



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:30 AM UTC

PDB ID : 3IFZ / pdb_00003ifz
Title : crystal structure of the first part of the Mycobacterium tuberculosis DNA gyrase reaction core: the breakage and reunion domain at 2.7 Å resolution
Authors : Piton, J.; Aubry, A.; Delarue, M.; Mayer, C.
Deposited on : 2009-07-27
Resolution : 2.70 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

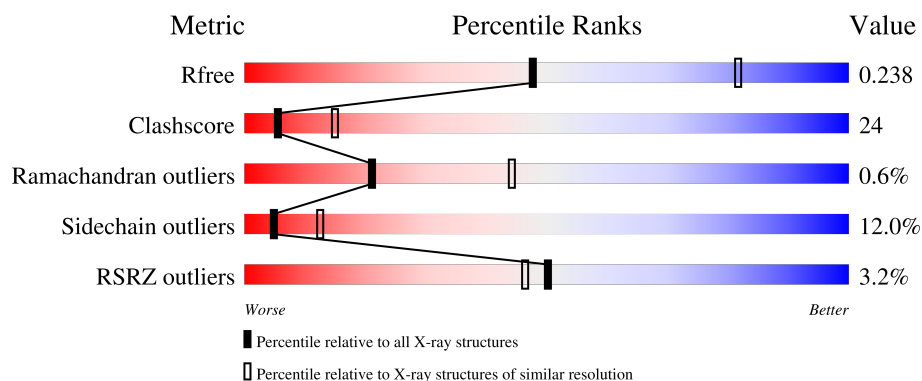
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
R_{free}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	508	4% 56% 33% 6% • • •
1	B	508	2% 58% 30% 5% 7%

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	MPD	A	509	-	-	X	-
2	MPD	B	509	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7774 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.

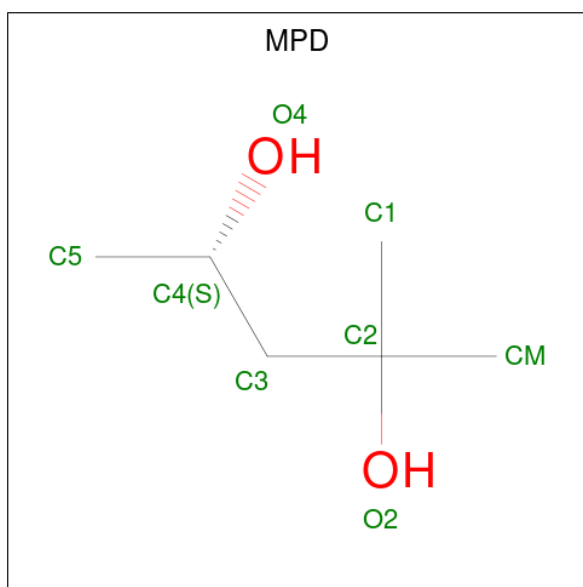
- Molecule 1 is a protein called DNA gyrase subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3834	2386	701	734	13			
1	B	473	Total	C	N	O	S	0	0	0
			3700	2303	682	703	12			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	502	GLU	-	expression tag	UNP Q07702
A	503	HIS	-	expression tag	UNP Q07702
A	504	HIS	-	expression tag	UNP Q07702
A	505	HIS	-	expression tag	UNP Q07702
A	506	HIS	-	expression tag	UNP Q07702
A	507	HIS	-	expression tag	UNP Q07702
A	508	HIS	-	expression tag	UNP Q07702
B	502	GLU	-	expression tag	UNP Q07702
B	503	HIS	-	expression tag	UNP Q07702
B	504	HIS	-	expression tag	UNP Q07702
B	505	HIS	-	expression tag	UNP Q07702
B	506	HIS	-	expression tag	UNP Q07702
B	507	HIS	-	expression tag	UNP Q07702
B	508	HIS	-	expression tag	UNP Q07702

- Molecule 2 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			8	6	2		
2	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		
3	B	1	Total	Na	0	0
			1	1		

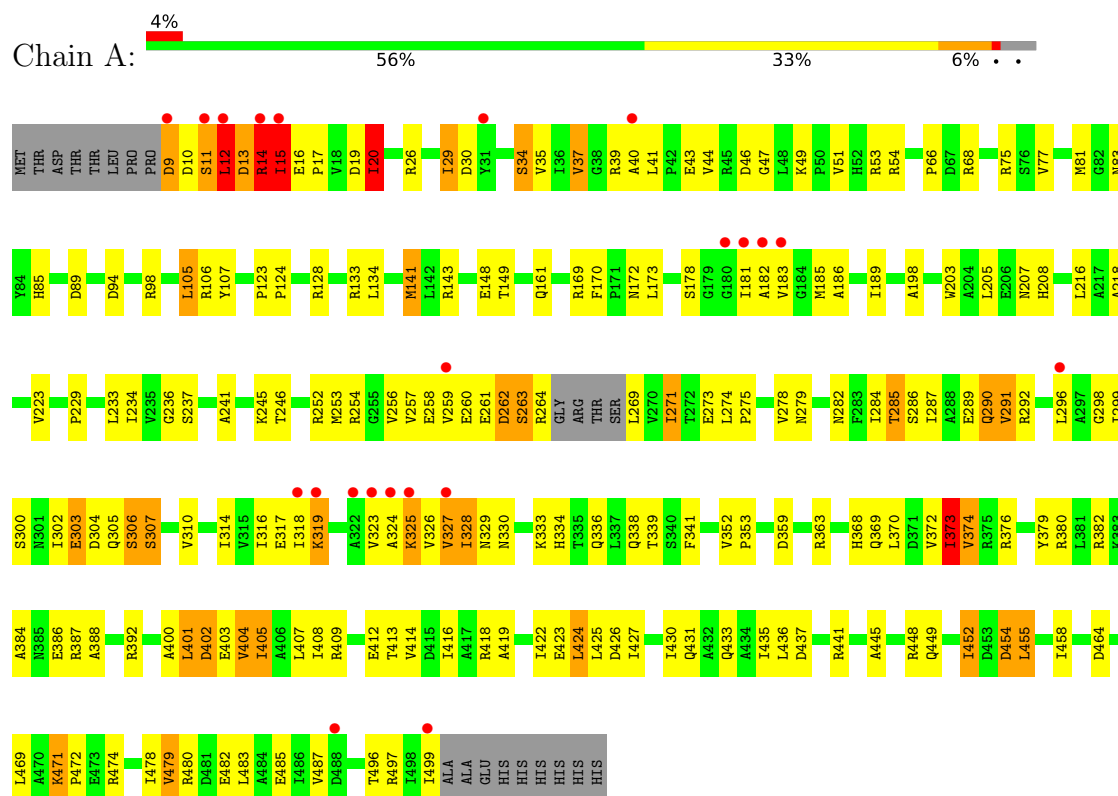
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	104	Total	O	0	0
			104	104		
4	B	118	Total	O	0	0
			118	118		

