



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:51 PM UTC

PDB ID : 3CMS / pdb\_00003cms  
Title : ENGINEERING ENZYME SUB-SITE SPECIFICITY: PREPARATION, KINETIC CHARACTERIZATION AND X-RAY ANALYSIS AT 2.0-ANGSTROMS RESOLUTION OF VAL111PHE SITE-MUTATED CALF CHYMOSIN  
Authors : Newman, M.; Frazao, C.; Shearer, A.; Tickle, I.J.; Blundell, T.L.  
Deposited on : 1990-02-26  
Resolution : 2.00 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

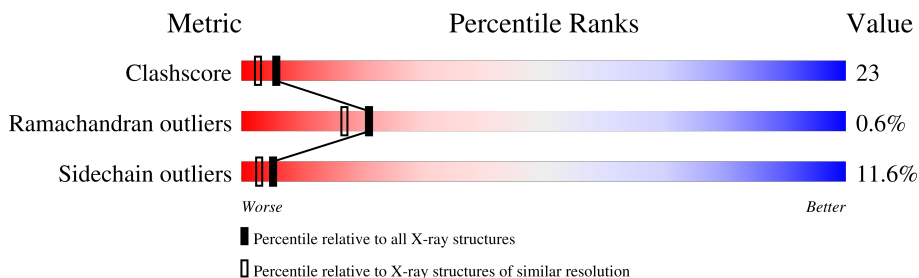
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

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	323	 46% 39% 11% ..

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2692 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 CHYMOSIN B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	320	2547	1624	405	504	14	0	8	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	111	PHE	VAL	conflict	UNP P00794

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	145	145	145	0	0

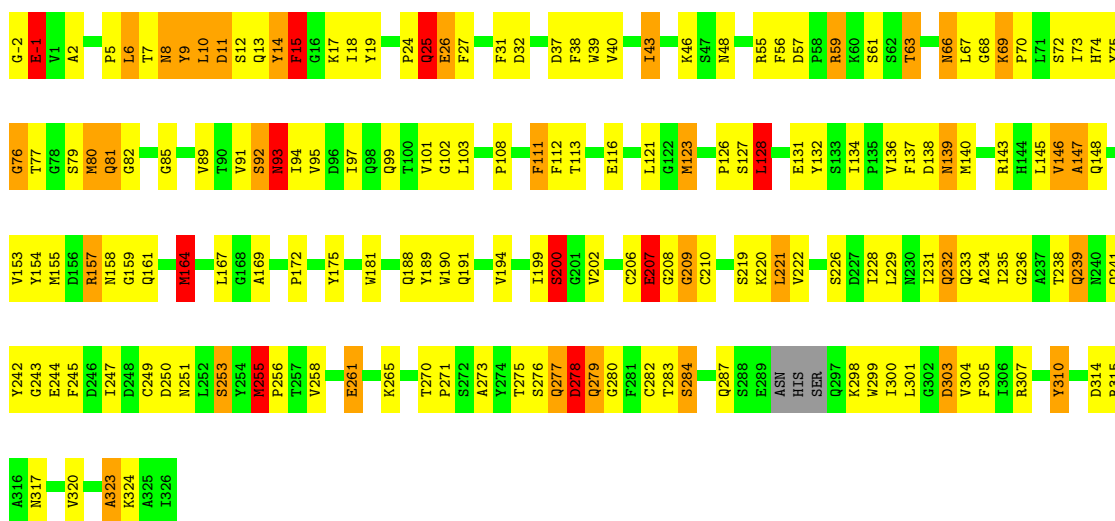
### 3 Residue-property plots

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: CHYMOSIN B

Chain A:  46% 39% 11% ..



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.21Å 114.56Å 72.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.00)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	RESTRAIN	Depositor
R, $R_{free}$	0.195 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2692	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	0.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

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	1.73	41/2611 (1.6%)	1.99	111/3555 (3.1%)

