



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 12:50 PM UTC

PDB ID : 1DXX / pdb_00001dxx
Title : N-terminal Actin-binding Domain of Human Dystrophin
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Deposited on : 2000-01-20
Resolution : 2.60 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	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

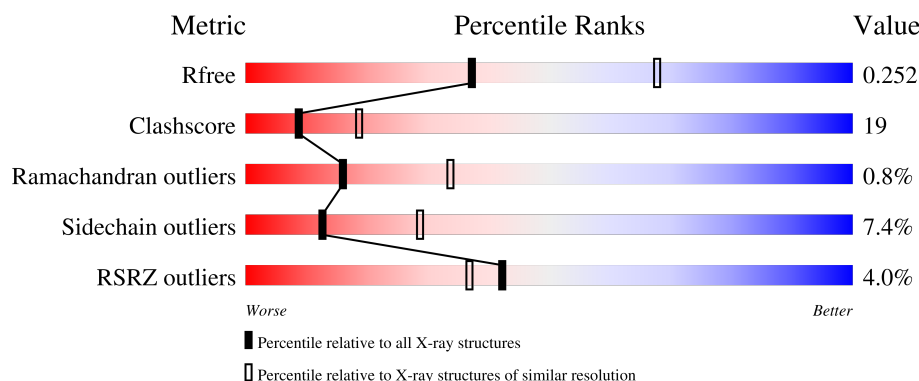
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	246	3% 48% 37% 9% ..
1	B	246	4% 49% 38% 7% ..
1	C	246	3% 48% 37% 9% ..
1	D	246	5% 49% 36% 9% ..

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7622 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 DYSTROPHIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	238	Total	C	N	O	S	0	0	0
			1887	1197	332	355	3			
1	B	238	Total	C	N	O	S	0	0	0
			1885	1194	333	355	3			
1	C	238	Total	C	N	O	S	0	0	0
			1891	1199	333	356	3			
1	D	238	Total	C	N	O	S	0	0	0
			1885	1193	333	356	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	10	SER	CYS	engineered mutation	UNP P11532
B	10	SER	CYS	engineered mutation	UNP P11532
C	10	SER	CYS	engineered mutation	UNP P11532
D	10	SER	CYS	engineered mutation	UNP P11532
A	188	SER	CYS	engineered mutation	UNP P11532
B	188	SER	CYS	engineered mutation	UNP P11532
C	188	SER	CYS	engineered mutation	UNP P11532
D	188	SER	CYS	engineered mutation	UNP P11532

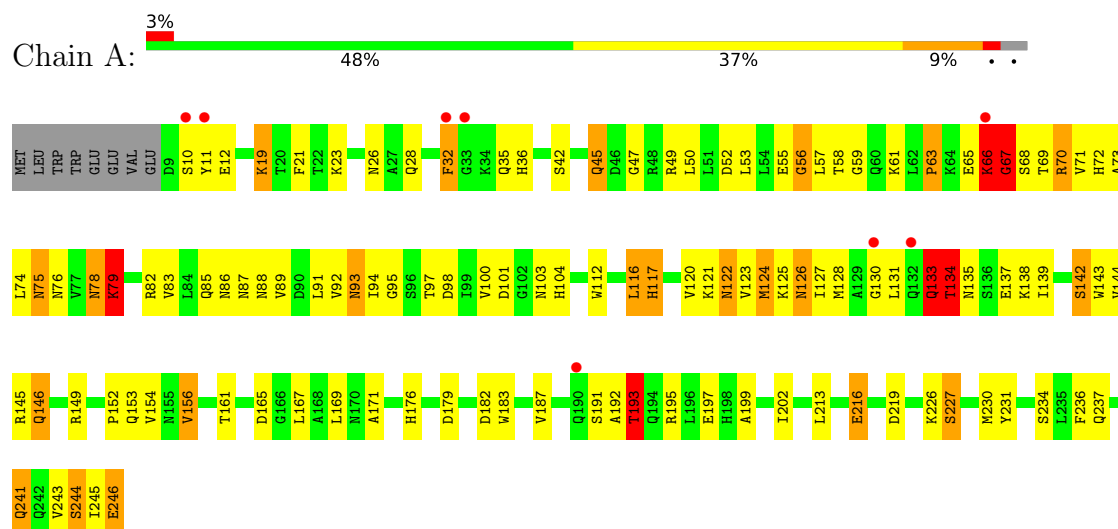
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	26	Total	O	0	0
			26	26		
2	B	19	Total	O	0	0
			19	19		
2	C	14	Total	O	0	0
			14	14		
2	D	15	Total	O	0	0
			15	15		

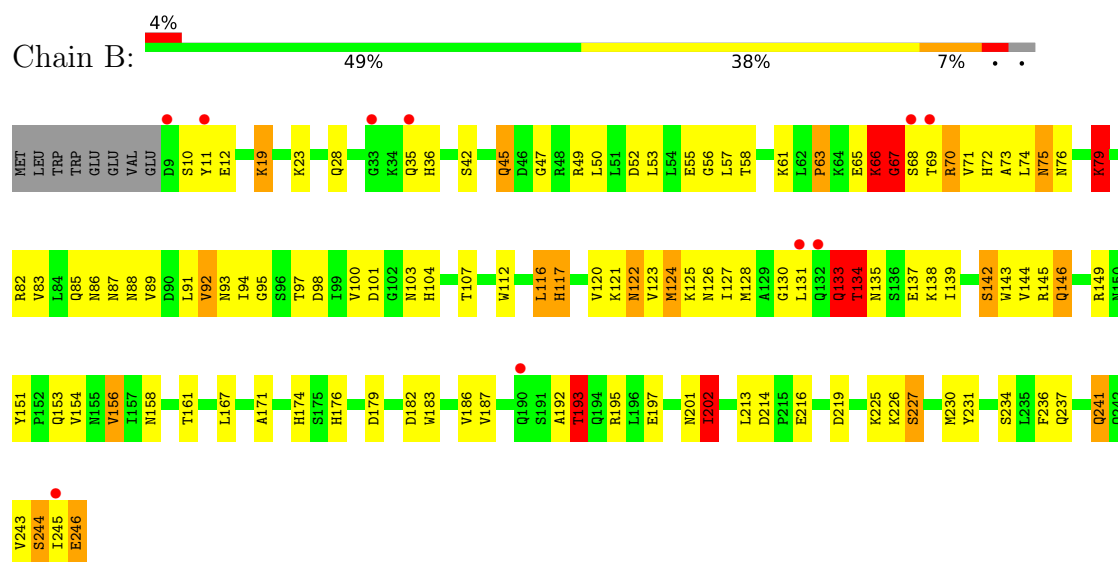
3 Residue-property plots [i](#)

