WORLDWIDE PDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:36 PM GMT

PDB ID	:	1UD1
Title	:	Crystal structure of proglycinin mutant C88S
Authors	:	Utsumi, S.; Adachi, M.
Deposited on	:	2003-04-24
Resolution	:	3.10 Å(reported)

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

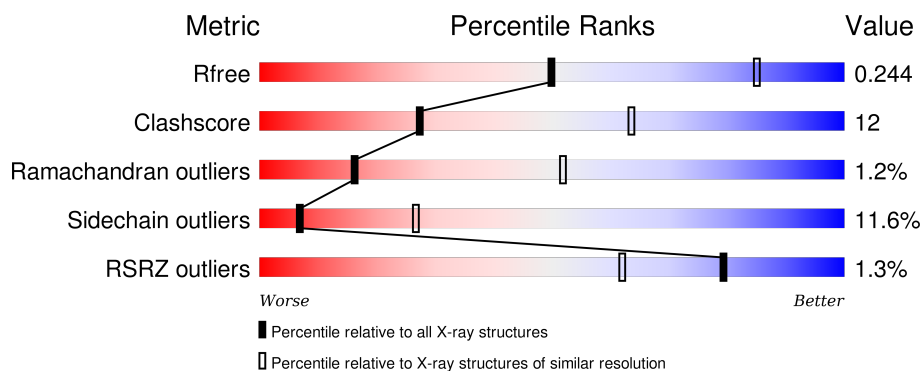|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.10 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	Percentile Ranks	Value
Rfree		0.244
Clashscore		12
Ramachandran outliers		1.2%
Sidechain outliers		11.6%
RSRZ outliers		1.3%

Worse *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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. 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	A	476	48% 24% · · 23%
1	B	476	45% 27% · · 23%
1	C	476	47% 27% · · 23%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 8649 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 Glycinin G1.

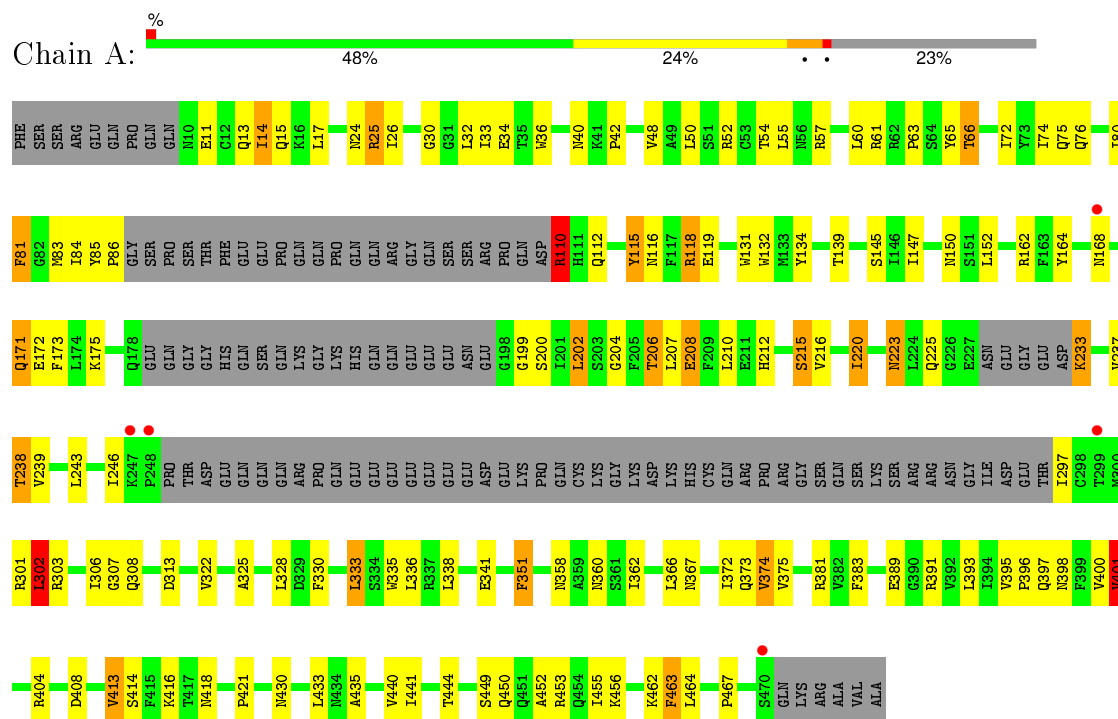| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	366	Total 2883	C 1821	N 510	O 541	S 11	0	0	0
1	B	366	Total 2883	C 1821	N 510	O 541	S 11	0	0	0
1	C	366	Total 2883	C 1821	N 510	O 541	S 11	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	SER	CYS	ENGINEERED	UNP P04776
B	88	SER	CYS	ENGINEERED	UNP P04776
C	88	SER	CYS	ENGINEERED	UNP P04776

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.

