



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:49 AM GMT

PDB ID : 3CBK
Title : chagasin-cathepsin B
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Deposited on : 2008-02-22
Resolution : 2.67 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

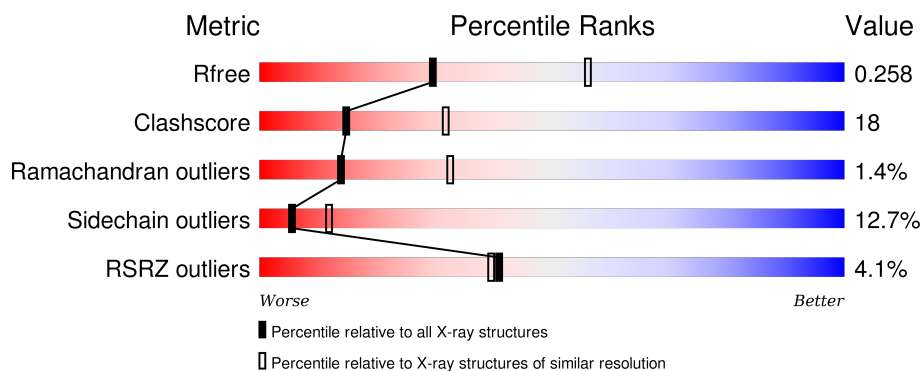
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.67 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	2780 (2.70-2.66)
Clashscore	102246	3138 (2.70-2.66)
Ramachandran outliers	100387	3089 (2.70-2.66)
Sidechain outliers	100360	3089 (2.70-2.66)
RSRZ outliers	91569	2789 (2.70-2.66)

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 $\leq 5\%$. 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	266	
2	B	110	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2890 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 Cathepsin B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	2	0
			1977	1239	339	382	17			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	29	ALA	CYS	ENGINEERED	UNP P07858
A	110	ALA	HIS	ENGINEERED	UNP P07858
A	115	ALA	SER	ENGINEERED	UNP P07858

- Molecule 2 is a protein called Chagasin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	110	Total	C	N	O	S	0	0	0
			850	542	144	161	3			

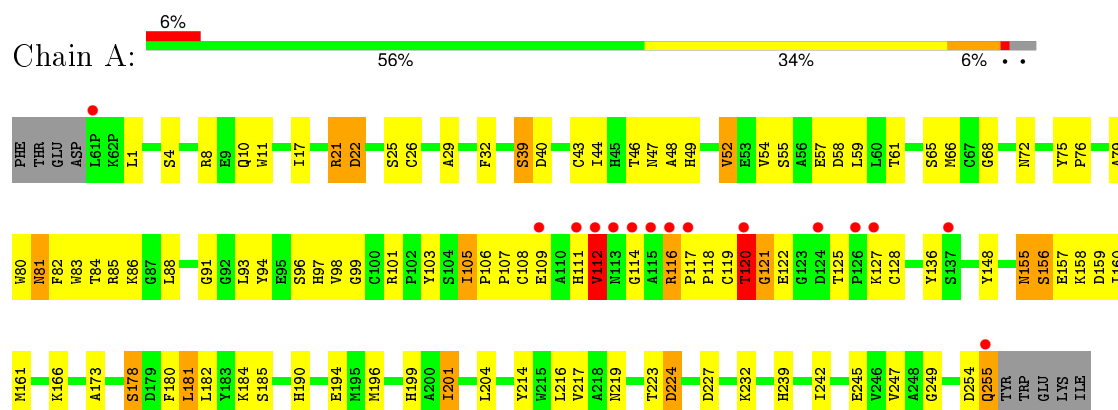
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	47	Total	O	0	0
			47	47		
3	B	16	Total	O	0	0
			16	16		

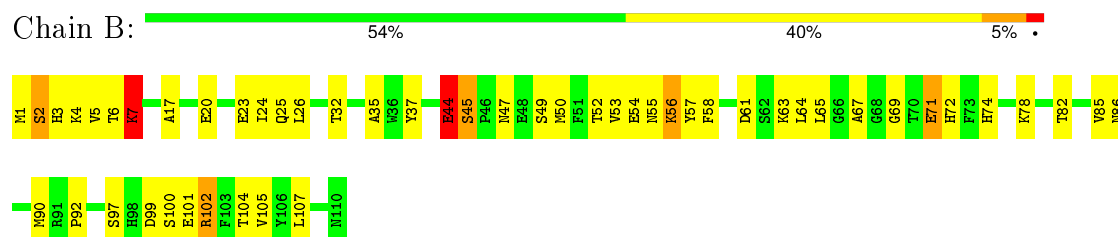
3 Residue-property plots [i](#)

