



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:17 PM GMT

PDB ID : 1EX3  
Title : CRYSTAL STRUCTURE OF BOVINE CHYMOTRYPSINOGEN A  
(TETRAGONAL)  
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Deposited on : 2000-04-28  
Resolution : 3.00 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

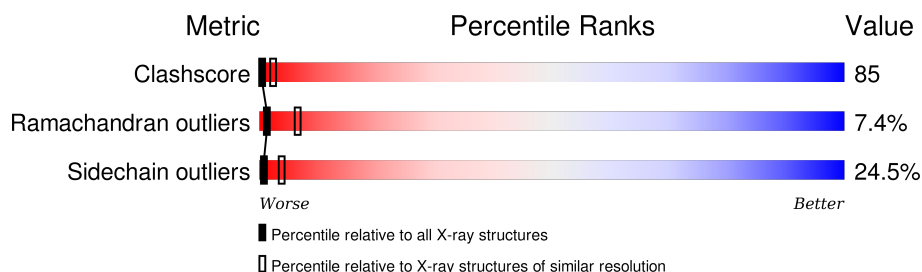
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

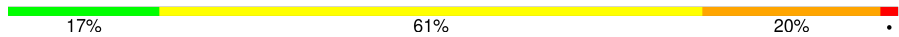
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	245	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1841 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 CHYMOTRYPSINOGEN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1799	1127	307	353	12			

- Molecule 2 is water.

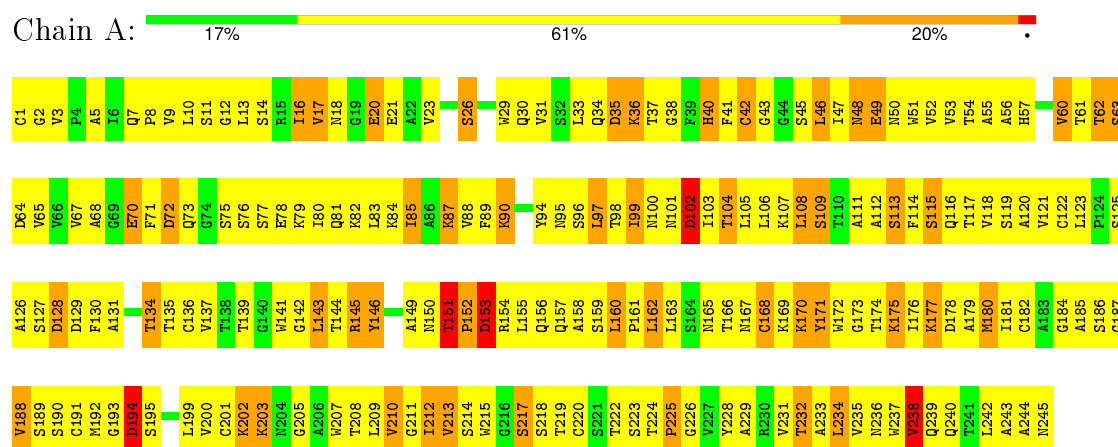
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	42	Total	O	0	0
			42	42		

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

#### • Molecule 1: CHYMOTRYPSINOGEN A



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.90 Å   114.90 Å   52.80 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	20.00 – 3.00	Depositor
% Data completeness (in resolution range)	100.0 (20.00-3.00)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	TNT	Depositor
R, $R_{free}$	0.204 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1841	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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	1.27	4/1835 (0.2%)	1.61	25/2502 (1.0%)

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	1	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	GLU	CD-OE2	9.03	1.35	1.25
1	A	20	GLU	CD-OE2	8.61	1.35	1.25
1	A	70	GLU	CD-OE2	8.39	1.34	1.25
1	A	49	GLU	CD-OE2	6.66	1.32	1.25

