



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 12, 2017 – 11:43 pm GMT

PDB ID : 1CGI  
Title : THREE-DIMENSIONAL STRUCTURE OF THE COMPLEXES BETWEEN BOVINE CHYMOTRYPSINOGEN\*A AND TWO RECOMBINANT VARIANTS OF HUMAN PANCREATIC SECRETORY TRYPSIN INHIBITOR (KAZAL-TYPE)  
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Deposited on : 1991-10-08  
Resolution : 2.30 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
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

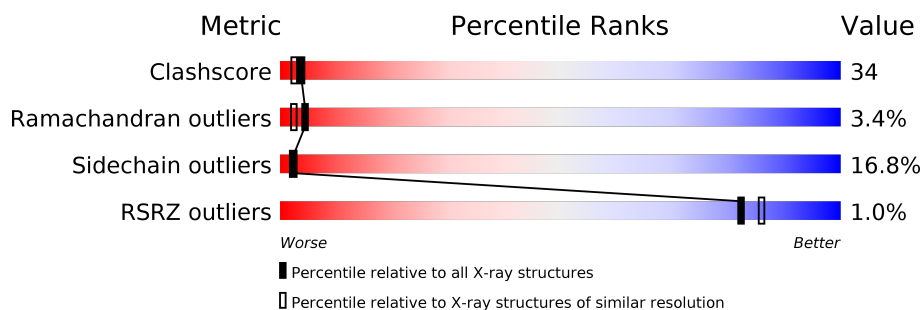
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	112137	4751 (2.30-2.30)
Ramachandran outliers	110173	4705 (2.30-2.30)
Sidechain outliers	110143	4704 (2.30-2.30)
RSRZ outliers	101464	4156 (2.30-2.30)

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.

Mol	Chain	Length	Quality of chain
1	E	245	<div> <div>32%</div> <div>46%</div> <div>20%</div> <div>•</div> </div>
2	I	56	<div> <div>29%</div> <div>43%</div> <div>25%</div> <div>•</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2291 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 ALPHA-CHYMOTRYPSINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	245	Total	C	N	O	S	20	0	0
			1799	1127	307	353	12			

- Molecule 2 is a protein called PANCREATIC SECRETORY TRYPSIN INHIBITOR (KAZAL TYPE) VARIANT 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	56	Total	C	N	O	S	24	0	0
			440	267	77	90	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	18	TYR	LYS	CONFLICT	UNP P00995
I	19	GLU	ILE	CONFLICT	UNP P00995
I	21	ARG	ASP	CONFLICT	UNP P00995
I	29	ASP	ASN	CONFLICT	UNP P00995

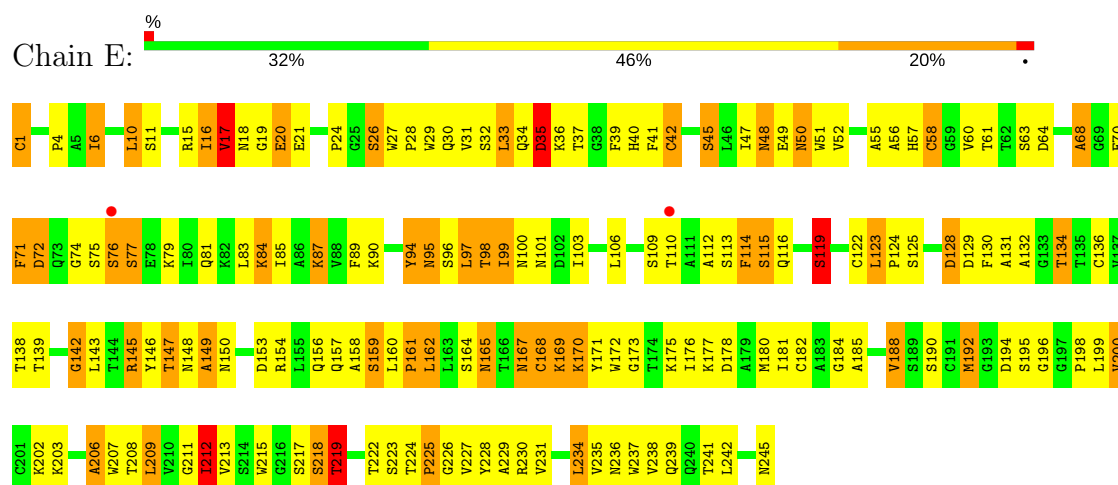
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	48	Total	O	0	0
			48	48		
3	I	4	Total	O	0	0
			4	4		