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	6

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	305	PHE	C-N	21.23	1.58	1.33
1	A	258	VAL	C-N	19.13	1.57	1.33
1	A	202	VAL	C-N	-18.75	1.12	1.33
1	A	273	ALA	C-N	17.34	1.56	1.33
1	A	6	LEU	C-N	-13.32	1.15	1.33
1	A	66	ASN	C-N	-13.12	1.13	1.33
1	A	15	PHE	C-N	12.69	1.51	1.33
1	A	11	ASP	C-N	11.81	1.51	1.33
1	A	12	SER	N-CA	10.80	1.60	1.46
1	A	243	GLY	C-N	-10.07	1.19	1.33
1	A	236	GLY	C-N	9.58	1.46	1.33
1	A	164	MET	C-N	9.16	1.46	1.33
1	A	251	ASN	C-N	-9.16	1.21	1.33
1	A	210	CYS	C-N	-9.08	1.20	1.33
1	A	255	MET	C-N	9.07	1.45	1.33
1	A	113	THR	C-N	8.50	1.46	1.33
1	A	278	ASP	C-N	-7.67	1.23	1.33
1	A	93	ASN	C-N	-7.61	1.24	1.33
1	A	12	SER	C-N	-7.41	1.23	1.33
1	A	85	GLY	C-N	-7.08	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	253	SER	C-N	-6.81	1.24	1.33
1	A	280	GLY	C-N	6.39	1.42	1.33
1	A	233	GLN	CD-OE1	6.29	1.35	1.23
1	A	148	GLN	CD-OE1	6.19	1.35	1.23
1	A	299	TRP	C-N	-5.95	1.25	1.33
1	A	181	TRP	NE1-CE2	-5.77	1.31	1.37
1	A	26	GLU	CA-CB	-5.71	1.44	1.53
1	A	190	TRP	NE1-CE2	-5.67	1.31	1.37
1	A	169	ALA	C-N	-5.66	1.25	1.33
1	A	256	PRO	C-N	-5.65	1.25	1.33
1	A	61	SER	C-N	-5.61	1.25	1.33
1	A	25	GLN	CD-OE1	5.60	1.34	1.23
1	A	131	GLU	C-N	-5.55	1.26	1.33
1	A	299	TRP	NE1-CE2	-5.53	1.31	1.37
1	A	210	CYS	N-CA	5.38	1.52	1.45
1	A	69	LYS	CA-C	5.38	1.58	1.53
1	A	89	VAL	CA-C	-5.32	1.46	1.52
1	A	32	ASP	N-CA	-5.29	1.39	1.46
1	A	277	GLN	C-N	-5.24	1.25	1.33
1	A	39	TRP	NE1-CE2	-5.20	1.31	1.37
1	A	63	THR	C-N	-5.04	1.26	1.33