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	ASP	CB-CG-OD2	-9.21	110.02	118.30
1	A	64	ASP	CB-CG-OD2	-9.16	110.05	118.30
1	A	35	ASP	CB-CG-OD2	-8.39	110.75	118.30
1	A	131	ALA	CB-CA-C	-8.01	98.09	110.10
1	A	35	ASP	CB-CG-OD1	7.25	124.83	118.30
1	A	128	ASP	CB-CG-OD1	7.15	124.73	118.30
1	A	146	TYR	CA-CB-CG	-6.84	100.39	113.40
1	A	26	SER	N-CA-CB	6.74	120.61	110.50
1	A	102	ASP	CB-CG-OD2	-6.65	112.32	118.30
1	A	217	SER	N-CA-CB	6.57	120.36	110.50
1	A	64	ASP	CB-CG-OD1	6.54	124.19	118.30
1	A	153	ASP	CB-CG-OD1	6.35	124.02	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	A	153	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	A	151	THR	N-CA-CB	5.98	121.66	110.30
1	A	129	ASP	CB-CG-OD2	-5.97	112.92	118.30
1	A	224	THR	C-N-CD	-5.68	108.09	120.60
1	A	117	THR	CA-CB-CG2	-5.43	104.80	112.40
1	A	225	PRO	N-CA-CB	5.27	109.63	103.30
1	A	151	THR	C-N-CD	-5.24	109.08	120.60
1	A	168	CYS	CA-CB-SG	-5.19	104.66	114.00
1	A	102	ASP	N-CA-C	5.10	124.78	111.00
1	A	178	ASP	CB-CG-OD1	5.05	122.85	118.30
1	A	210	VAL	CA-CB-CG1	-5.04	103.34	110.90
1	A	134	THR	N-CA-CB	5.04	119.87	110.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	102	ASP	CA

There are no planarity outliers.

## 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	1799	0	1777	304	0
2	A	42	0	0	2	0
All	All	1841	0	1777	304	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 85.

