



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 04:41 PM BST

PDB ID : 4FKB  
Title : An Organic solvent tolerant lipase 42  
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Deposited on : 2012-06-13  
Resolution : 1.22 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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13

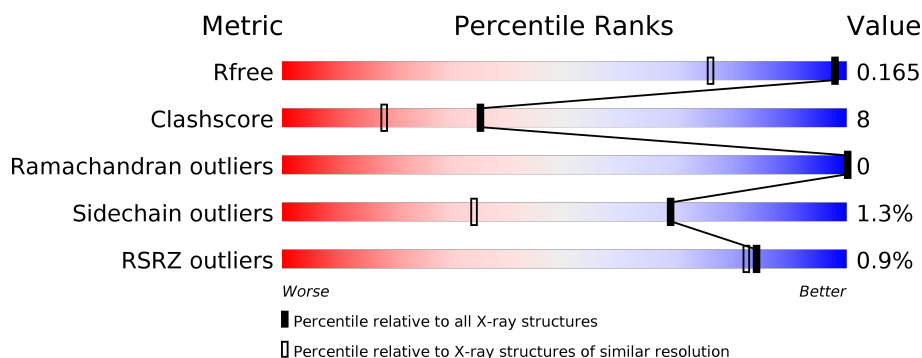
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.22 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))
$R_{free}$	130704	1232 (1.24-1.20)
Clashscore	141614	1294 (1.24-1.20)
Ramachandran outliers	138981	1251 (1.24-1.20)
Sidechain outliers	138945	1250 (1.24-1.20)
RSRZ outliers	127900	1209 (1.24-1.20)

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 on 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  $\leq 5\%$ . 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	388	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>%</span> <span>88%</span> <span>11%</span> </div> </div>
1	B	388	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 98%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> <span>%</span> <span>86%</span> <span>11%</span> </div> </div>

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
3	GOL	A	413	-	X	X	-
3	GOL	B	417	-	-	X	-
3	GOL	B	418	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7622 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 Thermostable organic solvent tolerant lipase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	21	0
			3154	2010	549	586	9			
1	B	387	Total	C	N	O	S	0	39	0
			3286	2099	575	601	11			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	LEU	TRP	engineered mutation	UNP Q5U780
A	202	GLU	GLN	engineered mutation	UNP Q5U780
B	147	LEU	TRP	engineered mutation	UNP Q5U780
B	202	GLU	GLN	engineered mutation	UNP Q5U780

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	A	1	Total C O 12 6 6	0	1
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 5 3 2	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	A	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 18 9 9	0	1
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0
3	B	1	Total C O 6 3 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	1
			12	6	6		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	5	Total	Na	0	0
			5	5		
4	A	4	Total	Na	0	0
			4	4		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	5	Total	Cl	0	0
			5	5		
5	A	5	Total	Cl	0	0
			5	5		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

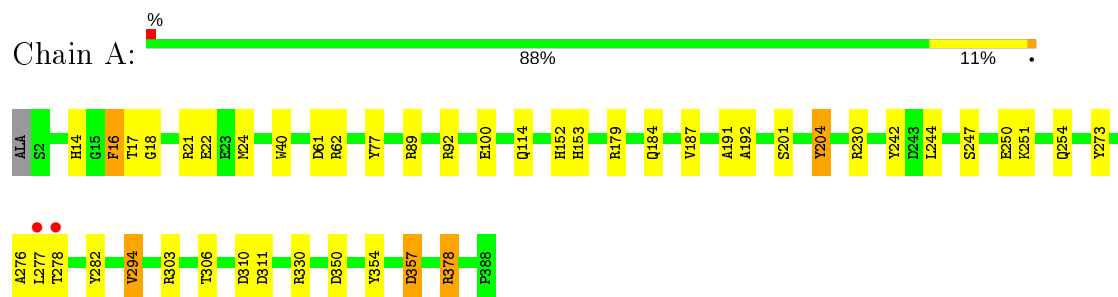
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	524	Total 524	O 524	0	0
7	B	491	Total 491	O 491	0	0

