Full wwPDB X-ray Structure Validation Report (i)

Nov 28, 2023 – 06:30 pm GMT

PDB ID	:	1DZB
Title	:	Crystal structure of phage library-derived single-chain Fv fragment 1F9 in complex with turkey egg-white lysozyme
Authors	:	Ay, J.; Keitel, T.; Kuettner, G.; Wessner, H.; Scholz, C.; Hahn, M.; Hoehne, W.
Deposited on	:	2000-02-23
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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

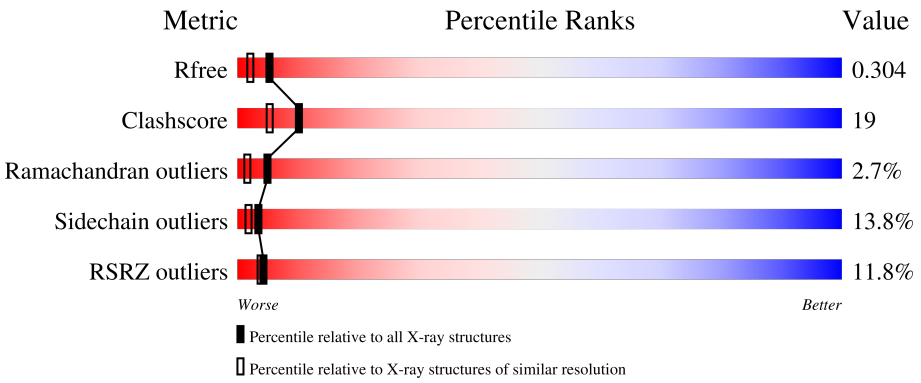
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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	253	7%; 50%; 27%; 9%; •; 11%
1	B	253	9%; 47%; 29%; 10%; •; 11%
2	X	129	%; 68%; 28%; •; •
2	Y	129	32%; 60%; 27%; 9%; •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5709 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 SCFV FRAGMENT 1F9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	224	1727	1086	284	351	6	0	0	2
1	B	224	1727	1086	284	351	6	0	0	2

- Molecule 2 is a protein called TURKEY EGG-WHITE LYSOZYME C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	X	129	1001	615	194	182	10	0	1	0
2	Y	129	994	611	191	182	10	0	0	0

- Molecule 3 is water.

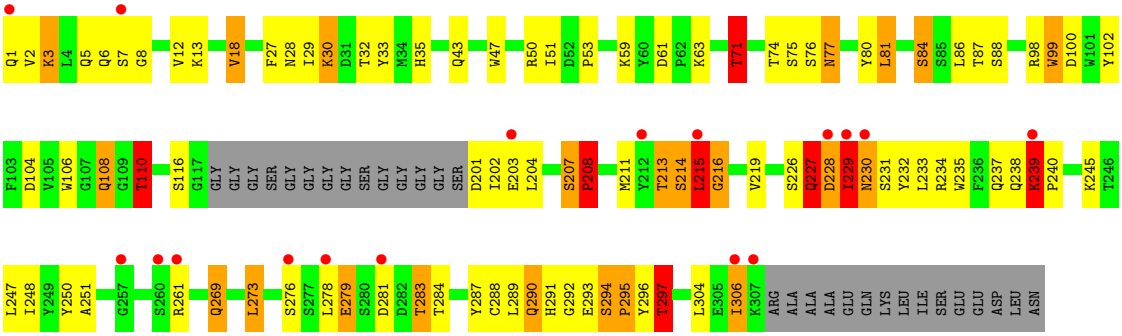
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	74	74	74	0	0
3	B	105	105	105	0	0
3	X	53	53	53	0	0
3	Y	28	28	28	0	0

3 Residue-property plots (i)

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

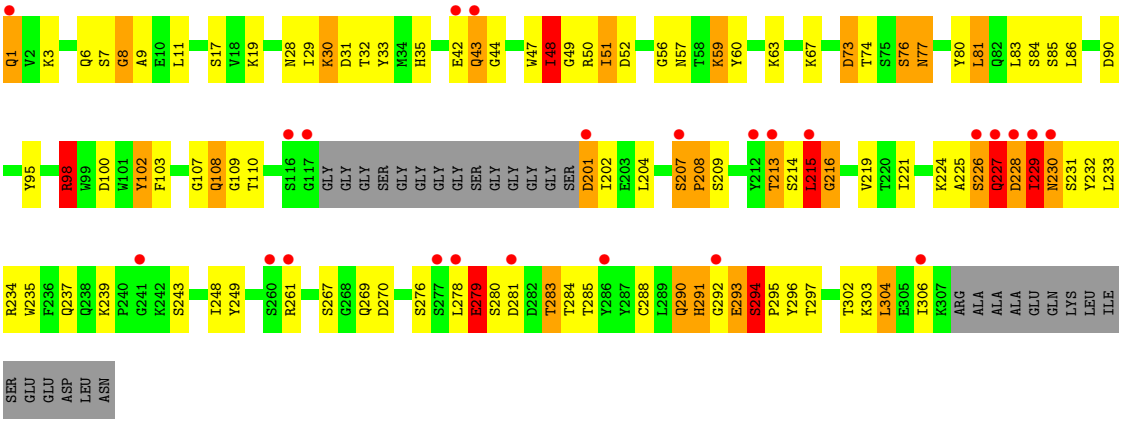
• Molecule 1: SCFV FRAGMENT 1F9

Chain A:



