



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 3, 2023 – 09:08 am GMT

PDB ID : 1GT9  
Title : High resolution crystal structure of a thermostable serine-carboxyl type proteinase, kumamolisin (kscp)  
Authors : Comellas-Bigler, M.; Fuentes-Prior, P.; Maskos, K.; Huber, R.; Oyama, H.; Uchida, K.; Dunn, B.M.; Oda, K.; Bode, W.  
Deposited on : 2002-01-14  
Resolution : 1.38 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 : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtrriage (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

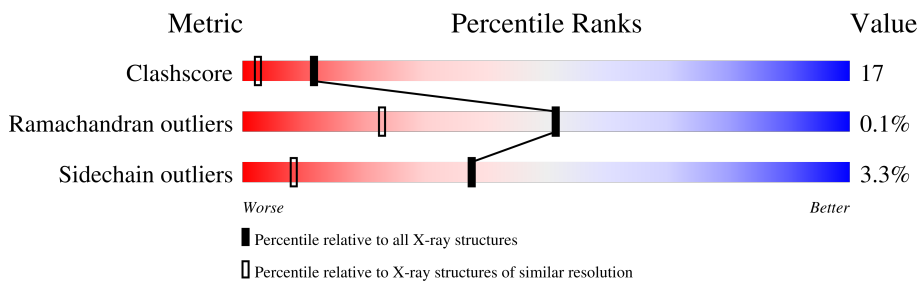
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.38 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	3037 (1.40-1.36)
Ramachandran outliers	138981	2970 (1.40-1.36)
Sidechain outliers	138945	2969 (1.40-1.36)

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	1	357	
1	2	357	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5928 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 KUMAMOLYSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	1	357	Total 2663	C 1674	N 453	O 531	S 5	20	14	0
1	2	357	Total 2687	C 1689	N 455	O 538	S 5	25	17	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	1	1	Total	O	S	0	0
			5	4	1		
3	2	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

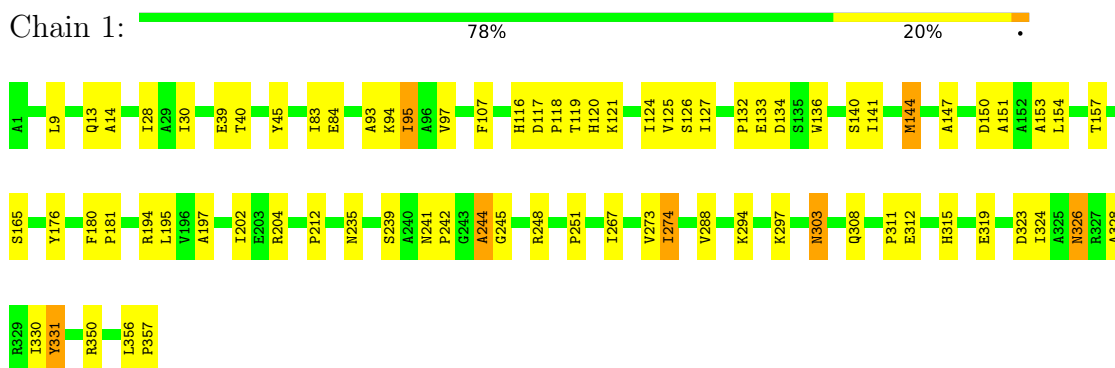
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	1	285	Total	O	0	0
			285	285		
4	2	281	Total	O	0	0
			281	281		

### 3 Residue-property plots

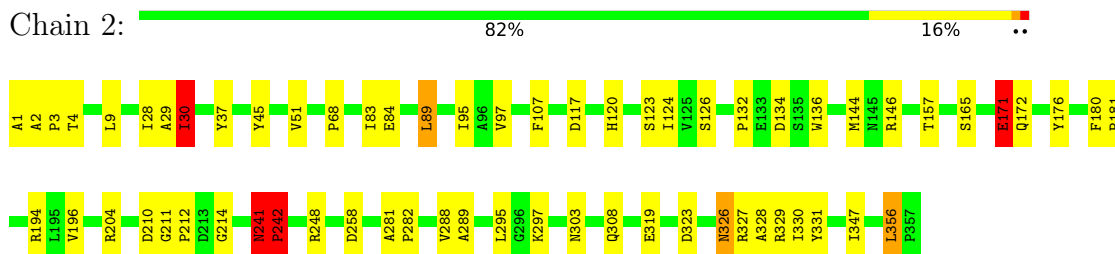
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



- Molecule 1: KUMAMOLYSIN



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.86Å 78.25Å 73.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.52 – 1.38	Depositor
% Data completeness (in resolution range)	95.4 (19.52-1.38)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.194 , 0.208	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	5928	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	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, SO4