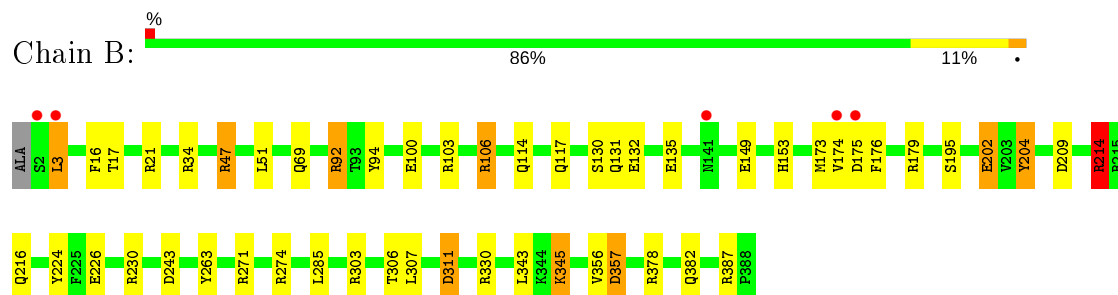
### 3 Residue-property plots [i](#)

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 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: Thermostable organic solvent tolerant lipase



- Molecule 1: Thermostable organic solvent tolerant lipase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.82Å 81.00Å 99.53Å 90.00° 96.69° 90.00°	Depositor
Resolution (Å)	50.00 – 1.22 26.31 – 1.22	Depositor EDS
% Data completeness (in resolution range)	93.7 (50.00-1.22) 93.7 (26.31-1.22)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.55 (at 1.22Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.127 , 0.165 0.127 , 0.165	Depositor DCC
$R_{free}$ test set	12959 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	7.3	Xtriage
Anisotropy	0.136	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 58.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	7622	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, CA, NA, CL

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	1.23	7/3298 (0.2%)	1.26	22/4483 (0.5%)
1	B	1.27	7/3475 (0.2%)	1.25	30/4711 (0.6%)
All	All	1.25	14/6773 (0.2%)	1.26	52/9194 (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

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	303	ARG	CZ-NH1	10.59	1.46	1.33
1	B	202	GLU	CD-OE2	10.02	1.36	1.25
1	A	100	GLU	CD-OE1	8.52	1.35	1.25
1	A	303	ARG	CZ-NH2	8.36	1.44	1.33
1	A	40	TRP	CD2-CE2	6.93	1.49	1.41
1	B	202	GLU	CB-CG	-6.85	1.39	1.52
1	B	202	GLU	CG-CD	-5.84	1.43	1.51
1	B	274	ARG	CD-NE	-5.68	1.36	1.46
1	B	132	GLU	CD-OE1	5.64	1.31	1.25
1	A	247[A]	SER	CA-CB	5.61	1.61	1.52
1	A	247[B]	SER	CA-CB	5.61	1.61	1.52
1	A	77	TYR	CE1-CZ	5.58	1.45	1.38
1	B	100	GLU	CG-CD	5.54	1.60	1.51
1	B	176	PHE	CE1-CZ	5.17	1.47	1.37