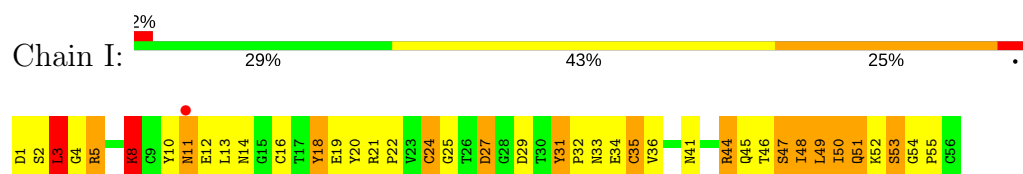
### 3 Residue-property plots

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



#### • Molecule 2: PANCREATIC SECRETORY TRYPSIN INHIBITOR (KAZAL TYPE) VARIANT 3



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.40Å 84.40Å 86.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.30 7.97 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.30) 71.2 (7.97-2.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.06 (at 2.30Å)	Xtriage
Refinement program	PROLSQ	Depositor
R, $R_{free}$	0.195 , (Not available) 0.194 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	16.0	Xtriage
Anisotropy	0.427	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 46.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.042 for -h,l,k 0.031 for -l,-k,-h	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	2291	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.44% 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

### 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	E	1.03	4/1835 (0.2%)	2.32	93/2502 (3.7%)
2	I	1.20	2/447 (0.4%)	2.69	33/601 (5.5%)
All	All	1.07	6/2282 (0.3%)	2.40	126/3103 (4.1%)

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
2	I	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	8	LYS	CD-CE	-9.74	1.26	1.51
2	I	3	LEU	C-N	7.42	1.46	1.33
1	E	26	SER	CB-OG	-5.39	1.35	1.42
1	E	136	CYS	CB-SG	-5.26	1.73	1.81
1	E	77	SER	CA-CB	5.15	1.60	1.52
1	E	182	CYS	CB-SG	-5.14	1.73	1.81

