Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 02:06 PM EDT

PDB ID	:	1S4I
Title	:	Crystal structure of a SOD-like protein from Bacillus subtilis
Authors	:	Banci, L.; Bertini, I.; Calderone, V.; Cramaro, F.; Del Conte, R.; Fantoni, A.; Mangani, S.; Quattrone, A.; Viezzoli, M.S.
Deposited on	:	2004-01-16
Resolution	:	1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ 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 ⓘ) were used in the production of this report:

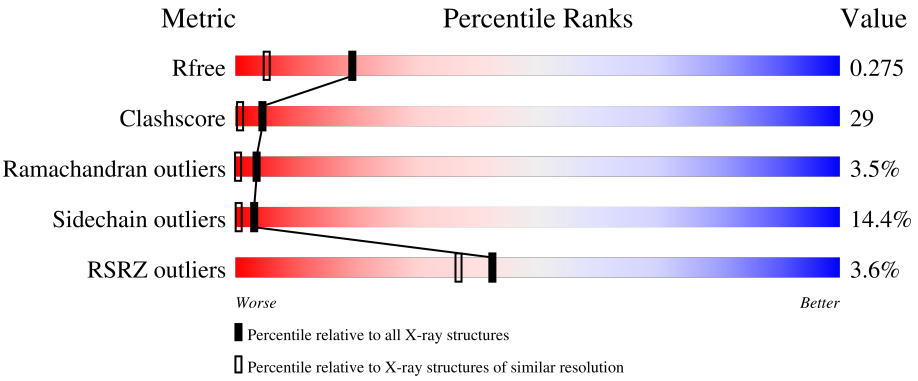
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	175	2% 48% 28% 8% • 14%
1	B	175	% 55% 19% 9% • 13%
1	C	175	4% 43% 30% 8% 5% 14%
1	D	175	5% 46% 30% 6% 5% 14%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4920 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 superoxide dismutase-like protein yojM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	152	Total	C	N	O	S	0	0	0
			1133	704	201	224	4			
1	A	151	Total	C	N	O	S	0	0	0
			1129	702	200	223	4			
1	C	151	Total	C	N	O	S	0	0	0
			1129	702	200	223	4			
1	D	151	Total	C	N	O	S	0	0	0
			1129	702	200	223	4			

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Zn	0	0
			2	2		
2	A	2	Total	Zn	0	0
			2	2		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Cl	0	0
			1	1		
3	A	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

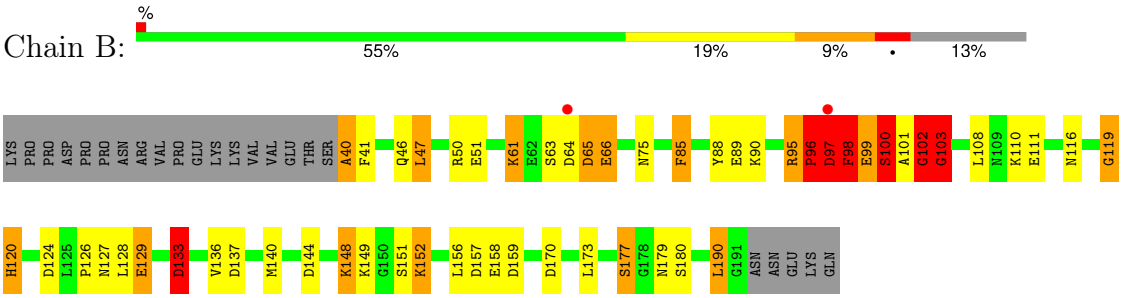
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	117	Total O 117 117	0	0
4	A	93	Total O 93 93	0	0
4	C	83	Total O 83 83	0	0
4	D	97	Total O 97 97	0	0

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.

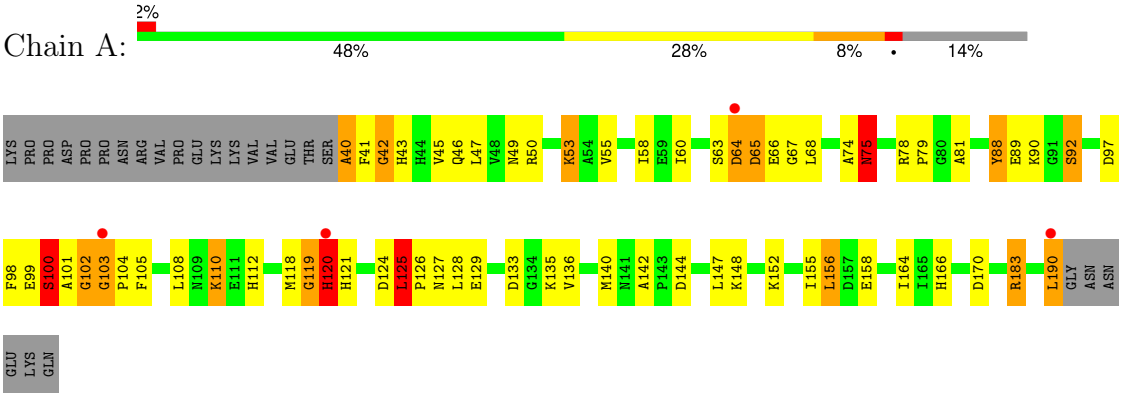
• Molecule 1: superoxide dismutase-like protein yojM

Chain B:



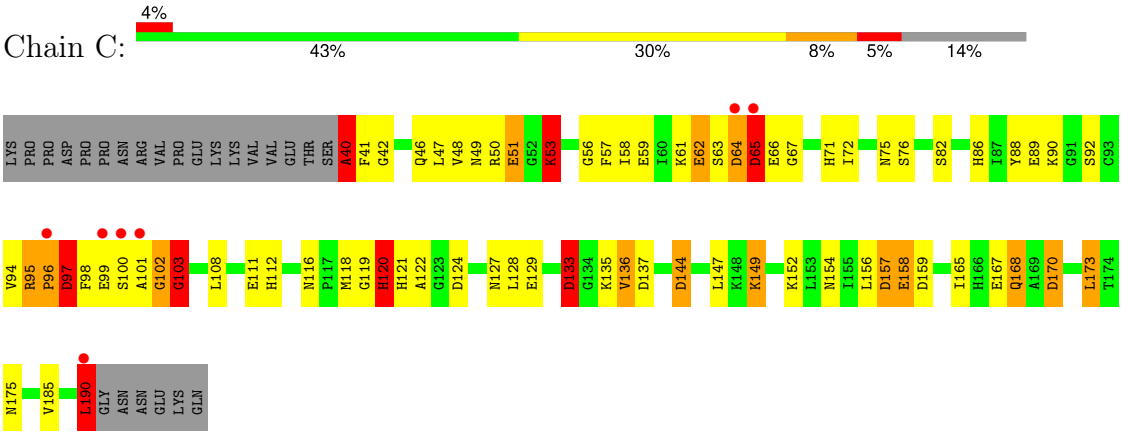
• Molecule 1: superoxide dismutase-like protein yojM

Chain A:



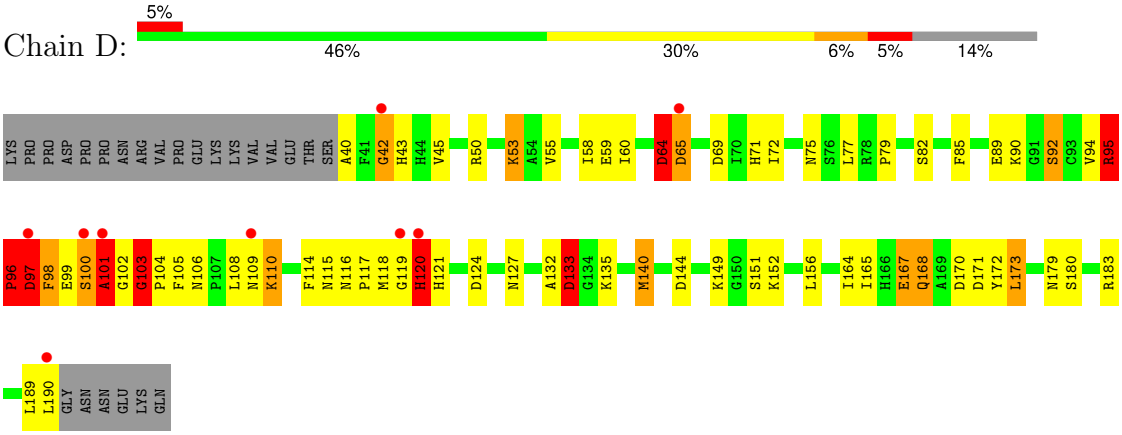
• Molecule 1: superoxide dismutase-like protein yojM

Chain C:



• Molecule 1: superoxide dismutase-like protein yojM

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	38.23Å 61.11Å 64.92Å 84.35° 76.02° 90.42°	Depositor
Resolution (Å)	37.01 – 1.80 37.07 – 1.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (37.01-1.80) 94.6 (37.07-1.80)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.03	Depositor
$< I/\sigma(I) >$ [1]	3.54 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.221 , 0.258 0.250 , 0.275	Depositor DCC
R_{free} test set	8080 reflections (8.35%)	wwPDB-VP
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	0.372	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 52.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4920	wwPDB-VP
Average B, all atoms (Å^2)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.09% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CL

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	1.19	4/1153 (0.3%)	1.35	12/1558 (0.8%)
1	B	1.43	7/1157 (0.6%)	1.66	24/1563 (1.5%)
1	C	1.17	2/1153 (0.2%)	1.49	22/1558 (1.4%)
1	D	1.39	12/1153 (1.0%)	1.62	29/1558 (1.9%)
All	All	1.30	25/4616 (0.5%)	1.54	87/6237 (1.4%)

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	1	7
1	B	0	7
1	C	0	4
1	D	1	10
All	All	2	28

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	120	HIS	C-N	10.92	1.59	1.34
1	D	96	PRO	N-CD	10.68	1.62	1.47
1	B	97	ASP	C-N	-9.45	1.12	1.34
1	B	96	PRO	C-N	-9.45	1.12	1.34
1	D	65	ASP	C-O	8.58	1.39	1.23
1	D	65	ASP	C-N	-8.52	1.14	1.34
1	D	102	GLY	C-N	-8.49	1.17	1.33
1	B	97	ASP	C-O	7.74	1.38	1.23
1	D	97	ASP	C-N	6.85	1.49	1.34
1	D	104	PRO	N-CD	6.78	1.57	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	96	PRO	C-O	6.71	1.36	1.23
1	C	41	PHE	C-N	6.38	1.44	1.33
1	D	59	GLU	CD-OE2	6.37	1.32	1.25
1	A	119	GLY	N-CA	-6.11	1.36	1.46
1	B	95	ARG	C-N	5.94	1.45	1.34
1	D	102	GLY	CA-C	-5.66	1.42	1.51
1	A	105	PHE	CG-CD2	5.53	1.47	1.38
1	D	59	GLU	CD-OE1	5.42	1.31	1.25
1	C	136	VAL	CB-CG1	-5.41	1.41	1.52
1	A	105	PHE	CE2-CZ	5.30	1.47	1.37
1	B	180	SER	CA-CB	5.30	1.60	1.52
1	B	100	SER	CB-OG	5.29	1.49	1.42
1	D	95	ARG	N-CA	-5.20	1.35	1.46
1	D	114	PHE	CE2-CZ	5.14	1.47	1.37
1	D	105	PHE	CE1-CZ	5.09	1.47	1.37