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	ARG	NE-CZ-NH2	-11.31	114.64	120.30
1	B	106	ARG	NE-CZ-NH1	-11.16	114.72	120.30
1	A	230	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	A	330[A]	ARG	NE-CZ-NH1	-10.61	115.00	120.30
1	A	330[B]	ARG	NE-CZ-NH1	-10.61	115.00	120.30
1	B	357	ASP	CB-CG-OD1	8.97	126.38	118.30
1	A	230	ARG	NE-CZ-NH2	-8.57	116.01	120.30
1	B	92[A]	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	B	92[B]	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	B	103[A]	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	B	103[B]	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	A	278	THR	C-N-CA	-8.26	104.96	122.30
1	B	271	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	B	303	ARG	NE-CZ-NH2	8.14	124.37	120.30
1	A	378[A]	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	A	378[B]	ARG	NE-CZ-NH1	7.87	124.23	120.30
1	B	3	LEU	CA-CB-CG	-7.60	97.81	115.30
1	A	357	ASP	CB-CG-OD1	7.54	125.09	118.30
1	B	214[A]	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	B	214[B]	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	A	62	ARG	NE-CZ-NH2	-6.97	116.81	120.30
1	A	21	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	A	89	ARG	NE-CZ-NH1	-6.90	116.85	120.30
1	A	354	TYR	CB-CG-CD2	-6.80	116.92	121.00
1	B	330	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	B	214[A]	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	B	214[B]	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	B	103[A]	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	B	103[B]	ARG	NE-CZ-NH1	6.53	123.57	120.30
1	A	330[A]	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	A	330[B]	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	A	277	LEU	CB-CG-CD2	-6.04	100.74	111.00
1	B	230	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	303	ARG	NE-CZ-NH1	-5.71	117.44	120.30
1	B	311	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	350	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	B	356[A]	VAL	CG1-CB-CG2	-5.49	102.12	110.90
1	B	356[B]	VAL	CG1-CB-CG2	-5.49	102.12	110.90
1	B	387	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	B	311	ASP	CB-CG-OD1	-5.42	113.42	118.30
1	A	294[A]	VAL	CA-CB-CG2	-5.30	102.95	110.90
1	A	294[B]	VAL	CA-CB-CG2	-5.30	102.95	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	GLU	CG-CD-OE2	-5.26	107.78	118.30
1	A	277	LEU	CB-CG-CD1	5.23	119.89	111.00
1	A	61	ASP	CB-CG-OD1	5.17	122.95	118.30
1	B	204	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	B	345[A]	LYS	CD-CE-NZ	5.15	123.55	111.70
1	B	345[B]	LYS	CD-CE-NZ	5.15	123.55	111.70
1	A	92	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	226	GLU	OE1-CD-OE2	-5.08	117.20	123.30
1	B	243	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	B	224	TYR	CD1-CE1-CZ	-5.01	115.29	119.80

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	16[A]	PHE	Peptide
1	B	16	PHE	Peptide

## 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	3154	0	3068	38	0
1	B	3286	0	3258	60	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	54	0	68	15	0
3	B	90	0	120	21	0
4	A	4	0	0	0	0
4	B	5	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	524	0	0	15	2
7	B	491	0	0	15	3
All	All	7622	0	6514	107	3

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 8.