All (304) 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:72:ASP:HB2	1:A:154:ARG:HG2	1.25	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LYS:HA	1:A:104:THR:HB	1.38	1.02
1:A:34:GLN:HE21	1:A:40:HIS:HB2	1.25	1.01
1:A:56:ALA:HA	1:A:104:THR:CG2	1.97	0.94
1:A:33:LEU:HD12	1:A:42:CYS:HB3	1.49	0.93
1:A:151:THR:HG22	1:A:152:PRO:HD3	1.51	0.93
1:A:72:ASP:HB2	1:A:154:ARG:CG	2.01	0.91
1:A:235:VAL:HA	1:A:238:VAL:HG23	1.50	0.90
1:A:152:PRO:HG3	1:A:156:GLN:NE2	1.86	0.90
1:A:67:VAL:CG1	1:A:80:ILE:HD12	2.04	0.88
1:A:94:TYR:CE1	1:A:102:ASP:HB2	2.09	0.87
1:A:41:PHE:HZ	1:A:60:VAL:HG13	1.38	0.86
1:A:34:GLN:NE2	1:A:40:HIS:HB2	1.90	0.86
1:A:114:PHE:HA	1:A:118:VAL:HG12	1.56	0.85
1:A:10:LEU:HD23	1:A:157:GLN:NE2	1.94	0.83
1:A:33:LEU:HD12	1:A:42:CYS:CB	2.09	0.83
1:A:151:THR:CG2	1:A:152:PRO:HD3	2.10	0.82
1:A:212:ILE:HG13	1:A:229:ALA:HB3	1.62	0.81
1:A:236:ASN:O	1:A:240:GLN:HG3	1.82	0.80
1:A:160:LEU:C	1:A:160:LEU:HD23	2.01	0.80
1:A:235:VAL:HA	1:A:238:VAL:CG2	2.11	0.80
1:A:146:TYR:C	1:A:149:ALA:O	2.21	0.79
1:A:67:VAL:HG11	1:A:80:ILE:HD12	1.63	0.78
1:A:29:TRP:HB3	1:A:120:ALA:HA	1.65	0.78
1:A:29:TRP:HA	1:A:119:SER:O	1.82	0.78
1:A:134:THR:H	1:A:162:LEU:HB2	1.48	0.78
1:A:211:GLY:HA2	1:A:231:VAL:HG23	1.64	0.78
1:A:151:THR:CB	1:A:152:PRO:HD3	2.14	0.78
1:A:34:GLN:HG3	1:A:40:HIS:HA	1.64	0.78
1:A:14:SER:HB3	1:A:20:GLU:OE1	1.83	0.77
1:A:8:PRO:HB3	1:A:26:SER:HB2	1.67	0.76
1:A:29:TRP:O	1:A:45:SER:HA	1.86	0.76
1:A:16:ILE:HG13	1:A:17:VAL:HG23	1.69	0.74
1:A:16:ILE:HA	1:A:188:VAL:HB	1.68	0.73
1:A:68:ALA:HB3	1:A:81:GLN:HB2	1.69	0.73
1:A:134:THR:O	1:A:161:PRO:HA	1.89	0.71
1:A:160:LEU:H	1:A:160:LEU:HD22	1.53	0.71
1:A:105:LEU:C	1:A:106:LEU:HD23	2.10	0.70
1:A:166:THR:HA	1:A:169:LYS:HD2	1.73	0.70
1:A:35:ASP:OD1	1:A:38:GLY:N	2.25	0.68
1:A:152:PRO:HG3	1:A:156:GLN:HE21	1.57	0.68
1:A:172:TRP:CZ3	1:A:215:TRP:HZ3	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:VAL:HG23	1:A:23:VAL:HG21	1.75	0.68
1:A:177:LYS:HD2	1:A:177:LYS:N	2.09	0.68
1:A:176:ILE:C	1:A:177:LYS:HD2	2.14	0.68
1:A:139:THR:HB	1:A:155:LEU:HD11	1.75	0.68
1:A:103:ILE:HB	1:A:234:LEU:HD12	1.76	0.68
1:A:174:THR:O	1:A:175:LYS:C	2.33	0.67
1:A:144:THR:C	1:A:146:TYR:H	1.98	0.67
1:A:34:GLN:CG	1:A:40:HIS:HA	2.24	0.67
1:A:115:SER:OG	1:A:116:GLN:N	2.24	0.67
1:A:234:LEU:HD23	1:A:234:LEU:N	2.09	0.66
1:A:85:ILE:HG21	1:A:88:VAL:HG22	1.77	0.66
1:A:80:ILE:O	1:A:80:ILE:HG13	1.94	0.66
1:A:47:ILE:HG21	1:A:53:VAL:CG2	2.25	0.66
1:A:40:HIS:HB3	2:A:327:HOH:O	1.95	0.65
1:A:114:PHE:CD1	1:A:118:VAL:HG12	2.31	0.65
1:A:61:THR:O	1:A:63:SER:N	2.30	0.65
1:A:146:TYR:HB3	1:A:149:ALA:C	2.17	0.65