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	145	ARG	NE-CZ-NH2	-16.85	111.88	120.30
2	I	5	ARG	NE-CZ-NH2	-14.73	112.93	120.30
2	I	5	ARG	NE-CZ-NH1	14.26	127.43	120.30
2	I	3	LEU	O-C-N	-13.44	100.35	123.20
2	I	8	LYS	CG-CD-CE	12.88	150.53	111.90
1	E	94	TYR	CB-CG-CD1	10.73	127.44	121.00
1	E	58	CYS	CA-CB-SG	10.68	133.23	114.00
2	I	44	ARG	CA-CB-CG	10.61	136.74	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	17	VAL	C-N-CA	10.38	147.64	121.70
1	E	236	ASN	CB-CA-C	9.94	130.28	110.40
1	E	234	LEU	CA-CB-CG	9.72	137.65	115.30
1	E	194	ASP	CB-CG-OD1	-9.60	109.67	118.30
2	I	3	LEU	CA-C-N	9.33	134.87	116.20
2	I	14	ASN	CB-CA-C	8.87	128.15	110.40
1	E	119	SER	N-CA-CB	8.64	123.46	110.50
1	E	35	ASP	CB-CA-C	-8.59	93.22	110.40
1	E	52	VAL	O-C-N	8.59	136.44	122.70
2	I	44	ARG	NE-CZ-NH1	-8.46	116.07	120.30
2	I	29	ASP	CB-CG-OD1	8.40	125.86	118.30
1	E	219	THR	OG1-CB-CG2	8.35	129.21	110.00
1	E	48	ASN	CB-CA-C	-8.22	93.96	110.40
1	E	168	CYS	CA-CB-SG	8.07	128.53	114.00
1	E	70	GLU	CG-CD-OE1	-7.87	102.55	118.30
2	I	2	SER	O-C-N	7.80	135.19	122.70
1	E	194	ASP	CB-CG-OD2	7.77	125.29	118.30
1	E	182	CYS	CA-CB-SG	7.66	127.78	114.00
1	E	70	GLU	OE1-CD-OE2	7.56	132.37	123.30
1	E	21	GLU	OE1-CD-OE2	7.55	132.37	123.30
2	I	33	ASN	CA-CB-CG	7.53	129.96	113.40
1	E	42	CYS	CA-CB-SG	7.46	127.44	114.00
1	E	17	VAL	CA-C-O	7.44	135.72	120.10
1	E	72	ASP	CB-CG-OD2	7.23	124.80	118.30
1	E	145	ARG	CD-NE-CZ	7.22	133.70	123.60
2	I	51	GLN	CA-C-O	7.21	135.25	120.10
1	E	217	SER	CA-CB-OG	7.20	130.64	111.20
1	E	35	ASP	O-C-N	7.17	134.17	122.70
1	E	50	ASN	CB-CA-C	-7.11	96.17	110.40
1	E	128	ASP	CB-CG-OD1	-7.09	111.92	118.30
1	E	219	THR	N-CA-CB	-7.08	96.84	110.30
1	E	224	THR	CA-CB-CG2	7.03	122.24	112.40
1	E	178	ASP	CB-CG-OD1	6.88	124.49	118.30
2	I	10	TYR	N-CA-C	-6.88	92.42	111.00
1	E	97	LEU	O-C-N	6.75	133.50	122.70
2	I	14	ASN	C-N-CA	6.67	136.31	122.30
2	I	35	CYS	CA-CB-SG	6.66	125.98	114.00
2	I	3	LEU	C-N-CA	-6.62	108.40	122.30
1	E	26	SER	N-CA-CB	6.53	120.29	110.50
1	E	35	ASP	CB-CG-OD1	-6.50	112.45	118.30
1	E	178	ASP	CB-CA-C	6.43	123.26	110.40
1	E	146	TYR	C-N-CA	6.38	137.66	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	134	THR	O-C-N	6.37	132.90	122.70
1	E	20	GLU	CA-CB-CG	6.37	127.42	113.40
1	E	145	ARG	NH1-CZ-NH2	6.32	126.35	119.40
1	E	47	ILE	C-N-CA	6.30	137.45	121.70
1	E	128	ASP	CA-CB-CG	-6.17	99.82	113.40
1	E	169	LYS	CA-CB-CG	-6.13	99.90	113.40
1	E	206	ALA	CB-CA-C	-6.08	100.98	110.10
1	E	162	LEU	CB-CG-CD2	-6.01	100.78	111.00
1	E	153	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	E	123	LEU	CA-CB-CG	5.98	129.05	115.30
1	E	200	VAL	CA-CB-CG2	5.97	119.86	110.90
1	E	153	ASP	CB-CG-OD1	5.96	123.66	118.30
1	E	226	GLY	CA-C-O	-5.95	109.89	120.60
1	E	30	GLN	OE1-CD-NE2	-5.93	108.27	121.90