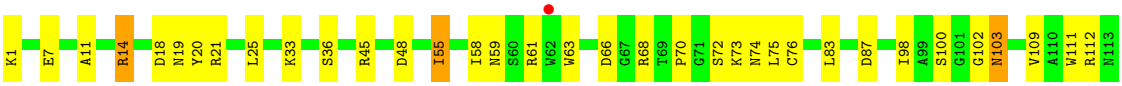
• Molecule 1: SCFV FRAGMENT 1F9

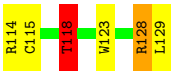
Chain B:



• Molecule 2: TURKEY EGG-WHITE LYSOZYME C

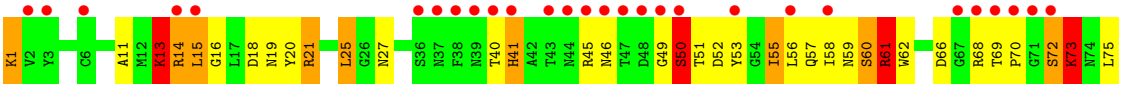
Chain X:

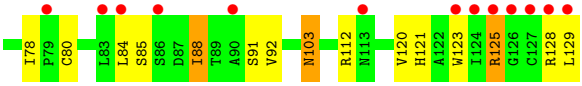




• Molecule 2: TURKEY EGG-WHITE LYSOZYME C

Chain Y:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	38.71Å 112.44Å 80.00Å 90.00° 97.67° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 19.77 – 2.00	Depositor EDS
% Data completeness (in resolution range)	87.9 (20.00-2.00) 87.9 (19.77-2.00)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.10 (at 2.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.225 , 0.306 0.227 , 0.304	Depositor DCC
R_{free} test set	2011 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	23.8	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 46.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5709	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	1.14	3/1768 (0.2%)	1.84	48/2404 (2.0%)
1	B	1.17	2/1768 (0.1%)	1.99	50/2404 (2.1%)
2	X	1.22	2/1026 (0.2%)	1.81	26/1385 (1.9%)
2	Y	0.98	0/1015	1.79	13/1371 (0.9%)
All	All	1.14	7/5577 (0.1%)	1.88	137/7564 (1.8%)

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	4
1	B	0	4
All	All	0	8

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	X	74	ASN	N-CA	6.42	1.59	1.46
1	A	231	SER	CA-CB	5.90	1.61	1.52
1	A	84	SER	CA-CB	5.70	1.61	1.52
1	A	208	PRO	N-CA	-5.53	1.37	1.47
1	B	98	ARG	NE-CZ	-5.46	1.25	1.33
1	B	243	SER	CB-OG	5.31	1.49	1.42
2	X	36	SER	CA-CB	5.04	1.60	1.52

