Full wwPDB X-ray Structure Validation Report (i)

May 26, 2020 – 12:22 pm BST

PDB ID	:	1CGJ
Title	:	THREE-DIMENSIONAL STRUCTURE OF THE COMPLEXES BETWEEN BOVINE CHYMOTRYPSINOGEN*A AND TWO RECOMBINANT VARIANTS OF HUMAN PANCREATIC SECRETORY TRYPSIN INHIBITOR (KAZAL-TYPE)
Authors	:	Hecht, H.J.; Szardenings, M.; Collins, J.; Schomburg, D.
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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

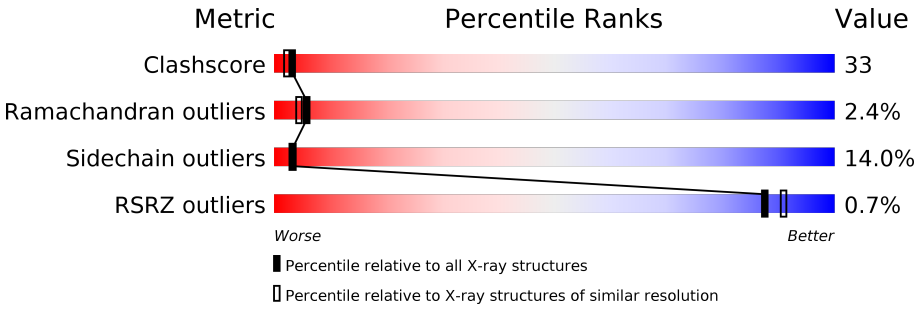
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 >=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 <=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	32% 44% 18% 5%
2	I	56	2% 30% 38% 29% .

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	16	0	0
			1799	1127	307	353	12			

- Molecule 2 is a protein called PANCREATIC SECRETORY TRYPSIN INHIBITOR (KAZAL TYPE) VARIANT 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	56	Total	C	N	O	S	24	0	0
			436	264	77	89	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	18	LEU	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.

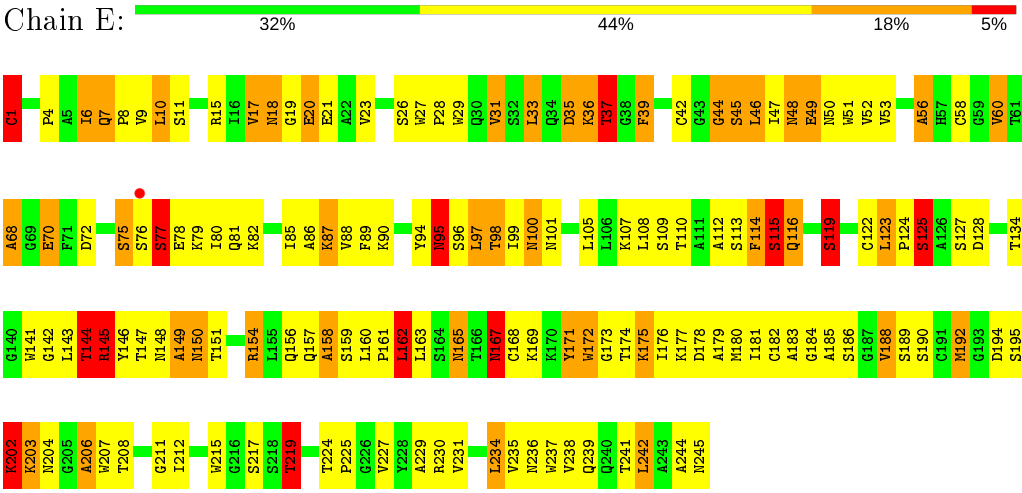
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	51	Total	O	0	0
			51	51		
3	I	5	Total	O	0	0
			5	5		

3 Residue-property plots (i)

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.

