



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 02:10 PM BST

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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

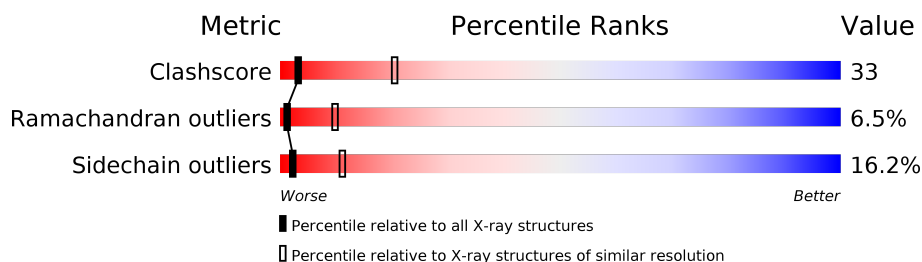
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	360	
1	B	360	
1	C	360	
1	D	360	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	IPT	A	400	-	X	-	-

2 Entry composition

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.

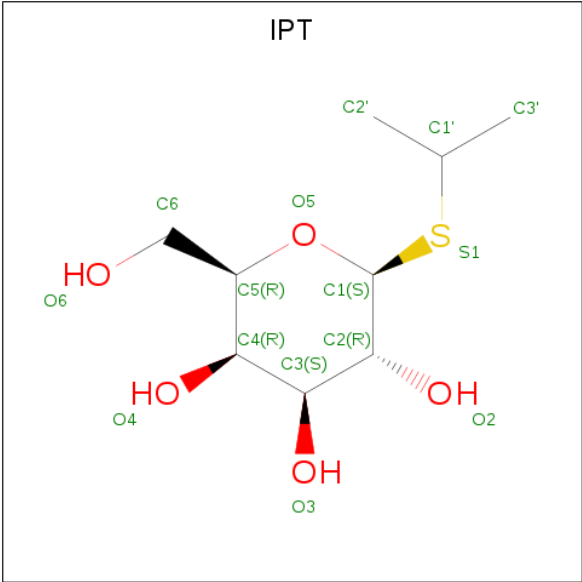
- Molecule 1 is a protein called INTACT LACTOSE OPERON REPRESSOR WITH GRATUITOUS INDUCER IPTG.

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 1-methylethyl 1-thio-beta-D-galactopyranoside (three-letter code: IPT) (formula: C₉H₁₈O₅S).



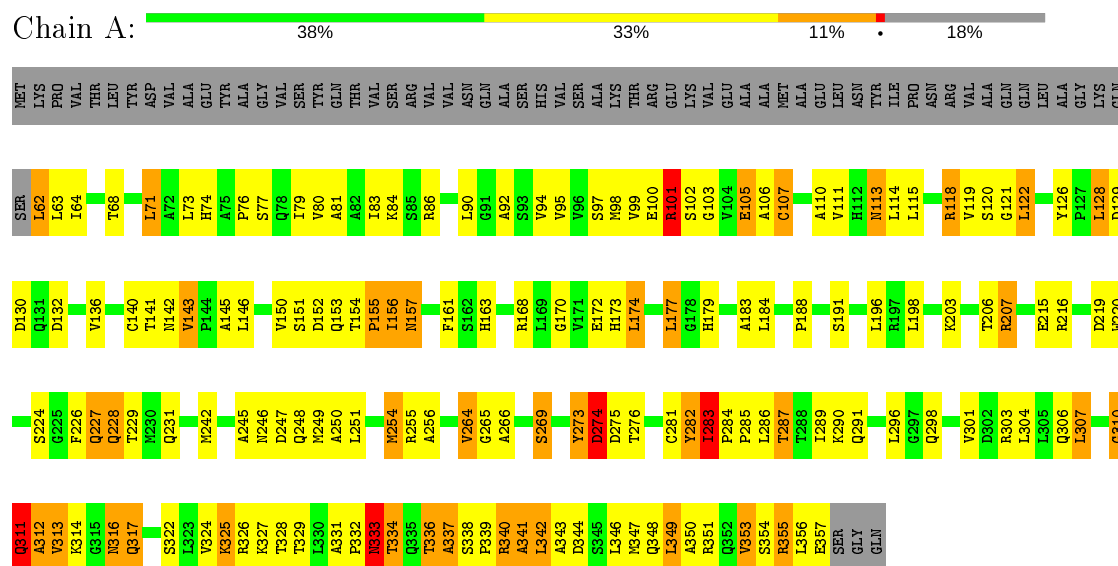
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			15	9	5	1		
2	B	1	Total	C	O	S	0	0
			15	9	5	1		
2	C	1	Total	C	O	S	0	0
			15	9	5	1		
2	D	1	Total	C	O	S	0	0
			15	9	5	1		

