Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 10:11 PM GMT

PDB ID	:	1SJI
Title	:	Comparing skeletal and cardiac calsequestrin structures and their calcium binding: a proposed mechanism for coupled calcium binding and protein polymerization
Authors	:	Park, H.J.; Park, I.Y.; Kim, E.J.; Youn, B.; Fields, K.; Dunker, A.K.; Kang, C.H.
Deposited on	:	2004-03-03
Resolution	:	2.40 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:

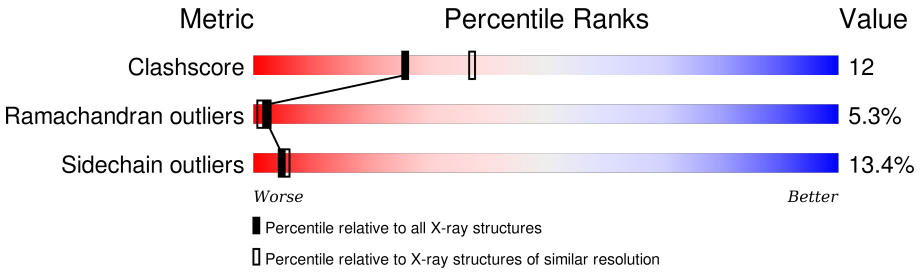
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.40 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	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)

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	350	53% 34% 12%
1	B	350	63% 26% 8%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5792 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 Calsequestrin, cardiac muscle isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2877	1865	443	563	6			
1	B	350	Total	C	N	O	S	0	0	0
			2877	1865	443	563	6			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	19	Total	O	0	0
			19	19		
2	B	19	Total	O	0	0
			19	19		

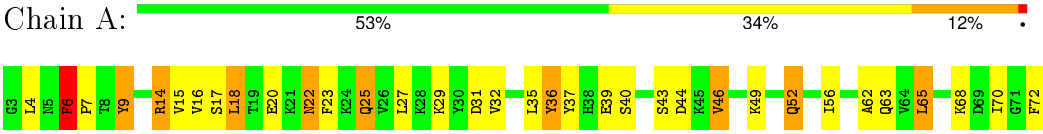
3 Residue-property plots (i)

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.

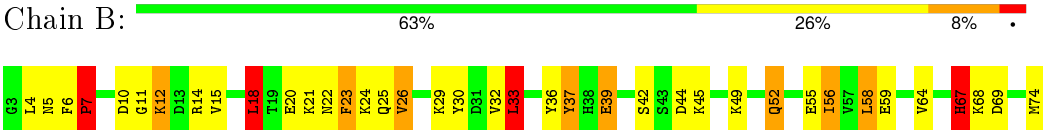
- Molecule 1: Calsequestrin, cardiac muscle isoform

Chain A:



- Molecule 1: Calsequestrin, cardiac muscle isoform

Chain B:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α, β, γ	145.19Å 145.19Å 99.82Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.40)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	0.04	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.192 , 0.241	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5792	wwPDB-VP
Average B, all atoms (Å^2)	41.0	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	0.93	0/2944	1.69	66/3986 (1.7%)
1	B	0.91	1/2944 (0.0%)	1.71	50/3986 (1.3%)
All	All	0.92	1/5888 (0.0%)	1.70	116/7972 (1.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
1	B	0	4
All	All	0	9

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	286	TRP	CG-CD2	-5.70	1.33	1.43