- Molecule 1: Glycinin G1

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R301 L302 R303 T309 D313 N316 A319 T324 S327 L333 S334 W335 L336 R337 L338 E341 F342 G343 M350 F351 V352 P353 S361 L366 N367 G368 R369 I372 Q373 V374 R381 V382 F383 E389 G390 R391 V392 V395 P396 Q397 N398 V401 A402 A403

Q406 S407 D408 E411 Y412 V413 D419 T425 L426 N430 S431 L432 L433 N434 A435 L436 P437 E438 E439 V440 I441 Q442 H443 T444 L447 N458 N459 F463 L464 E469 S470 GLN LYS ARG ALA VAL ALA

• Molecule 1: Glycinin G1

%

Chain C:

47% 27% • • 23%

PHE SER SER ARG GLU GLN PRO GLN GLN N10 E11 C12 K16 L20 N24 R25 G30 G31 L32 I33 E34 T35 W36 N37 P38 K41 V48 T54 L55 L60 R61 R62 P63 S64 Y65 T66 P69 Q70 E71 I72 Y73 I74 Q75 Q76 F81 G82 M83 I84 Y85 P86

GLY SER PRO SER THR PHE GLU GLU PRO GLN GLN PRO GLN GLN ARG GLY GLN GLN SER SER ARG PRO GLN GLN ASP R110 K113 F117 R118 E119 G120 D121 V125 W131 W132 V142 S145 I146 I147 L152 D157 Q158 M159 P160 R161 R162 N168 Q171 E172 F173 L174 K175

Q178 GLU GLN GLY GLY HIS GLN SER GLN LYS GLY LYS HIS GLN GLU GLU GLU ASN GLU G198 G199 S200 I201 G204 L210 E211 H212 I220 A221 K222 E227 ASN GLU GLY GLU ASP K233 T238 V239 L243 I246 K247 P248 PRO THR ASP GLU GLN GLN GLN ARG

PRO GLN GLU GLU GLU GLU GLU GLU GLU GLU ASP GLU LYS PRO GLN CYS LYS GLY LYS ASP LYS HIS CYS GLN ARG PRO ARG GLY SER GLU GLN SER LYS SER ARG ARG ASN GLY ILE ASP GLU THR I297 C298 T299 M300 R301 L302 R303 H304 N305 I306 G307 Q308 T309 S310 S311 P312 S321 T324

A325 F330 P331 A332 L333 S334 W335 L336 R337 L338 S339 A340 E341 F342 G343 M350 F351 L357 I362 A365 L366 N367 L371 I372 Q373 V374 R381 V382 F383 Q388 E389 G390 R391 V392 V395 P396 Q397 N398 F399 V400 V401 Q406 S407 D408 E411 Y412 V413 N418

T425 L426 A429 N430 S431 L432 L433 N434 A435 L436 P437 E438 E439 V440 T444 F445 N446 L447 K448 S449 Q450 R453 Q454 I455 F463 L464 V465 E469 S470 GLN LYS ARG ALA VAL ALA

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	114.34Å 114.34Å 145.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.10 14.84 – 2.59	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-3.10) 76.0 (14.84-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.22 (at 2.58Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.193 , 0.253 0.193 , 0.244	Depositor DCC
R_{free} test set	2848 reflections (10.10%)	DCC
Wilson B-factor (Å^2)	30.9	Xtriage
Anisotropy	0.001	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 40.4	EDS
Estimated twinning fraction	0.038 for h,-k,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Outliers	0 of 43871 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	8649	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.72	0/2940	1.44	33/3982 (0.8%)
1	B	0.72	0/2940	1.42	30/3982 (0.8%)
1	C	0.74	0/2940	1.44	38/3982 (1.0%)
All	All	0.72	0/8820	1.43	101/11946 (0.8%)

There are no bond length outliers.

