



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:50 PM UTC

PDB ID : 1NT4 / pdb_00001nt4
Title : Crystal structure of Escherichia coli periplasmic glucose-1-phosphatase H18A mutant complexed with glucose-1-phosphate
Authors : Lee, D.C.; Cottrill, M.A.; Forsberg, C.W.; Jia, Z.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on : 2003-01-28
Resolution : 2.40 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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
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

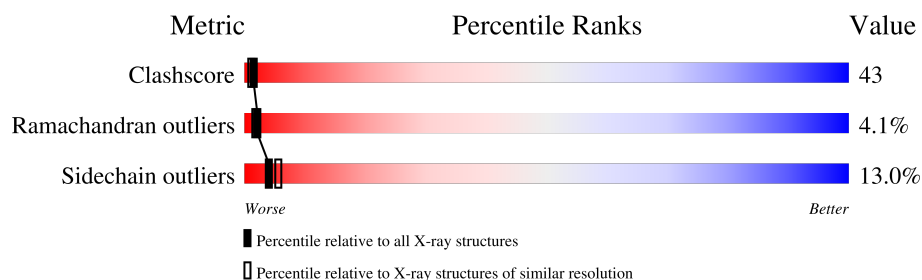
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

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	391	40% 47% 13% .
1	B	391	42% 45% 12% .

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	XGP	A	2000	-	-	X	-
2	XGP	B	2001	-	-	X	-

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6499 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.

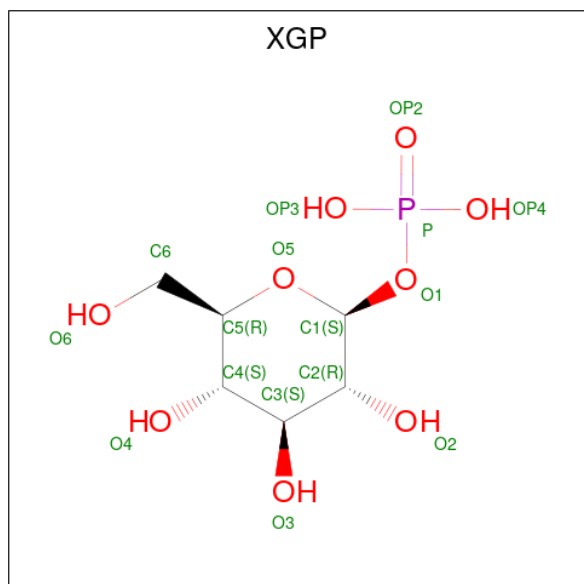
- Molecule 1 is a protein called Glucose-1-phosphatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	0	0
			3058	1935	513	593	17			
1	B	391	Total	C	N	O	S	0	0	0
			3058	1935	513	593	17			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	18	ALA	HIS	engineered mutation	UNP P19926
B	1018	ALA	HIS	engineered mutation	UNP P19926

- Molecule 2 is 1-O-phosphono-beta-D-glucopyranose (CCD ID: XGP) (formula: $C_6H_{13}O_9P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 3 is water.

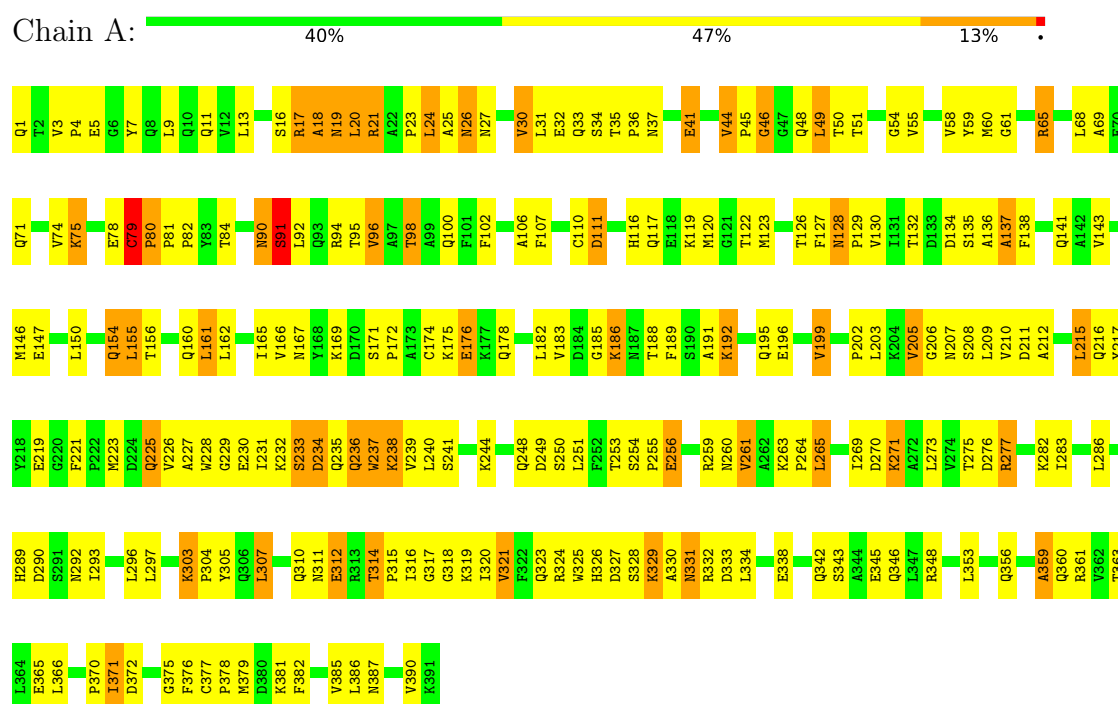
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	181	Total	O	0	0
			181	181		
3	B	170	Total	O	0	0
			170	170		

3 Residue-property plots

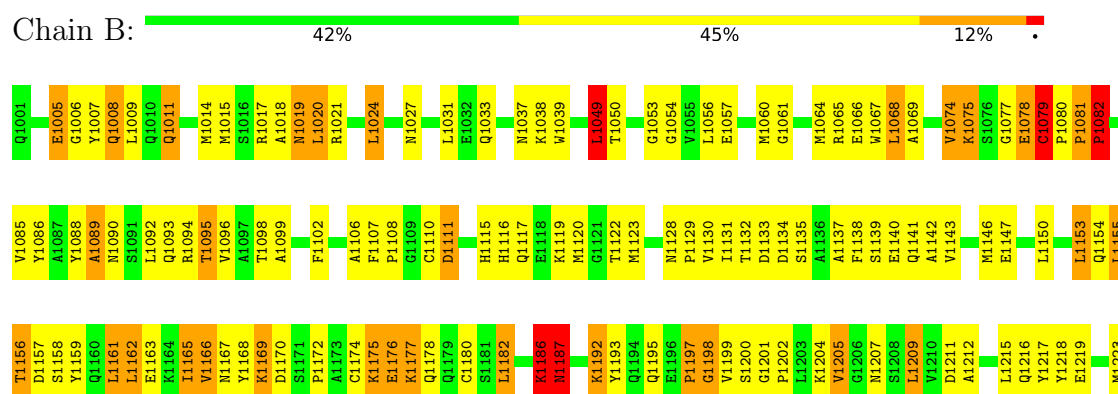
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: Glucose-1-phosphatase



• Molecule 1: Glucose-1-phosphatase





4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	156.26 Å 156.26 Å 84.58 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.40	Depositor
% Data completeness (in resolution range)	91.9 (30.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.218 , 0.284	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6499	wwPDB-VP
Average B, all atoms (Å ²)	30.0	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: XGP