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	1	0.89	10/2729 (0.4%)	0.95	12/3747 (0.3%)
1	2	1.58	18/2754 (0.7%)	2.66	19/3784 (0.5%)
All	All	1.29	28/5483 (0.5%)	2.00	31/7531 (0.4%)

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	1	0	4
1	2	1	4
All	All	1	8

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	171[A]	GLU	CD-OE1	36.98	1.66	1.25
1	2	171[B]	GLU	CD-OE1	36.98	1.66	1.25
1	2	242[A]	PRO	N-CD	22.17	1.78	1.47
1	2	242[B]	PRO	N-CD	22.17	1.78	1.47
1	2	242[A]	PRO	CA-CB	18.34	1.90	1.53
1	2	242[B]	PRO	CA-CB	18.34	1.90	1.53
1	2	165[A]	SER	CB-OG	-17.78	1.19	1.42
1	2	165[B]	SER	CB-OG	-17.78	1.19	1.42
1	1	244[A]	ALA	C-N	17.70	1.65	1.33
1	1	244[B]	ALA	C-N	17.70	1.65	1.33
1	1	245[A]	GLY	N-CA	14.08	1.67	1.46
1	1	245[B]	GLY	N-CA	14.08	1.67	1.46
1	2	146[A]	ARG	CZ-NH1	-13.31	1.15	1.33
1	2	146[B]	ARG	CZ-NH1	-13.31	1.15	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	2	242[A]	PRO	N-CA	12.21	1.68	1.47
1	2	242[B]	PRO	N-CA	12.21	1.68	1.47
1	2	241[A]	ASN	CA-CB	8.51	1.75	1.53
1	2	241[B]	ASN	CA-CB	8.51	1.75	1.53
1	1	13[A]	GLN	CG-CD	7.28	1.67	1.51
1	1	13[B]	GLN	CG-CD	7.28	1.67	1.51
1	2	146[A]	ARG	CG-CD	6.93	1.69	1.51
1	2	146[B]	ARG	CG-CD	6.93	1.69	1.51
1	2	30[A]	ILE	CB-CG1	-6.15	1.36	1.54
1	2	30[B]	ILE	CB-CG1	-6.15	1.36	1.54
1	1	140[A]	SER	C-N	6.12	1.48	1.34
1	1	140[B]	SER	C-N	6.12	1.48	1.34
1	1	194[A]	ARG	CG-CD	5.82	1.66	1.51
1	1	194[B]	ARG	CG-CD	5.82	1.66	1.51

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	146[A]	ARG	NH1-CZ-NH2	-104.76	4.17	119.40
1	2	146[B]	ARG	NH1-CZ-NH2	-104.76	4.17	119.40
1	2	242[A]	PRO	N-CA-CB	-18.05	81.64	103.30
1	2	242[B]	PRO	N-CA-CB	-18.05	81.64	103.30
1	2	242[A]	PRO	CA-N-CD	-16.25	88.76	111.50
1	2	242[B]	PRO	CA-N-CD	-16.25	88.76	111.50
1	1	244[A]	ALA	C-N-CA	-14.29	92.29	122.30
1	1	244[B]	ALA	C-N-CA	-14.29	92.29	122.30
1	2	171[A]	GLU	CG-CD-OE1	-12.61	93.08	118.30
1	2	171[B]	GLU	CG-CD-OE1	-12.61	93.08	118.30
1	2	242[A]	PRO	N-CD-CG	-12.31	84.74	103.20
1	2	242[B]	PRO	N-CD-CG	-12.31	84.74	103.20
1	2	242[A]	PRO	CB-CA-C	-8.61	90.49	112.00
1	2	242[B]	PRO	CB-CA-C	-8.61	90.49	112.00
1	1	144[A]	MET	CA-CB-CG	7.99	126.87	113.30
1	1	144[B]	MET	CA-CB-CG	7.99	126.87	113.30
1	1	274[A]	ILE	CG1-CB-CG2	-7.76	94.32	111.40
1	1	274[B]	ILE	CG1-CB-CG2	-7.76	94.32	111.40
1	2	146[A]	ARG	NE-CZ-NH1	-7.68	116.46	120.30
1	2	146[B]	ARG	NE-CZ-NH1	-7.68	116.46	120.30
1	2	242[A]	PRO	N-CA-C	-7.12	93.58	112.10
1	2	242[B]	PRO	N-CA-C	-7.12	93.58	112.10
1	2	241[A]	ASN	N-CA-CB	-6.75	98.45	110.60
1	2	241[B]	ASN	N-CA-CB	-6.75	98.45	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	1	244[A]	ALA	CA-C-N	-5.92	104.35	116.20
1	1	244[B]	ALA	CA-C-N	-5.92	104.35	116.20
1	2	356	LEU	CA-CB-CG	5.80	128.64	115.30
1	1	245[A]	GLY	N-CA-C	-5.46	99.46	113.10
1	1	245[B]	GLY	N-CA-C	-5.46	99.46	113.10
1	1	140[A]	SER	O-C-N	-5.07	114.59	122.70
1	1	140[B]	SER	O-C-N	-5.07	114.59	122.70

