Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:30 PM GMT

PDB ID	:	1FXZ
Title	:	CRYSTAL STRUCTURE OF SOYBEAN PROGLYCININ A1AB1B HOMOTRIMER
Authors	:	Adachi, M.; Takenaka, Y.; Gidamis, A.B.; Mikami, B.; Utsumi, S.
Deposited on	:	2000-09-28
Resolution	:	2.80 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

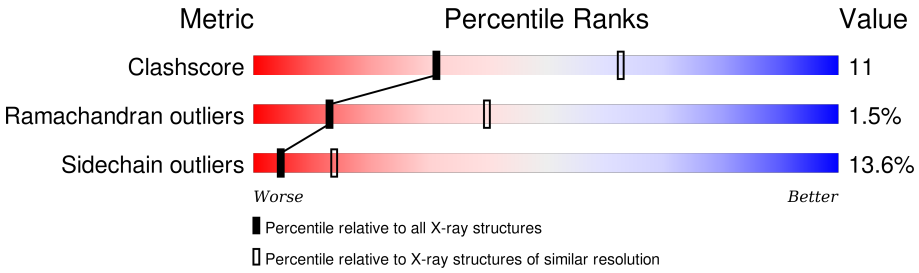
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	476	48% 25% • 22%
1	B	476	47% 24% 5% • 22%
1	C	476	51% 23% • 22%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8773 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	371	Total	C	N	O	S	0	0	0
			2913	1838	515	548	12			
1	B	371	Total	C	N	O	S	0	0	0
			2913	1838	515	548	12			
1	C	371	Total	C	N	O	S	0	0	0
			2913	1838	515	548	12			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	16	Total	O	0	0
			16	16		
2	B	6	Total	O	0	0
			6	6		
2	C	12	Total	O	0	0
			12	12		

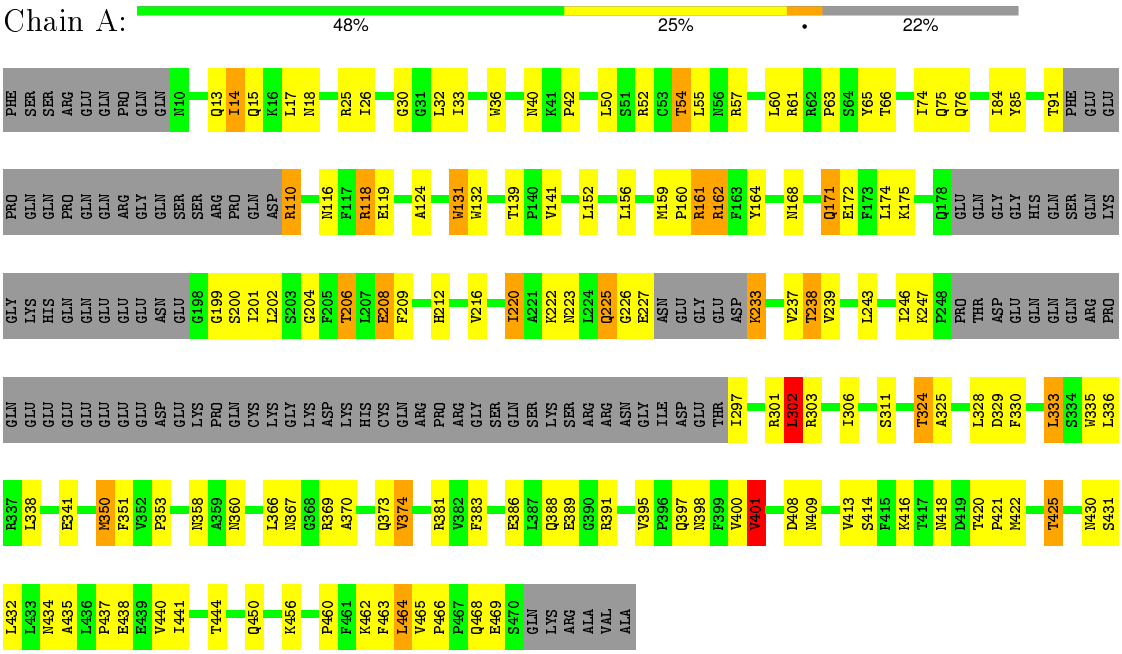
3 Residue-property plots (i)