All (107) 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:16[B]:PHE:CE2	7:A:710:HOH:O	1.83	1.29
1:B:214[A]:ARG:HH21	1:B:214[A]:ARG:CG	1.35	1.29
1:B:174[B]:VAL:HG23	7:B:968:HOH:O	1.30	1.26
1:A:306[B]:THR:HG22	7:A:683:HOH:O	1.04	1.22
1:B:173[B]:MET:CE	1:B:179[B]:ARG:HD2	1.71	1.20
3:B:418:GOL:H31	7:B:627:HOH:O	1.41	1.20
1:B:131[B]:GLN:NE2	1:B:135[B]:GLU:OE2	1.74	1.19
1:B:174[B]:VAL:O	1:B:175[B]:ASP:HB2	1.45	1.12
1:B:173[B]:MET:HE3	1:B:179[B]:ARG:HD2	1.24	1.10
1:B:378:ARG:HB3	3:B:417:GOL:O1	1.55	1.05
1:B:106:ARG:HH21	1:B:153:HIS:HE1	1.07	1.02
1:B:214[A]:ARG:HG2	1:B:214[A]:ARG:NH2	1.36	1.00
1:A:254[A]:GLN:NE2	7:A:935:HOH:O	1.96	0.98
1:A:153:HIS:HB3	3:A:412:GOL:H12	1.45	0.97
1:B:149[B]:GLU:OE2	7:B:938:HOH:O	1.85	0.94
1:B:214[A]:ARG:NH2	1:B:216:GLN:HE22	1.66	0.94
1:B:378:ARG:HG3	7:B:804:HOH:O	1.76	0.86
1:A:242:TYR:OH	1:A:251:LYS:HD3	1.76	0.85
1:B:174[B]:VAL:O	1:B:175[B]:ASP:CB	2.20	0.85
1:B:131[B]:GLN:OE1	7:B:977:HOH:O	1.95	0.84
1:A:16[B]:PHE:CZ	7:A:710:HOH:O	2.17	0.82
1:B:378:ARG:HE	3:B:417:GOL:C1	1.92	0.81
1:B:214[A]:ARG:NH2	1:B:216:GLN:NE2	2.29	0.81
1:B:173[B]:MET:HE1	1:B:179[B]:ARG:HD2	1.64	0.80
1:B:173[B]:MET:CE	1:B:179[B]:ARG:CD	2.58	0.79
1:A:179:ARG:HD3	1:A:294[B]:VAL:HG21	1.67	0.77
1:A:114:GLN:NE2	1:A:244[B]:LEU:HG	2.00	0.76
1:B:214[A]:ARG:NH2	7:B:749:HOH:O	2.19	0.76
1:B:214[A]:ARG:CG	1:B:214[A]:ARG:NH2	2.09	0.74
1:B:378:ARG:HE	3:B:417:GOL:H11	1.51	0.73
1:B:106:ARG:HH21	1:B:153:HIS:CE1	1.99	0.71
1:A:250[A]:GLU:OE1	7:A:947:HOH:O	2.11	0.69
1:B:195:SER:OG	3:B:418:GOL:H32	1.94	0.68
1:B:214[A]:ARG:HH21	1:B:214[A]:ARG:HG2	0.55	0.67
1:A:114:GLN:HE22	1:A:244[B]:LEU:HG	1.57	0.66
5:B:423:CL:CL	7:B:725:HOH:O	2.50	0.66
1:B:195:SER:OG	3:B:418:GOL:H12	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214[A]:ARG:CZ	1:B:216:GLN:HE22	2.11	0.64
1:A:311[A]:ASP:H	3:A:413:GOL:H31	1.63	0.63
1:B:92[A]:ARG:NH2	7:B:801:HOH:O	2.31	0.63
1:A:153:HIS:CG	7:A:839:HOH:O	2.52	0.62
1:B:378:ARG:CB	3:B:417:GOL:O1	2.38	0.61
1:B:106:ARG:NH2	1:B:153:HIS:HE1	1.89	0.61
3:A:413:GOL:H12	7:A:617:HOH:O	2.01	0.60
1:B:214[A]:ARG:HH22	1:B:216:GLN:NE2	1.99	0.60
1:B:378:ARG:NE	3:B:417:GOL:H11	2.17	0.60
1:A:311[A]:ASP:OD2	3:A:413:GOL:H32	2.03	0.58
1:B:51:LEU:HD22	1:B:69[B]:GLN:CG	2.33	0.58
1:B:131[B]:GLN:NE2	1:B:135[B]:GLU:CD	2.56	0.58
1:B:51:LEU:HD22	1:B:69[B]:GLN:HG3	1.86	0.58
1:B:378:ARG:HH21	3:B:417:GOL:H32	1.69	0.57
1:A:17[A]:THR:HG1	1:A:204:TYR:HH	1.49	0.57
1:A:311[B]:ASP:H	3:A:413:GOL:H31	1.68	0.57