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	2	242[B]	PRO	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	1	165[B]	SER	Mainchain
1	1	331	TYR	Mainchain
1	1	95[A]	ILE	Mainchain
1	1	95[B]	ILE	Mainchain
1	2	171[A]	GLU	Sidechain
1	2	241[B]	ASN	Peptide
1	2	30[A]	ILE	Mainchain
1	2	30[B]	ILE	Mainchain

## 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	1	2663	0	2559	90	83
1	2	2687	0	2581	92	54
2	1	1	0	0	0	0
2	2	1	0	0	0	0
3	1	5	0	0	0	0
3	2	5	0	0	0	0
4	1	285	0	0	32	4
4	2	281	0	0	14	7

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5928	0	5140	182	87

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 17.

All (182) 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)
1:2:241[A]:ASN:CA	1:2:241[A]:ASN:CB	1.75	1.64
1:1:95[A]:ILE:CD1	1:1:95[A]:ILE:CG1	1.76	1.59
1:2:242[A]:PRO:N	1:2:242[A]:PRO:CA	1.68	1.56
1:2:242[B]:PRO:CD	1:2:242[B]:PRO:N	1.75	1.49
1:2:144[B]:MET:CE	1:2:144[B]:MET:SD	2.03	1.47
1:2:242[A]:PRO:CA	1:2:242[A]:PRO:CB	1.90	1.47
1:2:242[A]:PRO:N	1:2:242[A]:PRO:CD	1.78	1.44
1:1:144[B]:MET:SD	1:1:144[B]:MET:CE	2.09	1.41
1:2:194:ARG:NE	4:2:2170:HOH:O	1.57	1.35
1:2:171[A]:GLU:CD	1:2:171[A]:GLU:OE1	1.66	1.34
1:2:1[A]:ALA:HA	4:2:2001:HOH:O	1.13	1.29
1:1:150:ASP:HA	4:1:2142:HOH:O	1.32	1.27
1:1:294:LYS:HE2	4:1:2237:HOH:O	1.37	1.25
1:1:117:ASP:N	4:1:2111:HOH:O	1.71	1.23
1:2:171[B]:GLU:OE1	1:2:171[B]:GLU:CD	1.81	1.18
1:1:154:LEU:CD1	4:1:2139:HOH:O	1.92	1.16
1:1:235:ASN:HB3	4:1:2209:HOH:O	1.53	1.07
1:1:118:PRO:HD2	4:1:2110:HOH:O	1.53	1.06
1:1:118:PRO:CD	4:1:2110:HOH:O	2.03	1.05
1:1:294:LYS:CE	4:1:2237:HOH:O	1.96	1.05
1:1:119:THR:HA	4:1:2113:HOH:O	1.56	1.04
1:1:116:HIS:C	4:1:2111:HOH:O	1.94	1.03
1:1:195:LEU:HD11	1:1:202:ILE:HD12	1.37	1.02
1:2:124[A]:ILE:HD11	1:2:288:VAL:HG11	1.41	1.01
1:1:356:LEU:CD2	4:1:2236:HOH:O	2.07	1.01
1:2:176:TYR:H	1:2:241[B]:ASN:HD21	1.06	0.99
1:1:154:LEU:HG	4:1:2139:HOH:O	1.61	0.98
1:1:117:ASP:OD2	4:1:2110:HOH:O	1.79	0.98
1:2:242[A]:PRO:CA	1:2:242[A]:PRO:CD	2.42	0.98
1:2:242[B]:PRO:CD	1:2:242[B]:PRO:CA	2.42	0.97
1:2:124[A]:ILE:HD13	1:2:157:THR:HB	1.45	0.96
1:2:124[A]:ILE:HD11	1:2:288:VAL:CG1	1.98	0.94
1:1:153:ALA:HB3	4:1:2142:HOH:O	1.67	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:242[A]:PRO:N	1:2:242[A]:PRO:CG	2.33	0.91
1:1:176:TYR:H	1:1:241[B]:ASN:HD21	1.12	0.90
1:1:176:TYR:H	1:1:241[A]:ASN:HD21	1.19	0.90
1:1:154:LEU:HD12	4:1:2139:HOH:O	1.59	0.90
1:2:242[A]:PRO:N	1:2:242[A]:PRO:CB	2.34	0.90
1:2:242[B]:PRO:CD	1:2:242[B]:PRO:CG	2.51	0.89
1:1:195:LEU:HD11	1:1:202:ILE:CD1	2.05	0.87
1:2:242[A]:PRO:CB	1:2:242[A]:PRO:C	2.45	0.85
1:1:30:ILE:HD12	1:1:83:ILE:HD13	1.59	0.84
1:2:241[A]:ASN:C	1:2:242[A]:PRO:CA	2.46	0.83
1:1:118:PRO:N	4:1:2110:HOH:O	2.11	0.82
1:2:176:TYR:H	1:2:241[A]:ASN:HD21	1.24	0.81
1:2:242[A]:PRO:N	1:2:242[A]:PRO:C	2.34	0.81
1:2:171[A]:GLU:OE1	1:2:171[A]:GLU:CG	2.30	0.80
1:2:241[A]:ASN:CB	1:2:241[A]:ASN:C	2.51	0.80
1:2:242[A]:PRO:CA	1:2:242[A]:PRO:CG	2.60	0.79
1:1:312:GLU:OE2	1:1:350:ARG:HD3	1.82	0.79