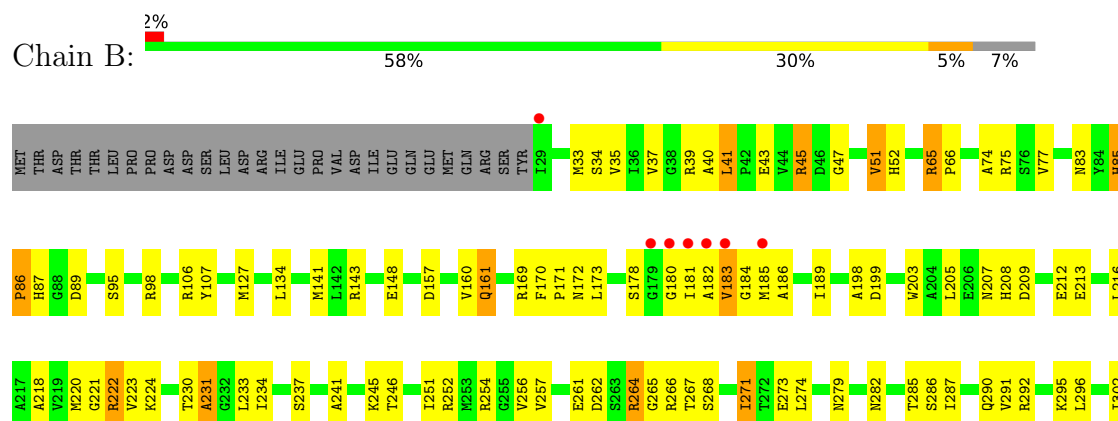
3 Residue-property plots

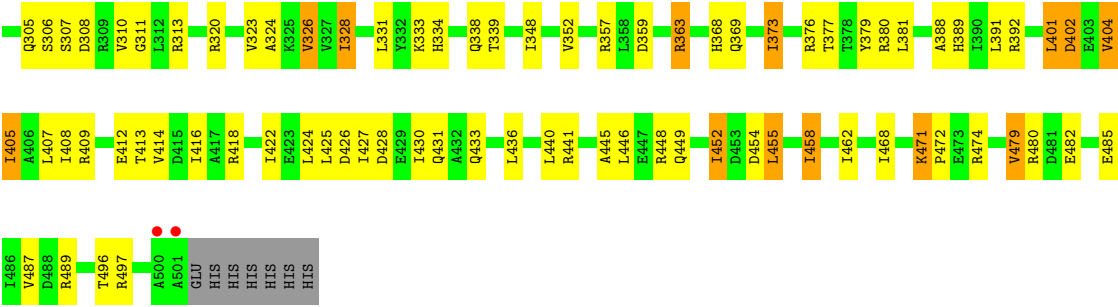
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: DNA gyrase subunit A



• Molecule 1: DNA gyrase subunit A





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.91Å 109.66Å 102.00Å 90.00° 120.40° 90.00°	Depositor
Resolution (Å)	19.90 – 2.70 19.90 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.90-2.70) 98.9 (19.90-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.71Å)	Xtriage
Refinement program	BUSTER-TNT 2.5.1	Depositor
R, R_{free}	0.192 , 0.233 0.200 , 0.238	Depositor DCC
R_{free} test set	2125 reflections (4.24%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for $-1/2^*h+1/2^*k+1, 1/2^*h-1/2^*k+1, 1/2^*h+1/2^*k$ 0.015 for $-1/2^*h-1/2^*k+1, -1/2^*h-1/2^*k-1, 1/2^*h-1/2^*k$	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7774	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.35	0/3892	0.88	12/5271 (0.2%)
1	B	0.37	0/3757	0.87	11/5090 (0.2%)
All	All	0.36	0/7649	0.87	23/10361 (0.2%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	ARG	N-CA-C	10.29	122.45	111.03
1	A	85	HIS	CA-C-N	7.98	129.81	119.84
1	A	85	HIS	C-N-CA	7.98	129.81	119.84
1	B	170	PHE	CA-C-N	7.76	129.54	119.84
1	B	170	PHE	C-N-CA	7.76	129.54	119.84
1	B	264	ARG	N-CA-C	7.70	119.75	111.36
1	B	85	HIS	CA-C-N	7.43	129.13	119.84
1	B	85	HIS	C-N-CA	7.43	129.13	119.84
1	A	471	LYS	CA-C-N	7.22	127.23	119.28
1	A	471	LYS	C-N-CA	7.22	127.23	119.28
1	B	471	LYS	CA-C-N	7.12	127.11	119.28
1	B	471	LYS	C-N-CA	7.12	127.11	119.28
1	A	20	ILE	N-CA-C	-7.00	103.95	110.53
1	A	373	ILE	N-CA-C	6.48	117.26	110.72
1	A	172	ASN	N-CA-C	5.63	117.87	111.11
1	A	170	PHE	CA-C-N	5.57	126.80	119.84
1	A	170	PHE	C-N-CA	5.57	126.80	119.84
1	B	45	ARG	N-CA-C	5.45	117.31	111.36
1	B	172	ASN	N-CA-C	5.37	117.55	111.11
1	B	65	ARG	CA-C-N	5.34	125.15	119.28
1	B	65	ARG	C-N-CA	5.34	125.15	119.28
1	A	325	LYS	N-CA-C	-5.14	106.98	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	LEU	N-CA-C	5.06	117.14	108.90

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	3834	0	3838	204	0
1	B	3700	0	3715	157	0
2	A	8	0	14	9	0
2	B	8	0	14	9	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	104	0	0	4	0
4	B	118	0	0	0	0
All	All	7774	0	7581	359	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 24.