All (111) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	258	VAL	CA-C-N	-12.79	106.39	123.14
1	A	258	VAL	C-N-CA	-12.79	106.39	123.14
1	A	11	ASP	O-C-N	-10.97	110.35	121.87
1	A	236	GLY	CA-C-N	-10.92	107.10	122.93
1	A	236	GLY	C-N-CA	-10.92	107.10	122.93
1	A	121	LEU	CA-C-N	10.46	141.90	121.41
1	A	121	LEU	C-N-CA	10.46	141.90	121.41
1	A	320	VAL	O-C-N	-9.87	112.08	123.03
1	A	200	SER	CB-CA-C	-9.63	98.06	111.73
1	A	26	GLU	O-C-N	9.43	134.22	123.19
1	A	95	VAL	CA-C-N	9.31	137.85	123.23
1	A	95	VAL	C-N-CA	9.31	137.85	123.23
1	A	148	GLN	OE1-CD-NE2	9.31	131.91	122.60
1	A	273	ALA	CA-C-N	-9.11	108.07	122.65
1	A	273	ALA	C-N-CA	-9.11	108.07	122.65
1	A	40	VAL	O-C-N	8.98	128.01	121.72
1	A	232	GLN	O-C-N	-8.95	112.42	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	GLU	CB-CG-CD	-8.91	97.46	112.60
1	A	207	GLU	CA-C-N	-8.79	109.50	123.31
1	A	207	GLU	C-N-CA	-8.79	109.50	123.31
1	A	305	PHE	CA-C-N	-8.71	106.36	120.64
1	A	305	PHE	C-N-CA	-8.71	106.36	120.64
1	A	9	TYR	O-C-N	8.54	134.20	122.41
1	A	236	GLY	O-C-N	8.42	131.82	122.47
1	A	207	GLU	O-C-N	-8.40	112.53	122.95
1	A	169	ALA	CA-C-N	8.26	133.75	123.10
1	A	169	ALA	C-N-CA	8.26	133.75	123.10
1	A	111	PHE	CA-CB-CG	-8.24	105.56	113.80
1	A	31	PHE	CA-C-N	8.04	135.85	123.23
1	A	31	PHE	C-N-CA	8.04	135.85	123.23
1	A	310	TYR	O-C-N	-7.96	112.42	123.01
1	A	123	MET	CG-SD-CE	7.93	118.36	100.90
1	A	38	PHE	O-C-N	-7.93	113.86	123.30
1	A	89	VAL	O-C-N	7.90	131.71	123.18
1	A	208	GLY	N-CA-C	7.66	124.21	114.25
1	A	101	VAL	CA-C-N	7.59	129.28	120.71
1	A	101	VAL	C-N-CA	7.59	129.28	120.71
1	A	108	PRO	CB-CA-C	-7.42	100.02	110.63
1	A	303	ASP	O-C-N	-7.41	114.27	122.12
1	A	317	ASN	CB-CG-ND2	7.24	127.27	116.40
1	A	-1	GLU	O-C-N	7.04	131.27	123.25
1	A	207	GLU	CB-CG-CD	6.87	124.28	112.60
1	A	32	ASP	CA-C-O	-6.81	112.74	121.11
1	A	146	VAL	O-C-N	6.68	129.93	122.98
1	A	315	ARG	NE-CZ-NH1	6.67	128.17	121.50
1	A	304	VAL	CA-CB-CG2	6.62	121.65	110.40
1	A	48	ASN	CA-CB-CG	6.58	119.18	112.60
1	A	40	VAL	CA-CB-CG2	6.48	121.42	110.40
1	A	233	GLN	OE1-CD-NE2	-6.45	116.15	122.60
1	A	-1	GLU	N-CA-C	6.43	118.84	109.07
1	A	251	ASN	CA-C-N	6.21	129.11	120.29
1	A	251	ASN	C-N-CA	6.21	129.11	120.29
1	A	67	LEU	N-CA-C	-6.17	106.73	114.56
1	A	146	VAL	CA-C-N	-6.13	110.49	120.72
1	A	146	VAL	C-N-CA	-6.13	110.49	120.72
1	A	305	PHE	CA-CB-CG	-6.08	107.72	113.80
1	A	154	TYR	O-C-N	-6.08	116.10	123.27
1	A	233	GLN	CG-CD-NE2	5.98	125.38	116.40
1	A	189	TYR	CA-C-N	-5.96	112.80	122.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	TYR	C-N-CA	-5.96	112.80	122.34
1	A	40	VAL	CA-C-O	-5.94	113.82	121.13
1	A	92	SER	CB-CA-C	-5.89	109.80	116.63
1	A	25	GLN	OE1-CD-NE2	-5.89	116.71	122.60
1	A	70	PRO	O-C-N	5.89	130.18	123.00
1	A	121	LEU	CA-C-O	-5.85	113.19	120.57
1	A	317	ASN	OD1-CG-ND2	-5.84	116.76	122.60
1	A	103	LEU	N-CA-C	-5.81	97.68	108.02
1	A	12	SER	CA-C-N	5.79	131.84	122.29
1	A	12	SER	C-N-CA	5.79	131.84	122.29
1	A	323	ALA	O-C-N	-5.78	117.01	123.48
1	A	305	PHE	N-CA-CB	-5.71	101.76	110.33
1	A	164	MET	CA-C-N	5.71	131.05	123.05
1	A	164	MET	C-N-CA	5.71	131.05	123.05
1	A	26	GLU	CB-CA-C	5.71	119.07	109.48
1	A	202	VAL	O-C-N	5.69	130.49	122.97
1	A	9	TYR	CA-C-N	5.69	132.40	121.54
1	A	9	TYR	C-N-CA	5.69	132.40	121.54
1	A	102	GLY	O-C-N	-5.68	117.17	122.96
1	A	37	ASP	O-C-N	-5.61	116.78	123.06
1	A	206	CYS	N-CA-C	-5.60	105.07	112.24
1	A	137	PHE	CA-C-N	-5.57	111.22	120.68
1	A	137	PHE	C-N-CA	-5.57	111.22	120.68
1	A	209	GLY	CA-C-N	-5.55	112.14	121.75
1	A	209	GLY	C-N-CA	-5.55	112.14	121.75
1	A	323	ALA	CA-C-N	-5.51	113.24	120.95
1	A	323	ALA	C-N-CA	-5.51	113.24	120.95
1	A	158	ASN	N-CA-C	-5.46	106.59	113.20
1	A	147	ALA	N-CA-C	-5.42	105.92	112.54
1	A	7	THR	CA-C-N	-5.40	115.37	122.99
1	A	7	THR	C-N-CA	-5.40	115.37	122.99
1	A	307	ARG	NE-CZ-NH2	5.40	124.06	119.20
1	A	209	GLY	O-C-N	-5.39	115.69	122.70
1	A	67	LEU	O-C-N	5.36	127.78	122.10
1	A	148	GLN	O-C-N	5.36	129.38	123.33
1	A	55	ARG	NE-CZ-NH2	5.35	124.02	119.20
1	A	157	ARG	NE-CZ-NH2	5.30	123.97	119.20
1	A	6	LEU	CA-C-N	5.29	130.60	122.93
1	A	6	LEU	C-N-CA	5.29	130.60	122.93
1	A	320	VAL	CA-CB-CG2	5.28	119.38	110.40
1	A	59	ARG	NE-CZ-NH2	5.26	123.93	119.20
1	A	143	ARG	NE-CZ-NH2	5.24	123.92	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	8	ASN	O-C-N	5.24	129.53	123.30
1	A	209	GLY	CA-C-O	5.19	129.61	120.57
1	A	256	PRO	CA-C-N	5.18	128.82	121.42
1	A	256	PRO	C-N-CA	5.18	128.82	121.42
1	A	208	GLY	CA-C-O	-5.17	113.97	119.55
1	A	239	GLN	CA-C-N	5.08	129.81	121.39
1	A	239	GLN	C-N-CA	5.08	129.81	121.39
1	A	315	ARG	N-CA-C	5.06	119.17	112.89
1	A	233	GLN	CA-CB-CG	-5.05	103.99	114.10
1	A	284	SER	O-C-N	5.03	128.99	123.16