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	101	ASP	CA-C-N	-15.47	83.17	117.20
1	B	14	ARG	NE-CZ-NH1	11.77	126.19	120.30
1	B	67	HIS	CA-C-N	-11.69	91.48	117.20
1	A	232	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	A	286	TRP	CD1-CG-CD2	9.41	113.83	106.30
1	A	242	TRP	CD1-CG-CD2	8.84	113.37	106.30
1	A	198	TYR	CB-CG-CD2	-8.48	115.91	121.00
1	A	286	TRP	CE2-CD2-CG	-8.36	100.61	107.30
1	A	286	TRP	CG-CD2-CE3	8.30	141.38	133.90
1	B	294	LEU	CA-C-N	-8.30	98.93	117.20
1	B	299	TRP	CD1-CG-CD2	8.30	112.94	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	324	TRP	CE2-CD2-CG	-8.15	100.78	107.30
1	B	342	TRP	CD1-CG-CD2	8.13	112.80	106.30
1	B	67	HIS	O-C-N	8.10	135.66	122.70
1	A	286	TRP	CB-CG-CD1	-8.09	116.48	127.00
1	A	242	TRP	CE2-CD2-CG	-8.00	100.90	107.30
1	B	299	TRP	CE2-CD2-CG	-7.95	100.94	107.30
1	B	101	ASP	O-C-N	7.93	135.39	122.70
1	B	324	TRP	CE2-CD2-CG	-7.86	101.01	107.30
1	B	294	LEU	N-CA-CB	-7.85	94.71	110.40
1	B	14	ARG	NE-CZ-NH2	-7.77	116.41	120.30
1	B	294	LEU	CA-C-O	7.72	136.31	120.10
1	B	324	TRP	CD1-CG-CD2	7.71	112.47	106.30
1	A	350	LYS	CA-C-N	-7.67	100.32	117.20
1	A	342	TRP	CE2-CD2-CG	-7.66	101.17	107.30
1	B	231	ARG	NE-CZ-NH2	-7.50	116.55	120.30
1	B	342	TRP	CE2-CD2-CG	-7.18	101.56	107.30
1	A	242	TRP	CG-CD2-CE3	7.17	140.35	133.90
1	B	286	TRP	CA-CB-CG	7.13	127.25	113.70
1	A	324	TRP	CD1-CG-CD2	7.13	112.00	106.30
1	B	242	TRP	CE2-CD2-CG	-7.10	101.62	107.30
1	A	227	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	B	286	TRP	NE1-CE2-CZ2	-7.03	122.67	130.40
1	A	137	GLN	C-N-CA	-6.93	104.36	121.70
1	A	136	VAL	CG1-CB-CG2	-6.87	99.91	110.90
1	A	342	TRP	CD1-CG-CD2	6.84	111.77	106.30
1	B	18	LEU	CA-C-N	-6.82	102.19	117.20
1	B	294	LEU	CB-CA-C	6.74	123.00	110.20
1	A	234	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	231	ARG	CB-CG-CD	-6.61	94.43	111.60
1	A	134	LEU	CA-C-N	-6.59	102.71	117.20
1	B	286	TRP	CE2-CD2-CG	-6.58	102.03	107.30
1	A	6	PHE	CA-CB-CG	6.53	129.58	113.90
1	B	238	MET	CA-CB-CG	6.52	124.38	113.30
1	A	299	TRP	CE2-CD2-CG	-6.51	102.09	107.30
1	A	325	MET	CA-C-N	-6.46	102.98	117.20
1	A	242	TRP	CB-CG-CD1	-6.36	118.73	127.00
1	B	286	TRP	NE1-CE2-CD2	6.32	113.62	107.30
1	A	134	LEU	CA-C-O	6.31	133.36	120.10
1	B	141	ARG	NE-CZ-NH1	6.29	123.44	120.30
1	B	347	LEU	CA-CB-CG	6.28	129.75	115.30
1	B	100	GLY	CA-C-N	-6.26	103.43	117.20
1	A	300	GLU	CA-CB-CG	6.21	127.06	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	33	LEU	CA-C-N	-6.20	103.56	117.20
1	B	293	PRO	CA-C-N	-6.20	103.56	117.20
1	A	318	THR	CA-CB-CG2	6.11	120.95	112.40
1	A	342	TRP	CG-CD2-CE3	6.07	139.36	133.90