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: Cathepsin B



• Molecule 2: Chagasin



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	85.07Å 85.07Å 115.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.67 19.77 – 2.67	Depositor EDS
% Data completeness (in resolution range)	94.1 (20.00-2.67) 94.5 (19.77-2.67)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.67Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.193 , 0.242 0.211 , 0.258	Depositor DCC
R_{free} test set	573 reflections (5.07%)	DCC
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 43.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 11884 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2890	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	1.13	1/2044 (0.0%)	1.26	18/2779 (0.6%)
2	B	1.23	4/876 (0.5%)	1.35	15/1193 (1.3%)
All	All	1.16	5/2920 (0.2%)	1.29	33/3972 (0.8%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	CYS	CB-SG	-8.51	1.67	1.82
2	B	23	GLU	CD-OE2	6.43	1.32	1.25
2	B	61	ASP	CB-CG	5.71	1.63	1.51
2	B	71	GLU	CD-OE2	5.26	1.31	1.25
2	B	44	GLU	CG-CD	5.05	1.59	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	VAL	N-CA-C	15.01	151.53	111.00
1	A	112	VAL	CB-CA-C	-10.03	92.35	111.40
1	A	156	SER	CB-CA-C	9.30	127.78	110.10
2	B	61	ASP	CB-CG-OD2	7.69	125.22	118.30
1	A	148	TYR	CB-CA-C	-7.63	95.13	110.40
2	B	23	GLU	CG-CD-OE2	7.27	132.83	118.30
2	B	24	ILE	N-CA-C	-7.11	91.82	111.00
2	B	61	ASP	N-CA-C	-7.01	92.06	111.00
1	A	109	GLU	N-CA-C	6.79	129.33	111.00
2	B	2	SER	CB-CA-C	6.71	122.84	110.10
2	B	74	HIS	N-CA-C	-6.57	93.27	111.00
2	B	17	ALA	CB-CA-C	6.38	119.67	110.10
2	B	7	LYS	CB-CA-C	-6.38	97.65	110.40
2	B	23	GLU	CG-CD-OE1	-6.33	105.63	118.30
2	B	63	LYS	CB-CA-C	-6.03	98.34	110.40
1	A	194	GLU	CB-CA-C	6.02	122.45	110.40
1	A	22	ASP	CB-CG-OD2	5.96	123.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	26	CYS	CB-CA-C	-5.93	98.55	110.40
1	A	109	GLU	CB-CA-C	-5.92	98.56	110.40
1	A	227	ASP	N-CA-C	-5.89	95.09	111.00
1	A	155	ASN	N-CA-C	-5.84	95.24	111.00
1	A	254	ASP	CB-CA-C	5.70	121.79	110.40
2	B	23	GLU	CA-CB-CG	5.58	125.68	113.40
1	A	182	LEU	CA-CB-CG	5.54	128.03	115.30
1	A	11	TRP	N-CA-C	-5.50	96.14	111.00
1	A	1	LEU	CA-CB-CG	5.40	127.72	115.30
2	B	65	LEU	N-CA-C	-5.36	96.54	111.00
2	B	102	ARG	NE-CZ-NH2	-5.36	117.62	120.30
2	B	56	LYS	CB-CA-C	5.33	121.06	110.40
1	A	245	GLU	N-CA-C	-5.32	96.65	111.00
1	A	156	SER	N-CA-C	-5.21	96.93	111.00
2	B	23	GLU	N-CA-CB	5.09	119.77	110.60
1	A	158	LYS	CB-CA-C	-5.08	100.23	110.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1977	0	1828	69	0
2	B	850	0	817	31	0
3	A	47	0	0	5	0
3	B	16	0	0	1	0
All	All	2890	0	2645	97	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 18.