3:B:418:GOL:H32	7:B:608:HOH:O	2.04	0.56
1:B:195:SER:OG	3:B:418:GOL:C3	2.54	0.56
1:A:310:ASP:CA	3:A:413:GOL:H31	2.36	0.55
1:A:378[A]:ARG:HG3	7:A:1023:HOH:O	2.07	0.55
1:B:131[B]:GLN:HE21	1:B:135[B]:GLU:CD	2.10	0.54
1:A:378[B]:ARG:NH1	7:A:1010:HOH:O	1.81	0.54
3:B:407:GOL:C3	7:B:916:HOH:O	2.51	0.54
1:A:152:HIS:HD2	7:A:561:HOH:O	1.91	0.54
1:A:153:HIS:CD2	7:A:839:HOH:O	2.61	0.53
1:B:17[B]:THR:HG1	1:B:204:TYR:HH	1.49	0.53
1:B:34:ARG:O	3:B:415:GOL:H31	2.09	0.53
1:B:173[B]:MET:HE1	1:B:179[B]:ARG:CD	2.32	0.52
1:A:184:GLN:O	1:A:187[B]:VAL:HG12	2.09	0.52
1:B:92[B]:ARG:HD2	1:B:94:TYR:OH	2.12	0.50
1:A:310:ASP:HB2	3:A:413:GOL:H31	1.93	0.50
1:B:263:TYR:CZ	1:B:345[B]:LYS:HE2	2.46	0.50
1:B:306:THR:HG23	7:B:747:HOH:O	2.12	0.50
1:A:276:ALA:O	7:A:996:HOH:O	2.20	0.49
1:B:378:ARG:HB2	3:B:417:GOL:H31	1.93	0.49
1:B:311:ASP:HB2	7:B:965:HOH:O	2.12	0.49
1:B:378:ARG:HB3	3:B:417:GOL:HO1	1.74	0.48
1:A:152:HIS:HE1	7:A:845:HOH:O	1.95	0.48
1:B:378:ARG:NH2	3:B:417:GOL:H32	2.28	0.48
1:A:311[A]:ASP:H	3:A:413:GOL:C3	2.24	0.48
1:B:47:ARG:HG2	7:B:824:HOH:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ALA:O	3:A:414:GOL:H2	2.15	0.47
1:A:14:HIS:CG	1:A:18:GLY:HA3	2.50	0.47
1:A:24[B]:MET:HG3	1:A:191:ALA:HB1	1.98	0.46
1:B:130:SER:OG	3:B:416:GOL:H12	2.17	0.45
1:B:21:ARG:HD3	3:B:413[A]:GOL:H2	1.99	0.45
1:B:130:SER:OG	3:B:416:GOL:C1	2.65	0.45
1:B:3:LEU:HD12	1:B:3:LEU:H	1.81	0.44
1:A:114:GLN:CD	1:A:244[B]:LEU:HG	2.37	0.44
1:A:311[B]:ASP:H	3:A:413:GOL:C3	2.28	0.44
1:A:273:TYR:CZ	1:A:282:TYR:HB2	2.53	0.44
1:A:201[A]:SER:HB2	3:A:411:GOL:HO2	1.82	0.44
1:A:201[B]:SER:OG	3:A:411:GOL:O2	1.81	0.43
3:B:418:GOL:C3	7:B:608:HOH:O	2.65	0.43
1:B:92[B]:ARG:HD2	1:B:94:TYR:CZ	2.53	0.43
1:A:251:LYS:HE2	1:A:251:LYS:HB3	1.65	0.43
1:B:263:TYR:CE1	1:B:345[B]:LYS:HE2	2.54	0.43
1:B:343:LEU:HD11	1:B:382[B]:GLN:HG2	1.99	0.43
1:A:24[A]:MET:CE	1:A:191:ALA:CB	2.97	0.42
1:A:153:HIS:HA	7:A:839:HOH:O	2.19	0.42
1:B:114[B]:GLN:HG3	1:B:117:GLN:OE1	2.19	0.42
1:B:17[B]:THR:OG1	1:B:204:TYR:OH	2.23	0.42
1:A:310:ASP:C	3:A:413:GOL:H31	2.40	0.41
1:B:214[A]:ARG:HH22	1:B:216:GLN:HE22	1.49	0.41
1:A:378[A]:ARG:NH2	7:A:776:HOH:O	2.54	0.41
1:B:3:LEU:HD12	1:B:3:LEU:N	2.36	0.40
3:B:407:GOL:H32	7:B:916:HOH:O	2.19	0.40
1:B:92[A]:ARG:HE	1:B:209[A]:ASP:CG	2.25	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:A:683:HOH:O	7:B:718:HOH:O[4_545]	2.03	0.17
7:B:736:HOH:O	7:B:761:HOH:O[4_545]	2.09	0.11
7:A:684:HOH:O	7:B:682:HOH:O[3_445]	2.16	0.04