1	B	100	GLY	C-N-CA	6.03	136.77	121.70
1	A	121	ASP	N-CA-CB	-5.95	99.89	110.60
1	B	37	TYR	CB-CG-CD2	-5.94	117.44	121.00
1	B	242	TRP	CD1-CG-CD2	5.89	111.01	106.30
1	B	232	ARG	CA-C-N	5.85	130.08	117.20
1	A	37	TYR	CB-CG-CD2	-5.84	117.50	121.00
1	A	340	GLU	CA-C-N	-5.81	104.42	117.20
1	A	232	ARG	CB-CG-CD	-5.77	96.59	111.60
1	B	242	TRP	CG-CD2-CE3	5.70	139.03	133.90
1	A	342	TRP	CB-CG-CD1	-5.70	119.59	127.00
1	B	238	MET	CG-SD-CE	5.68	109.30	100.20
1	A	39	GLU	CA-CB-CG	5.67	125.87	113.40
1	B	18	LEU	O-C-N	5.64	131.73	122.70
1	A	6	PHE	CB-CG-CD1	-5.63	116.86	120.80
1	A	117	GLU	CA-CB-CG	5.62	125.76	113.40
1	A	184	VAL	CG1-CB-CG2	-5.61	101.92	110.90
1	A	339	LEU	CA-CB-CG	5.61	128.19	115.30
1	B	303	PHE	CB-CG-CD2	-5.60	116.88	120.80
1	A	299	TRP	CD1-CG-CD2	5.57	110.75	106.30
1	A	46	VAL	CA-C-N	-5.56	104.97	117.20
1	A	242	TRP	CG-CD1-NE1	-5.53	104.57	110.10
1	A	134	LEU	N-CA-CB	-5.52	99.36	110.40
1	B	304	LYS	CA-C-N	-5.52	105.06	117.20
1	A	18	LEU	CA-C-N	-5.45	105.22	117.20
1	B	44	ASP	N-CA-C	-5.43	96.33	111.00
1	A	325	MET	CG-SD-CE	5.43	108.89	100.20
1	A	102	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	127	VAL	CG1-CB-CG2	-5.41	102.25	110.90
1	A	137	GLN	CA-CB-CG	5.39	125.27	113.40
1	A	36	TYR	CB-CG-CD1	-5.39	117.77	121.00
1	A	15	VAL	CA-C-N	-5.39	105.34	117.20
1	B	101	ASP	CA-C-O	5.38	131.39	120.10
1	A	324	TRP	CG-CD2-CE3	5.36	138.72	133.90
1	A	286	TRP	CG-CD1-NE1	-5.34	104.76	110.10
1	B	232	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	286	TRP	NE1-CE2-CZ2	-5.34	124.53	130.40
1	A	272	VAL	CA-CB-CG1	-5.27	103.00	110.90
1	B	320	ALA	N-CA-C	5.26	125.20	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	298	TYR	CA-C-N	-5.24	105.67	117.20
1	A	257	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	6	PHE	CB-CG-CD2	5.23	124.46	120.80
1	A	351	ILE	N-CA-CB	-5.20	98.84	110.80
1	A	291	ASP	CA-CB-CG	5.19	124.82	113.40
1	B	160	TYR	CB-CG-CD2	-5.19	117.89	121.00
1	B	26	VAL	CA-CB-CG2	-5.17	103.14	110.90
1	A	298	TYR	CA-C-O	5.17	130.95	120.10
1	A	324	TRP	CB-CG-CD1	-5.14	120.31	127.00
1	B	319	ASP	CA-C-N	-5.13	105.91	117.20
1	A	234	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	B	52	GLN	CA-CB-CG	5.13	124.69	113.40
1	A	141	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	74	MET	CG-SD-CE	-5.10	92.04	100.20
1	A	18	LEU	O-C-N	5.10	130.86	122.70
1	B	7	PRO	N-CA-C	5.09	125.34	112.10
1	B	247	ASN	CA-CB-CG	5.08	124.57	113.40
1	B	103	THR	CA-CB-OG1	-5.07	98.36	109.00
1	A	237	ASP	CA-CB-CG	5.06	124.53	113.40
1	A	37	TYR	CB-CG-CD1	5.03	124.02	121.00
1	B	103	THR	CA-CB-CG2	5.02	119.42	112.40