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

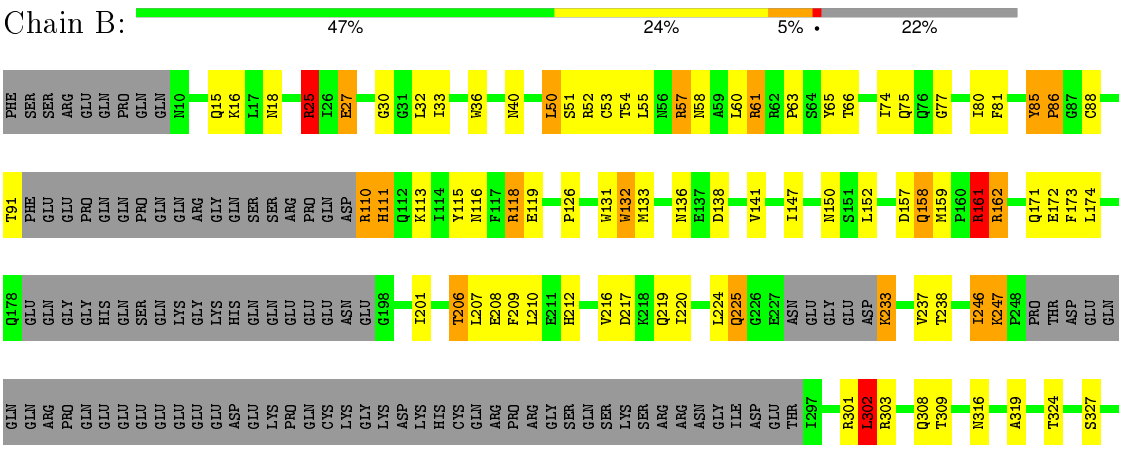
- Molecule 1: GLYCININ G1

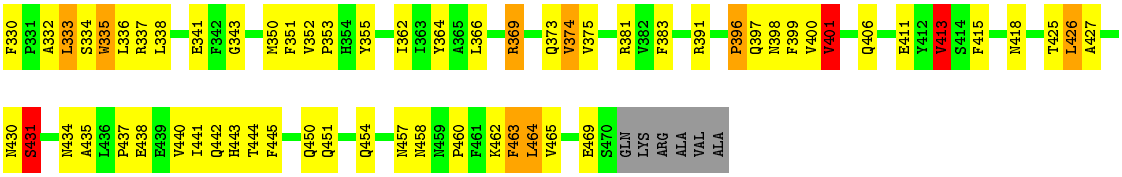
Chain A:



- Molecule 1: GLYCININ G1

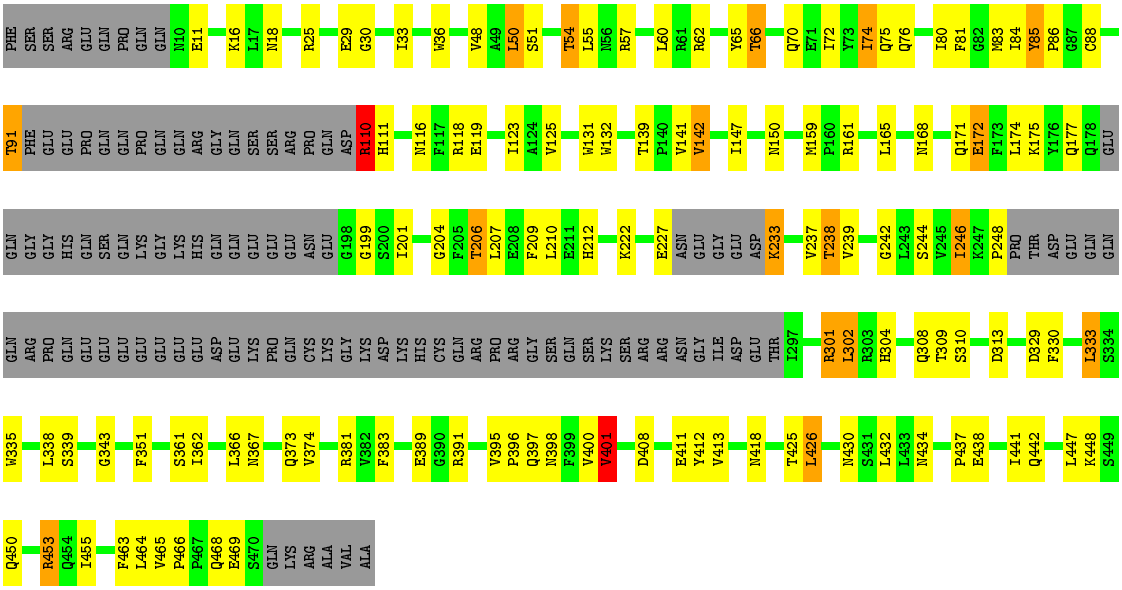
Chain B:





- Molecule 1: GLYCININ G1

Chain C:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α, β, γ	115.52Å 115.52Å 147.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.199 , 0.250	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8773	wwPDB-VP
Average B, all atoms (Å^2)	22.0	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	0.68	0/2971	1.37	32/4025 (0.8%)
1	B	0.68	0/2971	1.38	34/4025 (0.8%)
1	C	0.71	0/2971	1.40	34/4025 (0.8%)
All	All	0.69	0/8913	1.38	100/12075 (0.8%)

There are no bond length outliers.