## 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	406/388 (105%)	397 (98%)	9 (2%)	0	100	100
1	B	425/388 (110%)	414 (97%)	11 (3%)	0	100	100
All	All	831/776 (107%)	811 (98%)	20 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	337/318 (106%)	334 (99%)	3 (1%)	78	50
1	B	357/318 (112%)	350 (98%)	7 (2%)	55	17
All	All	694/636 (109%)	684 (99%)	10 (1%)	69	32

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	GLU
1	A	204	TYR
1	A	357	ASP
1	B	202	GLU
1	B	214[A]	ARG
1	B	214[B]	ARG
1	B	285[A]	LEU
1	B	285[B]	LEU

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Mol	Chain	Res	Type
1	B	307	LEU
1	B	357	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	152	HIS
1	A	172	ASN
1	B	44	ASN
1	B	153	HIS
1	B	172	ASN
1	B	216	GLN
1	B	257	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 48 ligands modelled in this entry, 1 is modelled with single atom and 23 are monoatomic - leaving 24 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
3	GOL	A	411	-	3,4,5	0.50	0	1,4,5	0.72	0
3	GOL	B	417	-	5,5,5	0.76	0	5,5,5	0.66	0
3	GOL	B	412	-	5,5,5	0.64	0	5,5,5	0.93	0
3	GOL	A	408	-	5,5,5	0.22	0	5,5,5	0.76	0
3	GOL	B	409	-	5,5,5	0.54	0	5,5,5	1.78	3 (60%)
3	GOL	A	413	-	5,5,5	1.03	0	5,5,5	2.67	2 (40%)
3	GOL	B	418	-	5,5,5	0.64	0	5,5,5	1.58	1 (20%)
3	GOL	B	407	-	5,5,5	0.90	0	5,5,5	0.91	0
3	GOL	A	409	-	5,5,5	0.98	0	5,5,5	1.10	0
3	GOL	B	410	-	5,5,5	0.96	0	5,5,5	0.63	0
3	GOL	A	410	-	5,5,5	0.79	0	5,5,5	1.26	0
3	GOL	A	414	-	5,5,5	0.66	0	5,5,5	0.82	0
3	GOL	A	412	-	5,5,5	0.77	0	5,5,5	1.12	1 (20%)
3	GOL	A	403[B]	-	5,5,5	0.44	0	5,5,5	1.08	0
3	GOL	B	416	-	5,5,5	0.83	0	5,5,5	1.20	0
3	GOL	A	403[A]	-	5,5,5	0.70	0	5,5,5	0.84	0
3	GOL	B	408[B]	-	5,5,5	0.51	0	5,5,5	0.88	0
3	GOL	B	408[C]	-	5,5,5	0.64	0	5,5,5	0.65	0
3	GOL	B	414	-	5,5,5	0.33	0	5,5,5	0.63	0
3	GOL	B	413[B]	-	5,5,5	1.12	1 (20%)	5,5,5	1.39	1 (20%)
3	GOL	B	408[A]	-	5,5,5	0.69	0	5,5,5	0.87	0
3	GOL	B	413[A]	-	5,5,5	1.18	0	5,5,5	1.22	0
3	GOL	B	411	-	5,5,5	1.22	1 (20%)	5,5,5	0.84	0
3	GOL	B	415	-	5,5,5	0.80	0	5,5,5	0.94	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
3	GOL	A	411	-	-	2/2/2/4	-
3	GOL	B	417	-	-	0/4/4/4	-
3	GOL	B	412	-	-	1/4/4/4	-
3	GOL	A	408	-	-	4/4/4/4	-
3	GOL	B	409	-	-	2/4/4/4	-
3	GOL	A	413	-	-	4/4/4/4	-
3	GOL	B	418	-	-	4/4/4/4	-
3	GOL	B	407	-	-	0/4/4/4	-
3	GOL	A	409	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	410	-	-	0/4/4/4	-
3	GOL	A	410	-	-	0/4/4/4	-
3	GOL	A	414	-	-	4/4/4/4	-
3	GOL	A	412	-	-	2/4/4/4	-
3	GOL	A	403[B]	-	-	2/4/4/4	-
3	GOL	B	416	-	-	2/4/4/4	-
3	GOL	A	403[A]	-	-	4/4/4/4	-
3	GOL	B	408[B]	-	-	0/4/4/4	-
3	GOL	B	408[C]	-	-	1/4/4/4	-
3	GOL	B	414	-	-	1/4/4/4	-
3	GOL	B	413[B]	-	-	0/4/4/4	-
3	GOL	B	408[A]	-	-	0/4/4/4	-
3	GOL	B	413[A]	-	-	0/4/4/4	-
3	GOL	B	411	-	-	0/4/4/4	-
3	GOL	B	415	-	-	2/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	411	GOL	O3-C3	2.44	1.52	1.42
3	B	413[B]	GOL	O2-C2	-2.07	1.37	1.43