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	0.47	0/3128	1.02	17/4248 (0.4%)
1	B	0.49	0/3128	1.08	23/4248 (0.5%)
All	All	0.48	0/6256	1.05	40/8496 (0.5%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	236	GLN	N-CA-C	-11.95	97.96	112.54
1	B	1236	GLN	N-CA-C	-10.68	99.92	113.16
1	B	1049	LEU	N-CA-C	9.83	123.23	111.33
1	B	1169	LYS	N-CA-C	-9.53	97.95	110.43
1	B	1081	PRO	CA-C-N	8.12	129.99	119.84
1	B	1081	PRO	C-N-CA	8.12	129.99	119.84
1	B	1356	GLN	N-CA-C	-7.68	97.06	109.96
1	A	79	CYS	CA-C-N	7.57	128.18	120.38
1	A	79	CYS	C-N-CA	7.57	128.18	120.38
1	B	1180	CYS	N-CA-C	7.01	121.14	112.59
1	B	1131	ILE	N-CA-C	-6.47	100.30	108.84
1	A	359	ALA	N-CA-C	-6.46	101.83	110.55
1	B	1079	CYS	CA-C-N	6.43	124.29	119.66
1	B	1079	CYS	C-N-CA	6.43	124.29	119.66
1	A	80	PRO	N-CA-C	6.42	118.53	110.70
1	B	1158	SER	N-CA-C	-6.33	104.48	111.82
1	A	137	ALA	N-CA-C	-6.16	104.68	111.82
1	B	1107	PHE	CA-C-N	6.15	127.53	119.84
1	B	1107	PHE	C-N-CA	6.15	127.53	119.84
1	B	1371	ILE	N-CA-C	5.97	116.56	110.05
1	B	1009	LEU	N-CA-C	-5.94	99.60	109.46
1	A	34	SER	N-CA-C	5.93	120.25	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	17	ARG	N-CA-C	5.71	119.92	111.87
1	A	318	GLY	N-CA-C	5.62	118.40	111.93
1	B	1130	VAL	N-CA-C	5.57	117.35	108.89
1	B	1177	LYS	N-CA-C	-5.50	104.49	113.19
1	A	81	PRO	CA-C-N	5.49	126.71	119.84
1	A	81	PRO	C-N-CA	5.49	126.71	119.84
1	B	1234	ASP	CB-CA-C	-5.43	109.33	115.79
1	A	37	ASN	N-CA-C	5.31	117.72	110.55
1	A	174	CYS	N-CA-C	-5.23	106.58	113.12
1	A	314	THR	CA-C-N	5.15	126.28	119.84
1	A	314	THR	C-N-CA	5.15	126.28	119.84
1	B	1082	PRO	N-CA-C	5.14	123.07	112.47
1	B	1165	ILE	CB-CA-C	-5.14	105.20	112.14
1	B	1008	GLN	N-CA-C	5.10	121.67	110.80
1	A	356	GLN	N-CA-C	-5.06	105.45	110.97
1	B	1137	ALA	N-CA-C	-5.04	105.78	111.28
1	B	1252	PHE	N-CA-C	5.03	120.26	113.72
1	A	283	ILE	N-CA-C	5.01	115.33	108.12

There are no chirality outliers.

There are no planarity outliers.

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	3058	0	2996	253	0
1	B	3058	0	2993	270	0
2	A	16	0	10	6	0
2	B	16	0	10	6	0
3	A	181	0	0	21	0
3	B	170	0	0	14	0
All	All	6499	0	6009	525	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 43.