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	128	LEU	Mainchain
1	A	261	GLU	Mainchain
1	A	278	ASP	Mainchain
1	A	310	TYR	Mainchain
1	A	323	ALA	Mainchain
1	A	80	MET	Mainchain

## 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	2547	0	2411	115	0
2	A	145	0	0	5	0
All	All	2692	0	2411	115	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 23.

All (115) 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:6:LEU:HD13	1:A:14:TYR:CE2	2.01	0.96
1:A:80:MET:HE2	1:A:81:GLN:C	1.94	0.91
1:A:270:THR:HB	1:A:271:PRO:HD2	1.53	0.90
1:A:247:ILE:HG23	1:A:255:MET:CE	2.06	0.86
1:A:6:LEU:HD13	1:A:14:TYR:CZ	2.11	0.85
1:A:73[B]:ILE:HG21	1:A:75[B]:TYR:CZ	2.11	0.84
1:A:9:TYR:HB2	1:A:15:PHE:HZ	1.45	0.79
1:A:247:ILE:HG23	1:A:255:MET:HE1	1.62	0.78
1:A:2:ALA:HB2	1:A:94:ILE:HG13	1.69	0.74
1:A:19:TYR:CE1	1:A:26:GLU:HB2	2.22	0.74
1:A:25:GLN:HE22	1:A:57:ASP:H	1.35	0.74
1:A:247:ILE:CG2	1:A:255:MET:HE1	2.18	0.74
1:A:128:LEU:HD13	1:A:188:GLN:CG	2.20	0.72
1:A:239:GLN:HA	1:A:244:GLU:O	1.89	0.72
1:A:77[B]:THR:HG22	1:A:111:PHE:CD1	2.25	0.71
1:A:77[B]:THR:HG21	1:A:111:PHE:CE1	2.24	0.71
1:A:278:ASP:O	1:A:279:GLN:C	2.32	0.70
1:A:140:MET:HA	1:A:145:LEU:HD12	1.75	0.69
1:A:9:TYR:HB2	1:A:15:PHE:CZ	2.25	0.68
1:A:155:MET:HE1	1:A:303:ASP:OD1	1.94	0.68
1:A:161:GLN:HG2	1:A:161:GLN:O	1.92	0.67
1:A:75[B]:TYR:O	1:A:76[B]:GLY:C	2.38	0.67
1:A:172:PRO:HA	1:A:175:TYR:CE2	2.29	0.66
1:A:247:ILE:HG23	1:A:255:MET:HE2	1.77	0.66
1:A:73[B]:ILE:HD13	2:A:1104:HOH:O	1.96	0.65
1:A:128:LEU:CD1	1:A:188:GLN:HG2	2.26	0.65
1:A:220:LYS:HD3	1:A:287:GLN:HB2	1.78	0.64
1:A:2:ALA:HB1	1:A:92:SER:HB3	1.79	0.64
1:A:250:ASP:OD1	1:A:250:ASP:O	2.16	0.64
1:A:270:THR:HB	1:A:271:PRO:CD	2.27	0.64
1:A:128:LEU:HD13	1:A:188:GLN:HG2	1.80	0.64
1:A:19:TYR:CD1	1:A:26:GLU:HB2	2.33	0.63
1:A:6:LEU:CD1	1:A:14:TYR:CZ	2.80	0.63
1:A:73[B]:ILE:CG2	1:A:75[B]:TYR:CZ	2.83	0.62
1:A:249:CYS:SG	1:A:282:CYS:N	2.72	0.62
1:A:73[A]:ILE:HD13	2:A:1104:HOH:O	2.00	0.61
1:A:80:MET:HE2	1:A:81:GLN:O	1.99	0.61
1:A:5:PRO:HA	1:A:164:MET:HE3	1.83	0.61
1:A:231:ILE:O	1:A:235:ILE:HG12	2.01	0.60
1:A:244:GLU:HG2	1:A:245:PHE:N	2.16	0.60
1:A:77[B]:THR:CG2	1:A:111:PHE:CD1	2.84	0.60
1:A:6:LEU:CD1	1:A:14:TYR:CE2	2.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:LEU:HD13	1:A:188:GLN:HG3	1.85	0.59
1:A:2:ALA:HB3	1:A:167:LEU:HD12	1.86	0.58
1:A:14:TYR:OH	1:A:153:VAL:HG13	2.02	0.58
1:A:247:ILE:CG2	1:A:255:MET:CE	2.78	0.57
1:A:57:ASP:OD1	1:A:59:ARG:HB2	2.05	0.57
1:A:-1:GLU:O	1:A:147:ALA:N	2.33	0.57
1:A:74[A]:HIS:HD2	1:A:79[A]:SER:OG	1.87	0.57
1:A:277:GLN:HB2	1:A:282:CYS:SG	2.45	0.57
1:A:14:TYR:CD2	1:A:155:MET:HG2	2.42	0.55
1:A:244:GLU:CG	1:A:245:PHE:N	2.69	0.55
1:A:75[B]:TYR:O	1:A:77[B]:THR:N	2.39	0.55
