



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:30 PM UTC

PDB ID : 1JI3 / pdb\_00001ji3  
Title : CRYSTAL STRUCTURE OF THE FIRST THERMOSTABLE BACTERIAL LIPASE FROM BACILLUS STEAROTHERMOPHILUS  
Authors : Tyndall, J.D.A.; Sinchaikul, S.; Fothergill-Gilmore, L.A.; Taylor, P.; Walkinshaw, M.D.  
Deposited on : 2001-06-29  
Resolution : 2.20 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](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (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

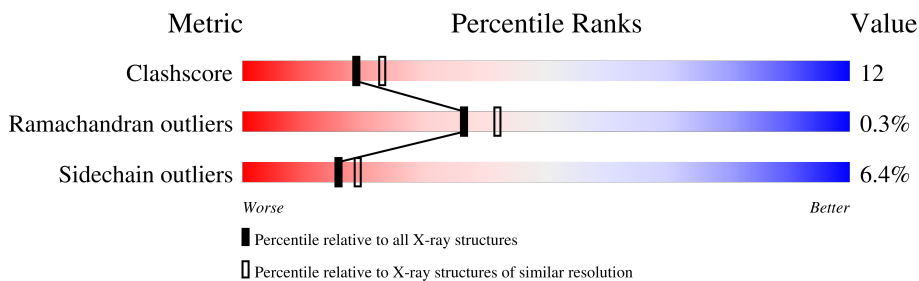
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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  $\geq 3$ , 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	388	
1	B	388	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6470 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 lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	388	3062	1940	541	573	8	0	0	0
1	B	388	3057	1936	540	573	8	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	63	VAL	ALA	conflict	UNP Q9L6D3
A	68	VAL	ALA	conflict	UNP Q9L6D3
B	63	VAL	ALA	conflict	UNP Q9L6D3
B	68	VAL	ALA	conflict	UNP Q9L6D3

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total 1	Ca 1	0	0
2	B	1	Total 1	Ca 1	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	168	Total 168	O 168	0	0
4	B	179	Total 179	O 179	0	0

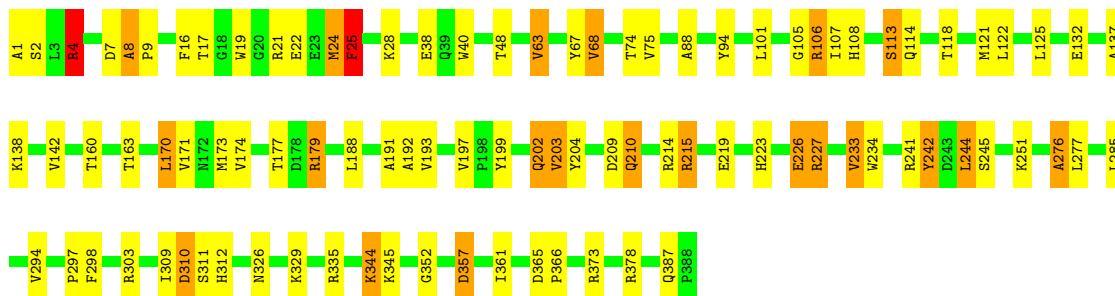
### 3 Residue-property plots

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.

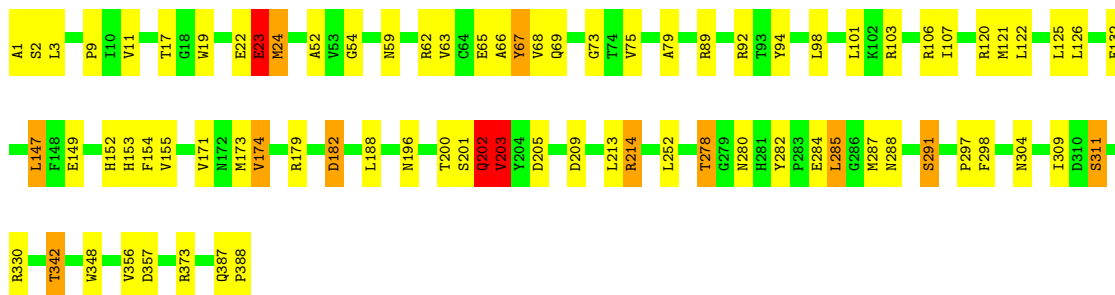
- Molecule 1: lipase

Chain A: 