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: DYSTROPHIN

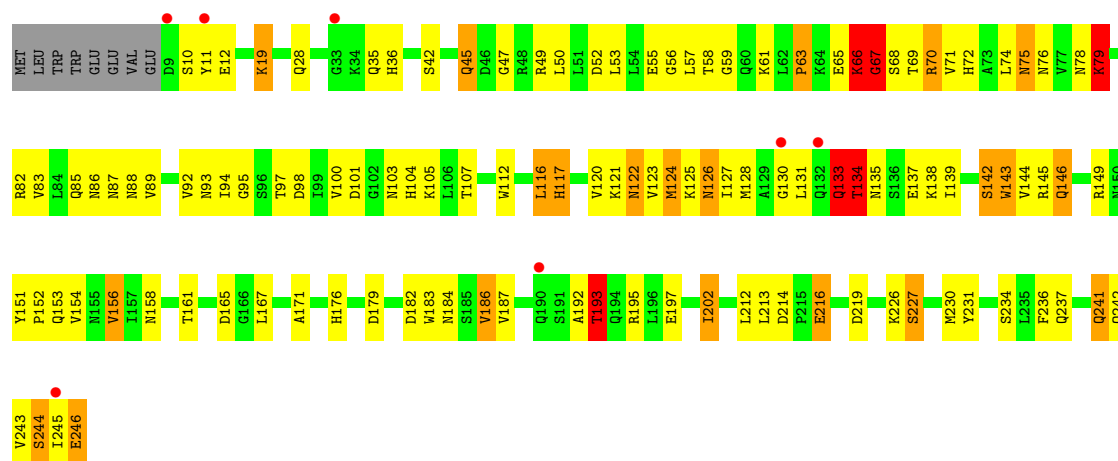


• Molecule 1: DYSTROPHIN

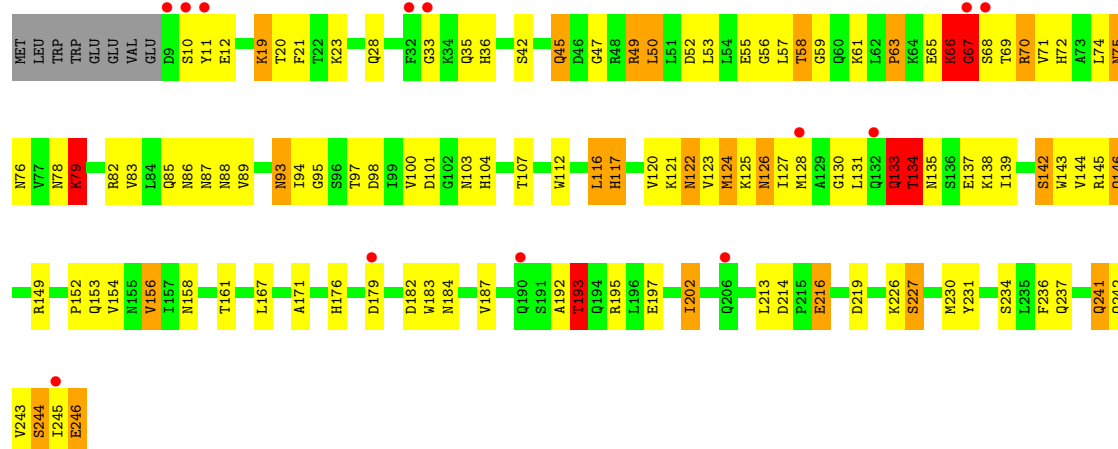


• Molecule 1: DYSTROPHIN





• Molecule 1: DYSTROPHIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.69Å 79.33Å 81.95Å 61.08° 78.22° 70.54°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.0 (20.00-2.60) 95.2 (20.00-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.29 (at 2.61Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.232 , 0.268 0.223 , 0.252	Depositor DCC
R_{free} test set	1799 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	38.7	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.130 for -h,-k,-k+l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7622	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.35 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.6765e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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

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	0.82	0/1923	2.22	83/2614 (3.2%)
1	B	0.84	0/1920	2.22	85/2609 (3.3%)
1	C	0.84	0/1927	2.23	93/2619 (3.6%)
1	D	0.82	0/1920	2.22	86/2610 (3.3%)
All	All	0.83	0/7690	2.22	347/10452 (3.3%)

There are no bond length outliers.

