Full wwPDB X-ray Structure Validation Report (i)

Jun 11, 2024 – 06:54 PM EDT

PDB ID	:	1C1G
Title	:	CRYSTAL STRUCTURE OF TROPOMYOSIN AT 7 ANGSTROMS RESOLUTION IN THE SPERMINE-INDUCED CRYSTAL FORM
Authors	:	Whitby, F.G.; Phillips Jr., G.N.
Deposited on	:	1999-07-22
Resolution	:	7.00 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:

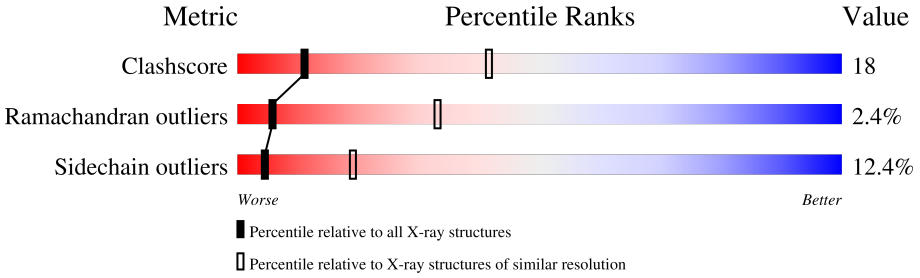
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.36.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 7.00 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))
Clashscore	141614	1069 (10.00-3.90)
Ramachandran outliers	138981	1002 (10.00-3.90)
Sidechain outliers	138945	1002 (10.00-3.86)

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%

Mol	Chain	Length	Quality of chain
1	A	284	64% 24% 8% •
1	B	284	68% 22% 8% •
1	C	284	62% 26% 8% •
1	D	284	60% 28% 8% •

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9160 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 TROPOMYOSIN.

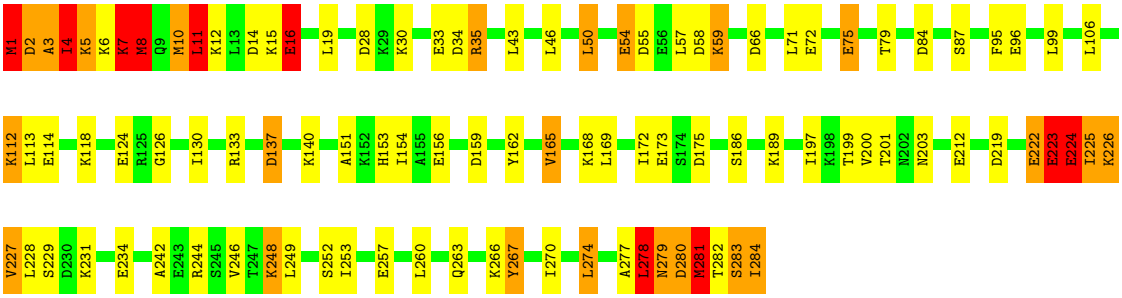
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	284	2290	1402	387	494	7	0	0	0
1	B	284	2290	1402	387	494	7	0	0	0
1	C	284	2290	1402	387	494	7	0	0	0
1	D	284	2290	1402	387	494	7	0	0	0

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. 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. 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.

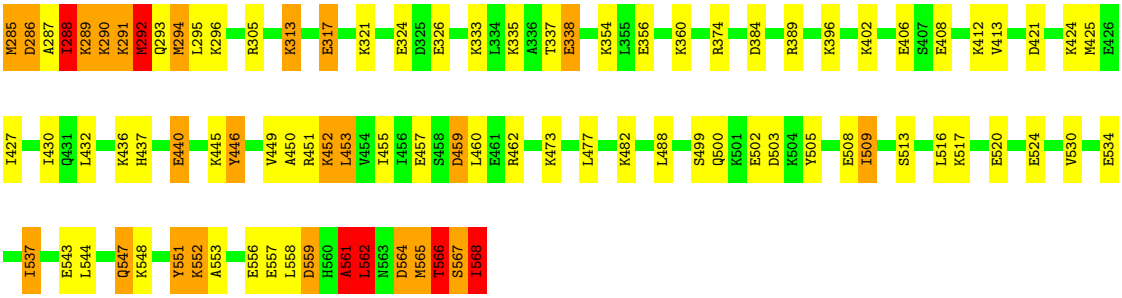
• Molecule 1: TROPOMYOSIN

Chain A:



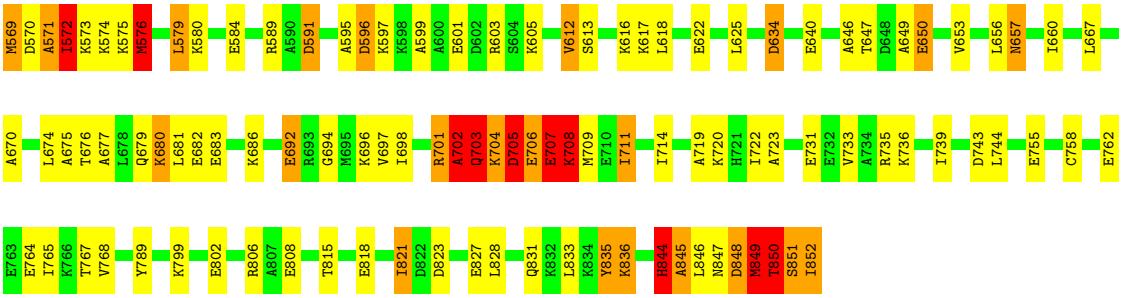
• Molecule 1: TROPOMYOSIN

Chain B:



• Molecule 1: TROPOMYOSIN

Chain C:



• Molecule 1: TROPOMYOSIN

Chain D:

M853 D854 A855 I856 K857 K858 K859 M860 Q861 M862 L863 K864 L865 D866 K867 E868 N869 E876 A877 E878 A879 D880 K881 K882 A883 A884 E885 D886 R887 S888 K889 E892 K901 T905 L909 D910 S913 D918 E924 T931 D936 N941 I944 F947 E950 L951

D952 R957 L958 L962 L965 E966 E969 D973 E976 K980 V981 I982 A986 Q987 K988 D989 E990 E991 K992 M993 E994 I995 I998 H1005 E1008 D1011 R1012 K1013 Y1014 V1017 A1018 R1019 K1020 L1021 V1022 I1023 I1024 E1025 S1026 D1027 S1038 E1048 I1049 K1050 T1051

V1052 T1053 L1056 K1057 E1060 E1064 Q1068 D1071 K1072 Y1073 E1074 E1075 E1076 I1077 K1078 V1079 L1080 S1081 D1082 K1083 L1084 K1085 E1086 A1087 E1088 V1098 T1099 I1105 L1108 E1111 L1112 E1125 L1126 D1127 H1128 A1129 L1130 N1131 D1132 M1133 T1134 S1135 I1136

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	259.74Å 55.30Å 136.26Å 90.00° 97.42° 90.00°	Depositor
Resolution (Å)	100.00 – 7.00 99.88 – 7.00	Depositor EDS
% Data completeness (in resolution range)	96.4 (100.00-7.00) 96.4 (99.88-7.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 6.73Å)	Xtriage
Refinement program	XTALVIEW, X-PLOR	Depositor
R, R_{free}	0.404 , (Not available) 0.449 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	210.9	Xtriage
Anisotropy	1.027	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.54 , 457.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.34$, $< L^2 > = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.67	EDS
Total number of atoms	9160	wwPDB-VP
Average B, all atoms (Å^2)	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.35% 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	0.86	3/2299 (0.1%)	1.79	56/3062 (1.8%)
1	B	0.80	2/2299 (0.1%)	1.63	41/3062 (1.3%)
1	C	1.28	11/2299 (0.5%)	1.86	59/3062 (1.9%)
1	D	0.91	8/2299 (0.3%)	1.82	67/3062 (2.2%)
All	All	0.98	24/9196 (0.3%)	1.78	223/12248 (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	3
1	C	0	5
1	D	0	5
All	All	0	13