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	61	ARG	NE-CZ-NH2	-10.95	114.83	120.30
1	A	162	ARG	NE-CZ-NH2	-9.82	115.39	120.30
1	A	132	TRP	CD1-CG-CD2	9.22	113.67	106.30
1	B	335	TRP	CD1-CG-CD2	8.73	113.28	106.30
1	C	36	TRP	CD1-CG-CD2	8.54	113.13	106.30
1	C	301	ARG	NE-CZ-NH1	8.50	124.55	120.30
1	A	52	ARG	NE-CZ-NH1	8.48	124.54	120.30
1	B	132	TRP	CD1-CG-CD2	8.47	113.08	106.30
1	C	335	TRP	CD1-CG-CD2	8.46	113.07	106.30
1	A	335	TRP	CD1-CG-CD2	8.45	113.06	106.30
1	B	36	TRP	CD1-CG-CD2	8.41	113.03	106.30
1	B	162	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	A	131	TRP	CD1-CG-CD2	8.19	112.86	106.30
1	A	132	TRP	CE2-CD2-CG	-7.95	100.94	107.30
1	C	36	TRP	CE2-CD2-CG	-7.87	101.00	107.30
1	A	131	TRP	CE2-CD2-CG	-7.80	101.06	107.30
1	B	36	TRP	CE2-CD2-CG	-7.67	101.16	107.30
1	C	132	TRP	CD1-CG-CD2	7.66	112.42	106.30
1	C	132	TRP	CE2-CD2-CG	-7.59	101.23	107.30
1	C	162	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	C	335	TRP	CE2-CD2-CG	-7.46	101.33	107.30
1	C	131	TRP	CE2-CD2-CG	-7.44	101.35	107.30
1	B	301	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	B	381	ARG	NE-CZ-NH1	7.42	124.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	36	TRP	CE2-CD2-CG	-7.41	101.37	107.30
1	A	36	TRP	CD1-CG-CD2	7.40	112.22	106.30
1	B	131	TRP	CD1-CG-CD2	7.37	112.19	106.30
1	B	132	TRP	CE2-CD2-CG	-7.34	101.43	107.30
1	C	401	VAL	CB-CA-C	-7.33	97.47	111.40
1	A	335	TRP	CE2-CD2-CG	-7.28	101.47	107.30
1	C	131	TRP	CD1-CG-CD2	7.27	112.11	106.30
1	B	131	TRP	CE2-CD2-CG	-7.25	101.50	107.30
1	B	335	TRP	CE2-CD2-CG	-6.97	101.73	107.30
1	C	36	TRP	CG-CD2-CE3	6.90	140.11	133.90
1	A	61	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	C	36	TRP	CB-CG-CD1	-6.78	118.19	127.00
1	A	36	TRP	CB-CG-CD1	-6.67	118.33	127.00
1	C	60	LEU	CA-CB-CG	6.67	130.63	115.30
1	C	25	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	C	110	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	C	301	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	B	131	TRP	CG-CD2-CE3	6.31	139.58	133.90
1	B	408	ASP	O-C-N	-6.20	112.79	122.70
1	B	381	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	B	174	LEU	CA-CB-CG	6.18	129.51	115.30
1	A	36	TRP	CG-CD2-CE3	6.10	139.39	133.90
1	C	131	TRP	CG-CD2-CE3	6.09	139.38	133.90
1	A	14	ILE	CA-C-N	-6.09	103.81	117.20
1	A	131	TRP	CG-CD2-CE3	6.05	139.35	133.90
1	C	351	PHE	CA-CB-CG	6.01	128.33	113.90
1	A	301	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	C	61	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	C	381	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	C	62	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	A	302	LEU	CA-CB-CG	5.96	129.00	115.30
1	B	131	TRP	CB-CG-CD1	-5.92	119.30	127.00
1	A	132	TRP	CB-CG-CD1	-5.88	119.36	127.00
1	B	50	LEU	CA-CB-CG	5.86	128.78	115.30
1	B	118	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	132	TRP	CG-CD2-CE3	5.81	139.13	133.90
1	A	110	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	C	351	PHE	CB-CG-CD2	-5.77	116.76	120.80
1	A	132	TRP	CG-CD1-NE1	-5.76	104.33	110.10
1	B	401	VAL	CB-CA-C	-5.76	100.46	111.40
1	C	131	TRP	CB-CG-CD1	-5.72	119.56	127.00
1	A	413	VAL	CB-CA-C	-5.64	100.68	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	131	TRP	CB-CG-CD1	-5.62	119.70	127.00
1	C	132	TRP	CG-CD2-CE3	5.61	138.95	133.90
1	A	375	VAL	CG1-CB-CG2	-5.56	102.00	110.90
1	B	110	ARG	NE-CZ-NH1	5.55	123.08	120.30
1	A	351	PHE	CA-CB-CG	5.54	127.19	113.90
1	B	301	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	C	302	LEU	CA-CB-CG	5.50	127.96	115.30
1	B	302	LEU	CA-CB-CG	5.46	127.87	115.30
1	B	431	SER	N-CA-C	5.45	125.71	111.00
1	B	335	TRP	CG-CD1-NE1	-5.41	104.69	110.10
1	C	132	TRP	CB-CG-CD1	-5.38	120.00	127.00
1	B	303	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	C	36	TRP	CG-CD1-NE1	-5.37	104.73	110.10
1	A	335	TRP	CG-CD1-NE1	-5.36	104.74	110.10
1	B	413	VAL	CB-CA-C	-5.35	101.23	111.40
1	B	351	PHE	CA-CB-CG	5.34	126.71	113.90
1	B	36	TRP	CG-CD2-CE3	5.32	138.69	133.90
1	B	36	TRP	CG-CD1-NE1	-5.29	104.81	110.10
1	C	41	LYS	CB-CG-CD	-5.26	97.93	111.60
1	A	401	VAL	CB-CA-C	-5.24	101.44	111.40
1	C	337	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	C	110	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	C	300	MET	CG-SD-CE	-5.16	91.94	100.20
1	C	425	THR	CA-CB-CG2	5.16	119.63	112.40
1	A	57	ARG	NE-CZ-NH2	-5.15	117.72	120.30
1	A	60	LEU	CA-CB-CG	5.15	127.15	115.30
1	B	36	TRP	CB-CG-CD1	-5.15	120.31	127.00
1	A	404	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	115	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	A	134	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	C	175	LYS	CA-CB-CG	5.12	124.66	113.40
1	C	118	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	C	335	TRP	CG-CD1-NE1	-5.06	105.04	110.10
1	C	74	ILE	CG1-CB-CG2	-5.02	100.36	111.40
1	C	413	VAL	CB-CA-C	-5.00	101.90	111.40