- Molecule 1: lipase

Chain B: 



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.50Å 81.24Å 99.78Å 90.00° 96.33° 90.00°	Depositor
Resolution (Å)	100.00 – 2.20	Depositor
% Data completeness (in resolution range)	98.7 (100.00-2.20)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.166 , 0.210	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	6470	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	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: ZN, CA

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	0.36	0/3147	1.55	36/4280 (0.8%)
1	B	0.36	0/3140	1.52	19/4271 (0.4%)
All	All	0.36	0/6287	1.53	55/8551 (0.6%)

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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	310	ASP	CB-CA-C	-10.25	91.10	111.60
1	A	2	SER	N-CA-C	10.12	125.02	110.14
1	B	202	GLN	N-CA-C	8.12	121.68	111.69
1	A	215	ARG	CG-CD-NE	-8.06	94.26	112.00
1	B	153	HIS	CB-CA-C	-8.00	99.14	110.34
1	A	276	ALA	CA-C-N	-7.81	110.23	122.49
1	A	276	ALA	C-N-CA	-7.81	110.23	122.49
1	B	23	GLU	CB-CA-C	7.51	124.70	110.51
1	A	310	ASP	CB-CG-OD1	-7.49	101.18	118.40
1	A	214	ARG	N-CA-C	-7.31	97.22	108.76
1	A	352	GLY	N-CA-C	7.26	119.45	112.04
1	B	174	VAL	CB-CA-C	-6.91	103.13	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	GLN	CA-CB-CG	-6.79	100.51	114.10
1	A	309	ILE	CA-C-N	6.77	134.63	122.64
1	A	309	ILE	C-N-CA	6.77	134.63	122.64
1	A	233	VAL	N-CA-C	-6.48	104.25	113.07
1	A	311	SER	CA-CB-OG	-6.32	98.47	111.10
1	A	310	ASP	CB-CG-OD2	6.29	132.86	118.40
1	B	17	THR	OG1-CB-CG2	-6.16	96.97	109.30
1	B	182	ASP	N-CA-C	-6.12	104.72	111.82
1	A	311	SER	CB-CA-C	-6.04	98.74	110.46
1	B	330	ARG	NE-CZ-NH1	-6.04	115.46	121.50
1	B	24	MET	CG-SD-CE	-6.00	87.71	100.90
1	A	227	ARG	NE-CZ-NH2	-5.84	113.94	119.20
1	A	8	ALA	CA-C-O	5.70	124.76	119.24
1	A	17	THR	OG1-CB-CG2	-5.69	97.91	109.30
1	A	67	TYR	CA-C-O	5.68	126.78	120.82
1	B	155	VAL	N-CA-C	5.67	115.96	107.51
1	B	67	TYR	N-CA-C	-5.66	105.01	111.07
1	A	215	ARG	NE-CZ-NH2	-5.64	114.13	119.20
1	A	310	ASP	N-CA-CB	-5.62	101.47	110.51
1	A	210	GLN	CB-CA-C	-5.57	101.21	110.68
1	B	356	VAL	N-CA-C	-5.53	100.98	108.06
1	A	242	TYR	N-CA-C	5.52	117.38	111.36
1	A	309	ILE	O-C-N	5.48	128.31	122.45
1	B	152	HIS	N-CA-C	-5.46	100.98	109.72
1	B	330	ARG	CA-CB-CG	-5.46	103.18	114.10
1	A	285	LEU	CA-C-N	-5.38	114.86	123.31
1	A	285	LEU	C-N-CA	-5.38	114.86	123.31
1	B	291	SER	CB-CA-C	5.38	119.72	110.79
1	B	23	GLU	CG-CD-OE1	5.38	130.77	118.40
1	B	342	THR	CB-CA-C	5.34	118.68	110.14
1	A	174	VAL	CA-C-N	-5.32	111.39	121.54
1	A	174	VAL	C-N-CA	-5.32	111.39	121.54
1	A	4	ARG	CG-CD-NE	5.31	123.68	112.00
1	A	63	VAL	CG1-CB-CG2	-5.17	99.42	110.80
1	B	311	SER	CA-CB-OG	-5.12	100.86	111.10
1	A	25	PHE	CB-CA-C	-5.10	100.27	110.42
1	B	66	ALA	N-CA-C	5.09	117.22	111.11
1	A	310	ASP	N-CA-C	5.09	117.85	110.17
1	A	138	LYS	N-CA-C	-5.08	105.65	111.14
1	A	197	VAL	CA-C-O	5.06	122.64	119.51
1	B	22	GLU	N-CA-C	-5.03	107.15	113.28
1	A	19	TRP	CA-C-N	5.02	125.91	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	19	TRP	C-N-CA	5.02	125.91	120.44