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	96	PRO	C-N-CA	19.17	169.61	121.70
1	B	97	ASP	O-C-N	-18.30	93.42	122.70
1	C	137	ASP	CB-CG-OD1	12.74	129.77	118.30
1	D	104	PRO	CA-N-CD	-10.21	97.21	111.50
1	D	65	ASP	CA-C-O	-10.05	98.99	120.10
1	D	96	PRO	CA-N-CD	-9.84	97.72	111.50
1	D	99	GLU	C-N-CA	9.84	146.30	121.70
1	D	95	ARG	NE-CZ-NH1	-9.33	115.64	120.30
1	D	171	ASP	CB-CG-OD1	9.23	126.61	118.30
1	C	133	ASP	CB-CG-OD2	9.22	126.60	118.30
1	B	96	PRO	CA-C-N	8.79	136.53	117.20
1	B	173	LEU	CB-CG-CD1	-8.54	96.48	111.00
1	C	41	PHE	O-C-N	-8.47	108.80	123.20
1	B	96	PRO	CA-C-O	-8.46	99.89	120.20
1	B	97	ASP	CA-C-N	8.21	135.27	117.20
1	A	120	HIS	CA-C-N	-8.21	99.13	117.20
1	C	157	ASP	CB-CG-OD2	8.19	125.67	118.30
1	C	41	PHE	CA-C-N	8.18	132.56	116.20
1	D	103	GLY	C-N-CD	8.08	145.36	128.40
1	D	101	ALA	CB-CA-C	8.05	122.17	110.10
1	C	144	ASP	CB-CG-OD2	8.02	125.52	118.30
1	B	97	ASP	CA-C-O	-8.00	103.30	120.10
1	B	144	ASP	CB-CG-OD2	7.81	125.33	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	102	GLY	O-C-N	-7.65	110.19	123.20
1	D	95	ARG	O-C-N	-7.64	106.58	121.10
1	C	64	ASP	CB-CG-OD2	7.53	125.08	118.30
1	D	95	ARG	CA-C-N	7.41	137.83	117.10
1	C	103	GLY	CA-C-O	-7.27	107.52	120.60
1	C	75	ASN	CB-CA-C	-7.24	95.92	110.40
1	D	95	ARG	N-CA-CB	7.19	123.54	110.60
1	D	104	PRO	O-C-N	-7.18	111.20	122.70
1	D	101	ALA	C-N-CA	-7.06	107.48	122.30
1	C	124	ASP	CB-CG-OD1	7.05	124.64	118.30
1	A	183	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	D	65	ASP	CA-C-N	6.89	132.35	117.20
1	D	97	ASP	CA-C-N	-6.72	102.41	117.20
1	D	98	PHE	O-C-N	-6.71	111.97	122.70
1	B	133	ASP	CB-CG-OD2	6.64	124.28	118.30
1	D	120	HIS	O-C-N	-6.62	112.11	122.70
1	C	97	ASP	CB-CG-OD2	6.61	124.25	118.30
1	D	144	ASP	CB-CG-OD2	6.58	124.22	118.30
1	D	96	PRO	CA-C-N	6.55	131.61	117.20
1	A	65	ASP	CB-CG-OD2	6.54	124.19	118.30
1	B	41	PHE	N-CA-C	-6.48	93.50	111.00
1	C	168	GLN	CB-CA-C	-6.47	97.46	110.40
1	A	120	HIS	CB-CA-C	6.39	123.18	110.40
1	D	102	GLY	CA-C-O	6.38	132.09	120.60
1	B	137	ASP	CB-CG-OD1	6.23	123.90	118.30
1	D	101	ALA	N-CA-CB	6.22	118.81	110.10
1	D	42	GLY	N-CA-C	6.20	128.60	113.10
1	A	64	ASP	CB-CG-OD2	6.17	123.86	118.30
1	B	129	GLU	CG-CD-OE1	-6.13	106.04	118.30
1	D	71	HIS	N-CA-C	-6.10	94.52	111.00
1	C	102	GLY	CA-C-N	6.08	128.36	116.20
1	D	101	ALA	O-C-N	-5.98	113.03	123.20
1	D	100	SER	O-C-N	-5.97	113.14	122.70
1	B	102	GLY	CA-C-N	5.95	128.09	116.20
1	C	41	PHE	CB-CG-CD1	5.84	124.89	120.80
1	C	102	GLY	C-N-CA	5.84	134.57	122.30
1	B	102	GLY	N-CA-C	5.79	127.59	113.10
1	B	98	PHE	O-C-N	-5.71	113.56	122.70
1	B	157	ASP	CB-CG-OD2	5.64	123.38	118.30
1	B	99	GLU	OE1-CD-OE2	-5.63	116.54	123.30
1	A	41	PHE	N-CA-C	-5.62	95.82	111.00
1	A	125	LEU	CB-CG-CD1	-5.55	101.57	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	129	GLU	OE1-CD-OE2	5.48	129.88	123.30
1	C	65	ASP	CB-CG-OD2	5.46	123.21	118.30
1	C	40	ALA	C-N-CA	5.46	135.34	121.70
1	A	119	GLY	N-CA-C	5.46	126.74	113.10
1	C	137	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	B	100	SER	N-CA-CB	-5.44	102.34	110.50
1	C	119	GLY	N-CA-C	5.39	126.57	113.10
1	B	47	LEU	CB-CG-CD1	-5.38	101.85	111.00
1	B	124	ASP	CB-CG-OD2	5.37	123.13	118.30
1	A	156	LEU	CA-CB-CG	5.37	127.65	115.30
1	B	133	ASP	CB-CA-C	-5.35	99.70	110.40
1	A	75	ASN	CB-CA-C	5.33	121.06	110.40
1	C	120	HIS	CB-CA-C	5.33	121.05	110.40
1	C	190	LEU	CA-CB-CG	5.31	127.51	115.30
1	B	85	PHE	CB-CG-CD1	5.25	124.48	120.80
1	A	144	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	104	PRO	N-CA-C	-5.17	98.65	112.10
1	D	64	ASP	CB-CG-OD2	5.14	122.93	118.30
1	D	69	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	85	PHE	CB-CG-CD2	-5.11	117.22	120.80
1	C	170	ASP	CB-CG-OD1	5.09	122.88	118.30
1	D	118	MET	CB-CG-SD	-5.02	97.33	112.40