All (100) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	61	ARG	NE-CZ-NH2	-9.69	115.45	120.30
1	A	61	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	C	132	TRP	CD1-CG-CD2	8.63	113.21	106.30
1	B	132	TRP	CD1-CG-CD2	8.62	113.20	106.30
1	B	301	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	C	118	ARG	NE-CZ-NH2	-8.37	116.12	120.30
1	B	335	TRP	CD1-CG-CD2	8.30	112.94	106.30
1	B	36	TRP	CD1-CG-CD2	8.28	112.92	106.30
1	C	335	TRP	CD1-CG-CD2	8.27	112.92	106.30
1	A	132	TRP	CD1-CG-CD2	8.22	112.87	106.30
1	A	162	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	A	335	TRP	CD1-CG-CD2	8.01	112.71	106.30
1	B	36	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	A	131	TRP	CD1-CG-CD2	7.83	112.56	106.30
1	C	36	TRP	CD1-CG-CD2	7.74	112.49	106.30
1	C	131	TRP	CD1-CG-CD2	7.67	112.43	106.30
1	A	132	TRP	CE2-CD2-CG	-7.60	101.22	107.30
1	C	132	TRP	CE2-CD2-CG	-7.58	101.24	107.30
1	C	36	TRP	CE2-CD2-CG	-7.57	101.24	107.30
1	A	335	TRP	CE2-CD2-CG	-7.43	101.36	107.30
1	A	131	TRP	CE2-CD2-CG	-7.40	101.38	107.30
1	B	132	TRP	CE2-CD2-CG	-7.31	101.45	107.30
1	C	335	TRP	CE2-CD2-CG	-7.28	101.47	107.30
1	C	131	TRP	CE2-CD2-CG	-7.23	101.52	107.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	36	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	C	25	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	B	131	TRP	CD1-CG-CD2	6.79	111.73	106.30
1	C	401	VAL	CB-CA-C	-6.67	98.72	111.40
1	A	302	LEU	CA-CB-CG	6.60	130.47	115.30
1	B	335	TRP	CE2-CD2-CG	-6.60	102.02	107.30
1	A	36	TRP	CD1-CG-CD2	6.59	111.57	106.30
1	C	36	TRP	CG-CD2-CE3	6.52	139.77	133.90
1	C	453	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	B	131	TRP	CE2-CD2-CG	-6.51	102.09	107.30
1	B	162	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	85	TYR	CB-CG-CD2	-6.46	117.13	121.00
1	C	60	LEU	CA-CB-CG	6.29	129.78	115.30
1	B	303	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	52	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	36	TRP	CB-CG-CD1	-6.25	118.88	127.00
1	B	57	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	C	110	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	C	36	TRP	CB-CG-CD1	-6.10	119.07	127.00
1	B	36	TRP	CG-CD2-CE3	6.08	139.37	133.90
1	A	60	LEU	CA-CB-CG	6.08	129.28	115.30
1	A	162	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	A	36	TRP	CG-CD2-CE3	5.99	139.29	133.90
1	B	174	LEU	CA-CB-CG	5.96	129.00	115.30
1	B	118	ARG	NE-CZ-NH2	-5.91	117.34	120.30
1	C	131	TRP	CG-CD2-CE3	5.91	139.21	133.90
1	A	413	VAL	CB-CA-C	-5.86	100.27	111.40
1	A	132	TRP	CG-CD2-CE3	5.84	139.16	133.90
1	C	57	ARG	NE-CZ-NH1	5.84	123.22	120.30
1	B	36	TRP	CB-CG-CD1	-5.84	119.41	127.00
1	C	132	TRP	CG-CD2-CE3	5.73	139.05	133.90
1	C	381	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	301	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	453	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	B	57	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	A	132	TRP	CB-CG-CD1	-5.58	119.74	127.00
1	A	14	ILE	CA-C-N	-5.53	105.03	117.20
1	A	351	PHE	CB-CG-CD2	-5.53	116.93	120.80
1	A	131	TRP	CG-CD2-CE3	5.51	138.86	133.90
1	C	132	TRP	CB-CG-CD1	-5.51	119.84	127.00
1	B	85	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	C	85	TYR	CB-CG-CD2	-5.50	117.70	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	132	TRP	CG-CD1-NE1	-5.47	104.63	110.10
1	C	425	THR	CA-CB-CG2	5.39	119.94	112.40
1	A	174	LEU	CA-CB-CG	5.37	127.66	115.30
1	B	401	VAL	CB-CA-C	-5.36	101.21	111.40
1	B	431	SER	N-CA-C	5.33	125.40	111.00
1	B	351	PHE	CA-CB-CG	5.33	126.69	113.90
1	B	61	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	C	131	TRP	CB-CG-CD1	-5.30	120.11	127.00
1	B	413	VAL	CB-CA-C	-5.30	101.33	111.40
1	C	62	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	57	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	401	VAL	CB-CA-C	-5.28	101.37	111.40
1	A	131	TRP	CB-CG-CD1	-5.27	120.15	127.00
1	B	335	TRP	CG-CD1-NE1	-5.27	104.83	110.10
1	C	413	VAL	CB-CA-C	-5.24	101.44	111.40
1	A	397	GLN	CA-C-N	5.20	128.65	117.20
1	B	161	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	C	74	ILE	CG1-CB-CG2	-5.18	99.99	111.40
1	B	25	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	B	36	TRP	CG-CD1-NE1	-5.17	104.93	110.10
1	C	301	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	B	302	LEU	CA-CB-CG	5.16	127.16	115.30
1	B	457	ASN	N-CA-C	5.14	124.89	111.00
1	B	131	TRP	CG-CD2-CE3	5.12	138.50	133.90
1	C	142	VAL	N-CA-C	-5.11	97.21	111.00
1	C	351	PHE	CA-CB-CG	5.11	126.15	113.90
1	B	50	LEU	CA-CB-CG	5.10	127.03	115.30
1	B	369	ARG	CB-CG-CD	-5.07	98.42	111.60
1	C	62	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	A	369	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	C	302	LEU	CA-CB-CG	5.03	126.88	115.30
1	B	52	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	B	301	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	A	335	TRP	CG-CD1-NE1	-5.02	105.08	110.10