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	208	ILE	Peptide
1	A	309	LYS	Peptide
1	A	327	ILE	Peptide
1	A	36	TYR	Sidechain
1	A	6	PHE	Peptide
1	B	101	ASP	Mainchain
1	B	327	ILE	Peptide
1	B	333	LEU	Peptide
1	B	67	HIS	Mainchain

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	2877	0	2799	85	0
1	B	2877	0	2799	61	0
2	A	19	0	0	4	0
2	B	19	0	0	3	0
All	All	5792	0	5598	141	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 (141) 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:B:39:GLU:HB2	1:B:77:ALA:HB3	1.58	0.84
1:A:346:VAL:HA	1:A:351:ILE:HA	1.63	0.81
1:A:314:VAL:HG23	1:A:323:VAL:HB	1.64	0.77
1:A:99:LYS:NZ	1:A:171:GLN:HE22	1.84	0.76
1:A:304:LYS:HE2	1:A:304:LYS:H	1.52	0.74
1:A:228:PRO:HG2	1:A:231:ARG:HB3	1.67	0.74
1:A:190:LEU:HD12	1:A:194:GLU:HG2	1.70	0.74
1:B:255:ALA:O	1:B:286:TRP:HZ3	1.74	0.71
1:A:246:LEU:HD22	1:A:283:SER:HB3	1.74	0.69
1:A:316:ASN:HD21	1:A:318:THR:HG22	1.55	0.69
1:A:303:PHE:HB3	1:A:305:ILE:HG12	1.74	0.68
1:A:183:GLY:HA2	1:A:186:LYS:HE2	1.75	0.67
1:B:30:TYR:HB2	1:B:33:LEU:HD12	1.77	0.67
1:A:128:GLU:HB3	2:A:1515:HOH:O	1.95	0.66
1:B:82:LYS:HA	1:B:85:LYS:HG2	1.78	0.65
1:B:79:LYS:HD2	1:B:80:GLU:HB2	1.79	0.64
1:A:295:LEU:HD22	1:B:7:PRO:HD2	1.78	0.63
1:B:108:GLY:H	1:B:239:PHE:HD1	1.47	0.63
1:B:36:TYR:HB2	1:B:95:LEU:HD12	1.81	0.63
1:A:20:GLU:HB3	1:A:83:LEU:HD11	1.81	0.62
1:A:99:LYS:HZ2	1:A:171:GLN:HE22	1.44	0.61
1:A:297:ALA:O	1:A:300:GLU:HB3	2.00	0.61
1:B:327:ILE:HB	1:B:331:ASP:HB3	1.82	0.61
1:A:313:GLY:HA2	1:A:342:TRP:CH2	2.35	0.61
1:B:339:LEU:O	1:B:343:ILE:HG13	2.00	0.61
1:B:282:LEU:HD12	1:B:343:ILE:HG21	1.83	0.60
1:B:18:LEU:HD21	1:B:26:VAL:HG11	1.84	0.60
1:A:133:LYS:O	1:A:136:VAL:HB	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:VAL:O	1:A:73:VAL:HA	2.02	0.59
1:A:6:PHE:HB2	2:B:1845:HOH:O	2.02	0.59
1:B:350:LYS:HG2	1:B:351:ILE:HG13	1.85	0.59
1:A:14:ARG:HH11	1:A:14:ARG:HG2	1.65	0.59
1:B:15:VAL:HG21	1:B:58:LEU:HB3	1.85	0.59
1:B:99:LYS:C	1:B:101:ASP:H	2.06	0.58
1:B:272:VAL:HG13	1:B:340:GLU:HG2	1.86	0.58
1:B:312:ILE:HG21	1:B:339:LEU:HD21	1.86	0.58
1:B:15:VAL:HG12	1:B:74:MET:HG2	1.85	0.58
1:A:18:LEU:HD11	1:A:23:PHE:HA	1.85	0.57
1:B:24:LYS:HG3	1:B:25:GLN:HG2	1.84	0.57
1:A:268:ILE:O	1:A:272:VAL:HG13	2.03	0.57
1:A:256:GLU:HB3	1:A:259:ASP:HB3	1.87	0.56