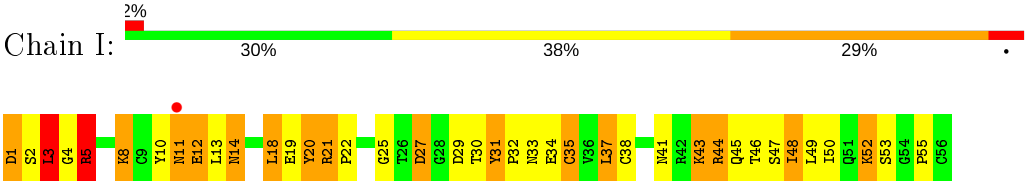
• Molecule 1: ALPHA-CHYMOTRYPSINOGEN

Chain E:



• Molecule 2: PANCREATIC SECRETORY TRYPSIN INHIBITOR (KAZAL TYPE) VARIANT 4

Chain I:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	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) 73.6 (7.97-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	12.48 (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.	wwPDB-VP
Wilson B-factor (Å^2)	20.1	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 30.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.041 for -h,l,k 0.020 for -l,-k,-h	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	2291	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	1.16	8/1835 (0.4%)	2.46	109/2502 (4.4%)
2	I	1.53	2/442 (0.5%)	2.83	34/594 (5.7%)
All	All	1.24	10/2277 (0.4%)	2.54	143/3096 (4.6%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	8	LYS	CD-CE	-21.97	0.96	1.51
1	E	162	LEU	CB-CG	10.76	1.83	1.52
1	E	36	LYS	CA-CB	-7.01	1.38	1.53
1	E	203	LYS	CG-CD	6.74	1.75	1.52
2	I	18	LEU	CB-CG	6.42	1.71	1.52
1	E	150	ASN	CA-CB	-5.89	1.37	1.53
1	E	1	CYS	CB-SG	-5.54	1.72	1.81
1	E	42	CYS	CB-SG	-5.16	1.73	1.81
1	E	125	SER	CB-OG	5.08	1.48	1.42
1	E	26	SER	CB-OG	-5.01	1.35	1.42