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1	ALA	Peptide
1	B	1	ALA	Peptide

## 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3062	0	2929	80	0
1	B	3057	0	2917	62	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	168	0	0	8	0
4	B	179	0	0	8	0
All	All	6470	0	5846	142	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 12.

All (142) 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:68:VAL:HG21	1:B:75:VAL:HA	1.21	1.09
1:A:344:LYS:HZ2	1:A:344:LYS:HB3	1.12	1.08
1:A:344:LYS:HB3	1:A:344:LYS:NZ	1.67	1.06
1:A:171:VAL:HG21	1:A:244:LEU:CD1	1.86	1.05
1:A:171:VAL:HG21	1:A:244:LEU:HD11	1.43	0.98
1:B:19:TRP:HB2	1:B:23:GLU:CG	1.93	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:GLU:HB2	4:A:467:HOH:O	1.64	0.96
1:B:19:TRP:HB2	1:B:23:GLU:HG2	1.51	0.92
1:B:285:LEU:C	1:B:285:LEU:HD23	2.00	0.87
1:A:171:VAL:CG2	1:A:244:LEU:HD11	2.04	0.87
1:A:24:MET:CE	1:A:193:VAL:HG21	2.04	0.87
1:B:68:VAL:HG21	1:B:75:VAL:CA	2.08	0.81
1:A:244:LEU:CD1	1:A:244:LEU:C	2.56	0.77
1:B:68:VAL:HG23	4:B:438:HOH:O	1.87	0.75
1:B:24:MET:HE1	1:B:188:LEU:HD23	1.69	0.74
1:A:171:VAL:CG2	1:A:244:LEU:CD1	2.60	0.74
1:A:68:VAL:HG11	1:A:75:VAL:HG22	1.69	0.74
1:A:244:LEU:C	1:A:244:LEU:HD12	2.12	0.73
1:B:19:TRP:HB2	1:B:23:GLU:CD	2.15	0.71
1:A:105:GLY:C	1:A:106:ARG:HG2	2.16	0.71
1:A:171:VAL:HG21	1:A:244:LEU:HD13	1.71	0.71
1:B:68:VAL:CG1	1:B:73:GLY:O	2.39	0.71
1:A:24:MET:HE3	1:A:193:VAL:HG21	1.72	0.70
1:B:59:ASN:O	1:B:63:VAL:HG23	1.91	0.70
1:B:202:GLN:O	1:B:203:VAL:HG13	1.92	0.70
1:B:209:ASP:HB2	4:B:526:HOH:O	1.90	0.70
1:B:63:VAL:HG21	1:B:121:MET:HB3	1.74	0.70
1:A:24:MET:HE1	1:A:193:VAL:HG21	1.74	0.69
1:B:68:VAL:CG2	4:B:438:HOH:O	2.41	0.69
1:A:344:LYS:NZ	1:A:344:LYS:CB	2.41	0.69
1:A:170:LEU:HD22	1:A:173:MET:HE2	1.73	0.68
1:A:344:LYS:HZ2	1:A:344:LYS:CB	1.95	0.68
1:B:68:VAL:HG22	4:B:451:HOH:O	1.94	0.68
1:A:177:THR:CG2	1:A:234:TRP:HE1	2.07	0.67
1:B:285:LEU:HD23	1:B:285:LEU:O	1.95	0.67
1:A:276:ALA:O	1:A:277:LEU:HD23	1.94	0.67
1:A:244:LEU:HD12	1:A:245:SER:N	2.10	0.66
1:A:188:LEU:HD21	1:A:204:TYR:HD2	1.61	0.66
1:A:177:THR:HG22	1:A:234:TRP:HE1	1.60	0.66
1:A:24:MET:HE1	1:A:193:VAL:CG2	2.26	0.65
1:B:202:GLN:C	1:B:203:VAL:CG1	2.69	0.65