1:2:241[A]:ASN:CB	1:2:241[A]:ASN:N	2.44	0.79
1:2:1[A]:ALA:CA	4:2:2001:HOH:O	1.89	0.78
1:1:241[B]:ASN:HB3	1:1:242[B]:PRO:HD2	1.66	0.77
1:1:154:LEU:CG	4:1:2139:HOH:O	2.09	0.76
1:2:241[B]:ASN:C	1:2:242[B]:PRO:CD	2.52	0.76
1:2:241[B]:ASN:HB3	1:2:242[B]:PRO:CD	2.16	0.75
1:1:95[A]:ILE:CD1	1:1:95[A]:ILE:CB	2.65	0.75
1:1:273:VAL:O	1:1:274[B]:ILE:HD13	1.88	0.74
1:2:30[A]:ILE:HD13	1:2:126:SER:HB3	1.69	0.74
1:1:125:VAL:HG12	1:1:127:ILE:HD11	1.70	0.72
1:1:197:ALA:HB2	1:1:202:ILE:HD13	1.70	0.72
1:2:30[B]:ILE:CD1	1:2:126:SER:HB3	2.19	0.72
1:2:28:ILE:HD13	1:2:124[A]:ILE:HB	1.73	0.71
1:2:171[B]:GLU:OE1	1:2:171[B]:GLU:CG	2.39	0.70
1:2:123:SER:O	1:2:124[B]:ILE:HD13	1.92	0.69
1:2:4[B]:THR:OG1	4:2:2008:HOH:O	2.11	0.69
1:1:117:ASP:C	4:1:2111:HOH:O	2.31	0.69
1:2:242[B]:PRO:CD	1:2:242[B]:PRO:CB	2.70	0.68
1:2:326:ASN:HD22	1:2:328:ALA:H	1.41	0.68
1:1:326:ASN:HD22	1:1:328:ALA:H	1.41	0.68
1:1:124:ILE:CD1	1:1:157:THR:HB	2.24	0.68
1:2:30[B]:ILE:HD12	1:2:126:SER:HB3	1.74	0.68
1:2:241[A]:ASN:C	1:2:242[A]:PRO:CD	2.60	0.67
1:2:83:ILE:HD11	1:2:97:VAL:HG22	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:194:ARG:CZ	4:2:2170:HOH:O	2.19	0.65
1:1:356:LEU:HD23	4:1:2236:HOH:O	1.82	0.65
1:1:144[B]:MET:CE	1:1:144[B]:MET:CG	2.75	0.64
1:1:195:LEU:CD1	1:1:202:ILE:HD12	2.22	0.64
1:2:176:TYR:H	1:2:241[B]:ASN:ND2	1.88	0.63
1:1:83:ILE:HD11	1:1:97:VAL:HG22	1.81	0.62
1:2:144[B]:MET:CE	1:2:144[B]:MET:CG	2.77	0.62
1:1:294:LYS:HD2	4:1:2235:HOH:O	2.00	0.61
1:2:28:ILE:CD1	1:2:124[A]:ILE:HB	2.31	0.60
1:2:176:TYR:N	1:2:241[B]:ASN:HD21	1.89	0.60
1:2:1[A]:ALA:N	4:2:2001:HOH:O	2.23	0.60
1:1:133:GLU:O	1:1:141[B]:ILE:HD11	2.02	0.59
1:2:258:ASP:OD2	4:2:2188:HOH:O	2.17	0.59
1:1:150:ASP:O	4:1:2141:HOH:O	0.59	0.58
1:1:294:LYS:HE3	4:1:2237:HOH:O	1.85	0.58
1:2:319:GLU:HG3	4:2:2254:HOH:O	2.02	0.58
1:1:303:ASN:N	1:1:303:ASN:HD22	2.02	0.56
1:2:3[B]:PRO:HD2	1:2:196:VAL:HG13	1.87	0.56
1:1:124:ILE:HD12	1:1:157:THR:HB	1.88	0.56
1:2:241[B]:ASN:HB3	1:2:242[B]:PRO:HD3	1.88	0.55
1:1:124:ILE:HD13	1:1:157:THR:HB	1.89	0.55
1:2:83:ILE:HD12	1:2:95[B]:ILE:HG21	1.89	0.54
1:1:30:ILE:HD12	1:1:83:ILE:CD1	2.36	0.54
1:2:326:ASN:ND2	1:2:328:ALA:H	2.04	0.54
1:2:68:PRO:HB3	4:2:2038:HOH:O	2.07	0.54
1:2:117:ASP:OD1	1:2:120:HIS:HD2	1.91	0.54
1:1:204:ARG:NH1	1:1:319:GLU:OE1	2.41	0.54
1:2:28:ILE:HD11	1:2:289:ALA:HB2	1.90	0.54
1:1:326:ASN:ND2	1:1:328:ALA:H	2.05	0.54
1:2:347:ILE:HD13	4:2:2017:HOH:O	2.07	0.54
1:1:127:ILE:HD12	1:1:127:ILE:N	2.23	0.53
1:1:14:ALA:HB1	1:1:202:ILE:HD11	1.90	0.53
1:1:83:ILE:HD12	1:1:95[A]:ILE:HG21	1.90	0.52
1:1:197:ALA:CB	1:1:202:ILE:HD13	2.39	0.52
1:2:132:PRO:O	1:2:136:TRP:HD1	1.92	0.52
1:1:235:ASN:CB	4:1:2209:HOH:O	2.29	0.52
1:1:204:ARG:HH12	1:1:319:GLU:CD	2.13	0.52
1:1:239:SER:HB3	1:1:244[B]:ALA:O	2.10	0.52
1:1:356:LEU:HD22	4:1:2236:HOH:O	1.92	0.52
1:1:117:ASP:OD1	1:1:120:HIS:HD2	1.93	0.52
1:2:241[A]:ASN:CA	1:2:241[A]:ASN:CG	2.67	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:83:ILE:HD12	1:2:95[A]:ILE:HG21	1.92	0.51