All (143) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	145	ARG	NE-CZ-NH2	-18.26	111.17	120.30
2	I	21	ARG	NE-CZ-NH1	17.67	129.13	120.30
2	I	5	ARG	NE-CZ-NH1	14.26	127.43	120.30
2	I	29	ASP	CB-CG-OD1	13.04	130.04	118.30
1	E	77	SER	C-N-CA	12.24	152.29	121.70
2	I	21	ARG	NE-CZ-NH2	-11.53	114.53	120.30
1	E	145	ARG	NE-CZ-NH1	10.60	125.60	120.30
1	E	236	ASN	CB-CA-C	10.56	131.53	110.40
2	I	5	ARG	NE-CZ-NH2	-10.18	115.21	120.30
2	I	27	ASP	CB-CG-OD1	-10.16	109.16	118.30
1	E	204	ASN	CA-CB-CG	9.83	135.02	113.40
1	E	35	ASP	CB-CA-C	-9.62	91.16	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	1	ASP	CB-CG-OD1	-9.59	109.67	118.30
1	E	1	CYS	CA-CB-SG	9.41	130.94	114.00
1	E	115	SER	O-C-N	9.19	137.41	122.70
1	E	36	LYS	N-CA-CB	9.01	126.81	110.60
1	E	154	ARG	NE-CZ-NH2	-8.95	115.82	120.30
1	E	42	CYS	CA-CB-SG	8.93	130.07	114.00
1	E	234	LEU	CA-CB-CG	8.91	135.79	115.30
1	E	17	VAL	C-N-CA	8.89	143.93	121.70
2	I	20	TYR	CB-CG-CD2	8.55	126.13	121.00
1	E	168	CYS	CA-CB-SG	8.47	129.25	114.00
1	E	48	ASN	CB-CA-C	-8.34	93.72	110.40
1	E	68	ALA	C-N-CA	8.27	139.67	122.30
2	I	38	CYS	CA-CB-SG	8.04	128.47	114.00
2	I	20	TYR	CB-CG-CD1	-7.99	116.20	121.00
1	E	219	THR	OG1-CB-CG2	7.98	128.35	110.00
2	I	31	TYR	CB-CG-CD1	7.94	125.77	121.00
1	E	162	LEU	CB-CG-CD2	-7.91	97.55	111.00
2	I	37	LEU	O-C-N	7.86	135.27	122.70
1	E	217	SER	O-C-N	7.82	135.21	122.70
1	E	115	SER	N-CA-CB	7.68	122.01	110.50
1	E	219	THR	N-CA-CB	-7.48	96.09	110.30
1	E	206	ALA	O-C-N	7.39	134.52	122.70
1	E	39	PHE	CB-CA-C	7.36	125.11	110.40
1	E	10	LEU	CA-CB-CG	7.23	131.92	115.30
1	E	178	ASP	CB-CA-C	7.16	124.71	110.40
1	E	167	ASN	CB-CA-C	7.06	124.52	110.40
1	E	149	ALA	CA-C-O	6.98	134.75	120.10
2	I	1	ASP	CB-CG-OD2	6.86	124.48	118.30
1	E	18	ASN	CB-CG-OD1	-6.77	108.07	121.60
1	E	60	VAL	O-C-N	6.71	133.43	122.70
2	I	35	CYS	CB-CA-C	6.68	123.77	110.40
2	I	10	TYR	N-CA-CB	6.67	122.61	110.60
2	I	10	TYR	N-CA-C	-6.64	93.06	111.00
1	E	6	ILE	CA-C-O	6.53	133.82	120.10
2	I	14	ASN	OD1-CG-ND2	-6.51	106.92	121.90
2	I	30	THR	O-C-N	-6.51	112.28	122.70
1	E	167	ASN	CB-CG-OD1	-6.46	108.68	121.60
1	E	159	SER	CA-CB-OG	6.43	128.56	111.20
1	E	146	TYR	N-CA-CB	-6.40	99.09	110.60
1	E	149	ALA	CB-CA-C	6.39	119.69	110.10
1	E	6	ILE	CA-C-N	-6.35	103.22	117.20
1	E	174	THR	O-C-N	6.32	132.81	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	178	ASP	CB-CG-OD1	6.32	123.99	118.30
2	I	49	LEU	O-C-N	6.31	132.79	122.70
1	E	146	TYR	CA-C-O	6.29	133.30	120.10
1	E	20	GLU	OE1-CD-OE2	6.27	130.82	123.30
1	E	149	ALA	C-N-CA	6.27	137.37	121.70
1	E	212	ILE	CA-C-O	-6.25	106.97	120.10
1	E	199	LEU	N-CA-CB	6.24	122.87	110.40
1	E	37	THR	CA-CB-CG2	-6.21	103.70	112.40
1	E	20	GLU	CA-CB-CG	6.19	127.02	113.40
1	E	48	ASN	CA-CB-CG	-6.14	99.90	113.40
1	E	1	CYS	C-N-CA	6.13	135.18	122.30
2	I	14	ASN	CB-CA-C	6.11	122.62	110.40
1	E	78	GLU	CA-CB-CG	6.09	126.79	113.40
1	E	49	GLU	CG-CD-OE2	6.05	130.40	118.30
2	I	33	ASN	CB-CA-C	6.02	122.45	110.40
1	E	70	GLU	CG-CD-OE1	-6.00	106.30	118.30
1	E	35	ASP	O-C-N	5.96	132.24	122.70