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	2913	0	2870	79	0
1	B	2913	0	2870	82	0
1	C	2913	0	2870	64	0
2	A	16	0	0	1	0
2	B	6	0	0	0	0
2	C	12	0	0	0	0
All	All	8773	0	8610	188	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 11.

All (188) 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:33:ILE:HG21	1:A:172:GLU:HG2	1.63	0.81
1:B:65:TYR:HE1	1:C:398:ASN:HB3	1.47	0.80
1:A:65:TYR:HE1	1:B:398:ASN:HB3	1.49	0.78
1:A:398:ASN:HB3	1:C:65:TYR:HE1	1.54	0.72
1:A:168:ASN:HA	1:A:199:GLY:HA2	1.73	0.70
1:A:75:GLN:HG3	1:A:366:LEU:HD22	1.74	0.70
1:A:425:THR:HG22	1:A:431:SER:HA	1.74	0.70
1:A:14:ILE:HG21	1:A:17:LEU:HD23	1.76	0.67
1:A:66:THR:HG22	1:A:161:ARG:O	1.94	0.67
1:A:373:GLN:HG2	1:A:381:ARG:HD2	1.75	0.66
1:A:110:ARG:HH12	1:B:438:GLU:H	1.43	0.66
1:A:438:GLU:HB2	1:C:110:ARG:NH2	2.10	0.66
1:B:33:ILE:HG21	1:B:172:GLU:HG2	1.76	0.66
1:B:66:THR:HG22	1:B:161:ARG:O	1.96	0.65
1:B:353:PRO:HA	1:B:401:VAL:O	1.96	0.65
1:C:33:ILE:HG21	1:C:172:GLU:HG2	1.79	0.64
1:A:395:VAL:HG11	1:A:401:VAL:HG22	1.80	0.64
1:B:333:LEU:HD12	1:B:336:LEU:HD12	1.82	0.61
1:A:438:GLU:HB2	1:C:110:ARG:HH22	1.65	0.61
1:B:333:LEU:HG	1:B:338:LEU:O	2.00	0.60
1:B:118:ARG:NH2	1:B:309:THR:HG21	2.15	0.60
1:A:381:ARG:HD3	1:C:204:GLY:O	2.02	0.60
1:A:302:LEU:H	1:A:302:LEU:HD22	1.67	0.60
1:C:374:VAL:CG1	1:C:383:PHE:HB3	2.32	0.58
1:B:324:THR:HG22	1:B:341:GLU:HG3	1.84	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:ARG:HG2	1:B:32:LEU:HD11	1.84	0.58
1:C:50:LEU:HD23	1:C:51:SER:H	1.69	0.57
1:B:75:GLN:HG3	1:B:366:LEU:HD22	1.86	0.57
1:C:333:LEU:HG	1:C:338:LEU:O	2.04	0.57
1:C:80:ILE:HG22	1:C:116:ASN:ND2	2.20	0.57
1:A:116:ASN:ND2	1:A:247:LYS:HG2	2.19	0.57
1:B:233:LYS:HB2	1:B:237:VAL:HG22	1.87	0.57
1:A:440:VAL:O	1:A:444:THR:HG23	2.05	0.57
1:B:350:MET:HG2	1:B:465:VAL:CG1	2.35	0.56
1:A:438:GLU:H	1:C:110:ARG:HH12	1.52	0.56
1:B:201:ILE:HD12	1:C:400:VAL:HG21	1.87	0.56
1:B:63:PRO:HG3	1:B:132:TRP:HB3	1.86	0.56
1:B:425:THR:HG23	1:B:431:SER:HA	1.88	0.56
1:C:233:LYS:HB2	1:C:237:VAL:HG22	1.87	0.56
1:B:212:HIS:HE1	1:C:466:PRO:O	1.89	0.56
1:A:373:GLN:HE22	1:C:206:THR:HB	1.71	0.56
1:A:243:LEU:HD21	1:B:440:VAL:HG12	1.87	0.55
1:B:118:ARG:HH22	1:B:309:THR:HG21	1.70	0.55