All (97) 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:58:PHE:CE1	2:B:72:HIS:NE2	2.36	0.94
2:B:58:PHE:CD1	2:B:72:HIS:NE2	2.38	0.91
1:A:66:MET:HE2	1:A:85:ARG:HH21	1.36	0.90
1:A:57:GLU:O	1:A:61:THR:HG23	1.76	0.84
1:A:91:GLY:HA3	1:A:101:ARG:O	1.79	0.82
1:A:55:SER:HB2	1:A:91:GLY:HA3	1.60	0.80
2:B:58:PHE:CE1	2:B:72:HIS:CD2	2.70	0.78
2:B:58:PHE:CD1	2:B:72:HIS:CD2	2.76	0.73
1:A:239:HIS:O	1:A:242:ILE:HG22	1.88	0.73
1:A:201:ILE:HD13	1:A:217:VAL:HG11	1.71	0.73
1:A:80:TRP:O	1:A:84:THR:HG23	1.89	0.72
1:A:199:HIS:HA	3:A:279:HOH:O	1.89	0.71
1:A:116:ARG:HB3	1:A:117:PRO:CD	2.21	0.71
1:A:17:ILE:HG22	1:A:17:ILE:O	1.90	0.69
2:B:56:LYS:HB2	3:B:125:HOH:O	1.93	0.69
1:A:82:PHE:CE1	1:A:86:LYS:HG3	2.30	0.67
2:B:86:ASN:OD1	2:B:104:THR:HG23	1.93	0.67
2:B:45:SER:HB3	2:B:53:VAL:HG23	1.76	0.66
1:A:224:ASP:N	1:A:224:ASP:OD1	2.29	0.65
1:A:80:TRP:O	1:A:83:TRP:HB3	1.98	0.64
2:B:50:MET:HE2	2:B:50:MET:HA	1.81	0.63
2:B:90:MET:HE3	2:B:92:PRO:HA	1.81	0.63
1:A:112:VAL:HG12	1:A:112:VAL:O	1.98	0.62
1:A:201:ILE:HD13	1:A:217:VAL:CG1	2.29	0.62
1:A:214:TYR:CZ	1:A:232:LYS:HD3	2.34	0.62
1:A:99:GLY:HA2	1:A:136:TYR:CE1	2.35	0.61
2:B:85:VAL:O	2:B:85:VAL:HG12	2.00	0.60
1:A:114:GLY:O	1:A:116:ARG:HG2	2.03	0.59
2:B:55:ASN:HA	2:B:72:HIS:O	2.03	0.59
1:A:10:GLN:HG3	1:A:10:GLN:O	2.01	0.59
2:B:44:GLU:HA	2:B:44:GLU:OE1	2.03	0.59
1:A:116:ARG:HB3	1:A:117:PRO:HD2	1.84	0.59
1:A:65:SER:HA	1:A:68:GLY:O	2.06	0.56
1:A:76:PRO:O	1:A:79:ALA:HB3	2.05	0.56
1:A:43:CYS:SG	1:A:48:ALA:HA	2.46	0.56
1:A:97:HIS:CD2	3:A:265:HOH:O	2.59	0.54
1:A:173:ALA:HA	1:A:199:HIS:O	2.08	0.54
1:A:156:SER:HB3	1:A:159:ASP:HB2	1.90	0.53
2:B:85:VAL:O	2:B:104:THR:HA	2.09	0.53
1:A:8:ARG:NH2	1:A:216:LEU:HD21	2.24	0.53
1:A:22:ASP:OD1	1:A:22:ASP:C	2.43	0.53
1:A:112:VAL:O	1:A:112:VAL:CG1	2.54	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:SER:HB2	1:A:98:VAL:HG23	1.92	0.51
1:A:255:GLN:C	1:A:255:GLN:NE2	2.63	0.51
1:A:17:ILE:CG2	1:A:17:ILE:O	2.57	0.51
1:A:214:TYR:CE1	1:A:232:LYS:HD3	2.45	0.51
1:A:8:ARG:HH21	1:A:216:LEU:HD21	1.76	0.50
2:B:7:LYS:NZ	2:B:7:LYS:HB3	2.27	0.49
1:A:93:LEU:O	1:A:96:SER:OG	2.22	0.49
1:A:106:PRO:HB2	1:A:107:PRO:O	2.13	0.48
1:A:66:MET:HE2	1:A:85:ARG:NH2	2.16	0.48
1:A:178:SER:O	1:A:180:PHE:N	2.47	0.47
1:A:120:THR:HG22	1:A:121:GLY:H	1.79	0.47
2:B:35:ALA:HB3	2:B:37:TYR:CZ	2.49	0.47
1:A:91:GLY:CA	1:A:101:ARG:O	2.58	0.47
2:B:57:TYR:OH	2:B:69:GLY:N	2.45	0.47
1:A:59:LEU:HB2	1:A:88:LEU:HD21	1.97	0.47
1:A:47:ASN:ND2	1:A:47:ASN:O	2.47	0.46
1:A:29:ALA:HA	1:A:32:PHE:HB2	1.97	0.46
2:B:25:GLN:HA	2:B:71:GLU:O	2.15	0.46
1:A:103:TYR:CZ	1:A:105:ILE:HG12	2.50	0.46
1:A:81:ASN:HA	1:A:84:THR:HG23	1.98	0.46
1:A:25:SER:O	2:B:32:THR:HG21	2.16	0.45
2:B:45:SER:OG	2:B:47:ASN:O	2.34	0.45
1:A:39:SER:HB3	1:A:52:VAL:O	2.17	0.45
2:B:104:THR:O	2:B:105:VAL:HG23	2.17	0.45
1:A:166:LYS:HE3	1:A:166:LYS:HB2	1.73	0.45
1:A:21:ARG:NH1	3:A:285:HOH:O	2.46	0.45
1:A:108:CYS:O	2:B:99:ASP:HB2	2.17	0.45
2:B:90:MET:CE	2:B:92:PRO:HA	2.47	0.44
1:A:58:ASP:OD2	1:A:88:LEU:HA	2.17	0.44
1:A:116:ARG:CB	1:A:117:PRO:CD	2.95	0.44
1:A:214:TYR:CD1	1:A:214:TYR:C	2.89	0.44
2:B:5:VAL:HG12	2:B:6:THR:N	2.30	0.44
1:A:75:TYR:O	1:A:76:PRO:C	2.56	0.44
1:A:61:THR:O	1:A:128:CYS:HB2	2.18	0.44
2:B:7:LYS:HB3	2:B:7:LYS:HZ3	1.83	0.44
1:A:94:TYR:CE1	1:A:106:PRO:HB3	2.53	0.43
2:B:1:MET:O	2:B:3:HIS:CD2	2.72	0.43
1:A:120:THR:HG23	2:B:101:GLU:HG3	2.00	0.43
1:A:156:SER:O	1:A:160:ILE:HD12	2.19	0.43
2:B:82:THR:HA	2:B:107:LEU:O	2.19	0.43
1:A:255:GLN:O	1:A:255:GLN:NE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:104:THR:HG22	2:B:105:VAL:N	2.35	0.42
1:A:21:ARG:NH2	1:A:54:VAL:O	2.53	0.42
1:A:80:TRP:CZ3	1:A:249:GLY:N	2.88	0.41
1:A:46:THR:O	1:A:49:HIS:HB2	2.20	0.41
1:A:181:LEU:HG	1:A:181:LEU:H	1.71	0.41
1:A:21:ARG:HB2	1:A:32:PHE:CE1	2.55	0.41
2:B:7:LYS:NZ	2:B:7:LYS:CB	2.84	0.41
1:A:219:ASN:HB3	3:A:282:HOH:O	2.21	0.41
1:A:72[B]:ASN:ND2	3:A:294:HOH:O	2.49	0.41
2:B:97:SER:OG	2:B:99:ASP:N	2.49	0.40
1:A:190:HIS:H	1:A:239:HIS:CE1	2.39	0.40
1:A:157:GLU:O	1:A:161:MET:HG3	2.21	0.40
1:A:40:ASP:O	1:A:44:ILE:HG13	2.21	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	257/266 (97%)	231 (90%)	21 (8%)	5 (2%)	10	23
2	B	108/110 (98%)	103 (95%)	5 (5%)	0	100	100
All	All	365/376 (97%)	334 (92%)	26 (7%)	5 (1%)	14	32