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	852	ILE	N-CA	30.96	2.08	1.46
1	C	852	ILE	CA-CB	21.53	2.04	1.54
1	C	851	SER	C-N	15.91	1.70	1.34
1	C	572	ILE	CA-CB	11.53	1.81	1.54
1	D	859	LYS	N-CA	10.74	1.67	1.46
1	C	705	ASP	N-CA	9.29	1.65	1.46
1	C	705	ASP	CA-C	9.07	1.76	1.52
1	D	860	MET	N-CA	8.86	1.64	1.46
1	C	705	ASP	C-N	8.60	1.53	1.34
1	A	224	GLU	CA-CB	8.43	1.72	1.53
1	D	858	LYS	C-N	8.01	1.52	1.34
1	C	851	SER	CA-C	7.28	1.71	1.52
1	D	858	LYS	C-O	6.26	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	859	LYS	CA-C	5.96	1.68	1.52
1	C	708	LYS	CB-CG	5.90	1.68	1.52
1	A	223	GLU	N-CA	5.76	1.57	1.46
1	C	708	LYS	CG-CD	5.56	1.71	1.52
1	B	568	ILE	CB-CG2	-5.52	1.35	1.52
1	A	224	GLU	CB-CG	5.34	1.62	1.52
1	D	860	MET	C-N	5.25	1.46	1.34
1	D	860	MET	CA-C	5.17	1.66	1.52
1	D	879	ALA	N-CA	5.14	1.56	1.46
1	B	565	MET	N-CA	5.06	1.56	1.46
1	C	704	LYS	C-N	5.03	1.45	1.34