All (137) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	98	ARG	NE-CZ-NH1	26.30	133.45	120.30
2	Y	21	ARG	CD-NE-CZ	21.04	153.05	123.60
1	B	98	ARG	CD-NE-CZ	19.00	150.20	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	45	ARG	NE-CZ-NH1	15.17	127.89	120.30
1	A	281	ASP	CA-CB-CG	13.57	143.26	113.40
1	A	294	SER	CA-C-O	-13.40	91.95	120.10
2	Y	125	ARG	CD-NE-CZ	13.15	142.02	123.60
1	A	8	GLY	N-CA-C	12.94	145.45	113.10
1	B	294	SER	CA-C-O	-12.73	93.36	120.10
1	A	207	SER	CA-C-O	-12.40	94.06	120.10
2	X	21	ARG	CD-NE-CZ	12.30	140.83	123.60
1	B	100	ASP	CB-CG-OD1	12.26	129.34	118.30
1	B	207	SER	CA-C-O	-11.73	95.47	120.10
1	B	227	GLN	N-CA-CB	11.26	130.86	110.60
1	A	208	PRO	CA-N-CD	-11.23	95.78	111.50
2	Y	112	ARG	CD-NE-CZ	10.85	138.78	123.60
1	B	98	ARG	NE-CZ-NH2	-10.74	114.93	120.30
1	A	295	PRO	N-CA-CB	10.42	115.80	103.30
1	B	226	SER	C-N-CA	10.17	147.13	121.70
1	A	81	LEU	CB-CG-CD2	10.02	128.04	111.00
2	X	68	ARG	CD-NE-CZ	9.87	137.42	123.60
2	Y	112	ARG	NE-CZ-NH1	9.61	125.11	120.30
2	X	45	ARG	NE-CZ-NH2	-9.33	115.64	120.30
1	B	208	PRO	N-CA-CB	9.27	114.43	103.30
1	A	99	TRP	CA-CB-CG	9.08	130.95	113.70
1	B	295	PRO	N-CA-CB	9.02	114.12	103.30
1	B	208	PRO	CA-N-CD	-8.98	98.92	111.50
2	Y	125	ARG	NE-CZ-NH1	8.96	124.78	120.30
2	X	18	ASP	CB-CG-OD1	8.95	126.35	118.30
1	B	295	PRO	N-CD-CG	8.89	116.53	103.20
1	A	295	PRO	CA-N-CD	-8.83	99.14	111.50
1	A	295	PRO	N-CD-CG	8.82	116.43	103.20
2	Y	61	ARG	CD-NE-CZ	8.78	135.89	123.60
1	B	208	PRO	N-CD-CG	8.65	116.17	103.20
1	B	234	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	B	42	GLU	CA-CB-CG	8.57	132.26	113.40
1	B	295	PRO	CA-N-CD	-8.53	99.56	111.50
1	B	50	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	B	227	GLN	CB-CG-CD	8.42	133.48	111.60
1	B	9	ALA	N-CA-CB	8.28	121.69	110.10
1	A	208	PRO	N-CA-CB	8.13	113.05	103.30
1	A	207	SER	O-C-N	8.06	136.41	121.10
2	X	114	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	B	63	LYS	CA-CB-CG	7.95	130.88	113.40
2	X	45	ARG	CD-NE-CZ	7.92	134.69	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	287	TYR	CB-CG-CD1	-7.92	116.25	121.00
1	B	48	ILE	CA-CB-CG2	7.89	126.67	110.90
1	A	239	LYS	CA-CB-CG	7.81	130.58	113.40
1	A	99	TRP	N-CA-CB	7.79	124.62	110.60
1	A	214	SER	C-N-CA	7.66	140.86	121.70
2	X	87	ASP	CB-CG-OD1	7.59	125.13	118.30
1	A	215	LEU	CB-CG-CD1	7.54	123.82	111.00
1	B	102	TYR	CB-CG-CD1	7.51	125.51	121.00
1	B	100	ASP	CA-CB-CG	7.47	129.83	113.40
1	B	90	ASP	CB-CG-OD2	7.39	124.95	118.30
1	B	291	HIS	CA-C-O	7.38	135.59	120.10
1	A	287	TYR	CB-CG-CD2	7.31	125.39	121.00
2	X	7	GLU	OE1-CD-OE2	-7.28	114.56	123.30
1	B	231	SER	N-CA-CB	-7.28	99.58	110.50
1	A	98	ARG	CD-NE-CZ	7.25	133.74	123.60
2	X	14[A]	ARG	CD-NE-CZ	7.13	133.58	123.60
2	X	14[B]	ARG	CD-NE-CZ	7.13	133.58	123.60
1	B	98	ARG	NH1-CZ-NH2	-7.12	111.56	119.40
1	B	8	GLY	O-C-N	-7.07	111.38	122.70
1	B	226	SER	O-C-N	-6.93	111.61	122.70
1	A	273	LEU	CA-CB-CG	6.86	131.08	115.30
1	A	226	SER	C-N-CA	6.85	138.83	121.70
1	B	234	ARG	CD-NE-CZ	6.83	133.16	123.60
2	Y	49	GLY	N-CA-C	-6.82	96.04	113.10
1	B	234	ARG	CA-CB-CG	6.72	128.19	113.40
2	Y	73	LYS	N-CA-C	-6.68	92.96	111.00
1	A	104	ASP	CB-CG-OD1	6.66	124.29	118.30
1	B	279	GLU	OE1-CD-OE2	-6.61	115.36	123.30
1	A	231	SER	N-CA-CB	-6.59	100.61	110.50
1	B	31	ASP	CB-CG-OD2	6.53	124.17	118.30
1	A	110	THR	CA-CB-CG2	6.52	121.53	112.40
1	B	201	ASP	CB-CG-OD1	6.51	124.16	118.30
1	A	229	ILE	N-CA-CB	6.50	125.76	110.80
1	B	8	GLY	C-N-CA	6.48	137.89	121.70
2	Y	21	ARG	NE-CZ-NH1	6.47	123.54	120.30
2	X	18	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	A	234	ARG	CD-NE-CZ	6.35	132.49	123.60
1	B	230	ASN	N-CA-C	-6.32	93.94	111.00
1	A	102	TYR	CB-CG-CD2	-6.30	117.22	121.00
1	A	234	ARG	CG-CD-NE	6.30	125.04	111.80
1	B	102	TYR	CB-CG-CD2	-6.28	117.23	121.00
1	B	100	ASP	OD1-CG-OD2	-6.15	111.61	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	50	SER	N-CA-CB	-6.07	101.39	110.50
2	X	55	ILE	CB-CA-C	-6.04	99.52	111.60
1	B	60	TYR	CB-CA-C	-6.03	98.35	110.40
2	X	55	ILE	N-CA-CB	6.00	124.61	110.80
1	A	201	ASP	N-CA-CB	5.95	121.32	110.60
1	B	73	ASP	CB-CG-OD2	5.93	123.63	118.30
2	X	55	ILE	O-C-N	5.87	132.10	122.70
2	X	55	ILE	CA-C-O	-5.85	107.82	120.10
2	Y	123	TRP	CA-CB-CG	-5.81	102.67	113.70
2	X	118	THR	N-CA-CB	-5.69	99.48	110.30
2	X	74	ASN	CB-CA-C	5.68	121.75	110.40
2	Y	13	LYS	CA-C-N	5.67	129.67	117.20
2	Y	72	SER	CA-C-O	5.66	131.98	120.10
1	A	228	ASP	C-N-CA	5.60	135.71	121.70
2	X	11	ALA	N-CA-CB	-5.55	102.33	110.10
1	A	228	ASP	O-C-N	-5.52	113.88	122.70
1	A	294	SER	CA-C-N	5.46	132.40	117.10
1	A	8	GLY	CA-C-N	5.45	129.19	117.20
1	A	71	THR	N-CA-CB	-5.43	99.99	110.30
1	B	215	LEU	CA-CB-CG	5.42	127.75	115.30
1	A	84	SER	N-CA-CB	-5.40	102.40	110.50
1	A	102	TYR	CB-CG-CD1	5.40	124.24	121.00
1	B	293	GLU	CA-CB-CG	5.39	125.27	113.40
1	A	3	LYS	CA-CB-CG	5.39	125.26	113.40
1	B	48	ILE	CB-CG1-CD1	-5.38	98.84	113.90
1	A	269	GLN	CA-CB-CG	5.33	125.12	113.40
1	A	61	ASP	N-CA-C	-5.31	96.66	111.00
2	X	68	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	A	228	ASP	CA-C-N	5.28	128.82	117.20
1	A	281	ASP	N-CA-CB	-5.25	101.14	110.60
1	A	18	VAL	CG1-CB-CG2	-5.24	102.52	110.90
1	B	281	ASP	CB-CA-C	-5.23	99.94	110.40
2	X	7	GLU	CA-CB-CG	5.20	124.84	113.40
1	B	267	SER	N-CA-CB	5.19	118.29	110.50
1	A	226	SER	O-C-N	-5.16	114.45	122.70
1	B	8	GLY	N-CA-C	5.15	125.98	113.10
1	A	8	GLY	O-C-N	-5.15	114.46	122.70
1	A	297	THR	N-CA-CB	-5.14	100.53	110.30
1	B	229	ILE	CG1-CB-CG2	5.14	122.70	111.40
2	X	48	ASP	CB-CG-OD2	5.13	122.92	118.30
1	B	229	ILE	N-CA-C	-5.13	97.15	111.00
2	X	66	ASP	CB-CG-OD2	-5.12	113.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	X	70	PRO	N-CA-C	5.12	125.40	112.10
2	X	114	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	8	GLY	CA-C-N	5.09	128.41	117.20
2	X	20	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	A	100	ASP	CB-CG-OD2	-5.05	113.76	118.30
1	A	214	SER	CA-C-O	5.05	130.70	120.10
1	A	110	THR	CA-C-O	5.04	130.67	120.10
1	B	76	SER	N-CA-CB	-5.02	102.97	110.50