All (359) 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)
2:B:509:MPD:H12	2:B:509:MPD:C5	1.61	1.22
2:B:509:MPD:H53	2:B:509:MPD:C1	1.57	1.21
1:B:74:ALA:HA	1:B:127:MET:HE2	1.22	1.18
1:A:298:GLY:HA2	1:A:319:LYS:HG2	1.32	1.08
1:A:259:VAL:HG12	1:A:269:LEU:HA	1.33	1.07
1:A:318:ILE:HD12	1:A:323:VAL:HA	1.39	1.05
2:A:509:MPD:H53	2:A:509:MPD:H12	1.40	1.03
2:B:509:MPD:C5	2:B:509:MPD:C1	2.30	0.98
1:A:424:LEU:HD13	1:A:425:LEU:HG	1.46	0.97
2:B:509:MPD:H52	2:B:509:MPD:O2	1.58	0.97
1:A:274:LEU:HB3	1:A:278:VAL:HG21	1.45	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:VAL:HB	1:B:127:MET:HE3	1.47	0.96
1:A:262:ASP:HB2	1:A:264:ARG:N	1.82	0.94
1:A:9:ASP:N	1:A:26:ARG:HD3	1.85	0.91
1:A:205:LEU:HD11	1:A:479:VAL:HG22	1.50	0.91
1:A:418:ARG:HH11	1:A:433:GLN:HE22	1.18	0.91
1:B:205:LEU:HD11	1:B:479:VAL:HG22	1.52	0.91
1:B:418:ARG:HH11	1:B:433:GLN:HE22	1.18	0.90
1:A:16:GLU:HG3	1:A:17:PRO:HD2	1.54	0.89
1:B:373:ILE:HD11	1:B:376:ARG:HH21	1.38	0.88
1:A:284:ILE:HD11	1:A:314:ILE:CD1	2.04	0.88
2:A:509:MPD:H53	2:A:509:MPD:C1	1.99	0.87
1:A:324:ALA:HB3	1:A:326:VAL:HG12	1.58	0.85
1:B:74:ALA:CA	1:B:127:MET:HE2	2.06	0.83
1:A:284:ILE:HD11	1:A:314:ILE:HD12	1.60	0.83
1:B:241:ALA:O	1:B:245:LYS:HG2	1.79	0.82
1:A:324:ALA:CB	1:A:326:VAL:HG12	2.10	0.82
1:A:291:VAL:CG2	1:A:299:ILE:HD12	2.10	0.81
1:A:287:ILE:HG22	1:A:302:ILE:HD11	1.60	0.81
1:A:292:ARG:HG3	1:A:292:ARG:HH11	1.45	0.80
1:B:77:VAL:CB	1:B:127:MET:HE3	2.10	0.80
1:A:424:LEU:CD1	1:A:425:LEU:HG	2.12	0.80
2:B:509:MPD:C5	2:B:509:MPD:O2	2.30	0.80
1:A:16:GLU:CG	1:A:17:PRO:HD2	2.12	0.80
1:B:485:GLU:HG2	1:B:489:ARG:HH22	1.47	0.80
2:A:509:MPD:O2	2:A:509:MPD:C5	2.30	0.79
1:B:405:ILE:O	1:B:409:ARG:HG3	1.81	0.79
1:A:405:ILE:O	1:A:409:ARG:HG3	1.83	0.79
1:B:373:ILE:CD1	1:B:376:ARG:HH21	1.96	0.78
1:A:274:LEU:HB3	1:A:278:VAL:CG2	2.12	0.78
1:A:83:ASN:ND2	1:B:75:ARG:HH12	1.82	0.77
1:A:318:ILE:CD1	1:A:323:VAL:HA	2.13	0.77
1:A:241:ALA:O	1:A:245:LYS:HG2	1.85	0.76
1:A:254:ARG:HH21	1:A:338:GLN:NE2	1.84	0.76
1:B:264:ARG:N	1:B:265:GLY:HA2	1.99	0.75
1:A:298:GLY:HA2	1:A:319:LYS:CG	2.14	0.75
1:B:148:GLU:HG3	1:B:379:TYR:CD1	2.21	0.75
1:A:275:PRO:O	1:A:278:VAL:HG22	1.86	0.75
1:A:205:LEU:HD11	1:A:479:VAL:CG2	2.16	0.75
1:A:262:ASP:HA	1:A:263:SER:CB	2.15	0.75
1:A:448:ARG:HD3	4:A:606:HOH:O	1.86	0.75
1:B:305:GLN:HB2	1:B:313:ARG:HG2	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:VAL:HB	1:B:326:VAL:HG13	1.69	0.74
1:B:254:ARG:HH21	1:B:338:GLN:NE2	1.86	0.74
1:B:205:LEU:HD11	1:B:479:VAL:CG2	2.18	0.74
1:A:148:GLU:HG3	1:A:379:TYR:CD1	2.23	0.74
1:A:259:VAL:CG1	1:A:269:LEU:HD12	2.17	0.73
1:B:74:ALA:HA	1:B:127:MET:CE	2.09	0.73
1:A:424:LEU:HD22	1:A:424:LEU:O	1.88	0.73
1:A:12:LEU:H	1:A:12:LEU:HD23	1.53	0.73
1:A:259:VAL:HG11	1:A:269:LEU:HD12	1.72	0.72
1:A:14:ARG:HD3	1:A:19:ASP:CG	2.14	0.72
1:A:330:ASN:HA	1:A:333:LYS:HD2	1.71	0.72
2:A:509:MPD:H12	2:A:509:MPD:C5	2.06	0.72
1:A:94:ASP:O	1:A:98:ARG:HG3	1.90	0.71
1:A:236:GLY:H	1:A:499:ILE:HD13	1.54	0.71
1:B:169:ARG:HE	1:B:369:GLN:HE22	1.37	0.71
1:B:418:ARG:HH11	1:B:433:GLN:NE2	1.89	0.71
1:A:169:ARG:HE	1:A:369:GLN:HE22	1.38	0.70
1:A:105:LEU:HD21	2:A:509:MPD:H53	1.73	0.70
1:A:14:ARG:O	1:A:15:ILE:HG22	1.91	0.69
1:A:418:ARG:HH11	1:A:433:GLN:NE2	1.89	0.69
1:B:87:HIS:C	1:B:89:ASP:H	1.99	0.69
1:A:236:GLY:H	1:A:499:ILE:CD1	2.06	0.69
1:A:413:THR:HG22	1:B:446:LEU:HD12	1.74	0.69
1:B:182:ALA:HB3	1:B:185:MET:CG	2.22	0.68
1:A:30:ASP:O	1:A:34:SER:HB3	1.94	0.68
1:A:271:ILE:HG13	1:A:271:ILE:O	1.94	0.68
1:A:40:ALA:HB3	1:A:182:ALA:HB2	1.77	0.67
1:A:284:ILE:HD11	1:A:314:ILE:HD11	1.76	0.67
1:A:287:ILE:HG22	1:A:302:ILE:CD1	2.24	0.66
1:B:271:ILE:HD11	1:B:274:LEU:HG	1.77	0.66
1:A:437:ASP:OD1	1:B:441:ARG:NH1	2.28	0.66
1:A:298:GLY:CA	1:A:319:LYS:HG2	2.19	0.66
1:A:419:ALA:O	1:A:423:GLU:HG3	1.96	0.66
2:A:509:MPD:H12	2:A:509:MPD:O4	1.95	0.66
1:A:445:ALA:HB3	1:B:412:GLU:HA	1.76	0.66
1:B:77:VAL:HB	1:B:127:MET:CE	2.25	0.65
1:A:37:VAL:HG22	1:A:182:ALA:HB1	1.79	0.65
1:A:271:ILE:HD11	1:A:274:LEU:HG	1.79	0.65