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	413	GOL	O2-C2-C3	3.88	126.21	109.12
3	A	413	GOL	O3-C3-C2	3.81	128.45	110.20
3	B	413[B]	GOL	O2-C2-C3	-2.34	98.83	109.12
3	A	412	GOL	O2-C2-C1	-2.28	99.09	109.12
3	B	409	GOL	C3-C2-C1	-2.16	103.31	111.70
3	B	418	GOL	C3-C2-C1	-2.15	103.36	111.70
3	B	409	GOL	O1-C1-C2	-2.09	100.16	110.20
3	B	409	GOL	O2-C2-C3	-2.08	99.97	109.12

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	411	GOL	O2-C2-C3-O3
3	B	418	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	414	GOL	O1-C1-C2-C3
3	A	412	GOL	C1-C2-C3-O3
3	A	412	GOL	O2-C2-C3-O3
3	A	403[B]	GOL	O1-C1-C2-C3
3	B	416	GOL	C1-C2-C3-O3
3	B	416	GOL	O2-C2-C3-O3
3	B	415	GOL	C1-C2-C3-O3
3	B	418	GOL	O1-C1-C2-O2
3	A	414	GOL	O1-C1-C2-O2
3	B	412	GOL	O1-C1-C2-C3
3	A	408	GOL	O1-C1-C2-C3
3	A	408	GOL	C1-C2-C3-O3
3	A	413	GOL	O1-C1-C2-C3
3	A	413	GOL	C1-C2-C3-O3
3	B	418	GOL	O1-C1-C2-C3
3	A	414	GOL	C1-C2-C3-O3
3	A	403[A]	GOL	O1-C1-C2-C3
3	A	408	GOL	O1-C1-C2-O2
3	A	413	GOL	O1-C1-C2-O2
3	A	413	GOL	O2-C2-C3-O3
3	B	418	GOL	O2-C2-C3-O3
3	A	403[A]	GOL	O1-C1-C2-O2
3	A	414	GOL	O2-C2-C3-O3
3	A	408	GOL	O2-C2-C3-O3
3	B	409	GOL	O2-C2-C3-O3
3	A	411	GOL	C1-C2-C3-O3
3	A	403[A]	GOL	O2-C2-C3-O3
3	B	415	GOL	O2-C2-C3-O3
3	B	408[C]	GOL	O1-C1-C2-C3
3	B	414	GOL	O1-C1-C2-C3
3	A	403[B]	GOL	O1-C1-C2-O2
3	B	409	GOL	C1-C2-C3-O3
3	A	403[A]	GOL	C1-C2-C3-O3

There are no ring outliers.