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	120	HIS	CA
1	D	101	ALA	CA

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	100	SER	Peptide
1	A	102	GLY	Peptide
1	A	103	GLY	Peptide
1	A	119	GLY	Mainchain
1	A	40	ALA	Peptide
1	A	42	GLY	Peptide
1	A	88	TYR	Peptide
1	B	102	GLY	Peptide
1	B	103	GLY	Peptide
1	B	119	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	B	40	ALA	Peptide
1	B	96	PRO	Peptide
1	B	97	ASP	Peptide,Mainchain
1	C	102	GLY	Peptide
1	C	103	GLY	Peptide,Mainchain
1	C	40	ALA	Peptide
1	D	101	ALA	Peptide,Mainchain
1	D	103	GLY	Mainchain
1	D	132	ALA	Peptide
1	D	40	ALA	Peptide
1	D	64	ASP	Peptide
1	D	95	ARG	Peptide,Mainchain
1	D	96	PRO	Peptide
1	D	97	ASP	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	1129	0	1075	81	0
1	B	1133	0	1076	58	0
1	C	1129	0	1075	63	0
1	D	1129	0	1072	55	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	93	0	0	24	0
4	B	117	0	0	18	0
4	C	83	0	0	17	0
4	D	97	0	0	4	0
All	All	4920	0	4298	253	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 29.

