Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:50 AM GMT

PDB ID	:	2UY1
Title	:	CRYSTAL STRUCTURE OF CSTF-77
Authors	:	Legrand, P.; Pinaud, N.; Minvielle-Sebastia, L.; Fribourg, S.
Deposited on	:	2007-04-02
Resolution	:	2.00 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 (1)) were used in the production of this report:

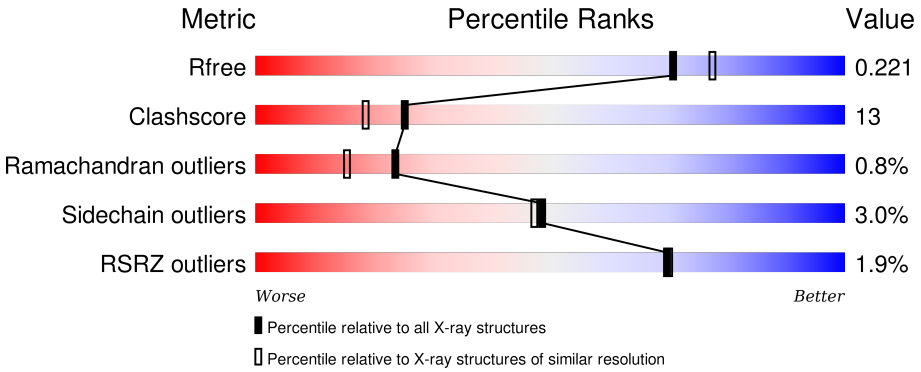
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

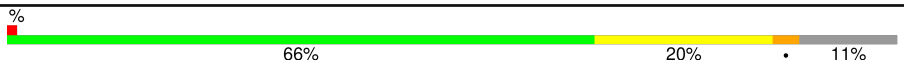
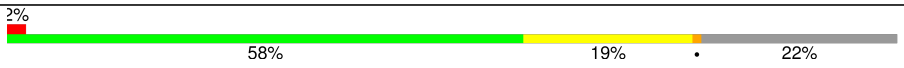
The reported resolution of this entry is 2.00 Å.

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))
R_{free}	91344	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	493	
2	B	493	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7223 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 CLEAVAGE STIMULATION FACTOR 77.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	2	0
			3668	2374	601	672	21			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	95	GLU	LEU	CONFLICT	UNP Q8SWC5

- Molecule 2 is a protein called CLEAVAGE STIMULATION FACTOR 77.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	384	Total	C	N	O	S	0	1	0
			3235	2112	530	574	19			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	42	TRP	LYS	CONFLICT	UNP Q8SWC5
B	68	PHE	TYR	CONFLICT	UNP Q8SWC5
B	88	PHE	TYR	CONFLICT	UNP Q8SWC5
B	152	LEU	ILE	CONFLICT	UNP Q8SWC5
B	210	PHE	TYR	CONFLICT	UNP Q8SWC5

- Molecule 3 is water.