All (347) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	12	GLU	CA-CB-CG	11.47	137.04	114.10
1	D	12	GLU	CA-CB-CG	11.42	136.94	114.10
1	A	12	GLU	CA-CB-CG	11.38	136.87	114.10
1	B	12	GLU	CA-CB-CG	11.25	136.60	114.10
1	A	68	SER	N-CA-C	-10.88	98.99	114.12
1	D	68	SER	N-CA-C	-10.68	99.27	114.12
1	B	68	SER	N-CA-C	-10.64	99.33	114.12
1	C	68	SER	N-CA-C	-10.49	99.54	114.12
1	C	145	ARG	NE-CZ-NH2	-10.20	110.02	119.20
1	A	145	ARG	NE-CZ-NH2	-9.74	110.44	119.20
1	B	145	ARG	NE-CZ-NH2	-9.69	110.48	119.20
1	D	93	ASN	CA-CB-CG	-9.42	103.18	112.60
1	B	104	HIS	CA-CB-CG	-9.26	104.54	113.80
1	D	145	ARG	NE-CZ-NH2	-9.09	111.02	119.20
1	D	82	ARG	CD-NE-CZ	9.05	137.07	124.40
1	A	145	ARG	CD-NE-CZ	8.92	136.88	124.40
1	D	145	ARG	CD-NE-CZ	8.88	136.82	124.40
1	D	104	HIS	CA-CB-CG	-8.83	104.97	113.80
1	C	145	ARG	CD-NE-CZ	8.82	136.75	124.40
1	B	145	ARG	CD-NE-CZ	8.80	136.72	124.40
1	A	93	ASN	CA-CB-CG	-8.78	103.82	112.60
1	B	93	ASN	CA-CB-CG	-8.73	103.87	112.60
1	A	82	ARG	CD-NE-CZ	8.58	136.41	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	82	ARG	CD-NE-CZ	8.50	136.30	124.40
1	C	93	ASN	CA-CB-CG	-8.49	104.11	112.60
1	B	82	ARG	CD-NE-CZ	8.41	136.17	124.40
1	A	89	VAL	O-C-N	-8.36	112.86	122.72
1	C	195	ARG	CD-NE-CZ	8.35	136.09	124.40
1	B	122	ASN	OD1-CG-ND2	8.24	130.84	122.60
1	C	104	HIS	CA-CB-CG	-8.20	105.60	113.80
1	A	122	ASN	OD1-CG-ND2	8.17	130.77	122.60
1	D	67	GLY	CA-C-O	8.16	134.77	120.57
1	C	133	GLN	OE1-CD-NE2	-8.14	114.46	122.60
1	A	195	ARG	CD-NE-CZ	8.10	135.74	124.40
1	B	195	ARG	CD-NE-CZ	8.10	135.74	124.40
1	A	67	GLY	CA-C-O	8.08	134.63	120.57
1	D	45	GLN	OE1-CD-NE2	-8.08	114.52	122.60
1	D	68	SER	CA-C-O	8.05	127.76	118.90
1	D	122	ASN	OD1-CG-ND2	8.02	130.62	122.60
1	C	67	GLY	CA-C-O	7.96	134.42	120.57
1	A	45	GLN	N-CA-C	7.93	120.83	111.71
1	A	68	SER	CA-C-O	7.93	127.62	118.90
1	B	67	GLY	CA-C-O	7.93	134.37	120.57
1	A	133	GLN	OE1-CD-NE2	-7.91	114.69	122.60
1	C	145	ARG	NE-CZ-NH1	7.91	129.41	121.50
1	D	195	ARG	CD-NE-CZ	7.88	135.44	124.40
1	D	45	GLN	N-CA-C	7.87	120.76	111.71
1	D	117	HIS	CA-CB-CG	-7.85	105.95	113.80
1	C	68	SER	CA-C-O	7.82	127.50	118.90
1	B	12	GLU	N-CA-CB	7.81	123.28	110.39
1	C	122	ASN	OD1-CG-ND2	7.81	130.41	122.60
1	B	45	GLN	N-CA-C	7.79	120.67	111.71
1	D	12	GLU	N-CA-CB	7.73	123.14	110.39
1	B	133	GLN	OE1-CD-NE2	-7.69	114.91	122.60
1	A	104	HIS	CA-CB-CG	-7.69	106.11	113.80
1	D	145	ARG	NE-CZ-NH1	7.67	129.17	121.50
1	B	68	SER	CA-C-O	7.65	127.31	118.90
1	A	45	GLN	OE1-CD-NE2	-7.63	114.97	122.60
1	C	12	GLU	N-CA-CB	7.61	122.95	110.39
1	A	12	GLU	N-CA-CB	7.61	122.95	110.39
1	D	79	LYS	CA-CB-CG	7.59	129.28	114.10
1	C	45	GLN	N-CA-C	7.56	120.41	111.71
1	B	145	ARG	NE-CZ-NH1	7.55	129.05	121.50
1	B	97	THR	CA-C-N	7.51	130.35	120.28
1	B	97	THR	C-N-CA	7.51	130.35	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	133	GLN	OE1-CD-NE2	-7.50	115.10	122.60
1	A	79	LYS	CA-CB-CG	7.47	129.04	114.10
1	A	145	ARG	NE-CZ-NH1	7.47	128.97	121.50
1	B	117	HIS	CA-CB-CG	-7.44	106.36	113.80
1	C	28	GLN	OE1-CD-NE2	7.42	130.02	122.60
1	C	154	VAL	CA-C-O	-7.41	112.63	120.48
1	B	79	LYS	CA-CB-CG	7.40	128.90	114.10
1	A	97	THR	CA-C-N	7.38	130.16	120.28
1	A	97	THR	C-N-CA	7.38	130.16	120.28
1	C	97	THR	CA-C-N	7.37	130.15	120.28
1	C	97	THR	C-N-CA	7.37	130.15	120.28
1	C	79	LYS	CA-CB-CG	7.32	128.75	114.10
1	B	45	GLN	OE1-CD-NE2	-7.20	115.40	122.60
1	D	182	ASP	N-CA-CB	-7.20	99.25	110.55
1	A	154	VAL	CA-C-O	-7.19	112.86	120.48
1	D	97	THR	CA-C-N	7.18	129.90	120.28
1	D	97	THR	C-N-CA	7.18	129.90	120.28
1	D	11	TYR	N-CA-C	-7.14	101.64	111.28
1	A	117	HIS	CA-CB-CG	-7.13	106.67	113.80
1	B	11	TYR	N-CA-C	-7.08	101.72	111.28
1	C	45	GLN	OE1-CD-NE2	-7.07	115.53	122.60
1	C	142	SER	N-CA-CB	7.05	120.23	110.01
1	C	117	HIS	CA-CB-CG	-7.04	106.76	113.80
1	B	89	VAL	O-C-N	-6.99	114.47	122.72
1	A	11	TYR	N-CA-C	-6.97	101.87	111.28
1	B	28	GLN	OE1-CD-NE2	6.97	129.57	122.60
1	D	156	VAL	N-CA-CB	-6.97	103.15	110.95
1	C	89	VAL	O-C-N	-6.94	114.53	122.72
1	C	182	ASP	N-CA-CB	-6.91	99.70	110.55
1	B	158	ASN	OD1-CG-ND2	-6.90	115.70	122.60
1	D	219	ASP	CB-CG-OD2	-6.90	102.54	118.40
1	A	63	PRO	CA-C-O	-6.87	113.60	121.36
1	B	154	VAL	CA-C-O	-6.87	113.20	120.48
1	C	63	PRO	CA-C-O	-6.86	113.60	121.36
1	B	142	SER	N-CA-CB	6.86	119.96	110.01
1	B	63	PRO	CA-C-O	-6.85	113.62	121.36
1	B	219	ASP	CB-CG-OD2	-6.84	102.67	118.40
1	B	58	THR	CA-C-O	-6.83	112.66	120.24
1	A	133	GLN	N-CA-C	-6.81	104.72	113.16
1	A	28	GLN	OE1-CD-NE2	6.79	129.39	122.60
1	C	156	VAL	N-CA-CB	-6.78	103.35	110.95
1	B	182	ASP	N-CA-CB	-6.78	99.91	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	ARG	CA-C-O	-6.76	113.33	120.63
1	C	161	THR	CA-C-O	-6.73	111.34	119.49
1	D	89	VAL	O-C-N	-6.73	114.78	122.72
1	D	213	LEU	N-CA-C	6.72	121.00	110.17
1	A	182	ASP	N-CA-CB	-6.72	100.00	110.55
1	C	11	TYR	N-CA-C	-6.66	102.29	111.28
1	D	134	THR	N-CA-C	6.65	120.24	109.40
1	D	142	SER	N-CA-CB	6.65	119.65	110.01
1	B	134	THR	N-CA-C	6.64	120.22	109.40
1	C	219	ASP	CB-CG-OD2	-6.62	103.17	118.40
1	C	193	THR	CB-CA-C	6.61	121.92	110.68
1	A	142	SER	N-CA-CB	6.61	119.59	110.01
1	B	19	LYS	CB-CA-C	-6.60	100.47	110.90
1	D	193	THR	CB-CA-C	6.59	121.88	110.68
1	B	156	VAL	N-CA-CB	-6.53	103.64	110.95
1	A	219	ASP	CB-CG-OD2	-6.52	103.41	118.40
1	A	58	THR	CA-C-O	-6.51	113.01	120.24
1	A	213	LEU	N-CA-C	6.50	120.64	110.17
1	A	156	VAL	N-CA-CB	-6.45	103.73	110.95
1	C	133	GLN	N-CA-C	-6.44	105.17	113.16
1	B	213	LEU	N-CA-C	6.42	120.51	110.17