All (253) 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:156:LEU:HD23	1:A:190:LEU:CD2	1.64	1.28
1:D:110:LYS:HE2	1:D:120:HIS:CB	1.66	1.25
1:D:156:LEU:HD21	1:D:189:LEU:HG	1.19	1.17
1:A:156:LEU:CD2	1:A:190:LEU:CD2	2.25	1.14
1:A:140:MET:HB3	4:A:894:HOH:O	1.46	1.12
1:C:156:LEU:CD1	1:C:190:LEU:HD21	1.80	1.11
1:A:156:LEU:CD2	1:A:190:LEU:HD22	1.80	1.11
1:B:89:GLU:HG2	1:B:103:GLY:HA3	1.32	1.10
1:B:120:HIS:HB3	4:B:918:HOH:O	1.49	1.10
1:C:156:LEU:HD11	1:C:190:LEU:CD2	1.81	1.10
1:B:88:TYR:HD1	1:B:103:GLY:O	1.34	1.07
1:D:110:LYS:HE2	1:D:120:HIS:HB3	1.37	1.06
1:A:156:LEU:HD23	1:A:190:LEU:HD21	1.35	1.05
1:D:110:LYS:HE2	1:D:120:HIS:HB2	1.35	1.05
1:C:50:ARG:O	1:C:51:GLU:HG3	1.58	1.02
1:A:88:TYR:HD1	1:A:103:GLY:HA3	1.28	0.99
1:C:62:GLU:HB2	4:C:681:HOH:O	1.63	0.99
1:C:167:GLU:HB3	4:C:684:HOH:O	1.63	0.96
1:C:156:LEU:HD11	1:C:190:LEU:HD21	1.01	0.96
1:A:140:MET:HE3	4:A:894:HOH:O	1.63	0.96
1:A:156:LEU:CD2	1:A:190:LEU:HD21	1.93	0.94
1:A:108:LEU:O	1:A:110:LYS:HE2	1.71	0.91
1:B:88:TYR:CD1	1:B:103:GLY:O	2.23	0.90
1:A:133:ASP:HB3	4:A:889:HOH:O	1.73	0.89
1:B:97:ASP:O	1:B:98:PHE:C	2.11	0.88
1:B:148:LYS:HD3	4:B:835:HOH:O	1.74	0.88
1:A:88:TYR:CD1	1:A:103:GLY:HA3	2.08	0.87
1:B:40:ALA:HB1	4:B:917:HOH:O	1.74	0.87
1:C:89:GLU:CD	1:C:103:GLY:HA3	1.95	0.86
1:A:133:ASP:OD1	1:A:135:LYS:HD2	1.75	0.86
1:C:156:LEU:CD1	1:C:190:LEU:CD2	2.48	0.86
1:B:190:LEU:HG	1:A:78:ARG:NH1	1.90	0.86
1:A:53:LYS:HG2	4:A:810:HOH:O	1.75	0.85
1:A:156:LEU:HD23	1:A:190:LEU:HD22	1.42	0.85
1:B:89:GLU:CG	1:B:103:GLY:HA3	2.06	0.85
1:A:100:SER:HB3	4:A:858:HOH:O	1.75	0.84
1:B:152:LYS:HD3	4:B:909:HOH:O	1.78	0.84
1:B:64:ASP:HA	1:B:65:ASP:CB	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:LEU:CD2	1:D:189:LEU:HG	2.06	0.82
1:D:156:LEU:HD21	1:D:189:LEU:CG	2.05	0.82
1:B:152:LYS:CD	1:B:152:LYS:H	1.94	0.81
1:A:43:HIS:HB2	1:A:60:ILE:HG12	1.64	0.80
1:C:120:HIS:HE1	4:C:680:HOH:O	1.63	0.80
1:A:147:LEU:HD22	1:A:156:LEU:HD12	1.65	0.79
1:D:133:ASP:HB3	1:D:135:LYS:H	1.47	0.79
1:B:101:ALA:HB1	1:B:102:GLY:HA2	1.65	0.78
1:C:97:ASP:HA	4:C:642:HOH:O	1.83	0.78
1:D:45:VAL:CG2	1:D:58:ILE:HB	2.12	0.78
1:A:127:ASN:HD21	1:A:170:ASP:HB3	1.48	0.78
1:C:97:ASP:HB2	4:C:661:HOH:O	1.84	0.78
1:C:90:LYS:HG3	1:C:159:ASP:HB3	1.64	0.78
1:D:115:ASN:HD22	1:D:173:LEU:HD21	1.48	0.78
1:D:133:ASP:OD2	1:D:135:LYS:HD2	1.86	0.76
1:A:89:GLU:H	1:A:103:GLY:HA2	1.50	0.76
1:A:66:GLU:HG3	1:A:67:GLY:H	1.51	0.76
1:D:92:SER:HB3	1:D:101:ALA:HB3	1.66	0.76
1:C:112:HIS:HB2	1:C:121:HIS:CE1	2.21	0.75
1:A:90:LYS:HD3	4:A:834:HOH:O	1.86	0.75
1:C:53:LYS:HA	4:C:609:HOH:O	1.85	0.75
1:D:167:GLU:HG2	1:D:168:GLN:HG2	1.69	0.74
1:B:64:ASP:HA	1:B:65:ASP:CG	2.08	0.74
1:D:115:ASN:HD22	1:D:173:LEU:CD2	1.99	0.73
1:A:66:GLU:HG3	1:A:67:GLY:N	2.04	0.73
1:D:89:GLU:HG2	1:D:103:GLY:O	1.89	0.73
1:C:95:ARG:HD3	4:C:655:HOH:O	1.89	0.72
1:A:46:GLN:HG2	4:A:809:HOH:O	1.87	0.72
1:D:94:VAL:HB	1:D:100:SER:HB2	1.71	0.72
1:D:45:VAL:HG23	1:D:45:VAL:O	1.90	0.71
1:C:118:MET:HG3	4:C:668:HOH:O	1.89	0.71
1:A:40:ALA:HB1	4:C:656:HOH:O	1.89	0.70
1:B:97:ASP:O	1:B:99:GLU:N	2.24	0.70
1:C:147:LEU:HD12	4:C:681:HOH:O	1.91	0.70
1:B:65:ASP:HB2	4:B:913:HOH:O	1.90	0.70
1:B:100:SER:CB	4:B:887:HOH:O	2.38	0.70
1:A:140:MET:CE	4:A:894:HOH:O	2.28	0.68
1:D:179:ASN:CG	4:D:797:HOH:O	2.32	0.68
1:A:156:LEU:HD21	1:A:190:LEU:HD22	1.70	0.68
1:D:110:LYS:CE	1:D:120:HIS:HB3	2.21	0.68
1:D:45:VAL:HG21	1:D:58:ILE:HB	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ALA:HB1	1:B:102:GLY:CA	2.26	0.66
1:B:111:GLU:HG3	1:B:116:ASN:ND2	2.12	0.65
1:C:96:PRO:HG2	1:C:97:ASP:OD1	1.97	0.65
1:C:149:LYS:HA	1:C:154:ASN:HD22	1.60	0.65
1:D:115:ASN:HB2	1:D:173:LEU:HD22	1.79	0.64
1:B:64:ASP:HA	1:B:65:ASP:HB3	1.78	0.64