3 Residue-property plots

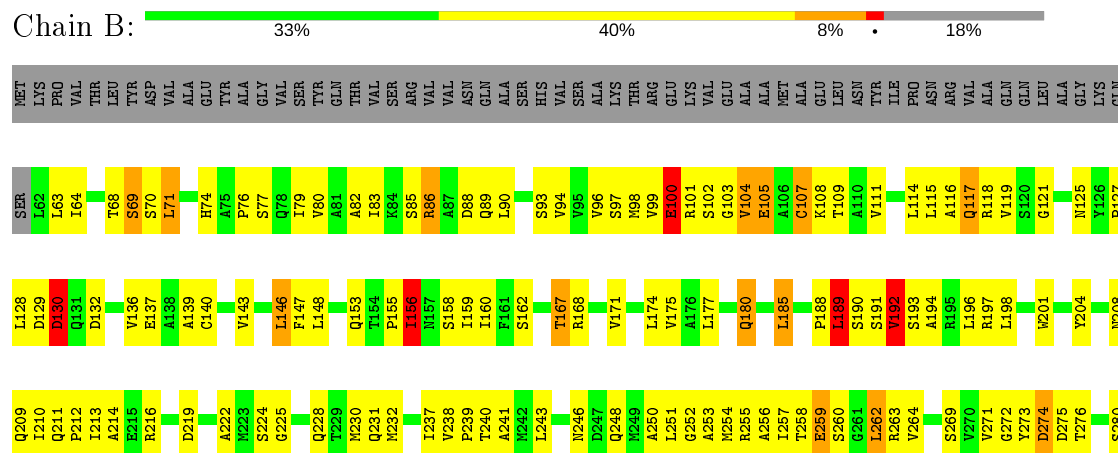
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



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



[illegible]

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

S300	A214	V143	SER	NET
V301	P144	A145	L62	PRO
D302	R216	P145	L63	LYS
R303		L146	I64	VAL
L304	D219	F147		THR
	W220	L148	S69	LEU
		D149	S70	TYR
S307	Q228	V150	P76	ASP
S308	R230	D152		VAL
Q309	Q231	Q153	I79	GLU
Q311	M232		V80	TYR
A312	L233	I156		ALA
V313	K314	M157	I83	GLY
S315	E235	S158	K84	VAL
G316	R236	I159	S85	SER
N316	G236	I160	R86	TYR
Q317	I237		A87	GLN
L318	V238	D165	D88	THR
	P239	G166	Q89	VAL
V321	T240	T167	L90	SER
S322	A241	R168		ARG
L323	M242	L169	S93	VAL
V324	L243	G170	V94	VAL
K325	V244	V171	V95	ASN
R326	A245	G172	V96	GLN
K327	M246	H173		ALA
T328	D247		E100	SER
T329		L177	F101	HIS
L330	L251	Q180	S102	VAL
R333	M254	Q181	E105	SER
T336	R255		A106	LYS
A337	A256	L184		THR
S338	T257	L185	M113	ARG
P339	E259		L114	GLU
R340		P188	L115	LYS
A341	L262	A189	A116	VAL
L342	R263	S190	Q117	GLU
V343	V264	S191	R118	ALA
D344	G265	V192	V119	ALA
S345		S193	S120	NET
L346	I268	A194	G121	ALA
M347	S269	R195	L122	GLU
Q348		L196	I123	LEU
L349	G272	R197		ASN
A350	Y273		Y126	TYR
	D274	G200	P127	ILE
V353		W201	L128	PRO
S354	I283		D129	ASN
R355	P284	Y204	D130	ARG
L356	P285	L205	Q131	VAL
E357	L286	T206	D132	ALA
SER	T287	R207		GLN
GLY	L288	N208	V136	LEU
GLN	T289	I210	E137	LEU
		I211		GLY
	G297	Q211	G140	ALA
	Q298	P212	T141	GLY
	E299	T213	V142	TYR

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α , β , γ	141.20 Å 75.10 Å 149.20 Å 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(°)	Ideal(°)
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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

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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:B:97:SER:HB2	1:B:114:LEU:HD21	1.53	0.89
1:D:86:ARG:HG3	1:D:298:GLN:HA	1.54	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:C:213:ILE:HD11	1:C:239:PRO:HB3	1.64	0.79
1:B:357:GLU:OE2	1:D:340:ARG:HA	1.82	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:A:350:ALA:HA	1:C:346:LEU:HD12	1.69	0.74
1:C:340:ARG:HD2	1:C:343:ALA:HB3	1.67	0.74
1:A:266:ALA:O	1:A:333:ASN:HB3	1.87	0.74

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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:B:86:ARG:HH11	1:B:86:ARG:HG2	1.52	0.73
1:D:353:VAL:O	1:D:356:LEU:HD13	1.87	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:A:118:ARG:HH11	1:A:118:ARG:HB2	1.57	0.70
1:A:81:ALA:O	1:A:84:LYS:HB3	1.92	0.70
1:B:216:ARG:HB3	1:B:228:GLN:NE2	2.07	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:C:76:PRO:O	1:C:80:VAL:HG23	1.93	0.69
1:D:152:ASP:HB3	1:D:160:ILE:HD11	1.74	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:B:283:ILE:HB	1:B:284:PRO:CD	2.25	0.66
1:C:283:ILE:CD1	1:C:284:PRO:HD3	2.24	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

