



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:19 AM UTC

PDB ID : 1LBH / pdb_00001lbh
Title : INTACT LACTOSE OPERON REPRESSOR WITH GRATUITOUS INDUCER IPTG
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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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

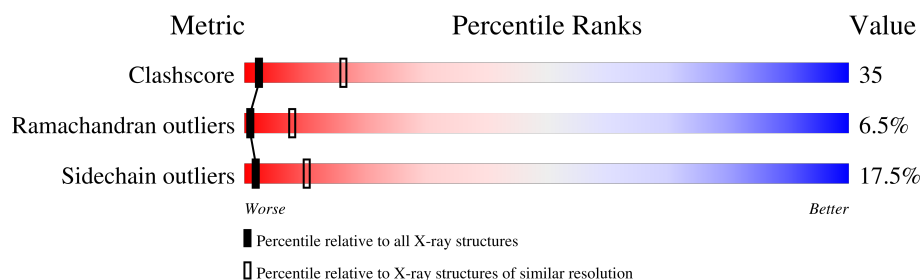
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	360	34% 33% 14% • 18%
1	B	360	28% 38% 13% • 18%
1	C	360	31% 36% 13% • 18%
1	D	360	30% 37% 13% • 18%

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.

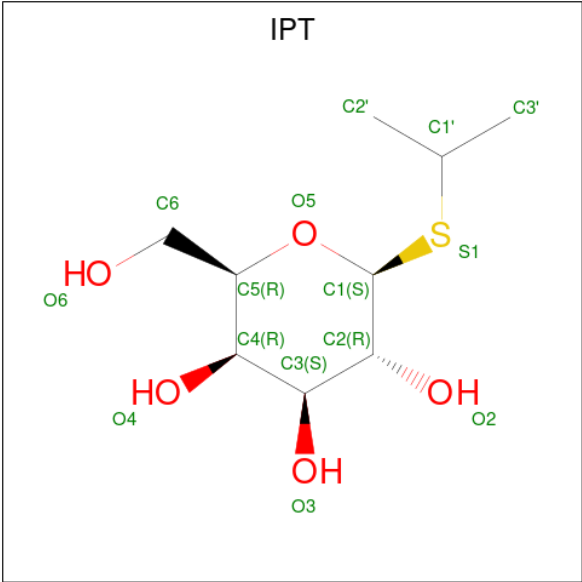
- Molecule 1 is a protein called INTACT LACTOSE OPERON REPRESSOR WITH GRATUITOUS INDUCER IPTG.

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 (CCD ID: IPT) (formula: C₉H₁₈O₅S).



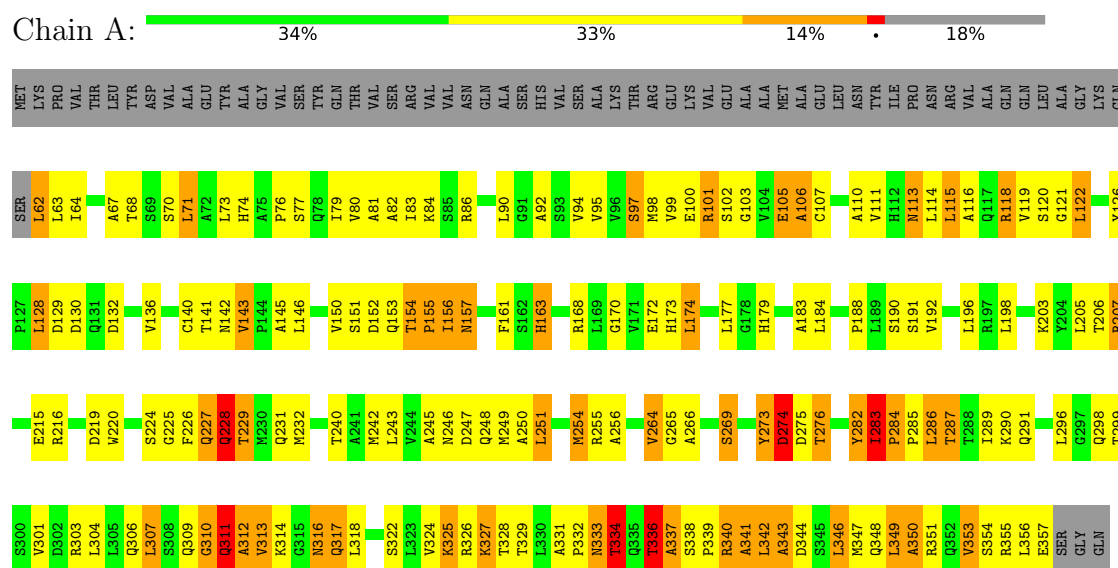
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			15	9	5	1		
2	B	1	Total	C	O	S	0	0
			15	9	5	1		
2	C	1	Total	C	O	S	0	0
			15	9	5	1		
2	D	1	Total	C	O	S	0	0
			15	9	5	1		