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	A	2883	0	2845	76	0
1	B	2883	0	2845	99	0
1	C	2883	0	2845	70	0
All	All	8649	0	8535	205	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 12.

All (205) 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:C:33:ILE:HG21	1:C:172:GLU:HG2	1.54	0.90
1:B:65:TYR:HE1	1:C:398:ASN:HB3	1.46	0.79
1:A:168:ASN:HA	1:A:199:GLY:HA2	1.66	0.77
1:A:398:ASN:HB3	1:C:65:TYR:HE1	1.50	0.76
1:B:206:THR:HB	1:C:373:GLN:HE22	1.51	0.74
1:B:25:ARG:HG2	1:B:32:LEU:HD11	1.70	0.73
1:C:395:VAL:HG11	1:C:401:VAL:HG22	1.72	0.71
1:A:65:TYR:HE1	1:B:398:ASN:HB3	1.55	0.71
1:B:116:ASN:HD21	1:B:247:LYS:HA	1.58	0.68
1:A:33:ILE:HG21	1:A:172:GLU:HG2	1.74	0.68
1:A:112:GLN:HB2	1:B:435:ALA:HB1	1.75	0.67
1:B:75:GLN:HG3	1:B:366:LEU:HD22	1.76	0.67
1:A:341:GLU:HB3	1:A:414:SER:HB3	1.76	0.67
1:B:66:THR:HG22	1:B:161:ARG:O	1.94	0.67
1:A:233:LYS:HB2	1:A:237:VAL:HG22	1.76	0.66
1:B:324:THR:HG22	1:B:341:GLU:HG3	1.78	0.66
1:C:447:LEU:HD11	1:C:455:ILE:HD12	1.78	0.66
1:B:81:PHE:CE1	1:B:115:TYR:HB2	2.30	0.65
1:C:168:ASN:HA	1:C:199:GLY:HA2	1.77	0.65
1:B:246:ILE:HG23	1:B:248:PRO:HD3	1.79	0.65
1:A:75:GLN:HG3	1:A:366:LEU:HD22	1.79	0.64
1:B:239:VAL:HG11	1:B:243:LEU:HD12	1.79	0.64
1:B:118:ARG:NH2	1:B:309:THR:HG21	2.13	0.64
1:B:425:THR:HG21	1:B:430:ASN:ND2	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:118:ARG:HH22	1:B:309:THR:HG21	1.63	0.63
1:B:374:VAL:HG13	1:B:383:PHE:HB3	1.82	0.62
1:B:33:ILE:HG21	1:B:172:GLU:HG2	1.81	0.61
1:C:75:GLN:HG3	1:C:366:LEU:HD22	1.84	0.60
1:C:306:ILE:HG21	1:C:325:ALA:HB2	1.84	0.60
1:C:66:THR:HG23	1:C:161:ARG:O	2.02	0.60
1:B:437:PRO:HB2	1:B:440:VAL:HG13	1.84	0.59
1:A:74:ILE:HG22	1:A:119:GLU:HA	1.84	0.59
1:B:353:PRO:HA	1:B:401:VAL:O	2.02	0.59
1:B:438:GLU:O	1:B:441:ILE:HG22	2.03	0.58
1:B:302:LEU:H	1:B:302:LEU:HD22	1.69	0.58
1:B:63:PRO:HG3	1:B:132:TRP:HB3	1.85	0.58
1:A:373:GLN:HG2	1:A:381:ARG:HD2	1.86	0.57
1:B:333:LEU:HG	1:B:338:LEU:O	2.04	0.57
1:C:239:VAL:HG21	1:C:243:LEU:HD13	1.87	0.56
1:A:449:SER:O	1:A:453:ARG:HG3	2.05	0.56
1:A:395:VAL:HG11	1:A:401:VAL:HG22	1.87	0.56
1:B:316:ASN:HB3	1:B:319:ALA:HB3	1.88	0.55
1:A:206:THR:HG23	1:A:208:GLU:HG2	1.87	0.55
1:C:333:LEU:HG	1:C:338:LEU:O	2.07	0.55
1:A:440:VAL:O	1:A:444:THR:HG23	2.06	0.55
1:A:216:VAL:HG12	1:B:458:ASN:ND2	2.21	0.55
1:A:306:ILE:HG21	1:A:325:ALA:HB2	1.88	0.54
1:B:25:ARG:HG3	1:B:34:GLU:HG2	1.89	0.54