2	I	47	SER	N-CA-CB	5.96	119.44	110.50
1	E	112	ALA	N-CA-CB	5.95	118.44	110.10
1	E	136	CYS	CB-CA-C	5.94	122.28	110.40
1	E	189	SER	O-C-N	-5.93	113.21	122.70
1	E	97	LEU	C-N-CA	5.90	136.44	121.70
1	E	167	ASN	OD1-CG-ND2	5.84	135.33	121.90
1	E	188	VAL	N-CA-CB	-5.76	98.82	111.50
2	I	43	LYS	N-CA-CB	-5.75	100.25	110.60
1	E	46	LEU	CA-CB-CG	5.75	128.52	115.30
1	E	48	ASN	CB-CG-ND2	-5.70	103.02	116.70
1	E	72	ASP	CB-CG-OD1	5.67	123.41	118.30
1	E	204	ASN	N-CA-CB	5.67	120.81	110.60
2	I	3	LEU	N-CA-CB	-5.67	99.07	110.40
1	E	20	GLU	CB-CG-CD	5.64	129.43	114.20
1	E	119	SER	N-CA-CB	5.64	118.95	110.50
1	E	114	PHE	O-C-N	5.63	131.72	122.70
1	E	33	LEU	CB-CG-CD1	-5.63	101.44	111.00
2	I	8	LYS	CB-CA-C	-5.61	99.19	110.40
1	E	186	SER	CA-C-N	5.59	127.39	116.20
1	E	20	GLU	CG-CD-OE2	-5.58	107.14	118.30
1	E	82	LYS	O-C-N	5.57	131.61	122.70
1	E	172	TRP	CG-CD1-NE1	5.52	115.62	110.10
1	E	56	ALA	CB-CA-C	-5.52	101.82	110.10
1	E	144	THR	N-CA-CB	-5.50	99.84	110.30
1	E	171	TYR	N-CA-CB	5.47	120.45	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	48	ASN	O-C-N	5.47	131.45	122.70
1	E	174	THR	CA-C-O	-5.45	108.65	120.10
1	E	200	VAL	CA-CB-CG2	5.44	119.06	110.90
2	I	37	LEU	CA-C-O	-5.42	108.73	120.10
2	I	29	ASP	CB-CG-OD2	-5.41	113.44	118.30
1	E	75	SER	CA-C-N	-5.39	105.35	117.20
1	E	115	SER	CB-CA-C	-5.36	99.91	110.10
1	E	136	CYS	N-CA-CB	-5.35	100.98	110.60
1	E	98	THR	CA-CB-CG2	5.32	119.85	112.40
1	E	227	VAL	C-N-CA	5.32	135.01	121.70
1	E	123	LEU	CA-CB-CG	5.32	127.53	115.30
1	E	163	LEU	CB-CG-CD2	-5.31	101.97	111.00
1	E	171	TYR	CB-CG-CD2	5.29	124.17	121.00
1	E	194	ASP	CB-CG-OD1	-5.27	113.56	118.30
1	E	44	GLY	O-C-N	5.27	131.13	122.70
2	I	43	LYS	CA-CB-CG	5.26	124.97	113.40
1	E	20	GLU	CA-C-N	-5.25	105.65	117.20
1	E	63	SER	CB-CA-C	-5.25	100.13	110.10
2	I	44	ARG	CA-CB-CG	5.25	124.95	113.40
1	E	244	ALA	O-C-N	5.24	131.08	122.70
2	I	31	TYR	CG-CD2-CE2	5.23	125.49	121.30
1	E	7	GLN	N-CA-CB	-5.23	101.19	110.60
1	E	17	VAL	N-CA-CB	5.21	122.96	111.50
1	E	157	GLN	C-N-CA	5.16	134.60	121.70
1	E	100	ASN	CB-CG-OD1	-5.16	111.28	121.60
1	E	115	SER	CA-C-N	-5.16	105.85	117.20
2	I	48	ILE	O-C-N	5.16	130.95	122.70
1	E	190	SER	N-CA-C	-5.15	97.10	111.00
1	E	171	TYR	CB-CA-C	-5.14	100.12	110.40
1	E	31	VAL	CA-C-N	-5.13	105.92	117.20
1	E	208	THR	CA-CB-CG2	5.13	119.58	112.40
1	E	202	LYS	CB-CA-C	5.12	120.65	110.40
1	E	174	THR	CA-CB-CG2	-5.12	105.23	112.40
1	E	183	ALA	CB-CA-C	-5.12	102.43	110.10
1	E	48	ASN	OD1-CG-ND2	5.11	133.66	121.90
1	E	1	CYS	CA-C-N	-5.11	105.98	116.20
1	E	172	TRP	CD1-NE1-CE2	-5.11	104.40	109.00
2	I	11	ASN	CB-CA-C	5.11	120.61	110.40
1	E	75	SER	N-CA-CB	5.09	118.14	110.50
1	E	95	ASN	CA-C-N	-5.09	106.00	117.20
1	E	138	THR	CA-CB-CG2	5.08	119.51	112.40
1	E	182	CYS	CA-CB-SG	5.08	123.14	114.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	19	GLU	OE1-CD-OE2	5.08	129.39	123.30
1	E	21	GLU	CB-CG-CD	-5.03	100.61	114.20
1	E	188	VAL	O-C-N	5.02	130.74	122.70
1	E	158	ALA	N-CA-CB	5.00	117.10	110.10
2	I	12	GLU	CA-CB-CG	5.00	124.40	113.40