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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:C:226:PHE:HD1	1:C:256:ALA:HB2	1.61	0.66
1:D:213:ILE:HD11	1:D:239:PRO:CB	2.24	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:203:LYS:O	1:A:207:ARG:HG2	1.97	0.64
1:A:121:GLY:HA3	1:A:304:LEU:HD21	1.79	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:A:163:HIS:CD2	1:A:163:HIS:H	2.16	0.63
1:C:114:LEU:O	1:C:119:VAL:HG22	1.98	0.63
1:C:290:LYS:HB2	1:C:324:VAL:HG23	1.79	0.63
1:A:226:PHE:CD1	1:A:256:ALA:HB2	2.32	0.63
1:B:189:LEU:HD21	1:B:198:LEU:HD22	1.79	0.63
1:A:283:ILE:CG1	1:B:283:ILE:HD12	2.19	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:B:333:ASN:C	1:B:335:GLN:H	2.02	0.63
1:D:254:MET:CE	1:D:284:PRO:HD2	2.28	0.63
1:C:86:ARG:HG2	1:C:298:GLN:HA	1.81	0.62
1:C:216:ARG:HB3	1:C:228:GLN:HG3	1.81	0.62
1:D:216:ARG:HD3	1:D:232:MET:HB2	1.81	0.62
1:D:173:HIS:O	1:D:177:LEU:HB2	2.00	0.62
1:D:208:ASN:O	1:D:209:GLN:HB2	2.00	0.62
1:D:247:ASP:OD2	1:D:286:LEU:HD13	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:A:353:VAL:O	1:A:356:LEU:HG	1.99	0.61
1:B:185:LEU:HD11	1:B:225:GLY:HA2	1.82	0.61
1:B:69:SER:HB2	1:B:76:PRO:HB3	1.82	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:ASN:HD22	1:A:113:ASN:N	1.97	0.61
1:A:343:ALA:HB3	1:C:354:SER:HB3	1.82	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:A:349:LEU:HD11	1:B:345:SER:HB2	1.84	0.60
1:C:285:PRO:CB	1:C:326:ARG:HD3	2.31	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: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: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:168:ARG:HG2	1:D:168:ARG:HH11	1.67	0.59
1:D:349:LEU:O	1:D:353:VAL:HG23	2.02	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:175:VAL:HG22	1:B:210:ILE:HD12	1.84	0.59
1:B:338:SER:OG	1:B:341:ALA:HB3	2.02	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:A:99:VAL:HG21	1:A:126:TYR:CD1	2.37	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:D:283:ILE:CG2	1:D:284:PRO:HD3	2.16	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

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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:A:216:ARG:HB3	1:A:228:GLN:HG3	1.86	0.57
1:A:245:ALA:HB3	1:A:249:MET:CE	2.35	0.57
1:B:285:PRO:O	1:B:326:ARG:HB3	2.05	0.57
1:B:351:ARG:HG3	1:B:351:ARG:HH11	1.69	0.57
1:C:140:CYS:SG	1:C:145:ALA:HB2	2.44	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:A:247:ASP:O	1:A:250:ALA:HB3	2.05	0.56
1:B:132:ASP:O	1:B:136:VAL:HG23	2.05	0.56
1:B:174:LEU:CD1	1:B:243:LEU:HD21	2.34	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:A:177:LEU:O	1:A:332:PRO:HD3	2.07	0.55
1:B:342:LEU:HD12	1:B:343:ALA:N	2.21	0.55
1:D:283:ILE:O	1:D:285:PRO:HD3	2.06	0.55
1:A:151:SER:OG	1:A:153:GLN:NE2	2.40	0.55
1:A:73:LEU:O	1:A:248:GLN:NE2	2.39	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:C:174:LEU:HD13	1:C:241:ALA:HB1	1.89	0.55
1:A:343:ALA:O	1:C:350:ALA:HB1	2.06	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:A:100:GLU:O	1:A:102:SER:N	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:286:LEU:O	1:C:326:ARG:HD2	2.08	0.54
1:A:341:ALA:O	1:A:344:ASP:N	2.40	0.54
1:A:340:ARG:HA	1:C:357:GLU:HG3	1.89	0.54
1:D:339:PRO:O	1:D:342:LEU:HG	2.08	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:B:287:THR:HG23	1:B:325:LYS:HA	1.89	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: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:B:293:PHE:HA	1:B:296:LEU:HB3	1.90	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: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:A:355:ARG:NH2	1:B:334:THR:HG22	2.24	0.53
1:C:331:ALA:HB3	1:C:339:PRO:HG3	1.91	0.53
1:B:147:PHE:CD1	1:B:156:ILE:HG13	2.43	0.53
1:C:107:CYS:O	1:C:108:LYS:HB2	2.09	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:C:340:ARG:O	1:C:342:LEU:N	2.42	0.52
1:D:232:MET:HG2	1:D:237:ILE:HD12	1.91	0.52
1:B:339:PRO:HD2	1:B:341:ALA:CB	2.39	0.52
1:B:192:VAL:O	1:B:196:LEU:HG	2.09	0.52
1:D:115:LEU:CD1	1:D:122:LEU:HD11	2.39	0.52
1:B:351:ARG:HA	1:B:351:ARG:NH1	2.25	0.52
1:C:356:LEU:HD23	1:D:338:SER:O	2.09	0.52
1:A:86:ARG:HH12	1:A:90:LEU:HD21	1.75	0.52
1:B:283:ILE:O	1:B:285:PRO:HD3	2.10	0.52
1:C:286:LEU:H	1:C:286:LEU:HD23	1.75	0.52
1:B:303:ARG:HH21	1:B:313:VAL:HB	1.74	0.51
1:C:345:SER:HB2	1:D:349:LEU:HD21	1.91	0.51