1:B:77:GLY:HA3	1:B:141:VAL:HG22	1.89	0.54
1:C:54:THR:HB	1:C:142:VAL:HG22	1.89	0.54
1:B:147:ILE:HD11	1:B:162:ARG:NH2	2.23	0.54
1:B:425:THR:HG21	1:B:430:ASN:CG	2.28	0.53
1:A:455:ILE:HG13	1:C:220:ILE:HD11	1.90	0.53
1:A:215:SER:HB3	1:B:459:ASN:HB2	1.91	0.53
1:B:425:THR:HG23	1:B:431:SER:HA	1.91	0.52
1:A:81:PHE:HE2	1:A:83:MET:SD	2.32	0.52
1:A:81:PHE:CE1	1:A:115:TYR:HB2	2.44	0.52
1:C:433:LEU:HA	1:C:436:LEU:HD12	1.91	0.52
1:C:343:GLY:O	1:C:411:GLU:HA	2.10	0.52
1:A:430:ASN:ND2	1:A:462:LYS:HE2	2.25	0.51
1:B:54:THR:HA	1:B:141:VAL:O	2.10	0.51
1:B:28:SER:HB3	1:B:236:ILE:HB	1.93	0.51
1:A:243:LEU:HD21	1:B:440:VAL:HG12	1.91	0.51
1:C:30:GLY:HA3	1:C:238:THR:HG23	1.91	0.51
1:C:85:TYR:CZ	1:C:297:ILE:HG12	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:85:TYR:CZ	1:A:297:ILE:HG12	2.46	0.51
1:A:302:LEU:H	1:A:302:LEU:HD22	1.76	0.51
1:A:367:ASN:HA	1:A:389:GLU:HG2	1.93	0.51
1:B:233:LYS:HB2	1:B:237:VAL:CG2	2.40	0.50
1:B:201:ILE:HD12	1:C:400:VAL:HG21	1.93	0.50
1:B:233:LYS:HB2	1:B:237:VAL:HG22	1.93	0.50
1:B:343:GLY:O	1:B:411:GLU:HA	2.12	0.50
1:B:27:GLU:HG3	1:B:32:LEU:HD13	1.94	0.49
1:A:223:ASN:HB3	1:B:447:LEU:HD21	1.94	0.49
1:C:449:SER:O	1:C:453:ARG:HG3	2.12	0.49
1:C:324:THR:HG22	1:C:341:GLU:HG3	1.95	0.48
1:A:444:THR:HG21	1:C:63:PRO:HD3	1.95	0.48
1:A:374:VAL:HG13	1:A:383:PHE:HB3	1.95	0.48
1:B:74:ILE:HG22	1:B:119:GLU:HA	1.94	0.48
1:A:206:THR:HB	1:B:373:GLN:HE22	1.77	0.48
1:A:204:GLY:O	1:B:381:ARG:HD3	2.13	0.48
1:A:216:VAL:HG12	1:B:458:ASN:HD22	1.79	0.48
1:A:306:ILE:CG2	1:A:325:ALA:HB2	2.43	0.48
1:C:367:ASN:HA	1:C:389:GLU:HG2	1.95	0.48
1:A:330:PHE:CD2	1:A:333:LEU:HD22	2.48	0.48
1:C:121:ASP:HA	1:C:305:ASN:HA	1.95	0.48
1:B:30:GLY:HA3	1:B:238:THR:HG23	1.95	0.48
1:A:233:LYS:HE2	1:A:237:VAL:HG13	1.96	0.48
1:B:203:SER:HB3	1:B:226:GLY:HA3	1.95	0.48
1:C:76:GLN:HA	1:C:119:GLU:HB3	1.96	0.48
1:A:322:VAL:HG21	1:A:463:PHE:CE2	2.49	0.48
1:A:171:GLN:HE21	1:A:173:PHE:HB2	1.80	0.47
1:B:63:PRO:HD3	1:C:444:THR:HG21	1.96	0.47
1:C:365:ALA:HB3	1:C:388:GLN:O	2.14	0.47
1:B:81:PHE:HE2	1:B:83:MET:SD	2.37	0.47
1:C:339:SER:HB2	1:C:418:ASN:O	2.14	0.47
1:A:239:VAL:HG13	1:B:443:HIS:CE1	2.49	0.47
1:C:371:LEU:HB2	1:C:406:GLN:NE2	2.29	0.47
1:B:433:LEU:HA	1:B:436:LEU:HD12	1.97	0.47
1:B:20:LEU:HB2	1:B:392:VAL:HG12	1.97	0.47
1:C:302:LEU:HD22	1:C:302:LEU:H	1.80	0.47
1:A:65:TYR:CE1	1:B:398:ASN:HB3	2.42	0.47