There are no chirality outliers.

There are no planarity outliers.

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	E	1799	0	1775	127	0
2	I	436	0	414	29	7
3	E	51	0	0	3	7
3	I	5	0	0	0	0
All	All	2291	0	2189	144	7

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 33.

All (144) 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:162:LEU:CG	1:E:162:LEU:CB	1.83	1.54
1:E:180:MET:O	1:E:230:ARG:NH1	1.92	1.01
1:E:172:TRP:CB	1:E:176:ILE:HD11	1.95	0.96
1:E:165:ASN:O	1:E:169:LYS:HG3	1.65	0.95
1:E:48:ASN:HB3	1:E:50:ASN:H	1.30	0.94
1:E:81:GLN:HE22	1:E:113:SER:H	1.02	0.93
1:E:224:THR:HG22	1:E:225:PRO:HD2	1.50	0.91
1:E:172:TRP:HB2	1:E:176:ILE:HD11	1.52	0.89
1:E:215:TRP:CE3	2:I:13:LEU:HD11	2.11	0.86
1:E:162:LEU:CB	1:E:162:LEU:CD2	2.55	0.84
1:E:87:LYS:HD3	1:E:88:VAL:N	1.94	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:11:SER:OG	1:E:20:GLU:OE1	1.99	0.80
1:E:95:ASN:ND2	1:E:97:LEU:H	1.79	0.80
1:E:76:SER:O	1:E:77:SER:HB2	1.83	0.77
1:E:95:ASN:HD22	1:E:97:LEU:H	1.33	0.76
1:E:224:THR:HG22	1:E:225:PRO:CD	2.16	0.75
1:E:98:THR:HG22	1:E:100:ASN:HB2	1.69	0.75
1:E:81:GLN:NE2	1:E:113:SER:H	1.83	0.74
1:E:48:ASN:HB2	1:E:51:TRP:H	1.52	0.74
1:E:4:PRO:HB2	1:E:6:ILE:O	1.87	0.73
1:E:87:LYS:HD3	1:E:88:VAL:H	1.52	0.73
1:E:169:LYS:O	1:E:173:GLY:HA2	1.90	0.72
1:E:215:TRP:CZ3	2:I:13:LEU:HD11	2.26	0.70
1:E:56:ALA:HB1	1:E:90:LYS:HD3	1.72	0.70
1:E:35:ASP:HB3	1:E:37:THR:N	2.08	0.68
2:I:22:PRO:HA	2:I:31:TYR:O	1.93	0.68
2:I:4:GLY:O	2:I:50:ILE:O	2.11	0.68
1:E:35:ASP:HB3	1:E:37:THR:H	1.57	0.68
1:E:215:TRP:CD2	2:I:13:LEU:HD11	2.30	0.67
1:E:125:SER:O	1:E:128:ASP:HB2	1.95	0.66
1:E:175:LYS:O	1:E:177:LYS:HD3	1.96	0.66
1:E:48:ASN:CB	1:E:50:ASN:H	2.08	0.66
1:E:35:ASP:HB2	1:E:39:PHE:H	1.62	0.65
1:E:29:TRP:O	1:E:45:SER:HA	1.97	0.65
2:I:8:LYS:HG3	2:I:34:GLU:OE2	1.96	0.64
1:E:175:LYS:HE3	2:I:14:ASN:HD22	1.63	0.64
1:E:172:TRP:HB3	1:E:176:ILE:HD11	1.78	0.64
1:E:181:ILE:HG13	1:E:230:ARG:NH2	2.14	0.63
2:I:52:LYS:HG3	2:I:53:SER:O	1.99	0.62
1:E:27:TRP:CD1	1:E:139:THR:HG21	2.35	0.62
1:E:27:TRP:HE3	1:E:29:TRP:CZ2	2.17	0.62
1:E:95:ASN:HD22	1:E:96:SER:N	1.98	0.61
1:E:67:VAL:O	3:E:255:HOH:O	2.16	0.60