All (223) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	4	ILE	CA-CB-CG2	-21.88	67.14	110.90
1	C	572	ILE	N-CA-CB	-21.77	60.73	110.80
1	B	568	ILE	N-CA-CB	-21.05	62.38	110.80
1	C	852	ILE	CB-CA-C	-18.23	75.14	111.60
1	A	223	GLU	CA-C-N	-17.61	78.46	117.20
1	C	708	LYS	CA-CB-CG	15.88	148.34	113.40
1	D	879	ALA	CA-C-N	-15.44	83.22	117.20
1	D	856	ILE	CB-CA-C	15.44	142.47	111.60
1	B	565	MET	CG-SD-CE	14.66	123.65	100.20
1	A	224	GLU	CA-CB-CG	14.30	144.85	113.40
1	D	880	ASP	N-CA-C	14.07	148.99	111.00
1	D	858	LYS	CA-C-O	-13.89	90.92	120.10
1	A	224	GLU	CA-C-N	-13.69	87.09	117.20
1	C	572	ILE	N-CA-C	-13.41	74.79	111.00
1	C	851	SER	CA-C-O	-13.23	92.32	120.10
1	D	856	ILE	N-CA-CB	-13.04	80.82	110.80
1	D	861	GLN	C-N-CA	-12.63	90.13	121.70
1	B	568	ILE	N-CA-C	-12.51	77.23	111.00
1	A	4	ILE	CA-CB-CG1	12.32	134.42	111.00
1	C	572	ILE	CA-CB-CG2	12.15	135.20	110.90
1	C	852	ILE	CG1-CB-CG2	-12.01	84.97	111.40
1	D	862	MET	CA-C-N	12.01	143.62	117.20
1	D	856	ILE	N-CA-C	-11.73	79.32	111.00
1	B	565	MET	CA-CB-CG	11.59	133.01	113.30
1	C	851	SER	CA-C-N	11.56	142.64	117.20
1	C	847	ASN	C-N-CA	-11.39	93.22	121.70
1	C	572	ILE	CG1-CB-CG2	-11.35	86.43	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	708	LYS	CG-CD-CE	11.17	145.40	111.90
1	C	851	SER	N-CA-C	11.11	141.00	111.00
1	D	880	ASP	CA-CB-CG	11.08	137.77	113.40
1	A	226	LYS	CA-C-N	11.07	141.55	117.20
1	A	7	LYS	CA-CB-CG	11.04	137.68	113.40
1	C	851	SER	C-N-CA	10.70	148.44	121.70
1	C	851	SER	N-CA-CB	-10.64	94.53	110.50
1	D	1014	TYR	CB-CG-CD2	-10.40	114.76	121.00
1	C	702	ALA	CA-C-N	-10.26	94.62	117.20
1	B	551	TYR	CB-CG-CD2	-10.25	114.85	121.00
1	A	224	GLU	N-CA-C	10.14	138.38	111.00
1	C	852	ILE	N-CA-CB	10.05	133.91	110.80
1	D	856	ILE	CA-C-N	9.97	139.13	117.20
1	D	859	LYS	O-C-N	-9.80	107.02	122.70
1	A	281	MET	CB-CA-C	-9.75	90.89	110.40
1	A	223	GLU	CA-C-O	9.67	140.41	120.10
1	C	708	LYS	CB-CG-CD	9.65	136.70	111.60
1	C	708	LYS	N-CA-CB	-9.59	93.34	110.60
1	D	882	LYS	CA-C-N	9.59	138.30	117.20
1	B	288	ILE	CA-CB-CG2	-9.56	91.78	110.90
1	D	880	ASP	CA-C-N	-9.51	96.29	117.20
1	C	852	ILE	N-CA-C	9.46	136.53	111.00
1	D	856	ILE	CG1-CB-CG2	-9.37	90.79	111.40
1	C	571	ALA	C-N-CA	9.30	144.96	121.70
1	C	589	ARG	NE-CZ-NH1	-9.07	115.77	120.30
1	A	281	MET	O-C-N	-9.03	108.26	122.70
1	A	35	ARG	NE-CZ-NH1	-8.91	115.84	120.30
1	D	861	GLN	N-CA-C	-8.88	87.03	111.00
1	A	1	MET	N-CA-C	-8.81	87.21	111.00
1	B	446	TYR	CB-CG-CD2	-8.80	115.72	121.00
1	A	281	MET	N-CA-CB	8.65	126.17	110.60
1	A	5	LYS	CA-CB-CG	8.61	132.35	113.40
1	B	564	ASP	CA-C-N	8.61	136.14	117.20
1	D	860	MET	CA-CB-CG	8.52	127.78	113.30
1	B	294	MET	CA-C-N	8.51	135.93	117.20
1	B	564	ASP	N-CA-CB	-8.47	95.36	110.60
1	B	565	MET	N-CA-CB	8.42	125.75	110.60
1	A	284	ILE	CG1-CB-CG2	-8.38	92.97	111.40
1	B	564	ASP	CA-CB-CG	8.32	131.69	113.40
1	A	284	ILE	CA-CB-CG2	-8.25	94.39	110.90
1	B	561	ALA	CA-C-N	-8.23	99.09	117.20
1	D	858	LYS	CA-C-N	8.23	135.31	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	280	ASP	N-CA-CB	-8.19	95.86	110.60
1	B	453	LEU	CA-CB-CG	8.19	134.13	115.30
1	D	858	LYS	C-N-CA	8.19	142.16	121.70
1	B	568	ILE	CB-CA-C	8.15	127.90	111.60
1	A	4	ILE	CG1-CB-CG2	-8.13	93.50	111.40
1	D	878	GLU	O-C-N	8.13	135.70	122.70
1	A	8	MET	CA-CB-CG	8.10	127.07	113.30
1	C	852	ILE	CA-CB-CG2	7.98	126.85	110.90
1	D	859	LYS	N-CA-C	7.94	132.43	111.00
1	D	878	GLU	C-N-CA	7.92	141.49	121.70
1	C	572	ILE	CB-CA-C	7.88	127.36	111.60
1	A	283	SER	CA-C-N	7.80	134.36	117.20
1	C	849	MET	N-CA-CB	7.75	124.55	110.60
1	D	857	LYS	CA-C-N	-7.75	100.15	117.20
1	D	879	ALA	CA-C-O	7.68	136.24	120.10
1	D	1014	TYR	CA-CB-CG	7.67	127.97	113.40
1	B	565	MET	CB-CA-C	-7.64	95.12	110.40
1	C	572	ILE	CA-C-N	7.58	133.88	117.20
1	A	284	ILE	CA-CB-CG1	7.58	125.41	111.00
1	A	7	LYS	C-N-CA	-7.58	102.76	121.70
1	B	446	TYR	CA-CB-CG	7.58	127.80	113.40
1	C	848	ASP	N-CA-CB	-7.58	96.97	110.60
1	C	705	ASP	CA-C-N	7.57	133.86	117.20
1	B	292	MET	CA-CB-CG	7.55	126.13	113.30
1	C	850	THR	CA-CB-CG2	7.53	122.94	112.40
1	A	222	GLU	O-C-N	7.50	134.70	122.70
1	A	3	ALA	CA-C-N	7.43	133.56	117.20
1	D	880	ASP	CB-CG-OD1	7.37	124.93	118.30
1	C	706	GLU	CA-C-N	7.33	133.31	117.20
1	D	1021	LEU	CA-CB-CG	7.22	131.91	115.30
1	D	862	MET	O-C-N	-7.21	111.16	122.70
1	C	708	LYS	N-CA-C	7.18	130.39	111.00
1	A	226	LYS	CA-C-O	-7.18	105.03	120.10
1	D	862	MET	CA-C-O	-7.15	105.09	120.10
1	B	564	ASP	CB-CA-C	7.13	124.67	110.40
1	A	225	ILE	N-CA-C	-7.11	91.80	111.00
1	A	5	LYS	CB-CA-C	-7.03	96.33	110.40
1	C	576	MET	N-CA-CB	7.00	123.20	110.60
1	C	576	MET	CB-CA-C	-6.95	96.50	110.40
1	D	853	MET	O-C-N	-6.94	111.59	122.70
1	C	702	ALA	O-C-N	6.94	133.80	122.70
1	B	288	ILE	CA-CB-CG1	6.91	124.13	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	858	LYS	N-CA-C	-6.90	92.36	111.00
