Full wwPDB X-ray Structure Validation Report (i)

Jan 30, 2024 – 08:10 PM EST

PDB ID	:	1JI3
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

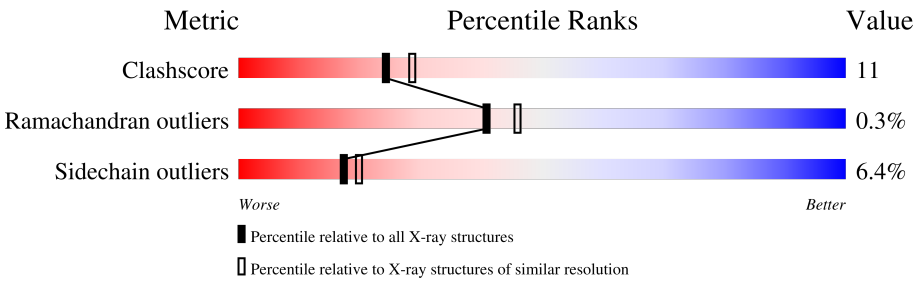
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (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 >=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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	388	75% 20% • •
1	B	388	79% 18% • •

2 Entry composition (i)

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 (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is water.

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

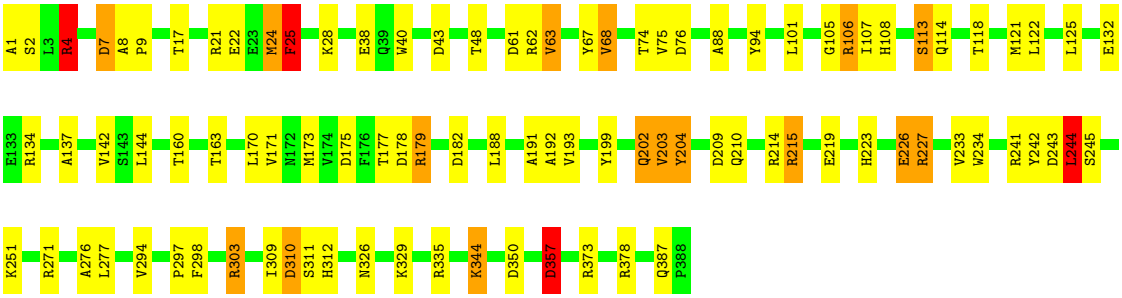
3 Residue-property plots (i)

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.

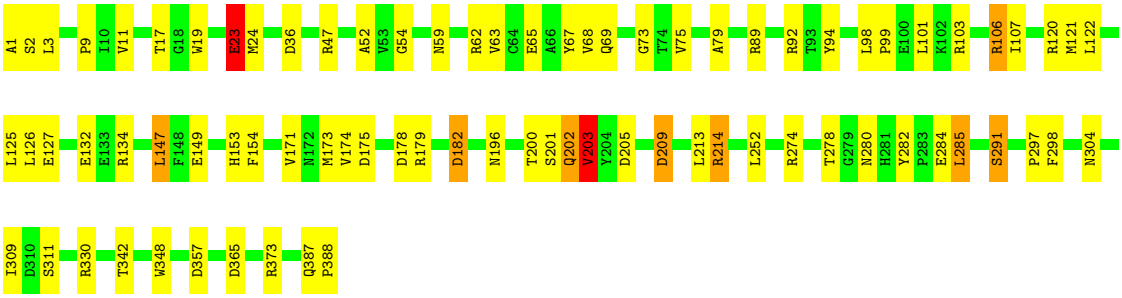
• Molecule 1: lipase

Chain A:



• Molecule 1: lipase

Chain B:



4 Data and refinement statistics (i)

Xtriage (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, α, β, γ	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.	Xtriage
Total number of atoms	6470	wwPDB-VP
Average B, all atoms (Å^2)	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: CA, ZN