3 Residue-property plots

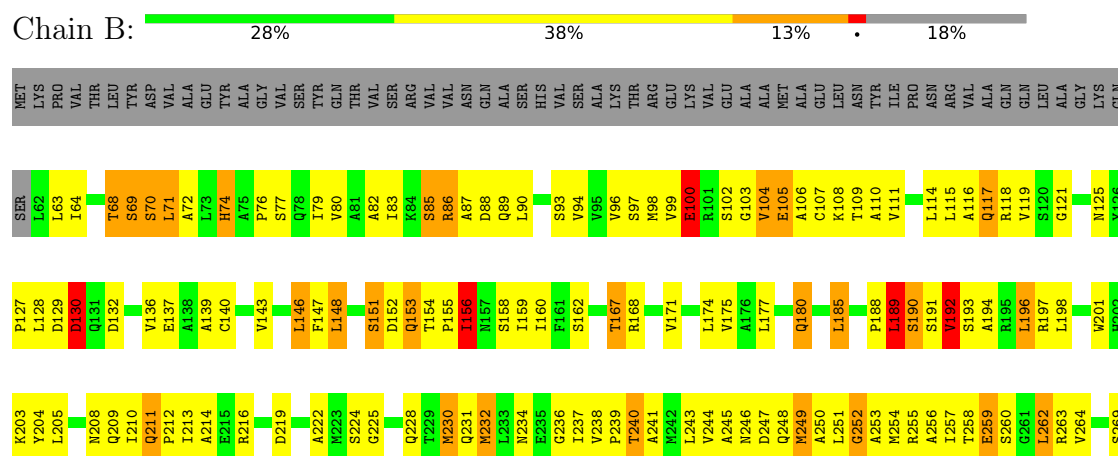
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



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 [i](#)

5.1 Standard geometry [i](#)

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	0.98	3/2247 (0.1%)	1.37	24/3055 (0.8%)
1	B	0.96	3/2247 (0.1%)	1.40	36/3055 (1.2%)
1	C	0.99	5/2247 (0.2%)	1.38	28/3055 (0.9%)
1	D	1.08	2/2247 (0.1%)	1.49	41/3055 (1.3%)
All	All	1.00	13/8988 (0.1%)	1.41	129/12220 (1.1%)

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 (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	230	MET	SD-CE	-22.50	1.23	1.79
1	B	230	MET	SD-CE	-10.26	1.53	1.79
1	B	334	THR	CA-CB	7.06	1.61	1.53
1	D	98	MET	SD-CE	6.72	1.96	1.79
1	C	353	VAL	CA-CB	6.68	1.62	1.54
1	A	343	ALA	CA-CB	-6.47	1.43	1.53
1	C	353	VAL	CA-C	6.02	1.59	1.52
1	A	336	THR	CA-CB	5.97	1.63	1.53
1	A	334	THR	CA-CB	5.85	1.62	1.53
1	C	75	ALA	CA-CB	-5.32	1.49	1.54
1	C	254	MET	SD-CE	-5.30	1.66	1.79
1	B	249	MET	SD-CE	-5.21	1.66	1.79
1	C	98	MET	SD-CE	5.05	1.92	1.79