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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:A:310:GLY:O	1:A:312:ALA:N	2.43	0.51
1:B:167:THR:HG21	1:B:197:ARG:O	2.10	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:B:64:ILE:CD1	1:B:301:VAL:HG13	2.40	0.51
1:D:216:ARG:HB3	1:D:228:GLN:HE21	1.76	0.51
1:B:254:MET:HE2	1:B:284:PRO:HD2	1.91	0.51
1:A:183:ALA:HB3	1:A:242:MET:HG2	1.93	0.51
1:D:246:ASN:HA	1:D:273:TYR:O	2.11	0.51
1:A:285:PRO:CB	1:A:326:ARG:HD3	2.41	0.51
1:B:159:ILE:O	1:B:160:ILE:HD13	2.11	0.51
1:B:177:LEU:O	1:B:332:PRO:HD3	2.11	0.51
1:C:154:THR:CG2	1:C:156:ILE:HG12	2.39	0.51
1:C:117:GLN:OE1	1:D:117:GLN:HB3	2.10	0.51
1:A:303:ARG:O	1:A:307:LEU:HD23	2.10	0.50
1:A:76:PRO:O	1:A:80:VAL:HG23	2.10	0.50
1:D:122:LEU:HD12	1:D:140:CYS:SG	2.51	0.50
1:D:201:TRP:CD1	1:D:243:LEU:HD13	2.45	0.50
1:D:272:GLY:H	1:D:286:LEU:HD22	1.76	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:229:THR:O	1:D:233:LEU:HB2	2.11	0.50
1:D:344:ASP:O	1:D:347:MET:HB2	2.12	0.50
1:A:255:ARG:NH1	1:B:280:SER:O	2.45	0.50
1:A:71:LEU:HD23	1:A:98:MET:HG2	1.94	0.50
1:C:255:ARG:O	1:C:259:GLU:HB2	2.12	0.50
1:D:216:ARG:NH2	1:D:231:GLN:HE21	2.09	0.50
1:B:271:VAL:HG22	1:B:329:THR:CG2	2.41	0.50
1:D:149:ASP:O	1:D:150:VAL:HG13	2.11	0.50
1:D:273:TYR:O	1:D:274:ASP:HB2	2.12	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:146:LEU:HD22	1:B:147:PHE:N	2.28	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