1:A:152:PRO:CG	1:A:156:GLN:HG2	2.27	0.64
1:A:29:TRP:CA	1:A:119:SER:O	2.44	0.64
1:A:160:LEU:O	1:A:160:LEU:HD23	1.96	0.64
1:A:167:ASN:CG	1:A:170:LYS:HE3	2.18	0.64
1:A:195:SER:HA	1:A:213:VAL:CG1	2.28	0.64
1:A:3:VAL:HG12	1:A:3:VAL:O	1.97	0.64
1:A:152:PRO:HG3	1:A:156:GLN:CD	2.17	0.64
1:A:50:ASN:HA	1:A:108:LEU:HD12	1.80	0.64
1:A:141:TRP:HB3	1:A:144:THR:HG21	1.79	0.63
1:A:152:PRO:CG	1:A:156:GLN:HE21	2.10	0.63
1:A:134:THR:HG22	1:A:135:THR:N	2.13	0.63
1:A:174:THR:O	1:A:176:ILE:N	2.32	0.63
1:A:182:CYS:HA	1:A:226:GLY:O	1.98	0.63
1:A:172:TRP:CH2	1:A:215:TRP:HZ3	2.16	0.63
1:A:78:GLU:HB2	1:A:80:ILE:CG2	2.29	0.62
1:A:175:LYS:O	1:A:177:LYS:HD3	1.98	0.62
1:A:85:ILE:HD13	1:A:106:LEU:HB3	1.81	0.62
1:A:49:GLU:HB2	1:A:112:ALA:O	1.98	0.62
1:A:152:PRO:HG3	1:A:156:GLN:CG	2.29	0.62
1:A:243:ALA:O	1:A:245:ASN:N	2.33	0.62
1:A:56:ALA:HA	1:A:104:THR:HG22	1.80	0.61
1:A:172:TRP:HB2	1:A:176:ILE:HD11	1.82	0.61
1:A:47:ILE:CG2	1:A:53:VAL:HG23	2.31	0.61
1:A:72:ASP:CB	1:A:154:ARG:HG2	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:TRP:HB3	1:A:120:ALA:CA	2.30	0.61
1:A:167:ASN:HA	1:A:170:LYS:HG3	1.81	0.61
1:A:184:GLY:O	1:A:185:ALA:HB3	2.00	0.60
1:A:202:LYS:O	1:A:203:LYS:HB2	2.00	0.60
1:A:235:VAL:O	1:A:238:VAL:HG23	2.01	0.60
1:A:160:LEU:HD22	1:A:160:LEU:N	2.13	0.60
1:A:142:GLY:O	1:A:145:ARG:HG3	2.02	0.60
1:A:16:ILE:C	1:A:188:VAL:HG23	2.22	0.60
1:A:130:PHE:N	1:A:130:PHE:CD1	2.68	0.60
1:A:151:THR:HG22	1:A:152:PRO:CD	2.29	0.59
1:A:41:PHE:CZ	1:A:60:VAL:HG13	2.28	0.59
1:A:146:TYR:HB3	1:A:149:ALA:HB3	1.83	0.59
1:A:194:ASP:O	1:A:213:VAL:HG11	2.03	0.59
1:A:211:GLY:HA2	1:A:229:ALA:O	2.02	0.59
1:A:34:GLN:HG2	1:A:40:HIS:N	2.18	0.58
1:A:8:PRO:CB	1:A:26:SER:HB2	2.32	0.58
1:A:95:ASN:OD1	1:A:97:LEU:N	2.35	0.58
1:A:52:VAL:HB	1:A:106:LEU:HB2	1.84	0.58
1:A:233:ALA:C	1:A:234:LEU:HD23	2.24	0.58
1:A:145:ARG:NH2	2:A:319:HOH:O	2.26	0.58
1:A:236:ASN:O	1:A:237:TRP:C	2.37	0.58
1:A:152:PRO:CG	1:A:156:GLN:NE2	2.65	0.58
1:A:146:TYR:HB3	1:A:149:ALA:CB	2.34	0.58
1:A:10:LEU:HD23	1:A:157:GLN:CD	2.23	0.57
1:A:136:CYS:HB3	1:A:200:VAL:O	2.04	0.57
1:A:95:ASN:OD1	1:A:96:SER:N	2.38	0.57
1:A:17:VAL:O	1:A:189:SER:N	2.29	0.57
1:A:61:THR:C	1:A:63:SER:H	2.08	0.57
1:A:152:PRO:HG2	1:A:156:GLN:HG2	1.87	0.57
1:A:167:ASN:ND2	1:A:170:LYS:HE3	2.20	0.57
1:A:146:TYR:CD1	1:A:146:TYR:N	2.73	0.56
1:A:141:TRP:O	1:A:144:THR:HG23	2.05	0.56
1:A:51:TRP:CZ2	1:A:107:LYS:HD2	2.40	0.56
1:A:125:SER:O	1:A:232:THR:HG22	2.06	0.56
1:A:146:TYR:O	1:A:149:ALA:O	2.23	0.56
1:A:177:LYS:O	1:A:180:MET:HG3	2.05	0.56
1:A:47:ILE:HG21	1:A:53:VAL:HG23	1.87	0.55
1:A:107:LYS:NZ	1:A:245:ASN:O	2.39	0.55