1	D	176	HIS	CA-CB-CG	-6.42	107.38	113.80
1	D	145	ARG	CA-C-O	-6.39	114.11	120.82
1	D	154	VAL	CA-C-O	-6.38	113.71	120.48
1	D	133	GLN	N-CA-C	-6.37	105.26	113.16
1	A	193	THR	CB-CA-C	6.37	121.50	110.68
1	D	63	PRO	CA-C-O	-6.34	114.19	121.36
1	A	134	THR	N-CA-C	6.34	119.73	109.40
1	A	55	GLU	CA-C-O	-6.30	114.38	121.00
1	C	50	LEU	CA-C-O	-6.29	114.21	120.82
1	B	193	THR	CB-CA-C	6.29	121.37	110.68
1	B	145	ARG	CA-C-O	-6.29	114.22	120.82
1	B	176	HIS	CA-CB-CG	-6.24	107.56	113.80
1	D	19	LYS	CB-CA-C	-6.21	101.08	110.90
1	A	85	GLN	OE1-CD-NE2	-6.21	116.39	122.60
1	C	134	THR	N-CA-C	6.20	119.51	109.40
1	C	213	LEU	N-CA-C	6.20	120.16	110.17
1	B	61	LYS	N-CA-CB	6.19	120.27	110.55
1	B	94	ILE	CA-C-N	-6.18	115.12	122.16
1	B	94	ILE	C-N-CA	-6.18	115.12	122.16
1	B	55	GLU	CA-C-O	-6.17	114.52	121.00
1	C	58	THR	CA-C-O	-6.16	113.40	120.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	19	LYS	CB-CA-C	-6.16	101.40	110.95
1	A	70	ARG	CB-CA-C	6.15	120.65	110.81
1	B	167	LEU	N-CA-C	6.13	117.76	111.14
1	C	176	HIS	CA-CB-CG	-6.12	107.68	113.80
1	B	133	GLN	N-CA-C	-6.12	105.58	113.16
1	A	19	LYS	CB-CA-C	-6.10	101.26	110.90
1	D	58	THR	CA-C-O	-6.10	113.47	120.24
1	C	55	GLU	CA-C-O	-6.09	114.60	121.00
1	C	52	ASP	CA-CB-CG	-6.08	106.52	112.60
1	C	74	LEU	CA-C-O	6.08	126.97	120.10
1	A	74	LEU	CA-C-O	6.07	126.96	120.10
1	D	61	LYS	N-CA-CB	6.06	120.07	110.55
1	A	61	LYS	N-CA-CB	6.06	120.09	110.57
1	D	74	LEU	CA-C-O	6.06	126.95	120.10
1	C	85	GLN	OE1-CD-NE2	-6.05	116.55	122.60
1	C	70	ARG	CB-CA-C	6.05	120.48	110.81
1	A	176	HIS	CA-CB-CG	-6.02	107.78	113.80
1	D	28	GLN	OE1-CD-NE2	6.00	128.60	122.60
1	A	83	VAL	N-CA-CB	6.00	117.57	110.55
1	D	161	THR	CA-C-O	-5.97	112.56	119.61
1	D	116	LEU	CA-C-O	5.97	127.09	120.82
1	A	103	ASN	N-CA-C	-5.96	98.01	108.20
1	D	94	ILE	CA-C-N	-5.96	115.37	122.16
1	D	94	ILE	C-N-CA	-5.96	115.37	122.16
1	D	146	GLN	N-CA-CB	5.96	118.65	110.01
1	B	52	ASP	CA-CB-CG	-5.95	106.65	112.60
1	B	138	LYS	CA-C-N	-5.94	111.98	120.42
1	B	138	LYS	C-N-CA	-5.94	111.98	120.42
1	C	12	GLU	CB-CA-C	-5.94	101.33	111.31
1	C	61	LYS	N-CA-CB	5.93	119.86	110.55
1	C	105	LYS	CA-CB-CG	5.92	125.93	114.10
1	A	94	ILE	CA-C-N	-5.91	115.42	122.16
1	A	94	ILE	C-N-CA	-5.91	115.42	122.16
1	A	32	PHE	CB-CG-CD2	-5.89	110.68	120.70
1	A	145	ARG	CA-C-O	-5.89	114.64	120.82
1	D	12	GLU	CB-CA-C	-5.88	101.43	111.31
1	D	55	GLU	CA-C-O	-5.88	114.83	121.00
1	C	125	LYS	N-CA-CB	5.87	118.85	110.16
1	A	125	LYS	N-CA-CB	5.84	118.80	110.16
1	A	146	GLN	N-CA-CB	5.84	118.54	110.07
1	D	167	LEU	N-CA-C	5.84	117.44	111.14
1	D	138	LYS	CA-C-N	-5.82	112.15	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	138	LYS	C-N-CA	-5.82	112.15	120.42
1	B	146	GLN	N-CA-CB	5.81	118.44	110.01
1	B	73	ALA	N-CA-C	-5.81	104.85	111.07
1	B	161	THR	CA-C-O	-5.81	112.46	119.49
1	A	52	ASP	CA-CB-CG	-5.80	106.80	112.60
1	A	138	LYS	CA-C-N	-5.79	112.19	120.42
1	A	138	LYS	C-N-CA	-5.79	112.19	120.42
1	A	73	ALA	N-CA-C	-5.79	104.88	111.07
1	B	50	LEU	CA-C-O	-5.79	114.75	120.82
1	B	12	GLU	CB-CA-C	-5.78	101.60	111.31
1	B	125	LYS	N-CA-CB	5.77	118.71	110.16
1	D	125	LYS	N-CA-CB	5.76	118.69	110.16
1	A	12	GLU	CB-CA-C	-5.75	101.65	111.31
1	C	156	VAL	N-CA-C	5.75	117.05	108.54
1	C	146	GLN	N-CA-CB	5.74	118.40	110.07
1	C	138	LYS	CA-C-N	-5.74	112.27	120.42
1	C	138	LYS	C-N-CA	-5.74	112.27	120.42
1	B	195	ARG	O-C-N	-5.73	116.05	122.12
1	C	94	ILE	CA-C-N	-5.72	115.64	122.16
1	C	94	ILE	C-N-CA	-5.72	115.64	122.16
1	A	75	ASN	O-C-N	5.70	128.25	122.09
1	B	195	ARG	CA-C-O	5.70	126.59	120.55
1	A	58	THR	N-CA-C	5.69	118.69	111.69
1	A	156	VAL	N-CA-C	5.69	116.96	108.54
1	C	93	ASN	CA-C-N	-5.68	115.39	123.11
1	C	93	ASN	C-N-CA	-5.68	115.39	123.11
1	A	167	LEU	N-CA-C	5.66	117.26	111.14
1	D	75	ASN	O-C-N	5.66	128.20	122.09
1	C	103	ASN	N-CA-C	-5.65	98.54	108.20
1	B	75	ASN	O-C-N	5.64	128.19	122.09
1	C	145	ARG	CA-C-O	-5.64	114.90	120.82
1	A	161	THR	CA-C-O	-5.61	112.70	119.49
1	B	56	GLY	CA-C-O	5.61	126.46	120.40
1	A	195	ARG	O-C-N	-5.61	116.18	122.12
1	C	75	ASN	O-C-N	5.60	128.13	122.09
1	D	21	PHE	CA-C-O	-5.59	114.62	120.55
1	D	70	ARG	CB-CA-C	5.58	119.73	110.81
1	D	83	VAL	N-CA-CB	5.57	117.07	110.55
1	D	50	LEU	CA-C-O	-5.56	114.98	120.82
1	B	70	ARG	CB-CA-C	5.56	119.70	110.81
1	A	191	SER	CA-C-O	5.55	126.93	120.49
1	D	182	ASP	N-CA-C	5.55	117.56	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	85	GLN	OE1-CD-NE2	-5.54	117.06	122.60
1	C	143	TRP	CA-C-O	-5.54	114.68	120.55
1	D	149	ARG	CA-C-O	-5.54	113.84	120.10
1	B	74	LEU	CA-C-O	5.54	126.36	120.10
1	C	83	VAL	N-CA-CB	5.53	117.02	110.55
1	A	182	ASP	N-CA-C	5.52	117.51	108.52
1	B	93	ASN	CA-C-N	-5.50	115.63	123.11
1	B	93	ASN	C-N-CA	-5.50	115.63	123.11
1	C	195	ARG	O-C-N	-5.50	116.29	122.12
1	A	83	VAL	CA-C-N	-5.49	113.31	120.44
1	A	83	VAL	C-N-CA	-5.49	113.31	120.44
1	C	213	LEU	CA-C-O	5.49	127.75	121.28
1	A	149	ARG	CA-C-O	-5.47	114.07	120.20
1	C	152	PRO	N-CA-C	5.47	120.95	113.84
1	D	213	LEU	CA-C-O	5.47	127.73	121.28
1	C	116	LEU	CA-C-O	5.46	126.55	120.82
1	D	58	THR	N-CA-C	5.45	118.40	111.69
1	D	52	ASP	CA-CB-CG	-5.45	107.15	112.60
1	C	158	ASN	OD1-CG-ND2	-5.45	117.16	122.60
1	D	152	PRO	N-CA-C	5.45	120.92	113.84
1	C	126	ASN	CA-CB-CG	5.44	118.04	112.60
1	C	50	LEU	N-CA-C	-5.43	105.26	111.07
1	C	78	ASN	OD1-CG-ND2	-5.43	117.17	122.60
1	A	195	ARG	CA-C-O	5.43	126.31	120.55
1	C	167	LEU	N-CA-C	5.43	117.00	111.14
1	A	152	PRO	N-CA-C	5.43	120.89	113.84
1	C	83	VAL	CA-C-N	-5.42	113.39	120.44