All (525) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:ARG:HH12	1:A:334:LEU:HD11	1.17	1.08
1:A:223:MET:HB3	1:A:232:LYS:HD2	1.37	1.07
1:A:186:LYS:H	1:A:186:LYS:HD2	1.19	1.03
1:B:1231:ILE:CD1	1:B:1232:LYS:H	1.73	1.02
1:B:1277:ARG:HD2	1:B:1324:ARG:HH21	1.26	1.00
1:B:1231:ILE:HD13	1:B:1232:LYS:H	1.25	1.00
1:B:1031:LEU:HD13	1:B:1209:LEU:HD12	1.44	0.98
1:B:1186:LYS:HG2	1:B:1187:ASN:H	1.29	0.98
1:A:199:VAL:HG22	1:A:251:LEU:HD21	1.48	0.96
1:A:92:LEU:O	1:A:96:VAL:HG12	1.67	0.95
1:B:1186:LYS:O	1:B:1187:ASN:HB2	1.67	0.94
1:B:1343:SER:H	1:B:1346:GLN:HE21	1.00	0.93
1:B:1310:GLN:HG2	1:B:1315:PRO:HG3	1.50	0.92
1:B:1227:ALA:HB3	1:B:1231:ILE:HG13	1.51	0.92
1:B:1343:SER:H	1:B:1346:GLN:NE2	1.68	0.91
1:B:1293:ILE:HG23	1:B:1320:ILE:HD11	1.51	0.91
1:B:1289:HIS:CG	2:B:2001:XGP:O6	2.24	0.91
1:A:223:MET:HE2	1:A:223:MET:HA	1.52	0.91
1:A:49:LEU:HD23	1:A:98:THR:HG22	1.55	0.89
1:A:199:VAL:HG11	1:A:203:LEU:HD23	1.56	0.87
1:B:1005:GLU:CD	1:B:1006:GLY:H	1.81	0.87
1:A:169:LYS:O	1:A:169:LYS:HD3	1.75	0.86
2:A:2000:XGP:H6	3:A:3181:HOH:O	1.74	0.86
1:B:1011:GLN:HE21	1:B:1277:ARG:HD3	1.41	0.85
1:B:1277:ARG:HD2	1:B:1324:ARG:NH2	1.91	0.85
1:B:1343:SER:N	1:B:1346:GLN:HE21	1.75	0.85
1:B:1146:MET:HE1	1:B:1197:PRO:O	1.77	0.85
1:B:1019:ASN:HD22	1:B:1020:LEU:H	1.19	0.84
1:A:90:ASN:H	1:A:90:ASN:HD22	1.22	0.84
1:A:5:GLU:CD	1:A:5:GLU:H	1.85	0.83
1:B:1234:ASP:OD2	1:B:1236:GLN:HG3	1.79	0.83
1:A:332:ARG:NH1	1:A:334:LEU:HD11	1.95	0.81
1:A:132:THR:H	1:A:260:ASN:HD21	1.27	0.80
1:A:310:GLN:HG2	1:A:315:PRO:HG3	1.62	0.79
1:A:35:THR:HB	1:A:166:VAL:HG13	1.65	0.79
1:B:1226:VAL:O	1:B:1231:ILE:HD11	1.83	0.78
1:B:1289:HIS:ND1	2:B:2001:XGP:OP4	2.15	0.78
1:A:79:CYS:SG	1:A:80:PRO:HD2	2.25	0.77
1:A:192:LYS:CD	1:A:195:GLN:HB2	2.14	0.77
1:A:289:HIS:CG	2:A:2000:XGP:O6	2.37	0.77
1:B:1238:LYS:HD2	1:B:1311:ASN:ND2	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:LYS:H	1:A:186:LYS:CD	1.89	0.77
1:B:1332:ARG:HE	1:B:1334:LEU:HD21	1.50	0.76
1:B:1132:THR:H	1:B:1260:ASN:HD21	1.33	0.76
1:B:1192:LYS:HD3	1:B:1195:GLN:NE2	2.01	0.76
1:A:366:LEU:HD23	1:A:385:VAL:HG11	1.68	0.75
1:B:1031:LEU:HD12	1:B:1039:TRP:CZ2	2.21	0.74
1:A:303:LYS:HG3	1:A:304:PRO:HD2	1.69	0.74
1:A:19:ASN:HD22	1:A:20:LEU:H	1.33	0.74
1:A:227:ALA:HB3	1:A:231:ILE:HG22	1.68	0.73
1:B:1169:LYS:O	1:B:1170:ASP:HB2	1.88	0.73
1:A:90:ASN:HB3	1:A:127:PHE:CD2	2.24	0.73
1:A:119:LYS:HE2	1:A:122:THR:HG21	1.69	0.73
1:B:1238:LYS:HD2	1:B:1311:ASN:HD21	1.50	0.72
1:B:1265:LEU:O	1:B:1269:ILE:HG12	1.89	0.72
1:A:186:LYS:HD2	1:A:186:LYS:N	1.98	0.72
1:B:1186:LYS:HD2	1:B:1186:LYS:N	2.05	0.72
1:B:1231:ILE:CD1	1:B:1232:LYS:N	2.52	0.72
1:B:1270:ASP:O	1:B:1274:VAL:HG13	1.90	0.72
1:A:161:LEU:HD11	1:A:236:GLN:HB3	1.71	0.71
1:A:265:LEU:O	1:A:269:ILE:HG12	1.90	0.71
1:A:17:ARG:HD2	1:A:314:THR:HG22	1.73	0.71
1:A:25:ALA:HB2	1:A:46:GLY:HA2	1.73	0.71
1:A:233:SER:HB3	1:A:236:GLN:NE2	2.06	0.71
1:B:1186:LYS:HD2	1:B:1186:LYS:H	1.54	0.71
1:A:90:ASN:HB3	1:A:127:PHE:HD2	1.56	0.71
1:B:1146:MET:CE	1:B:1197:PRO:HB2	2.21	0.71
1:A:51:THR:O	1:A:55:VAL:HG23	1.90	0.71
1:A:377:CYS:SG	1:A:378:PRO:HD2	2.30	0.70
1:B:1186:LYS:CG	1:B:1187:ASN:H	2.03	0.70
1:B:1293:ILE:HG23	1:B:1320:ILE:CD1	2.22	0.70
1:A:44:VAL:HG13	1:A:48:GLN:HB2	1.74	0.70
1:B:1088:TYR:O	1:B:1089:ALA:HB3	1.91	0.69
1:B:1135:SER:HB3	1:B:1138:PHE:HB3	1.72	0.69
1:A:249:ASP:O	1:A:253:THR:HB	1.92	0.69
1:B:1031:LEU:HD12	1:B:1039:TRP:CH2	2.27	0.69
1:A:166:VAL:HG21	1:A:209:LEU:HD23	1.75	0.69
1:B:1231:ILE:O	1:B:1233:SER:N	2.26	0.69
1:A:17:ARG:O	1:A:17:ARG:HG2	1.93	0.68
1:A:165:ILE:HG23	1:A:230:GLU:CB	2.24	0.68
1:A:18:ALA:HA	1:A:98:THR:HG21	1.76	0.68
1:B:1249:ASP:O	1:B:1253:THR:HB	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1289:HIS:CB	2:B:2001:XGP:O6	2.41	0.68
1:A:192:LYS:HD3	1:A:195:GLN:HB2	1.75	0.68
1:B:1110:CYS:O	1:B:1111:ASP:HB2	1.93	0.68
1:A:123:MET:HE3	1:A:128:ASN:HA	1.77	0.67
1:B:1049:LEU:HD13	1:B:1050:THR:O	1.93	0.67
1:A:143:VAL:O	1:A:147:GLU:HG3	1.95	0.67
1:B:1314:THR:O	1:B:1314:THR:HG22	1.95	0.67
1:B:1018:ALA:O	1:B:1316:ILE:O	2.12	0.66
1:B:1227:ALA:CB	1:B:1231:ILE:HG13	2.24	0.66
1:B:1020:LEU:O	1:B:1049:LEU:O	2.13	0.66
1:B:1098:THR:HG23	1:B:1287:VAL:HG11	1.78	0.66
1:B:1186:LYS:H	1:B:1186:LYS:HZ3	1.43	0.66
1:A:94:ARG:O	1:A:98:THR:HG23	1.96	0.66
1:B:1290:ASP:HB2	1:B:1314:THR:HG21	1.78	0.66
1:B:1186:LYS:HG2	1:B:1187:ASN:N	2.08	0.65
1:A:226:VAL:HG23	1:A:226:VAL:O	1.96	0.65
1:A:18:ALA:O	1:A:316:ILE:O	2.15	0.65
1:B:1015:MET:HG3	1:B:1293:ILE:CD1	2.26	0.65
1:B:1371:ILE:HD11	3:B:3175:HOH:O	1.96	0.65
1:A:270:ASP:HB2	1:A:386:LEU:HB3	1.79	0.65
1:A:233:SER:HB3	1:A:236:GLN:HE21	1.61	0.65
1:A:175:LYS:O	1:A:176:GLU:HB2	1.97	0.65
1:A:19:ASN:ND2	1:A:20:LEU:H	1.95	0.65
1:B:1011:GLN:NE2	1:B:1277:ARG:NH1	2.45	0.65
1:B:1128:ASN:HD22	1:B:1129:PRO:HD2	1.61	0.65
1:A:96:VAL:O	1:A:100:GLN:HG3	1.95	0.64
1:B:1119:LYS:HD3	1:B:1122:THR:HG21	1.79	0.64
1:A:20:LEU:HD11	1:A:219:GLU:HA	1.78	0.64
1:A:65:ARG:HH21	1:A:74:VAL:HG11	1.61	0.64
1:A:192:LYS:HD2	1:A:192:LYS:O	1.98	0.64
1:A:324:ARG:HD3	1:A:379:MET:HE2	1.78	0.64
1:B:1186:LYS:H	1:B:1186:LYS:CD	2.11	0.64
1:B:1172:PRO:O	1:B:1176:GLU:HB3	1.98	0.63
1:A:20:LEU:HD23	1:A:215:LEU:HD12	1.81	0.63
1:B:1384:SER:O	1:B:1388:GLU:HB2	1.99	0.63
1:B:1175:LYS:HD2	1:B:1175:LYS:O	1.98	0.63
1:A:156:THR:O	1:A:160:GLN:HG3	1.99	0.62
1:A:212:ALA:O	1:A:216:GLN:HG3	1.98	0.62
1:A:5:GLU:CD	1:A:5:GLU:N	2.57	0.62
1:B:1015:MET:HE3	1:B:1265:LEU:HG	1.81	0.62
1:A:175:LYS:O	1:A:176:GLU:CB	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:PRO:HG2	1:A:256:GLU:OE2	1.99	0.62
1:A:254:SER:HB3	3:A:3061:HOH:O	2.00	0.62
1:B:1366:LEU:HD23	1:B:1385:VAL:HG11	1.81	0.62
1:A:221:PHE:HB3	1:A:225:GLN:HB3	1.82	0.62
1:A:343:SER:H	1:A:346:GLN:NE2	1.98	0.62
1:B:1088:TYR:O	1:B:1115:HIS:O	2.18	0.61
1:B:1202:PRO:HA	1:B:1205:VAL:CG1	2.30	0.61