1:B:15:GLN:HG3	1:B:16:LYS:H	1.70	0.55
1:B:206:THR:HB	1:C:373:GLN:HE22	1.72	0.55
1:A:156:LEU:HD21	1:B:397:GLN:H	1.70	0.55
1:C:395:VAL:HG11	1:C:401:VAL:HG22	1.88	0.55
1:A:84:ILE:HG23	1:B:435:ALA:HB3	1.88	0.55
1:A:40:ASN:HB3	1:A:42:PRO:HD2	1.89	0.54
1:B:53:CYS:SG	1:B:61:ARG:NH2	2.79	0.54
1:A:118:ARG:HH11	1:A:303:ARG:HH22	1.54	0.54
1:A:110:ARG:NH2	1:B:438:GLU:HB2	2.22	0.54
1:A:435:ALA:HB3	1:C:84:ILE:HG23	1.90	0.54
1:A:437:PRO:HB2	1:A:440:VAL:HG13	1.89	0.53
1:A:425:THR:HG21	2:A:487:HOH:O	2.08	0.53
1:B:369:ARG:HE	1:B:406:GLN:NE2	2.07	0.53
1:A:233:LYS:HE2	1:A:237:VAL:HG13	1.91	0.53
1:A:74:ILE:HG22	1:A:119:GLU:HA	1.90	0.53
1:A:63:PRO:HD3	1:B:444:THR:HG21	1.91	0.53
1:C:66:THR:HG23	1:C:161:ARG:O	2.09	0.52
1:C:54:THR:HB	1:C:142:VAL:HG22	1.90	0.52
1:B:343:GLY:O	1:B:411:GLU:HA	2.09	0.52
1:B:27:GLU:HG3	1:B:32:LEU:HD13	1.91	0.52
1:C:367:ASN:HA	1:C:389:GLU:HG2	1.92	0.52
1:C:70:GLN:HB3	1:C:125:VAL:HB	1.92	0.52
1:C:330:PHE:CD2	1:C:333:LEU:HD22	2.44	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:201:ILE:HD11	1:C:426:LEU:HD21	1.92	0.52
1:B:55:LEU:HD11	1:B:133:MET:HG2	1.92	0.51
1:B:246:ILE:HG13	1:B:247:LYS:H	1.76	0.51
1:B:81:PHE:HZ	1:B:302:LEU:HD23	1.76	0.51
1:A:110:ARG:HH22	1:B:438:GLU:HB2	1.76	0.50
1:A:216:VAL:HG12	1:B:458:ASN:ND2	2.26	0.50
1:B:463:PHE:HD2	1:B:464:LEU:HD13	1.76	0.50
1:B:201:ILE:CD1	1:C:426:LEU:HD21	2.42	0.50
1:A:367:ASN:HA	1:A:389:GLU:HG2	1.94	0.50
1:A:456:LYS:HZ3	1:C:110:ARG:NH2	2.10	0.50
1:B:74:ILE:HG22	1:B:119:GLU:HA	1.93	0.49
1:A:456:LYS:NZ	1:C:110:ARG:NH2	2.60	0.49
1:C:80:ILE:HG22	1:C:116:ASN:HD22	1.77	0.49
1:B:441:ILE:HG13	1:B:445:PHE:CD2	2.47	0.49
1:B:374:VAL:CG1	1:B:383:PHE:HB3	2.41	0.49
1:A:76:GLN:HA	1:A:119:GLU:HG2	1.93	0.49
1:B:30:GLY:HA2	1:B:238:THR:HG23	1.95	0.49
1:B:330:PHE:CE2	1:B:333:LEU:HD13	2.48	0.48
1:B:147:ILE:HD11	1:B:162:ARG:NH2	2.29	0.48
1:B:440:VAL:O	1:B:444:THR:HG23	2.13	0.48
1:B:364:TYR:HB3	1:B:413:VAL:HG23	1.95	0.48
1:C:339:SER:HB2	1:C:418:ASN:O	2.13	0.48
1:C:50:LEU:HD23	1:C:51:SER:N	2.27	0.48
1:C:246:ILE:O	1:C:248:PRO:HD3	2.14	0.48
1:A:63:PRO:HA	1:A:131:TRP:O	2.13	0.48
1:C:447:LEU:HD11	1:C:455:ILE:HD12	1.94	0.48
1:C:81:PHE:HE2	1:C:83:MET:SD	2.37	0.48