2:I:20:TYR:CE2	2:I:22:PRO:HG3	2.36	0.60
1:E:211:GLY:HA2	1:E:229:ALA:O	2.03	0.59
1:E:95:ASN:HD22	1:E:95:ASN:C	2.05	0.58
1:E:177:LYS:HG2	1:E:180:MET:CE	2.33	0.58
1:E:67:VAL:HG13	1:E:80:ILE:HD12	1.85	0.57
1:E:51:TRP:CZ3	1:E:107:LYS:HB2	2.40	0.57
1:E:58:CYS:O	2:I:21:ARG:NH2	2.37	0.56
1:E:47:ILE:HG21	1:E:123:LEU:HD21	1.87	0.56
1:E:4:PRO:CB	1:E:6:ILE:O	2.53	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:LEU:CD1	1:E:60:VAL:HG21	2.35	0.56
1:E:49:GLU:HA	1:E:114:PHE:CE1	2.40	0.56
2:I:37:LEU:O	2:I:37:LEU:HD12	2.05	0.56
1:E:160:LEU:N	1:E:160:LEU:HD23	2.21	0.55
1:E:75:SER:C	1:E:77:SER:N	2.59	0.55
1:E:148:ASN:O	1:E:149:ALA:C	2.45	0.54
1:E:200:VAL:HG23	1:E:207:TRP:CE3	2.43	0.54
1:E:50:ASN:O	1:E:108:LEU:HG	2.07	0.54
1:E:215:TRP:HA	2:I:18:LEU:HG	1.89	0.53
1:E:184:GLY:O	1:E:185:ALA:HB3	2.09	0.53
1:E:177:LYS:HG2	1:E:180:MET:HE1	1.92	0.52
1:E:62:THR:HG22	1:E:85:ILE:HG22	1.92	0.51
1:E:1:CYS:C	1:E:122:CYS:SG	2.88	0.51
1:E:158:ALA:HB1	1:E:188:VAL:HG11	1.92	0.51
1:E:162:LEU:CD1	1:E:162:LEU:CB	2.83	0.51
1:E:142:GLY:HA2	1:E:192:MET:O	2.10	0.51
1:E:28:PRO:HB2	1:E:119:SER:N	2.26	0.51
1:E:94:TYR:HB2	1:E:101:ASN:O	2.11	0.51
1:E:81:GLN:HE22	1:E:113:SER:N	1.87	0.50
1:E:239:GLN:OE1	1:E:239:GLN:HA	2.11	0.50
2:I:52:LYS:O	2:I:52:LYS:HG2	2.11	0.50
2:I:52:LYS:NZ	2:I:55:PRO:O	2.43	0.50
1:E:215:TRP:CZ3	2:I:13:LEU:CD1	2.94	0.49
1:E:171:TYR:CD2	1:E:225:PRO:HD3	2.47	0.49
1:E:27:TRP:CE3	1:E:29:TRP:CZ2	3.00	0.49
1:E:172:TRP:HB2	1:E:176:ILE:CD1	2.35	0.49
1:E:98:THR:CG2	1:E:100:ASN:HB2	2.42	0.49
1:E:95:ASN:O	1:E:99:ILE:N	2.46	0.48
1:E:124:PRO:CG	1:E:231:VAL:HG12	2.43	0.48
1:E:9:VAL:HG23	1:E:23:VAL:HG21	1.94	0.48
1:E:224:THR:CG2	1:E:225:PRO:CD	2.90	0.48
1:E:115:SER:HB2	1:E:116:GLN:H	1.27	0.48
1:E:68:ALA:N	1:E:81:GLN:O	2.41	0.48
1:E:224:THR:CG2	1:E:225:PRO:HD2	2.35	0.47
2:I:27:ASP:HB3	2:I:48:ILE:HD12	1.96	0.47
1:E:179:ALA:O	3:E:250:HOH:O	2.20	0.47
1:E:158:ALA:HB1	1:E:188:VAL:CG1	2.44	0.47
1:E:46:LEU:HD23	1:E:52:VAL:HG22	1.97	0.47
1:E:86:ALA:HB2	1:E:109:SER:HB2	1.96	0.47
2:I:44:ARG:O	2:I:45:GLN:C	2.49	0.47
1:E:64:ASP:O	1:E:85:ILE:HD12	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:LEU:CG	1:E:162:LEU:CA	2.83	0.46