All (129) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	283	ILE	CA-C-N	-16.52	103.36	120.38
1	D	283	ILE	C-N-CA	-16.52	103.36	120.38
1	C	283	ILE	CA-C-N	-15.99	103.91	120.38
1	C	283	ILE	C-N-CA	-15.99	103.91	120.38
1	B	283	ILE	CA-C-N	-12.71	107.29	120.38
1	B	283	ILE	C-N-CA	-12.71	107.29	120.38
1	D	230	MET	N-CA-C	-10.63	99.66	111.14
1	B	277	GLU	N-CA-C	10.45	122.25	111.07
1	C	284	PRO	N-CA-C	-10.41	98.00	110.70
1	A	283	ILE	CA-C-N	-10.32	109.75	120.38
1	A	283	ILE	C-N-CA	-10.32	109.75	120.38
1	D	236	GLY	N-CA-C	10.18	129.03	115.59
1	D	286	LEU	N-CA-C	9.53	124.16	109.96
1	B	355	ARG	N-CA-C	-9.50	101.11	112.89
1	D	327	LYS	N-CA-C	9.40	125.00	112.88
1	A	154	THR	CA-C-N	9.34	131.52	119.84
1	A	154	THR	C-N-CA	9.34	131.52	119.84
1	D	334	THR	N-CA-C	-9.24	99.25	113.02
1	D	352	GLN	N-CA-C	-9.18	101.17	111.82
1	D	154	THR	N-CA-C	-8.84	98.68	109.72
1	D	287	THR	N-CA-C	-8.73	94.35	108.41
1	B	72	ALA	N-CA-C	-8.50	101.96	111.14
1	A	287	THR	N-CA-C	-8.50	96.25	109.76
1	B	236	GLY	N-CA-C	8.44	124.73	114.69
1	A	327	LYS	N-CA-C	8.28	123.60	113.17
1	A	346	LEU	N-CA-C	-8.25	102.36	111.36
1	C	282	TYR	N-CA-C	-8.20	98.34	110.23
1	A	225	GLY	N-CA-C	-7.97	102.69	113.37
1	B	282	TYR	N-CA-C	-7.97	98.22	110.10
1	D	338	SER	CA-C-N	7.75	129.53	119.84
1	D	338	SER	C-N-CA	7.75	129.53	119.84
1	C	287	THR	N-CA-C	-7.70	98.03	110.20
1	B	340	ARG	N-CA-C	-7.45	104.23	112.72
1	C	106	ALA	N-CA-C	-7.37	101.73	111.24
1	A	192	VAL	N-CA-C	-7.32	102.61	110.23
1	A	205	LEU	N-CA-C	-7.24	103.39	111.28
1	B	334	THR	N-CA-C	-7.20	103.41	113.20
1	D	98	MET	N-CA-C	7.20	121.22	109.85
1	C	349	LEU	N-CA-C	-7.19	103.53	111.36
1	B	343	ALA	N-CA-C	-7.10	103.47	111.14
1	D	154	THR	CA-C-N	7.07	128.68	119.84
1	D	154	THR	C-N-CA	7.07	128.68	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	327	LYS	N-CA-C	7.06	121.72	113.18
1	B	154	THR	CA-C-N	6.96	128.54	119.84
1	B	154	THR	C-N-CA	6.96	128.54	119.84
1	A	318	LEU	N-CA-C	6.93	119.85	109.25
1	C	87	ALA	N-CA-C	-6.90	103.45	110.97
1	B	286	LEU	N-CA-C	6.89	120.64	110.30
1	C	154	THR	CA-C-N	6.83	128.38	119.84
1	C	154	THR	C-N-CA	6.83	128.38	119.84
1	A	291	GLN	N-CA-C	-6.82	97.29	108.41
1	C	208	ASN	N-CA-C	-6.73	102.39	111.87
1	A	67	ALA	N-CA-C	-6.72	98.29	109.24
1	D	333	ASN	N-CA-C	6.66	124.99	110.80
1	D	355	ARG	N-CA-C	6.64	121.13	112.89
1	A	334	THR	N-CA-C	-6.57	105.57	112.93
1	B	331	ALA	N-CA-C	-6.51	101.37	109.64
1	C	261	GLY	N-CA-C	6.46	124.88	115.32
1	D	308	SER	N-CA-C	-6.45	104.25	111.28
1	C	281	CYS	N-CA-C	6.45	121.94	113.30
1	B	330	LEU	N-CA-C	6.33	117.78	108.86
1	D	318	LEU	N-CA-C	6.28	119.14	108.90
1	B	87	ALA	N-CA-C	-6.27	104.89	112.54
1	B	230	MET	N-CA-C	-6.25	104.00	111.69
1	C	73	LEU	N-CA-C	6.19	120.43	112.26
1	D	319	LEU	CA-C-N	6.16	126.35	120.31
1	D	319	LEU	C-N-CA	6.16	126.35	120.31
1	B	287	THR	N-CA-C	-6.12	99.19	108.67
1	D	336	THR	N-CA-C	6.11	120.47	107.70
1	B	205	LEU	N-CA-C	-6.10	104.18	111.69
1	C	347	MET	N-CA-C	6.08	118.41	111.11
1	B	70	SER	N-CA-C	-6.04	100.15	109.76
1	C	209	GLN	N-CA-C	6.04	119.75	111.54
1	A	313	VAL	N-CA-C	-5.98	96.89	109.34
1	B	110	ALA	N-CA-C	-5.97	103.94	111.11
1	B	337	ALA	N-CA-C	5.93	123.42	110.80
1	A	286	LEU	N-CA-C	5.92	118.30	109.59
1	B	291	GLN	N-CA-C	-5.87	97.56	108.02
1	A	240	THR	N-CA-C	-5.87	105.88	114.39
1	C	108	LYS	N-CA-C	-5.83	98.37	110.80
1	B	247	ASP	N-CA-C	5.83	118.58	111.82
1	D	284	PRO	N-CA-C	-5.83	103.59	110.70
1	A	106	ALA	N-CA-C	-5.83	104.12	111.11
1	C	105	GLU	N-CA-C	-5.79	106.05	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	193	SER	N-CA-C	-5.73	104.03	111.02
1	D	74	HIS	N-CA-C	5.66	117.53	111.36
1	D	96	VAL	N-CA-C	5.64	116.34	108.89
1	D	163	HIS	N-CA-C	-5.61	105.31	111.82
1	B	327	LYS	N-CA-C	5.59	122.00	113.61
1	D	337	ALA	N-CA-C	-5.56	106.26	113.16
1	A	276	THR	N-CA-C	-5.56	103.19	110.53
1	C	167	THR	N-CA-C	-5.54	107.06	113.88
1	D	146	LEU	N-CA-C	-5.53	100.69	109.59
1	D	155	PRO	N-CA-C	5.51	123.83	112.47
1	C	109	THR	N-CA-C	-5.51	105.18	111.07
1	B	148	LEU	N-CA-C	5.49	120.11	113.41
1	B	315	GLY	N-CA-C	5.47	121.03	111.78
1	B	85	SER	N-CA-C	5.46	117.31	111.36
1	B	152	ASP	N-CA-C	-5.46	106.66	113.15
1	C	245	ALA	N-CA-C	5.42	119.15	112.54
1	A	228	GLN	N-CA-C	5.42	117.26	111.36
1	C	96	VAL	N-CA-C	5.41	116.37	108.53
1	C	196	LEU	N-CA-C	-5.39	105.48	111.36
1	D	70	SER	N-CA-C	-5.36	101.24	109.76
1	D	282	TYR	N-CA-C	-5.35	103.43	110.33
1	D	283	ILE	CB-CA-C	5.34	121.08	111.36
1	A	116	ALA	N-CA-C	-5.31	106.97	113.50
1	D	312	ALA	N-CA-C	5.31	122.10	110.80
1	C	278	ASP	N-CA-C	5.29	119.22	112.34
1	B	252	GLY	N-CA-C	-5.28	106.38	112.50
1	A	251	LEU	N-CA-C	-5.26	105.44	111.07
1	C	279	SER	N-CA-C	5.22	118.44	111.75
1	B	196	LEU	N-CA-C	5.20	118.72	112.38
1	D	340	ARG	N-CA-C	5.20	117.36	111.02
1	D	133	ALA	N-CA-C	-5.19	105.53	111.14
1	D	177	LEU	N-CA-C	-5.18	106.91	113.18
1	D	138	ALA	N-CA-C	-5.18	105.53	111.07
1	B	68	THR	N-CA-C	5.18	117.75	110.14
1	B	151	SER	N-CA-C	-5.17	103.22	110.50
1	B	190	SER	N-CA-C	-5.14	106.86	112.72
1	C	67	ALA	N-CA-C	-5.14	100.79	108.96
1	C	210	ILE	CB-CA-C	-5.14	102.74	110.55
1	B	106	ALA	N-CA-C	-5.13	105.38	110.97
1	D	205	LEU	N-CA-C	-5.10	105.63	111.14
1	B	339	PRO	N-CA-C	-5.08	102.00	112.47
1	D	279	SER	N-CA-C	5.08	118.25	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	97	SER	N-CA-C	-5.08	100.97	109.24
1	D	247	ASP	N-CA-C	5.02	118.67	112.54
1	A	350	ALA	N-CA-C	-5.01	105.71	111.07