1:B:1346:GLN:NE2	1:B:1360:GLN:HE21	1.98	0.61
1:B:1289:HIS:CD2	2:B:2001:XGP:O6	2.53	0.61
1:B:1086:TYR:HB2	1:B:1281:PRO:HG3	1.82	0.61
1:A:231:ILE:HG13	1:A:240:LEU:HD12	1.83	0.61
1:B:1310:GLN:NE2	1:B:1312:GLU:HG2	2.15	0.61
1:A:232:LYS:O	1:A:233:SER:HB3	1.99	0.61
1:A:146:MET:HG2	1:A:250:SER:O	2.00	0.61
1:A:146:MET:HE2	1:A:189:PHE:CD1	2.36	0.61
1:B:1212:ALA:O	1:B:1216:GLN:HG3	2.00	0.61
1:A:21:ARG:HA	1:A:49:LEU:HA	1.82	0.61
1:A:165:ILE:HG23	1:A:230:GLU:HB2	1.83	0.61
1:B:1015:MET:HG3	1:B:1293:ILE:HD13	1.83	0.60
1:B:1060:MET:HE1	1:B:1341:TYR:HA	1.83	0.60
1:B:1165:ILE:HG23	1:B:1230:GLU:HB2	1.83	0.60
1:B:1310:GLN:HE21	1:B:1312:GLU:H	1.50	0.60
1:A:21:ARG:NH2	1:A:24:LEU:HD13	2.17	0.60
1:B:1090:ASN:N	1:B:1095:THR:HG21	2.16	0.60
1:B:1253:THR:O	1:B:1298:THR:HG21	2.01	0.60
1:B:1219:GLU:HA	1:B:1219:GLU:OE1	2.02	0.59
1:A:277:ARG:HB3	1:A:324:ARG:HH12	1.66	0.59
1:B:1011:GLN:HB3	1:B:1277:ARG:NH1	2.17	0.59
1:A:192:LYS:HD3	1:A:195:GLN:OE1	2.02	0.59
1:B:1098:THR:CG2	1:B:1287:VAL:HG11	2.33	0.59
1:B:1255:PRO:O	1:B:1259:ARG:HG2	2.01	0.59
1:B:1123:MET:HE2	1:B:1128:ASN:HA	1.84	0.59
1:A:273:LEU:O	1:A:277:ARG:HG2	2.03	0.59
1:B:1019:ASN:ND2	1:B:1020:LEU:H	1.97	0.59
1:A:21:ARG:HD2	1:A:94:ARG:HD2	1.85	0.59
1:A:71:GLN:OE1	1:A:325:TRP:HH2	1.86	0.59
1:B:1146:MET:HE1	1:B:1197:PRO:HB2	1.84	0.58
1:A:165:ILE:HG23	1:A:230:GLU:HB3	1.84	0.58
1:A:232:LYS:HG3	3:A:3040:HOH:O	2.02	0.58
1:A:126:THR:O	1:A:265:LEU:HD13	2.03	0.58
1:B:1232:LYS:O	1:B:1233:SER:C	2.46	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:LYS:HB2	1:A:303:LYS:NZ	2.19	0.58
1:B:1138:PHE:HA	1:B:1141:GLN:NE2	2.19	0.58
1:A:227:ALA:HB3	1:A:231:ILE:CG2	2.33	0.58
1:A:334:LEU:HD23	1:A:378:PRO:HA	1.86	0.58
1:B:1192:LYS:HD2	1:B:1192:LYS:O	2.04	0.58
1:B:1078:GLU:O	1:B:1079:CYS:HB2	2.02	0.58
1:B:1316:ILE:CG2	1:B:1317:GLY:N	2.67	0.58
1:B:1192:LYS:CD	1:B:1195:GLN:HB2	2.34	0.57
1:B:1135:SER:HB3	1:B:1138:PHE:CB	2.33	0.57
1:B:1290:ASP:CB	1:B:1314:THR:HG21	2.34	0.57
1:B:1316:ILE:HG23	1:B:1317:GLY:N	2.18	0.57
1:B:1379:MET:HE3	1:B:1383:ASP:OD2	2.05	0.57
1:A:231:ILE:HG13	1:A:240:LEU:CD1	2.35	0.57
1:B:1098:THR:HB	3:B:3183:HOH:O	2.04	0.57
1:A:110:CYS:O	1:A:111:ASP:CB	2.53	0.57
1:B:1020:LEU:O	1:B:1049:LEU:HD22	2.04	0.57
1:B:1057:GLU:OE2	1:B:1102:PHE:HB2	2.05	0.57
1:B:1217:TYR:CE2	1:B:1348:ARG:HG3	2.39	0.57
1:A:223:MET:HE3	1:A:348:ARG:NH2	2.19	0.57
1:A:65:ARG:HH21	1:A:74:VAL:CG1	2.18	0.57
1:B:1174:CYS:O	1:B:1178:GLN:HA	2.04	0.57
1:B:1343:SER:OG	1:B:1346:GLN:HG3	2.05	0.56
1:A:17:ARG:NH2	1:A:316:ILE:HA	2.21	0.56
1:A:49:LEU:HD13	1:A:50:THR:O	2.04	0.56
1:A:269:ILE:CG2	1:A:273:LEU:HD22	2.36	0.56
1:B:1021:ARG:NH1	1:B:1024:LEU:HD13	2.20	0.56
1:A:74:VAL:HG12	1:A:75:LYS:N	2.21	0.56
1:A:84:THR:HG23	1:A:282:LYS:HD2	1.86	0.56
1:A:21:ARG:CZ	1:A:24:LEU:HD13	2.36	0.56
1:B:1011:GLN:HE21	1:B:1277:ARG:CD	2.16	0.56
1:B:1134:ASP:HB3	1:B:1193:TYR:CG	2.41	0.56
1:B:1186:LYS:N	1:B:1186:LYS:HZ3	2.03	0.56
1:B:1223:MET:HE2	1:B:1232:LYS:HD3	1.87	0.56
1:B:1142:ALA:O	1:B:1146:MET:HG3	2.07	0.56
1:B:1227:ALA:HB3	1:B:1231:ILE:CG1	2.32	0.55
1:B:1165:ILE:HG23	1:B:1230:GLU:CB	2.36	0.55
1:A:27:ASN:O	1:A:31:LEU:HD13	2.06	0.55
1:A:165:ILE:HD13	1:A:231:ILE:HA	1.87	0.55
1:A:271:LYS:HA	1:A:275:THR:OG1	2.07	0.55
1:A:4:PRO:HG2	1:A:7:TYR:CE1	2.41	0.55
1:A:381:LYS:O	1:A:385:VAL:HG23	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:ASP:HA	1:A:314:THR:HG21	1.89	0.55
2:A:2000:XGP:C6	3:A:3181:HOH:O	2.44	0.55
1:B:1202:PRO:HA	1:B:1205:VAL:HG13	1.89	0.55
1:B:1075:LYS:HE2	1:B:1075:LYS:HA	1.89	0.54
1:B:1005:GLU:CD	1:B:1006:GLY:N	2.60	0.54
1:A:90:ASN:HD21	1:A:95:THR:HG21	1.71	0.54
1:A:146:MET:HE2	1:A:189:PHE:HD1	1.71	0.54
1:B:1011:GLN:CB	1:B:1277:ARG:NH1	2.70	0.54
1:B:1192:LYS:HD3	1:B:1195:GLN:CD	2.32	0.54
1:A:167:ASN:C	1:A:167:ASN:HD22	2.16	0.54
1:B:1231:ILE:O	1:B:1232:LYS:C	2.50	0.54
1:B:1223:MET:SD	1:B:1348:ARG:NH2	2.80	0.54
1:A:189:PHE:CE1	1:A:199:VAL:HG13	2.42	0.54
1:A:202:PRO:HA	1:A:205:VAL:CG1	2.38	0.54
1:A:303:LYS:HG3	1:A:304:PRO:CD	2.37	0.54
1:B:1006:GLY:O	1:B:1007:TYR:HB2	2.08	0.54
1:B:1297:LEU:CD1	1:B:1320:ILE:HD13	2.38	0.53
1:B:1086:TYR:CB	1:B:1281:PRO:HG3	2.39	0.53
1:B:1065:ARG:HG2	1:B:1065:ARG:HH11	1.73	0.53
1:A:321:VAL:O	1:A:321:VAL:CG2	2.56	0.53
1:A:365:GLU:OE1	1:A:370:PRO:HA	2.09	0.53
1:A:17:ARG:O	1:A:17:ARG:CG	2.56	0.53
1:A:248:GLN:HE22	1:A:290:ASP:HB2	1.73	0.53
1:A:21:ARG:HH21	1:A:23:PRO:HA	1.73	0.53
1:A:91:SER:HB2	1:A:120:MET:HA	1.91	0.53
1:B:1271:LYS:HA	1:B:1275:THR:OG1	2.08	0.53
1:B:1085:VAL:HG13	1:B:1283:ILE:HG22	1.91	0.52
1:A:263:LYS:HE2	1:A:264:PRO:HD3	1.90	0.52
1:B:1186:LYS:NZ	1:B:1186:LYS:HB3	2.24	0.52
1:A:175:LYS:NZ	1:A:175:LYS:HB3	2.24	0.52
1:A:310:GLN:HE21	1:A:312:GLU:HG2	1.74	0.52
1:B:1153:LEU:HB3	1:B:1155:LEU:HD13	1.91	0.52
1:A:45:PRO:O	1:A:46:GLY:C	2.52	0.52
1:A:75:LYS:N	1:A:75:LYS:HD3	2.25	0.52
1:A:13:LEU:HD23	1:A:13:LEU:C	2.34	0.52
1:A:41:GLU:HG2	3:A:3057:HOH:O	2.10	0.52
1:A:44:VAL:CG1	1:A:48:GLN:HB2	2.39	0.52
1:B:1199:VAL:HG22	1:B:1200:SER:N	2.25	0.52
1:B:1162:LEU:O	1:B:1166:VAL:HB	2.09	0.52
1:A:74:VAL:CG1	1:A:75:LYS:N	2.73	0.52
1:A:74:VAL:HG13	3:A:3030:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1011:GLN:HB3	1:B:1277:ARG:HH12	1.73	0.52
1:B:1015:MET:CE	1:B:1265:LEU:HG	2.40	0.52
1:B:1116:HIS:HD2	1:B:1117:GLN:O	1.91	0.52
1:A:90:ASN:HD22	1:A:90:ASN:N	1.94	0.52
1:B:1146:MET:HE3	1:B:1197:PRO:HB2	1.92	0.52
1:A:24:LEU:HG	1:A:26:ASN:ND2	2.25	0.52
1:A:75:LYS:HG2	3:A:3030:HOH:O	2.08	0.52
1:A:235:GLN:OE1	1:A:235:GLN:HA	2.10	0.51
1:A:320:ILE:N	1:A:320:ILE:HD12	2.25	0.51
1:B:1186:LYS:N	1:B:1186:LYS:CD	2.73	0.51
1:A:17:ARG:CZ	1:A:316:ILE:HD12	2.40	0.51
1:A:165:ILE:HD12	1:A:240:LEU:HD11	1.92	0.51
1:A:69:ALA:HA	1:A:74:VAL:O	2.09	0.51
1:B:1088:TYR:O	1:B:1089:ALA:CB	2.56	0.51
1:A:137:ALA:O	1:A:141:GLN:HG3	2.11	0.51
1:A:205:VAL:O	1:A:209:LEU:HD13	2.11	0.51