1:C:33:ILE:HG21	1:C:172:GLU:CG	2.42	0.48
1:A:360:ASN:O	1:A:416:LYS:HA	2.13	0.48
1:C:91:THR:HG23	1:C:111:HIS:O	2.14	0.48
1:A:370:ALA:O	1:A:386:GLU:HA	2.14	0.47
1:A:330:PHE:CD2	1:A:333:LEU:HD22	2.49	0.47
1:C:343:GLY:HA3	1:C:412:TYR:CE1	2.48	0.47
1:B:171:GLN:HE21	1:B:173:PHE:HB2	1.79	0.47
1:A:341:GLU:HB3	1:A:414:SER:HB3	1.96	0.47
1:B:430:ASN:ND2	1:B:462:LYS:HE2	2.29	0.47
1:A:463:PHE:CD2	1:A:464:LEU:HD13	2.49	0.47
1:A:225:GLN:HE21	1:A:227:GLU:HG2	1.79	0.47
1:B:15:GLN:HG3	1:B:16:LYS:N	2.30	0.47
1:A:118:ARG:HH11	1:A:303:ARG:NH2	2.12	0.47
1:C:30:GLY:HA3	1:C:238:THR:HG23	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:430:ASN:ND2	1:A:462:LYS:HE2	2.30	0.47
1:A:233:LYS:HB2	1:A:237:VAL:HG22	1.96	0.46
1:B:57:ARG:HD2	1:B:138:ASP:HA	1.97	0.46
1:A:400:VAL:HG21	1:C:201:ILE:HB	1.98	0.46
1:B:362:ILE:HB	1:B:415:PHE:HB2	1.97	0.46
1:B:30:GLY:CA	1:B:238:THR:HG23	2.45	0.46
1:A:353:PRO:HA	1:A:401:VAL:O	2.16	0.46
1:C:374:VAL:HB	1:C:401:VAL:HG13	1.97	0.46
1:A:422:MET:SD	1:C:85:TYR:OH	2.61	0.46
1:A:116:ASN:HD21	1:A:247:LYS:HG2	1.80	0.46
1:B:437:PRO:HB2	1:B:440:VAL:HG13	1.98	0.46
1:A:239:VAL:HG13	1:B:443:HIS:CE1	2.50	0.46
1:C:66:THR:HG21	1:C:147:ILE:HD13	1.98	0.45
1:A:216:VAL:HG11	1:A:220:ILE:HD11	1.98	0.45
1:C:85:TYR:HB3	1:C:88:CYS:SG	2.56	0.45
1:B:57:ARG:HG2	1:B:58:ASN:OD1	2.17	0.45
1:A:350:MET:HG2	1:A:465:VAL:CG1	2.46	0.45
1:A:201:ILE:HD12	1:B:426:LEU:HD21	1.98	0.45
1:C:168:ASN:HA	1:C:199:GLY:HA2	1.99	0.45
1:B:57:ARG:HG3	1:B:136:ASN:O	2.16	0.45
1:C:438:GLU:O	1:C:441:ILE:HG22	2.17	0.45
1:B:332:ALA:O	1:B:335:TRP:HB2	2.17	0.45
1:A:110:ARG:HH12	1:B:438:GLU:N	2.13	0.45
1:A:162:ARG:H	1:A:171:GLN:HG3	1.82	0.44
1:A:26:ILE:O	1:A:32:LEU:HD12	2.18	0.44
1:C:330:PHE:O	1:C:333:LEU:HB2	2.18	0.44
1:C:301:ARG:NH2	1:C:304:HIS:ND1	2.65	0.44
1:B:224:LEU:HD13	1:C:455:ILE:HD13	2.00	0.44
1:A:13:GLN:NE2	1:C:177:GLN:HG3	2.33	0.44
1:C:72:ILE:HB	1:C:123:ILE:HB	2.00	0.44
1:B:217:ASP:OD2	1:B:219:GLN:HB3	2.17	0.44
1:C:76:GLN:HA	1:C:119:GLU:HB3	2.00	0.43
1:B:374:VAL:HG12	1:B:383:PHE:HB3	2.01	0.43
1:A:330:PHE:HD2	1:A:333:LEU:HD22	1.83	0.43
1:B:157:ASP:OD1	1:B:159:MET:HB2	2.17	0.43
1:B:327:SER:HB2	1:B:334:SER:HB3	1.99	0.43