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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:A:71:LEU:HD23	1:A:98:MET:CG	2.41	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: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:A:347:MET:HG2	1:C:350:ALA:CB	2.42	0.49
1:B:222:ALA:HA	1:B:248:GLN:O	2.13	0.49
1:C:338:SER:O	1:C:339:PRO:C	2.51	0.49
1:D:230:MET:HG2	1:D:231:GLN:N	2.28	0.49
1:D:303:ARG:O	1:D:307:LEU:HD23	2.13	0.49
1:C:133:ALA:HB1	1:C:156:ILE:HD13	1.94	0.49
1:D:338:SER:HA	1:D:342:LEU:HD11	1.94	0.49
1:A:273:TYR:O	1:A:274:ASP:CB	2.61	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:119:VAL:HG21	1:C:122:LEU:HD21	1.94	0.48
1:D:200:GLY:O	1:D:204:TYR:HD1	1.96	0.48
1:A:161:PHE:HE2	1:A:296:LEU:HD22	1.78	0.48
1:C:273:TYR:O	1:C:274:ASP:CB	2.61	0.48
1:C:338:SER:N	1:C:339:PRO:CD	2.75	0.48
1:B:282:TYR:O	1:B:283:ILE:C	2.52	0.48
1:A:99:VAL:CG2	1:A:126:TYR:CD1	2.96	0.48
1:A:303:ARG:HG2	1:A:307:LEU:HD23	1.95	0.48
1:A:73:LEU:HB2	1:A:76:PRO:HG3	1.94	0.48
1:C:173:HIS:ND1	1:C:323:LEU:HD21	2.28	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:B:271:VAL:HA	1:B:287:THR:O	2.14	0.48
1:D:289:ILE:HG23	1:D:321:VAL:CG1	2.43	0.48
1:C:198:LEU:HD13	1:C:198:LEU:O	2.14	0.48
1:C:148:LEU:HD11	1:C:296:LEU:HD11	1.95	0.48
1:D:146:LEU:HD11	1:D:159:ILE:HG13	1.95	0.48
1:B:160:ILE:HB	1:B:318:LEU:CD1	2.44	0.48
1:D:122:LEU:CD1	1:D:140:CYS:SG	3.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:GLY:O	1:B:105:GLU:N	2.47	0.47
1:B:180:GLN:O	1:B:210:ILE:HG23	2.14	0.47
1:C:90:LEU:HD23	1:C:90:LEU:N	2.28	0.47
1:D:273:TYR:O	1:D:274:ASP:CB	2.62	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:107:CYS:O	1:A:111:VAL:HG23	2.15	0.47
1:A:224:SER:O	1:A:228:GLN:HB2	2.13	0.47
1:C:129:ASP:H	1:C:132:ASP:HB2	1.79	0.47
1:D:83:ILE:HD12	1:D:123:ILE:HD12	1.96	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: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:A:265:GLY:HA2	1:A:328:THR:O	2.14	0.47
1:B:211:GLN:HG3	1:B:212:PRO:HD2	1.95	0.47
1:A:346:LEU:HB2	1:C:350:ALA:HB2	1.97	0.47
1:B:333:ASN:C	1:B:335:GLN:N	2.68	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:A:287:THR:HG23	1:A:325:LYS:HA	1.95	0.47
1:B:114:LEU:O	1:B:119:VAL:HG13	2.15	0.47
1:C:100:GLU:C	1:C:102:SER:H	2.18	0.47
1:C:185:LEU:HD23	1:C:244:VAL:CG1	2.44	0.47
1:C:342:LEU:N	1:C:342:LEU:HD23	2.30	0.47
1:A:122:LEU:O	1:A:145:ALA:HA	2.14	0.46
1:A:156:ILE:H	1:A:156:ILE:HG12	1.56	0.46
1:D:113:ASN:O	1:D:116:ALA:HB3	2.15	0.46
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:A:157:ASN:N	1:A:157:ASN:OD1	2.48	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:332:PRO:O	1:A:334:THR:N	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:C:331:ALA:HB3	1:C:339:PRO:CB	2.45	0.46
1:C:342:LEU:H	1:C:342:LEU:HD23	1.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:283:ILE:O	1:D:285:PRO:CD	2.63	0.46
1:C:96:VAL:HB	1:D:96:VAL:HB	1.97	0.46
1:C:192:VAL:O	1:C:196:LEU:N	2.45	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:B:191:SER:O	1:B:194:ALA:N	2.49	0.46
1:C:347:MET:O	1:C:350:ALA:HB3	2.16	0.46
1:A:71:LEU:O	1:A:77:SER:OG	2.31	0.46
1:D:168:ARG:HG2	1:D:168:ARG:NH1	2.31	0.46
1:D:241:ALA:HA	1:D:269:SER:O	2.16	0.46
1:A:354:SER:HB3	1:C:343:ALA:HB2	1.97	0.46
1:A:342:LEU:HD23	1:B:349:LEU:HD23	1.97	0.46
1:D:180:GLN:O	1:D:210:ILE:HG21	2.16	0.46
1:A:332:PRO:C	1:A:334:THR:H	2.18	0.46
1:C:286:LEU:HA	1:C:328:THR:OG1	2.16	0.46
1:C:87:ALA:HB1	1:C:92:ALA:O	2.16	0.46
1:D:79:ILE:O	1:D:83:ILE:HG12	2.15	0.46
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:115:LEU:HD11	1:D:122:LEU:HD11	1.98	0.45
1:D:185:LEU:HD23	1:D:244:VAL:HG13	1.98	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:C:219:ASP:O	1:C:220:TRP:CB	2.64	0.45
1:B:63:LEU:HD12	1:B:93:SER:HB3	1.99	0.45
1:B:116:ALA:C	1:B:118:ARG:H	2.18	0.45
1:C:340:ARG:O	1:C:342:LEU:HG	2.16	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:356:LEU:HD13	1:D:356:LEU:H	1.81	0.45
1:A:273:TYR:HA	1:A:289:ILE:HB	1.98	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:D:283:ILE:HD13	1:D:283:ILE:HA	1.61	0.45
1:D:325:LYS:CB	1:D:325:LYS:NZ	2.79	0.45
1:A:283:ILE:O	1:A:285:PRO:N	2.50	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:D:338:SER:N	1:D:339:PRO:HD3	2.31	0.45
1:B:136:VAL:O	1:B:139:ALA:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:232:MET:HG2	1:B:237:ILE:HB	1.97	0.45
1:B:283:ILE:O	1:B:285:PRO:N	2.50	0.45
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:A:163:HIS:H	1:A:163:HIS:HD2	1.64	0.45
1:A:188:PRO:HD2	1:A:220:TRP:CE2	2.52	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:B:96:VAL:CG1	1:B:97:SER:N	2.80	0.45
1:C:100:GLU:O	1:C:102:SER:N	2.50	0.45
1:C:184:LEU:HD13	1:C:201:TRP:CE3	2.50	0.45
1:C:336:THR:C	1:C:338:SER:H	2.19	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:77:SER:HB3	1:B:71:LEU:O	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:HD23	1:D:243:LEU:HA	1.73	0.44
1:B:115:LEU:HD11	1:B:140:CYS:HA	1.99	0.44
1:B:70:SER:HA	1:B:98:MET:HE1	1.98	0.44
1:C:287:THR:HA	1:C:324:VAL:O	2.18	0.44
1:A:336:THR:CG2	1:A:337:ALA:N	2.80	0.44
1:A:63:LEU:O	1:A:120:SER:N	2.50	0.44
1:B:216:ARG:HH21	1:B:231:GLN:HE21	1.66	0.44
1:B:283:ILE:N	1:B:283:ILE:CD1	2.81	0.44
1:B:332:PRO:O	1:B:333:ASN:C	2.56	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:C:282:TYR:O	1:C:283:ILE:C	2.56	0.44
1:C:71:LEU:H	1:C:98:MET:HE1	1.82	0.44
1:D:191:SER:O	1:D:194:ALA:N	2.50	0.44
1:A:343:ALA:CB	1:C:354:SER:CB	2.92	0.44
1:B:198:LEU:HA	1:B:201:TRP:CE3	2.53	0.44
1:B:240:THR:HG22	1:B:334:THR:HG23	2.00	0.44
1:B:351:ARG:HA	1:B:351:ARG:CZ	2.48	0.44
1:C:331:ALA:HB3	1:C:339:PRO:CG	2.47	0.44
1:A:118:ARG:CB	1:A:118:ARG:NH1	2.80	0.44
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:140:CYS:HB3	1:B:143:VAL:CG2	2.48	0.44
1:B:271:VAL:HG22	1:B:329:THR:HG21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:346:LEU:HA	1:B:349:LEU:HD13	1.99	0.44
1:C:148:LEU:O	1:C:160:ILE:HG22	2.17	0.44
1:C:210:ILE:CG2	1:C:211:GLN:N	2.80	0.44
1:B:346:LEU:HD11	1:C:346:LEU:HD11	2.00	0.44
1:A:152:ASP:OD1	1:A:152:ASP:N	2.51	0.44
1:A:184:LEU:O	1:A:215:GLU:HA	2.17	0.44
1:B:198:LEU:O	1:B:201:TRP:HB2	2.18	0.44
1:B:284:PRO:O	1:B:286:LEU:N	2.51	0.44
1:C:174:LEU:HD21	1:C:271:VAL:CG2	2.48	0.44
1:D:298:GLN:HG2	1:D:302:ASP:OD2	2.18	0.44
1:B:211:GLN:OE1	1:B:211:GLN:HA	2.17	0.44
1:A:129:ASP:HB2	1:A:132:ASP:OD2	2.18	0.43
1:A:339:PRO:HA	1:C:357:GLU:OE1	2.17	0.43
1:D:257:ILE:HG21	1:D:268:ILE:HB	1.99	0.43
1:A:170:GLY:O	1:A:174:LEU:HD23	2.18	0.43
1:A:303:ARG:HG3	1:A:313:VAL:HG11	2.00	0.43
1:A:177:LEU:HD22	1:A:331:ALA:N	2.33	0.43
1:A:105:GLU:O	1:A:106:ALA:C	2.57	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:B:284:PRO:O	1:B:285:PRO:C	2.54	0.43
1:A:254:MET:HG3	1:A:264:VAL:HG21	2.00	0.43
1:A:246:ASN:HA	1:A:273:TYR:O	2.18	0.43
1:B:191:SER:O	1:B:194:ALA:HB3	2.19	0.43
1:C:123:ILE:HG23	1:C:148:LEU:HD23	2.01	0.43
1:A:340:ARG:N	1:C:357:GLU:CD	2.71	0.43
1:D:208:ASN:O	1:D:209:GLN:CB	2.66	0.43
1:D:213:ILE:CD1	1:D:239:PRO:HB3	2.35	0.43
1:B:148:LEU:HD13	1:B:296:LEU:HD21	1.99	0.43
1:B:89:GLN:H	1:B:89:GLN:HG2	1.59	0.43
1:C:73:LEU:HD23	1:C:73:LEU:HA	1.74	0.43
1:D:64:ILE:CD1	1:D:301:VAL:HG13	2.48	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:283:ILE:CD1	1:B:283:ILE:HG23	2.42	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:227:GLN:O	1:A:231:GLN:HG3	2.19	0.43
1:A:275:ASP:HB3	1:A:290:LYS:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:GLN:O	1:A:313:VAL:HG23	2.19	0.43
1:B:116:ALA:C	1:B:118:ARG:N	2.72	0.43
1:C:246:ASN:HA	1:C:273:TYR:O	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:95:VAL:HG22	1:D:95:VAL:CG2	2.48	0.43
1:A:269:SER:HB3	1:A:329:THR:HA	2.01	0.42
1:A:351:ARG:HG2	1:B:262:LEU:HD13	2.01	0.42
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:B:258:THR:C	1:B:260:SER:H	2.21	0.42
1:D:188:PRO:HD3	1:D:219:ASP:HA	2.01	0.42
1:D:286:LEU:O	1:D:288:THR:HG22	2.19	0.42
1:A:355:ARG:NH2	1:B:262:LEU:HD11	2.34	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:C:352:GLN:NE2	1:D:337:ALA:O	2.53	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:288:THR:OG1	1:D:289:ILE:N	2.51	0.42
1:A:79:ILE:O	1:A:83:ILE:HG13	2.19	0.42
1:D:126:TYR:HA	1:D:127:PRO:HD3	1.90	0.42
1:D:356:LEU:HD22	1:D:357:GLU:CD	2.40	0.42
1:C:179:HIS:O	1:C:180:GLN:HG3	2.20	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:D:86:ARG:NH1	1:D:302:ASP:OD2	2.52	0.42
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.83	0.42
1:B:117:GLN:N	1:B:117:GLN:OE1	2.53	0.42
1:B:250:ALA:HA	1:B:253:ALA:HB3	2.01	0.42
1:B:273:TYR:O	1:B:274:ASP:CB	2.68	0.42
1:C:161:PHE:HE2	1:C:296:LEU:HD22	1.85	0.42
1:D:165:ASP:O	1:D:169:LEU:HG	2.19	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:283:ILE:N	1:C:283:ILE:HD13	2.35	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:63:LEU:HA	1:C:93:SER:O	2.20	0.42
1:A:68:THR:HG22	1:A:97:SER:O	2.19	0.42