1:A:14:ILE:HG21	1:A:17:LEU:CD2	2.45	0.47
1:C:343:GLY:HA3	1:C:412:TYR:CE1	2.50	0.46
1:C:374:VAL:CG1	1:C:383:PHE:HB3	2.46	0.46
1:A:360:ASN:O	1:A:416:LYS:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:435:ALA:HB3	1:C:84:ILE:HG23	1.98	0.46
1:A:164:TYR:O	1:A:200:SER:HB2	2.16	0.46
1:A:63:PRO:HD3	1:B:444:THR:HG21	1.97	0.46
1:B:64:SER:HB2	1:B:162:ARG:HG2	1.98	0.46
1:B:373:GLN:HA	1:B:383:PHE:O	2.16	0.46
1:A:358:ASN:OD1	1:A:421:PRO:HA	2.15	0.46
1:B:440:VAL:O	1:B:444:THR:HG23	2.16	0.45
1:C:396:PRO:HD2	1:C:399:PHE:CD2	2.51	0.45
1:A:76:GLN:HA	1:A:119:GLU:HG2	1.98	0.45
1:A:110:ARG:HH12	1:B:438:GLU:H	1.62	0.45
1:A:30:GLY:HA3	1:A:238:THR:HG23	1.98	0.45
1:A:333:LEU:HD12	1:A:336:LEU:HD12	1.98	0.45
1:B:85:TYR:CZ	1:B:297:ILE:HG12	2.52	0.45
1:C:301:ARG:NH2	1:C:304:HIS:ND1	2.65	0.45
1:B:62:ARG:HG2	1:C:444:THR:HG22	1.98	0.45
1:A:381:ARG:HD3	1:C:204:GLY:O	2.17	0.45
1:B:35:THR:HG22	1:B:51:SER:HB2	1.98	0.45
1:B:201:ILE:CD1	1:C:426:LEU:HD21	2.47	0.45
1:A:80:ILE:HG22	1:A:116:ASN:HD22	1.81	0.45
1:B:369:ARG:HE	1:B:406:GLN:NE2	2.15	0.45
1:A:333:LEU:HG	1:A:338:LEU:O	2.17	0.45
1:B:202:LEU:HA	1:B:202:LEU:HD12	1.81	0.45
1:B:76:GLN:O	1:B:141:VAL:HA	2.15	0.44
1:C:333:LEU:HD12	1:C:336:LEU:HD12	1.99	0.44
1:B:367:ASN:HA	1:B:389:GLU:HG2	1.99	0.44
1:A:85:TYR:HA	1:A:86:PRO:HD2	1.84	0.44
1:C:48:VAL:HG21	1:C:362:ILE:HG12	2.00	0.44
1:A:13:GLN:HE21	1:C:159:MET:HG3	1.82	0.43
1:A:433:LEU:O	1:A:441:ILE:HD11	2.18	0.43
1:A:430:ASN:HD21	1:A:462:LYS:HE2	1.83	0.43
1:B:53:CYS:SG	1:B:61:ARG:NH2	2.86	0.43
1:C:81:PHE:CZ	1:C:83:MET:SD	3.11	0.43
1:A:11:GLU:HG3	1:C:157:ASP:HB3	2.00	0.43
1:B:32:LEU:HB3	1:B:54:THR:HG23	2.00	0.43
1:A:456:LYS:NZ	1:C:110:ARG:NH2	2.67	0.43
1:B:159:MET:HE3	1:B:160:PRO:O	2.19	0.43
1:C:246:ILE:O	1:C:248:PRO:HD3	2.19	0.43
1:A:24:ASN:O	1:A:34:GLU:HA	2.18	0.43
1:B:33:ILE:HG21	1:B:172:GLU:CG	2.47	0.43
1:C:69:PRO:HB3	1:C:336:LEU:HD22	2.01	0.43
1:A:216:VAL:HG11	1:A:220:ILE:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:THR:HB	1:C:373:GLN:NE2	2.28	0.43
1:A:84:ILE:HG21	1:B:432:LEU:HA	2.01	0.43
1:C:70:GLN:HB3	1:C:125:VAL:HB	2.01	0.43
1:C:72:ILE:HG23	1:C:145:SER:HB3	2.00	0.43
1:B:374:VAL:CG1	1:B:383:PHE:HB3	2.48	0.42
1:C:171:GLN:HE21	1:C:173:PHE:HB2	1.84	0.42
1:B:395:VAL:HG21	1:B:401:VAL:HG11	2.00	0.42
1:C:330:PHE:O	1:C:333:LEU:HB2	2.19	0.42
1:A:452:ALA:O	1:A:456:LYS:HG3	2.19	0.42
1:A:40:ASN:HB3	1:A:42:PRO:HD2	2.01	0.42