1	C	83	VAL	C-N-CA	-5.42	113.39	120.44
1	D	195	ARG	O-C-N	-5.42	116.38	122.12
1	B	50	LEU	N-CA-C	-5.42	105.28	111.07
1	C	202	ILE	CA-C-O	-5.41	115.43	121.17
1	B	156	VAL	N-CA-C	5.41	116.54	108.54
1	B	213	LEU	CA-C-O	5.40	127.65	121.28
1	B	182	ASP	N-CA-C	5.39	117.31	108.52
1	B	225	LYS	CA-C-O	-5.39	115.34	121.00
1	A	78	ASN	OD1-CG-ND2	-5.39	117.21	122.60
1	D	156	VAL	N-CA-C	5.39	116.51	108.54
1	C	149	ARG	CA-C-O	-5.36	114.20	120.20
1	B	85	GLN	OE1-CD-NE2	-5.35	117.25	122.60
1	D	93	ASN	CA-C-N	-5.35	115.83	123.11
1	D	93	ASN	C-N-CA	-5.35	115.83	123.11
1	C	182	ASP	N-CA-C	5.34	117.23	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	83	VAL	N-CA-CB	5.34	116.80	110.55
1	A	116	LEU	CA-C-O	5.34	126.43	120.82
1	C	195	ARG	CA-C-O	5.33	126.20	120.55
1	B	134	THR	CA-C-O	5.32	126.45	120.70
1	A	134	THR	CA-C-O	5.31	126.43	120.70
1	A	126	ASN	CA-CB-CG	5.30	117.90	112.60
1	B	202	ILE	N-CA-C	-5.28	105.35	110.42
1	A	50	LEU	CA-C-O	-5.28	115.28	120.82
1	B	103	ASN	N-CA-C	-5.28	99.17	108.20
1	D	134	THR	CA-C-O	5.28	126.40	120.70
1	A	216	GLU	CB-CG-CD	5.28	121.57	112.60
1	B	116	LEU	CA-C-O	5.25	126.34	120.82
1	A	61	LYS	N-CA-C	-5.23	100.65	109.07
1	A	213	LEU	CA-C-O	5.22	127.44	121.28
1	B	126	ASN	CA-CB-CG	5.21	117.81	112.60
1	B	107	THR	N-CA-C	-5.20	105.69	111.36
1	D	49	ARG	NH1-CZ-NH2	-5.20	112.54	119.30
1	C	216	GLU	CB-CG-CD	5.19	121.42	112.60
1	C	59	GLY	CA-C-N	5.19	130.82	121.06
1	C	59	GLY	C-N-CA	5.19	130.82	121.06
1	B	142	SER	CA-C-O	-5.18	115.38	120.82
1	A	59	GLY	CA-C-N	5.17	130.79	121.06
1	A	59	GLY	C-N-CA	5.17	130.79	121.06
1	B	52	ASP	CB-CA-C	-5.17	102.20	110.79
1	D	52	ASP	CB-CA-C	-5.17	102.21	110.79
1	D	67	GLY	CA-C-N	5.17	130.35	122.23
1	D	67	GLY	C-N-CA	5.17	130.35	122.23
1	D	142	SER	CA-C-O	-5.17	115.40	120.82
1	D	59	GLY	CA-C-N	5.16	130.76	121.06
1	D	59	GLY	C-N-CA	5.16	130.76	121.06
1	D	216	GLU	CB-CG-CD	5.16	121.37	112.60
1	D	202	ILE	CA-C-O	-5.16	115.70	121.17
1	A	21	PHE	CA-C-O	-5.15	115.09	120.55
1	D	86	ASN	N-CA-CB	5.15	118.27	110.28
1	A	50	LEU	N-CA-C	-5.15	105.56	111.07
1	C	92	VAL	CA-CB-CG2	-5.14	101.66	110.40
1	C	142	SER	CB-CA-C	-5.13	102.82	110.88
1	A	56	GLY	CA-C-O	5.13	125.94	120.40
1	A	165	ASP	O-C-N	-5.13	115.77	122.59
1	C	56	GLY	CA-C-O	5.12	125.93	120.40
1	C	86	ASN	CA-C-O	-5.12	114.08	119.97
1	D	158	ASN	OD1-CG-ND2	-5.12	117.48	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	214	ASP	N-CA-C	-5.12	103.08	110.40
1	B	58	THR	N-CA-C	5.12	117.98	111.69
1	D	103	ASN	N-CA-C	-5.12	99.45	108.20
1	A	86	ASN	N-CA-CB	5.11	118.19	110.28
1	B	70	ARG	NE-CZ-NH1	-5.11	116.39	121.50
1	D	107	THR	N-CA-C	-5.11	105.80	111.36
1	C	58	THR	N-CA-C	5.10	117.97	111.69
1	C	107	THR	N-CA-C	-5.10	105.80	111.36
1	C	184	ASN	CA-CB-CG	-5.09	107.51	112.60
1	C	134	THR	CA-C-O	5.09	126.20	120.70
1	B	225	LYS	O-C-N	5.09	127.32	122.03
1	C	151	TYR	CA-C-N	5.09	124.75	119.56
1	C	151	TYR	C-N-CA	5.09	124.75	119.56
1	A	26	ASN	O-C-N	-5.09	116.73	122.12
1	D	56	GLY	CA-C-O	5.09	125.89	120.40
1	B	86	ASN	N-CA-CB	5.08	118.16	110.28
1	C	67	GLY	CA-C-N	5.08	130.21	122.23
1	C	67	GLY	C-N-CA	5.08	130.21	122.23
1	D	125	LYS	CA-C-O	-5.08	115.03	120.42
1	D	184	ASN	CA-CB-CG	-5.08	107.52	112.60
1	C	165	ASP	O-C-N	-5.07	115.85	122.59
1	C	186	VAL	N-CA-C	-5.07	106.21	111.58
1	C	116	LEU	O-C-N	-5.06	116.85	122.07
1	B	151	TYR	CA-C-N	5.06	124.72	119.56
1	B	151	TYR	C-N-CA	5.06	124.72	119.56
1	B	92	VAL	CA-CB-CG2	-5.04	101.84	110.40
1	D	126	ASN	CA-CB-CG	5.02	117.62	112.60
1	D	142	SER	CB-CA-C	-5.01	103.01	110.88
1	D	202	ILE	N-CA-C	-5.01	105.61	110.42
1	B	174	HIS	CA-CB-CG	-5.00	108.80	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1887	0	1861	84	0
1	B	1885	0	1865	79	0
1	C	1891	0	1867	85	0
1	D	1885	0	1860	89	0
2	A	26	0	0	1	0
2	B	19	0	0	0	0
2	C	14	0	0	1	0
2	D	15	0	0	2	0
All	All	7622	0	7453	280	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 (280) 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:245:ILE:HD12	1:D:245:ILE:HD12	1.29	1.12
1:A:245:ILE:HD12	1:B:245:ILE:HD12	1.29	1.11
1:A:69:THR:HB	1:A:72:HIS:HD2	1.34	0.91
1:C:69:THR:HB	1:C:72:HIS:HD2	1.36	0.91
1:D:69:THR:HB	1:D:72:HIS:HD2	1.35	0.90
1:B:69:THR:HB	1:B:72:HIS:HD2	1.35	0.89
1:C:69:THR:HG22	1:C:71:VAL:H	1.44	0.81
1:C:237:GLN:NE2	1:D:122:ASN:HD22	1.79	0.81
1:B:69:THR:HG22	1:B:71:VAL:H	1.46	0.80
1:A:69:THR:HG22	1:A:71:VAL:H	1.45	0.80
1:D:69:THR:HG22	1:D:71:VAL:H	1.46	0.79
1:A:128:MET:HG2	1:B:131:LEU:CD1	2.13	0.79
1:C:122:ASN:HD22	1:D:237:GLN:NE2	1.82	0.78
1:A:146:GLN:HE22	1:A:244:SER:HB2	1.51	0.76
1:A:131:LEU:CD1	1:B:128:MET:HG2	2.16	0.75
1:D:146:GLN:HE22	1:D:244:SER:HB2	1.52	0.75
1:D:33:GLY:HA2	2:D:2002:HOH:O	1.87	0.75
1:A:122:ASN:HD22	1:B:237:GLN:NE2	1.85	0.75
1:B:146:GLN:HE22	1:B:244:SER:HB2	1.52	0.74
1:C:146:GLN:HE22	1:C:244:SER:HB2	1.52	0.74
1:C:237:GLN:HE22	1:D:122:ASN:HD22	1.35	0.73
1:C:131:LEU:CD1	1:D:128:MET:HG2	2.20	0.72
1:C:135:ASN:HD21	1:C:137:GLU:HB2	1.55	0.71
1:D:69:THR:HG22	1:D:71:VAL:N	2.07	0.70
1:A:135:ASN:HD21	1:A:137:GLU:HB2	1.55	0.70
1:C:146:GLN:NE2	1:C:244:SER:HB2	2.07	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:GLN:NE2	1:B:244:SER:HB2	2.06	0.70
1:C:69:THR:HG22	1:C:71:VAL:N	2.06	0.70
1:D:146:GLN:NE2	1:D:244:SER:HB2	2.07	0.70
1:B:135:ASN:HD21	1:B:137:GLU:HB2	1.56	0.69
1:D:135:ASN:HD21	1:D:137:GLU:HB2	1.55	0.69
1:C:122:ASN:HD22	1:D:237:GLN:HE22	1.37	0.69
1:A:69:THR:HG22	1:A:71:VAL:N	2.07	0.69
1:A:146:GLN:NE2	1:A:244:SER:HB2	2.06	0.69
1:A:237:GLN:NE2	1:B:122:ASN:HD22	1.89	0.69