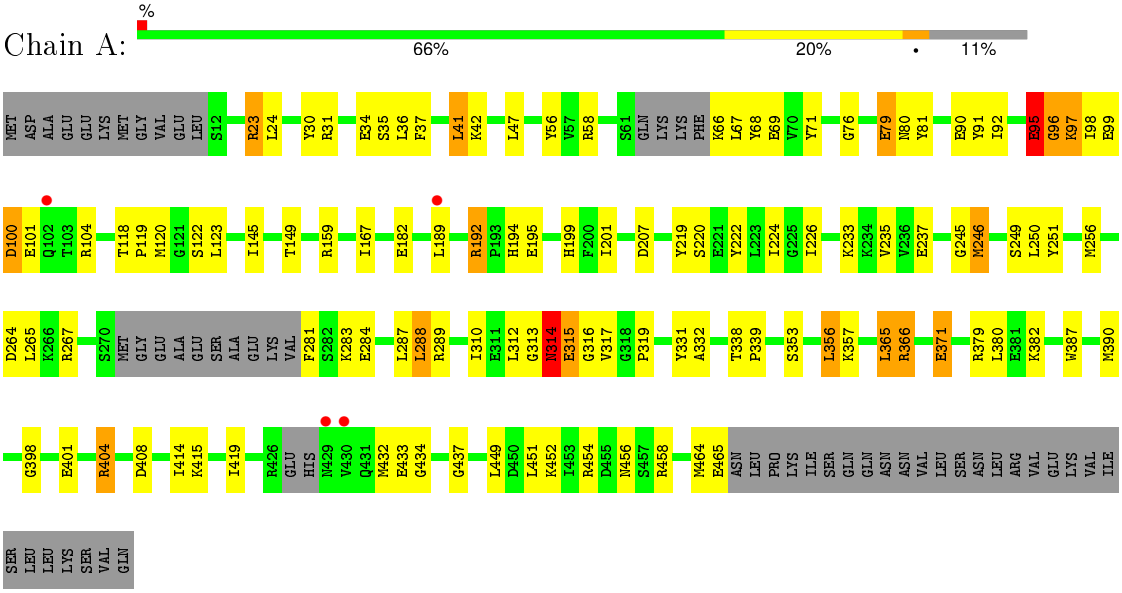
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	221	Total	O	0	0
			221	221		
3	B	99	Total	O	0	0
			99	99		

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.

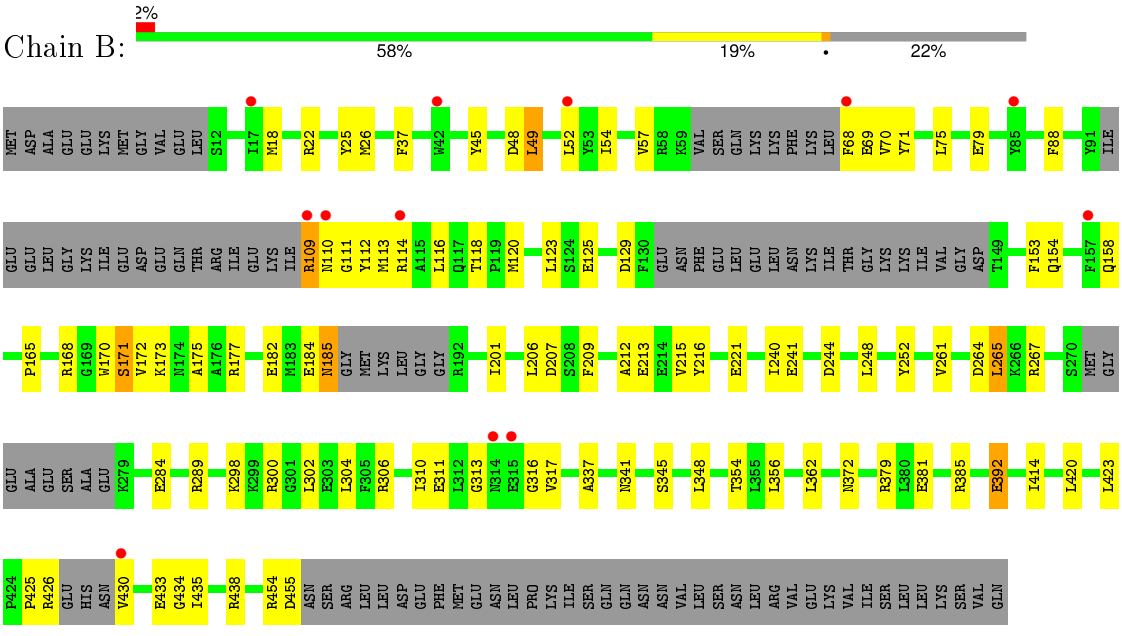
- Molecule 1: CLEAVAGE STIMULATION FACTOR 77

Chain A:



- Molecule 2: CLEAVAGE STIMULATION FACTOR 77

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.44Å 148.28Å 91.44Å 90.00° 92.15° 90.00°	Depositor
Resolution (Å)	91.29 – 2.00 29.84 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.7 (91.29-2.00) 99.4 (29.84-2.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.60 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.225 , 0.280 0.227 , 0.221	Depositor DCC
R_{free} test set	3954 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	23.8	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 30.1	EDS
Estimated twinning fraction	0.075 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.25$	Xtriage
Outliers	0 of 79075 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	7223	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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, 0.375 respectively for untwinned datasets, and 0.333, 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	A	1.16	7/3757 (0.2%)	0.99	11/5041 (0.2%)
2	B	0.98	3/3319 (0.1%)	0.91	3/4455 (0.1%)
All	All	1.08	10/7076 (0.1%)	0.95	14/9496 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
2	B	0	4
All	All	0	12

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	251	TYR	C-N	-13.68	1.02	1.34
1	A	331	TYR	CD2-CE2	6.55	1.49	1.39
1	A	95[A]	GLU	CA-C	6.08	1.68	1.52
1	A	95[B]	GLU	CA-C	6.08	1.68	1.52
2	B	372	ASN	CG-OD1	5.93	1.36	1.24
1	A	122	SER	CB-OG	5.75	1.49	1.42
1	A	456	ASN	CG-OD1	5.75	1.36	1.24
2	B	392	GLU	CB-CG	5.68	1.62	1.52
2	B	185	ASN	CG-OD1	5.22	1.35	1.24
1	A	332	ALA	CA-CB	5.13	1.63	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	356	LEU	CA-CB-CG	9.93	138.13	115.30
1	A	404	ARG	NE-CZ-NH2	-8.03	116.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	95[A]	GLU	CA-C-O	-6.97	105.46	120.10
1	A	95[B]	GLU	CA-C-O	-6.97	105.46	120.10
1	A	404	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	365	LEU	CA-CB-CG	6.58	130.42	115.30
1	A	356	LEU	CA-CB-CG	6.56	130.39	115.30
2	B	302	LEU	CB-CG-CD2	-6.04	100.73	111.00
2	B	302	LEU	CA-CB-CG	5.36	127.62	115.30
1	A	458	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	A	95[A]	GLU	CA-C-N	5.17	126.54	116.20
1	A	95[B]	GLU	CA-C-N	5.17	126.54	116.20
1	A	41	LEU	CB-CG-CD1	5.12	119.70	111.00
1	A	449	LEU	CB-CG-CD1	-5.00	102.49	111.00

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	312	LEU	Peptide
1	A	314	ASN	Peptide
1	A	95[A]	GLU	Mainchain,Peptide
1	A	95[B]	GLU	Mainchain,Peptide
1	A	96	GLY	Peptide
1	A	97	LYS	Peptide
2	B	109	ARG	Peptide
2	B	114	ARG	Peptide
2	B	170	TRP	Peptide
2	B	171	SER	Peptide

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	3668	0	3621	83	0
2	B	3235	0	3180	98	0
3	A	221	0	0	12	0
3	B	99	0	0	11	0
All	All	7223	0	6801	173	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 13.