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	SER	Mainchain,Peptide
1	A	294	SER	Mainchain,Peptide
1	B	207	SER	Mainchain,Peptide
1	B	294	SER	Mainchain,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	1727	0	1646	69	0
1	B	1727	0	1646	89	0
2	X	1001	0	965	21	0
2	Y	994	0	956	34	0
3	A	74	0	0	6	0
3	B	105	0	0	4	0
3	X	53	0	0	3	0
3	Y	28	0	0	0	0
All	All	5709	0	5213	202	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 19.

All (202) 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:30:LYS:HE3	1:A:74:THR:HB	1.43	1.01
1:A:71:THR:HG22	1:A:80:TYR:HB2	1.42	0.99
1:A:278:LEU:HD21	1:A:306:ILE:HD12	1.47	0.96
1:A:35:HIS:HD2	1:A:47:TRP:HE1	1.10	0.95
1:B:29:ILE:H	1:B:77:ASN:HD21	1.11	0.94
1:B:43:GLN:HE21	1:B:44:GLY:H	1.15	0.94
1:B:229:ILE:HG21	1:B:232:TYR:HB2	1.49	0.92
1:B:229:ILE:HG12	1:B:232:TYR:HD2	1.34	0.91
1:B:35:HIS:HD2	1:B:47:TRP:HE1	1.14	0.90
1:B:6:GLN:H	1:B:108:GLN:HE22	1.19	0.89
1:B:29:ILE:H	1:B:77:ASN:ND2	1.71	0.88
1:B:1:GLN:HE22	1:B:3:LYS:HE3	1.38	0.87
1:A:108:GLN:HE21	1:A:108:GLN:H	1.23	0.87
2:Y:13:LYS:O	2:Y:14:ARG:HB3	1.75	0.86
1:B:229:ILE:HG12	1:B:232:TYR:CD2	2.10	0.86
1:B:83:LEU:HB3	1:B:86:LEU:HD21	1.56	0.85
1:A:233:LEU:HD11	1:A:288:CYS:HB2	1.60	0.84
1:B:229:ILE:CG2	1:B:232:TYR:H	1.90	0.83
1:B:290:GLN:NE2	1:B:292:GLY:H	1.78	0.81
1:A:6:GLN:H	1:A:108:GLN:HE22	1.28	0.80
1:A:261:ARG:HH11	1:A:279:GLU:HG2	1.48	0.78
1:A:290:GLN:NE2	1:A:292:GLY:H	1.81	0.77
1:A:290:GLN:HG3	1:A:297:THR:HG22	1.64	0.77
1:A:35:HIS:CD2	1:A:47:TRP:HE1	2.01	0.76
1:B:43:GLN:NE2	1:B:44:GLY:H	1.85	0.75
1:B:290:GLN:HG3	1:B:297:THR:HG22	1.69	0.75
1:A:290:GLN:HE22	1:A:293:GLU:H	1.35	0.75
1:B:228:ASP:O	1:B:229:ILE:HB	1.87	0.74
1:B:229:ILE:HG23	1:B:232:TYR:H	1.51	0.74
2:Y:1:LYS:HD3	2:Y:41:HIS:ND1	2.02	0.74
1:B:35:HIS:CD2	1:B:47:TRP:HE1	2.04	0.73
1:B:290:GLN:HE22	1:B:293:GLU:H	1.37	0.71
1:A:87:THR:CG2	1:B:67:LYS:HG3	2.20	0.70
1:B:227:GLN:HB2	3:B:2095:HOH:O	1.89	0.70
1:B:29:ILE:N	1:B:77:ASN:HD21	1.86	0.70
1:B:81:LEU:HD12	1:B:83:LEU:HD22	1.72	0.69
1:A:2:VAL:HG13	3:A:2009:HOH:O	1.92	0.69
2:X:63:TRP:O	2:X:76:CYS:HB2	1.95	0.67
1:A:239:LYS:HA	1:A:284:THR:HG22	1.75	0.67
1:B:229:ILE:HG21	1:B:232:TYR:CB	2.24	0.67
1:B:98:ARG:O	1:B:98:ARG:HG3	1.95	0.66
1:A:29:ILE:H	1:A:77:ASN:HD21	1.41	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:LYS:H	1:A:30:LYS:NZ	1.93	0.65
2:Y:59:ASN:ND2	2:Y:61:ARG:HB3	2.12	0.65
1:A:87:THR:HG21	1:B:67:LYS:HG3	1.78	0.65
2:Y:50:SER:HB2	2:Y:60:SER:OG	1.97	0.65
1:A:33:TYR:H	2:X:103:ASN:ND2	1.94	0.65
1:A:261:ARG:NH1	1:A:279:GLU:HG2	2.11	0.65
1:A:290:GLN:CG	1:A:297:THR:HG22	2.28	0.63
2:Y:61:ARG:O	2:Y:72:SER:HA	1.98	0.63
1:A:230:ASN:HB2	3:A:2065:HOH:O	1.99	0.63
1:B:30:LYS:H	1:B:30:LYS:CD	2.13	0.62
1:A:290:GLN:HE21	1:A:292:GLY:H	1.45	0.62
1:B:290:GLN:HE21	1:B:292:GLY:H	1.45	0.62
1:A:237:GLN:HB2	1:A:247:LEU:HD11	1.81	0.62
2:Y:50:SER:HB3	2:Y:69:THR:HG21	1.81	0.61
1:A:18:VAL:HG22	1:A:86:LEU:HD11	1.82	0.61
1:B:30:LYS:HE2	3:B:2050:HOH:O	2.00	0.61
2:X:25:LEU:HD23	2:X:129:LEU:HD21	1.82	0.61
1:A:227:GLN:H	1:A:269:GLN:HG2	1.65	0.61
1:B:290:GLN:CG	1:B:297:THR:HG22	2.31	0.60
2:Y:50:SER:HB3	2:Y:69:THR:CG2	2.31	0.60