1:A:227:SER:HA	1:A:230:MET:HE2	1.75	0.68
1:B:69:THR:HG22	1:B:71:VAL:N	2.07	0.68
1:A:69:THR:HB	1:A:72:HIS:CD2	2.25	0.68
1:C:128:MET:HG2	1:D:131:LEU:CD1	2.23	0.68
1:B:130:GLY:O	1:B:133:GLN:NE2	2.27	0.67
1:A:130:GLY:O	1:A:133:GLN:NE2	2.28	0.67
1:D:130:GLY:O	1:D:133:GLN:NE2	2.28	0.66
1:D:63:PRO:HD2	1:D:79:LYS:NZ	2.11	0.66
1:D:227:SER:HA	1:D:230:MET:HE2	1.75	0.66
1:B:227:SER:HA	1:B:230:MET:HE2	1.77	0.66
1:D:69:THR:HB	1:D:72:HIS:CD2	2.26	0.66
1:A:124:MET:CE	1:B:131:LEU:HD22	2.25	0.66
1:A:131:LEU:HD13	1:B:124:MET:HE2	1.78	0.66
1:B:69:THR:HB	1:B:72:HIS:CD2	2.26	0.65
1:C:227:SER:HA	1:C:230:MET:HE2	1.78	0.65
1:C:130:GLY:O	1:C:133:GLN:NE2	2.29	0.65
1:A:63:PRO:HD2	1:A:79:LYS:NZ	2.12	0.64
1:B:63:PRO:HD2	1:B:79:LYS:NZ	2.10	0.64
1:A:124:MET:HE2	1:B:131:LEU:HD13	1.78	0.64
1:C:63:PRO:HD2	1:C:79:LYS:NZ	2.12	0.64
1:A:122:ASN:HD22	1:B:237:GLN:HE22	1.45	0.64
1:A:131:LEU:HD22	1:B:124:MET:CE	2.28	0.63
1:B:87:ASN:O	1:B:88:ASN:HB2	1.97	0.63
1:C:144:VAL:HG11	1:C:156:VAL:HG11	1.82	0.62
1:A:128:MET:HG2	1:B:131:LEU:HD12	1.81	0.62
1:D:144:VAL:HG11	1:D:156:VAL:HG11	1.83	0.61
1:A:87:ASN:O	1:A:88:ASN:HB2	2.00	0.61
1:B:144:VAL:HG11	1:B:156:VAL:HG11	1.82	0.61
1:C:87:ASN:O	1:C:88:ASN:HB2	2.00	0.61
1:A:127:ILE:HG21	1:B:245:ILE:HD11	1.83	0.60
1:B:63:PRO:HD2	1:B:79:LYS:HZ2	1.65	0.60
1:A:237:GLN:HE22	1:B:122:ASN:HD22	1.48	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:PRO:HD2	1:D:79:LYS:HZ2	1.66	0.60
1:A:131:LEU:HD12	1:B:128:MET:HG2	1.82	0.59
1:C:131:LEU:HD13	1:D:124:MET:HE2	1.84	0.59
1:A:144:VAL:HG11	1:A:156:VAL:HG11	1.83	0.59
1:A:245:ILE:HD11	1:B:127:ILE:HG21	1.85	0.59
1:A:49:ARG:HG2	2:A:2006:HOH:O	2.01	0.59
1:D:87:ASN:O	1:D:88:ASN:HB2	2.02	0.59
1:A:63:PRO:HD2	1:A:79:LYS:HZ2	1.67	0.59
1:C:131:LEU:HD22	1:D:124:MET:CE	2.33	0.58
1:C:124:MET:HE2	1:D:131:LEU:HD13	1.84	0.58
1:D:35:GLN:O	1:D:49:ARG:NH2	2.37	0.58
1:C:67:GLY:HA3	1:C:72:HIS:HB2	1.86	0.58
1:D:67:GLY:HA3	1:D:72:HIS:HB2	1.87	0.56
1:C:69:THR:HB	1:C:72:HIS:CD2	2.27	0.56
1:C:124:MET:CE	1:D:131:LEU:HD22	2.35	0.56
1:D:143:TRP:HB2	1:D:243:VAL:HG12	1.87	0.56
1:B:67:GLY:HA3	1:B:72:HIS:HB2	1.86	0.56
1:C:130:GLY:HA3	1:C:246:GLU:HG2	1.88	0.56
1:B:130:GLY:HA3	1:B:246:GLU:HG2	1.88	0.56
1:A:67:GLY:HA3	1:A:72:HIS:HB2	1.87	0.56
1:D:130:GLY:HA3	1:D:246:GLU:HG2	1.88	0.55
1:C:116:LEU:HD12	1:C:120:VAL:HB	1.88	0.55
1:C:143:TRP:HB2	1:C:243:VAL:HG12	1.87	0.55
1:D:231:TYR:O	1:D:234:SER:HB2	2.06	0.55
1:A:130:GLY:HA3	1:A:246:GLU:HG2	1.89	0.55
1:A:143:TRP:HB2	1:A:243:VAL:HG12	1.88	0.55
1:C:35:GLN:O	1:C:49:ARG:NH2	2.39	0.55
1:B:35:GLN:O	1:B:49:ARG:NH2	2.40	0.55
1:A:53:LEU:HG	1:A:57:LEU:HD12	1.89	0.54
1:B:143:TRP:HB2	1:B:243:VAL:HG12	1.88	0.54
1:A:116:LEU:HD12	1:A:120:VAL:HB	1.90	0.54
1:A:35:GLN:O	1:A:49:ARG:NH2	2.41	0.54
1:C:53:LEU:HG	1:C:57:LEU:HD12	1.90	0.54
1:C:65:GLU:CD	1:C:75:ASN:HD22	2.16	0.54
1:D:53:LEU:HG	1:D:57:LEU:CD1	2.38	0.54
1:B:231:TYR:O	1:B:234:SER:HB2	2.08	0.54
1:C:53:LEU:HG	1:C:57:LEU:CD1	2.37	0.54
1:D:53:LEU:HG	1:D:57:LEU:HD12	1.89	0.54
1:B:53:LEU:HG	1:B:57:LEU:HD12	1.90	0.54
1:B:65:GLU:CD	1:B:75:ASN:HD22	2.16	0.53
1:B:53:LEU:HG	1:B:57:LEU:CD1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:112:TRP:CZ2	1:D:226:LYS:HG2	2.44	0.53
1:D:116:LEU:HD12	1:D:120:VAL:HB	1.90	0.53
1:A:53:LEU:HG	1:A:57:LEU:CD1	2.39	0.53
1:B:67:GLY:HA3	1:B:72:HIS:CB	2.38	0.53
1:B:116:LEU:HD12	1:B:120:VAL:HB	1.91	0.53
1:C:231:TYR:O	1:C:234:SER:HB2	2.09	0.53
1:D:67:GLY:HA3	1:D:72:HIS:CB	2.39	0.53
1:A:231:TYR:O	1:A:234:SER:HB2	2.09	0.52
1:D:65:GLU:CD	1:D:75:ASN:HD22	2.17	0.52
1:D:133:GLN:HG2	1:D:133:GLN:O	2.10	0.52
1:B:133:GLN:O	1:B:133:GLN:HG2	2.09	0.52
1:C:67:GLY:HA3	1:C:72:HIS:CB	2.39	0.52
1:A:65:GLU:CD	1:A:75:ASN:HD22	2.17	0.52
1:A:67:GLY:HA3	1:A:72:HIS:CB	2.39	0.52
1:B:66:LYS:HE2	1:B:66:LYS:N	2.26	0.51
1:C:69:THR:O	1:C:70:ARG:C	2.54	0.51
1:A:69:THR:O	1:A:70:ARG:C	2.53	0.51
1:A:133:GLN:O	1:A:133:GLN:HG2	2.10	0.51
1:B:69:THR:O	1:B:70:ARG:C	2.53	0.51
1:A:123:VAL:O	1:A:127:ILE:HG12	2.11	0.51
1:C:133:GLN:O	1:C:133:GLN:HG2	2.10	0.50
1:C:241:GLN:HE22	1:D:126:ASN:HD22	1.58	0.50
1:D:123:VAL:O	1:D:127:ILE:HG12	2.12	0.50
1:A:226:LYS:HG2	1:B:112:TRP:CZ2	2.46	0.50
1:C:66:LYS:N	1:C:66:LYS:HE2	2.27	0.50
1:C:126:ASN:HD22	1:D:241:GLN:HE22	1.60	0.50
1:C:131:LEU:HD12	1:D:128:MET:HG2	1.93	0.50
1:C:226:LYS:HG2	1:D:112:TRP:CZ2	2.46	0.50
1:C:135:ASN:HD21	1:C:137:GLU:CB	2.24	0.50
1:B:135:ASN:HD21	1:B:137:GLU:CB	2.24	0.49
1:A:112:TRP:CZ2	1:B:226:LYS:HG2	2.46	0.49
1:D:66:LYS:HE2	1:D:66:LYS:N	2.27	0.49
1:B:123:VAL:O	1:B:127:ILE:HG12	2.12	0.49
1:A:66:LYS:N	1:A:66:LYS:HE2	2.27	0.49
1:B:47:GLY:HA3	1:B:76:ASN:HB3	1.95	0.49
1:C:123:VAL:O	1:C:127:ILE:HG12	2.12	0.48
1:C:128:MET:HG2	1:D:131:LEU:HD12	1.95	0.48
1:D:69:THR:O	1:D:70:ARG:C	2.55	0.48
1:D:47:GLY:HA3	1:D:76:ASN:HB3	1.96	0.48
1:D:42:SER:O	1:D:45:GLN:HB2	2.14	0.48
1:A:47:GLY:HA3	1:A:76:ASN:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:ILE:HD11	1:D:127:ILE:HG21	1.94	0.48
1:D:135:ASN:HD21	1:D:137:GLU:CB	2.24	0.48
1:B:216:GLU:CD	1:B:216:GLU:H	2.22	0.48
1:C:47:GLY:HA3	1:C:76:ASN:HB3	1.95	0.48
1:B:144:VAL:CG1	1:B:156:VAL:HG11	2.45	0.47
1:A:66:LYS:HB2	1:A:67:GLY:H	1.39	0.47
1:C:144:VAL:CG1	1:C:156:VAL:HG11	2.44	0.47
1:D:216:GLU:H	1:D:216:GLU:CD	2.22	0.47
1:C:63:PRO:HD2	1:C:79:LYS:HZ2	1.76	0.47
1:C:245:ILE:CD1	1:D:245:ILE:HD12	2.21	0.47
1:D:193:THR:O	1:D:197:GLU:HG3	2.15	0.47
1:A:135:ASN:HD21	1:A:137:GLU:CB	2.25	0.47