1:B:1167:ASN:O	1:B:1169:LYS:O	2.28	0.51
1:A:110:CYS:O	1:A:111:ASP:HB2	2.10	0.51
1:A:128:ASN:HD22	1:A:129:PRO:HD2	1.74	0.51
1:B:1065:ARG:HE	1:B:1074:VAL:CG1	2.23	0.51
1:A:49:LEU:CD2	1:A:98:THR:HG22	2.35	0.51
1:A:263:LYS:HE2	3:A:3038:HOH:O	2.10	0.51
1:A:217:TYR:CE2	1:A:348:ARG:HD2	2.46	0.51
1:B:1074:VAL:HG22	1:B:1080:PRO:HB3	1.93	0.51
1:A:134:ASP:HA	3:A:3154:HOH:O	2.10	0.50
1:A:192:LYS:HD3	1:A:195:GLN:CB	2.41	0.50
1:A:371:ILE:HG13	1:A:375:GLY:C	2.35	0.50
1:A:4:PRO:HG2	1:A:7:TYR:CD1	2.46	0.50
1:B:1138:PHE:C	1:B:1138:PHE:CD1	2.89	0.50
1:A:327:ASP:OD2	1:A:327:ASP:C	2.53	0.50
1:B:1365:GLU:HB2	1:B:1371:ILE:HD12	1.93	0.50
1:A:154:GLN:C	1:A:155:LEU:HD13	2.36	0.50
1:A:155:LEU:N	1:A:155:LEU:HD22	2.27	0.50
1:B:1066:GLU:HB3	1:B:1355:LEU:HG	1.93	0.50
1:B:1277:ARG:CZ	1:B:1324:ARG:HE	2.25	0.50
1:A:11:GLN:NE2	1:A:324:ARG:NH1	2.60	0.50
1:A:256:GLU:H	1:A:256:GLU:CD	2.19	0.50
1:B:1326:HIS:HE1	1:B:1328:SER:HA	1.76	0.50
1:A:333:ASP:O	1:A:334:LEU:HD23	2.11	0.50
1:A:17:ARG:O	1:A:18:ALA:O	2.29	0.50
1:A:18:ALA:CA	1:A:98:THR:HG21	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1231:ILE:HD12	1:B:1232:LYS:H	1.72	0.50
1:A:256:GLU:HA	1:A:259:ARG:NH2	2.27	0.49
1:B:1011:GLN:NE2	1:B:1277:ARG:HD3	2.20	0.49
1:B:1155:LEU:HG	1:B:1243:LEU:HD23	1.93	0.49
1:B:1088:TYR:HB3	1:B:1286:LEU:HD12	1.93	0.49
1:B:1377:CYS:SG	1:B:1378:PRO:HD2	2.52	0.49
1:B:1139:SER:O	1:B:1143:VAL:HG23	2.12	0.49
1:B:1143:VAL:O	1:B:1147:GLU:HG3	2.12	0.49
1:B:1155:LEU:O	1:B:1157:ASP:N	2.46	0.49
1:B:1335:MET:HG2	1:B:1382:PHE:CD1	2.48	0.49
1:A:3:VAL:HG21	1:A:325:TRP:CZ3	2.48	0.49
1:A:226:VAL:O	1:A:226:VAL:CG2	2.60	0.49
1:B:1133:ASP:C	1:B:1135:SER:H	2.20	0.49
1:A:343:SER:H	1:A:346:GLN:HE21	1.59	0.49
1:B:1011:GLN:CD	1:B:1277:ARG:NH1	2.70	0.49
1:B:1291:SER:OG	2:B:2001:XGP:H5	2.13	0.49
1:A:232:LYS:O	1:A:236:GLN:NE2	2.46	0.49
1:B:1207:ASN:O	1:B:1211:ASP:HB2	2.13	0.49
1:B:1231:ILE:HD12	1:B:1232:LYS:N	2.28	0.48
1:A:221:PHE:O	1:A:348:ARG:NH2	2.46	0.48
1:B:1226:VAL:O	1:B:1226:VAL:HG13	2.13	0.48
1:B:1106:ALA:C	1:B:1108:PRO:HD3	2.38	0.48
1:B:1310:GLN:HE21	1:B:1312:GLU:HG2	1.77	0.48
1:A:206:GLY:O	1:A:210:VAL:HG23	2.13	0.48
1:A:59:TYR:HB3	1:A:353:LEU:HB2	1.96	0.48
1:B:1169:LYS:HG2	3:B:3186:HOH:O	2.14	0.48
1:A:20:LEU:HD11	1:A:219:GLU:CA	2.43	0.48
1:A:79:CYS:SG	1:A:107:PHE:HB3	2.53	0.48
1:B:1049:LEU:O	1:B:1050:THR:HG23	2.14	0.48
1:B:1031:LEU:HD21	3:B:3012:HOH:O	2.14	0.48
1:B:1186:LYS:O	1:B:1187:ASN:CB	2.49	0.48
1:A:248:GLN:NE2	1:A:290:ASP:HB2	2.29	0.48
1:B:1020:LEU:HA	1:B:1316:ILE:HG12	1.96	0.48
1:B:1159:TYR:O	1:B:1163:GLU:HG3	2.14	0.48
1:B:1186:LYS:H	1:B:1186:LYS:NZ	2.10	0.47
1:A:21:ARG:O	1:A:215:LEU:HG	2.14	0.47
1:A:305:TYR:CD1	1:A:307:LEU:HD13	2.49	0.47
1:B:1049:LEU:C	1:B:1050:THR:HG23	2.39	0.47
1:B:1192:LYS:HD2	1:B:1195:GLN:HB2	1.96	0.47
1:A:30:VAL:HG12	3:A:3091:HOH:O	2.14	0.47
1:B:1049:LEU:HD23	3:B:3183:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:GLN:O	1:A:171:SER:HB2	2.14	0.47
1:A:35:THR:HA	1:A:171:SER:HB3	1.96	0.47
1:A:303:LYS:CG	1:A:304:PRO:HD2	2.42	0.47
1:A:155:LEU:HD22	1:A:155:LEU:H	1.79	0.47
1:A:326:HIS:NE2	1:A:331:ASN:ND2	2.63	0.47
1:A:332:ARG:NH1	1:A:334:LEU:HD21	2.30	0.47
1:B:1094:ARG:O	1:B:1098:THR:HG22	2.14	0.47
1:B:1037:ASN:C	1:B:1038:LYS:HE2	2.39	0.47
1:B:1146:MET:CE	1:B:1251:LEU:HA	2.45	0.47
1:B:1270:ASP:OD1	1:B:1386:LEU:HB3	2.14	0.47
1:B:1310:GLN:HG2	1:B:1315:PRO:CG	2.34	0.47
1:A:130:VAL:HB	1:A:195:GLN:N	2.30	0.47
1:A:289:HIS:CB	2:A:2000:XGP:O6	2.62	0.47
1:A:321:VAL:CG2	1:A:323:GLN:HE21	2.28	0.47
1:B:1033:GLN:HA	1:B:1172:PRO:HG2	1.97	0.47
1:B:1357:ALA:N	1:B:1358:PRO:HD3	2.29	0.47
1:A:271:LYS:O	1:A:276:ASP:HB2	2.15	0.47
1:A:342:GLN:HA	1:A:346:GLN:NE2	2.30	0.47
1:B:1168:TYR:C	1:B:1169:LYS:O	2.53	0.47
1:A:135:SER:C	1:A:137:ALA:H	2.23	0.47
1:B:1161:LEU:O	1:B:1165:ILE:HG12	2.15	0.47
1:B:1326:HIS:ND1	1:B:1326:HIS:C	2.73	0.47
1:A:21:ARG:HD2	1:A:94:ARG:CD	2.44	0.47
1:A:116:HIS:CE1	1:A:120:MET:HE1	2.50	0.47
1:A:223:MET:HE2	1:A:223:MET:CA	2.35	0.47
1:A:314:THR:HG22	1:A:314:THR:O	2.15	0.47
1:A:231:ILE:HG12	1:A:231:ILE:O	2.15	0.46
1:A:386:LEU:O	1:A:390:VAL:HG23	2.15	0.46
1:B:1146:MET:HE2	1:B:1251:LEU:HD23	1.96	0.46
1:B:1289:HIS:HB2	2:B:2001:XGP:O6	2.14	0.46
1:B:1326:HIS:CE1	1:B:1328:SER:HA	2.49	0.46
1:B:1264:PRO:HG2	3:B:3065:HOH:O	2.14	0.46
1:B:1014:MET:HE1	1:B:1064:MET:CE	2.45	0.46
1:B:1168:TYR:O	1:B:1169:LYS:C	2.59	0.46
1:B:1297:LEU:HD11	1:B:1320:ILE:HD13	1.97	0.46
1:A:74:VAL:HG12	1:A:75:LYS:O	2.14	0.46
1:B:1049:LEU:HD11	1:B:1054:GLY:N	2.30	0.46
1:B:1331:ASN:OD1	1:B:1331:ASN:O	2.33	0.46
1:B:1017:ARG:HG2	1:B:1018:ALA:N	2.30	0.46
1:B:1293:ILE:CG2	1:B:1320:ILE:HD11	2.35	0.46
1:B:1309:ASP:HB3	1:B:1343:SER:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1357:ALA:N	1:B:1358:PRO:CD	2.78	0.46
1:B:1011:GLN:CB	1:B:1277:ARG:HH11	2.27	0.46
1:A:207:ASN:O	1:A:211:ASP:HB2	2.16	0.46
1:B:1014:MET:HE1	1:B:1064:MET:HE3	1.98	0.46
1:B:1354:THR:OG1	1:B:1356:GLN:O	2.30	0.46
1:A:138:PHE:CD1	1:A:138:PHE:C	2.94	0.46
1:A:238:LYS:O	1:A:238:LYS:NZ	2.38	0.46
1:B:1064:MET:O	1:B:1068:LEU:HB2	2.16	0.46
1:B:1186:LYS:HZ3	1:B:1186:LYS:HB3	1.78	0.46
1:B:1254:SER:HB3	1:B:1257:VAL:HG13	1.98	0.46
1:B:1274:VAL:HG22	1:B:1275:THR:N	2.31	0.45
1:B:1359:ALA:HA	3:B:3191:HOH:O	2.16	0.45
1:A:192:LYS:HD2	1:A:195:GLN:HB2	1.93	0.45
1:B:1356:GLN:O	1:B:1357:ALA:HB3	2.16	0.45
1:A:35:THR:OG1	1:A:36:PRO:HD2	2.16	0.45
1:A:196:GLU:OE2	2:A:2000:XGP:O4	2.35	0.45
1:A:316:ILE:CG2	1:A:317:GLY:N	2.79	0.45
1:A:292:ASN:O	1:A:296:LEU:HB2	2.17	0.45
1:B:1310:GLN:NE2	1:B:1312:GLU:CG	2.78	0.45
1:A:31:LEU:HD11	1:A:208:SER:HB3	1.98	0.45
1:A:32:GLU:HA	3:A:3218:HOH:O	2.17	0.45
1:B:1233:SER:HB2	1:B:1236:GLN:OE1	2.17	0.45
1:B:1067:TRP:CE3	1:B:1068:LEU:HD12	2.52	0.45
1:A:227:ALA:O	1:A:230:GLU:HB2	2.17	0.45
1:A:310:GLN:NE2	1:A:312:GLU:CG	2.80	0.45