1:B:179:ARG:NH1	1:B:182:ASP:OD2	2.30	0.64
1:B:65:GLU:O	1:B:69:GLN:HG3	1.98	0.63
1:A:63:VAL:HG21	1:A:121:MET:HB3	1.79	0.63
1:B:63:VAL:HG13	1:B:122:LEU:HB2	1.79	0.63
1:A:344:LYS:HB3	1:A:344:LYS:HZ3	1.62	0.63
1:A:242:TYR:OH	1:A:251:LYS:HD2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:MET:CE	1:A:193:VAL:CG2	2.75	0.62
1:A:68:VAL:HG11	1:A:75:VAL:CG2	2.28	0.62
1:B:67:TYR:CE1	1:B:147:LEU:HD23	2.34	0.62
1:A:68:VAL:HG13	1:A:94:TYR:HD2	1.65	0.61
1:B:68:VAL:CG2	1:B:75:VAL:HA	2.14	0.60
1:B:63:VAL:HG11	1:B:125:LEU:HD12	1.83	0.60
1:B:202:GLN:C	1:B:203:VAL:HG12	2.27	0.59
1:B:285:LEU:C	1:B:285:LEU:CD2	2.74	0.59
1:B:278:THR:HB	1:B:280:ASN:H	1.68	0.59
1:B:202:GLN:O	1:B:203:VAL:CG1	2.51	0.58
1:A:244:LEU:C	1:A:244:LEU:HD13	2.28	0.58
1:A:68:VAL:HG13	1:A:94:TYR:CD2	2.39	0.57
1:A:105:GLY:O	1:A:106:ARG:HG2	2.04	0.56
1:A:177:THR:HG23	4:A:430:HOH:O	2.05	0.56
1:A:226:GLU:HG3	4:A:530:HOH:O	2.05	0.56
1:A:310:ASP:HB3	1:A:312:HIS:H	1.72	0.55
1:B:120:ARG:HD2	1:B:348:TRP:CZ2	2.43	0.54
1:A:171:VAL:CG2	1:A:244:LEU:HD13	2.36	0.53
1:A:173:MET:HG2	1:A:298:PHE:CG	2.44	0.53
1:A:199:TYR:O	1:A:215:ARG:NH2	2.36	0.53
1:A:63:VAL:HG11	1:A:125:LEU:HD12	1.90	0.53
1:B:214:ARG:HG2	1:B:214:ARG:NH1	2.24	0.52
1:B:252:LEU:HD23	1:B:252:LEU:C	2.35	0.51
1:B:284:GLU:OE2	4:B:578:HOH:O	2.18	0.51
1:B:173:MET:HG2	1:B:298:PHE:CG	2.45	0.50
1:B:79:ALA:HB2	1:B:89:ARG:HD2	1.94	0.50
1:A:137:ALA:HA	1:A:142:VAL:HG22	1.94	0.50
1:A:114:GLN:NE2	1:A:244:LEU:HB3	2.27	0.50
1:B:92:ARG:NH2	1:B:205:ASP:OD2	2.42	0.49
1:B:24:MET:HE1	1:B:188:LEU:CD2	2.40	0.49
1:B:213:LEU:C	1:B:214:ARG:HD3	2.37	0.49
1:A:68:VAL:CG1	1:A:75:VAL:HG22	2.39	0.49
1:B:67:TYR:CD1	1:B:147:LEU:CD2	2.96	0.49
1:B:373:ARG:HG3	4:B:512:HOH:O	2.12	0.49
1:A:7:ASP:HB2	4:A:490:HOH:O	2.12	0.48
1:A:179:ARG:HG2	1:A:294:VAL:CG1	2.43	0.48
1:A:38:GLU:HG3	1:A:48:THR:HG22	1.96	0.48
1:B:3:LEU:HD12	1:B:3:LEU:HA	1.65	0.48
1:A:63:VAL:HG11	1:A:122:LEU:HA	1.96	0.48
1:A:63:VAL:CG1	1:A:122:LEU:HA	2.43	0.48
1:A:215:ARG:HD3	4:A:495:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ALA:HB1	4:A:412:HOH:O	2.13	0.47
1:A:357:ASP:OD1	1:A:357:ASP:C	2.56	0.47
1:B:52:ALA:O	1:B:69:GLN:NE2	2.41	0.47