1:A:244:GLU:CG	1:A:245:PHE:H	2.20	0.54
1:A:278:ASP:O	1:A:279:GLN:O	2.26	0.54
1:A:43:ILE:HG23	1:A:56:PHE:O	2.08	0.54
1:A:126:PRO:HG3	1:A:138:ASP:OD2	2.07	0.54
1:A:283:THR:HG22	1:A:284:SER:N	2.22	0.54
1:A:221:LEU:HD21	1:A:301:LEU:HD23	1.90	0.53
1:A:199:ILE:O	1:A:200:SER:HB2	2.07	0.52
1:A:80:MET:C	1:A:80:MET:SD	2.93	0.52
1:A:93:ASN:ND2	1:A:94:ILE:HG13	2.25	0.52
1:A:247:ILE:O	1:A:282:CYS:HB2	2.10	0.52
1:A:199:ILE:HD12	1:A:234:ALA:HB1	1.92	0.51
1:A:112:PHE:HD2	2:A:1121:HOH:O	1.91	0.51
1:A:228:ILE:O	1:A:232:GLN:HG2	2.09	0.51
1:A:235:ILE:O	1:A:255:MET:HG2	2.10	0.51
1:A:69:LYS:HD2	1:A:132:TYR:CE2	2.46	0.51
1:A:93:ASN:HD22	1:A:94:ILE:N	2.08	0.51
1:A:238:THR:O	1:A:245:PHE:HA	2.11	0.50
1:A:77[B]:THR:CG2	1:A:111:PHE:CE1	2.94	0.50
1:A:222:VAL:HB	1:A:300:ILE:HB	1.93	0.50
1:A:238:THR:HG22	1:A:239:GLN:N	2.27	0.49
1:A:-2:GLY:C	1:A:-1:GLU:HG2	2.37	0.49
1:A:194:VAL:O	1:A:209:GLY:HA2	2.11	0.49
1:A:5:PRO:CA	1:A:164:MET:HE3	2.43	0.48
1:A:10:LEU:O	1:A:11:ASP:HB2	2.13	0.48
1:A:19:TYR:HB3	1:A:24:PRO:HB2	1.94	0.48
1:A:14:TYR:CZ	1:A:153:VAL:HG13	2.48	0.48
1:A:19:TYR:HE1	1:A:26:GLU:HB2	1.75	0.47
1:A:271:PRO:O	1:A:275:THR:HB	2.15	0.47
1:A:13:GLN:HB2	1:A:15:PHE:CE2	2.50	0.47
1:A:191:GLN:HE22	1:A:298:LYS:CE	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ILE:O	1:A:200:SER:CB	2.59	0.47
1:A:191:GLN:NE2	1:A:298:LYS:CE	2.78	0.46
1:A:-1:GLU:O	1:A:146:VAL:HA	2.16	0.46
1:A:80:MET:HE2	1:A:82:GLY:N	2.28	0.46
1:A:93:ASN:HD22	1:A:94:ILE:HG13	1.81	0.46
1:A:19:TYR:CE1	1:A:26:GLU:HG3	2.51	0.45
1:A:66:ASN:ND2	1:A:68:GLY:H	2.15	0.45
1:A:157:ARG:C	1:A:159:GLY:H	2.25	0.44
1:A:26:GLU:HG2	1:A:27:PHE:N	2.32	0.44
1:A:221:LEU:HD21	1:A:301:LEU:CD2	2.47	0.44
1:A:207:GLU:H	1:A:207:GLU:HG3	1.18	0.44
1:A:283:THR:CG2	1:A:284:SER:N	2.81	0.44
1:A:14:TYR:CD1	1:A:14:TYR:O	2.71	0.44
1:A:80:MET:CE	1:A:81:GLN:C	2.80	0.43
1:A:99:GLN:NE2	1:A:136:VAL:HA	2.33	0.43
1:A:-1:GLU:HB2	1:A:145:LEU:O	2.18	0.43
1:A:261:GLU:HB2	2:A:1089:HOH:O	2.18	0.43
1:A:161:GLN:O	1:A:161:GLN:CG	2.65	0.43
1:A:9:TYR:CB	1:A:15:PHE:CZ	2.99	0.43
1:A:128:LEU:CD1	1:A:188:GLN:CG	2.88	0.43
1:A:74[A]:HIS:CD2	1:A:79[A]:SER:OG	2.70	0.42
1:A:324:LYS:HE2	2:A:1108:HOH:O	2.20	0.42
1:A:229:LEU:HA	1:A:229:LEU:HD12	1.63	0.42
1:A:43:ILE:HG21	1:A:43:ILE:HD13	1.73	0.42
1:A:127:SER:OG	1:A:188:GLN:HA	2.19	0.42
1:A:238:THR:CG2	1:A:239:GLN:N	2.83	0.41
1:A:250:ASP:O	1:A:250:ASP:CG	2.63	0.41
1:A:80:MET:CE	1:A:82:GLY:HA3	2.50	0.41
1:A:134:ILE:HG21	1:A:139:ASN:ND2	2.35	0.41
1:A:73[B]:ILE:HG21	1:A:75[B]:TYR:OH	2.19	0.40
1:A:80:MET:CE	1:A:82:GLY:N	2.84	0.40
1:A:314:ASP:OD1	1:A:314:ASP:C	2.65	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	324/323 (100%)	308 (95%)	13 (4%)	3 (1%)	14 9