1:A:441:ARG:NH1	1:B:433:GLN:OE1	2.30	0.65
1:A:75:ARG:NH1	1:B:157:ASP:OD1	2.30	0.65
1:A:234:ILE:CD1	1:A:496:THR:HG21	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:509:MPD:H53	2:A:509:MPD:O2	1.97	0.64
1:B:37:VAL:HG12	1:B:348:ILE:HD11	1.80	0.64
1:B:271:ILE:HG13	1:B:271:ILE:O	1.96	0.63
1:A:307:SER:O	1:A:310:VAL:HG12	1.99	0.63
1:A:263:SER:O	1:A:264:ARG:HG3	1.97	0.63
1:A:286:SER:HA	1:A:289:GLU:OE1	1.98	0.63
1:B:264:ARG:NH2	1:B:267:THR:O	2.31	0.63
1:B:389:HIS:CE1	1:B:430:ILE:HD11	2.34	0.63
1:A:291:VAL:HG22	1:A:299:ILE:HD12	1.80	0.63
1:B:182:ALA:HB3	1:B:185:MET:HG2	1.81	0.62
1:B:307:SER:O	1:B:311:GLY:N	2.30	0.62
1:A:40:ALA:HB3	1:A:182:ALA:CB	2.29	0.62
1:A:292:ARG:HG3	1:A:292:ARG:NH1	2.13	0.62
1:B:391:LEU:HD12	1:B:458:ILE:HD12	1.82	0.62
1:A:169:ARG:HE	1:A:369:GLN:NE2	1.98	0.61
1:B:169:ARG:HE	1:B:369:GLN:NE2	1.98	0.61
2:A:509:MPD:C1	2:A:509:MPD:O4	2.48	0.61
1:B:287:ILE:HG22	1:B:302:ILE:CD1	2.31	0.61
1:A:256:VAL:HB	1:A:273:GLU:HB2	1.82	0.61
1:A:424:LEU:HD13	1:A:425:LEU:CG	2.27	0.60
1:A:262:ASP:HA	1:A:263:SER:OG	2.01	0.60
1:B:324:ALA:O	1:B:328:ILE:HG13	2.01	0.60
1:B:41:LEU:HD21	1:B:182:ALA:HB2	1.84	0.60
1:A:16:GLU:HG3	1:A:17:PRO:CD	2.30	0.60
1:A:106:ARG:HG3	1:A:107:TYR:CE2	2.37	0.60
1:B:33:MET:HE1	1:B:183:VAL:HB	1.84	0.59
2:A:509:MPD:O2	2:A:509:MPD:H52	2.03	0.59
1:A:106:ARG:HA	1:A:229:PRO:HB3	1.86	0.58
1:A:298:GLY:O	1:A:318:ILE:HA	2.03	0.58
1:B:256:VAL:HB	1:B:273:GLU:HB2	1.84	0.58
1:A:285:THR:HG22	1:A:289:GLU:OE1	2.03	0.58
1:B:33:MET:CE	1:B:183:VAL:HG11	2.34	0.58
1:B:106:ARG:HG3	1:B:107:TYR:CE2	2.38	0.58
1:A:234:ILE:HD12	1:A:496:THR:CG2	2.34	0.58
1:A:10:ASP:CG	1:A:11:SER:H	2.10	0.57
1:B:468:ILE:HG13	1:B:474:ARG:NH1	2.19	0.57
1:A:16:GLU:CD	1:A:17:PRO:HD2	2.29	0.57
1:A:234:ILE:HD12	1:A:496:THR:HG21	1.87	0.57
1:B:182:ALA:HB3	1:B:185:MET:HG3	1.85	0.57
1:A:183:VAL:C	1:A:185:MET:H	2.12	0.57
1:A:262:ASP:HA	1:A:263:SER:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:LEU:C	1:B:407:LEU:HD23	2.29	0.57
1:B:485:GLU:CG	1:B:489:ARG:HH22	2.16	0.57
1:A:418:ARG:HD3	1:A:433:GLN:NE2	2.19	0.57
1:A:169:ARG:NH2	1:A:373:ILE:HD11	2.20	0.56
1:B:418:ARG:HD3	1:B:433:GLN:NE2	2.20	0.56
1:A:407:LEU:C	1:A:407:LEU:HD23	2.30	0.56
1:A:323:VAL:HG12	1:A:323:VAL:O	2.04	0.56
1:B:252:ARG:HG3	1:B:252:ARG:NH1	2.20	0.56
2:B:509:MPD:H52	2:B:509:MPD:HO2	1.68	0.56
1:A:12:LEU:HD23	1:A:12:LEU:N	2.20	0.56
1:A:499:ILE:HD12	4:A:599:HOH:O	2.06	0.56
1:A:252:ARG:NH1	1:A:252:ARG:HG3	2.21	0.55
1:B:485:GLU:HG2	1:B:489:ARG:NH2	2.20	0.55
1:A:15:ILE:HG23	1:A:15:ILE:O	2.05	0.55
1:B:373:ILE:HD11	1:B:376:ARG:NH2	2.17	0.55
1:B:266:ARG:HG3	1:B:320:ARG:HG2	1.89	0.55
1:A:412:GLU:HA	1:B:445:ALA:HB3	1.87	0.55
1:B:39:ARG:HH12	1:B:51:VAL:HG22	1.71	0.55
1:B:422:ILE:HG23	1:B:427:ILE:O	2.07	0.55
1:B:404:VAL:O	1:B:408:ILE:HG13	2.07	0.54
1:B:216:LEU:O	1:B:220:MET:HG3	2.07	0.54
1:A:296:LEU:HG	1:A:299:ILE:HD11	1.88	0.54
1:A:422:ILE:HG23	1:A:427:ILE:O	2.08	0.54
2:B:509:MPD:H12	2:B:509:MPD:H53	0.69	0.54
1:A:404:VAL:O	1:A:408:ILE:HG13	2.08	0.54
1:B:160:VAL:HG12	1:B:161:GLN:N	2.21	0.54
1:A:40:ALA:CB	1:A:182:ALA:HA	2.38	0.54
1:A:262:ASP:HB2	1:A:263:SER:C	2.33	0.54
1:A:12:LEU:O	1:A:13:ASP:HB3	2.08	0.53
1:A:269:LEU:HD21	1:A:327:VAL:HG12	1.91	0.53
1:B:183:VAL:HG13	1:B:183:VAL:O	2.08	0.53
1:B:287:ILE:HG22	1:B:302:ILE:HD13	1.90	0.53
1:A:169:ARG:HG3	1:A:169:ARG:HH11	1.73	0.53
1:A:254:ARG:HE	1:A:338:GLN:HE21	1.56	0.53
1:B:373:ILE:O	1:B:377:THR:HG23	2.09	0.53
1:A:300:SER:N	1:A:317:GLU:O	2.34	0.53
1:A:290:GLN:HE22	1:A:334:HIS:HB3	1.74	0.53
1:B:295:LYS:HE3	1:B:334:HIS:CD2	2.44	0.53
1:A:17:PRO:HA	1:A:20:ILE:HD12	1.91	0.52
1:B:182:ALA:HB3	1:B:185:MET:O	2.09	0.52
1:B:323:VAL:HB	1:B:326:VAL:CG1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:GLU:O	1:A:261:GLU:HG3	2.09	0.52
1:A:39:ARG:HH22	1:A:54:ARG:HH12	1.58	0.52
1:B:233:LEU:HD23	1:B:497:ARG:HB2	1.91	0.52
1:B:254:ARG:HE	1:B:338:GLN:HE21	1.55	0.52
1:A:304:ASP:OD1	1:A:306:SER:OG	2.28	0.52
1:A:324:ALA:HB3	1:A:326:VAL:CG1	2.35	0.52
1:B:328:ILE:O	1:B:331:LEU:HB2	2.09	0.52