1	B	551	TYR	CB-CG-CD1	6.90	125.14	121.00
1	A	244	ARG	NE-CZ-NH1	-6.88	116.86	120.30
1	A	224	GLU	O-C-N	6.86	133.68	122.70
1	B	338	GLU	OE1-CD-OE2	-6.82	115.11	123.30
1	D	1133	MET	CA-CB-CG	6.80	124.87	113.30
1	C	573	LYS	CA-CB-CG	6.80	128.37	113.40
1	B	505	TYR	CB-CG-CD2	-6.79	116.93	121.00
1	A	280	ASP	CB-CA-C	6.76	123.91	110.40
1	D	860	MET	O-C-N	-6.76	111.89	122.70
1	D	854	ASP	N-CA-C	6.70	129.10	111.00
1	C	701	ARG	O-C-N	6.70	133.42	122.70
1	C	789	TYR	CB-CG-CD2	-6.68	116.99	121.00
1	B	566	THR	O-C-N	-6.65	112.06	122.70
1	A	173	GLU	CA-CB-CG	6.63	127.98	113.40
1	D	1014	TYR	CB-CG-CD1	6.60	124.96	121.00
1	A	7	LYS	N-CA-CB	6.60	122.48	110.60
1	C	705	ASP	N-CA-C	6.56	128.71	111.00
1	C	705	ASP	O-C-N	-6.52	112.27	122.70
1	B	374	ARG	NE-CZ-NH2	6.44	123.52	120.30
1	D	862	MET	CA-CB-CG	6.42	124.21	113.30
1	D	858	LYS	O-C-N	6.40	132.94	122.70
1	D	887	ARG	NE-CZ-NH1	-6.40	117.10	120.30
1	C	848	ASP	N-CA-C	6.38	128.23	111.00
1	C	847	ASN	CA-C-N	-6.37	103.19	117.20
1	C	849	MET	CB-CA-C	-6.33	97.75	110.40
1	A	280	ASP	CB-CG-OD1	6.32	123.99	118.30
1	B	446	TYR	CB-CG-CD1	6.30	124.78	121.00
1	C	569	MET	O-C-N	-6.28	112.66	122.70
1	D	860	MET	N-CA-C	6.28	127.94	111.00
1	A	279	ASN	CA-C-N	-6.24	103.47	117.20
1	D	857	LYS	N-CA-C	6.22	127.78	111.00
1	A	212	GLU	OE1-CD-OE2	-6.21	115.85	123.30
1	D	1073	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	A	4	ILE	CA-C-N	-6.15	103.66	117.20
1	C	704	LYS	CA-C-O	-6.15	107.19	120.10
1	D	856	ILE	CA-C-O	-6.13	107.23	120.10
1	D	1132	ASP	CA-C-N	-6.12	103.75	117.20
1	B	294	MET	O-C-N	-6.07	112.99	122.70
1	D	882	LYS	CA-C-O	-6.04	107.42	120.10
1	A	223	GLU	N-CA-C	6.01	127.23	111.00
1	D	880	ASP	O-C-N	6.01	132.32	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	2	ASP	CA-C-N	-6.01	103.98	117.20
1	D	965	LEU	CA-CB-CG	6.00	129.09	115.30
1	D	854	ASP	O-C-N	-5.99	113.11	122.70
1	C	849	MET	CA-CB-CG	5.98	123.46	113.30
1	B	564	ASP	CA-C-O	-5.95	107.60	120.10
1	A	283	SER	CA-C-O	-5.95	107.61	120.10
1	A	278	LEU	CA-CB-CG	5.93	128.95	115.30
1	B	305	ARG	NE-CZ-NH2	5.91	123.25	120.30
1	D	990	GLU	N-CA-C	-5.91	95.05	111.00
1	D	855	ALA	O-C-N	-5.90	113.26	122.70
1	A	226	LYS	O-C-N	-5.89	113.27	122.70
1	A	222	GLU	C-N-CA	5.83	136.28	121.70
1	D	857	LYS	CB-CA-C	-5.82	98.76	110.40
1	A	267	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	C	569	MET	CA-C-N	5.79	129.94	117.20
1	B	561	ALA	O-C-N	5.78	131.95	122.70
1	D	879	ALA	N-CA-C	5.78	126.60	111.00
1	B	482	LYS	CA-CB-CG	5.78	126.11	113.40
1	C	848	ASP	O-C-N	-5.78	113.45	122.70
1	C	572	ILE	CA-C-O	-5.76	108.00	120.10
1	D	881	LYS	CA-CB-CG	5.75	126.06	113.40
1	B	440	GLU	OE1-CD-OE2	-5.75	116.41	123.30
1	C	806	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	A	35	ARG	NE-CZ-NH2	5.71	123.16	120.30
1	C	701	ARG	C-N-CA	5.69	135.92	121.70
1	C	802	GLU	OE1-CD-OE2	-5.68	116.49	123.30
1	D	856	ILE	O-C-N	-5.67	113.62	122.70
1	A	11	LEU	CA-CB-CG	-5.64	102.33	115.30
1	D	858	LYS	CB-CA-C	5.63	121.67	110.40
1	D	1131	ASN	CA-C-N	5.59	129.50	117.20
1	C	703	GLN	CA-C-O	-5.58	108.38	120.10
1	B	566	THR	CA-CB-CG2	5.56	120.18	112.40
1	B	562	LEU	CA-CB-CG	5.54	128.04	115.30
1	C	650	GLU	OE1-CD-OE2	-5.54	116.65	123.30
1	C	835	TYR	CB-CG-CD2	-5.53	117.68	121.00
1	A	75	GLU	CA-CB-CG	-5.53	101.24	113.40
1	D	853	MET	N-CA-C	5.51	125.87	111.00
1	D	882	LYS	O-C-N	-5.51	113.89	122.70
1	C	848	ASP	CB-CA-C	5.50	121.39	110.40
1	B	289	LYS	CA-CB-CG	5.49	125.47	113.40
1	D	854	ASP	CA-C-N	5.47	129.24	117.20
1	D	887	ARG	NE-CZ-NH2	5.44	123.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	10	MET	CA-C-N	5.44	129.16	117.20
1	D	860	MET	N-CA-CB	-5.42	100.85	110.60
1	A	3	ALA	CA-C-O	-5.41	108.74	120.10
1	C	849	MET	N-CA-C	-5.38	96.47	111.00
1	C	572	ILE	CA-CB-CG1	-5.36	100.81	111.00
1	B	290	LYS	C-N-CA	-5.36	108.31	121.70
1	D	853	MET	CA-CB-CG	5.35	122.40	113.30
1	D	1098	VAL	N-CA-C	-5.35	96.55	111.00
1	A	156	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	B	567	SER	C-N-CA	5.31	134.98	121.70
1	D	860	MET	CA-C-N	5.28	128.82	117.20
1	A	2	ASP	CA-C-O	5.26	131.15	120.10
1	B	565	MET	N-CA-C	-5.23	96.87	111.00
1	D	1086	GLU	OE1-CD-OE2	-5.18	117.08	123.30
1	B	566	THR	CA-C-N	5.18	128.59	117.20
1	A	14	ASP	CB-CG-OD1	5.17	122.96	118.30
1	D	880	ASP	CA-C-O	5.17	130.95	120.10
1	C	707	GLU	C-N-CA	-5.16	108.80	121.70
1	A	16	GLU	CA-C-N	5.14	128.51	117.20
1	C	703	GLN	C-N-CA	5.11	134.47	121.70
1	A	225	ILE	C-N-CA	-5.11	108.94	121.70
1	C	706	GLU	O-C-N	-5.10	114.54	122.70
1	B	292	MET	CB-CA-C	-5.08	100.25	110.40
1	D	856	ILE	CA-CB-CG2	5.07	121.03	110.90
1	D	1076	GLU	OE1-CD-OE2	-5.05	117.24	123.30
1	A	224	GLU	CA-C-O	5.03	130.67	120.10
1	B	547	GLN	CA-CB-CG	-5.03	102.34	113.40
1	A	1	MET	CA-CB-CG	5.02	121.83	113.30