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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:C:356:LEU:HD12	1:C:356:LEU:N	2.23	0.42
1:D:201:TRP:NE1	1:D:243:LEU:HD13	2.35	0.42
1:D:321:VAL:CG1	1:D:322:SER:N	2.83	0.42
1:A:338:SER:CB	1:A:342:LEU:HD12	2.50	0.42
1:B:77:SER:HA	1:B:80:VAL:HG22	2.02	0.42
1:C:281:CYS:O	1:D:251:LEU:HD22	2.20	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:D:325:LYS:HZ2	1:D:325:LYS:HB2	1.81	0.42
1:A:132:ASP:O	1:A:136:VAL:HG23	2.19	0.41
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:C:272:GLY:H	1:C:288:THR:HA	1.84	0.41
1:A:154:THR:HA	1:A:155:PRO:HD2	1.70	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:250:ALA:HB3	1:A:286:LEU:HD11	2.03	0.41
1:A:342:LEU:HD11	1:B:352:GLN:CB	2.50	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:108:LYS:O	1:C:112:HIS:ND1	2.53	0.41
1:C:229:THR:O	1:C:233:LEU:HG	2.20	0.41
1:C:285:PRO:HB3	1:C:326:ARG:HD3	2.01	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:A:173:HIS:CD2	1:A:329:THR:HG21	2.56	0.41
1:B:127:PRO:C	1:B:128:LEU:HD22	2.40	0.41
1:B:255:ARG:O	1:B:259:GLU:HG2	2.19	0.41
1:C:90:LEU:HD12	1:C:305:LEU:CD1	2.51	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: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: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:D:265:GLY:N	1:D:268:ILE:O	2.51	0.41
1:D:283:ILE:HG23	1:D:283:ILE:HD12	1.81	0.41
1:A:250:ALA:CB	1:A:286:LEU:HD11	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:GLN:CG	1:B:212:PRO:HD2	2.51	0.41
1:B:216:ARG:NH2	1:B:231:GLN:HE21	2.18	0.41
1:B:68:THR:O	1:B:99:VAL:HG12	2.21	0.41
1:C:153:GLN:HB2	1:C:153:GLN:HE21	1.71	0.41
1:A:126:TYR:O	1:A:128:LEU:HD22	2.21	0.41
1:A:62:LEU:CD2	1:A:64:ILE:HG13	2.38	0.41
1:B:311:GLN:HB3	1:B:312:ALA:H	1.50	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:D:283:ILE:O	1:D:285:PRO:N	2.54	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:A:286:LEU:HA	1:A:286:LEU:HD23	1.85	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:D:193:SER:O	1:D:197:ARG:HB2	2.21	0.40
1:B:214:ALA:HB2	1:B:237:ILE:HG21	2.02	0.40
1:C:290:LYS:HB2	1:C:324:VAL:CG2	2.48	0.40
1:A:312:ALA:HA	1:A:314:LYS:HG3	2.04	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: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