2:I:5:ARG:HG2	2:I:50:ILE:HD12	1.98	0.46
1:E:219:THR:O	1:E:219:THR:HG23	2.15	0.46
1:E:161:PRO:HG2	1:E:161:PRO:O	2.16	0.45
1:E:167:ASN:ND2	1:E:167:ASN:O	2.49	0.45
1:E:202:LYS:HA	1:E:206:ALA:O	2.15	0.45
1:E:181:ILE:CG1	1:E:230:ARG:NH2	2.79	0.45
1:E:70:GLU:HG3	1:E:80:ILE:HG21	1.97	0.45
1:E:51:TRP:CH2	1:E:107:LYS:HB2	2.51	0.45
1:E:99:ILE:HG13	2:I:13:LEU:CD2	2.47	0.45
1:E:192:MET:HG2	2:I:32:PRO:HB2	1.98	0.44
1:E:138:THR:HG22	1:E:160:LEU:CD2	2.48	0.44
1:E:31:VAL:HG22	1:E:44:GLY:C	2.38	0.44
1:E:144:THR:C	1:E:145:ARG:HG2	2.39	0.43
1:E:144:THR:HG22	1:E:148:ASN:ND2	2.33	0.43
1:E:7:GLN:HA	1:E:8:PRO:HD3	1.81	0.43
1:E:156:GLN:HB2	3:E:251:HOH:O	2.16	0.43
1:E:99:ILE:HG13	2:I:13:LEU:HD22	2.00	0.43
1:E:37:THR:HG23	1:E:37:THR:H	1.43	0.43
1:E:124:PRO:HG3	1:E:231:VAL:HG12	2.00	0.43
1:E:138:THR:HG22	1:E:160:LEU:HD21	1.99	0.43
1:E:162:LEU:HB2	1:E:162:LEU:CD2	2.47	0.43
2:I:37:LEU:HD11	2:I:48:ILE:HB	2.00	0.43
1:E:137:VAL:HG12	1:E:138:THR:N	2.33	0.43
1:E:144:THR:O	1:E:145:ARG:HG2	2.18	0.43
1:E:51:TRP:CE2	1:E:242:LEU:HD12	2.53	0.43
2:I:34:GLU:O	2:I:35:CYS:C	2.56	0.43
1:E:94:TYR:HA	1:E:100:ASN:O	2.19	0.42
2:I:4:GLY:O	2:I:5:ARG:HB3	2.18	0.42
1:E:141:TRP:O	1:E:151:THR:HB	2.19	0.42
1:E:162:LEU:HD11	1:E:199:LEU:HD21	2.01	0.42
1:E:203:LYS:N	1:E:206:ALA:O	2.27	0.42
1:E:47:ILE:HD12	1:E:123:LEU:HD11	2.02	0.42
1:E:134:THR:O	1:E:161:PRO:HA	2.19	0.42
1:E:162:LEU:HA	1:E:162:LEU:HD12	2.00	0.42
1:E:89:PHE:O	1:E:237:TRP:HH2	2.03	0.42
2:I:41:ASN:OD1	2:I:46:THR:OG1	2.31	0.42
1:E:105:LEU:HD11	1:E:238:VAL:HA	2.01	0.42
1:E:241:THR:O	1:E:245:ASN:HB2	2.20	0.41
1:E:138:THR:HA	1:E:198:PRO:O	2.20	0.41
1:E:235:VAL:O	1:E:239:GLN:HG2	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:THR:HG23	1:E:177:LYS:HE2	2.01	0.41
2:I:43:LYS:HB2	2:I:43:LYS:HE3	1.69	0.41
1:E:15:ARG:HH11	1:E:15:ARG:HD3	1.63	0.41
1:E:195:SER:OG	2:I:18:LEU:C	2.59	0.41
1:E:169:LYS:O	1:E:173:GLY:CA	2.65	0.41
1:E:162:LEU:HG	1:E:181:ILE:HD11	2.03	0.41
1:E:97:LEU:O	2:I:12:GLU:HB2	2.20	0.41
1:E:95:ASN:HD21	1:E:97:LEU:HB2	1.85	0.40
1:E:160:LEU:H	1:E:160:LEU:HD23	1.86	0.40
2:I:25:GLY:C	2:I:27:ASP:H	2.24	0.40