1:D:179:ASN:HB3	4:D:797:HOH:O	1.96	0.64
1:C:120:HIS:CE1	4:C:680:HOH:O	2.42	0.64
1:B:127:ASN:HD21	1:B:170:ASP:HB3	1.63	0.63
1:B:177:SER:CB	4:B:830:HOH:O	2.47	0.63
1:A:99:GLU:O	1:A:101:ALA:HA	1.99	0.63
1:A:99:GLU:HB2	4:A:865:HOH:O	1.99	0.63
1:C:112:HIS:H	1:C:175:ASN:HD21	1.46	0.62
1:A:43:HIS:HB2	1:A:60:ILE:CG1	2.29	0.62
1:C:127:ASN:HD21	1:C:170:ASP:HB3	1.64	0.62
1:A:99:GLU:CB	4:A:865:HOH:O	2.48	0.62
1:A:63:SER:C	1:A:65:ASP:HA	2.22	0.61
1:A:78:ARG:NH2	4:A:864:HOH:O	2.33	0.61
1:B:152:LYS:HD2	1:B:152:LYS:N	2.15	0.60
1:C:86:HIS:HB2	1:C:88:TYR:CE2	2.35	0.60
1:D:115:ASN:HB2	1:D:173:LEU:CD2	2.32	0.60
1:D:127:ASN:HD21	1:D:170:ASP:HB3	1.65	0.60
1:A:127:ASN:HD21	1:A:170:ASP:CB	2.13	0.60
1:D:110:LYS:HG3	1:D:120:HIS:HB3	1.83	0.60
1:A:125:LEU:HB3	1:A:126:PRO:CD	2.33	0.59
1:B:100:SER:HB3	4:B:887:HOH:O	2.00	0.59
1:B:66:GLU:HB3	4:B:913:HOH:O	2.03	0.59
1:B:129:GLU:CG	4:B:873:HOH:O	2.50	0.58
1:A:110:LYS:CD	4:A:861:HOH:O	2.51	0.58
1:C:133:ASP:HB3	1:C:135:LYS:H	1.68	0.58
1:B:152:LYS:HG2	4:B:894:HOH:O	2.03	0.58
1:C:50:ARG:O	1:C:51:GLU:CG	2.44	0.58
1:D:168:GLN:HB3	4:D:770:HOH:O	2.02	0.58
1:C:53:LYS:HG2	4:C:609:HOH:O	2.04	0.58
1:D:116:ASN:HB3	1:D:119:GLY:HA3	1.86	0.58
1:A:156:LEU:HD22	1:A:190:LEU:HD21	1.84	0.57
1:A:147:LEU:HD22	1:A:156:LEU:CD1	2.32	0.57
1:D:106:ASN:ND2	1:D:109:ASN:HA	2.19	0.57
1:C:111:GLU:O	1:C:120:HIS:N	2.34	0.57
1:B:127:ASN:HD21	1:B:170:ASP:H	1.53	0.56
1:C:62:GLU:CA	4:C:681:HOH:O	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:179:ASN:CB	4:D:797:HOH:O	2.52	0.56
1:A:92:SER:OG	1:A:100:SER:O	2.23	0.56
1:A:90:LYS:CE	4:A:873:HOH:O	2.53	0.56
1:A:90:LYS:HE3	4:A:873:HOH:O	2.06	0.56
1:D:45:VAL:CG2	1:D:45:VAL:O	2.54	0.56
1:D:110:LYS:CE	1:D:120:HIS:HB2	2.23	0.56
1:B:151:SER:HA	4:B:909:HOH:O	2.05	0.56
1:C:49:ASN:O	1:C:51:GLU:N	2.34	0.56
1:A:125:LEU:HB3	1:A:126:PRO:HD3	1.87	0.55
1:B:190:LEU:HG	1:A:78:ARG:HH12	1.67	0.55
1:D:106:ASN:HD21	1:D:109:ASN:HA	1.72	0.55
1:B:99:GLU:O	1:B:101:ALA:HA	2.07	0.54
1:A:110:LYS:HD3	4:A:861:HOH:O	2.07	0.54
1:C:65:ASP:CB	1:C:66:GLU:HA	2.38	0.54
1:A:140:MET:CG	4:A:894:HOH:O	2.54	0.53
1:A:121:HIS:HB2	1:A:124:ASP:CG	2.29	0.53
1:B:177:SER:HB2	4:B:830:HOH:O	2.08	0.53
1:A:50:ARG:HD3	4:A:820:HOH:O	2.08	0.53
1:C:127:ASN:HD21	1:C:170:ASP:CB	2.21	0.53
1:C:99:GLU:O	1:C:101:ALA:HA	2.08	0.53
1:D:50:ARG:HG2	1:D:96:PRO:O	2.09	0.53
1:A:66:GLU:CG	1:A:67:GLY:N	2.72	0.52
1:A:47:LEU:HD21	1:A:58:ILE:HD12	1.91	0.52
1:D:127:ASN:HD21	1:D:170:ASP:H	1.58	0.52
1:C:62:GLU:HA	4:C:681:HOH:O	2.07	0.52
1:B:66:GLU:HG2	4:B:891:HOH:O	2.09	0.52
1:A:112:HIS:HB2	1:A:121:HIS:CE1	2.46	0.51
1:B:63:SER:O	1:B:65:ASP:HB3	2.11	0.51
1:C:64:ASP:HA	1:C:65:ASP:OD2	2.11	0.51
1:A:63:SER:O	1:A:65:ASP:HA	2.10	0.51
1:A:158:GLU:HB2	4:A:887:HOH:O	2.10	0.51
1:C:127:ASN:HD21	1:C:170:ASP:H	1.57	0.51
1:D:168:GLN:HG3	1:D:180:SER:O	2.10	0.51
1:D:172:TYR:C	1:D:173:LEU:HD23	2.31	0.51
1:A:97:ASP:O	1:A:99:GLU:N	2.44	0.51
1:B:152:LYS:HD3	1:B:152:LYS:H	1.73	0.51
1:C:40:ALA:N	1:C:61:LYS:HG3	2.26	0.50
1:C:62:GLU:CB	4:C:681:HOH:O	2.34	0.50
1:A:100:SER:CB	4:A:858:HOH:O	2.45	0.50
1:C:92:SER:OG	1:C:94:VAL:HG23	2.12	0.50
1:C:57:PHE:CE2	1:C:59:GLU:HG3	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:127:ASN:HD21	1:B:170:ASP:CB	2.25	0.50
1:C:156:LEU:CD1	1:C:190:LEU:HD23	2.39	0.50
1:D:116:ASN:O	1:D:119:GLY:N	2.40	0.49
1:B:97:ASP:C	4:B:892:HOH:O	2.50	0.49
1:C:108:LEU:N	1:C:108:LEU:HD12	2.27	0.49
1:C:159:ASP:HB2	4:C:677:HOH:O	2.12	0.49
1:D:77:LEU:O	1:D:79:PRO:HD3	2.13	0.49
1:A:126:PRO:HD2	1:A:140:MET:SD	2.53	0.49
1:C:89:GLU:CG	1:C:103:GLY:HA3	2.43	0.49
1:B:158:GLU:HB2	4:B:866:HOH:O	2.12	0.48
1:C:49:ASN:OD1	1:C:51:GLU:HB2	2.14	0.48
1:C:63:SER:OG	1:C:64:ASP:N	2.46	0.48