2	I	27	ASP	CB-CG-OD2	5.90	123.61	118.30
1	E	1	CYS	C-N-CA	5.87	134.63	122.30
1	E	154	ARG	CD-NE-CZ	-5.86	115.40	123.60
1	E	222	THR	O-C-N	-5.86	113.33	122.70
1	E	212	ILE	CA-C-O	-5.85	107.81	120.10
2	I	5	ARG	N-CA-CB	5.85	121.13	110.60
1	E	227	VAL	CA-CB-CG1	5.85	119.67	110.90
1	E	146	TYR	CA-C-O	5.84	132.37	120.10
1	E	154	ARG	NE-CZ-NH2	5.83	123.21	120.30
1	E	84	LYS	CB-CG-CD	5.80	126.69	111.60
2	I	2	SER	CA-C-N	-5.78	104.49	117.20
1	E	225	PRO	C-N-CA	5.75	134.37	122.30
2	I	33	ASN	CB-CA-C	5.73	121.86	110.40
1	E	227	VAL	CG1-CB-CG2	-5.71	101.76	110.90
1	E	129	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	E	199	LEU	N-CA-C	-5.69	95.64	111.00
1	E	55	ALA	O-C-N	5.68	131.79	122.70
2	I	36	VAL	O-C-N	5.67	131.77	122.70
1	E	149	ALA	CB-CA-C	5.64	118.56	110.10
1	E	34	GLN	C-N-CA	5.61	135.73	121.70
1	E	68	ALA	C-N-CA	5.60	134.05	122.30
1	E	222	THR	C-N-CA	5.59	135.68	121.70
1	E	71	PHE	N-CA-CB	5.59	120.66	110.60
1	E	52	VAL	CA-C-N	-5.58	104.92	117.20
1	E	1	CYS	CA-CB-SG	5.57	124.03	114.00
1	E	149	ALA	CA-C-O	5.56	131.77	120.10
1	E	115	SER	N-CA-CB	5.53	118.80	110.50
1	E	219	THR	CA-CB-OG1	-5.51	97.44	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	149	ALA	C-N-CA	5.49	135.43	121.70
1	E	142	GLY	CA-C-O	-5.47	110.75	120.60
1	E	167	ASN	CB-CA-C	5.47	121.34	110.40
1	E	55	ALA	N-CA-CB	5.46	117.74	110.10
2	I	19	GLU	CB-CG-CD	5.44	128.88	114.20
1	E	42	CYS	O-C-N	-5.41	114.00	123.20
2	I	51	GLN	CA-C-N	-5.41	105.29	117.20
1	E	217	SER	O-C-N	5.40	131.35	122.70
1	E	98	THR	N-CA-CB	-5.39	100.06	110.30
2	I	31	TYR	CB-CG-CD1	5.38	124.23	121.00
1	E	132	ALA	CB-CA-C	5.38	118.17	110.10
1	E	33	LEU	CB-CG-CD1	-5.35	101.91	111.00
1	E	147	THR	CA-CB-CG2	5.31	119.83	112.40
2	I	47	SER	CA-CB-OG	-5.30	96.89	111.20
1	E	1	CYS	CB-CA-C	5.29	120.98	110.40
1	E	17	VAL	CA-C-N	-5.27	105.60	117.20
2	I	18	TYR	N-CA-C	5.26	125.20	111.00
2	I	33	ASN	C-N-CA	5.25	134.81	121.70
1	E	71	PHE	O-C-N	5.23	131.07	122.70
1	E	72	ASP	O-C-N	5.22	131.06	122.70
2	I	24	CYS	N-CA-CB	5.22	119.99	110.60
1	E	146	TYR	N-CA-CB	-5.20	101.24	110.60
2	I	19	GLU	OE1-CD-OE2	5.20	129.54	123.30
1	E	31	VAL	CA-CB-CG1	5.18	118.67	110.90
2	I	36	VAL	CA-CB-CG2	-5.15	103.17	110.90
1	E	114	PHE	CB-CG-CD1	-5.15	117.19	120.80
2	I	18	TYR	CG-CD1-CE1	5.14	125.41	121.30
1	E	234	LEU	CB-CG-CD1	5.09	119.65	111.00
1	E	159	SER	N-CA-CB	5.08	118.12	110.50
1	E	190	SER	CA-C-O	-5.08	109.44	120.10
2	I	48	ILE	O-C-N	5.07	130.80	122.70
1	E	6	ILE	CA-C-N	-5.06	106.08	117.20
2	I	50	ILE	O-C-N	5.06	130.79	122.70
1	E	106	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	I	3	LEU	Mainchain,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	E	1799	0	1775	121	0
2	I	440	0	412	36	0
3	E	48	0	0	1	0
3	I	4	0	0	0	0
All	All	2291	0	2187	146	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 34.