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	169	1
1	B	2218	0	2269	181	0
1	C	2218	0	2269	188	0
1	D	2218	0	2269	158	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	637	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 35.

All (637) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ARG:HH11	1:B:168:ARG:HG2	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:HH11	1:B:340:ARG:HB2	1.45	0.80
1:C:356:LEU:HD12	1:C:356:LEU:H	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: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:C:62:LEU:HG	1:C:63:LEU:N	1.96	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
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:C:230:MET:SD	1:C:230:MET:C	2.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ARG:HG2	1:B:168:ARG:NH1	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:B:86:ARG:HH12	1:B:302:ASP:CG	1.96	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:B:354:SER:OG	1:D:343:ALA:HB3	1.89	0.70
1:D:137:GLU:O	1:D:140:CYS:HB3	1.91	0.70
1:B:349:LEU:HD12	1:B:349:LEU:H	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: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: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: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: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:O	1:D:235:GLU:HG2	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:B:333:ASN:C	1:B:335:GLN:H	2.02	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HB2	1:D:325:LYS:NZ	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: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: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: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: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: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: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: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
1:A:113:ASN:N	1:A:113:ASN:HD22	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:D:208:ASN:O	1:D:209:GLN:HB2	2.00	0.61
1:A:346:LEU:HD22	1:D:346:LEU:HD22	1.80	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:ALA:CB	1:C:347:MET:HG3	2.31	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:B:339:PRO:O	1:D:357:GLU:HG2	2.02	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: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:HH11	1:D:168:ARG:HG2	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:86:ARG:HG2	1:A:298:GLN:HA	1.84	0.58
1:A:101:ARG:HA	1:A:126:TYR:OH	2.03	0.58
1:A:283:ILE:O	1:A:284:PRO:C	2.45	0.58
1:B:171:VAL:HG11	1:B:204:TYR:C	2.28	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:A:70:SER:HA	1:A:98:MET:HE3	1.86	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
1:C:337:ALA:C	1:C:339:PRO:HD2	2.27	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:HD13	1:D:90:LEU:N	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:B:245:ALA:HB3	1:B:249:MET:HE1	1.86	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:A:343:ALA:HB2	1:C:353:VAL:C	2.30	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:183:ALA:HB1	1:D:232:MET:HE2	1.89	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:D:254:MET:HE3	1:D:264:VAL:HG21	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:LEU:O	1:C:332:PRO:HD3	2.08	0.54
1:A:347:MET:HE1	1:C:351:ARG:HH21	1.72	0.54
1:A:283:ILE:CG2	1:A:284:PRO:HD3	2.36	0.54
1:B:100:GLU:H	1:B:100:GLU:CD	2.14	0.54
1:C:283:ILE:O	1:C:285:PRO:HD3	2.07	0.54
1:D:187:GLY:HA2	1:D:249:MET:HE1	1.89	0.54
1:A:100:GLU:O	1:A:102:SER:N	2.41	0.54
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:HG13	1:D:313:VAL:O	2.08	0.54
1:C:68:THR:O	1:C:99:VAL:HB	2.07	0.54
1:C:338:SER:O	1:C:339:PRO:C	2.51	0.53
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:A:347:MET:HE1	1:C:351:ARG:NH2	2.23	0.53
1:B:282:TYR:O	1:B:283:ILE:C	2.52	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: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: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:254:MET:HE2	1:B:284:PRO:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:115:LEU:CD1	1:D:122:LEU:HD11	2.39	0.52
1:B:351:ARG:NH1	1:B:351:ARG:HA	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:A:229:THR:HG22	1:A:232:MET:HE2	1.90	0.52
1:B:283:ILE:O	1:B:285:PRO:HD3	2.10	0.52
1:C:286:LEU:HD23	1:C:286:LEU:H	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
1:B:197:ARG:NH2	2:B:400:IPT:O4	2.41	0.51
1:C:100:GLU:C	1:C:102:SER:H	2.18	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:310:GLY:O	1:A:312:ALA:N	2.43	0.51
1:B:70:SER:HA	1:B:98:MET:HE3	1.92	0.51