All (173) 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)
2:B:109:ARG:HA	2:B:111:GLY:N	1.37	1.37
2:B:109:ARG:CA	2:B:111:GLY:H	1.37	1.35
2:B:45:TYR:HB2	2:B:207:ASP:OD2	1.42	1.19
1:A:192:ARG:HH11	1:A:192:ARG:HG2	1.09	1.12
2:B:171:SER:HB3	2:B:175:ALA:H	1.08	1.09
2:B:171:SER:HB2	2:B:172:VAL:C	1.79	1.03
1:A:414:ILE:HG12	2:B:430:VAL:HG22	1.43	1.00
2:B:171:SER:CB	2:B:175:ALA:H	1.75	1.00
2:B:171:SER:HB3	2:B:175:ALA:N	1.83	0.94
2:B:171:SER:HA	3:B:2016:HOH:O	1.69	0.92
1:A:314:ASN:HA	1:A:316:GLY:N	1.88	0.88
2:B:212:ALA:O	2:B:215:VAL:HG22	1.73	0.87
2:B:45:TYR:CB	2:B:207:ASP:OD2	2.23	0.87
2:B:165:PRO:O	2:B:168:ARG:O	1.96	0.84
2:B:116:LEU:HD22	2:B:153:PHE:HB2	1.61	0.79
1:A:58:ARG:HG2	1:A:67:LEU:HD11	1.63	0.79
2:B:48:ASP:O	2:B:49:LEU:HB3	1.83	0.78
2:B:48:ASP:O	2:B:49:LEU:CB	2.28	0.78
1:A:315:GLU:HG3	1:A:315:GLU:O	1.85	0.76
1:A:310:ILE:O	1:A:313:GLY:HA3	1.87	0.75
1:A:314:ASN:HA	1:A:316:GLY:H	1.51	0.75
2:B:171:SER:HB2	2:B:173:LYS:N	2.02	0.74
1:A:42:LYS:HG2	3:A:2010:HOH:O	1.87	0.74
2:B:425:PRO:O	2:B:426:ARG:HB2	1.88	0.74
1:A:192:ARG:NH1	1:A:192:ARG:HG2	1.87	0.74
2:B:109:ARG:HA	2:B:111:GLY:CA	2.17	0.74
1:A:246:MET:O	1:A:250:LEU:HG	1.88	0.73
2:B:109:ARG:HA	2:B:111:GLY:H	0.58	0.72
1:A:99:GLU:O	1:A:100:ASP:CB	2.38	0.71
1:A:433:GLU:HB3	2:B:414:ILE:HG21	1.73	0.71
2:B:18:MET:HE2	2:B:48:ASP:HB3	1.71	0.70
1:A:233:LYS:O	1:A:237:GLU:HG3	1.90	0.70
2:B:18:MET:CE	2:B:48:ASP:HB3	2.22	0.70
1:A:96:GLY:HA3	1:A:97:LYS:CB	2.22	0.69
2:B:289:ARG:HH11	2:B:317:VAL:HG12	1.57	0.67
2:B:18:MET:HE1	2:B:52:LEU:HD12	1.76	0.66
2:B:171:SER:OG	2:B:172:VAL:HA	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLU:HG3	1:A:201:ILE:CD1	2.25	0.66
2:B:171:SER:CB	2:B:172:VAL:CA	2.74	0.66
2:B:289:ARG:NH1	2:B:317:VAL:HG12	2.10	0.65
1:A:366:ARG:HD2	3:A:2146:HOH:O	1.96	0.64
2:B:171:SER:HB2	2:B:172:VAL:CA	2.27	0.64
2:B:241:GLU:HG2	3:B:2026:HOH:O	1.97	0.62
2:B:379:ARG:HD3	3:B:2059:HOH:O	1.99	0.62
1:A:34:GLU:OE2	1:A:56:TYR:OH	2.13	0.62
1:A:264:ASP:OD1	1:A:267:ARG:NH2	2.33	0.62
1:A:145:ILE:O	1:A:149:THR:HG23	2.00	0.61
2:B:109:ARG:CA	2:B:111:GLY:N	2.23	0.60
2:B:182:GLU:HG3	2:B:201:ILE:CD1	2.31	0.59
2:B:125:GLU:OE1	2:B:125:GLU:N	2.37	0.58
1:A:353:SER:O	1:A:357:LYS:HG3	2.03	0.58
1:A:47:LEU:HD22	1:A:81:TYR:HE2	1.68	0.58
2:B:18:MET:CE	2:B:52:LEU:HD12	2.34	0.57
1:A:99:GLU:O	1:A:100:ASP:HB2	2.04	0.57
1:A:404:ARG:NH2	2:B:221:GLU:OE1	2.36	0.57
1:A:408:ASP:OD1	2:B:438:ARG:NH1	2.30	0.56
1:A:80:ASN:HA	1:A:118:THR:HG23	1.88	0.56
2:B:158:GLN:HG2	3:B:2013:HOH:O	2.07	0.55
1:A:432:MET:HB2	1:A:437:GLY:HA2	1.89	0.54