1:A:30:LYS:H	1:A:30:LYS:HZ2	1.47	0.60
1:B:30:LYS:HD2	1:B:74:THR:HB	1.83	0.59
1:B:1:GLN:NE2	1:B:3:LYS:HE3	2.13	0.59
1:B:219:VAL:HG11	1:B:304:LEU:HD11	1.85	0.59
1:A:202:ILE:O	1:A:297:THR:HG21	2.04	0.58
1:B:28:ASN:HB3	1:B:30:LYS:HG2	1.84	0.58
2:Y:20:TYR:CE1	2:Y:21:ARG:HG2	2.39	0.58
1:B:6:GLN:N	1:B:108:GLN:HE22	1.98	0.58
1:B:6:GLN:HB3	1:B:110:THR:CG2	2.33	0.58
2:X:14[B]:ARG:NH2	3:X:2009:HOH:O	2.26	0.57
1:A:84:SER:HB3	1:B:85:SER:OG	2.04	0.57
2:Y:60:SER:HB2	2:Y:80:CYS:SG	2.45	0.57
2:Y:121:HIS:CE1	2:Y:125:ARG:HH11	2.22	0.57
1:B:6:GLN:HB3	1:B:110:THR:HG23	1.86	0.56
2:X:115:CYS:O	2:X:118:THR:HB	2.05	0.56
1:B:221:ILE:HG12	1:B:302:THR:HG21	1.87	0.56
1:A:229:ILE:HG13	1:A:230:ASN:H	1.71	0.56
1:B:7:SER:O	1:B:110:THR:HG22	2.07	0.55
2:Y:59:ASN:HD21	2:Y:61:ARG:HB3	1.69	0.55
1:A:29:ILE:H	1:A:77:ASN:ND2	2.04	0.55
1:B:233:LEU:HD11	1:B:288:CYS:HB2	1.87	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:261:ARG:HH11	1:B:279:GLU:HG2	1.72	0.54
1:B:290:GLN:NE2	1:B:292:GLY:N	2.54	0.54
2:Y:18:ASP:HB2	2:Y:25:LEU:HD23	1.89	0.54
1:B:227:GLN:HA	1:B:269:GLN:HG3	1.89	0.54
1:B:48:ILE:HG13	1:B:49:GLY:N	2.23	0.53
1:B:81:LEU:HD12	1:B:83:LEU:CD2	2.37	0.53
2:Y:61:ARG:HA	2:Y:69:THR:HG21	1.91	0.53
1:A:99:TRP:CH2	1:A:106:TRP:CZ2	2.97	0.53
1:A:283:THR:O	1:A:284:THR:HG23	2.09	0.52
1:B:30:LYS:H	1:B:30:LYS:HD3	1.75	0.52
2:X:59:ASN:ND2	2:X:61:ARG:H	2.07	0.51
1:A:6:GLN:HB3	1:A:110:THR:HG22	1.92	0.51
1:A:6:GLN:H	1:A:108:GLN:NE2	2.01	0.51
1:B:33:TYR:H	2:Y:103:ASN:ND2	2.08	0.51
1:B:59:LYS:HG3	3:B:2102:HOH:O	2.11	0.51
1:B:81:LEU:HD11	1:B:83:LEU:HD13	1.93	0.51
1:B:228:ASP:O	1:B:229:ILE:CB	2.48	0.50
1:B:204:LEU:HG	1:B:297:THR:HG23	1.94	0.50
1:A:27:PHE:CE1	1:A:32:THR:HG21	2.47	0.50
2:Y:11:ALA:HB1	2:Y:88:ILE:HD13	1.93	0.49
2:Y:15:LEU:HD13	2:Y:92:VAL:HG21	1.94	0.49
1:A:30:LYS:CE	1:A:74:THR:HB	2.29	0.49
1:A:28:ASN:HB3	1:A:30:LYS:NZ	2.27	0.49
1:A:214:SER:O	1:A:216:GLY:N	2.42	0.49
2:X:61:ARG:HH11	2:X:61:ARG:HG3	1.77	0.49
1:A:35:HIS:HE1	2:X:102:GLY:O	1.95	0.49
2:X:111:TRP:CD1	2:X:115:CYS:HB2	2.47	0.49
1:A:204:LEU:HG	1:A:297:THR:HG23	1.94	0.49
1:B:28:ASN:HB3	1:B:30:LYS:CG	2.42	0.49
2:X:61:ARG:HD2	3:X:2029:HOH:O	2.11	0.49
1:A:290:GLN:NE2	1:A:292:GLY:N	2.56	0.48
1:A:229:ILE:HG13	1:A:230:ASN:N	2.28	0.48
1:A:30:LYS:HE3	1:A:74:THR:CB	2.30	0.48
1:B:48:ILE:HD11	1:B:81:LEU:HD21	1.95	0.48
1:B:204:LEU:CD2	1:B:225:ALA:HB2	2.44	0.48
1:B:103:PHE:HE2	2:Y:62:TRP:HH2	1.60	0.48
1:B:229:ILE:HD13	1:B:292:GLY:O	2.13	0.48
2:Y:45:ARG:HD3	2:Y:68:ARG:HH12	1.79	0.48
1:B:261:ARG:HD2	1:B:279:GLU:OE2	2.14	0.47
1:B:290:GLN:HG3	1:B:297:THR:CG2	2.41	0.47
2:Y:66:ASP:HB3	2:Y:80:CYS:SG	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:GLN:O	1:A:284:THR:HB	2.14	0.47
2:X:33:LYS:HG2	2:X:123:TRP:CH2	2.49	0.47
1:A:33:TYR:H	2:X:103:ASN:HD21	1.59	0.47
1:A:239:LYS:HB3	1:A:240:PRO:HD2	1.95	0.47
2:Y:15:LEU:CD1	2:Y:88:ILE:HG12	2.45	0.47
2:Y:14:ARG:O	2:Y:16:GLY:N	2.48	0.47
1:B:215:LEU:HD13	1:B:280:SER:HB2	1.97	0.47
1:A:219:VAL:HG21	1:A:278:LEU:HD13	1.97	0.47
1:B:284:THR:HB	1:B:285:THR:H	1.65	0.47
2:Y:27:ASN:ND2	2:Y:120:VAL:HG21	2.29	0.47
2:Y:73:LYS:HD2	2:Y:73:LYS:N	2.30	0.46