1:B:167:THR:HG21	1:B:197:ARG:O	2.10	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:333:ASN:C	1:B:335:GLN:N	2.68	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: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:117:GLN:OE1	1:D:117:GLN:HB3	2.10	0.51
1:C:154:THR:CG2	1:C:156:ILE:HG12	2.39	0.51
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: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:232:MET:HE1	1:C:242:MET:HE3	1.94	0.50
1:C:71:LEU:H	1:C:98:MET:HE1	1.76	0.50
1:A:332:PRO:C	1:A:334:THR:H	2.18	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:157:ASN:H	1:D:157:ASN:ND2	2.09	0.50
1:D:229:THR:O	1:D:233:LEU:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:344:ASP:O	1:D:347:MET: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: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:116:ALA:C	1:B:118:ARG:H	2.18	0.50
1:B:271:VAL:HG22	1:B:329:THR:CG2	2.41	0.50
1:C:177:LEU:HD22	1:C:330:LEU:C	2.36	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: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
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:C:336:THR:C	1:C:338:SER:H	2.19	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:B:332:PRO:O	1:B:333:ASN:C	2.56	0.49
1:C:282:TYR:O	1:C:283:ILE:C	2.56	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:D:273:TYR:O	1:D:274:ASP:HB2	2.12	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:A:73:LEU:HB2	1:A:76:PRO:HG3	1.94	0.48
1:A:99:VAL:CG2	1:A:126:TYR:CD1	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ARG:HG2	1:A:307:LEU:HD23	1.95	0.48
1:C:173:HIS:ND1	1:C:323:LEU:HD21	2.28	0.48
1:C:342:LEU:CD1	1:D:356:LEU:HD11	2.44	0.48
1:D:257:ILE:O	1:D:262:LEU:HB2	2.14	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: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:A:105:GLU:O	1:A:106:ALA:C	2.57	0.48
1:B:284:PRO:O	1:B:285:PRO:C	2.54	0.48
1:D:146:LEU:HD11	1:D:159:ILE:HG13	1.95	0.48
1:A:340:ARG:N	1:C:357:GLU:CD	2.71	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:B:129:ASP:O	1:B:130:ASP:C	2.56	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:B:258:THR:C	1:B:260:SER:N	2.72	0.48
1:C:345:SER:HA	1:C:348:GLN:HE21	1.79	0.48
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:C:336:THR:C	1:C:338:SER:N	2.71	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:HD2	1:C:86:ARG:HA	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:211:GLN:HG3	1:B:212:PRO:HD2	1.95	0.47
1:B:258:THR:C	1:B:260:SER:H	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:ALA:C	1:D:118:ARG:H	2.23	0.47
1:D:356:LEU:HD22	1:D:357:GLU:CD	2.40	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:HD12	1:D:349:LEU:HA	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:D:242:MET:HE2	1:D:242:MET:HB3	1.61	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:350:ALA:CB	1:C:346:LEU:HB2	2.45	0.46
1:B:116:ALA:C	1:B:118:ARG:N	2.72	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:CD2	1:C:342:LEU:H	2.28	0.46
1:B:188:PRO:C	1:B:190:SER:H	2.23	0.46
1:C:96:VAL:HB	1:D:96:VAL:HB	1.97	0.46
1:C:331:ALA:HB3	1:C:339:PRO:CB	2.45	0.46
1:C:342:LEU:HD23	1:C:342:LEU:H	1.78	0.46
1:D:283:ILE:O	1:D:285:PRO:CD	2.63	0.46
1:C:192:VAL:O	1:C:196:LEU:N	2.45	0.46
1:D:76:PRO:O	1:D:80:VAL:HG23	2.15	0.46
1:D:287:THR:HG23	1:D:325:LYS:HA	1.96	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:B:127:PRO:C	1:B:128:LEU:HD22	2.40	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: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:A:242:MET:HB3	1:A:242:MET:HE2	1.64	0.46
1:C:87:ALA:HB1	1:C:92:ALA:O	2.16	0.46
1:C:286:LEU:HA	1:C:328:THR:OG1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:340:ARG:O	1:C:342:LEU:HG	2.16	0.45
1:C:345:SER:O	1:C:346:LEU:C	2.59	0.45
1:A:73:LEU:O	1:A:74:HIS:HB2	2.16	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:HA	1:D:283:ILE:HD13	1.61	0.45
1:D:325:LYS:NZ	1:D:325:LYS:CB	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:86:ARG:CG	1:B:86:ARG:NH1	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:N	2.50	0.45
1:B:349:LEU:O	1:B:352:GLN:HB2	2.16	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:O5	2:B:400:IPT:C3'	2.64	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: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:282:TYR:C	1:A:283:ILE:O	2.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:LEU:HD11	1:B:140:CYS:HA	1.99	0.44
1:A:188:PRO:C	1:A:190:SER:H	2.24	0.44
1:C:287:THR:HA	1:C:324:VAL:O	2.18	0.44
1:A:63:LEU:O	1:A:120:SER:N	2.50	0.44
1:A:336:THR:CG2	1:A:337:ALA:N	2.80	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: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: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:86:ARG:HE	1:A:298:GLN:HB2	1.83	0.44