1:C:127:ASN:ND2	1:C:170:ASP:H	2.11	0.48
1:A:65:ASP:HB3	1:A:66:GLU:HA	1.95	0.48
1:D:115:ASN:O	1:D:117:PRO:HD3	2.14	0.48
1:C:65:ASP:HB3	1:C:66:GLU:HA	1.95	0.48
1:A:98:PHE:C	1:A:100:SER:H	2.16	0.48
1:D:164:ILE:HG21	1:D:183:ARG:HB3	1.95	0.48
1:D:121:HIS:HB2	1:D:124:ASP:CG	2.35	0.47
1:A:125:LEU:CB	1:A:126:PRO:CD	2.92	0.47
1:A:127:ASN:ND2	1:A:170:ASP:HB3	2.25	0.47
1:D:45:VAL:HG22	1:D:58:ILE:O	2.13	0.47
1:C:165:ILE:HB	1:C:185:VAL:HB	1.95	0.47
1:B:89:GLU:CD	1:B:103:GLY:CA	2.83	0.47
1:C:82:SER:OG	1:C:129:GLU:OE2	2.26	0.47
1:A:110:LYS:HD2	4:A:861:HOH:O	2.13	0.47
1:B:111:GLU:HG3	1:B:116:ASN:HD21	1.80	0.47
1:B:65:ASP:HB2	1:B:66:GLU:CB	2.45	0.47
1:A:156:LEU:HD22	1:A:190:LEU:CD2	2.33	0.46
1:B:95:ARG:HG3	4:A:830:HOH:O	2.15	0.46
1:A:90:LYS:NZ	4:A:873:HOH:O	2.48	0.46
1:A:147:LEU:CD2	1:A:156:LEU:HD12	2.41	0.46
1:A:140:MET:CB	4:A:894:HOH:O	2.24	0.46
1:D:43:HIS:HB2	1:D:60:ILE:HG12	1.98	0.45
1:A:102:GLY:O	1:A:183:ARG:NH1	2.42	0.45
1:C:89:GLU:OE2	1:C:103:GLY:HA3	2.13	0.45
1:D:110:LYS:CG	1:D:120:HIS:HB3	2.44	0.45
1:A:49:ASN:C	1:A:49:ASN:OD1	2.54	0.45
1:B:119:GLY:O	1:B:120:HIS:HB2	2.15	0.45
1:B:120:HIS:CG	4:B:918:HOH:O	2.65	0.45
1:C:48:VAL:O	1:C:185:VAL:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:119:GLY:O	1:D:120:HIS:HB2	2.17	0.45
1:C:63:SER:HB3	1:C:67:GLY:O	2.18	0.44
1:C:116:ASN:HA	1:C:173:LEU:HD23	1.99	0.44
1:A:88:TYR:HB3	1:A:103:GLY:HA3	2.00	0.44
1:D:53:LYS:HD2	1:D:55:VAL:HG12	1.99	0.44
1:A:133:ASP:CB	4:A:889:HOH:O	2.49	0.44
1:D:85:PHE:CE2	1:D:140:MET:SD	3.11	0.44
1:B:89:GLU:CD	1:B:103:GLY:HA3	2.37	0.44
1:C:128:LEU:HD22	1:C:136:VAL:HG21	1.99	0.44
1:D:45:VAL:HG22	1:D:58:ILE:HB	1.98	0.43
1:D:72:ILE:HD11	1:D:165:ILE:HD11	2.00	0.43
1:B:128:LEU:HD22	1:B:136:VAL:HG21	1.99	0.43
1:B:85:PHE:HE2	1:B:140:MET:SD	2.41	0.43
1:A:128:LEU:HD22	1:A:136:VAL:HG21	2.01	0.43
1:B:47:LEU:HD23	1:B:47:LEU:HA	1.75	0.43
1:C:49:ASN:C	1:C:51:GLU:N	2.72	0.43
1:A:55:VAL:HA	1:A:75:ASN:HD21	1.84	0.43
1:D:90:LYS:HB2	1:D:101:ALA:HB1	2.00	0.43
1:B:120:HIS:CB	4:B:918:HOH:O	2.31	0.43
1:A:127:ASN:HD21	1:A:170:ASP:H	1.67	0.43
1:C:98:PHE:C	1:C:100:SER:N	2.72	0.43
1:D:110:LYS:HG3	1:D:120:HIS:O	2.19	0.42
1:A:125:LEU:CD2	1:A:142:ALA:HB2	2.49	0.42
1:B:64:ASP:O	1:D:64:ASP:OD2	2.38	0.42
1:C:100:SER:HA	1:C:101:ALA:HB2	2.01	0.42
1:A:78:ARG:HE	1:A:81:ALA:HB2	1.84	0.42
1:A:121:HIS:HB2	1:A:124:ASP:OD2	2.19	0.42
1:C:53:LYS:CA	4:C:609:HOH:O	2.56	0.42
1:D:127:ASN:HD21	1:D:170:ASP:CB	2.30	0.42
1:B:65:ASP:HB2	1:B:66:GLU:HB3	2.01	0.42
1:A:74:ALA:HB3	1:A:136:VAL:CG1	2.50	0.42
1:C:47:LEU:HG	1:C:56:GLY:C	2.40	0.42
1:B:65:ASP:CB	1:B:66:GLU:HA	2.49	0.42
1:C:58:ILE:HA	1:C:71:HIS:O	2.20	0.42
1:B:64:ASP:CA	1:B:65:ASP:CB	2.90	0.41
1:B:127:ASN:ND2	1:B:170:ASP:H	2.18	0.41
1:A:78:ARG:HA	1:A:79:PRO:HD3	1.94	0.41
1:B:110:LYS:HE3	1:B:110:LYS:HB3	1.87	0.41
1:B:190:LEU:CG	1:A:78:ARG:NH1	2.74	0.41
1:D:95:ARG:HH11	1:D:95:ARG:HD2	1.54	0.41
1:A:88:TYR:OH	1:A:166:HIS:NE2	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:ALA:HB1	1:C:144:ASP:O	2.21	0.41
1:C:149:LYS:HA	1:C:154:ASN:ND2	2.33	0.41
1:D:50:ARG:HE	1:D:50:ARG:HB2	1.59	0.41
1:D:58:ILE:HD11	1:D:72:ILE:HD12	2.03	0.41
1:B:61:LYS:HZ3	1:B:61:LYS:HG3	1.25	0.41
1:A:68:LEU:CD1	1:A:155:ILE:HD11	2.51	0.41
1:C:157:ASP:O	1:C:158:GLU:C	2.58	0.41
1:B:152:LYS:H	1:B:152:LYS:HD2	1.68	0.40
1:A:88:TYR:HB3	1:A:103:GLY:CA	2.52	0.40
1:A:164:ILE:HD13	1:A:183:ARG:HD3	2.04	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	149/175 (85%)	132 (89%)	15 (10%)	2 (1%)	12 3
1	B	150/175 (86%)	134 (89%)	10 (7%)	6 (4%)	3 0
1	C	149/175 (85%)	125 (84%)	15 (10%)	9 (6%)	1 0
1	D	149/175 (85%)	136 (91%)	9 (6%)	4 (3%)	5 1
All	All	597/700 (85%)	527 (88%)	49 (8%)	21 (4%)	3 0