1:B:6:GLN:HE21	1:B:107:GLY:HA3	1.80	0.46
1:B:209:SER:HB2	3:B:2071:HOH:O	2.16	0.46
1:B:214:SER:O	1:B:216:GLY:N	2.42	0.46
2:X:109:VAL:O	2:X:112:ARG:HB2	2.15	0.46
1:B:237:GLN:HG2	1:B:284:THR:HG21	1.98	0.46
1:B:19:LYS:HE2	1:B:80:TYR:CD2	2.51	0.46
1:B:6:GLN:NE2	1:B:109:GLY:H	2.14	0.45
1:A:35:HIS:CD2	1:A:50:ARG:HB3	2.52	0.45
2:X:25:LEU:CD2	2:X:129:LEU:HD21	2.47	0.45
1:B:81:LEU:CD1	1:B:83:LEU:HD13	2.46	0.45
1:A:27:PHE:HD2	3:A:2009:HOH:O	2.00	0.45
2:X:61:ARG:O	2:X:72:SER:HA	2.15	0.45
1:B:98:ARG:HH11	1:B:103:PHE:HB3	1.81	0.45
1:A:289:LEU:HD11	1:A:296:TYR:HB3	1.97	0.45
2:X:14[B]:ARG:NH1	3:X:2009:HOH:O	2.50	0.45
2:Y:56:LEU:HB2	2:Y:58:ILE:HD11	1.99	0.45
1:A:295:PRO:HD2	3:A:2070:HOH:O	2.16	0.45
1:B:235:TRP:HB2	1:B:248:ILE:HB	1.99	0.45
1:A:261:ARG:HD2	1:A:279:GLU:CD	2.38	0.44
2:Y:59:ASN:ND2	2:Y:61:ARG:H	2.14	0.44
1:A:99:TRP:HH2	1:A:106:TRP:CZ2	2.34	0.44
1:B:51:ILE:HD12	1:B:52:ASP:N	2.32	0.44
1:B:59:LYS:HD2	1:B:59:LYS:HA	1.62	0.44
1:B:213:THR:HG21	1:B:219:VAL:HG21	1.98	0.44
1:B:261:ARG:NH1	1:B:279:GLU:HG2	2.33	0.44
1:B:32:THR:HB	2:Y:103:ASN:HD21	1.81	0.44
2:Y:88:ILE:HG13	2:Y:92:VAL:HG23	1.99	0.44
1:A:27:PHE:HE1	1:A:32:THR:HG21	1.82	0.43
1:A:227:GLN:HA	1:A:269:GLN:HG3	1.99	0.43
1:B:108:GLN:NE2	1:B:108:GLN:H	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:ASN:HA	1:B:77:ASN:HD21	1.82	0.43
2:Y:55:ILE:H	2:Y:55:ILE:HG13	1.45	0.43
2:Y:40:THR:O	2:Y:84:LEU:HA	2.17	0.43
1:A:3:LYS:NZ	1:A:5:GLN:HB2	2.33	0.43
1:B:33:TYR:H	2:Y:103:ASN:HD21	1.65	0.43
1:B:102:TYR:HA	1:B:249:TYR:CE2	2.53	0.43
1:B:202:ILE:O	1:B:297:THR:HG21	2.18	0.43
2:Y:51:THR:HB	2:Y:53:TYR:CE2	2.53	0.43
1:B:73:ASP:CG	1:B:76:SER:HB3	2.39	0.43
1:A:208:PRO:HG2	1:A:211:MET:CE	2.49	0.43
1:B:204:LEU:HD23	1:B:225:ALA:HB2	2.00	0.43
2:X:58:ILE:HB	2:X:83:LEU:HD13	2.01	0.43
1:B:51:ILE:HD13	1:B:57:ASN:O	2.19	0.42
1:B:227:GLN:HA	1:B:269:GLN:CG	2.48	0.42
1:A:239:LYS:CA	1:A:284:THR:HG22	2.44	0.42
1:A:12:VAL:HG11	1:A:18:VAL:CG1	2.49	0.42
1:B:6:GLN:HE22	1:B:95:TYR:HA	1.85	0.42
1:A:229:ILE:HG23	1:A:232:TYR:CD2	2.54	0.42
2:X:19:ASN:HD22	2:X:19:ASN:HA	1.69	0.42
1:A:51:ILE:O	1:A:53:PRO:HD3	2.20	0.42
1:A:213:THR:OG1	1:A:278:LEU:HD22	2.20	0.42
1:B:283:THR:O	1:B:284:THR:HG23	2.19	0.42
1:B:291:HIS:HA	1:B:296:TYR:CD1	2.54	0.42
2:X:63:TRP:CE2	2:X:98:ILE:HG12	2.54	0.42
1:A:250:TYR:O	1:A:251:ALA:HB3	2.20	0.41
2:Y:60:SER:HG	2:Y:69:THR:HG1	1.66	0.41
1:A:239:LYS:HG3	1:A:284:THR:CG2	2.50	0.41
1:B:51:ILE:HD11	1:B:56:GLY:HA2	2.02	0.41
1:A:291:HIS:HE1	3:A:2064:HOH:O	2.03	0.41
2:Y:69:THR:HA	2:Y:70:PRO:HD3	1.77	0.41
1:B:227:GLN:O	1:B:228:ASP:C	2.58	0.41
1:A:291:HIS:HD2	2:X:100:SER:O	2.03	0.41
1:B:224:LYS:HG2	1:B:270:ASP:OD1	2.22	0.40
1:A:71:THR:HB	3:A:2030:HOH:O	2.21	0.40
2:X:59:ASN:ND2	2:X:61:ARG:HB3	2.36	0.40
2:Y:52:ASP:HB3	2:Y:57:GLN:HB3	2.02	0.40
1:A:235:TRP:HB2	1:A:248:ILE:HB	2.03	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	220/253 (87%)	200 (91%)	13 (6%)	7 (3%)	4 1
1	B	220/253 (87%)	202 (92%)	10 (4%)	8 (4%)	3 1
2	X	128/129 (99%)	123 (96%)	4 (3%)	1 (1%)	19 13
2	Y	127/129 (98%)	106 (84%)	18 (14%)	3 (2%)	6 2
All	All	695/764 (91%)	631 (91%)	45 (6%)	19 (3%)	5 1