1:A:118:ARG:CB	1:A:118:ARG:NH1	2.80	0.44
1:A:157:ASN:OD1	1:A:157:ASN:N	2.48	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
1:B:346:LEU:HA	1:B:349:LEU:HD13	1.99	0.44
1:B:346:LEU:HD11	1:C:346:LEU:HD11	2.00	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: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:86:ARG:HD3	1:D:86:ARG:C	2.42	0.44
1:D:298:GLN:HG2	1:D:302:ASP:OD2	2.18	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: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:113:ASN:N	1:A:113:ASN:ND2	2.65	0.43
1:B:180:GLN:HA	1:B:210:ILE:HD13	2.01	0.43
1:A:246:ASN:HA	1:A:273:TYR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:MET:HG3	1:A:264:VAL:HG21	2.00	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: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:89:GLN:H	1:B:89:GLN:HG2	1.59	0.43
1:B:148:LEU:HD13	1:B:296:LEU:HD21	1.99	0.43
1:C:73:LEU:HD23	1:C:73:LEU:HA	1.74	0.43
1:C:142:ASN:O	1:C:143:VAL:C	2.61	0.43
1:D:64:ILE:CD1	1:D:301:VAL:HG13	2.48	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: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
1:A:311:GLN:O	1:A:313:VAL:HG23	2.19	0.43
1:C:95:VAL:HG22	1:D:95:VAL:CG2	2.48	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:331:ALA:CB	1:C:339:PRO:HB3	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:B:96:VAL:CG1	1:B:97:SER:N	2.80	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:A:245:ALA:HB3	1:A:249:MET:HE1	2.00	0.42
1:C:301:VAL:O	1:C:302:ASP:C	2.62	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:341:ALA:O	1:A:342:LEU:C	2.62	0.42
1:A:355:ARG:NH2	1:B:262:LEU:HD11	2.34	0.42
1:B:151:SER:C	1:B:153:GLN:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ILE:O	1:A:83:ILE:HG13	2.19	0.42
1:A:151:SER:C	1:A:153:GLN:N	2.75	0.42
1:D:126:TYR:HA	1:D:127:PRO:HD3	1.90	0.42
1:C:179:HIS:O	1:C:180:GLN:HG3	2.20	0.42
1:D:86:ARG:NH1	1:D:302:ASP:OD2	2.52	0.42
1:D:210:ILE:HG22	1:D:211:GLN:N	2.34	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:C:206:THR:HG22	1:C:211:GLN:CD	2.44	0.42
1:D:165:ASP:O	1:D:169:LEU:HG	2.19	0.42
1:B:79:ILE:O	1:B:83:ILE:HG12	2.19	0.42
1:B:180:GLN:HA	1:B:210:ILE:CD1	2.50	0.42
1:C:283:ILE:HD13	1:C:283:ILE:N	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:B:201:TRP:C	1:B:203:LYS:H	2.28	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
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:D:333:ASN:ND2	1:D:333:ASN:C	2.77	0.42
1:A:82:ALA:C	1:A:84:LYS:N	2.76	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:HB2	1:D:325:LYS:HZ2	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:SER:HA	1:B:98:MET:CE	2.50	0.41
1:B:79:ILE:O	1:B:82:ALA:HB3	2.19	0.41
1:C:108:LYS:O	1:C:112:HIS:ND1	2.53	0.41
1:C:200:GLY:O	1:C:201:TRP:C	2.61	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:C:299:THR:O	1:C:300:SER:C	2.62	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: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:D:188:PRO:C	1:D:190:SER:H	2.28	0.41
1:A:115:LEU:CD1	1:A:140:CYS:HA	2.50	0.41
1:B:331:ALA:O	1:B:332:PRO:C	2.63	0.41
1:C:100:GLU:C	1:C:102:SER:N	2.75	0.41
1:C:146:LEU:HD12	1:C:146:LEU:HA	1.81	0.41
1:C:275:ASP:HB3	1:C:290:LYS:HG2	2.03	0.41
1:D:70:SER:O	1:D:76:PRO:HG3	2.21	0.41
1:D:212:PRO:C	1:D:214:ALA:H	2.28	0.41
1:D:220:TRP:HZ3	1:D:245:ALA:O	2.03	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:HD12	1:D:283:ILE:HG23	1.81	0.41
1:A:250:ALA:CB	1:A:286:LEU:HD11	2.51	0.41
1:B:68:THR:O	1:B:99:VAL:HG12	2.21	0.41
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:C:153:GLN:HE21	1:C:153:GLN:HB2	1.71	0.41
1:D:86:ARG:HH11	1:D:302:ASP:CG	2.28	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:355:ARG:C	1:D:357:GLU:H	2.29	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:D:166:GLY:HA3	1:D:273:TYR:OH	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:86:ARG:CZ	1:B:90:LEU:HD11	2.50	0.40
1:B:174:LEU:HD23	1:B:174:LEU:HA	1.87	0.40
1:C:73:LEU:O	1:C:76:PRO:HD2	2.20	0.40
1:C:296:LEU:O	1:C:300:SER:OG	2.35	0.40
1:D:193:SER:O	1:D:197:ARG:HB2	2.21	0.40
1:D:340:ARG:O	1:D:341:ALA:C	2.64	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:309:GLN:C	1:A:311:GLN:H	2.29	0.40
1:A:312:ALA:HA	1:A:314:LYS:HG3	2.04	0.40
1:B:188:PRO:C	1:B:190:SER:N	2.79	0.40
1:B:274:ASP:HA	1:B:291:GLN:HG3	2.03	0.40
1:B:283:ILE:CB	1:B:284:PRO:CD	2.96	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%)	1	12
1	B	294/360 (82%)	231 (79%)	41 (14%)	22 (8%)	1	5
1	C	294/360 (82%)	244 (83%)	33 (11%)	17 (6%)	1	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	294/360 (82%)	242 (82%)	31 (10%)	21 (7%)	1	6
All	All	1176/1440 (82%)	954 (81%)	146 (12%)	76 (6%)	1	8