2:B:109:ARG:C	2:B:111:GLY:H	2.01	0.54
2:B:215:VAL:HG23	2:B:216:TYR:CD2	2.43	0.54
1:A:30:TYR:O	1:A:34:GLU:HG3	2.08	0.54
2:B:45:TYR:N	2:B:207:ASP:OD2	2.41	0.53
1:A:189:LEU:HD23	1:A:194:HIS:HA	1.89	0.53
1:A:118:THR:HB	1:A:120:MET:HE3	1.89	0.53
1:A:76:GLY:O	1:A:79:GLU:HG2	2.08	0.53
2:B:311:GLU:HG3	3:B:2040:HOH:O	2.08	0.53
1:A:452:LYS:HE2	3:A:2194:HOH:O	2.08	0.52
2:B:70:VAL:O	2:B:70:VAL:HG12	2.09	0.52
2:B:116:LEU:HA	2:B:123:LEU:HD11	1.91	0.52
1:A:281:PHE:HA	1:A:284:GLU:OE2	2.09	0.52
1:A:68:TYR:HB2	1:A:95[B]:GLU:OE2	2.09	0.52
2:B:171:SER:OG	2:B:172:VAL:CA	2.57	0.52
3:A:2189:HOH:O	2:B:433:GLU:HG3	2.09	0.51
1:A:219:TYR:HB3	1:A:235:VAL:HG11	1.91	0.51
2:B:68:PHE:HA	2:B:71:TYR:HD2	1.75	0.51
1:A:192:ARG:HH11	1:A:192:ARG:CG	2.00	0.51
2:B:392:GLU:OE2	3:B:2068:HOH:O	2.19	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:GLY:C	1:A:98:ILE:H	2.14	0.51
2:B:45:TYR:CA	2:B:207:ASP:OD2	2.59	0.51
2:B:79:GLU:O	2:B:118:THR:HG21	2.10	0.51
2:B:54:ILE:HA	2:B:57:VAL:HG12	1.91	0.51
2:B:18:MET:CE	2:B:52:LEU:CD1	2.90	0.50
1:A:233:LYS:HB2	1:A:256:MET:HE2	1.93	0.50
1:A:357:LYS:HB3	1:A:380:LEU:HD13	1.92	0.50
2:B:154:GLN:O	2:B:158:GLN:HG3	2.11	0.50
2:B:213:GLU:HB2	2:B:248:LEU:HG	1.93	0.50
2:B:252:TYR:HD2	2:B:261:VAL:HG11	1.76	0.50
2:B:454:ARG:O	2:B:455:ASP:OD1	2.30	0.49
1:A:182:GLU:HG3	1:A:201:ILE:HD11	1.94	0.49
2:B:306:ARG:O	2:B:310:ILE:HG13	2.12	0.49
1:A:96:GLY:HA3	1:A:97:LYS:HB3	1.94	0.49
2:B:264:ASP:OD1	2:B:267:ARG:NH2	2.45	0.49
1:A:233:LYS:HB2	1:A:256:MET:CE	2.42	0.49
2:B:109:ARG:HD2	2:B:112:TYR:CD1	2.48	0.48
1:A:101:GLU:HG3	1:A:104:ARG:NH2	2.27	0.48
2:B:171:SER:CA	3:B:2016:HOH:O	2.42	0.48
1:A:96:GLY:HA3	1:A:97:LYS:HB2	1.93	0.48
2:B:49:LEU:CD2	3:B:2001:HOH:O	2.63	0.47
1:A:99:GLU:O	1:A:100:ASP:HB3	2.12	0.47
2:B:284:GLU:HG2	2:B:284:GLU:H	1.33	0.47
1:A:246:MET:HG3	1:A:246:MET:O	2.14	0.47
1:A:118:THR:HB	1:A:120:MET:CE	2.44	0.47
1:A:464:MET:O	1:A:465:GLU:HB2	2.12	0.47
2:B:311:GLU:C	2:B:313:GLY:H	2.17	0.47
2:B:433:GLU:CG	2:B:434:GLY:N	2.79	0.47
2:B:433:GLU:HG2	2:B:434:GLY:N	2.31	0.46
1:A:379:ARG:NH2	3:A:2169:HOH:O	2.37	0.46
1:A:119:PRO:HD3	1:A:159:ARG:NH2	2.30	0.46
2:B:381:GLU:HG3	3:B:2060:HOH:O	2.14	0.46
2:B:354:THR:HG22	2:B:423:LEU:HD21	1.98	0.46
1:A:371:GLU:HG3	3:A:2166:HOH:O	2.15	0.46
2:B:18:MET:HE1	2:B:48:ASP:HB3	1.97	0.46
2:B:337:ALA:O	2:B:341:ASN:ND2	2.43	0.46
1:A:195[A]:GLU:HG2	1:A:199:HIS:CD2	2.51	0.46
1:A:404:ARG:HH22	2:B:221:GLU:CD	2.19	0.46
1:A:319:PRO:HB3	1:A:356:LEU:HD22	1.97	0.46
2:B:265:LEU:HA	2:B:265:LEU:HD12	1.77	0.46