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	223	GLU	Mainchain,Peptide
1	A	224	GLU	Mainchain
1	C	702	ALA	Mainchain
1	C	703	GLN	Mainchain
1	C	705	ASP	Peptide
1	C	707	GLU	Peptide
1	C	850	THR	Peptide
1	D	1135	SER	Mainchain
1	D	859	LYS	Mainchain,Peptide

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Mol	Chain	Res	Type	Group
1	D	879	ALA	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	2290	0	2295	96	0
1	B	2290	0	2292	87	0
1	C	2290	0	2291	120	3
1	D	2290	0	2292	84	3
All	All	9160	0	9170	330	3

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 (330) 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:C:572:ILE:CB	1:C:572:ILE:CA	1.81	1.58
1:D:859:LYS:N	1:D:859:LYS:CA	1.67	1.51
1:C:705:ASP:C	1:C:705:ASP:CA	1.76	1.50
1:C:572:ILE:CB	1:C:572:ILE:N	1.71	1.46
1:C:851:SER:C	1:C:852:ILE:N	1.70	1.44
1:C:852:ILE:CB	1:C:852:ILE:CA	2.04	1.35
1:C:572:ILE:N	1:C:572:ILE:HB	1.29	1.29
1:A:280:ASP:HB3	1:B:565:MET:SD	1.80	1.22
1:C:852:ILE:N	1:C:852:ILE:CA	2.08	1.17
1:C:852:ILE:CB	1:C:852:ILE:C	2.27	1.03
1:C:705:ASP:N	1:C:708:LYS:HD2	1.74	1.02
1:D:880:ASP:HB3	1:D:882:LYS:N	1.74	1.01
1:B:567:SER:HB2	1:B:568:ILE:HD12	1.44	0.97
1:C:852:ILE:N	1:C:852:ILE:HA	1.79	0.97
1:C:572:ILE:HB	1:C:572:ILE:H	1.28	0.95
1:D:860:MET:HA	1:D:863:LEU:H	1.32	0.93
1:C:705:ASP:HB3	1:D:993:MET:HB2	1.50	0.90
1:C:703:GLN:C	1:C:708:LYS:HG2	1.92	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:702:ALA:HA	1:C:708:LYS:HE2	1.53	0.88
1:D:880:ASP:HB2	1:D:883:ALA:N	1.90	0.87
1:A:224:GLU:HB2	1:A:227:VAL:N	1.90	0.86
1:A:8:MET:SD	1:B:292:MET:HA	2.15	0.86
1:A:4:ILE:HD12	1:B:288:ILE:HB	1.58	0.86
1:C:576:MET:SD	1:D:859:LYS:HE2	2.16	0.85
1:C:571:ALA:C	1:C:572:ILE:HB	1.96	0.85
1:A:224:GLU:HB2	1:A:227:VAL:H	1.44	0.82
1:C:572:ILE:CA	1:C:572:ILE:CG1	2.57	0.81
1:A:223:GLU:HA	1:A:224:GLU:HG2	1.64	0.79
1:D:880:ASP:HB2	1:D:883:ALA:H	1.46	0.78
1:C:703:GLN:O	1:C:708:LYS:HG2	1.85	0.77
1:C:569:MET:C	1:C:572:ILE:HG22	2.05	0.76
1:C:571:ALA:C	1:C:572:ILE:CB	2.53	0.74
1:C:707:GLU:N	1:C:708:LYS:HG3	2.03	0.74
1:D:1017:VAL:HA	1:D:1020:LYS:HB2	1.71	0.73
1:A:8:MET:HE1	1:B:296:LYS:N	2.04	0.73
1:C:706:GLU:H	1:C:708:LYS:HE3	1.54	0.73
1:C:705:ASP:CA	1:C:708:LYS:HB3	2.20	0.72
1:D:860:MET:SD	1:D:864:LYS:HB2	2.29	0.72
1:C:571:ALA:O	1:C:575:LYS:HB3	1.89	0.72
1:B:449:VAL:HA	1:B:452:LYS:HB2	1.72	0.71
1:A:1:MET:H2	1:A:4:ILE:H	1.38	0.71
1:C:707:GLU:H	1:C:708:LYS:HG3	1.53	0.70
1:A:4:ILE:HD12	1:B:288:ILE:CB	2.22	0.70
1:D:859:LYS:N	1:D:859:LYS:HA	1.95	0.69
1:A:43:LEU:HD11	1:B:326:GLU:HB3	1.76	0.68
1:C:705:ASP:C	1:C:705:ASP:CB	2.60	0.68
1:A:224:GLU:HB2	1:A:226:LYS:C	2.14	0.67
1:A:219:ASP:HA	1:A:222:GLU:HG3	1.77	0.67
1:A:222:GLU:O	1:A:224:GLU:HB3	1.94	0.67
1:C:848:ASP:HA	1:C:851:SER:H	1.60	0.67
1:C:705:ASP:H	1:C:708:LYS:HD2	1.56	0.67
1:A:57:LEU:HD22	1:B:337:THR:HG22	1.77	0.66
1:B:558:LEU:O	1:B:561:ALA:HB3	1.96	0.66
1:D:856:ILE:O	1:D:859:LYS:N	2.28	0.65
1:D:855:ALA:O	1:D:858:LYS:HB2	1.97	0.65
1:A:2:ASP:O	1:A:5:LYS:HB3	1.97	0.65
1:A:8:MET:SD	1:B:292:MET:CA	2.84	0.65
1:C:702:ALA:O	1:C:708:LYS:HG3	1.96	0.64
1:C:706:GLU:H	1:C:708:LYS:CE	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:706:GLU:C	1:C:708:LYS:HB2	2.18	0.64
1:C:706:GLU:N	1:C:708:LYS:CG	2.60	0.64
1:C:852:ILE:CA	1:C:852:ILE:HB	2.21	0.64
1:D:860:MET:HA	1:D:863:LEU:N	2.09	0.64
1:A:277:ALA:O	1:A:280:ASP:HB2	1.97	0.64
1:D:854:ASP:O	1:D:857:LYS:HB3	1.98	0.63
1:B:286:ASP:O	1:B:289:LYS:HB3	1.97	0.63
1:C:704:LYS:N	1:C:708:LYS:HG2	2.13	0.63
1:A:7:LYS:CE	1:B:292:MET:HB2	2.27	0.63
1:C:846:LEU:O	1:C:849:MET:N	2.31	0.63
1:C:828:LEU:HD11	1:D:1111:GLU:HG3	1.80	0.63
1:C:831:GLN:HE22	1:D:1112:LEU:HG	1.64	0.62
1:D:989:ASP:HA	1:D:992:LYS:HB2	1.81	0.62
1:D:859:LYS:N	1:D:859:LYS:CB	2.58	0.62
1:C:703:GLN:O	1:C:707:GLU:HB3	2.00	0.62
1:C:705:ASP:N	1:C:708:LYS:CD	2.59	0.61
1:C:852:ILE:HG22	1:D:1136:ILE:HD13	1.81	0.61
1:B:291:LYS:NZ	1:B:291:LYS:HB3	2.16	0.61
1:D:1130:LEU:HA	1:D:1133:MET:SD	2.40	0.61
1:A:224:GLU:HB3	1:A:226:LYS:H	1.66	0.61
1:C:705:ASP:O	1:C:709:MET:HB2	2.00	0.61
1:A:4:ILE:HD11	1:B:288:ILE:HD12	1.83	0.60
1:B:285:MET:O	1:B:288:ILE:HG13	2.01	0.60
1:C:702:ALA:C	1:C:708:LYS:HD3	2.22	0.60
1:D:857:LYS:O	1:D:858:LYS:O	2.20	0.60
1:C:848:ASP:O	1:C:851:SER:N	2.35	0.60
1:B:421:ASP:O	1:B:425:MET:HB2	2.03	0.59
1:D:880:ASP:HB3	1:D:882:LYS:H	1.66	0.59
1:B:285:MET:C	1:B:288:ILE:HG13	2.23	0.59
1:B:287:ALA:O	1:B:290:LYS:HB2	2.02	0.59
1:D:856:ILE:HA	1:D:859:LYS:HB3	1.84	0.59
1:B:557:GLU:O	1:B:561:ALA:HB2	2.02	0.59
1:A:7:LYS:CD	1:A:8:MET:HG2	2.33	0.59
1:A:253:ILE:O	1:A:257:GLU:HB2	2.02	0.59
1:B:530:VAL:O	1:B:534:GLU:HB2	2.02	0.59
1:A:3:ALA:O	1:A:6:LYS:N	2.36	0.59
1:B:459:ASP:OD1	1:B:462:ARG:NH2	2.36	0.58
1:C:731:GLU:O	1:C:735:ARG:HB2	2.02	0.58
1:A:4:ILE:CD1	1:B:288:ILE:HD12	2.33	0.58
1:A:8:MET:HE1	1:B:295:LEU:C	2.23	0.58
1:A:186:SER:HA	1:A:189:LYS:HB2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:N	1:A:4:ILE:HG12	2.19	0.57
1:A:267:TYR:HE2	1:B:547:GLN:HB3	1.69	0.57