1:2:171[B]:GLU:OE1	1:2:171[B]:GLU:HG3	2.09	0.51
1:1:241[B]:ASN:CB	1:1:242[B]:PRO:HD2	2.39	0.51
1:1:28:ILE:HD12	1:1:93:ALA:HB1	1.92	0.50
1:2:51:VAL:HA	4:2:2047:HOH:O	2.11	0.50
1:2:295:LEU:HD23	1:2:356:LEU:HD23	1.93	0.50
1:2:347:ILE:CD1	4:2:2017:HOH:O	2.59	0.50
1:2:28:ILE:CD1	1:2:124[B]:ILE:HB	2.42	0.50
1:1:83:ILE:HD11	1:1:97:VAL:CG2	2.42	0.49
1:1:45:TYR:CE1	1:1:84:GLU:HB3	2.48	0.49
1:2:2[B]:ALA:O	1:2:3[B]:PRO:C	2.50	0.49
1:2:204:ARG:HH12	1:2:319:GLU:CD	2.16	0.49
1:2:242[A]:PRO:N	1:2:242[A]:PRO:O	2.45	0.49
1:2:28:ILE:HD13	1:2:124[B]:ILE:HB	1.95	0.49
1:1:9:LEU:HD22	1:1:9:LEU:N	2.28	0.49
1:1:132:PRO:O	1:1:136:TRP:HD1	1.96	0.48
1:2:45:TYR:CE1	1:2:84:GLU:HB3	2.48	0.48
1:2:241[A]:ASN:O	1:2:242[A]:PRO:CA	2.61	0.47
1:2:281:ALA:HB3	1:2:282:PRO:HD3	1.95	0.47
1:1:315:HIS:CE1	4:1:2183:HOH:O	2.67	0.47
1:2:323:ASP:OD1	1:2:326:ASN:ND2	2.46	0.47
1:2:29:ALA:O	1:2:30[B]:ILE:HD13	2.14	0.47
1:2:241[B]:ASN:HD22	1:2:241[B]:ASN:HA	1.58	0.47
1:2:330:ILE:HA	1:2:331:TYR:HA	1.65	0.46
1:1:319:GLU:HG2	4:1:2083:HOH:O	2.14	0.46
1:2:303:ASN:HD22	1:2:303:ASN:N	2.12	0.46
1:1:204:ARG:NH1	1:1:319:GLU:CD	2.69	0.45
1:1:125:VAL:HG12	1:1:127:ILE:CD1	2.40	0.45
1:1:311:PRO:HG2	4:1:2249:HOH:O	2.15	0.45
1:1:324:ILE:C	1:1:324:ILE:HD12	2.36	0.45
1:1:141[B]:ILE:HD12	4:1:2128:HOH:O	2.16	0.45
1:2:83:ILE:HD11	1:2:97:VAL:CG2	2.45	0.45
1:1:212:PRO:HD2	4:1:2192:HOH:O	2.17	0.44
1:1:274[A]:ILE:HD13	1:1:274[A]:ILE:HA	1.90	0.44
1:1:326:ASN:HD22	1:1:326:ASN:C	2.21	0.44
1:2:30[B]:ILE:HD13	1:2:126:SER:HB3	1.98	0.44
1:1:204:ARG:HH21	1:1:204:ARG:HG3	1.82	0.44
1:1:30:ILE:CD1	1:1:83:ILE:HD13	2.37	0.44
1:1:323:ASP:OD1	1:1:326:ASN:ND2	2.50	0.43
1:1:126:SER:C	1:1:127:ILE:HD12	2.38	0.43
1:1:274[A]:ILE:HD12	1:1:274[A]:ILE:HG23	1.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:153:ALA:CB	4:1:2142:HOH:O	2.46	0.43
1:1:180:PHE:CG	1:1:181:PRO:HA	2.54	0.43
1:1:267:ILE:HD11	1:1:274[B]:ILE:HG13	2.01	0.43
1:2:37:TYR:HA	4:2:2038:HOH:O	2.17	0.43
1:2:117:ASP:OD1	1:2:120:HIS:CD2	2.72	0.43
1:2:241[A]:ASN:CA	1:2:241[A]:ASN:ND2	2.81	0.43
1:2:180:PHE:CG	1:2:181:PRO:HA	2.54	0.43
1:2:241[B]:ASN:CA	1:2:242[B]:PRO:CD	2.96	0.43
1:1:124:ILE:HD11	1:1:288:VAL:CG1	2.49	0.42
1:1:14:ALA:HB1	1:1:202:ILE:CD1	2.49	0.42
1:2:212:PRO:HD2	4:2:2192:HOH:O	2.19	0.42
1:2:136:TRP:CZ3	1:2:144[B]:MET:SD	3.13	0.42
1:1:136:TRP:CZ3	1:1:144[B]:MET:SD	3.13	0.42
1:1:83:ILE:CD1	1:1:95[A]:ILE:HG21	2.50	0.42
1:1:124:ILE:HD11	1:1:288:VAL:HG11	2.01	0.42
1:1:176:TYR:N	1:1:241[B]:ASN:HD21	1.96	0.41
1:2:171[A]:GLU:OE1	1:2:171[A]:GLU:HG2	2.12	0.41
1:2:2[B]:ALA:HB1	1:2:3[B]:PRO:CD	2.50	0.41
1:1:141[B]:ILE:CD1	4:1:2128:HOH:O	2.67	0.41
1:2:241[B]:ASN:CB	1:2:242[B]:PRO:CD	2.92	0.41
1:1:357:PRO:CD	4:1:2282:HOH:O	2.67	0.41
1:1:124:ILE:CD1	1:1:288:VAL:HG11	2.51	0.41
1:1:330:ILE:HA	1:1:331:TYR:HA	1.81	0.41
1:2:124[B]:ILE:HD12	1:2:157:THR:HB	2.02	0.41
1:2:326:ASN:HD22	1:2:326:ASN:C	2.24	0.41
1:2:9:LEU:HD23	1:2:89:LEU:HD12	2.04	0.40