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	116	ARG
1	A	121	GLY
1	A	120	THR
1	A	118	PRO
1	A	201	ILE

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	211/218 (97%)	187 (89%)	24 (11%)	7	15
2	B	91/91 (100%)	77 (85%)	14 (15%)	3	7
All	All	302/309 (98%)	264 (87%)	38 (13%)	5	12

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	21	ARG
1	A	39	SER
1	A	52	VAL
1	A	81	ASN
1	A	105	ILE
1	A	111	HIS
1	A	112	VAL
1	A	119	CYS
1	A	120	THR
1	A	122	GLU
1	A	125	THR
1	A	127	LYS
1	A	155	ASN
1	A	178	SER
1	A	181	LEU
1	A	184	LYS
1	A	185	SER
1	A	196	MET
1	A	204	LEU
1	A	223	THR
1	A	224	ASP
1	A	247	VAL
1	A	255	GLN
2	B	2	SER
2	B	4	LYS
2	B	7	LYS

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Mol	Chain	Res	Type
2	B	20	GLU
2	B	26	LEU
2	B	44	GLU
2	B	45	SER
2	B	49	SER
2	B	52	THR
2	B	54	GLU
2	B	64	LEU
2	B	78	LYS
2	B	100	SER
2	B	102	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	ASN
1	A	97	HIS
1	A	155	ASN
2	B	3	HIS

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

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 [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(Å ²)	Q<0.9
1	A	257/266 (96%)	0.27	15 (5%) 26 24	36, 53, 75, 92	0
2	B	110/110 (100%)	0.21	0 100 100	38, 48, 61, 72	0
All	All	367/376 (97%)	0.25	15 (4%) 41 39	36, 51, 70, 92	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	112	VAL	8.5
1	A	113	ASN	4.5
1	A	114	GLY	3.9
1	A	61(P)	LEU	3.8
1	A	117	PRO	3.5
1	A	116	ARG	3.4
1	A	111	HIS	3.3
1	A	137	SER	2.7
1	A	120	THR	2.5
1	A	127	LYS	2.5
1	A	255	GLN	2.5
1	A	115	ALA	2.4
1	A	124	ASP	2.2
1	A	126	PRO	2.2
1	A	109	GLU	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.