1:A:291:VAL:HG22	1:A:296:LEU:O	2.10	0.51
1:A:83:ASN:HD21	1:B:75:ARG:HH12	1.57	0.51
1:B:262:ASP:O	1:B:265:GLY:HA2	2.10	0.51
1:B:402:ASP:N	1:B:402:ASP:OD2	2.43	0.51
1:A:269:LEU:HB2	1:A:316:ILE:O	2.11	0.51
1:B:198:ALA:CB	1:B:487:VAL:HG21	2.40	0.51
1:A:183:VAL:HG12	1:A:183:VAL:O	2.09	0.51
1:B:407:LEU:HD13	1:B:424:LEU:HD22	1.93	0.51
1:A:203:TRP:CE2	1:A:207:ASN:ND2	2.79	0.51
1:B:262:ASP:OD2	1:B:266:ARG:N	2.44	0.51
1:B:287:ILE:HG22	1:B:302:ILE:HD11	1.93	0.51
1:A:402:ASP:OD2	1:A:402:ASP:N	2.44	0.50
1:A:448:ARG:NH1	4:A:606:HOH:O	2.24	0.50
1:A:455:LEU:O	1:A:458:ILE:HG22	2.11	0.50
1:B:203:TRP:CE2	1:B:207:ASN:ND2	2.79	0.50
1:A:233:LEU:HD23	1:A:497:ARG:HB2	1.94	0.50
1:B:169:ARG:HG3	1:B:169:ARG:HH11	1.76	0.50
1:A:325:LYS:O	1:A:328:ILE:HB	2.12	0.50
1:A:373:ILE:HG13	1:A:376:ARG:HH21	1.76	0.50
1:A:373:ILE:CG1	1:A:376:ARG:HH21	2.25	0.50
1:B:45:ARG:HG2	1:B:368:HIS:HB2	1.94	0.50
1:B:391:LEU:CD1	1:B:458:ILE:HD12	2.42	0.50
1:B:418:ARG:NH1	1:B:433:GLN:HE22	1.99	0.50
1:B:252:ARG:HG3	1:B:252:ARG:HH11	1.76	0.50
1:A:205:LEU:CD1	1:A:479:VAL:HG22	2.33	0.49
1:A:259:VAL:HG12	1:A:269:LEU:CA	2.24	0.49
1:A:259:VAL:CG1	1:A:269:LEU:HA	2.24	0.49
1:B:359:ASP:O	1:B:363:ARG:HG3	2.12	0.49
1:A:75:ARG:NH2	1:B:83:ASN:ND2	2.60	0.49
1:A:424:LEU:HD22	1:A:424:LEU:C	2.37	0.49
1:B:290:GLN:HB3	1:B:296:LEU:HD12	1.93	0.49
1:A:205:LEU:HD13	1:A:480:ARG:HB2	1.95	0.49
1:A:284:ILE:CD1	1:A:314:ILE:HD12	2.39	0.49
1:A:252:ARG:HG3	1:A:252:ARG:HH11	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:MET:HE1	1:B:183:VAL:CB	2.42	0.49
1:A:216:LEU:HD13	1:A:359:ASP:OD1	2.13	0.49
1:B:37:VAL:CG1	1:B:348:ILE:HD11	2.42	0.49
1:B:212:GLU:OE1	1:B:357:ARG:NH2	2.42	0.49
1:B:39:ARG:NH2	1:B:85:HIS:HE1	2.11	0.48
1:A:169:ARG:HG3	1:A:169:ARG:NH1	2.28	0.48
1:A:401:LEU:O	1:A:405:ILE:HG13	2.12	0.48
1:A:455:LEU:O	1:A:455:LEU:HD12	2.13	0.48
1:B:40:ALA:HB1	1:B:181:ILE:O	2.14	0.48
1:B:47:GLY:CA	1:B:173:LEU:HB2	2.43	0.48
1:A:173:LEU:HD11	1:A:189:ILE:HD13	1.96	0.48
1:A:368:HIS:HD2	4:A:544:HOH:O	1.95	0.48
1:B:407:LEU:CD1	1:B:424:LEU:HD22	2.44	0.48
1:B:455:LEU:HD12	1:B:455:LEU:O	2.13	0.48
1:A:412:GLU:HG3	1:B:446:LEU:HG	1.96	0.48
1:A:425:LEU:O	1:A:426:ASP:HB3	2.14	0.48
1:A:258:GLU:HG3	1:A:258:GLU:O	2.13	0.48
1:A:262:ASP:CA	1:A:263:SER:CB	2.89	0.48
1:B:33:MET:HE2	1:B:183:VAL:HG11	1.95	0.48
1:B:182:ALA:O	1:B:184:GLY:N	2.47	0.48
1:A:286:SER:O	1:A:290:GLN:HB2	2.13	0.48
1:B:205:LEU:CD1	1:B:479:VAL:HG22	2.35	0.47
1:B:389:HIS:ND1	1:B:430:ILE:HD11	2.29	0.47
1:A:37:VAL:HG22	1:A:182:ALA:CB	2.43	0.47
1:B:454:ASP:O	1:B:458:ILE:HG13	2.14	0.47
1:A:66:PRO:HG3	1:A:134:LEU:O	2.13	0.47
1:A:149:THR:HB	1:A:372:VAL:HG13	1.97	0.47
1:B:173:LEU:HD11	1:B:189:ILE:HD13	1.97	0.47
1:B:205:LEU:HD13	1:B:480:ARG:HB2	1.97	0.47
1:A:328:ILE:HG22	1:A:329:ASN:N	2.29	0.47
1:B:77:VAL:CG1	1:B:127:MET:HE3	2.45	0.47
1:B:286:SER:O	1:B:290:GLN:HB2	2.14	0.47
1:B:401:LEU:O	1:B:405:ILE:HG13	2.15	0.47
1:A:435:ILE:O	1:B:440:LEU:HD12	2.14	0.47
1:B:254:ARG:HH21	1:B:338:GLN:HE22	1.59	0.47
1:B:448:ARG:O	1:B:452:ILE:HD12	2.15	0.47
1:A:387:ARG:NH2	1:A:454:ASP:OD2	2.47	0.46
1:A:436:LEU:HB3	1:B:441:ARG:HB3	1.97	0.46
1:B:425:LEU:O	1:B:426:ASP:HB3	2.14	0.46
1:B:230:THR:O	1:B:231:ALA:HB3	2.15	0.46
1:A:37:VAL:HG11	1:A:353:PRO:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:VAL:HG23	1:A:278:VAL:O	2.15	0.46
1:A:252:ARG:HH11	1:A:252:ARG:CG	2.29	0.46
1:A:471:LYS:HA	1:A:472:PRO:HD2	1.72	0.46
1:A:430:ILE:CG2	1:A:431:GLN:N	2.78	0.46
1:A:324:ALA:HB1	1:A:326:VAL:HG12	1.90	0.46
1:B:52:HIS:CD2	1:B:95:SER:HB3	2.51	0.46
1:A:75:ARG:NH2	1:B:83:ASN:HD22	2.14	0.46
1:A:474:ARG:O	1:A:478:ILE:HG13	2.16	0.45
1:B:160:VAL:CG1	1:B:161:GLN:N	2.78	0.45
1:B:376:ARG:O	1:B:380:ARG:HG3	2.17	0.45
1:A:77:VAL:HG11	1:A:89:ASP:HB2	1.99	0.45
1:A:198:ALA:CB	1:A:487:VAL:HG21	2.47	0.45
1:A:441:ARG:HB3	1:B:436:LEU:HB3	1.98	0.45
1:A:303:GLU:OE1	1:A:303:GLU:HA	2.17	0.45
1:A:329:ASN:O	1:A:333:LYS:HG3	2.16	0.45
1:B:252:ARG:HH11	1:B:252:ARG:CG	2.29	0.45
1:B:234:ILE:CD1	1:B:496:THR:HG21	2.47	0.45