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	0.30	0/3147	1.41	37/4280 (0.9%)
1	B	0.30	0/3140	1.29	18/4271 (0.4%)
All	All	0.30	0/6287	1.35	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(^{o})	Ideal(^{o})
1	A	310	ASP	CB-CG-OD1	-19.02	101.18	118.30
1	A	310	ASP	CB-CG-OD2	16.18	132.86	118.30
1	A	227	ARG	NE-CZ-NH2	-12.72	113.94	120.30
1	A	215	ARG	NE-CZ-NH2	-12.35	114.13	120.30
1	A	62	ARG	NE-CZ-NH2	-11.10	114.75	120.30
1	A	227	ARG	NE-CZ-NH1	10.94	125.77	120.30
1	A	134	ARG	NE-CZ-NH1	9.85	125.23	120.30
1	A	134	ARG	NE-CZ-NH2	-9.83	115.38	120.30
1	B	330	ARG	NE-CZ-NH1	-9.68	115.46	120.30
1	A	310	ASP	CB-CA-C	-9.65	91.10	110.40
1	A	350	ASP	CB-CG-OD1	9.39	126.75	118.30
1	A	215	ARG	CG-CD-NE	-8.35	94.26	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	182	ASP	CB-CG-OD2	7.85	125.36	118.30
1	B	365	ASP	CB-CG-OD2	7.83	125.35	118.30
1	B	24	MET	CG-SD-CE	-7.80	87.71	100.20
1	A	63	VAL	CG1-CB-CG2	-7.17	99.42	110.90
1	B	23	GLU	CB-CA-C	7.15	124.70	110.40
1	A	243	ASP	CB-CG-OD1	7.09	124.68	118.30
1	A	175	ASP	CB-CG-OD2	6.88	124.49	118.30
1	B	182	ASP	CB-CG-OD1	6.63	124.27	118.30
1	B	134	ARG	NE-CZ-NH2	-6.47	117.07	120.30
1	A	76	ASP	CB-CG-OD1	6.46	124.12	118.30
1	A	61	ASP	CB-CG-OD2	6.40	124.06	118.30
1	B	178	ASP	CB-CG-OD1	6.35	124.01	118.30
1	A	303	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	B	23	GLU	CG-CD-OE1	6.24	130.77	118.30
1	A	244	LEU	CB-CG-CD1	-6.08	100.66	111.00
1	A	311	SER	CB-CA-C	-5.98	98.74	110.10
1	A	271	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	A	202	GLN	CA-CB-CG	-5.86	100.51	113.40
1	A	215	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	B	17	THR	OG1-CB-CG2	-5.66	96.97	110.00
1	A	4	ARG	CG-CD-NE	5.66	123.68	111.80
1	B	153	HIS	CB-CA-C	-5.63	99.14	110.40
1	B	175	ASP	CB-CG-OD2	5.63	123.36	118.30
1	B	36	ASP	CB-CG-OD1	5.54	123.29	118.30
1	B	127	GLU	OE1-CD-OE2	5.52	129.92	123.30
1	A	62	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	144	LEU	CB-CG-CD1	5.39	120.17	111.00
1	A	67	TYR	CB-CG-CD2	-5.30	117.82	121.00
1	A	178	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	17	THR	OG1-CB-CG2	-5.25	97.91	110.00
1	B	209	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	43	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	2	SER	N-CA-C	5.19	125.02	111.00
1	B	106	ARG	NE-CZ-NH1	-5.19	117.71	120.30
1	A	309	ILE	C-N-CA	5.17	134.63	121.70
1	A	214	ARG	N-CA-C	-5.11	97.22	111.00
1	A	310	ASP	N-CA-CB	-5.07	101.47	110.60
1	A	25	PHE	CB-CA-C	-5.07	100.27	110.40
1	B	291	SER	CB-CA-C	5.06	119.72	110.10
1	B	274	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	A	357	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	7	ASP	CB-CG-OD2	5.03	122.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	ASP	CB-CG-OD1	5.03	122.83	118.30

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	76	0
1	B	3057	0	2917	56	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	132	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 11.