All (7) 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)
2:I:2:SER:OG	3:E:290:HOH:O[6_555]	0.93	1.27
2:I:2:SER:CB	3:E:290:HOH:O[6_555]	0.95	1.25
2:I:2:SER:CA	3:E:289:HOH:O[6_555]	0.97	1.23
2:I:2:SER:N	3:E:289:HOH:O[6_555]	1.17	1.03
2:I:2:SER:C	3:E:289:HOH:O[6_555]	1.43	0.77
2:I:2:SER:O	3:E:289:HOH:O[6_555]	1.88	0.32
2:I:2:SER:CB	3:E:289:HOH:O[6_555]	1.99	0.21

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%)	229 (94%)	9 (4%)	5 (2%)	7	5
2	I	54/56 (96%)	48 (89%)	4 (7%)	2 (4%)	3	2
All	All	297/301 (99%)	277 (93%)	13 (4%)	7 (2%)	6	4

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	17	VAL
1	E	19	GLY
1	E	77	SER
2	I	3	LEU
1	E	150	ASN
1	E	18	ASN
2	I	5	ARG

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%)	170 (85%)	30 (15%)	3 3
2	I	50/50 (100%)	45 (90%)	5 (10%)	7 9
All	All	250/250 (100%)	215 (86%)	35 (14%)	3 3

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	1	CYS
1	E	10	LEU
1	E	36	LYS
1	E	37	THR
1	E	45	SER
1	E	53	VAL
1	E	77	SER
1	E	79	LYS
1	E	87	LYS
1	E	95	ASN
1	E	110	THR
1	E	115	SER
1	E	116	GLN
1	E	119	SER
1	E	125	SER
1	E	127	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	143	LEU
1	E	144	THR
1	E	145	ARG
1	E	147	THR
1	E	154	ARG
1	E	162	LEU
1	E	165	ASN
1	E	167	ASN
1	E	175	LYS
1	E	192	MET
1	E	202	LYS
1	E	219	THR
1	E	234	LEU
1	E	242	LEU
2	I	1	ASP
2	I	3	LEU
2	I	5	ARG
2	I	11	ASN
2	I	52	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	34	GLN
1	E	48	ASN
1	E	73	GLN
1	E	81	GLN
1	E	95	ASN
1	E	165	ASN
1	E	167	ASN
2	I	14	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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^{th} 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^2)	Q<0.9
1	E	245/245 (100%)	-0.41	1 (0%)	92	95	2, 11, 31, 48	4 (1%)
2	I	53/56 (94%)	-0.30	1 (1%)	66	73	2, 8, 43, 50	1 (1%)
All	All	298/301 (99%)	-0.39	2 (0%)	87	91	2, 10, 36, 50	5 (1%)

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	11	ASN	2.8
1	E	76	SER	2.7

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

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.