1:A:448:ARG:O	1:A:452:ILE:HD12	2.17	0.44
1:A:455:LEU:HA	1:A:458:ILE:HG22	1.98	0.44
1:B:98:ARG:HE	2:B:509:MPD:HM3	1.82	0.44
1:A:81:MET:HE3	1:B:127:MET:HE1	1.99	0.44
1:A:253:MET:HE2	1:A:341:PHE:HB2	1.99	0.44
1:B:381:LEU:HD11	1:B:462:ILE:HG23	2.00	0.44
1:A:384:ALA:HA	1:A:458:ILE:HD11	1.99	0.44
1:A:413:THR:OG1	1:A:416:ILE:HD12	2.17	0.44
1:B:290:GLN:NE2	1:B:334:HIS:HB3	2.33	0.44
1:A:47:GLY:CA	1:A:173:LEU:HB2	2.47	0.44
1:A:208:HIS:CD2	1:A:208:HIS:H	2.35	0.44
1:A:483:LEU:O	1:A:487:VAL:HG23	2.18	0.44
1:B:279:ASN:HB3	1:B:282:ASN:HB2	2.00	0.44
1:A:254:ARG:HH21	1:A:338:GLN:HE22	1.59	0.44
1:B:203:TRP:CE2	1:B:218:ALA:CB	3.01	0.43
1:A:418:ARG:NH1	1:A:433:GLN:HE22	1.99	0.43
1:B:373:ILE:HD12	1:B:373:ILE:HA	1.78	0.43
1:A:259:VAL:HG11	1:A:269:LEU:CD1	2.46	0.43
1:B:413:THR:OG1	1:B:416:ILE:HD12	2.18	0.43
1:A:271:ILE:HD12	1:A:273:GLU:O	2.19	0.43
1:B:87:HIS:C	1:B:89:ASP:N	2.69	0.43
1:B:169:ARG:HG3	1:B:169:ARG:NH1	2.32	0.43
1:B:271:ILE:HD12	1:B:273:GLU:O	2.19	0.43
1:B:290:GLN:HG3	1:B:295:LYS:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:ARG:HB2	1:B:66:PRO:HD2	2.01	0.43
1:B:66:PRO:HG3	1:B:134:LEU:O	2.19	0.43
1:A:254:ARG:HH21	1:A:338:GLN:HE21	1.65	0.43
1:A:291:VAL:CG2	1:A:296:LEU:HB3	2.49	0.43
1:B:169:ARG:NH2	1:B:482:GLU:OE1	2.41	0.43
1:A:29:ILE:HG22	1:A:30:ASP:N	2.33	0.42
1:B:376:ARG:HD3	1:B:380:ARG:CZ	2.49	0.42
1:A:9:ASP:HB3	1:A:10:ASP:H	1.60	0.42
1:B:306:SER:O	1:B:307:SER:HB3	2.18	0.42
1:B:471:LYS:HA	1:B:472:PRO:HD2	1.76	0.42
1:A:40:ALA:O	1:A:49:LYS:HD3	2.19	0.42
1:A:279:ASN:HB3	1:A:282:ASN:HB2	2.00	0.42
1:B:221:GLY:O	1:B:224:LYS:NZ	2.47	0.42
1:A:181:ILE:HD12	1:A:186:ALA:HB2	2.01	0.42
1:A:388:ALA:O	1:A:392:ARG:HG3	2.19	0.42
1:A:10:ASP:CG	1:A:11:SER:N	2.77	0.42
1:A:141:MET:HE3	1:A:141:MET:HB3	1.65	0.42
1:A:430:ILE:HG23	1:A:431:GLN:N	2.34	0.42
1:A:128:ARG:HB3	1:B:86:PRO:HB2	2.00	0.42
1:A:169:ARG:NH2	1:A:482:GLU:OE1	2.41	0.42
1:B:391:LEU:CD1	1:B:458:ILE:CD1	2.98	0.42
1:A:376:ARG:O	1:A:380:ARG:HG3	2.20	0.42
1:A:412:GLU:O	1:B:446:LEU:HG	2.19	0.42
1:B:52:HIS:HD2	1:B:95:SER:HB3	1.85	0.42
1:B:198:ALA:HB2	1:B:487:VAL:HG21	2.02	0.42
1:B:208:HIS:CD2	1:B:208:HIS:H	2.36	0.42
1:B:216:LEU:O	1:B:216:LEU:HD12	2.20	0.42
1:B:388:ALA:O	1:B:392:ARG:HG3	2.20	0.42
1:A:68:ARG:O	1:A:133:ARG:NH1	2.43	0.41
1:B:333:LYS:HG2	1:B:334:HIS:CE1	2.54	0.41
1:A:236:GLY:CA	1:A:499:ILE:HD11	2.50	0.41
1:A:46:ASP:OD1	1:A:53:ARG:NH1	2.53	0.41
1:B:262:ASP:OD2	1:B:264:ARG:HB2	2.20	0.41
1:A:370:LEU:O	1:A:374:VAL:HG13	2.20	0.41
1:B:430:ILE:HG13	1:B:431:GLN:N	2.35	0.41
1:A:262:ASP:HB2	1:A:264:ARG:HB2	2.01	0.41
1:B:199:ASP:HB3	1:B:222:ARG:HG2	2.02	0.41
1:B:216:LEU:HA	1:B:359:ASP:HB3	2.03	0.41
1:B:65:ARG:HB2	1:B:66:PRO:CD	2.51	0.41
1:B:98:ARG:HE	2:B:509:MPD:CM	2.34	0.41
1:B:234:ILE:HD12	1:B:496:THR:CG2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:VAL:HG12	1:A:269:LEU:HD12	1.97	0.41
1:A:336:GLN:C	1:A:338:GLN:N	2.77	0.41
1:B:74:ALA:CB	1:B:127:MET:HE2	2.51	0.41
1:A:123:PRO:HA	1:A:124:PRO:HD3	1.89	0.41
1:A:252:ARG:NH1	1:A:252:ARG:CG	2.84	0.41
1:A:262:ASP:HB2	1:A:264:ARG:H	1.73	0.41
1:A:376:ARG:HD3	1:A:380:ARG:CZ	2.51	0.41
1:B:180:GLY:O	1:B:186:ALA:HB1	2.21	0.41
1:A:234:ILE:HD12	1:A:496:THR:HG22	2.03	0.41
1:A:262:ASP:CB	1:A:264:ARG:HB2	2.51	0.41
1:B:389:HIS:HE1	1:B:428:ASP:OD2	2.03	0.41
1:A:203:TRP:CE2	1:A:218:ALA:CB	3.04	0.40
1:A:400:ALA:O	1:A:404:VAL:HG13	2.21	0.40
1:A:464:ASP:OD1	1:A:474:ARG:NH2	2.38	0.40
1:A:260:GLU:HG2	1:A:261:GLU:H	1.85	0.40
1:A:16:GLU:HB3	1:A:19:ASP:OD2	2.22	0.40
1:A:382:ARG:O	1:A:386:GLU:HG3	2.22	0.40
1:B:313:ARG:HG2	1:B:313:ARG:O	2.20	0.40
1:B:471:LYS:O	1:B:474:ARG:HB2	2.21	0.40
1:A:203:TRP:CE2	1:A:218:ALA:HB1	2.57	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	483/508 (95%)	449 (93%)	32 (7%)	2 (0%)	30	54
1	B	471/508 (93%)	445 (94%)	22 (5%)	4 (1%)	16	37
All	All	954/1016 (94%)	894 (94%)	54 (6%)	6 (1%)	21	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	13	ASP
1	B	171	PRO
1	B	86	PRO
1	B	231	ALA
1	B	183	VAL
1	A	15	ILE

