
1	A	325	LYS
1	A	333	ASN
1	A	334	THR
1	A	336	THR
1	A	348	GLN
1	A	349	LEU
1	A	353	VAL
1	A	355	ARG
1	B	71	LEU
1	B	86	ARG
1	B	100	GLU
1	B	101	ARG
1	B	105	GLU
1	B	109	THR
1	B	117	GLN
1	B	130	ASP
1	B	146	LEU
1	B	153	GLN
1	B	155	PRO
1	B	156	ILE
1	B	167	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	180	GLN
1	B	185	LEU
1	B	189	LEU
1	B	192	VAL
1	B	193	SER
1	B	208	ASN
1	B	209	GLN
1	B	230	MET
1	B	238	VAL
1	B	251	LEU
1	B	259	GLU
1	B	262	LEU
1	B	264	VAL
1	B	276	THR
1	B	283	ILE
1	B	298	GLN
1	B	334	THR
1	B	340	ARG
1	B	342	LEU
1	B	344	ASP
1	B	348	GLN
1	B	351	ARG
1	B	356	LEU
1	B	357	GLU
1	C	71	LEU
1	C	78	GLN
1	C	89	GLN
1	C	95	VAL
1	C	97	SER
1	C	104	VAL
1	C	119	VAL
1	C	128	LEU
1	C	130	ASP
1	C	141	THR
1	C	151	SER
1	C	153	GLN
1	C	190	SER
1	C	192	VAL
1	C	196	LEU
1	C	202	HIS
1	C	228	GLN
1	C	230	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	231	GLN
1	C	251	LEU
1	C	259	GLU
1	C	264	VAL
1	C	273	TYR
1	C	276	THR
1	C	283	ILE
1	C	298	GLN
1	C	303	ARG
1	C	311	GLN
1	C	316	ASN
1	C	333	ASN
1	C	335	GLN
1	C	349	LEU
1	C	356	LEU
1	D	62	LEU
1	D	63	LEU
1	D	86	ARG
1	D	88	ASP
1	D	90	LEU
1	D	102	SER
1	D	105	GLU
1	D	113	ASN
1	D	115	LEU
1	D	120	SER
1	D	130	ASP
1	D	136	VAL
1	D	143	VAL
1	D	146	LEU
1	D	150	VAL
1	D	153	GLN
1	D	156	ILE
1	D	157	ASN
1	D	180	GLN
1	D	184	LEU
1	D	192	VAL
1	D	206	THR
1	D	207	ARG
1	D	230	MET
1	D	235	GLU
1	D	246	ASN
1	D	247	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	251	LEU
1	D	262	LEU
1	D	264	VAL
1	D	288	THR
1	D	307	LEU
1	D	309	GLN
1	D	311	GLN
1	D	313	VAL
1	D	318	LEU
1	D	324	VAL
1	D	327	LYS
1	D	333	ASN
1	D	347	MET
1	D	355	ARG
1	D	356	LEU
1	D	357	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	153	GLN
1	A	163	HIS
1	A	209	GLN
1	A	231	GLN
1	A	309	GLN
1	B	125	ASN
1	B	202	HIS
1	B	227	GLN
1	B	228	GLN
1	B	231	GLN
1	B	306	GLN
1	B	316	ASN
1	C	153	GLN
1	C	163	HIS
1	C	234	ASN
1	C	335	GLN
1	C	348	GLN
1	D	153	GLN
1	D	202	HIS
1	D	211	GLN
1	D	227	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	228	GLN
1	D	231	GLN
1	D	306	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

4 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	$\#\|Z\| > 2$
2	IPT	A	400	-	15,15,15	6.16	9 (60%)	19,21,21	3.75	15 (78%)
2	IPT	B	400	-	15,15,15	6.85	7 (46%)	19,21,21	3.11	11 (57%)
2	IPT	C	400	-	15,15,15	6.49	8 (53%)	19,21,21	3.66	10 (52%)
2	IPT	D	400	-	15,15,15	6.82	6 (40%)	19,21,21	3.43	9 (47%)

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
2	IPT	A	400	-	-	0/6/26/26	0/1/1/1
2	IPT	B	400	-	-	0/6/26/26	0/1/1/1
2	IPT	C	400	-	-	0/6/26/26	0/1/1/1
2	IPT	D	400	-	-	0/6/26/26	0/1/1/1