All (146) 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:E:35:ASP:OD2	1:E:37:THR:HB	1.58	1.04
1:E:180:MET:O	1:E:230:ARG:NH1	1.92	1.01
1:E:4:PRO:HB2	1:E:6:ILE:O	1.74	0.87
2:I:27:ASP:HB3	2:I:48:ILE:HD12	1.60	0.82
2:I:44:ARG:HB2	2:I:46:THR:HG23	1.63	0.81
1:E:158:ALA:HB1	1:E:188:VAL:HG11	1.63	0.80
1:E:33:LEU:HD23	1:E:33:LEU:N	1.96	0.80
1:E:95:ASN:ND2	1:E:97:LEU:H	1.80	0.79
1:E:95:ASN:HD22	1:E:97:LEU:H	1.31	0.78
1:E:241:THR:O	1:E:245:ASN:HB2	1.85	0.77
1:E:158:ALA:HB1	1:E:188:VAL:CG1	2.16	0.76
1:E:94:TYR:HB2	1:E:101:ASN:O	1.86	0.74
2:I:27:ASP:HB3	2:I:48:ILE:CD1	2.17	0.74
1:E:33:LEU:CD1	1:E:60:VAL:HG21	2.17	0.74
1:E:81:GLN:HE22	1:E:113:SER:H	1.35	0.73
2:I:22:PRO:HA	2:I:31:TYR:O	1.88	0.72
1:E:4:PRO:CB	1:E:6:ILE:O	2.40	0.69
1:E:198:PRO:HB2	1:E:200:VAL:HG13	1.72	0.69
1:E:123:LEU:HD11	1:E:238:VAL:HG11	1.75	0.69
1:E:99:ILE:HG13	2:I:13:LEU:HD22	1.75	0.69
1:E:35:ASP:HB3	1:E:37:THR:H	1.58	0.68
1:E:35:ASP:HB3	1:E:37:THR:N	2.08	0.68
1:E:64:ASP:O	1:E:85:ILE:HD12	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:35:ASP:HB2	1:E:39:PHE:H	1.57	0.67
1:E:35:ASP:OD2	1:E:37:THR:CB	2.41	0.65
1:E:192:MET:HG2	2:I:32:PRO:HB2	1.77	0.65
1:E:239:GLN:OE1	1:E:239:GLN:HA	1.97	0.64
1:E:165:ASN:O	1:E:169:LYS:HG3	1.98	0.63
1:E:172:TRP:CB	1:E:176:ILE:HD11	2.27	0.63
1:E:219:THR:O	1:E:219:THR:HG23	1.99	0.61
1:E:198:PRO:HB2	1:E:200:VAL:CG1	2.30	0.61
2:I:8:LYS:HG3	2:I:34:GLU:OE2	2.00	0.61
2:I:11:ASN:HD22	2:I:11:ASN:C	1.98	0.60
1:E:97:LEU:O	2:I:12:GLU:HB2	2.01	0.60
1:E:98:THR:HG22	1:E:100:ASN:HB2	1.82	0.60
1:E:215:TRP:CD2	2:I:13:LEU:HD11	2.36	0.60
1:E:184:GLY:O	1:E:185:ALA:HB3	2.01	0.59
1:E:68:ALA:HB3	1:E:81:GLN:HB2	1.84	0.59
1:E:215:TRP:CE2	2:I:13:LEU:HD11	2.39	0.58
1:E:29:TRP:O	1:E:45:SER:HA	2.04	0.58
1:E:99:ILE:HG13	2:I:13:LEU:CD2	2.34	0.58
2:I:52:LYS:NZ	2:I:55:PRO:O	2.36	0.58
1:E:161:PRO:HG2	1:E:161:PRO:O	2.03	0.58
1:E:171:TYR:CD2	1:E:225:PRO:HD3	2.38	0.57
2:I:27:ASP:CB	2:I:48:ILE:HD12	2.34	0.57
1:E:125:SER:O	1:E:128:ASP:HB2	2.04	0.57
1:E:131:ALA:O	1:E:134:THR:OG1	2.09	0.57
1:E:32:SER:OG	1:E:40:HIS:ND1	2.30	0.56
2:I:24:CYS:HB3	2:I:52:LYS:HG2	1.85	0.56