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	409/427 (96%)	354 (87%)	55 (13%)	4	9
1	B	391/427 (92%)	350 (90%)	41 (10%)	6	17
All	All	800/854 (94%)	704 (88%)	96 (12%)	5	12

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	11	SER
1	A	12	LEU
1	A	14	ARG
1	A	15	ILE
1	A	20	ILE
1	A	29	ILE
1	A	34	SER
1	A	35	VAL
1	A	37	VAL
1	A	41	LEU
1	A	43	GLU
1	A	44	VAL
1	A	51	VAL
1	A	105	LEU
1	A	141	MET
1	A	143	ARG
1	A	161	GLN

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Mol	Chain	Res	Type
1	A	178	SER
1	A	223	VAL
1	A	237	SER
1	A	246	THR
1	A	257	VAL
1	A	262	ASP
1	A	263	SER
1	A	271	ILE
1	A	285	THR
1	A	290	GLN
1	A	291	VAL
1	A	303	GLU
1	A	305	GLN
1	A	306	SER
1	A	307	SER
1	A	319	LYS
1	A	327	VAL
1	A	328	ILE
1	A	339	THR
1	A	352	VAL
1	A	363	ARG
1	A	373	ILE
1	A	374	VAL
1	A	401	LEU
1	A	402	ASP
1	A	403	GLU
1	A	404	VAL
1	A	405	ILE
1	A	414	VAL
1	A	424	LEU
1	A	449	GLN
1	A	452	ILE
1	A	454	ASP
1	A	455	LEU
1	A	469	LEU
1	A	479	VAL
1	A	485	GLU
1	B	34	SER
1	B	35	VAL
1	B	41	LEU
1	B	43	GLU
1	B	51	VAL