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
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

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Mol	Chain	Res	Type
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
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%)	198 (82%)	45 (18%)	1	9
1	B	243/295 (82%)	204 (84%)	39 (16%)	2	13
1	C	243/295 (82%)	202 (83%)	41 (17%)	2	11
1	D	243/295 (82%)	198 (82%)	45 (18%)	1	9
All	All	972/1180 (82%)	802 (82%)	170 (18%)	2	10

All (170) 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	105	GLU
1	A	113	ASN
1	A	115	LEU
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	163	HIS
1	A	174	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	243	LEU
1	A	251	LEU

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Mol	Chain	Res	Type
1	A	254	MET
1	A	264	VAL
1	A	269	SER
1	A	274	ASP
1	A	276	THR
1	A	283	ILE
1	A	284	PRO
1	A	299	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	334	THR
1	A	336	THR
1	A	348	GLN
1	A	349	LEU
1	A	353	VAL
1	B	71	LEU
1	B	74	HIS
1	B	86	ARG
1	B	100	GLU
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
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	211	GLN

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Mol	Chain	Res	Type
1	B	230	MET
1	B	232	MET
1	B	234	ASN
1	B	238	VAL
1	B	240	THR
1	B	244	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	334	THR
1	B	340	ARG
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	90	LEU
1	C	95	VAL
1	C	96	VAL
1	C	97	SER
1	C	104	VAL
1	C	119	VAL
1	C	122	LEU
1	C	128	LEU
1	C	130	ASP
1	C	141	THR
1	C	151	SER
1	C	153	GLN
1	C	175	VAL
1	C	190	SER
1	C	192	VAL
1	C	196	LEU
1	C	202	HIS
1	C	211	GLN
1	C	228	GLN
1	C	230	MET
1	C	231	GLN

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Mol	Chain	Res	Type
1	C	251	LEU
1	C	259	GLU
1	C	264	VAL
1	C	270	VAL
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	330	LEU
1	C	333	ASN
1	C	335	GLN
1	C	342	LEU
1	C	348	GLN
1	C	349	LEU
1	C	356	LEU
1	D	62	LEU
1	D	63	LEU
1	D	74	HIS
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	117	GLN
1	D	120	SER
1	D	128	LEU
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

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Mol	Chain	Res	Type
1	D	230	MET
1	D	235	GLU
1	D	246	ASN
1	D	251	LEU
1	D	262	LEU
1	D	264	VAL
1	D	288	THR
1	D	309	GLN
1	D	311	GLN
1	D	313	VAL
1	D	314	LYS
1	D	318	LEU
1	D	321	VAL
1	D	324	VAL
1	D	325	LYS
1	D	327	LYS
1	D	333	ASN
1	D	347	MET
1	D	355	ARG
1	D	356	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	113	ASN
1	A	153	GLN
1	A	163	HIS
1	A	228	GLN
1	A	309	GLN
1	A	317	GLN
1	B	125	ASN
1	B	157	ASN
1	B	227	GLN
1	B	228	GLN
1	B	231	GLN
1	B	234	ASN
1	B	248	GLN
1	B	306	GLN
1	B	316	ASN
1	B	317	GLN
1	C	153	GLN
1	C	163	HIS

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Mol	Chain	Res	Type
1	C	228	GLN
1	C	234	ASN
1	C	248	GLN
1	C	335	GLN
1	D	113	ASN
1	D	202	HIS
1	D	211	GLN
1	D	227	GLN
1	D	228	GLN
1	D	231	GLN
1	D	306	GLN
1	D	335	GLN
1	D	352	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	B	400	-	15,15,15	6.22	7 (46%)	18,21,21	3.29	12 (66%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	IPT	A	400	-	15,15,15	5.74	8 (53%)	18,21,21	3.86	16 (88%)
2	IPT	C	400	-	15,15,15	5.94	8 (53%)	18,21,21	4.11	11 (61%)
2	IPT	D	400	-	15,15,15	6.26	6 (40%)	18,21,21	3.70	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	B	400	-	-	4/6/26/26	0/1/1/1
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	D	400	-	-	5/6/26/26	0/1/1/1