1:B:86:PRO:HG2	1:C:357:LEU:HD11	2.00	0.42
1:B:76:GLN:HA	1:B:119:GLU:HB3	2.01	0.42
1:A:400:VAL:HG21	1:C:201:ILE:HB	2.01	0.42
1:B:80:ILE:HG22	1:B:116:ASN:ND2	2.35	0.42
1:C:66:THR:HG21	1:C:147:ILE:HD13	2.02	0.42
1:C:24:ASN:HB3	1:C:35:THR:OG1	2.20	0.42
1:A:66:THR:HG21	1:A:147:ILE:HD13	2.02	0.42
1:B:214:PHE:CD2	1:B:224:LEU:HD21	2.54	0.42
1:B:206:THR:HG22	1:B:209:PHE:H	1.84	0.42
1:B:24:ASN:HB3	1:B:35:THR:OG1	2.20	0.42
1:B:327:SER:HB3	1:B:419:ASP:HB2	2.01	0.42
1:A:26:ILE:HD11	1:A:172:GLU:HA	2.01	0.42
1:B:441:ILE:HD13	1:B:441:ILE:HG21	1.85	0.42
1:A:13:GLN:NE2	1:C:159:MET:HG3	2.35	0.42
1:B:156:LEU:HA	1:C:12:CYS:SG	2.60	0.42
1:C:350:MET:HB3	1:C:465:VAL:HG13	2.02	0.42
1:A:202:LEU:HD12	1:A:202:LEU:HA	1.77	0.42
1:B:68:GLY:N	1:B:127:THR:HG23	2.34	0.42
1:A:48:VAL:HG21	1:A:362:ILE:HG12	2.01	0.42
1:C:32:LEU:HB3	1:C:54:THR:HG23	2.02	0.42
1:B:168:ASN:HA	1:B:199:GLY:HA2	2.01	0.42
1:B:57:ARG:HG2	1:B:58:ASN:OD1	2.20	0.42
1:B:110:ARG:HH12	1:C:438:GLU:H	1.68	0.42
1:A:84:ILE:HD11	1:B:436:LEU:HD21	2.01	0.41
1:B:207:LEU:O	1:B:211:GLU:HG3	2.19	0.41
1:A:440:VAL:HG12	1:C:243:LEU:HD21	2.02	0.41
1:B:201:ILE:HD11	1:C:426:LEU:HD21	2.01	0.41
1:A:313:ASP:HB2	1:A:322:VAL:O	2.20	0.41
1:B:70:GLN:HE22	1:B:162:ARG:HH22	1.67	0.41
1:B:463:PHE:HD2	1:B:464:LEU:HD13	1.86	0.41
1:C:74:ILE:HG12	1:C:117:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:166:ALA:HB2	1:C:445:PHE:CE1	2.55	0.41
1:B:426:LEU:HD13	1:B:432:LEU:HD22	2.03	0.41
1:C:437:PRO:HB2	1:C:440:VAL:HG22	2.02	0.41
1:A:25:ARG:HG2	1:A:32:LEU:HD11	2.02	0.41
1:B:63:PRO:HB2	1:B:165:LEU:HD22	2.03	0.41
1:A:118:ARG:HH11	1:A:303:ARG:NH2	2.19	0.41
1:B:163:PHE:CZ	1:C:398:ASN:HB2	2.56	0.41
1:B:463:PHE:CD2	1:B:464:LEU:HD13	2.56	0.41
1:C:300:MET:HE1	1:C:332:ALA:HA	2.02	0.41
1:B:35:THR:HG21	1:B:172:GLU:HB3	2.03	0.40
1:C:20:LEU:HB2	1:C:392:VAL:HG13	2.02	0.40
1:C:312:PRO:HB3	1:C:321:SER:HB2	2.03	0.40
1:A:72:ILE:HG23	1:A:145:SER:HB3	2.03	0.40
1:B:372:ILE:HG12	1:B:403:ALA:CB	2.52	0.40
1:B:11:GLU:HA	1:B:41:LYS:HE2	2.03	0.40
1:A:398:ASN:HB3	1:C:65:TYR:CE1	2.40	0.40
1:A:372:ILE:HG21	1:A:393:LEU:CD2	2.52	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	356/476 (75%)	331 (93%)	19 (5%)	6 (2%)	11	43
1	B	356/476 (75%)	324 (91%)	29 (8%)	3 (1%)	24	63
1	C	356/476 (75%)	326 (92%)	26 (7%)	4 (1%)	17	55
All	All	1068/1428 (75%)	981 (92%)	74 (7%)	13 (1%)	16	52