1:C:438:GLU:O	1:C:442:GLN:HG3	2.18	0.43
1:B:85:TYR:HB3	1:B:88:CYS:SG	2.59	0.43
1:A:206:THR:HG22	1:A:209:PHE:H	1.84	0.43
1:A:164:TYR:O	1:A:200:SER:HB2	2.19	0.43
1:B:80:ILE:HG22	1:B:116:ASN:HD22	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:ARG:HH22	1:C:438:GLU:HB2	1.83	0.43
1:B:91:THR:HG23	1:B:111:HIS:O	2.19	0.43
1:A:220:ILE:HG22	1:B:451:GLN:HE21	1.84	0.42
1:A:204:GLY:O	1:B:381:ARG:HD3	2.19	0.42
1:A:408:ASP:HA	1:A:409:ASN:HA	1.88	0.42
1:A:206:THR:HB	1:B:373:GLN:HE22	1.84	0.42
1:B:77:GLY:HA3	1:B:141:VAL:HG22	2.01	0.42
1:C:343:GLY:O	1:C:411:GLU:HA	2.19	0.42
1:A:324:THR:HG23	1:A:341:GLU:HG3	2.00	0.42
1:A:418:ASN:O	1:A:421:PRO:HG3	2.19	0.42
1:C:330:PHE:CE2	1:C:333:LEU:HD13	2.54	0.42
1:B:355:TYR:HB3	1:B:400:VAL:HG22	2.02	0.42
1:B:352:VAL:HG21	1:B:427:ALA:O	2.19	0.42
1:A:465:VAL:HA	1:A:466:PRO:HD3	1.76	0.42
1:A:206:THR:CG2	1:A:208:GLU:HG2	2.49	0.42
1:C:75:GLN:HG3	1:C:366:LEU:HD22	2.01	0.42
1:C:465:VAL:HA	1:C:466:PRO:HD3	1.85	0.41
1:A:54:THR:HA	1:A:141:VAL:O	2.19	0.41
1:B:396:PRO:HB2	1:B:399:PHE:CD1	2.55	0.41
1:B:111:HIS:CD2	1:C:437:PRO:HG3	2.54	0.41
1:C:29:GLU:HB2	1:C:233:LYS:HA	2.02	0.41
1:C:165:LEU:HD12	1:C:201:ILE:HD11	2.02	0.41
1:A:30:GLY:CA	1:A:238:THR:HG23	2.51	0.41
1:B:81:PHE:CE1	1:B:115:TYR:HB2	2.55	0.41
1:A:159:MET:SD	1:A:160:PRO:HD2	2.60	0.41
1:C:54:THR:HA	1:C:141:VAL:O	2.20	0.41
1:A:25:ARG:HD2	1:A:25:ARG:HH11	1.76	0.41
1:B:65:TYR:CE1	1:C:398:ASN:HB3	2.39	0.41
1:A:374:VAL:CG1	1:A:383:PHE:HB3	2.50	0.41
1:B:216:VAL:CG1	1:B:220:ILE:HD11	2.51	0.41
1:B:207:LEU:HD22	1:B:225:GLN:OE1	2.21	0.40
1:B:316:ASN:HB3	1:B:319:ALA:HB3	2.03	0.40
1:C:239:VAL:HG12	1:C:242:GLY:H	1.85	0.40
1:C:206:THR:HG22	1:C:209:PHE:H	1.86	0.40
1:A:306:ILE:HG21	1:A:325:ALA:HB2	2.04	0.40
1:A:333:LEU:HG	1:A:338:LEU:O	2.21	0.40
1:C:48:VAL:HG21	1:C:362:ILE:HG12	2.04	0.40
1:B:438:GLU:O	1:B:442:GLN:HG3	2.21	0.40
1:A:358:ASN:OD1	1:A:421:PRO:HA	2.20	0.40
1:A:124:ALA:HB1	1:A:336:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	361/476 (76%)	333 (92%)	26 (7%)	2 (1%)	30	65
1	B	361/476 (76%)	333 (92%)	21 (6%)	7 (2%)	10	32
1	C	361/476 (76%)	327 (91%)	27 (8%)	7 (2%)	10	32
All	All	1083/1428 (76%)	993 (92%)	74 (7%)	16 (2%)	13	40