1:A:160:LEU:C	1:A:160:LEU:CD2	2.71	0.55
1:A:56:ALA:N	1:A:102:ASP:OD2	2.40	0.55
1:A:145:ARG:HH12	1:A:191:CYS:CA	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:LYS:O	1:A:171:TYR:N	2.40	0.54
1:A:152:PRO:HG3	1:A:156:GLN:HG2	1.90	0.54
1:A:17:VAL:N	1:A:188:VAL:HA	2.23	0.54
1:A:137:VAL:HA	1:A:158:ALA:O	2.07	0.54
1:A:212:ILE:CG1	1:A:229:ALA:HB3	2.36	0.54
1:A:75:SER:HB3	1:A:78:GLU:HG3	1.90	0.54
1:A:2:GLY:HA2	1:A:29:TRP:CZ3	2.42	0.54
1:A:194:ASP:O	1:A:213:VAL:HG21	2.08	0.54
1:A:151:THR:HB	1:A:152:PRO:HD3	1.90	0.54
1:A:12:GLY:O	1:A:13:LEU:C	2.45	0.54
1:A:234:LEU:CD2	1:A:234:LEU:N	2.71	0.54
1:A:114:PHE:HD1	1:A:118:VAL:HG12	1.71	0.53
1:A:46:LEU:HD23	1:A:48:ASN:O	2.08	0.53
1:A:134:THR:CG2	1:A:135:THR:N	2.71	0.53
1:A:105:LEU:O	1:A:106:LEU:HD23	2.07	0.53
1:A:144:THR:C	1:A:146:TYR:N	2.61	0.53
1:A:213:VAL:N	1:A:228:TYR:HD2	2.07	0.53
1:A:141:TRP:HB3	1:A:144:THR:CG2	2.39	0.52
1:A:145:ARG:HH12	1:A:191:CYS:HA	1.74	0.52
1:A:29:TRP:CB	1:A:120:ALA:HA	2.38	0.52
1:A:166:THR:O	1:A:169:LYS:HB2	2.10	0.52
1:A:61:THR:C	1:A:63:SER:N	2.63	0.52
1:A:46:LEU:HD22	1:A:114:PHE:CE1	2.45	0.52
1:A:142:GLY:O	1:A:144:THR:N	2.42	0.52
1:A:160:LEU:HB2	1:A:161:PRO:HD2	1.90	0.52
1:A:57:HIS:N	1:A:102:ASP:OD2	2.32	0.51
1:A:99:ILE:O	1:A:99:ILE:HG22	2.09	0.51
1:A:89:PHE:O	1:A:237:TRP:HH2	1.93	0.51
1:A:121:VAL:HG22	1:A:122:CYS:N	2.26	0.51
1:A:195:SER:HA	1:A:213:VAL:HG11	1.92	0.51
1:A:172:TRP:O	1:A:173:GLY:C	2.48	0.51
1:A:167:ASN:O	1:A:168:CYS:C	2.49	0.51
1:A:105:LEU:HD11	1:A:238:VAL:HG13	1.92	0.51
1:A:30:GLN:NE2	1:A:141:TRP:CZ3	2.78	0.51
1:A:212:ILE:N	1:A:228:TYR:HB3	2.26	0.51
1:A:16:ILE:O	1:A:17:VAL:HB	2.10	0.51
1:A:46:LEU:O	1:A:120:ALA:HA	2.12	0.50
1:A:188:VAL:N	1:A:222:THR:HB	2.25	0.50
1:A:177:LYS:H	1:A:180:MET:HG3	1.77	0.50
1:A:67:VAL:HG12	1:A:68:ALA:N	2.25	0.50
1:A:185:ALA:HB2	1:A:225:PRO:HG3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TRP:CZ3	1:A:215:TRP:CZ3	2.97	0.50
1:A:20:GLU:O	1:A:157:GLN:HG2	2.11	0.50
1:A:40:HIS:CG	1:A:73:GLN:HE22	2.28	0.50
1:A:17:VAL:HG12	1:A:18:ASN:N	2.27	0.50
1:A:187:GLY:HA2	1:A:222:THR:HB	1.94	0.50
1:A:190:SER:C	1:A:192:MET:H	2.13	0.50
1:A:94:TYR:HA	1:A:101:ASN:HB2	1.94	0.50
1:A:210:VAL:HG12	1:A:210:VAL:O	2.11	0.50
1:A:181:ILE:O	1:A:228:TYR:N	2.44	0.49
1:A:200:VAL:HG23	1:A:207:TRP:CE3	2.47	0.49
1:A:103:ILE:HG23	1:A:103:ILE:O	2.11	0.49
1:A:160:LEU:HB2	1:A:161:PRO:CD	2.43	0.49
1:A:202:LYS:O	1:A:203:LYS:CB	2.61	0.49
1:A:8:PRO:CA	1:A:26:SER:HB2	2.42	0.49
1:A:40:HIS:CD2	1:A:73:GLN:HE22	2.31	0.48
1:A:243:ALA:C	1:A:245:ASN:H	2.15	0.48
1:A:48:ASN:OD1	1:A:49:GLU:N	2.46	0.48
1:A:211:GLY:CA	1:A:231:VAL:HG23	2.38	0.48