1:B:152:PHE:HB2	1:B:180:PHE:HE1	1.71	0.56
1:B:32:VAL:HG22	1:B:99:LYS:HG3	1.88	0.56
1:B:292:PHE:O	1:B:296:VAL:HG23	2.06	0.56
1:A:313:GLY:HA2	1:A:342:TRP:HH2	1.71	0.55
1:A:18:LEU:HD12	1:A:22:ASN:HD21	1.71	0.55
1:A:306:ASP:H	1:A:311:GLN:HE22	1.55	0.55
1:A:326:GLU:O	1:A:329:ASP:HB3	2.07	0.54
1:A:68:LYS:HB3	1:A:70:ILE:HG13	1.89	0.54
1:A:9:TYR:HD1	1:A:63:GLN:OE1	1.91	0.54
1:B:229:THR:HG22	1:B:282:LEU:HD23	1.89	0.53
1:A:295:LEU:HD12	1:A:299:TRP:CE2	2.43	0.53
1:A:306:ASP:HB3	2:A:1565:HOH:O	2.07	0.53
1:A:269:LEU:HD21	1:A:312:ILE:HD12	1.91	0.52
1:B:45:LYS:HE2	1:B:49:LYS:HD2	1.91	0.52
1:A:65:LEU:HD11	1:A:120:LEU:HD21	1.91	0.52
1:B:149:ILE:HD13	1:B:188:LEU:HD13	1.91	0.52
1:A:263:TYR:O	1:A:267:GLU:HG2	2.09	0.52
1:A:25:GLN:NE2	1:A:25:GLN:H	2.07	0.52
1:B:22:ASN:HA	2:B:1983:HOH:O	2.08	0.51
1:B:25:GLN:O	1:B:29:LYS:HB2	2.10	0.51
1:A:99:LYS:HZ3	1:A:171:GLN:HE22	1.59	0.51
1:B:36:TYR:HE1	1:B:93:GLY:O	1.94	0.51
1:A:316:ASN:ND2	1:A:318:THR:HG22	2.24	0.50
1:A:76:ASP:HB3	1:A:79:LYS:HG3	1.94	0.50
1:A:215:GLU:O	1:A:219:VAL:HG23	2.12	0.50
1:B:253:ALA:HA	1:B:312:ILE:HA	1.94	0.50
1:B:10:ASP:HB3	1:B:12:LYS:HG3	1.94	0.49
1:B:347:LEU:H	1:B:347:LEU:HD13	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:ASN:HD22	1:B:317:VAL:N	2.11	0.48
1:A:304:LYS:HD2	1:A:305:ILE:HG23	1.95	0.48
1:A:18:LEU:HD12	1:A:22:ASN:ND2	2.28	0.48
1:A:314:VAL:HG21	1:A:351:ILE:HG23	1.96	0.48
1:A:151:PHE:CZ	1:A:182:LYS:HD2	2.48	0.48
1:A:100:GLY:HA3	2:A:1485:HOH:O	2.13	0.48
1:A:294:LEU:HD22	1:B:64:VAL:HG21	1.95	0.48
1:A:149:ILE:HG13	1:A:150:GLY:N	2.28	0.48
1:B:37:TYR:CD2	1:B:89:PHE:HB3	2.49	0.47
1:A:338:GLU:O	1:A:341:ASP:HB3	2.15	0.47
1:B:294:LEU:HD12	2:B:1537:HOH:O	2.14	0.47
1:A:35:LEU:HD13	1:A:89:PHE:HZ	1.78	0.47
1:B:266:LEU:HD11	1:B:286:TRP:CZ3	2.49	0.47
1:B:136:VAL:HG23	1:B:188:LEU:HD11	1.97	0.47
1:A:265:PHE:CD1	1:A:268:ILE:HD11	2.49	0.46
1:B:246:LEU:HD21	1:B:283:SER:H	1.80	0.46
1:B:108:GLY:N	1:B:239:PHE:HD1	2.13	0.46
1:A:279:ASN:HA	1:A:280:PRO:HD3	1.62	0.46
1:A:97:VAL:HG21	1:A:122:LEU:HD13	1.96	0.46
1:A:265:PHE:O	1:A:268:ILE:HG12	2.16	0.46
1:B:107:ASP:HB3	1:B:239:PHE:HB2	1.98	0.46
1:A:233:LEU:HD22	1:A:287:ILE:HG12	1.97	0.45
1:A:299:TRP:O	1:A:303:PHE:HB2	2.15	0.45
1:A:44:ASP:HB2	2:A:1770:HOH:O	2.15	0.45