1:C:848:ASP:CA	1:C:851:SER:H	2.17	0.57
1:A:260:LEU:HD11	1:B:543:GLU:HB3	1.86	0.57
1:C:601:GLU:HB3	1:C:605:LYS:NZ	2.19	0.57
1:C:706:GLU:H	1:C:708:LYS:CD	2.17	0.57
1:C:848:ASP:O	1:C:851:SER:CA	2.53	0.57
1:A:278:LEU:O	1:A:281:MET:HB3	2.04	0.57
1:B:408:GLU:O	1:B:412:LYS:HG3	2.05	0.57
1:D:986:ALA:HA	1:D:989:ASP:OD1	2.05	0.57
1:A:224:GLU:CB	1:A:227:VAL:H	2.17	0.56
1:C:852:ILE:C	1:C:852:ILE:CG2	2.73	0.56
1:A:224:GLU:HB3	1:A:226:LYS:N	2.20	0.56
1:D:1133:MET:HG2	1:D:1134:THR:N	2.19	0.56
1:C:706:GLU:N	1:C:708:LYS:HE3	2.21	0.56
1:D:1019:ARG:HA	1:D:1022:VAL:HG12	1.87	0.56
1:D:1084:LEU:O	1:D:1088:GLU:HB2	2.05	0.56
1:A:7:LYS:HD2	1:A:8:MET:HG2	1.88	0.55
1:C:705:ASP:C	1:C:708:LYS:HB3	2.26	0.55
1:C:706:GLU:N	1:C:708:LYS:CD	2.69	0.55
1:D:1056:LEU:HG	1:D:1060:GLU:OE2	2.07	0.55
1:A:8:MET:SD	1:B:291:LYS:O	2.65	0.55
1:C:569:MET:O	1:C:572:ILE:HG22	2.07	0.55
1:B:445:LYS:O	1:B:449:VAL:HG12	2.07	0.55
1:C:572:ILE:CA	1:C:572:ILE:HG13	2.37	0.55
1:D:1131:ASN:O	1:D:1135:SER:HB2	2.07	0.55
1:B:289:LYS:HB2	1:B:289:LYS:NZ	2.22	0.54
1:B:499:SER:HA	1:B:502:GLU:HB3	1.88	0.54
1:A:7:LYS:HE3	1:B:292:MET:HB2	1.89	0.54
1:A:165:VAL:HG23	1:B:453:LEU:HD23	1.90	0.54
1:A:224:GLU:CB	1:A:226:LYS:N	2.71	0.54
1:C:711:ILE:O	1:C:714:ILE:HG22	2.08	0.54
1:A:225:ILE:HD11	1:B:508:GLU:HB3	1.89	0.53
1:B:500:GLN:HA	1:B:503:ASP:OD1	2.09	0.53
1:C:677:ALA:O	1:C:681:LEU:HB2	2.08	0.53
1:D:880:ASP:CG	1:D:882:LYS:HB2	2.29	0.53
1:A:8:MET:CG	1:B:292:MET:HA	2.38	0.53
1:A:137:ASP:CG	1:A:140:LYS:HZ1	2.11	0.53
1:C:625:LEU:HD22	1:D:905:THR:HG22	1.90	0.53
1:C:701:ARG:O	1:C:708:LYS:CD	2.56	0.53
1:D:1048:GLU:HA	1:D:1051:THR:OG1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:705:ASP:C	1:C:708:LYS:CB	2.78	0.52
1:A:223:GLU:HA	1:A:224:GLU:CG	2.36	0.52
1:B:548:LYS:O	1:B:552:LYS:HD2	2.10	0.52
1:B:565:MET:CA	1:B:568:ILE:HG22	2.40	0.52
1:A:263:GLN:NE2	1:B:544:LEU:HG	2.25	0.52
1:B:285:MET:HA	1:B:288:ILE:HD12	1.91	0.51
1:C:571:ALA:HA	1:C:574:LYS:HB3	1.92	0.51
1:C:702:ALA:CA	1:C:708:LYS:HD3	2.41	0.51
1:C:848:ASP:C	1:C:850:THR:N	2.62	0.51
1:D:995:ILE:O	1:D:998:ILE:HG22	2.10	0.51
1:A:55:ASP:O	1:A:59:LYS:HG2	2.11	0.51
1:A:283:SER:O	1:A:284:ILE:HD13	2.10	0.51
1:A:274:LEU:O	1:A:277:ALA:HB3	2.11	0.50
1:C:827:GLU:HG3	1:C:831:GLN:NE2	2.25	0.50
1:A:4:ILE:HG13	1:B:288:ILE:HG21	1.94	0.50
1:A:263:GLN:HE22	1:B:544:LEU:HG	1.75	0.50
1:B:291:LYS:HE2	1:B:294:MET:HB3	1.93	0.50
1:D:876:GLU:O	1:D:879:ALA:HB3	2.11	0.50
1:D:1050:LYS:HA	1:D:1053:THR:OG1	2.11	0.50
1:A:242:ALA:O	1:A:246:VAL:HG23	2.12	0.50
1:C:764:GLU:O	1:C:768:VAL:HG12	2.11	0.50
1:D:880:ASP:CB	1:D:883:ALA:N	2.70	0.50
1:B:564:ASP:O	1:B:568:ILE:HB	2.12	0.49
1:C:733:VAL:HG22	1:D:1021:LEU:HD23	1.94	0.49
1:A:1:MET:O	1:A:4:ILE:N	2.45	0.49
1:A:114:GLU:HG2	1:A:118:LYS:NZ	2.27	0.49
1:B:402:LYS:O	1:B:406:GLU:HG3	2.11	0.49
1:C:656:LEU:O	1:C:660:ILE:HD13	2.12	0.49
1:C:705:ASP:HA	1:C:708:LYS:HB3	1.94	0.49
1:D:976:GLU:O	1:D:980:LYS:HG3	2.13	0.49
1:A:172:ILE:HD11	1:B:460:LEU:HD22	1.95	0.49
1:A:114:GLU:HG2	1:A:118:LYS:HZ2	1.78	0.49
1:C:667:LEU:HD11	1:D:950:GLU:HB3	1.95	0.49
1:C:680:LYS:HA	1:C:683:GLU:HB2	1.94	0.49
1:B:317:GLU:O	1:B:321:LYS:HG3	2.13	0.48
1:B:558:LEU:O	1:B:562:LEU:HB2	2.12	0.48
1:C:596:ASP:CG	1:D:881:LYS:HZ3	2.17	0.48
1:A:7:LYS:HG3	1:A:8:MET:H	1.79	0.48
1:A:8:MET:HE2	1:B:295:LEU:HB2	1.95	0.48
1:A:280:ASP:HB3	1:B:565:MET:CE	2.43	0.48
1:C:597:LYS:NZ	1:C:601:GLU:OE2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:702:ALA:O	1:C:708:LYS:CD	2.62	0.48
1:B:451:ARG:O	1:B:455:ILE:HB	2.14	0.48
1:C:702:ALA:HA	1:C:708:LYS:CE	2.34	0.48
1:D:987:GLN:HA	1:D:990:GLU:HB2	1.95	0.48
1:D:854:ASP:C	1:D:857:LYS:HB3	2.33	0.48
1:D:1064:GLU:O	1:D:1068:GLN:HG3	2.14	0.47
1:D:941:ASN:O	1:D:944:ILE:HG22	2.14	0.47
1:D:1126:LEU:O	1:D:1129:ALA:HB3	2.14	0.47
1:C:705:ASP:CA	1:C:705:ASP:O	2.51	0.47
1:A:133:ARG:O	1:A:137:ASP:HB2	2.14	0.47
1:A:162:TYR:HA	1:A:165:VAL:HG12	1.97	0.47
1:A:228:LEU:HD12	1:B:509:ILE:HG12	1.96	0.47
1:C:576:MET:HG3	1:D:859:LYS:HG3	1.95	0.47
1:D:856:ILE:HA	1:D:859:LYS:CB	2.44	0.47
1:A:225:ILE:HD12	1:B:509:ILE:HG13	1.95	0.47
1:B:543:GLU:HG3	1:B:547:GLN:HE21	1.80	0.47
1:C:703:GLN:O	1:C:708:LYS:N	2.48	0.47
1:D:879:ALA:O	1:D:880:ASP:CB	2.63	0.47
1:C:646:ALA:O	1:C:650:GLU:HB2	2.15	0.47
1:C:670:ALA:O	1:C:674:LEU:HB2	2.14	0.47
1:D:866:ASP:HA	1:D:869:ASN:HB3	1.97	0.47
1:A:222:GLU:O	1:A:224:GLU:CB	2.63	0.46
1:A:249:LEU:HD22	1:B:537:ILE:HG21	1.97	0.46
1:A:280:ASP:C	1:A:282:THR:H	2.18	0.46
1:A:203:ASN:HB3	1:B:488:LEU:HD11	1.98	0.46
1:B:564:ASP:C	1:B:566:THR:N	2.69	0.46
1:C:701:ARG:O	1:C:708:LYS:HD3	2.16	0.46
1:A:106:LEU:HD21	1:B:389:ARG:HD3	1.96	0.46
1:C:601:GLU:O	1:C:605:LYS:HG3	2.15	0.46
1:B:473:LYS:HZ3	1:B:477:LEU:HD11	1.81	0.46
1:C:818:GLU:O	1:C:821:ILE:HG22	2.16	0.46
1:C:579:LEU:HG	1:D:860:MET:HG3	1.96	0.46
1:D:880:ASP:HB3	1:D:882:LYS:CA	2.45	0.46
1:C:674:LEU:HD21	1:D:957:ARG:HD3	1.97	0.46
1:C:705:ASP:CA	1:C:708:LYS:HD2	2.45	0.46
1:B:436:LYS:HZ3	1:B:440:GLU:CD	2.19	0.46