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

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

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

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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

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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 ⓘ

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%)	1	8
1	B	243/295 (82%)	206 (85%)	37 (15%)	3	13
1	C	243/295 (82%)	210 (86%)	33 (14%)	3	17
1	D	243/295 (82%)	200 (82%)	43 (18%)	2	9
All	All	972/1180 (82%)	815 (84%)	157 (16%)	2	11

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

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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

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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

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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

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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

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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 monosaccharides 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	-	14,15,15	3.64	8 (57%)	18,21,21	4.12	16 (88%)
2	IPT	C	400	-	14,15,15	3.41	7 (50%)	18,21,21	4.34	12 (66%)
2	IPT	B	400	-	14,15,15	3.30	6 (42%)	18,21,21	3.41	11 (61%)
2	IPT	D	400	-	14,15,15	3.67	5 (35%)	18,21,21	3.75	10 (55%)

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	-	-	5/6/26/26	0/1/1/1
2	IPT	C	400	-	-	0/6/26/26	0/1/1/1
2	IPT	B	400	-	-	4/6/26/26	0/1/1/1
2	IPT	D	400	-	-	5/6/26/26	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	400	IPT	C1'-S1	-8.34	1.46	1.83
2	D	400	IPT	C1'-S1	-7.97	1.48	1.83
2	B	400	IPT	C1'-S1	-7.84	1.49	1.83
2	C	400	IPT	C1'-S1	-7.53	1.50	1.83
2	A	400	IPT	O5-C1	7.13	1.53	1.42
2	D	400	IPT	C4-C3	6.90	1.69	1.52
2	D	400	IPT	O5-C1	6.80	1.52	1.42
2	C	400	IPT	O5-C1	6.58	1.52	1.42
2	B	400	IPT	O5-C1	5.38	1.50	1.42
2	A	400	IPT	C4-C5	-5.07	1.42	1.53
2	C	400	IPT	C4-C3	4.52	1.63	1.52
2	B	400	IPT	O4-C4	-4.42	1.32	1.43
2	B	400	IPT	C2'-C1'	4.16	1.69	1.51
2	C	400	IPT	C3'-C1'	3.58	1.67	1.51
2	D	400	IPT	C2'-C1'	3.50	1.66	1.51
2	B	400	IPT	O3-C3	-3.27	1.35	1.43
2	A	400	IPT	C3-C2	-3.07	1.44	1.52
2	C	400	IPT	C4-C5	-3.04	1.46	1.53
2	B	400	IPT	C3'-C1'	2.70	1.63	1.51
2	A	400	IPT	C4-C3	2.65	1.59	1.52
2	C	400	IPT	O3-C3	-2.58	1.36	1.43
2	D	400	IPT	C3'-C1'	2.44	1.62	1.51
2	A	400	IPT	C3'-C1'	2.35	1.61	1.51
2	A	400	IPT	C2'-C1'	2.34	1.61	1.51
2	C	400	IPT	C3-C2	-2.12	1.46	1.52
2	A	400	IPT	O3-C3	-2.08	1.38	1.43