1:E:134:THR:O	1:E:161:PRO:HA	2.06	0.56
1:E:181:ILE:HG13	1:E:230:ARG:NH2	2.20	0.56
1:E:97:LEU:HB3	2:I:12:GLU:HG3	1.88	0.56
1:E:11:SER:OG	1:E:20:GLU:OE1	2.22	0.55
1:E:27:TRP:CD1	1:E:139:THR:HG21	2.42	0.55
1:E:103:ILE:HG23	1:E:237:TRP:CZ3	2.42	0.55
1:E:81:GLN:NE2	1:E:113:SER:H	2.02	0.54
1:E:72:ASP:OD1	1:E:74:GLY:N	2.41	0.53
1:E:41:PHE:O	1:E:42:CYS:SG	2.66	0.53
2:I:4:GLY:O	2:I:50:ILE:O	2.26	0.53
1:E:138:THR:HA	1:E:198:PRO:O	2.09	0.53
1:E:33:LEU:HD12	1:E:60:VAL:CG2	2.39	0.53
1:E:94:TYR:HA	1:E:100:ASN:O	2.08	0.53
1:E:1:CYS:C	1:E:122:CYS:SG	2.87	0.53
1:E:124:PRO:CG	1:E:231:VAL:HG12	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:48:ASN:HB2	1:E:50:ASN:H	1.74	0.52
1:E:81:GLN:HE22	1:E:113:SER:N	2.03	0.52
1:E:130:PHE:CZ	1:E:203:LYS:CE	2.93	0.52
1:E:114:PHE:HD1	1:E:114:PHE:N	2.08	0.51
1:E:172:TRP:HB2	1:E:176:ILE:CG1	2.41	0.51
1:E:56:ALA:HB1	1:E:90:LYS:HD2	1.93	0.51
1:E:238:VAL:O	1:E:242:LEU:HB2	2.11	0.51
1:E:32:SER:C	1:E:33:LEU:HD23	2.30	0.50
1:E:95:ASN:HD22	1:E:95:ASN:C	2.14	0.50
2:I:52:LYS:HG3	2:I:53:SER:O	2.12	0.50
1:E:24:PRO:HG3	1:E:71:PHE:CE2	2.46	0.50
1:E:33:LEU:CD1	1:E:60:VAL:CG2	2.88	0.50
1:E:27:TRP:HE3	1:E:29:TRP:CZ2	2.29	0.50
1:E:124:PRO:HG3	1:E:231:VAL:HG12	1.93	0.49
1:E:172:TRP:CG	1:E:176:ILE:HD11	2.47	0.49
1:E:169:LYS:O	1:E:173:GLY:N	2.45	0.49
1:E:167:ASN:HA	1:E:170:LYS:HD2	1.94	0.49
1:E:95:ASN:HD22	1:E:96:SER:N	2.11	0.49
1:E:35:ASP:CG	1:E:37:THR:HB	2.29	0.49
1:E:113:SER:O	1:E:114:PHE:C	2.52	0.49
1:E:20:GLU:O	1:E:156:GLN:HA	2.13	0.48
1:E:130:PHE:CZ	1:E:203:LYS:HE2	2.48	0.48
2:I:41:ASN:OD1	2:I:46:THR:OG1	2.31	0.48
1:E:16:ILE:O	1:E:17:VAL:C	2.52	0.48
1:E:200:VAL:HG23	1:E:207:TRP:CE3	2.49	0.48
1:E:49:GLU:HB3	1:E:112:ALA:O	2.14	0.48
2:I:20:TYR:CE2	2:I:22:PRO:HG3	2.49	0.48
1:E:114:PHE:CD1	1:E:114:PHE:N	2.80	0.47
1:E:20:GLU:O	1:E:157:GLN:N	2.44	0.47
1:E:20:GLU:HG3	1:E:157:GLN:HE21	1.79	0.47
2:I:52:LYS:O	2:I:52:LYS:HG2	2.14	0.47
2:I:52:LYS:O	2:I:52:LYS:CG	2.60	0.47
1:E:87:LYS:HB3	1:E:89:PHE:CE1	2.50	0.47
1:E:168:CYS:SG	1:E:172:TRP:HD1	2.37	0.46
1:E:130:PHE:HZ	1:E:203:LYS:CE	2.28	0.46
1:E:158:ALA:HB1	1:E:188:VAL:HG13	1.95	0.46