1:A:310:GLN:NE2	1:A:312:GLU:HG2	2.32	0.45
1:B:1197:PRO:O	1:B:1198:GLY:O	2.35	0.45
1:A:54:GLY:O	1:A:58:VAL:HG23	2.17	0.45
1:A:65:ARG:HD2	1:A:106:ALA:O	2.17	0.45
1:A:269:ILE:O	1:A:273:LEU:HB2	2.17	0.45
1:A:293:ILE:HG21	1:A:320:ILE:HD11	1.98	0.45
1:A:310:GLN:HE21	1:A:312:GLU:CG	2.29	0.45
1:A:61:GLY:HA2	1:A:102:PHE:CE1	2.52	0.44
1:A:136:ALA:N	3:A:3203:HOH:O	2.49	0.44
1:A:189:PHE:CD1	1:A:199:VAL:HG13	2.52	0.44
1:A:229:GLY:O	1:A:232:LYS:HB2	2.17	0.44
1:A:321:VAL:O	1:A:321:VAL:HG23	2.17	0.44
1:B:1057:GLU:HG2	1:B:1098:THR:O	2.16	0.44
1:B:1177:LYS:HD2	3:B:3287:HOH:O	2.17	0.44
1:A:377:CYS:SG	1:A:378:PRO:CD	3.05	0.44
1:B:1146:MET:HE2	1:B:1251:LEU:HA	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:LEU:HD13	1:A:273:LEU:HD13	1.98	0.44
1:B:1305:TYR:CD2	1:B:1307:LEU:HD13	2.53	0.44
1:B:1363:THR:HG22	3:B:3151:HOH:O	2.17	0.44
1:A:223:MET:O	1:A:226:VAL:HG22	2.17	0.44
1:B:1085:VAL:HG13	1:B:1283:ILE:CG2	2.48	0.44
1:A:129:PRO:C	1:A:261:VAL:HG22	2.43	0.44
1:B:1027:ASN:O	1:B:1031:LEU:HD23	2.17	0.44
1:B:1138:PHE:C	1:B:1140:GLU:N	2.73	0.44
1:B:1201:GLY:O	1:B:1205:VAL:HG12	2.17	0.44
1:A:9:LEU:HD13	1:A:325:TRP:CE2	2.52	0.44
1:B:1074:VAL:HG22	3:B:3070:HOH:O	2.17	0.44
1:A:60:MET:HE1	1:A:359:ALA:CB	2.48	0.44
1:B:1090:ASN:ND2	1:B:1092:LEU:HG	2.33	0.44
1:B:1090:ASN:H	1:B:1095:THR:HG21	1.82	0.44
1:B:1249:ASP:HA	1:B:1253:THR:OG1	2.17	0.44
1:A:20:LEU:HD13	1:A:219:GLU:OE2	2.17	0.44
1:A:33:GLN:HA	1:A:172:PRO:HG2	1.99	0.44
1:A:175:LYS:HE2	3:A:3307:HOH:O	2.17	0.44
1:A:35:THR:HB	1:A:166:VAL:CG1	2.43	0.43
1:B:1270:ASP:HA	1:B:1386:LEU:HD23	2.00	0.43
1:A:79:CYS:N	3:A:3277:HOH:O	2.49	0.43
1:A:234:ASP:OD1	1:A:236:GLN:HG3	2.18	0.43
1:B:1329:LYS:HG2	3:B:3214:HOH:O	2.17	0.43
1:A:290:ASP:OD2	2:A:2000:XGP:C1	2.66	0.43
1:B:1011:GLN:NE2	1:B:1277:ARG:HH11	2.15	0.43
1:B:1017:ARG:NH2	1:B:1314:THR:O	2.51	0.43
1:A:110:CYS:O	1:A:111:ASP:CG	2.61	0.43
1:A:327:ASP:O	1:A:330:ALA:O	2.37	0.43
1:B:1169:LYS:O	1:B:1170:ASP:CB	2.60	0.43
1:B:1231:ILE:HD12	1:B:1231:ILE:N	2.33	0.43
1:B:1252:PHE:CE2	1:B:1291:SER:HB3	2.53	0.43
1:A:235:GLN:C	1:A:237:TRP:N	2.70	0.43
1:B:1335:MET:HE3	1:B:1382:PHE:CZ	2.54	0.43
1:A:325:TRP:CG	1:A:376:PHE:HE2	2.37	0.43
1:A:90:ASN:N	1:A:90:ASN:ND2	2.65	0.43
1:B:1186:LYS:HZ3	1:B:1186:LYS:CB	2.32	0.43
1:B:1268:TYR:C	1:B:1268:TYR:CD2	2.97	0.43
1:A:316:ILE:HG23	1:A:317:GLY:N	2.32	0.43
1:B:1065:ARG:HG2	1:B:1065:ARG:NH1	2.33	0.43
1:B:1265:LEU:HD12	1:B:1265:LEU:HA	1.73	0.43
1:B:1277:ARG:HD2	1:B:1324:ARG:CZ	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1061:GLY:HA2	1:B:1102:PHE:CE1	2.54	0.43
1:B:1273:LEU:CB	1:B:1277:ARG:NH2	2.82	0.43
1:A:361:ARG:CZ	3:A:3059:HOH:O	2.67	0.42
1:B:1049:LEU:HD11	1:B:1053:GLY:C	2.44	0.42
1:B:1168:TYR:CE1	1:B:1182:LEU:HD13	2.54	0.42
1:B:1216:GLN:OE1	1:B:1226:VAL:HA	2.19	0.42
1:A:65:ARG:NH2	1:A:74:VAL:HG11	2.32	0.42
1:A:273:LEU:HD23	1:A:382:PHE:CZ	2.54	0.42
1:B:1075:LYS:HG3	1:B:1077:GLY:H	1.85	0.42
1:A:16:SER:CB	1:A:319:LYS:HG2	2.50	0.42
1:B:1099:ALA:HB2	1:B:1287:VAL:HG21	2.01	0.42
1:B:1226:VAL:HG13	1:B:1231:ILE:HD11	2.01	0.42
1:A:217:TYR:CZ	1:A:348:ARG:HD2	2.54	0.42
1:A:310:GLN:CG	1:A:315:PRO:HG3	2.42	0.42
1:B:1277:ARG:NH1	1:B:1324:ARG:HE	2.17	0.42
1:B:1338:GLU:OE2	1:B:1361:ARG:NH1	2.53	0.42
1:B:1232:LYS:HE3	3:B:3098:HOH:O	2.18	0.42
1:A:328:SER:O	1:A:329:LYS:C	2.63	0.42
1:A:330:ALA:O	1:A:332:ARG:N	2.45	0.42
1:B:1308:HIS:O	1:B:1309:ASP:HB2	2.20	0.42
1:A:116:HIS:NE2	1:A:120:MET:HE1	2.34	0.42
1:A:138:PHE:HB3	3:A:3203:HOH:O	2.20	0.42
1:A:211:ASP:OD2	1:A:244:LYS:HE2	2.20	0.42
1:B:1132:THR:N	1:B:1260:ASN:HD21	2.11	0.42
1:A:265:LEU:HD12	1:A:265:LEU:HA	1.91	0.42
1:A:241:SER:HB3	3:A:3265:HOH:O	2.20	0.41
1:B:1081:PRO:HA	1:B:1082:PRO:HD3	1.93	0.41
1:B:1093:GLN:C	1:B:1093:GLN:CD	2.89	0.41
1:A:1:GLN:HG2	3:A:3171:HOH:O	2.20	0.41
1:A:185:GLY:HA3	1:A:202:PRO:HG3	2.02	0.41
1:A:270:ASP:OD1	1:A:387:ASN:OD1	2.38	0.41
1:A:346:GLN:NE2	1:A:360:GLN:HE21	2.18	0.41
1:B:1168:TYR:CZ	1:B:1182:LEU:HD13	2.56	0.41
1:B:1290:ASP:HB2	1:B:1314:THR:CG2	2.48	0.41
1:B:1218:TYR:CE1	1:B:1347:LEU:HD12	2.56	0.41
1:A:244:LYS:NZ	1:A:312:GLU:HB3	2.36	0.41
1:B:1069:ALA:HA	1:B:1074:VAL:O	2.20	0.41
1:A:25:ALA:HB2	1:A:46:GLY:CA	2.47	0.41
1:A:21:ARG:NH2	1:A:23:PRO:HA	2.35	0.41
1:A:116:HIS:HD2	1:A:117:GLN:O	2.03	0.41
1:B:1129:PRO:C	1:B:1261:VAL:HG13	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1319:LYS:HE2	1:B:1319:LYS:HB3	1.94	0.41
1:A:91:SER:HA	1:A:120:MET:SD	2.61	0.41
1:A:175:LYS:HD2	3:A:3253:HOH:O	2.19	0.41
1:A:228:TRP:C	1:A:230:GLU:H	2.28	0.41
1:A:269:ILE:HG22	1:A:273:LEU:HD22	2.02	0.41
1:A:338:GLU:HG2	1:A:363:THR:HG22	2.02	0.41
1:B:1201:GLY:O	1:B:1204:LYS:HB3	2.20	0.41
1:B:1233:SER:O	1:B:1234:ASP:OD2	2.37	0.41
1:A:269:ILE:HG23	1:A:273:LEU:HD22	2.03	0.41
1:B:1056:LEU:HB3	1:B:1342:GLN:HE22	1.86	0.41
1:B:1128:ASN:HD22	1:B:1129:PRO:CD	2.31	0.41
1:B:1259:ARG:HD2	3:B:3254:HOH:O	2.21	0.41
1:B:1281:PRO:O	1:B:1282:LYS:C	2.65	0.41
1:A:311:ASN:HB2	3:A:3205:HOH:O	2.20	0.40
1:B:1093:GLN:HA	3:B:3258:HOH:O	2.21	0.40
1:B:1095:THR:O	1:B:1098:THR:CG2	2.69	0.40
1:B:1096:VAL:HG21	1:B:1120:MET:HE1	2.03	0.40
1:B:1049:LEU:O	1:B:1050:THR:CB	2.69	0.40
1:B:1297:LEU:HD12	1:B:1297:LEU:HA	1.85	0.40
1:B:1303:LYS:O	1:B:1304:PRO:C	2.63	0.40
1:B:1049:LEU:CD1	1:B:1050:THR:O	2.67	0.40
1:B:1134:ASP:HB3	1:B:1193:TYR:CD2	2.57	0.40
1:A:26:ASN:ND2	3:A:3105:HOH:O	2.54	0.40
1:A:175:LYS:O	1:A:176:GLU:CG	2.69	0.40
1:B:1065:ARG:NE	1:B:1074:VAL:HG11	2.36	0.40
1:B:1132:THR:HG22	1:B:1260:ASN:OD1	2.21	0.40
1:B:1296:LEU:HD13	1:B:1296:LEU:C	2.46	0.40
1:B:1307:LEU:HD23	1:B:1315:PRO:HD3	2.02	0.40
1:B:1310:GLN:NE2	1:B:1311:ASN:H	2.19	0.40
1:A:372:ASP:OD2	1:A:372:ASP:C	2.63	0.40
1:B:1020:LEU:HD11	1:B:1219:GLU:HA	2.03	0.40
1:B:1297:LEU:HD13	1:B:1320:ILE:HD13	2.03	0.40
1:B:1307:LEU:HD23	1:B:1315:PRO:CD	2.51	0.40