1:A:401:GLU:HG2	3:A:2185:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:ARG:HD3	1:A:317:VAL:HG12	1.98	0.45
2:B:109:ARG:HD2	2:B:112:TYR:HD1	1.81	0.45
2:B:48:ASP:O	2:B:49:LEU:HB2	2.14	0.45
2:B:109:ARG:C	2:B:111:GLY:N	2.65	0.45
2:B:430:VAL:O	2:B:430:VAL:HG12	2.16	0.45
2:B:454:ARG:O	2:B:455:ASP:CG	2.56	0.45
2:B:209:PHE:HB2	2:B:215:VAL:HG11	1.99	0.45
1:A:80:ASN:HB2	3:A:2024:HOH:O	2.15	0.44
2:B:22:ARG:HH11	2:B:22:ARG:HG3	1.82	0.44
1:A:419:ILE:HG13	2:B:430:VAL:HG21	1.99	0.44
2:B:88:PHE:CD1	2:B:120:MET:HE1	2.52	0.44
1:A:249:SER:HB3	1:A:265:LEU:HD11	1.99	0.44
1:A:23:ARG:HD3	3:A:2006:HOH:O	2.17	0.44
2:B:300:ARG:HB3	2:B:304:LEU:HD12	1.99	0.44
2:B:184:GLU:HG3	2:B:185:ASN:H	1.82	0.44
2:B:435:ILE:HD12	2:B:438:ARG:HD2	1.99	0.43
2:B:171:SER:CB	2:B:172:VAL:C	2.66	0.43
2:B:240:ILE:O	3:B:2027:HOH:O	2.21	0.43
1:A:91:TYR:CE1	1:A:95[B]:GLU:OE2	2.72	0.43
2:B:381:GLU:HB2	2:B:420:LEU:HD11	1.99	0.43
2:B:25:TYR:CD2	2:B:26:MET:HE2	2.53	0.43
2:B:345:SER:HA	2:B:348:LEU:HD12	2.01	0.43
2:B:37:PHE:HE1	2:B:49:LEU:HD12	1.83	0.43
2:B:75:LEU:O	2:B:79:GLU:HB3	2.19	0.43
1:A:338:THR:HB	1:A:339:PRO:CD	2.49	0.42
1:A:42:LYS:HG2	1:A:42:LYS:H	1.51	0.42
1:A:220:SER:O	1:A:224:ILE:HG13	2.19	0.42
1:A:36:LEU:C	1:A:36:LEU:HD23	2.40	0.42
1:A:287:LEU:HG	1:A:451:LEU:HB3	1.99	0.42
3:A:2178:HOH:O	2:B:298:LYS:HE2	2.19	0.42
1:A:419:ILE:HG13	2:B:430:VAL:CG2	2.50	0.42
2:B:173:LYS:NZ	2:B:177:ARG:NH2	2.68	0.41
1:A:398:GLY:O	2:B:298:LYS:HE3	2.20	0.41
1:A:37:PHE:O	1:A:41:LEU:HB2	2.20	0.41
1:A:66:LYS:O	1:A:69:GLU:HB2	2.20	0.41
1:A:167:ILE:HG23	1:A:167:ILE:HD12	1.88	0.41
1:A:382:LYS:HD3	1:A:387:TRP:CE2	2.56	0.41
1:A:120:MET:HG2	1:A:123:LEU:HD13	2.02	0.41
2:B:70:VAL:O	2:B:70:VAL:CG1	2.68	0.41
1:A:314:ASN:CA	1:A:316:GLY:H	2.25	0.41
2:B:379:ARG:HB3	2:B:379:ARG:HE	1.57	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:ARG:HD3	3:A:2170:HOH:O	2.21	0.41
1:A:96:GLY:C	1:A:98:ILE:N	2.74	0.41
1:A:92:ILE:HA	1:A:95[A]:GLU:OE1	2.21	0.41
1:A:288:LEU:HD23	1:A:289:ARG:HG3	2.01	0.41
1:A:245:GLY:HA3	3:A:2110:HOH:O	2.20	0.41
1:A:192:ARG:NH1	1:A:192:ARG:CG	2.67	0.40
1:A:222:TYR:CZ	1:A:226:ILE:HD13	2.56	0.40
1:A:71:TYR:OH	1:A:90:GLU:OE1	2.27	0.40
1:A:24:LEU:HD23	1:A:24:LEU:HA	1.87	0.40
2:B:362:LEU:HD11	2:B:385:ARG:HD3	2.03	0.40
2:B:171:SER:C	3:B:2016:HOH:O	2.59	0.40
2:B:88:PHE:HD1	2:B:120:MET:HE1	1.87	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	432/493 (88%)	412 (95%)	17 (4%)	3 (1%)	26	19
2	B	371/493 (75%)	358 (96%)	10 (3%)	3 (1%)	24	15
All	All	803/986 (81%)	770 (96%)	27 (3%)	6 (1%)	24	19