2:I:11:ASN:ND2	2:I:11:ASN:O	2.31	0.46
1:E:51:TRP:CE2	1:E:242:LEU:HD12	2.50	0.46
1:E:33:LEU:HD12	1:E:60:VAL:HG21	1.92	0.46
1:E:142:GLY:HA2	1:E:192:MET:O	2.15	0.45
1:E:160:LEU:N	1:E:160:LEU:HD23	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:181:ILE:CG1	1:E:230:ARG:NH2	2.79	0.45
1:E:99:ILE:CG1	2:I:13:LEU:HD22	2.46	0.45
1:E:156:GLN:HG3	3:E:252:HOH:O	2.17	0.44
1:E:177:LYS:HG2	1:E:180:MET:CE	2.47	0.44
1:E:218:SER:HA	2:I:16:CYS:HB2	2.00	0.44
1:E:148:ASN:O	1:E:149:ALA:C	2.55	0.44
1:E:27:TRP:CE3	1:E:29:TRP:CZ2	3.06	0.44
1:E:203:LYS:NZ	1:E:208:THR:HG21	2.32	0.44
1:E:124:PRO:HD3	1:E:209:LEU:O	2.18	0.43
1:E:196:GLY:HA2	1:E:212:ILE:HG23	2.01	0.43
1:E:172:TRP:HB2	1:E:176:ILE:HD11	1.98	0.43
2:I:25:GLY:HA2	2:I:49:LEU:O	2.18	0.43
1:E:10:LEU:HD12	1:E:10:LEU:HA	1.84	0.43
1:E:211:GLY:HA2	1:E:229:ALA:O	2.19	0.43
1:E:57:HIS:CD2	1:E:57:HIS:C	2.91	0.43
2:I:41:ASN:O	2:I:45:GLN:N	2.52	0.43
2:I:44:ARG:HD3	2:I:44:ARG:HH11	1.56	0.43
1:E:28:PRO:HB2	1:E:119:SER:N	2.34	0.43
1:E:123:LEU:HD11	1:E:238:VAL:CG1	2.46	0.43
1:E:115:SER:HB2	1:E:116:GLN:H	1.53	0.42
1:E:95:ASN:O	1:E:99:ILE:N	2.51	0.42
1:E:202:LYS:HA	1:E:206:ALA:O	2.18	0.42
2:I:27:ASP:HB3	2:I:48:ILE:HD11	2.01	0.42
1:E:203:LYS:HE3	1:E:203:LYS:HB2	1.82	0.42
1:E:213:VAL:HG22	1:E:228:TYR:HE2	1.85	0.42
2:I:44:ARG:HB2	2:I:46:THR:CG2	2.42	0.42
1:E:124:PRO:O	1:E:235:VAL:HG21	2.19	0.42
1:E:15:ARG:HG2	1:E:159:SER:HB2	2.01	0.42
2:I:53:SER:OG	2:I:54:GLY:N	2.52	0.42
2:I:44:ARG:NE	2:I:46:THR:HG21	2.35	0.41
1:E:56:ALA:HB1	1:E:90:LYS:CD	2.50	0.41
1:E:83:LEU:CD1	1:E:112:ALA:HB2	2.51	0.41
1:E:209:LEU:HD12	1:E:209:LEU:HA	1.80	0.41
2:I:27:ASP:OD1	2:I:27:ASP:N	2.49	0.41
2:I:4:GLY:HA2	2:I:49:LEU:HD13	2.03	0.41
1:E:195:SER:OG	2:I:18:TYR:C	2.59	0.41
1:E:58:CYS:O	2:I:21:ARG:NH2	2.31	0.41
1:E:172:TRP:HB2	1:E:176:ILE:HG12	2.03	0.41
1:E:35:ASP:CB	1:E:37:THR:HB	2.51	0.41
1:E:95:ASN:HD22	1:E:97:LEU:N	2.08	0.40
1:E:169:LYS:O	1:E:173:GLY:HA2	2.21	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	E	243/245 (99%)	224 (92%)	11 (4%)	8 (3%)	4	2
2	I	54/56 (96%)	51 (94%)	1 (2%)	2 (4%)	4	2
All	All	297/301 (99%)	275 (93%)	12 (4%)	10 (3%)	4	2