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	IPT	C1-S1	-23.91	1.39	1.80
2	D	400	IPT	C1-S1	-23.08	1.40	1.80
2	C	400	IPT	C1-S1	-22.12	1.42	1.80
2	A	400	IPT	C1-S1	-20.17	1.45	1.80
2	A	400	IPT	C1'-S1	-7.80	1.46	1.83
2	D	400	IPT	C1'-S1	-7.45	1.48	1.83
2	B	400	IPT	C1'-S1	-7.33	1.49	1.83
2	C	400	IPT	C1'-S1	-7.04	1.50	1.83
2	A	400	IPT	C4-C5	-5.05	1.42	1.53
2	B	400	IPT	O4-C4	-4.34	1.32	1.43
2	B	400	IPT	O3-C3	-3.21	1.35	1.43
2	C	400	IPT	C4-C5	-3.03	1.46	1.53
2	A	400	IPT	C3-C2	-3.00	1.44	1.52
2	C	400	IPT	O3-C3	-2.53	1.36	1.43
2	C	400	IPT	C3-C2	-2.08	1.46	1.52
2	A	400	IPT	O3-C3	-2.04	1.38	1.43
2	A	400	IPT	C2'-C1'	2.08	1.61	1.51
2	A	400	IPT	C3'-C1'	2.09	1.61	1.51
2	D	400	IPT	C3'-C1'	2.16	1.62	1.51
2	B	400	IPT	C3'-C1'	2.39	1.63	1.51
2	A	400	IPT	C4-C3	2.55	1.59	1.52
2	D	400	IPT	C2'-C1'	3.07	1.66	1.51
2	C	400	IPT	C3'-C1'	3.15	1.67	1.51
2	B	400	IPT	C2'-C1'	3.65	1.69	1.51
2	C	400	IPT	C4-C3	4.36	1.63	1.52
2	B	400	IPT	O5-C1	4.87	1.50	1.42
2	C	400	IPT	O5-C1	5.95	1.52	1.42
2	D	400	IPT	O5-C1	6.14	1.52	1.42
2	A	400	IPT	O5-C1	6.45	1.53	1.42
2	D	400	IPT	C4-C3	6.66	1.69	1.52

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	400	IPT	O3-C3-C2	-8.00	92.32	110.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	400	IPT	O5-C5-C4	-7.19	96.18	109.68
2	A	400	IPT	O5-C5-C4	-5.97	98.48	109.68
2	B	400	IPT	O4-C4-C3	-5.06	98.95	110.34
2	D	400	IPT	C1-C2-C3	-4.81	100.04	110.69
2	D	400	IPT	O5-C5-C4	-4.69	100.87	109.68
2	B	400	IPT	O5-C5-C4	-4.36	101.49	109.68
2	C	400	IPT	C1-C2-C3	-4.07	101.67	110.69
2	B	400	IPT	C1-C2-C3	-3.87	102.13	110.69
2	D	400	IPT	O3-C3-C2	-3.81	101.77	110.34
2	A	400	IPT	C1-C2-C3	-3.47	102.99	110.69
2	C	400	IPT	O3-C3-C2	-3.47	102.53	110.34
2	C	400	IPT	O4-C4-C5	-3.15	100.88	109.24
2	B	400	IPT	O3-C3-C2	-2.98	103.64	110.34
2	D	400	IPT	O4-C4-C5	-2.73	102.00	109.24
2	C	400	IPT	C3'-C1'-C2'	-2.70	101.96	111.72
2	A	400	IPT	O4-C4-C5	-2.48	102.67	109.24
2	A	400	IPT	O2-C2-C3	-2.42	104.89	110.34
2	B	400	IPT	O4-C4-C5	-2.18	103.47	109.24
2	A	400	IPT	O4-C4-C3	-2.10	105.60	110.34
2	A	400	IPT	O6-C6-C5	2.18	118.55	111.33
2	B	400	IPT	C1-O5-C5	2.20	116.93	112.74
2	B	400	IPT	O5-C5-C6	2.35	112.29	106.36
2	C	400	IPT	O4-C4-C3	2.38	115.70	110.34
2	A	400	IPT	C3-C4-C5	2.49	114.53	110.20
2	D	400	IPT	O5-C1-S1	2.98	117.58	110.01
2	A	400	IPT	C4-C3-C2	3.08	116.54	110.79
2	C	400	IPT	O3-C3-C4	3.15	117.43	110.34
2	A	400	IPT	O5-C5-C6	3.16	114.34	106.36
2	A	400	IPT	O3-C3-C4	3.22	117.59	110.34
2	B	400	IPT	C3-C4-C5	3.31	115.97	110.20
2	B	400	IPT	O5-C1-S1	3.31	118.40	110.01
2	A	400	IPT	O2-C2-C1	3.67	117.57	110.43
2	A	400	IPT	C1-O5-C5	4.04	120.43	112.74
2	C	400	IPT	C4-C3-C2	4.68	119.53	110.79
2	D	400	IPT	C4-C3-C2	4.70	119.56	110.79
2	A	400	IPT	O5-C1-S1	4.72	121.97	110.01
2	B	400	IPT	C4-C3-C2	5.48	121.01	110.79
2	D	400	IPT	C3-C4-C5	5.92	120.51	110.20
2	B	400	IPT	O5-C1-C2	5.99	118.33	110.19
2	D	400	IPT	O5-C1-C2	6.25	118.68	110.19
2	A	400	IPT	O5-C1-C2	6.39	118.86	110.19
2	D	400	IPT	C1-O5-C5	6.42	124.97	112.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	400	IPT	C1-O5-C5	6.81	125.73	112.74
2	C	400	IPT	O5-C1-C2	7.69	120.64	110.19

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
2	B	400	IPT	3	0
2	C	400	IPT	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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.