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	400	IPT	C1-S1	-20.18	1.39	1.80
2	D	400	IPT	C1-S1	-19.47	1.40	1.80
2	C	400	IPT	C1-S1	-18.66	1.42	1.80
2	A	400	IPT	C1-S1	-17.02	1.45	1.80
2	A	400	IPT	C1'-S1	-9.45	1.46	1.83
2	D	400	IPT	C1'-S1	-9.02	1.48	1.83
2	B	400	IPT	C1'-S1	-8.88	1.49	1.83
2	C	400	IPT	C1'-S1	-8.52	1.50	1.83
2	A	400	IPT	O5-C1	7.05	1.53	1.42
2	D	400	IPT	C4-C3	6.76	1.69	1.52
2	D	400	IPT	O5-C1	6.71	1.52	1.42
2	C	400	IPT	O5-C1	6.50	1.52	1.42
2	B	400	IPT	O5-C1	5.30	1.50	1.42
2	A	400	IPT	C4-C5	-4.99	1.42	1.53
2	B	400	IPT	C2'-C1'	4.77	1.69	1.51
2	C	400	IPT	C4-C3	4.43	1.63	1.52
2	B	400	IPT	O4-C4	-4.19	1.32	1.43
2	C	400	IPT	C3'-C1'	4.10	1.67	1.51
2	D	400	IPT	C2'-C1'	4.00	1.66	1.51
2	B	400	IPT	O3-C3	-3.10	1.35	1.43
2	B	400	IPT	C3'-C1'	3.08	1.63	1.51
2	A	400	IPT	C3-C2	-3.02	1.44	1.52
2	C	400	IPT	C4-C5	-2.99	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	400	IPT	C3'-C1'	2.78	1.62	1.51
2	A	400	IPT	C3'-C1'	2.68	1.61	1.51
2	A	400	IPT	C2'-C1'	2.67	1.61	1.51
2	A	400	IPT	C4-C3	2.60	1.59	1.52
2	C	400	IPT	O3-C3	-2.44	1.36	1.43
2	C	400	IPT	C3-C2	-2.08	1.46	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	IPT	O3-C3-C2	-7.66	92.32	110.38
2	C	400	IPT	O5-C5-C4	-7.50	96.18	109.70
2	C	400	IPT	O5-C1-C2	7.49	120.64	110.32
2	C	400	IPT	C1-O5-C5	7.34	125.73	112.56
2	D	400	IPT	C1-O5-C5	6.92	124.97	112.56
2	C	400	IPT	C3'-C1'-S1	6.30	128.26	110.12
2	A	400	IPT	O5-C5-C4	-6.23	98.48	109.70
2	A	400	IPT	O5-C1-C2	6.20	118.86	110.32
2	D	400	IPT	O5-C1-C2	6.07	118.68	110.32
2	B	400	IPT	O5-C1-C2	5.81	118.33	110.32
2	B	400	IPT	C4-C3-C2	5.80	121.01	110.83
2	D	400	IPT	C3-C4-C5	5.67	120.51	110.23
2	D	400	IPT	C1-C2-C3	-5.38	100.04	110.55
2	D	400	IPT	C4-C3-C2	4.98	119.56	110.83
2	C	400	IPT	C4-C3-C2	4.96	119.53	110.83
2	D	400	IPT	O5-C5-C4	-4.90	100.87	109.70
2	B	400	IPT	O4-C4-C3	-4.85	98.95	110.38
2	B	400	IPT	O5-C5-C4	-4.56	101.49	109.70
2	C	400	IPT	C1-C2-C3	-4.54	101.67	110.55
2	A	400	IPT	C1-O5-C5	4.39	120.43	112.56
2	B	400	IPT	C1-C2-C3	-4.31	102.13	110.55
2	A	400	IPT	O2-C2-C1	4.09	117.57	110.30
2	D	400	IPT	C2'-C1'-S1	4.08	121.85	110.12
2	A	400	IPT	C1-C2-C3	-3.86	102.99	110.55
2	A	400	IPT	C2'-C1'-S1	3.78	120.99	110.12
2	D	400	IPT	O3-C3-C2	-3.65	101.77	110.38
2	B	400	IPT	C2'-C1'-S1	3.54	120.30	110.12
2	C	400	IPT	O4-C4-C5	-3.43	100.88	109.32
2	C	400	IPT	O3-C3-C2	-3.33	102.53	110.38
2	A	400	IPT	C4-C3-C2	3.25	116.54	110.83
2	A	400	IPT	O5-C5-C6	3.19	114.34	106.44
2	B	400	IPT	C3-C4-C5	3.16	115.97	110.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	400	IPT	O3-C3-C4	3.06	117.59	110.38
2	C	400	IPT	O3-C3-C4	2.99	117.43	110.38
2	D	400	IPT	O4-C4-C5	-2.97	102.00	109.32
2	B	400	IPT	O3-C3-C2	-2.86	103.64	110.38
2	A	400	IPT	O4-C4-C5	-2.70	102.67	109.32
2	B	400	IPT	C3'-C1'-S1	2.66	117.79	110.12
2	C	400	IPT	C3'-C1'-C2'	-2.65	101.96	111.61
2	A	400	IPT	C3'-C1'-S1	2.54	117.42	110.12
2	D	400	IPT	C3'-C1'-S1	2.49	117.30	110.12
2	B	400	IPT	C1-O5-C5	2.44	116.93	112.56
2	B	400	IPT	O4-C4-C5	-2.38	103.47	109.32
2	A	400	IPT	C3-C4-C5	2.37	114.53	110.23
2	B	400	IPT	O5-C5-C6	2.36	112.29	106.44
2	A	400	IPT	O2-C2-C3	-2.33	104.89	110.38
2	C	400	IPT	O4-C4-C3	2.26	115.70	110.38
2	A	400	IPT	O6-C6-C5	2.12	118.55	111.33
2	A	400	IPT	O4-C4-C3	-2.03	105.60	110.38

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	B	400	IPT	O5-C1-S1-C1'
2	D	400	IPT	O5-C1-S1-C1'
2	D	400	IPT	O5-C5-C6-O6
2	B	400	IPT	O5-C5-C6-O6
2	A	400	IPT	C3'-C1'-S1-C1
2	B	400	IPT	C3'-C1'-S1-C1
2	D	400	IPT	C2'-C1'-S1-C1
2	D	400	IPT	C3'-C1'-S1-C1
2	A	400	IPT	C4-C5-C6-O6
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	B	400	IPT	3	0
2	C	400	IPT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section 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.