1:C:612:VAL:HG22	1:C:616:LYS:NZ	2.31	0.46
1:C:694:GLY:O	1:C:697:VAL:HG12	2.16	0.46
1:D:1014:TYR:O	1:D:1018:ALA:HB2	2.15	0.46
1:A:4:ILE:CG1	1:B:288:ILE:HG21	2.45	0.45
1:A:16:GLU:O	1:A:19:LEU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:MET:HG2	1:B:293:GLN:HG3	1.99	0.45
1:A:7:LYS:NZ	1:B:292:MET:HB2	2.31	0.45
1:A:75:GLU:CD	1:B:354:LYS:HZ3	2.20	0.45
1:A:224:GLU:HB2	1:A:226:LYS:CA	2.47	0.45
1:B:290:LYS:O	1:B:293:GLN:HB2	2.15	0.45
1:C:653:VAL:O	1:C:657:ASN:HB2	2.16	0.45
1:B:356:GLU:OE2	1:B:360:LYS:NZ	2.49	0.45
1:B:450:ALA:O	1:B:453:LEU:HG	2.17	0.45
1:A:95:PHE:O	1:A:99:LEU:HD13	2.16	0.45
1:C:622:GLU:OE1	1:D:901:LYS:NZ	2.50	0.45
1:D:880:ASP:CB	1:D:883:ALA:H	2.23	0.45
1:D:958:LEU:O	1:D:962:LEU:HB2	2.16	0.45
1:A:223:GLU:O	1:A:227:VAL:HB	2.16	0.45
1:A:266:LYS:O	1:A:270:ILE:HG13	2.17	0.45
1:A:112:LYS:HB2	1:A:112:LYS:NZ	2.32	0.45
1:B:285:MET:N	1:B:288:ILE:HD11	2.32	0.45
1:D:859:LYS:CA	1:D:859:LYS:H	2.07	0.45
1:A:4:ILE:HG22	1:A:7:LYS:HG2	1.99	0.45
1:A:248:LYS:NZ	1:A:252:SER:OG	2.50	0.45
1:B:424:LYS:HA	1:B:427:ILE:HB	1.99	0.44
1:C:704:LYS:O	1:C:708:LYS:CA	2.65	0.44
1:A:7:LYS:HD3	1:A:8:MET:HG2	1.99	0.44
1:D:856:ILE:HD13	1:D:856:ILE:HG21	1.62	0.44
1:D:885:GLU:O	1:D:889:LYS:HG3	2.17	0.44
1:D:1021:LEU:HD12	1:D:1022:VAL:N	2.33	0.44
1:B:285:MET:SD	1:B:289:LYS:NZ	2.88	0.44
1:C:675:ALA:O	1:C:679:GLN:HB2	2.18	0.44
1:D:864:LYS:NZ	1:D:868:GLU:OE2	2.51	0.44
1:C:844:HIS:O	1:C:845:ALA:C	2.56	0.44
1:C:848:ASP:HA	1:C:851:SER:N	2.30	0.44
1:A:8:MET:CE	1:B:295:LEU:HB2	2.48	0.44
1:B:534:GLU:O	1:B:537:ILE:HG22	2.17	0.44
1:A:169:LEU:O	1:A:172:ILE:HG22	2.18	0.43
1:C:744:LEU:HD11	1:D:1027:ASP:HB3	2.00	0.43
1:C:762:GLU:O	1:C:765:ILE:HG22	2.18	0.43
1:D:1108:LEU:O	1:D:1112:LEU:HD13	2.18	0.43
1:C:704:LYS:NZ	1:C:705:ASP:OD2	2.52	0.43
1:A:168:LYS:NZ	1:B:457:GLU:OE2	2.52	0.43
1:B:513:SER:O	1:B:517:LYS:NZ	2.52	0.43
1:C:649:ALA:O	1:C:653:VAL:HG23	2.19	0.43
1:C:704:LYS:O	1:C:708:LYS:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ARG:NH1	1:B:324:GLU:OE2	2.51	0.43
1:C:698:ILE:HG21	1:D:982:ILE:HG23	2.01	0.43
1:D:1008:GLU:HB3	1:D:1012:ARG:HH11	1.83	0.43
1:D:1011:ASP:O	1:D:1014:TYR:HB3	2.19	0.43
1:D:1068:GLN:HA	1:D:1071:ASP:OD1	2.18	0.43
1:D:1083:LYS:NZ	1:D:1086:GLU:OE1	2.51	0.43
1:D:1126:LEU:O	1:D:1130:LEU:HD13	2.18	0.43
1:B:292:MET:HG2	1:B:293:GLN:N	2.33	0.43
1:B:516:LEU:O	1:B:520:GLU:HB2	2.19	0.43
1:C:682:GLU:OE1	1:C:686:LYS:NZ	2.51	0.43
1:D:988:LYS:O	1:D:992:LYS:HD2	2.18	0.43
1:A:3:ALA:O	1:A:4:ILE:C	2.57	0.43
1:A:54:GLU:OE1	1:B:333:LYS:NZ	2.51	0.43
1:A:96:GLU:O	1:A:99:LEU:HB2	2.19	0.43
1:A:151:ALA:O	1:A:154:ILE:HG22	2.19	0.43
1:A:4:ILE:O	1:A:7:LYS:HG3	2.18	0.43
1:C:701:ARG:O	1:C:708:LYS:HD2	2.18	0.43
1:C:848:ASP:C	1:C:851:SER:N	2.72	0.43
1:B:562:LEU:O	1:B:566:THR:HB	2.19	0.42
1:B:313:LYS:NZ	1:B:317:GLU:HG3	2.33	0.42
1:C:736:LYS:HA	1:C:739:ILE:HG22	2.01	0.42
1:A:11:LEU:HD23	1:B:295:LEU:O	2.19	0.42
1:A:12:LYS:NZ	1:A:16:GLU:OE1	2.52	0.42
1:C:580:LYS:NZ	1:C:584:GLU:OE2	2.52	0.42
1:C:698:ILE:HD11	1:D:986:ALA:HB3	2.01	0.42
1:B:565:MET:HA	1:B:568:ILE:CG2	2.48	0.42
1:C:719:ALA:O	1:C:722:ILE:HG22	2.18	0.42
1:C:833:LEU:O	1:C:836:LYS:HB2	2.19	0.42
1:C:591:ASP:O	1:C:595:ALA:HB2	2.18	0.42
1:C:736:LYS:NZ	1:D:1025:GLU:OE1	2.53	0.42
1:B:285:MET:HA	1:B:288:ILE:CD1	2.50	0.42
1:D:1074:GLU:OE2	1:D:1078:LYS:NZ	2.49	0.42
1:B:559:ASP:O	1:B:562:LEU:HB3	2.20	0.42
1:C:755:GLU:O	1:C:758:CYS:HB2	2.20	0.42
1:D:1053:THR:O	1:D:1057:LYS:HD2	2.20	0.42
1:C:702:ALA:O	1:C:708:LYS:CG	2.66	0.42
1:C:707:GLU:N	1:C:708:LYS:CG	2.79	0.42
1:D:879:ALA:O	1:D:880:ASP:HB2	2.19	0.42
1:D:991:GLU:OE1	1:D:992:LYS:NZ	2.52	0.42
1:D:965:LEU:O	1:D:969:GLU:HG3	2.19	0.42
1:B:565:MET:HA	1:B:568:ILE:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1020:LYS:O	1:D:1023:ILE:HG22	2.20	0.41
1:A:279:ASN:HA	1:A:282:THR:OG1	2.20	0.41
1:A:7:LYS:O	1:A:10:MET:N	2.54	0.41
1:C:705:ASP:N	1:C:708:LYS:CG	2.83	0.41
1:A:12:LYS:NZ	1:A:16:GLU:OE2	2.53	0.41
1:A:46:LEU:O	1:A:50:LEU:HB2	2.20	0.41
1:A:50:LEU:HD21	1:B:333:LYS:HB3	2.02	0.41
1:C:682:GLU:HG2	1:C:686:LYS:NZ	2.36	0.41
1:A:1:MET:H2	1:A:4:ILE:HG12	1.83	0.41
1:C:692:GLU:OE2	1:C:696:LYS:NZ	2.53	0.41
1:C:704:LYS:C	1:C:708:LYS:CG	2.89	0.41
1:D:976:GLU:OE1	1:D:980:LYS:NZ	2.53	0.41
1:D:910:ASP:O	1:D:913:SER:HB3	2.21	0.41
1:D:1125:GLU:O	1:D:1129:ALA:HB2	2.20	0.41
1:D:905:THR:O	1:D:909:LEU:HB2	2.21	0.40
1:B:335:LYS:NZ	1:B:338:GLU:OE2	2.53	0.40
1:A:126:GLY:O	1:A:130:ILE:HG22	2.21	0.40
1:C:599:ALA:O	1:C:603:ARG:HB2	2.22	0.40
1:C:720:LYS:O	1:C:723:ALA:HB3	2.21	0.40
1:D:1081:SER:O	1:D:1085:LYS:NZ	2.54	0.40
1:A:223:GLU:O	1:A:224:GLU:CB	2.69	0.40
1:C:613:SER:O	1:C:617:LYS:HG2	2.21	0.40
1:A:168:LYS:O	1:A:172:ILE:HB	2.22	0.40
1:C:612:VAL:HG22	1:C:616:LYS:HZ2	1.86	0.40
1:C:680:LYS:HZ3	1:D:965:LEU:HA	1.87	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:851:SER:O	1:D:857:LYS:O[3_364]	2.14	0.06
1:C:848:ASP:O	1:D:856:ILE:O[3_364]	2.16	0.04
1:C:852:ILE:N	1:D:860:MET:N[3_364]	2.17	0.03