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76[A]	GLY
1	A	76[B]	GLY
1	A	279	GLN

### 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	283/280 (101%)	250 (88%)	33 (12%)	5 3

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-1	GLU
1	A	8	ASN
1	A	10	LEU
1	A	14	TYR
1	A	15	PHE
1	A	17	LYS
1	A	18	ILE
1	A	25	GLN
1	A	43	ILE
1	A	46	LYS
1	A	63	THR
1	A	72[A]	SER
1	A	72[B]	SER
1	A	81	GLN

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Mol	Chain	Res	Type
1	A	91	VAL
1	A	93	ASN
1	A	97	ILE
1	A	116	GLU
1	A	123	MET
1	A	128	LEU
1	A	139	ASN
1	A	164	MET
1	A	200	SER
1	A	207	GLU
1	A	219	SER
1	A	221	LEU
1	A	226	SER
1	A	241	GLN
1	A	242	TYR
1	A	253	SER
1	A	255	MET
1	A	265	LYS
1	A	276	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	66	ASN
1	A	93	ASN
1	A	99	GLN
1	A	139	ASN
1	A	142	ASN
1	A	180	HIS
1	A	191	GLN
1	A	230	ASN
1	A	297	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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	A	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	210:CYS	C	211:GLN	N	1.20
1	A	243:GLY	C	244:GLU	N	1.19
1	A	6:LEU	C	7:THR	N	1.15
1	A	66:ASN	C	67:LEU	N	1.13
1	A	202:VAL	C	203:VAL	N	1.12

## 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.