All (87) 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)
1:1:39:GLU:CA	1:1:357:PRO:C[2_556]	0.43	1.77
1:1:153:ALA:O	1:2:329:ARG:NH2[1_556]	0.46	1.74
1:1:154:LEU:N	1:2:329:ARG:NH1[1_556]	0.48	1.72
1:1:150:ASP:OD1	1:2:327:ARG:CG[1_556]	0.51	1.69
1:1:40:THR:N	1:1:357:PRO:CB[2_556]	0.53	1.67
1:1:153:ALA:C	1:2:329:ARG:CZ[1_556]	0.74	1.46
1:1:151:ALA:N	1:2:327:ARG:NH2[1_556]	0.75	1.45
1:1:150:ASP:OD2	1:2:327:ARG:CB[1_556]	0.77	1.43
1:1:147:ALA:O	1:2:327:ARG:NH1[1_556]	0.81	1.39

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:118:PRO:CB	1:2:210:ASP:CB[1_556]	0.83	1.37
1:1:153:ALA:O	1:2:329:ARG:CZ[1_556]	0.87	1.33
1:1:150:ASP:CG	1:2:327:ARG:CB[1_556]	0.88	1.32
1:1:118:PRO:CD	1:2:210:ASP:O[1_556]	0.89	1.31
1:1:154:LEU:CD2	4:2:2258:HOH:O[1_556]	0.90	1.30
1:1:150:ASP:CB	1:2:327:ARG:NE[1_556]	0.93	1.27
1:1:150:ASP:CG	1:2:327:ARG:CG[1_556]	0.96	1.24
1:1:153:ALA:C	1:2:329:ARG:NH1[1_556]	1.07	1.13
4:1:2107:HOH:O	4:2:2192:HOH:O[1_556]	1.07	1.13
1:1:40:THR:N	1:1:357:PRO:CG[2_556]	1.19	1.01
1:1:39:GLU:C	1:1:357:PRO:CA[2_556]	1.22	0.98
1:1:39:GLU:CA	1:1:357:PRO:O[2_556]	1.27	0.93
1:1:39:GLU:CA	1:1:357:PRO:CA[2_556]	1.32	0.88
1:1:39:GLU:C	1:1:357:PRO:CB[2_556]	1.36	0.84
1:1:39:GLU:C	1:1:357:PRO:C[2_556]	1.37	0.83
1:1:154:LEU:CG	4:2:2258:HOH:O[1_556]	1.42	0.78
1:1:40:THR:CA	1:1:357:PRO:CB[2_556]	1.44	0.76
1:1:118:PRO:CA	1:2:210:ASP:CB[1_556]	1.46	0.74
1:1:147:ALA:C	1:2:327:ARG:NH1[1_556]	1.47	0.73
1:1:118:PRO:N	1:2:210:ASP:O[1_556]	1.51	0.69
1:1:39:GLU:N	1:1:357:PRO:C[2_556]	1.54	0.66
1:1:39:GLU:CB	1:1:356:LEU:O[2_556]	1.55	0.65
1:1:154:LEU:CA	1:2:329:ARG:NH1[1_556]	1.56	0.64
1:1:150:ASP:OD1	1:2:327:ARG:CD[1_556]	1.57	0.63
1:1:154:LEU:N	1:2:329:ARG:CZ[1_556]	1.57	0.63
1:1:150:ASP:C	1:2:327:ARG:NH2[1_556]	1.59	0.61
1:1:39:GLU:CB	1:1:357:PRO:CA[2_556]	1.63	0.57
1:1:150:ASP:OD1	1:2:327:ARG:CB[1_556]	1.63	0.57
1:1:153:ALA:C	1:2:329:ARG:NH2[1_556]	1.63	0.57
4:1:2140:HOH:O	4:2:2263:HOH:O[1_556]	1.63	0.57
1:1:40:THR:N	1:1:357:PRO:CA[2_556]	1.64	0.56
1:1:118:PRO:CB	1:2:210:ASP:CA[1_556]	1.64	0.56
1:1:150:ASP:CB	1:2:327:ARG:CD[1_556]	1.64	0.56
1:1:118:PRO:CG	1:2:210:ASP:O[1_556]	1.75	0.45