1:B:45:GLN:HG2	1:B:100:VAL:O	2.14	0.47
1:B:66:LYS:HE2	1:B:66:LYS:H	1.80	0.47
1:B:42:SER:O	1:B:45:GLN:HB2	2.15	0.47
1:B:192:ALA:O	1:B:193:THR:C	2.57	0.47
1:D:192:ALA:O	1:D:193:THR:C	2.56	0.47
1:A:131:LEU:HD21	1:A:245:ILE:CD1	2.44	0.47
1:C:127:ILE:HG21	1:D:245:ILE:HD11	1.96	0.47
1:A:124:MET:O	1:A:124:MET:HG3	2.15	0.46
1:C:131:LEU:HD21	1:C:245:ILE:CD1	2.45	0.46
1:D:124:MET:O	1:D:124:MET:HG3	2.13	0.46
1:D:131:LEU:HD21	1:D:245:ILE:CD1	2.45	0.46
1:A:32:PHE:CE2	1:A:56:GLY:HA3	2.50	0.46
1:D:183:TRP:O	1:D:187:VAL:HG23	2.15	0.46
1:A:192:ALA:O	1:A:193:THR:C	2.58	0.46
1:C:242:GLN:HA	1:D:245:ILE:O	2.15	0.46
1:D:144:VAL:CG1	1:D:156:VAL:HG11	2.45	0.46
1:B:124:MET:O	1:B:124:MET:HG3	2.16	0.46
1:A:144:VAL:CG1	1:A:156:VAL:HG11	2.46	0.46
1:B:131:LEU:HD21	1:B:245:ILE:CD1	2.46	0.46
1:C:183:TRP:O	1:C:187:VAL:HG23	2.15	0.46
1:D:66:LYS:HE2	1:D:66:LYS:H	1.80	0.46
1:A:193:THR:O	1:A:197:GLU:HG3	2.16	0.46
1:B:66:LYS:HB2	1:B:67:GLY:H	1.39	0.46
1:C:66:LYS:HE2	1:C:66:LYS:H	1.81	0.46
1:C:131:LEU:CD2	1:C:245:ILE:HD13	2.46	0.46
1:A:66:LYS:HE2	1:A:66:LYS:H	1.80	0.45
1:C:245:ILE:HD12	1:D:245:ILE:CD1	2.21	0.45
1:A:245:ILE:HG22	1:A:246:GLU:N	2.31	0.45
1:B:193:THR:O	1:B:197:GLU:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:ILE:HG22	1:C:246:GLU:N	2.32	0.45
1:A:216:GLU:H	1:A:216:GLU:CD	2.22	0.45
1:A:124:MET:HE1	1:B:131:LEU:HD22	1.96	0.45
1:A:131:LEU:CD2	1:A:245:ILE:HD13	2.46	0.45
1:B:95:GLY:O	1:B:98:ASP:HB2	2.17	0.45
1:B:245:ILE:HG22	1:B:246:GLU:N	2.32	0.45
1:A:45:GLN:HG2	1:A:100:VAL:O	2.16	0.45
1:A:183:TRP:O	1:A:187:VAL:HG23	2.16	0.45
1:A:70:ARG:NH2	1:A:101:ASP:OD2	2.49	0.44
1:B:183:TRP:O	1:B:187:VAL:HG23	2.16	0.44
1:C:245:ILE:CG2	1:C:246:GLU:N	2.80	0.44
1:D:45:GLN:HG2	1:D:100:VAL:O	2.17	0.44
1:C:171:ALA:HB2	1:C:183:TRP:CH2	2.53	0.44
1:A:245:ILE:CG2	1:A:246:GLU:N	2.80	0.44
1:C:42:SER:O	1:C:45:GLN:HB2	2.17	0.44
1:A:42:SER:O	1:A:45:GLN:HB2	2.17	0.44
1:B:131:LEU:CD2	1:B:245:ILE:HD13	2.47	0.44
1:B:245:ILE:CG2	1:B:246:GLU:N	2.81	0.44
1:C:193:THR:O	1:C:197:GLU:HG3	2.17	0.44
1:D:131:LEU:CD2	1:D:245:ILE:HD13	2.47	0.44
1:C:66:LYS:HB2	1:C:67:GLY:H	1.39	0.44
1:C:216:GLU:CD	1:C:216:GLU:H	2.23	0.44
1:D:245:ILE:CG2	1:D:246:GLU:N	2.81	0.44
1:A:93:ASN:ND2	1:D:78:ASN:OD1	2.42	0.43
1:C:192:ALA:O	1:C:193:THR:C	2.57	0.43
1:A:131:LEU:HD13	1:B:128:MET:HG2	1.99	0.43
1:C:45:GLN:HG2	1:C:100:VAL:O	2.18	0.43
1:A:127:ILE:CG2	1:B:245:ILE:HD11	2.46	0.43
1:B:134:THR:CG2	1:B:139:ILE:HD11	2.48	0.43
1:A:78:ASN:OD1	1:D:93:ASN:ND2	2.44	0.43
1:A:126:ASN:HD22	1:B:241:GLN:HE22	1.67	0.43
1:A:171:ALA:HB2	1:A:183:TRP:CH2	2.54	0.43
1:B:153:GLN:NE2	1:B:183:TRP:HE1	2.17	0.43
1:C:236:PHE:CE2	1:C:241:GLN:HB3	2.53	0.43
1:C:245:ILE:O	1:D:242:GLN:HA	2.19	0.43
1:A:32:PHE:CD2	1:A:56:GLY:HA3	2.54	0.43
1:C:124:MET:O	1:C:124:MET:HG3	2.15	0.43
1:D:70:ARG:HH21	1:D:101:ASP:CG	2.26	0.43
1:C:131:LEU:HD22	1:D:124:MET:HE1	2.00	0.43
1:D:67:GLY:HA3	1:D:72:HIS:CG	2.54	0.43
1:D:70:ARG:NH2	1:D:101:ASP:OD2	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:THR:HA	2:D:2008:HOH:O	2.19	0.42
1:D:66:LYS:HB2	1:D:67:GLY:H	1.38	0.42
1:A:67:GLY:HA3	1:A:72:HIS:CG	2.54	0.42
1:A:70:ARG:HH21	1:A:101:ASP:CG	2.26	0.42
1:C:134:THR:CG2	1:C:139:ILE:HD11	2.49	0.42
1:D:245:ILE:HG22	1:D:246:GLU:N	2.33	0.42
1:A:245:ILE:HD11	1:B:127:ILE:CG2	2.48	0.42
1:A:128:MET:HG2	1:B:131:LEU:HD13	1.96	0.42
1:C:63:PRO:HD2	1:C:79:LYS:HZ1	1.81	0.42
1:A:112:TRP:CE2	1:B:226:LYS:HG2	2.54	0.42
1:A:236:PHE:CE2	1:A:241:GLN:HB3	2.54	0.42
1:D:117:HIS:HA	1:D:121:LYS:HE3	2.02	0.42
1:B:67:GLY:HA3	1:B:72:HIS:CG	2.54	0.42
1:B:236:PHE:CE2	1:B:241:GLN:HB3	2.55	0.42
1:C:128:MET:HG2	1:D:131:LEU:HD13	2.02	0.42
1:D:153:GLN:NE2	1:D:183:TRP:HE1	2.18	0.42
1:D:171:ALA:HB2	1:D:183:TRP:CH2	2.54	0.42
1:B:201:ASN:O	1:B:202:ILE:C	2.63	0.42
1:C:117:HIS:HA	1:C:121:LYS:HE3	2.02	0.42
1:C:153:GLN:NE2	1:C:183:TRP:HE1	2.18	0.42
1:C:241:GLN:OE1	1:D:126:ASN:HB3	2.19	0.42
1:D:134:THR:CG2	1:D:139:ILE:HD11	2.49	0.42
1:C:19:LYS:NZ	1:D:214:ASP:OD2	2.53	0.42
1:C:95:GLY:O	1:C:98:ASP:HB2	2.20	0.42
1:A:95:GLY:O	1:A:98:ASP:HB2	2.20	0.42
1:C:67:GLY:HA3	1:C:72:HIS:CG	2.55	0.42
1:D:236:PHE:CE2	1:D:241:GLN:HB3	2.55	0.42
1:A:117:HIS:HA	1:A:121:LYS:HE3	2.02	0.41
1:A:153:GLN:NE2	1:A:183:TRP:HE1	2.18	0.41
1:B:70:ARG:NH2	1:B:101:ASP:OD2	2.52	0.41
1:B:117:HIS:HA	1:B:121:LYS:HE3	2.01	0.41
1:B:171:ALA:HB2	1:B:183:TRP:CH2	2.55	0.41
1:C:70:ARG:HH21	1:C:101:ASP:CG	2.28	0.41
1:C:226:LYS:NZ	2:C:2012:HOH:O	2.54	0.41
1:D:19:LYS:O	1:D:23:LYS:HG3	2.20	0.41
1:C:212:LEU:O	1:D:20:THR:HG22	2.21	0.41
1:D:50:LEU:HD23	1:D:50:LEU:HA	1.91	0.41
1:A:19:LYS:O	1:A:23:LYS:HG3	2.21	0.41
1:A:91:LEU:O	1:A:92:VAL:C	2.62	0.41
1:C:112:TRP:CE2	1:D:226:LYS:HG2	2.55	0.41
1:A:134:THR:CG2	1:A:139:ILE:HD11	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:LYS:O	1:B:23:LYS:HG3	2.20	0.41
1:D:95:GLY:O	1:D:98:ASP:HB2	2.20	0.41
1:C:57:LEU:HD23	1:C:57:LEU:HA	1.96	0.41
1:C:226:LYS:HG2	1:D:112:TRP:CE2	2.56	0.41
1:B:70:ARG:HH21	1:B:101:ASP:CG	2.27	0.40
1:C:214:ASP:OD2	1:D:19:LYS:NZ	2.54	0.40
1:A:169:LEU:HG	1:A:199:ALA:HB1	2.04	0.40
1:B:91:LEU:O	1:B:92:VAL:C	2.64	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	236/246 (96%)	219 (93%)	15 (6%)	2 (1%)	16	34
1	B	236/246 (96%)	221 (94%)	13 (6%)	2 (1%)	16	34
1	C	236/246 (96%)	220 (93%)	14 (6%)	2 (1%)	16	34
1	D	236/246 (96%)	220 (93%)	14 (6%)	2 (1%)	16	34
All	All	944/984 (96%)	880 (93%)	56 (6%)	8 (1%)	16	34