1:A:62:THR:HG22	1:A:88:VAL:CG2	2.42	0.48
1:A:200:VAL:HG12	1:A:209:LEU:HA	1.95	0.48
1:A:145:ARG:NH1	1:A:191:CYS:HB3	2.28	0.48
1:A:50:ASN:OD1	1:A:111:ALA:HB2	2.14	0.48
1:A:105:LEU:HG	1:A:237:TRP:HZ3	1.79	0.48
1:A:103:ILE:CB	1:A:234:LEU:HD12	2.43	0.48
1:A:36:LYS:C	1:A:38:GLY:N	2.67	0.48
1:A:128:ASP:HB3	1:A:130:PHE:CE1	2.48	0.48
1:A:103:ILE:HG21	1:A:234:LEU:CD1	2.43	0.48
1:A:121:VAL:CG2	1:A:122:CYS:N	2.76	0.48
1:A:87:LYS:C	1:A:88:VAL:HG23	2.33	0.48
1:A:52:VAL:HG12	1:A:52:VAL:O	2.14	0.47
1:A:56:ALA:HA	1:A:104:THR:HG21	1.92	0.47
1:A:1:CYS:C	1:A:122:CYS:SG	2.92	0.47
1:A:95:ASN:C	1:A:95:ASN:OD1	2.52	0.47
1:A:29:TRP:C	1:A:29:TRP:CD1	2.86	0.47
1:A:53:VAL:HG12	1:A:54:THR:N	2.28	0.47
1:A:103:ILE:CG2	1:A:234:LEU:CD1	2.92	0.47
1:A:231:VAL:O	1:A:232:THR:C	2.51	0.47
1:A:235:VAL:O	1:A:236:ASN:C	2.53	0.47
1:A:106:LEU:N	1:A:106:LEU:HD23	2.27	0.47
1:A:46:LEU:O	1:A:121:VAL:HG12	2.15	0.47
1:A:172:TRP:CE3	1:A:215:TRP:CZ3	3.03	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:VAL:O	1:A:54:THR:HB	2.15	0.47
1:A:139:THR:HG22	1:A:157:GLN:HA	1.97	0.46
1:A:62:THR:HG22	1:A:88:VAL:HG23	1.96	0.46
1:A:123:LEU:HA	1:A:123:LEU:HD23	1.64	0.46
1:A:34:GLN:CG	1:A:40:HIS:CA	2.91	0.46
1:A:162:LEU:HD23	1:A:162:LEU:N	2.27	0.46
1:A:125:SER:O	1:A:126:ALA:C	2.53	0.46
1:A:12:GLY:C	1:A:14:SER:N	2.68	0.46
1:A:169:LYS:C	1:A:171:TYR:N	2.68	0.46
1:A:36:LYS:O	1:A:38:GLY:N	2.49	0.46
1:A:114:PHE:CD1	1:A:118:VAL:CG1	2.98	0.45
1:A:29:TRP:HB3	1:A:120:ALA:C	2.35	0.45
1:A:36:LYS:H	1:A:36:LYS:HG3	1.50	0.45
1:A:72:ASP:OD2	1:A:153:ASP:HB2	2.15	0.45
1:A:103:ILE:CG2	1:A:234:LEU:HD12	2.46	0.45
1:A:143:LEU:O	1:A:146:TYR:HD1	1.99	0.45
1:A:235:VAL:C	1:A:238:VAL:HG23	2.37	0.45
1:A:61:THR:OG1	1:A:63:SER:OG	2.30	0.45
1:A:20:GLU:O	1:A:157:GLN:N	2.46	0.45
1:A:118:VAL:HG12	1:A:118:VAL:O	2.15	0.45
1:A:212:ILE:O	1:A:213:VAL:C	2.55	0.45
1:A:17:VAL:H	1:A:188:VAL:HA	1.80	0.45
1:A:201:CYS:SG	1:A:210:VAL:HG21	2.56	0.45
1:A:65:VAL:O	1:A:65:VAL:HG13	2.15	0.45
1:A:78:GLU:HB2	1:A:80:ILE:HG23	1.97	0.45
1:A:98:THR:O	1:A:99:ILE:HB	2.17	0.45
1:A:232:THR:O	1:A:235:VAL:HG12	2.17	0.45
1:A:105:LEU:HG	1:A:237:TRP:CZ3	2.52	0.45
1:A:229:ALA:O	1:A:231:VAL:N	2.51	0.44
1:A:195:SER:HA	1:A:213:VAL:HG12	2.00	0.44
1:A:9:VAL:HG23	1:A:23:VAL:CG2	2.44	0.44
1:A:84:LYS:O	1:A:108:LEU:HB3	2.17	0.44
1:A:189:SER:OG	1:A:220:CYS:HB3	2.18	0.44
1:A:174:THR:C	1:A:176:ILE:N	2.69	0.44
1:A:47:ILE:HG23	1:A:53:VAL:HG23	1.99	0.44
1:A:34:GLN:HG2	1:A:40:HIS:CA	2.47	0.44
1:A:115:SER:N	1:A:118:VAL:O	2.50	0.44
1:A:30:GLN:O	1:A:30:GLN:HG3	2.13	0.44
1:A:190:SER:C	1:A:192:MET:N	2.70	0.44