1:A:219:GLU:OE2	1:A:227:ARG:HD3	2.15	0.47
1:B:68:VAL:HG13	1:B:73:GLY:C	2.40	0.47
1:A:63:VAL:HG13	1:A:122:LEU:HD13	1.96	0.47
1:A:170:LEU:CD2	1:A:173:MET:HE2	2.41	0.47
1:A:63:VAL:HG23	1:A:118:THR:HG23	1.97	0.46
1:A:68:VAL:HG21	1:A:74:THR:C	2.41	0.46
1:A:202:GLN:O	1:A:203:VAL:HG13	2.15	0.46
1:B:9:PRO:HD2	1:B:106:ARG:O	2.15	0.46
1:B:214:ARG:CG	1:B:214:ARG:HH11	2.28	0.46
1:B:98:LEU:O	1:B:101:LEU:HG	2.16	0.46
1:A:4:ARG:NH1	4:A:475:HOH:O	2.49	0.46
1:A:219:GLU:OE2	1:A:223:HIS:ND1	2.38	0.45
1:A:24:MET:O	1:A:25:PHE:C	2.60	0.45
1:B:120:ARG:HD2	1:B:348:TRP:CH2	2.52	0.45
1:A:297:PRO:HD2	4:A:486:HOH:O	2.16	0.45
1:A:8:ALA:HA	1:A:9:PRO:HD2	1.57	0.45
1:B:304:ASN:HB3	1:B:309:ILE:HD12	1.98	0.44
1:A:191:ALA:O	1:A:192:ALA:HB3	2.17	0.44
1:B:171:VAL:O	1:B:171:VAL:HG12	2.16	0.44
1:A:101:LEU:HD11	1:A:107:ILE:CG2	2.47	0.44
1:B:297:PRO:HD2	4:B:509:HOH:O	2.16	0.44
1:A:40:TRP:CE2	1:A:373:ARG:HD3	2.52	0.44
1:A:173:MET:HG3	1:A:298:PHE:CD1	2.53	0.44
1:B:92:ARG:HH22	1:B:205:ASP:CG	2.25	0.44
1:A:21:ARG:CZ	1:A:28:LYS:HE3	2.48	0.43
1:B:287:MET:O	1:B:288:ASN:C	2.62	0.43
1:A:173:MET:HG2	1:A:298:PHE:CD2	2.54	0.43
1:B:63:VAL:CG1	1:B:122:LEU:HA	2.50	0.42
1:B:214:ARG:HG2	1:B:214:ARG:HH11	1.84	0.42
1:A:16:PHE:C	1:A:16:PHE:CD1	2.96	0.42
1:A:113:SER:HB2	1:A:114:GLN:H	1.42	0.42
1:A:8:ALA:O	1:A:108:HIS:HD2	2.02	0.42
1:A:344:LYS:CB	1:A:344:LYS:HZ3	2.21	0.42
1:B:68:VAL:HG11	1:B:73:GLY:O	2.17	0.42
1:A:63:VAL:HG13	1:A:122:LEU:HB2	2.01	0.41
1:A:114:GLN:HE22	1:A:244:LEU:HB3	1.85	0.41
1:A:234:TRP:CE2	1:A:241:ARG:HD2	2.55	0.41
1:A:303:ARG:HH11	1:A:303:ARG:HD3	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:VAL:CG1	1:B:73:GLY:C	2.93	0.41
1:B:357:ASP:OD1	1:B:357:ASP:C	2.64	0.41
1:B:54:GLY:O	1:B:62:ARG:HD2	2.21	0.41
1:B:282:TYR:CD1	1:B:282:TYR:N	2.89	0.41
1:A:326:ASN:OD1	1:A:329:LYS:HE2	2.21	0.41
1:B:9:PRO:HG2	1:B:107:ILE:HG22	2.03	0.41
1:A:365:ASP:CG	1:A:366:PRO:HD2	2.46	0.41
1:A:8:ALA:O	1:A:108:HIS:CD2	2.74	0.41
1:B:126:LEU:HD23	1:B:126:LEU:HA	1.90	0.41
1:A:160:THR:HB	1:A:163:THR:OG1	2.21	0.41
1:B:154:PHE:C	1:B:154:PHE:CD1	2.99	0.40
1:B:94:TYR:HB3	4:B:446:HOH:O	2.21	0.40
1:B:387:GLN:HA	1:B:388:PRO:HD3	1.88	0.40