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	396	PRO
1	B	431	SER
1	B	158	GLN
1	B	246	ILE
1	C	172	GLU
1	C	310	SER
1	C	397	GLN
1	A	226	GLY
1	A	246	ILE
1	B	86	PRO
1	C	396	PRO
1	C	246	ILE
1	B	418	ASN
1	B	463	PHE
1	C	463	PHE
1	C	86	PRO

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	319/414 (77%)	274 (86%)	45 (14%)	4	12
1	B	319/414 (77%)	279 (88%)	40 (12%)	6	17
1	C	319/414 (77%)	274 (86%)	45 (14%)	4	12
All	All	957/1242 (77%)	827 (86%)	130 (14%)	5	14

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	18	ASN
1	A	50	LEU
1	A	54	THR
1	A	55	LEU
1	A	91	THR
1	A	110	ARG
1	A	118	ARG
1	A	139	THR
1	A	152	LEU
1	A	161	ARG
1	A	171	GLN
1	A	175	LYS
1	A	202	LEU
1	A	206	THR
1	A	208	GLU
1	A	212	HIS
1	A	220	ILE
1	A	222	LYS
1	A	223	ASN
1	A	225	GLN
1	A	233	LYS
1	A	238	THR
1	A	297	ILE
1	A	302	LEU
1	A	311	SER
1	A	324	THR
1	A	328	LEU
1	A	329	ASP
1	A	333	LEU
1	A	350	MET
1	A	374	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	388	GLN
1	A	391	ARG
1	A	401	VAL
1	A	420	THR
1	A	425	THR
1	A	432	LEU
1	A	434	ASN
1	A	441	ILE
1	A	450	GLN
1	A	460	PRO
1	A	464	LEU
1	A	468	GLN
1	A	469	GLU
1	B	18	ASN
1	B	25	ARG
1	B	27	GLU
1	B	40	ASN
1	B	50	LEU
1	B	51	SER
1	B	54	THR
1	B	60	LEU
1	B	86	PRO
1	B	110	ARG
1	B	111	HIS
1	B	113	LYS
1	B	126	PRO
1	B	150	ASN
1	B	152	LEU
1	B	158	GLN
1	B	161	ARG
1	B	206	THR
1	B	208	GLU
1	B	209	PHE
1	B	210	LEU
1	B	225	GLN
1	B	233	LYS
1	B	247	LYS
1	B	302	LEU
1	B	308	GLN
1	B	333	LEU
1	B	337	ARG
1	B	374	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	375	VAL
1	B	391	ARG
1	B	401	VAL
1	B	413	VAL
1	B	426	LEU
1	B	434	ASN
1	B	450	GLN
1	B	454	GLN
1	B	460	PRO
1	B	464	LEU
1	B	469	GLU
1	C	11	GLU
1	C	16	LYS
1	C	18	ASN
1	C	50	LEU
1	C	54	THR
1	C	55	LEU
1	C	66	THR
1	C	74	ILE
1	C	91	THR
1	C	110	ARG
1	C	139	THR
1	C	150	ASN
1	C	159	MET
1	C	171	GLN
1	C	174	LEU
1	C	175	LYS
1	C	206	THR
1	C	207	LEU
1	C	210	LEU
1	C	212	HIS
1	C	222	LYS
1	C	227	GLU
1	C	233	LYS
1	C	238	THR
1	C	244	SER
1	C	302	LEU
1	C	308	GLN
1	C	309	THR
1	C	313	ASP
1	C	329	ASP
1	C	333	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	361	SER
1	C	391	ARG
1	C	401	VAL
1	C	408	ASP
1	C	426	LEU
1	C	430	ASN
1	C	432	LEU
1	C	434	ASN
1	C	448	LYS
1	C	450	GLN
1	C	453	ARG
1	C	464	LEU
1	C	468	GLN
1	C	469	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	56	ASN
1	A	58	ASN
1	A	116	ASN
1	A	171	GLN
1	A	177	GLN
1	A	223	ASN
1	A	225	GLN
1	A	378	ASN
1	A	450	GLN
1	A	454	GLN
1	A	468	GLN
1	B	116	ASN
1	B	171	GLN
1	B	212	HIS
1	B	348	ASN
1	B	367	ASN
1	B	378	ASN
1	B	443	HIS
1	B	446	ASN
1	B	451	GLN
1	C	39	ASN
1	C	116	ASN
1	C	171	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	177	GLN
1	C	178	GLN
1	C	212	HIS
1	C	367	ASN
1	C	378	ASN
1	C	454	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

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.