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	17	VAL
1	E	19	GLY
1	E	75	SER
1	E	76	SER
2	I	3	LEU
1	E	150	ASN
1	E	209	LEU
2	I	5	ARG
1	E	18	ASN
1	E	99	ILE

### 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	E	200/200 (100%)	167 (84%)	33 (16%)	2	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	50/50 (100%)	41 (82%)	9 (18%)	2	2
All	All	250/250 (100%)	208 (83%)	42 (17%)	2	2

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	10	LEU
1	E	16	ILE
1	E	26	SER
1	E	35	ASP
1	E	36	LYS
1	E	45	SER
1	E	61	THR
1	E	63	SER
1	E	76	SER
1	E	77	SER
1	E	79	LYS
1	E	84	LYS
1	E	87	LYS
1	E	95	ASN
1	E	109	SER
1	E	110	THR
1	E	119	SER
1	E	143	LEU
1	E	145	ARG
1	E	147	THR
1	E	161	PRO
1	E	162	LEU
1	E	164	SER
1	E	165	ASN
1	E	170	LYS
1	E	175	LYS
1	E	188	VAL
1	E	192	MET
1	E	212	ILE
1	E	218	SER
1	E	219	THR
1	E	223	SER
1	E	234	LEU
2	I	1	ASP
2	I	3	LEU
2	I	8	LYS

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Mol	Chain	Res	Type
2	I	11	ASN
2	I	35	CYS
2	I	47	SER
2	I	49	LEU
2	I	51	GLN
2	I	53	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	34	GLN
1	E	73	GLN
1	E	81	GLN
1	E	95	ASN
1	E	116	GLN
1	E	165	ASN
1	E	167	ASN
2	I	11	ASN
2	I	51	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 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 [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	E	245/245 (100%)	-0.43	2 (0%) 86 89	2, 11, 33, 48	6 (2%)
2	I	53/56 (94%)	-0.29	1 (1%) 67 73	2, 8, 40, 47	1 (1%)
All	All	298/301 (99%)	-0.40	3 (1%) 82 86	2, 10, 35, 48	7 (2%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	11	ASN	3.7
1	E	110	THR	2.7
1	E	76	SER	2.5

### 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 carbohydrates in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.