1:1:153:ALA:C	1:2:329:ARG:NE[1_556]	1.77	0.43
1:1:154:LEU:CB	4:2:2258:HOH:O[1_556]	1.78	0.42
1:1:116:HIS:O	1:2:211:GLY:CA[1_556]	1.79	0.41
1:1:150:ASP:CG	1:2:327:ARG:CD[1_556]	1.79	0.41
4:1:2139:HOH:O	4:2:2265:HOH:O[1_556]	1.80	0.40
1:1:118:PRO:CG	1:2:214:GLY:CA[1_556]	1.81	0.39
1:1:94:LYS:CE	1:2:2[A]:ALA:CA[1_556]	1.82	0.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:1:147:ALA:O	1:2:327:ARG:CZ[1_556]	1.82	0.38
1:1:150:ASP:CB	1:2:327:ARG:CZ[1_556]	1.84	0.36
1:1:118:PRO:CA	1:2:210:ASP:CA[1_556]	1.85	0.35
1:1:40:THR:CA	1:1:357:PRO:CG[2_556]	1.89	0.31
1:1:153:ALA:O	1:2:329:ARG:NH1[1_556]	1.89	0.31
1:1:118:PRO:O	1:2:210:ASP:CG[1_556]	1.90	0.30
1:1:121:LYS:CG	4:2:2189:HOH:O[1_556]	1.90	0.30
1:1:39:GLU:CB	1:1:357:PRO:C[2_556]	1.93	0.27
1:1:153:ALA:O	1:2:329:ARG:NE[1_556]	1.94	0.26
1:1:150:ASP:OD2	1:2:327:ARG:CG[1_556]	1.96	0.24
1:1:39:GLU:CB	1:1:356:LEU:C[2_556]	1.97	0.23
1:1:39:GLU:CB	1:1:357:PRO:O[2_556]	1.97	0.23
1:1:151:ALA:CA	1:2:327:ARG:NH2[1_556]	1.98	0.22
1:1:94:LYS:CE	1:2:2[A]:ALA:N[1_556]	1.99	0.21
1:1:118:PRO:CB	1:2:210:ASP:C[1_556]	2.01	0.19
1:1:39:GLU:OE1	1:1:356:LEU:CB[2_556]	2.02	0.18
1:1:39:GLU:CG	1:1:356:LEU:O[2_556]	2.03	0.17
1:1:151:ALA:N	1:2:327:ARG:CZ[1_556]	2.03	0.17
1:1:39:GLU:CB	1:1:357:PRO:N[2_556]	2.05	0.15
1:1:150:ASP:CB	1:2:327:ARG:CG[1_556]	2.06	0.14
1:1:39:GLU:N	1:1:357:PRO:N[2_556]	2.07	0.13
1:1:40:THR:CB	1:1:357:PRO:CG[2_556]	2.07	0.13
1:1:150:ASP:CA	1:2:327:ARG:NE[1_556]	2.08	0.12
1:1:116:HIS:O	1:2:211:GLY:N[1_556]	2.10	0.10
1:1:118:PRO:CB	1:2:210:ASP:O[1_556]	2.10	0.10
1:2:327:ARG:CD	4:1:2143:HOH:O[1_554]	2.10	0.10
1:1:153:ALA:CA	1:2:329:ARG:CZ[1_556]	2.11	0.09
1:1:118:PRO:CD	1:2:210:ASP:C[1_556]	2.13	0.07
1:1:118:PRO:N	1:2:210:ASP:C[1_556]	2.13	0.07
1:1:39:GLU:CA	1:1:357:PRO:N[2_556]	2.14	0.06
1:1:150:ASP:OD2	1:2:327:ARG:CA[1_556]	2.14	0.06
1:1:39:GLU:O	1:1:357:PRO:CB[2_556]	2.15	0.05
1:1:118:PRO:O	1:2:210:ASP:OD1[1_556]	2.15	0.05
1:1:150:ASP:CA	1:2:327:ARG:CZ[1_556]	2.15	0.05
1:1:39:GLU:O	1:1:357:PRO:C[2_556]	2.17	0.03
1:1:39:GLU:N	1:1:357:PRO:CA[2_556]	2.18	0.02
1:1:118:PRO:CG	1:2:214:GLY:N[1_556]	2.18	0.02