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Mol	Chain	Res	Type
1	B	141	MET
1	B	143	ARG
1	B	161	GLN
1	B	178	SER
1	B	209	ASP
1	B	213	GLU
1	B	222	ARG
1	B	223	VAL
1	B	237	SER
1	B	246	THR
1	B	251	ILE
1	B	257	VAL
1	B	261	GLU
1	B	268	SER
1	B	271	ILE
1	B	285	THR
1	B	291	VAL
1	B	292	ARG
1	B	308	ASP
1	B	310	VAL
1	B	326	VAL
1	B	328	ILE
1	B	339	THR
1	B	352	VAL
1	B	363	ARG
1	B	373	ILE
1	B	401	LEU
1	B	402	ASP
1	B	404	VAL
1	B	405	ILE
1	B	414	VAL
1	B	449	GLN
1	B	452	ILE
1	B	455	LEU
1	B	458	ILE
1	B	479	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	52	HIS

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Mol	Chain	Res	Type
1	A	83	ASN
1	A	85	HIS
1	A	113	GLN
1	A	161	GLN
1	A	208	HIS
1	A	280	HIS
1	A	329	ASN
1	A	338	GLN
1	A	368	HIS
1	A	369	GLN
1	A	385	ASN
1	A	389	HIS
1	A	433	GLN
1	B	52	HIS
1	B	83	ASN
1	B	85	HIS
1	B	113	GLN
1	B	161	GLN
1	B	208	HIS
1	B	238	GLN
1	B	290	GLN
1	B	338	GLN
1	B	344	ASN
1	B	368	HIS
1	B	369	GLN
1	B	385	ASN
1	B	389	HIS

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

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	MPD	B	509	-	7,7,7	0.72	0	9,10,10	0.60	0
2	MPD	A	509	-	7,7,7	0.59	0	9,10,10	0.88	0

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	MPD	B	509	-	-	2/5/5/5	-
2	MPD	A	509	-	-	1/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	509	MPD	C2-C3-C4-C5
2	B	509	MPD	C2-C3-C4-C5
2	B	509	MPD	C2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	509	MPD	9	0
2	A	509	MPD	9	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 ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	487/508 (95%)	0.09	22 (4%) 38 34	29, 56, 109, 144	0
1	B	473/508 (93%)	-0.19	9 (1%) 66 63	26, 50, 80, 121	0
All	All	960/1016 (94%)	-0.05	31 (3%) 50 46	26, 53, 103, 144	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	182	ALA	6.4
1	A	322	ALA	5.4
1	A	15	ILE	5.1
1	A	12	LEU	4.7
1	A	324	ALA	3.7
1	B	181	ILE	3.7
1	B	182	ALA	3.5
1	A	318	ILE	3.3
1	A	319	LYS	3.0
1	A	259	VAL	2.9
1	A	183	VAL	2.9
1	B	183	VAL	2.9
1	A	11	SER	2.8
1	A	9	ASP	2.8
1	B	180	GLY	2.8
1	A	323	VAL	2.8
1	A	325	LYS	2.7
1	A	181	ILE	2.7
1	A	499	ILE	2.6
1	B	29	ILE	2.6
1	B	501	ALA	2.5
1	A	180	GLY	2.5
1	A	31	TYR	2.4
1	A	296	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	179	GLY	2.4
1	A	327	VAL	2.3
1	A	488	ASP	2.3
1	B	185	MET	2.2
1	B	500	ALA	2.1
1	A	14	ARG	2.1
1	A	40	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MPD	A	509	8/8	0.80	0.22	96,97,99,99	0
3	NA	B	510	1/1	0.87	0.36	77,77,77,77	0
2	MPD	B	509	8/8	0.90	0.15	63,65,67,67	0
3	NA	A	510	1/1	0.95	0.34	54,54,54,54	0

6.5 Other polymers [i](#)

There are no such residues in this entry.