1:A:55:ALA:HA	1:A:102:ASP:O	2.17	0.44
1:A:80:ILE:HD11	1:A:82:LYS:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:HIS:CB	1:A:73:GLN:HE22	2.30	0.44
1:A:145:ARG:HH12	1:A:191:CYS:CB	2.30	0.44
1:A:95:ASN:O	1:A:99:ILE:HA	2.18	0.44
1:A:103:ILE:C	1:A:104:THR:HG22	2.38	0.43
1:A:162:LEU:HD22	1:A:162:LEU:HA	1.66	0.43
1:A:2:GLY:HA2	1:A:29:TRP:HZ3	1.82	0.43
1:A:154:ARG:O	1:A:155:LEU:C	2.54	0.43
1:A:103:ILE:HG21	1:A:234:LEU:HD13	2.00	0.43
1:A:108:LEU:O	1:A:109:SER:O	2.36	0.43
1:A:33:LEU:HD12	1:A:42:CYS:HB2	1.97	0.43
1:A:20:GLU:CG	1:A:157:GLN:HE21	2.31	0.43
1:A:143:LEU:O	1:A:146:TYR:CD1	2.71	0.43
1:A:43:GLY:N	1:A:195:SER:O	2.40	0.42
1:A:145:ARG:NH1	1:A:191:CYS:CB	2.82	0.42
1:A:12:GLY:O	1:A:14:SER:N	2.52	0.42
1:A:121:VAL:HG21	1:A:209:LEU:HB2	2.00	0.42
1:A:145:ARG:NH2	1:A:193:GLY:O	2.53	0.42
1:A:18:ASN:HA	1:A:18:ASN:HD22	1.47	0.42
1:A:172:TRP:HB2	1:A:176:ILE:CD1	2.48	0.42
1:A:51:TRP:CG	1:A:242:LEU:HD11	2.54	0.42
1:A:85:ILE:HG21	1:A:88:VAL:CG2	2.47	0.42
1:A:5:ALA:HB1	1:A:116:GLN:HG2	2.02	0.42
1:A:166:THR:O	1:A:169:LYS:N	2.53	0.42
1:A:87:LYS:C	1:A:88:VAL:CG2	2.87	0.41
1:A:81:GLN:HE22	1:A:113:SER:N	2.18	0.41
1:A:172:TRP:HB2	1:A:176:ILE:CG1	2.50	0.41
1:A:184:GLY:O	1:A:185:ALA:CB	2.67	0.41
1:A:100:ASN:OD1	1:A:179:ALA:HB3	2.19	0.41
1:A:56:ALA:HA	1:A:104:THR:HG23	1.92	0.41
1:A:71:PHE:N	1:A:78:GLU:OE2	2.44	0.41
1:A:143:LEU:O	1:A:146:TYR:HB2	2.20	0.41
1:A:219:THR:O	1:A:220:CYS:C	2.58	0.41
1:A:169:LYS:O	1:A:173:GLY:N	2.52	0.41
1:A:172:TRP:CE3	1:A:215:TRP:HZ3	2.38	0.41
1:A:89:PHE:CD1	1:A:89:PHE:N	2.89	0.41
1:A:234:LEU:O	1:A:238:VAL:HG23	2.19	0.41
1:A:61:THR:HG1	1:A:63:SER:HG	1.66	0.41
1:A:210:VAL:O	1:A:210:VAL:CG1	2.67	0.41
1:A:166:THR:O	1:A:167:ASN:C	2.57	0.41
1:A:177:LYS:N	1:A:180:MET:HG3	2.35	0.41
1:A:146:TYR:CB	1:A:149:ALA:O	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:SER:HB3	1:A:78:GLU:CG	2.51	0.41
1:A:114:PHE:HD1	1:A:118:VAL:CG1	2.34	0.41
1:A:50:ASN:ND2	1:A:111:ALA:HB2	2.36	0.41
1:A:17:VAL:N	1:A:188:VAL:HG23	2.35	0.41
1:A:20:GLU:CD	1:A:157:GLN:HE21	2.25	0.41
1:A:105:LEU:HA	1:A:105:LEU:HD23	1.76	0.41
1:A:48:ASN:OD1	1:A:50:ASN:N	2.29	0.41
1:A:7:GLN:HA	1:A:8:PRO:HD3	1.87	0.41
1:A:57:HIS:CD2	1:A:57:HIS:O	2.74	0.40
1:A:163:LEU:HA	1:A:163:LEU:HD23	1.94	0.40
1:A:57:HIS:HB3	1:A:94:TYR:OH	2.21	0.40
1:A:67:VAL:HG11	1:A:80:ILE:CD1	2.42	0.40
1:A:142:GLY:O	1:A:143:LEU:C	2.59	0.40
1:A:67:VAL:HG12	1:A:68:ALA:H	1.87	0.40
1:A:68:ALA:O	1:A:80:ILE:HB	2.20	0.40
1:A:243:ALA:O	1:A:245:ASN:OXT	2.39	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	243/245 (99%)	192 (79%)	33 (14%)	18 (7%)	<b>1</b> <b>6</b>