There are no symmetry-related clashes.

## 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	386/388 (100%)	375 (97%)	10 (3%)	1 (0%)	36	42
1	B	386/388 (100%)	376 (97%)	9 (2%)	1 (0%)	36	42
All	All	772/776 (100%)	751 (97%)	19 (2%)	2 (0%)	36	42

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	PHE
1	B	203	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	320/320 (100%)	298 (93%)	22 (7%)	14	16
1	B	319/320 (100%)	300 (94%)	19 (6%)	17	21
All	All	639/640 (100%)	598 (94%)	41 (6%)	16	19

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ARG
1	A	24	MET
1	A	25	PHE
1	A	68	VAL
1	A	106	ARG
1	A	113	SER
1	A	132	GLU
1	A	170	LEU
1	A	179	ARG
1	A	203	VAL
1	A	209	ASP
1	A	210	GLN
1	A	226	GLU
1	A	233	VAL
1	A	244	LEU
1	A	335	ARG
1	A	344	LYS
1	A	345	LYS
1	A	357	ASP
1	A	361	ILE
1	A	378	ARG
1	A	387	GLN
1	B	2	SER
1	B	11	VAL
1	B	23	GLU
1	B	103	ARG
1	B	132	GLU

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Mol	Chain	Res	Type
1	B	147	LEU
1	B	149	GLU
1	B	174	VAL
1	B	196	ASN
1	B	200	THR
1	B	201	SER
1	B	202	GLN
1	B	203	VAL
1	B	214	ARG
1	B	278	THR
1	B	285	LEU
1	B	291	SER
1	B	311	SER
1	B	342	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	B	59	ASN
1	B	128	ASN
1	B	141	ASN
1	B	196	ASN

### 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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.