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	282/284 (99%)	241 (86%)	32 (11%)	9 (3%)	4 26
1	B	282/284 (99%)	250 (89%)	28 (10%)	4 (1%)	11 46
1	C	282/284 (99%)	246 (87%)	30 (11%)	6 (2%)	7 36
1	D	282/284 (99%)	246 (87%)	28 (10%)	8 (3%)	5 30
All	All	1128/1136 (99%)	983 (87%)	118 (10%)	27 (2%)	6 33

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	570	ASP
1	C	845	ALA
1	D	854	ASP
1	D	880	ASP
1	D	1133	MET
1	A	4	ILE
1	A	59	LYS
1	A	66	ASP
1	A	72	GLU
1	B	288	ILE
1	C	640	GLU
1	C	708	LYS
1	D	1079	VAL
1	D	1099	THR
1	A	7	LYS
1	C	844	HIS
1	D	879	ALA
1	D	986	ALA
1	A	71	LEU
1	A	224	GLU
1	B	286	ASP
1	B	553	ALA
1	A	58	ASP
1	A	113	LEU
1	B	561	ALA
1	C	634	ASP
1	D	1098	VAL

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	245/245 (100%)	209 (85%)	36 (15%)	3	15
1	B	245/245 (100%)	220 (90%)	25 (10%)	7	25
1	C	245/245 (100%)	217 (89%)	28 (11%)	5	21
1	D	245/245 (100%)	212 (86%)	33 (14%)	4	17
All	All	980/980 (100%)	858 (88%)	122 (12%)	4	19

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	ILE
1	A	7	LYS
1	A	8	MET
1	A	11	LEU
1	A	15	LYS
1	A	16	GLU
1	A	28	ASP
1	A	30	LYS
1	A	33	GLU
1	A	34	ASP
1	A	50	LEU
1	A	54	GLU
1	A	79	THR
1	A	84	ASP
1	A	87	SER
1	A	112	LYS
1	A	124	GLU
1	A	137	ASP
1	A	153	HIS
1	A	159	ASP
1	A	165	VAL
1	A	175	ASP
1	A	197	ILE

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Mol	Chain	Res	Type
1	A	199	THR
1	A	200	VAL
1	A	201	THR
1	A	224	GLU
1	A	227	VAL
1	A	229	SER
1	A	231	LYS
1	A	234	GLU
1	A	248	LYS
1	A	274	LEU
1	A	278	LEU
1	A	281	MET
1	B	285	MET
1	B	288	ILE
1	B	291	LYS
1	B	292	MET
1	B	313	LYS
1	B	317	GLU
1	B	384	ASP
1	B	396	LYS
1	B	413	VAL
1	B	430	ILE
1	B	432	LEU
1	B	437	HIS
1	B	446	TYR
1	B	452	LYS
1	B	459	ASP
1	B	509	ILE
1	B	524	GLU
1	B	537	ILE
1	B	551	TYR
1	B	552	LYS
1	B	556	GLU
1	B	559	ASP
1	B	562	LEU
1	B	566	THR
1	B	568	ILE
1	C	572	ILE
1	C	576	MET
1	C	579	LEU
1	C	591	ASP
1	C	596	ASP

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Mol	Chain	Res	Type
1	C	612	VAL
1	C	618	LEU
1	C	634	ASP
1	C	647	THR
1	C	657	ASN
1	C	676	THR
1	C	680	LYS
1	C	692	GLU
1	C	705	ASP
1	C	708	LYS
1	C	711	ILE
1	C	743	ASP
1	C	767	THR
1	C	799	LYS
1	C	808	GLU
1	C	815	THR
1	C	821	ILE
1	C	823	ASP
1	C	835	TYR
1	C	836	LYS
1	C	844	HIS
1	C	849	MET
1	C	850	THR
1	D	853	MET
1	D	857	LYS
1	D	881	LYS
1	D	882	LYS
1	D	892	GLU
1	D	905	THR
1	D	910	ASP
1	D	918	ASP
1	D	924	GLU
1	D	931	THR
1	D	936	ASP
1	D	947	PHE
1	D	952	ASP
1	D	965	LEU
1	D	966	GLU
1	D	973	ASP
1	D	989	ASP
1	D	992	LYS
1	D	1005	HIS

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Mol	Chain	Res	Type
1	D	1014	TYR
1	D	1020	LYS
1	D	1022	VAL
1	D	1025	GLU
1	D	1038	SER
1	D	1049	ILE
1	D	1057	LYS
1	D	1071	ASP
1	D	1086	GLU
1	D	1105	ILE
1	D	1125	GLU
1	D	1128	HIS
1	D	1134	THR
1	D	1136	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	B	431	GLN
1	D	1055	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)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	851:SER	C	852:ILE	N	1.70

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands (i)

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers (i)

Unable to reproduce the depositors R factor - this section is therefore empty.