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	109	SER
1	A	151	THR
1	A	152	PRO
1	A	203	LYS
1	A	244	ALA

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Mol	Chain	Res	Type
1	A	17	VAL
1	A	62	THR
1	A	217	SER
1	A	102	ASP
1	A	143	LEU
1	A	170	LYS
1	A	186	SER
1	A	188	VAL
1	A	175	LYS
1	A	213	VAL
1	A	238	VAL
1	A	99	ILE
1	A	205	GLY

### 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	200/200 (100%)	151 (76%)	49 (24%)	<b>1</b> <b>4</b>

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	SER
1	A	16	ILE
1	A	31	VAL
1	A	36	LYS
1	A	37	THR
1	A	40	HIS
1	A	42	CYS
1	A	46	LEU
1	A	48	ASN
1	A	60	VAL
1	A	63	SER
1	A	70	GLU
1	A	72	ASP

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Mol	Chain	Res	Type
1	A	76	SER
1	A	77	SER
1	A	79	LYS
1	A	83	LEU
1	A	85	ILE
1	A	87	LYS
1	A	90	LYS
1	A	97	LEU
1	A	102	ASP
1	A	104	THR
1	A	108	LEU
1	A	113	SER
1	A	115	SER
1	A	127	SER
1	A	145	ARG
1	A	150	ASN
1	A	153	ASP
1	A	159	SER
1	A	160	LEU
1	A	162	LEU
1	A	165	ASN
1	A	171	TYR
1	A	177	LYS
1	A	180	MET
1	A	194	ASP
1	A	199	LEU
1	A	202	LYS
1	A	208	THR
1	A	212	ILE
1	A	214	SER
1	A	218	SER
1	A	223	SER
1	A	232	THR
1	A	234	LEU
1	A	238	VAL
1	A	239	GLN

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

Mol	Chain	Res	Type
1	A	18	ASN
1	A	30	GLN

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Mol	Chain	Res	Type
1	A	34	GLN
1	A	40	HIS
1	A	73	GLN
1	A	81	GLN
1	A	150	ASN
1	A	156	GLN
1	A	157	GLN
1	A	165	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 carbohydrates 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](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.