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	LEU
1	A	229	ILE
1	A	276	SER
1	B	8	GLY
1	B	215	LEU
1	B	228	ASP
1	B	229	ILE
2	Y	15	LEU
2	Y	50	SER
1	A	227	GLN
1	A	228	ASP
1	B	276	SER
2	Y	14	ARG
1	B	216	GLY
2	X	128	ARG
1	A	208	PRO
1	B	208	PRO
1	A	216	GLY
1	B	306	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	191/207 (92%)	161 (84%)	30 (16%)	2 1
1	B	191/207 (92%)	165 (86%)	26 (14%)	3 2
2	X	104/103 (101%)	97 (93%)	7 (7%)	16 11
2	Y	103/103 (100%)	85 (82%)	18 (18%)	2 1
All	All	589/620 (95%)	508 (86%)	81 (14%)	3 2

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	GLN
1	A	7	SER
1	A	13	LYS
1	A	30	LYS
1	A	43	GLN
1	A	59	LYS
1	A	63	LYS
1	A	71	THR
1	A	75	SER
1	A	76	SER
1	A	77	ASN
1	A	81	LEU
1	A	88	SER
1	A	108	GLN
1	A	110	THR
1	A	116	SER
1	A	203	GLU
1	A	213	THR
1	A	215	LEU
1	A	227	GLN
1	A	230	ASN
1	A	239	LYS
1	A	245	LYS
1	A	273	LEU