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	100	ASP
1	A	314	ASN
2	B	49	LEU
2	B	110	ASN
2	B	316	GLY
1	A	434	GLY

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	395/444 (89%)	379 (96%)	16 (4%)	37 32
2	B	346/444 (78%)	340 (98%)	6 (2%)	68 71
All	All	741/888 (83%)	719 (97%)	22 (3%)	48 47

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ARG
1	A	31	ARG
1	A	35	SER
1	A	79	GLU
1	A	192	ARG
1	A	207	ASP
1	A	246	MET
1	A	283	LYS
1	A	288	LEU
1	A	315	GLU
1	A	365	LEU
1	A	366	ARG
1	A	371	GLU
1	A	390	MET
1	A	415	LYS
1	A	454	ARG
2	B	69	GLU
2	B	113	MET
2	B	129	ASP
2	B	206	LEU
2	B	244	ASP
2	B	265	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	409	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

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	A	438/493 (88%)	-0.14	4 (0%)	85	86	11, 22, 44, 58	0
2	B	384/493 (77%)	0.07	12 (3%)	52	53	12, 31, 52, 61	0
All	All	822/986 (83%)	-0.05	16 (1%)	70	70	11, 26, 50, 61	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	430	VAL	5.8
2	B	42	TRP	5.5
2	B	315	GLU	3.7
2	B	68	PHE	3.5
1	A	430	VAL	3.5
2	B	314	ASN	3.2
1	A	102	GLN	3.1
2	B	17	ILE	2.8
2	B	114	ARG	2.7
2	B	85	TYR	2.5
2	B	157	PHE	2.4
1	A	429	ASN	2.3
2	B	52	LEU	2.2
1	A	189	LEU	2.2
2	B	109	ARG	2.1
2	B	110	ASN	2.0

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.