10 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	411	GOL	2	0
3	B	417	GOL	9	0
3	A	413	GOL	11	0
3	B	418	GOL	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	407	GOL	2	0
3	A	414	GOL	1	0
3	A	412	GOL	1	0
3	B	416	GOL	2	0
3	B	413[A]	GOL	1	0
3	B	415	GOL	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	387/388 (99%)	-0.80	2 (0%) 91 90	5, 11, 23, 33	0
1	B	387/388 (99%)	-0.75	5 (1%) 77 75	4, 9, 22, 49	0
All	All	774/776 (99%)	-0.77	7 (0%) 84 82	4, 10, 23, 49	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	3	LEU	6.2
1	B	2	SER	5.2
1	B	174[A]	VAL	4.3
1	A	277	LEU	2.3
1	A	278	THR	2.3
1	B	141	ASN	2.2
1	B	175[A]	ASP	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 monosaccharides 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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
4	NA	A	406	1/1	0.83	0.21	64,64,64,64	0
3	GOL	A	410	6/6	0.88	0.14	31,35,38,41	0
3	GOL	A	414	6/6	0.88	0.20	43,51,82,94	0
3	GOL	B	409	6/6	0.89	0.14	34,39,49,60	0
3	GOL	B	418	6/6	0.90	0.26	24,35,44,46	0
3	GOL	B	414	6/6	0.90	0.17	44,50,60,71	0
3	GOL	B	416	6/6	0.91	0.15	20,35,50,56	0
3	GOL	B	415	6/6	0.91	0.14	27,33,35,53	0
3	GOL	A	403[A]	6/6	0.92	0.19	21,34,37,39	6
3	GOL	A	403[B]	6/6	0.92	0.19	21,25,27,34	6
3	GOL	B	417	6/6	0.92	0.19	20,31,43,51	0
3	GOL	B	407	6/6	0.94	0.17	16,22,25,28	0
4	NA	B	405	1/1	0.94	0.17	42,42,42,42	0
4	NA	A	407	1/1	0.95	0.33	37,37,37,37	0
3	GOL	A	408	6/6	0.96	0.15	41,43,57,72	0
3	GOL	A	411	5/6	0.96	0.14	30,33,43,44	0
3	GOL	A	413	6/6	0.96	0.18	16,22,32,44	0
3	GOL	B	410	6/6	0.96	0.09	14,17,24,32	0
3	GOL	A	412	6/6	0.97	0.21	19,42,51,61	0
3	GOL	B	413[B]	6/6	0.97	0.17	8,17,24,30	6
4	NA	B	404	1/1	0.97	0.11	31,31,31,31	0
3	GOL	B	413[A]	6/6	0.97	0.17	13,17,21,23	6
3	GOL	B	412	6/6	0.97	0.08	15,21,25,25	0
4	NA	B	403	1/1	0.98	0.18	40,40,40,40	0
4	NA	A	405	1/1	0.98	0.11	25,25,25,25	0
3	GOL	B	408[C]	6/6	0.99	0.07	6,14,18,18	6
3	GOL	A	402	1/6	0.99	0.04	15,15,15,15	0
4	NA	A	404	1/1	0.99	0.17	26,26,26,26	0
3	GOL	B	408[A]	6/6	0.99	0.07	7,14,18,24	6
4	NA	B	402	1/1	0.99	0.10	26,26,26,26	0
3	GOL	A	409	6/6	0.99	0.04	12,14,15,19	0
3	GOL	B	411	6/6	0.99	0.07	11,14,20,23	0
3	GOL	B	408[B]	6/6	0.99	0.07	8,12,13,14	6
5	CL	A	415	1/1	1.00	0.10	20,20,20,20	0
5	CL	B	419	1/1	1.00	0.03	12,12,12,12	0
2	ZN	A	401	1/1	1.00	0.01	7,7,7,7	0
5	CL	B	421	1/1	1.00	0.01	13,13,13,13	0
5	CL	B	423	1/1	1.00	0.06	16,16,16,16	0
5	CL	B	420	1/1	1.00	0.02	14,14,14,14	0
5	CL	A	419	1/1	1.00	0.06	18,18,18,18	0
6	CA	B	424	1/1	1.00	0.05	7,7,7,7	1
5	CL	A	418	1/1	1.00	0.02	18,18,18,18	0
6	CA	A	420	1/1	1.00	0.05	8,8,8,8	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CL	A	417	1/1	1.00	0.03	14,14,14,14	0
5	CL	B	422	1/1	1.00	0.03	15,15,15,15	0
2	ZN	B	401	1/1	1.00	0.01	6,6,6,6	0
5	CL	A	416	1/1	1.00	0.04	15,15,15,15	1
4	NA	B	406	1/1	1.00	0.02	12,12,12,12	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.