All (132) 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:NZ	1:A:344:LYS:HB3	1.67	1.08
1:A:171:VAL:HG21	1:A:244:LEU:CD1	1.86	1.05
1:A:344:LYS:HB3	1:A:344:LYS:HZ2	1.19	1.04
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:47:ARG:NH2	1:B:47:ARG:NH1	2.17	0.93
1:B:19:TRP:HB2	1:B:23:GLU:HG2	1.51	0.92
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:285:LEU:C	1:B:285:LEU:HD23	2.00	0.82
1:B:68:VAL:HG21	1:B:75:VAL:CA	2.08	0.81
1:B:68:VAL:HG23	4:B:438:HOH:O	1.87	0.75
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:CD1	1:A:244:LEU:C	2.56	0.73
1:A:24:MET:HE3	1:A:193:VAL:HG21	1.69	0.72
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: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:A:344:LYS:HB3	1:A:344:LYS:HZ3	1.54	0.70
1:B:63:VAL:HG21	1:B:121:MET:HB3	1.74	0.70
1:B:68:VAL:CG2	4:B:438:HOH:O	2.41	0.69
1:A:244:LEU:C	1:A:244:LEU:HD12	2.12	0.69
1:A:344:LYS:NZ	1:A:344:LYS:CB	2.41	0.69
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:B:19:TRP:HB2	1:B:23:GLU:CD	2.15	0.67
1:A:24:MET:HE1	1:A:193:VAL:HG21	1.77	0.66
1:A:105:GLY:C	1:A:106:ARG:HG2	2.16	0.66
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	2.27	0.64
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:242:TYR:OH	1:A:251:LYS:HD2	1.99	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:VAL:HG13	1:A:94:TYR:HD2	1.65	0.61
1:B:202:GLN:C	1:B:203:VAL:CG1	2.69	0.60
1:A:344:LYS:HZ2	1:A:344:LYS:CB	2.04	0.60
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: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: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:B:285:LEU:C	1:B:285:LEU:CD2	2.74	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:202:GLN:C	1:B:203:VAL:HG12	2.27	0.55
1:B:120:ARG:HD2	1:B:348:TRP:CZ2	2.43	0.54
1:A:244:LEU:C	1:A:244:LEU:HD13	2.28	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:284:GLU:OE2	4:B:578:HOH:O	2.18	0.51
1:A:344:LYS:HZ3	1:A:344:LYS:CB	2.12	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: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
1:A:88:ALA:HB1	4:A:412:HOH:O	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:VAL:HG13	1:A:122:LEU:HD13	1.96	0.47
1:B:252:LEU:HD23	1:B:252:LEU:C	2.35	0.47
1:A:63:VAL:HG23	1:A:118:THR:HG23	1.97	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: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:B:213:LEU:C	1:B:214:ARG:HD3	2.37	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:A:21:ARG:CZ	1:A:28:LYS:HE3	2.48	0.43
1:A:173:MET:HG2	1:A:298:PHE:CD2	2.54	0.43
1:A:357:ASP:OD1	1:A:357:ASP:C	2.56	0.42
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: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:B:68:VAL:HG13	1:B:73:GLY:C	2.40	0.42
1:A:68:VAL:HG21	1:A:74:THR:C	2.41	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:MET:O	1:A:25:PHE:C	2.60	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%)	41	46
1	B	386/388 (100%)	376 (97%)	9 (2%)	1 (0%)	41	46
All	All	772/776 (100%)	751 (97%)	19 (2%)	2 (0%)	41	46

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%)	299 (93%)	21 (7%)	16	19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	319/320 (100%)	299 (94%)	20 (6%)	18 20
All	All	639/640 (100%)	598 (94%)	41 (6%)	17 20

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	204	TYR
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	357	ASP
1	A	378	ARG
1	A	387	GLN
1	B	2	SER
1	B	11	VAL
1	B	23	GLU
1	B	99	PRO
1	B	103	ARG
1	B	132	GLU
1	B	147	LEU
1	B	149	GLU
1	B	154	PHE
1	B	174	VAL
1	B	196	ASN
1	B	200	THR
1	B	201	SER
1	B	202	GLN
1	B	203	VAL

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Mol	Chain	Res	Type
1	B	214	ARG
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 (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	HIS
1	A	172	ASN
1	B	131	GLN
1	B	141	ASN
1	B	172	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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.