1:A:297:ALA:HA	1:A:300:GLU:HB3	1.98	0.44
1:B:230:LEU:HD12	1:B:284:ILE:HB	2.00	0.44
1:B:282:LEU:HD11	1:B:343:ILE:HD13	1.98	0.44
1:A:164:GLU:O	1:A:167:ALA:HB3	2.18	0.44
1:B:300:GLU:HA	1:B:307:LEU:HD13	1.99	0.44
1:B:246:LEU:CD2	1:B:283:SER:H	2.31	0.44
1:A:115:LEU:O	1:A:119:LEU:HD22	2.17	0.44
1:A:35:LEU:HD13	1:A:89:PHE:CZ	2.53	0.43
1:A:79:LYS:HD2	1:A:80:GLU:OE1	2.18	0.43
1:B:18:LEU:HD21	1:B:26:VAL:CG1	2.47	0.43
1:A:104:ILE:HD13	1:A:122:LEU:HD21	1.99	0.43
1:B:260:PRO:O	1:B:264:GLU:HB2	2.18	0.43
1:A:56:ILE:HG21	1:B:56:ILE:HG21	2.01	0.43
1:B:312:ILE:HD13	1:B:339:LEU:HD21	1.99	0.42
1:B:18:LEU:HA	1:B:18:LEU:HD23	1.91	0.42
1:A:22:ASN:HA	1:A:25:GLN:NE2	2.34	0.42
1:B:26:VAL:HG13	1:B:33:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:108:GLY:HA3	1:B:236:GLU:O	2.19	0.42
1:A:148:LEU:HD13	1:A:176:PHE:CE1	2.54	0.42
1:B:105:GLU:HG3	1:B:105:GLU:H	1.69	0.42
1:A:343:ILE:HG22	1:A:347:LEU:HD22	2.01	0.42
1:A:265:PHE:HD1	1:A:268:ILE:HD11	1.83	0.42
1:A:144:ASP:HB3	1:A:201:PHE:CZ	2.54	0.42
1:A:330:ASP:CG	1:A:331:ASP:H	2.23	0.42
1:A:316:ASN:HD21	1:A:318:THR:CG2	2.28	0.42
1:A:109:GLU:HB2	1:A:238:MET:SD	2.59	0.42
1:A:62:ALA:HA	1:A:72:PHE:CE1	2.55	0.42
1:A:298:TYR:HB2	1:B:7:PRO:HD3	2.01	0.42
1:A:325:MET:HG3	1:A:342:TRP:CD1	2.55	0.42
1:B:333:LEU:HG	1:B:334:PRO:HA	2.02	0.42
1:A:49:LYS:HB2	1:B:11:GLY:HA2	2.02	0.42
1:A:271:GLN:HA	1:A:274:ARG:HE	1.84	0.41
1:B:23:PHE:CE2	1:B:83:LEU:HD21	2.54	0.41
1:B:52:GLN:O	1:B:56:ILE:HB	2.20	0.41
1:A:214:THR:CG2	1:A:217:GLU:HB2	2.50	0.41
1:A:152:PHE:O	1:A:180:PHE:HD1	2.04	0.41
1:A:303:PHE:CE1	1:A:324:TRP:HH2	2.39	0.41
1:A:303:PHE:CD1	1:A:324:TRP:HH2	2.39	0.41
1:A:32:VAL:HB	1:A:70:ILE:HG23	2.02	0.41
1:B:303:PHE:HD2	1:B:305:ILE:HD11	1.85	0.41
1:B:218:LEU:O	1:B:222:VAL:HG23	2.21	0.41
1:A:52:GLN:O	1:A:56:ILE:HB	2.20	0.41
1:A:304:LYS:N	1:A:304:LYS:HE2	2.27	0.40
1:B:229:THR:O	1:B:283:SER:HA	2.21	0.40
1:B:215:GLU:O	1:B:219:VAL:HG23	2.21	0.40
1:A:136:VAL:HG11	1:A:187:LYS:HD3	2.03	0.40
1:A:151:PHE:CE2	1:A:182:LYS:HD2	2.57	0.40
1:A:130:ILE:HG21	1:A:130:ILE:HD13	1.90	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	348/350 (99%)	294 (84%)	37 (11%)	17 (5%)	3 1
1	B	348/350 (99%)	303 (87%)	25 (7%)	20 (6%)	2 1
All	All	696/700 (99%)	597 (86%)	62 (9%)	37 (5%)	2 1