There are no symmetry-related clashes.

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	389/391 (100%)	352 (90%)	22 (6%)	15 (4%)	2	2
1	B	389/391 (100%)	347 (89%)	25 (6%)	17 (4%)	2	1
All	All	778/782 (100%)	699 (90%)	47 (6%)	32 (4%)	2	2

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	79	CYS
1	A	91	SER
1	A	111	ASP
1	A	176	GLU
1	A	234	ASP
1	B	1186	LYS
1	B	1187	ASN
1	B	1198	GLY
1	B	1232	LYS
1	A	18	ALA
1	A	46	GLY
1	A	78	GLU
1	A	271	LYS
1	A	329	LYS
1	A	331	ASN
1	B	1156	THR
1	B	1231	ILE
1	A	82	PRO
1	A	178	GLN
1	B	1078	GLU
1	B	1176	GLU
1	B	1008	GLN
1	B	1079	CYS
1	B	1233	SER
1	B	1329	LYS

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Mol	Chain	Res	Type
1	A	191	ALA
1	B	1082	PRO
1	B	1089	ALA
1	B	1111	ASP
1	B	1343	SER
1	A	233	SER
1	B	1197	PRO

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	335/335 (100%)	288 (86%)	47 (14%)	3	4
1	B	335/335 (100%)	295 (88%)	40 (12%)	5	7
All	All	670/670 (100%)	583 (87%)	87 (13%)	4	5

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	20	LEU
1	A	21	ARG
1	A	24	LEU
1	A	26	ASN
1	A	30	VAL
1	A	41	GLU
1	A	44	VAL
1	A	49	LEU
1	A	65	ARG
1	A	68	LEU
1	A	75	LYS
1	A	79	CYS
1	A	90	ASN
1	A	91	SER
1	A	96	VAL

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Mol	Chain	Res	Type
1	A	98	THR
1	A	128	ASN
1	A	150	LEU
1	A	154	GLN
1	A	155	LEU
1	A	161	LEU
1	A	162	LEU
1	A	182	LEU
1	A	183	VAL
1	A	186	LYS
1	A	188	THR
1	A	192	LYS
1	A	199	VAL
1	A	205	VAL
1	A	215	LEU
1	A	225	GLN
1	A	237	TRP
1	A	238	LYS
1	A	239	VAL
1	A	256	GLU
1	A	261	VAL
1	A	265	LEU
1	A	277	ARG
1	A	286	LEU
1	A	297	LEU
1	A	303	LYS
1	A	307	LEU
1	A	312	GLU
1	A	321	VAL
1	A	345	GLU
1	A	371	ILE
1	B	1005	GLU
1	B	1011	GLN
1	B	1019	ASN
1	B	1020	LEU
1	B	1024	LEU
1	B	1049	LEU
1	B	1068	LEU
1	B	1074	VAL
1	B	1075	LYS
1	B	1082	PRO
1	B	1095	THR

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Mol	Chain	Res	Type
1	B	1150	LEU
1	B	1153	LEU
1	B	1154	GLN
1	B	1155	LEU
1	B	1156	THR
1	B	1161	LEU
1	B	1162	LEU
1	B	1166	VAL
1	B	1175	LYS
1	B	1182	LEU
1	B	1186	LYS
1	B	1187	ASN
1	B	1192	LYS
1	B	1205	VAL
1	B	1209	LEU
1	B	1215	LEU
1	B	1231	ILE
1	B	1237	TRP
1	B	1257	VAL
1	B	1265	LEU
1	B	1274	VAL
1	B	1286	LEU
1	B	1297	LEU
1	B	1306	GLN
1	B	1307	LEU
1	B	1312	GLU
1	B	1363	THR
1	B	1369	CYS
1	B	1371	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	19	ASN
1	A	26	ASN
1	A	33	GLN
1	A	71	GLN
1	A	90	ASN
1	A	93	GLN
1	A	116	HIS
1	A	117	GLN

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Mol	Chain	Res	Type
1	A	128	ASN
1	A	141	GLN
1	A	167	ASN
1	A	179	GLN
1	A	194	GLN
1	A	236	GLN
1	A	248	GLN
1	A	260	ASN
1	A	292	ASN
1	A	306	GLN
1	A	308	HIS
1	A	310	GLN
1	A	311	ASN
1	A	331	ASN
1	A	346	GLN
1	A	349	ASN
1	A	360	GLN
1	A	387	ASN
1	B	1010	GLN
1	B	1011	GLN
1	B	1019	ASN
1	B	1062	HIS
1	B	1071	GLN
1	B	1116	HIS
1	B	1128	ASN
1	B	1141	GLN
1	B	1167	ASN
1	B	1194	GLN
1	B	1195	GLN
1	B	1248	GLN
1	B	1260	ASN
1	B	1306	GLN
1	B	1310	GLN
1	B	1311	ASN
1	B	1331	ASN
1	B	1342	GLN
1	B	1346	GLN
1	B	1349	ASN
1	B	1356	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

2 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	XGP	B	2001	-	15,16,16	1.35	2 (13%)	24,24,24	0.82	1 (4%)
2	XGP	A	2000	-	15,16,16	1.11	1 (6%)	24,24,24	0.81	1 (4%)

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	XGP	B	2001	-	-	1/7/27/27	0/1/1/1
2	XGP	A	2000	-	-	1/7/27/27	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	XGP	P-OP2	2.89	1.59	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	XGP	C4-C3	2.02	1.57	1.52
2	A	2000	XGP	C4-C3	2.01	1.57	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	XGP	O5-C1-O1	-2.71	107.82	111.36
2	A	2000	XGP	O5-C1-O1	-2.70	107.83	111.36

There are no chirality outliers.