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	400	IPT	O5-C1-C2	8.21	120.64	110.31
2	A	400	IPT	O3-C3-C2	-7.80	92.32	110.35
2	C	400	IPT	O5-C5-C4	-7.44	96.18	109.69
2	C	400	IPT	C1-O5-C5	7.13	125.73	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	IPT	O5-C1-C2	6.80	118.86	110.31
2	D	400	IPT	C1-O5-C5	6.72	124.97	112.58
2	D	400	IPT	O5-C1-C2	6.65	118.68	110.31
2	B	400	IPT	O5-C1-C2	6.37	118.33	110.31
2	C	400	IPT	C1-S1-C1'	6.30	119.56	100.26
2	A	400	IPT	C1-S1-C1'	6.24	119.38	100.26
2	A	400	IPT	O5-C5-C4	-6.17	98.48	109.69
2	B	400	IPT	C4-C3-C2	5.84	121.01	110.82
2	D	400	IPT	C3-C4-C5	5.76	120.51	110.24
2	D	400	IPT	C1-C2-C3	-5.34	100.04	110.59
2	C	400	IPT	C2-C1-S1	-5.07	103.48	111.30
2	D	400	IPT	C4-C3-C2	5.01	119.56	110.82
2	C	400	IPT	C4-C3-C2	4.99	119.53	110.82
2	B	400	IPT	C1-S1-C1'	4.93	115.36	100.26
2	B	400	IPT	O4-C4-C3	-4.93	98.95	110.35
2	D	400	IPT	O5-C5-C4	-4.86	100.87	109.69
2	B	400	IPT	O5-C5-C4	-4.52	101.49	109.69
2	C	400	IPT	C1-C2-C3	-4.51	101.67	110.59
2	B	400	IPT	C1-C2-C3	-4.29	102.13	110.59
2	A	400	IPT	C1-O5-C5	4.26	120.43	112.58
2	D	400	IPT	C1-S1-C1'	4.15	112.97	100.26
2	A	400	IPT	O2-C2-C1	3.97	117.57	110.27
2	A	400	IPT	C1-C2-C3	-3.85	102.99	110.59
2	D	400	IPT	O3-C3-C2	-3.71	101.77	110.35
2	C	400	IPT	O4-C4-C5	-3.39	100.88	109.30
2	C	400	IPT	O3-C3-C2	-3.38	102.53	110.35
2	A	400	IPT	C4-C3-C2	3.27	116.54	110.82
2	B	400	IPT	C3-C4-C5	3.21	115.97	110.24
2	A	400	IPT	O5-C5-C6	3.18	114.34	106.44
2	A	400	IPT	C2-C1-S1	-3.18	106.41	111.30
2	A	400	IPT	O3-C3-C4	3.13	117.59	110.35
2	C	400	IPT	O3-C3-C4	3.06	117.43	110.35
2	D	400	IPT	O4-C4-C5	-2.94	102.00	109.30
2	B	400	IPT	O3-C3-C2	-2.90	103.64	110.35
2	C	400	IPT	C3'-C1'-C2'	-2.83	101.96	111.73
2	A	400	IPT	O4-C4-C5	-2.67	102.67	109.30
2	D	400	IPT	C2-C1-S1	-2.50	107.44	111.30
2	A	400	IPT	C3-C4-C5	2.41	114.53	110.24
2	A	400	IPT	O2-C2-C3	-2.36	104.89	110.35
2	B	400	IPT	C1-O5-C5	2.36	116.93	112.58
2	B	400	IPT	O5-C5-C6	2.36	112.29	106.44
2	B	400	IPT	O4-C4-C5	-2.35	103.47	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	C	400	IPT	O4-C4-C3	2.31	115.70	110.35
2	A	400	IPT	O6-C6-C5	2.12	118.55	111.29
2	A	400	IPT	O4-C4-C3	-2.05	105.60	110.35

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	400	IPT	O5-C1-S1-C1'
2	A	400	IPT	C2'-C1'-S1-C1
2	A	400	IPT	C3'-C1'-S1-C1
2	B	400	IPT	O5-C1-S1-C1'
2	D	400	IPT	O5-C1-S1-C1'
2	D	400	IPT	C3'-C1'-S1-C1
2	D	400	IPT	O5-C5-C6-O6
2	B	400	IPT	O5-C5-C6-O6
2	A	400	IPT	C4-C5-C6-O6
2	B	400	IPT	C3'-C1'-S1-C1
2	D	400	IPT	C2'-C1'-S1-C1
2	A	400	IPT	C2-C1-S1-C1'
2	D	400	IPT	C2-C1-S1-C1'
2	B	400	IPT	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	400	IPT	1	0
2	B	400	IPT	3	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 is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.