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	246	ILE
1	B	396	PRO
1	B	431	SER
1	A	397	GLN
1	C	397	GLN
1	A	463	PHE
1	B	156	LEU
1	C	429	ALA
1	C	463	PHE
1	A	418	ASN
1	A	307	GLY
1	A	396	PRO
1	C	246	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	A	315/414 (76%)	276 (88%)	39 (12%)	6	23
1	B	315/414 (76%)	278 (88%)	37 (12%)	7	26
1	C	315/414 (76%)	281 (89%)	34 (11%)	8	30
All	All	945/1242 (76%)	835 (88%)	110 (12%)	7	27

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	25	ARG
1	A	50	LEU
1	A	54	THR
1	A	55	LEU
1	A	66	THR
1	A	81	PHE
1	A	110	ARG
1	A	118	ARG
1	A	139	THR

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Mol	Chain	Res	Type
1	A	150	ASN
1	A	152	LEU
1	A	171	GLN
1	A	175	LYS
1	A	202	LEU
1	A	206	THR
1	A	207	LEU
1	A	208	GLU
1	A	210	LEU
1	A	212	HIS
1	A	215	SER
1	A	220	ILE
1	A	223	ASN
1	A	225	GLN
1	A	233	LYS
1	A	238	THR
1	A	302	LEU
1	A	308	GLN
1	A	328	LEU
1	A	333	LEU
1	A	351	PHE
1	A	374	VAL
1	A	391	ARG
1	A	401	VAL
1	A	408	ASP
1	A	413	VAL
1	A	450	GLN
1	A	464	LEU
1	A	467	PRO
1	B	18	ASN
1	B	27	GLU
1	B	28	SER
1	B	40	ASN
1	B	50	LEU
1	B	54	THR
1	B	60	LEU
1	B	67	ASN
1	B	81	PHE
1	B	110	ARG
1	B	113	LYS
1	B	118	ARG
1	B	150	ASN

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Mol	Chain	Res	Type
1	B	158	GLN
1	B	171	GLN
1	B	202	LEU
1	B	209	PHE
1	B	210	LEU
1	B	215	SER
1	B	225	GLN
1	B	238	THR
1	B	247	LYS
1	B	299	THR
1	B	302	LEU
1	B	313	ASP
1	B	337	ARG
1	B	350	MET
1	B	361	SER
1	B	374	VAL
1	B	391	ARG
1	B	401	VAL
1	B	408	ASP
1	B	413	VAL
1	B	433	LEU
1	B	434	ASN
1	B	464	LEU
1	B	469	GLU
1	C	11	GLU
1	C	16	LYS
1	C	38	PRO
1	C	54	THR
1	C	55	LEU
1	C	81	PHE
1	C	110	ARG
1	C	113	LYS
1	C	152	LEU
1	C	171	GLN
1	C	174	LEU
1	C	175	LYS
1	C	210	LEU
1	C	212	HIS
1	C	220	ILE
1	C	222	LYS
1	C	233	LYS
1	C	238	THR

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Mol	Chain	Res	Type
1	C	302	LEU
1	C	308	GLN
1	C	311	SER
1	C	333	LEU
1	C	367	ASN
1	C	374	VAL
1	C	391	ARG
1	C	401	VAL
1	C	408	ASP
1	C	430	ASN
1	C	432	LEU
1	C	434	ASN
1	C	448	LYS
1	C	450	GLN
1	C	464	LEU
1	C	469	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	116	ASN
1	A	171	GLN
1	A	177	GLN
1	A	212	HIS
1	A	450	GLN
1	A	454	GLN
1	B	10	ASN
1	B	116	ASN
1	B	177	GLN
1	B	378	ASN
1	C	116	ASN
1	C	367	ASN
1	C	378	ASN
1	C	458	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 (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, 95th 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(Å²)	Q<0.9
1	A	366/476 (76%)	-0.75	5 (1%)	78	60	3, 15, 37, 47	0
1	B	366/476 (76%)	-0.63	6 (1%)	74	55	4, 19, 37, 50	0
1	C	366/476 (76%)	-0.73	3 (0%)	87	75	3, 15, 36, 47	0
All	All	1098/1428 (76%)	-0.70	14 (1%)	79	62	3, 16, 37, 50	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	248	PRO	3.8
1	A	470	SER	3.7
1	B	248	PRO	3.2
1	B	298	CYS	3.0
1	B	227	GLU	2.9
1	B	247	LYS	2.8
1	C	298	CYS	2.6
1	B	111	HIS	2.6
1	A	247	LYS	2.4
1	C	310	SER	2.4
1	A	299	THR	2.2
1	B	85	TYR	2.2
1	A	168	ASN	2.1
1	C	168	ASN	2.0

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.