## 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	1	369/357 (103%)	364 (99%)	5 (1%)	0	100	100
1	2	371/357 (104%)	362 (98%)	7 (2%)	2 (0%)	29	9
All	All	740/714 (104%)	726 (98%)	12 (2%)	2 (0%)	51	18

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	242[A]	PRO
1	2	242[B]	PRO

### 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	1	271/260 (104%)	263 (97%)	8 (3%)	41	10
1	2	274/260 (105%)	264 (96%)	10 (4%)	35	7
All	All	545/520 (105%)	527 (97%)	18 (3%)	38	8

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1	107	PHE
1	1	134	ASP
1	1	248	ARG
1	1	251	PRO

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Mol	Chain	Res	Type
1	1	297	LYS
1	1	303	ASN
1	1	308	GLN
1	1	326	ASN
1	2	89	LEU
1	2	107	PHE
1	2	134	ASP
1	2	172	GLN
1	2	242[A]	PRO
1	2	242[B]	PRO
1	2	248	ARG
1	2	297	LYS
1	2	308	GLN
1	2	326	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	109	ASN
1	1	120	HIS
1	1	145	ASN
1	1	235	ASN
1	1	303	ASN
1	1	326	ASN
1	2	13	GLN
1	2	24	GLN
1	2	67	GLN
1	2	109	ASN
1	2	120	HIS
1	2	145	ASN
1	2	235	ASN
1	2	303	ASN
1	2	315	HIS
1	2	326	ASN
1	2	332	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 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	$\# Z  > 2$
3	SO4	2	1359	-	4,4,4	0.26	0	6,6,6	0.30	0
3	SO4	1	1359	-	4,4,4	0.32	0	6,6,6	0.20	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	1	3

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	1	244[A]:ALA	C	245[A]:GLY	N	1.64
1	1	140[B]:SER	C	141[B]:ILE	N	1.18
1	1	244[B]:ALA	C	245[B]:GLY	N	1.09

## 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.