All (2) torsion outliers are listed below:

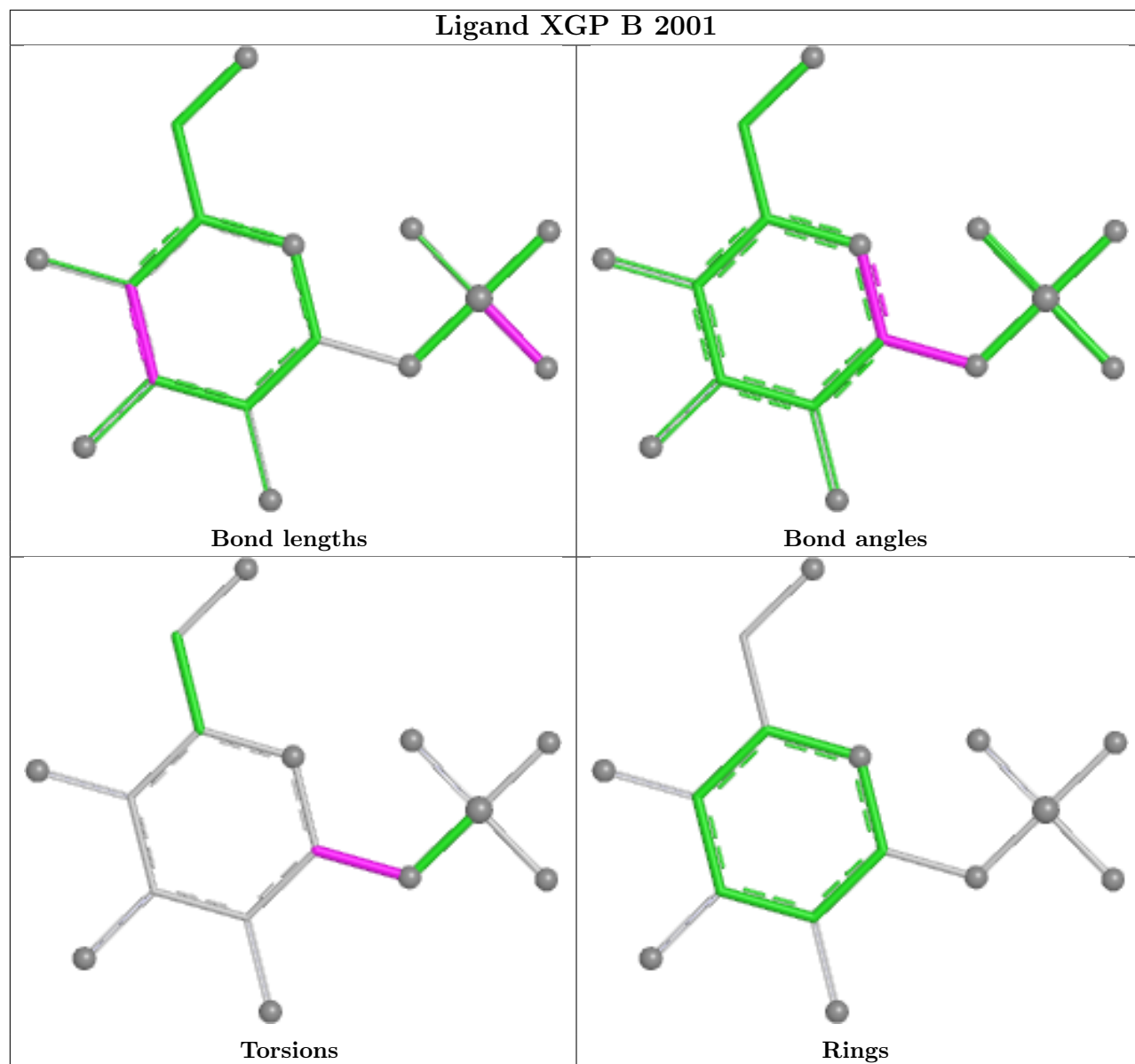
Mol	Chain	Res	Type	Atoms
2	A	2000	XGP	C2-C1-O1-P
2	B	2001	XGP	C2-C1-O1-P

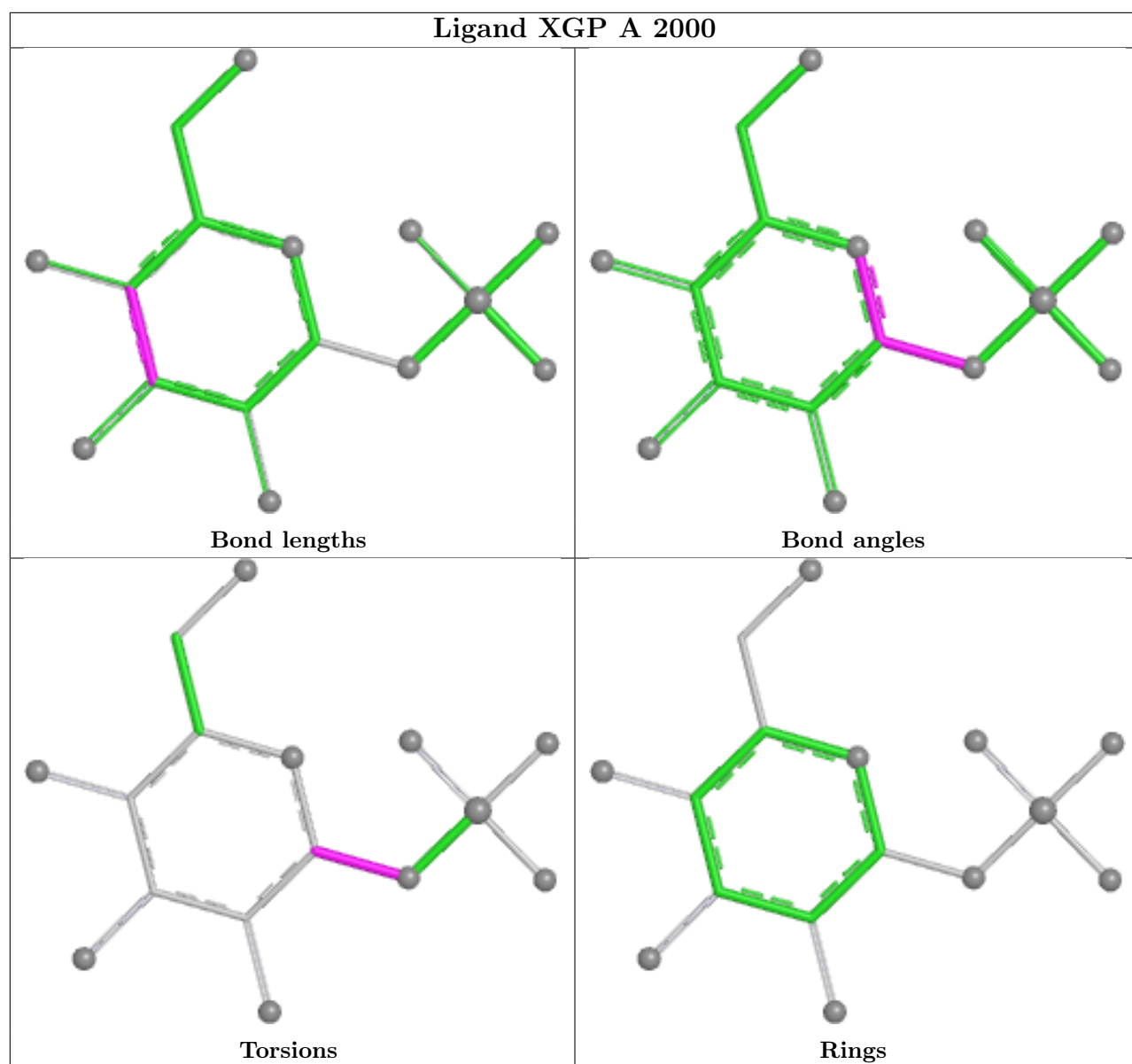
There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2001	XGP	6	0
2	A	2000	XGP	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.