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Mol	Chain	Res	Type
1	A	279	GLU
1	A	283	THR
1	A	290	GLN
1	A	297	THR
1	A	304	LEU
1	A	306	ILE
1	B	1	GLN
1	B	11	LEU
1	B	17	SER
1	B	30	LYS
1	B	43	GLN
1	B	48	ILE
1	B	51	ILE
1	B	59	LYS
1	B	77	ASN
1	B	81	LEU
1	B	84	SER
1	B	98	ARG
1	B	108	GLN
1	B	201	ASP
1	B	213	THR
1	B	226	SER
1	B	227	GLN
1	B	230	ASN
1	B	239	LYS
1	B	278	LEU
1	B	279	GLU
1	B	283	THR
1	B	290	GLN
1	B	294	SER
1	B	303	LYS
1	B	304	LEU
2	X	1	LYS
2	X	55	ILE
2	X	73	LYS
2	X	75	LEU
2	X	103	ASN
2	X	118	THR
2	X	128	ARG
2	Y	1	LYS
2	Y	13	LYS
2	Y	19	ASN

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Mol	Chain	Res	Type
2	Y	25	LEU
2	Y	41	HIS
2	Y	46	ASN
2	Y	55	ILE
2	Y	60	SER
2	Y	61	ARG
2	Y	73	LYS
2	Y	75	LEU
2	Y	78	ILE
2	Y	85	SER
2	Y	88	ILE
2	Y	91	SER
2	Y	103	ASN
2	Y	128	ARG
2	Y	129	LEU

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

Mol	Chain	Res	Type
1	A	1	GLN
1	A	35	HIS
1	A	43	GLN
1	A	77	ASN
1	A	82	GLN
1	A	108	GLN
1	A	227	GLN
1	A	237	GLN
1	A	290	GLN
1	A	291	HIS
1	B	1	GLN
1	B	6	GLN
1	B	35	HIS
1	B	43	GLN
1	B	77	ASN
1	B	108	GLN
1	B	237	GLN
1	B	290	GLN
1	B	291	HIS
2	X	19	ASN
2	X	44	ASN
2	X	46	ASN
2	X	57	GLN

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Mol	Chain	Res	Type
2	X	59	ASN
2	X	65	ASN
2	X	93	ASN
2	X	103	ASN
2	Y	59	ASN
2	Y	93	ASN
2	Y	103	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 monosaccharides 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(Å^2)	Q<0.9
1	A	224/253 (88%)	0.46	17 (7%)	13	13	15, 27, 70, 80	0
1	B	224/253 (88%)	0.40	24 (10%)	6	5	11, 24, 68, 79	0
2	X	129/129 (100%)	-0.25	1 (0%)	86	85	12, 20, 32, 51	0
2	Y	129/129 (100%)	1.46	41 (31%)	0	0	15, 43, 73, 80	0
All	All	706/764 (92%)	0.49	83 (11%)	4	4	11, 27, 69, 80	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Y	48	ASP	8.3
1	B	117	GLY	7.6
2	Y	129	LEU	6.6
1	B	229	ILE	6.3
1	A	215	LEU	5.9
2	Y	46	ASN	5.5
1	B	228	ASP	5.4
2	Y	67	GLY	5.1
1	B	306	ILE	5.1
1	A	228	ASP	4.9
1	B	116	SER	4.8
2	Y	47	THR	4.8
1	B	230	ASN	4.8
1	A	1	GLN	4.7
1	A	7	SER	4.7
2	Y	70	PRO	4.6
2	Y	128	ARG	4.5
1	A	230	ASN	4.3
1	A	212	TYR	4.3
2	Y	126	GLY	4.2
2	Y	83	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	261	ARG	4.0
1	B	212	TYR	3.9
1	A	307	LYS	3.9
2	Y	84	LEU	3.8
2	Y	2	VAL	3.8
2	Y	72	SER	3.8
1	A	276	SER	3.7
1	A	306	ILE	3.6
2	Y	68	ARG	3.6
1	A	229	ILE	3.6
1	A	260	SER	3.5
1	B	277	SER	3.5
2	Y	127	CYS	3.4
2	Y	71	GLY	3.2
2	Y	36	SER	3.1
2	Y	3	TYR	3.0
2	Y	14	ARG	2.9
1	B	215	LEU	2.9
2	Y	69	THR	2.7
1	A	257	GLY	2.7
1	B	278	LEU	2.7
2	Y	56	LEU	2.7
2	Y	39	ASN	2.7
2	Y	124	ILE	2.7
1	B	213	THR	2.7
2	Y	45	ARG	2.7
1	B	1	GLN	2.7
2	Y	90	ALA	2.6
2	Y	86	SER	2.6
2	Y	125	ARG	2.6
2	Y	37	ASN	2.6
1	A	261	ARG	2.6
2	Y	41	HIS	2.6
2	Y	53	TYR	2.6
1	A	239	LYS	2.6
1	B	281	ASP	2.5
1	A	281	ASP	2.5
1	B	201	ASP	2.5
2	Y	58	ILE	2.5
2	Y	50	SER	2.5
2	Y	15	LEU	2.5
1	B	260	SER	2.4

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Mol	Chain	Res	Type	RSRZ
2	Y	38	PHE	2.4
2	Y	44	ASN	2.3
1	B	241	GLY	2.3
1	B	227	GLN	2.3
1	A	278	LEU	2.3
1	B	292	GLY	2.3
2	Y	43	THR	2.2
2	Y	6	CYS	2.2
1	B	286	TYR	2.2
2	Y	49	GLY	2.2
1	B	226	SER	2.2
2	Y	79	PRO	2.2
1	A	203	GLU	2.2
1	B	42	GLU	2.2
1	B	207	SER	2.1
2	Y	40	THR	2.1
2	X	62	TRP	2.1
2	Y	113	ASN	2.1
1	B	43	GLN	2.0
2	Y	123	TRP	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 monosaccharides 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.