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	TYR
1	A	326	GLU
1	A	346	VAL
1	A	351	ILE
1	B	320	ALA
1	B	330	ASP
1	B	331	ASP
1	B	333	LEU
1	A	43	SER
1	A	320	ALA
1	B	5	ASN
1	B	6	PHE
1	B	42	SER
1	B	84	ALA
1	B	89	PHE
1	B	106	PHE
1	B	247	ASN
1	A	255	ALA
1	B	4	LEU
1	B	7	PRO
1	B	21	LYS
1	B	350	LYS
1	B	334	PRO
1	A	40	SER
1	A	310	PRO
1	A	329	ASP
1	B	12	LYS
1	B	68	LYS
1	A	6	PHE
1	A	318	THR
1	A	321	ASP
1	B	23	PHE
1	B	101	ASP

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Mol	Chain	Res	Type
1	A	7	PRO
1	A	305	ILE
1	A	46	VAL
1	A	327	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	317/317 (100%)	272 (86%)	45 (14%)	4 4
1	B	317/317 (100%)	277 (87%)	40 (13%)	5 6
All	All	634/634 (100%)	549 (87%)	85 (13%)	5 6

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	6	PHE
1	A	14	ARG
1	A	17	SER
1	A	22	ASN
1	A	25	GLN
1	A	27	LEU
1	A	29	LYS
1	A	31	ASP
1	A	52	GLN
1	A	65	LEU
1	A	73	VAL
1	A	75	VAL
1	A	87	LEU
1	A	92	GLU
1	A	98	LEU
1	A	117	GLU
1	A	119	LEU
1	A	122	LEU

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Mol	Chain	Res	Type
1	A	124	GLU
1	A	144	ASP
1	A	147	LYS
1	A	149	ILE
1	A	168	GLU
1	A	172	PRO
1	A	188	LEU
1	A	213	TYR
1	A	246	LEU
1	A	257	ARG
1	A	258	SER
1	A	259	ASP
1	A	266	LEU
1	A	295	LEU
1	A	301	LYS
1	A	304	LYS
1	A	310	PRO
1	A	311	GLN
1	A	314	VAL
1	A	316	ASN
1	A	318	THR
1	A	321	ASP
1	A	324	TRP
1	A	339	LEU
1	A	340	GLU
1	A	350	LYS
1	B	7	PRO
1	B	18	LEU
1	B	20	GLU
1	B	33	LEU
1	B	39	GLU
1	B	55	GLU
1	B	56	ILE
1	B	58	LEU
1	B	59	GLU
1	B	67	HIS
1	B	69	ASP
1	B	79	LYS
1	B	80	GLU
1	B	83	LEU
1	B	85	LYS
1	B	91	GLU

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Mol	Chain	Res	Type
1	B	95	LEU
1	B	105	GLU
1	B	110	PHE
1	B	120	LEU
1	B	131	ASN
1	B	165	GLU
1	B	181	ASP
1	B	199	GLU
1	B	213	TYR
1	B	229	THR
1	B	232	ARG
1	B	266	LEU
1	B	268	ILE
1	B	285	VAL
1	B	286	TRP
1	B	311	GLN
1	B	315	VAL
1	B	316	ASN
1	B	321	ASP
1	B	324	TRP
1	B	327	ILE
1	B	339	LEU
1	B	345	ASP
1	B	347	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	25	GLN
1	A	38	HIS
1	A	50	GLN
1	A	171	GLN
1	A	226	GLN
1	A	250	HIS
1	A	311	GLN
1	A	316	ASN
1	B	48	GLN
1	B	171	GLN
1	B	226	GLN
1	B	247	ASN
1	B	316	ASN

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.