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	97	ASP
1	B	98	PHE
1	B	120	HIS
1	B	133	ASP
1	A	120	HIS

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Mol	Chain	Res	Type
1	D	120	HIS
1	D	133	ASP
1	C	51	GLU
1	C	97	ASP
1	C	133	ASP
1	C	158	GLU
1	C	53	LYS
1	C	120	HIS
1	D	98	PHE
1	C	103	GLY
1	D	42	GLY
1	A	42	GLY
1	C	42	GLY
1	C	96	PRO
1	B	103	GLY
1	B	96	PRO

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	120/143 (84%)	106 (88%)	14 (12%)	5	1
1	B	120/143 (84%)	100 (83%)	20 (17%)	2	0
1	C	120/143 (84%)	105 (88%)	15 (12%)	4	1
1	D	120/143 (84%)	100 (83%)	20 (17%)	2	0
All	All	480/572 (84%)	411 (86%)	69 (14%)	3	0

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	46	GLN
1	B	50	ARG
1	B	51	GLU
1	B	61	LYS
1	B	65	ASP

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Mol	Chain	Res	Type
1	B	66	GLU
1	B	75	ASN
1	B	90	LYS
1	B	100	SER
1	B	108	LEU
1	B	126	PRO
1	B	133	ASP
1	B	148	LYS
1	B	149	LYS
1	B	152	LYS
1	B	156	LEU
1	B	159	ASP
1	B	177	SER
1	B	179	ASN
1	B	190	LEU
1	A	45	VAL
1	A	53	LYS
1	A	64	ASP
1	A	75	ASN
1	A	92	SER
1	A	100	SER
1	A	110	LYS
1	A	118	MET
1	A	120	HIS
1	A	125	LEU
1	A	129	GLU
1	A	148	LYS
1	A	152	LYS
1	A	190	LEU
1	C	46	GLN
1	C	53	LYS
1	C	62	GLU
1	C	65	ASP
1	C	72	ILE
1	C	76	SER
1	C	95	ARG
1	C	97	ASP
1	C	120	HIS
1	C	133	ASP
1	C	149	LYS
1	C	152	LYS
1	C	168	GLN

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Mol	Chain	Res	Type
1	C	173	LEU
1	C	190	LEU
1	D	53	LYS
1	D	64	ASP
1	D	65	ASP
1	D	75	ASN
1	D	82	SER
1	D	92	SER
1	D	95	ARG
1	D	97	ASP
1	D	108	LEU
1	D	110	LYS
1	D	120	HIS
1	D	133	ASP
1	D	140	MET
1	D	149	LYS
1	D	151	SER
1	D	152	LYS
1	D	167	GLU
1	D	168	GLN
1	D	173	LEU
1	D	190	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	46	GLN
1	B	75	ASN
1	B	127	ASN
1	A	75	ASN
1	A	127	ASN
1	C	75	ASN
1	C	127	ASN
1	C	175	ASN
1	D	75	ASN
1	D	115	ASN
1	D	127	ASN

5.3.3 RNA

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)

Of 10 ligands modelled in this entry, 10 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	2
1	B	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	102:GLY	C	103:GLY	N	1.17
1	D	65:ASP	C	66:GLU	N	1.14
1	B	96:PRO	C	97:ASP	N	1.12
1	B	97:ASP	C	98:PHE	N	1.12

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	151/175 (86%)	0.16	4 (2%)	56	51	17, 39, 51, 61	0
1	B	152/175 (86%)	0.12	2 (1%)	77	74	16, 33, 50, 63	0
1	C	151/175 (86%)	0.37	7 (4%)	32	26	17, 40, 58, 70	0
1	D	151/175 (86%)	0.27	9 (5%)	21	17	17, 38, 51, 57	0
All	All	605/700 (86%)	0.23	22 (3%)	42	37	16, 38, 54, 70	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	120	HIS	5.1
1	A	120	HIS	3.9
1	C	96	PRO	3.8
1	D	97	ASP	3.6
1	C	64	ASP	3.5
1	D	101	ALA	3.4
1	D	65	ASP	3.3
1	B	97	ASP	3.1
1	C	99	GLU	2.8
1	D	100	SER	2.7
1	A	64	ASP	2.6
1	A	190	LEU	2.6
1	C	100	SER	2.6
1	C	65	ASP	2.5
1	B	64	ASP	2.4
1	C	190	LEU	2.3
1	D	109	ASN	2.3
1	A	103	GLY	2.2
1	D	42	GLY	2.2
1	D	119	GLY	2.1
1	D	190	LEU	2.1
1	C	101	ALA	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ZN	A	802	1/1	0.89	0.09	32,32,32,32	0
3	CL	D	702	1/1	0.92	0.04	38,38,38,38	0
2	ZN	A	501	1/1	0.94	0.06	36,36,36,36	0
3	CL	A	502	1/1	0.95	0.13	34,34,34,34	0
2	ZN	B	801	1/1	0.95	0.10	27,27,27,27	0
3	CL	B	402	1/1	0.96	0.06	28,28,28,28	0
2	ZN	B	401	1/1	0.98	0.04	33,33,33,33	0
2	ZN	C	601	1/1	0.98	0.06	33,33,33,33	0
2	ZN	D	701	1/1	0.98	0.04	38,38,38,38	0
3	CL	C	602	1/1	0.99	0.13	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.