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	66	LYS
1	A	67	GLY
1	B	66	LYS
1	B	67	GLY
1	C	66	LYS
1	C	67	GLY
1	D	66	LYS

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Mol	Chain	Res	Type
1	D	67	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	208/226 (92%)	193 (93%)	15 (7%)	13	30
1	B	208/226 (92%)	192 (92%)	16 (8%)	12	27
1	C	209/226 (92%)	193 (92%)	16 (8%)	12	27
1	D	208/226 (92%)	193 (93%)	15 (7%)	13	30
All	All	833/904 (92%)	771 (93%)	62 (7%)	13	29

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	SER
1	A	36	HIS
1	A	66	LYS
1	A	79	LYS
1	A	124	MET
1	A	133	GLN
1	A	134	THR
1	A	142	SER
1	A	179	ASP
1	A	193	THR
1	A	202	ILE
1	A	227	SER
1	A	241	GLN
1	A	244	SER
1	A	246	GLU
1	B	10	SER
1	B	36	HIS
1	B	66	LYS
1	B	79	LYS
1	B	124	MET

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Mol	Chain	Res	Type
1	B	133	GLN
1	B	134	THR
1	B	142	SER
1	B	179	ASP
1	B	186	VAL
1	B	193	THR
1	B	202	ILE
1	B	227	SER
1	B	241	GLN
1	B	244	SER
1	B	246	GLU
1	C	10	SER
1	C	36	HIS
1	C	66	LYS
1	C	79	LYS
1	C	124	MET
1	C	133	GLN
1	C	134	THR
1	C	142	SER
1	C	179	ASP
1	C	186	VAL
1	C	193	THR
1	C	202	ILE
1	C	227	SER
1	C	241	GLN
1	C	244	SER
1	C	246	GLU
1	D	10	SER
1	D	36	HIS
1	D	66	LYS
1	D	79	LYS
1	D	124	MET
1	D	133	GLN
1	D	134	THR
1	D	142	SER
1	D	179	ASP
1	D	193	THR
1	D	202	ILE
1	D	227	SER
1	D	241	GLN
1	D	244	SER
1	D	246	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	72	HIS
1	A	117	HIS
1	A	126	ASN
1	A	146	GLN
1	A	184	ASN
1	A	237	GLN
1	B	72	HIS
1	B	117	HIS
1	B	126	ASN
1	B	146	GLN
1	B	184	ASN
1	B	237	GLN
1	C	45	GLN
1	C	72	HIS
1	C	117	HIS
1	C	126	ASN
1	C	146	GLN
1	C	237	GLN
1	D	72	HIS
1	D	117	HIS
1	D	126	ASN
1	D	133	GLN
1	D	146	GLN
1	D	237	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	238/246 (96%)	-0.01	8 (3%) 48 42	18, 35, 60, 74	0
1	B	238/246 (96%)	-0.04	10 (4%) 40 35	19, 35, 60, 75	0
1	C	238/246 (96%)	-0.07	7 (2%) 53 48	19, 35, 60, 75	0
1	D	238/246 (96%)	0.09	13 (5%) 30 25	19, 35, 60, 75	0
All	All	952/984 (96%)	-0.01	38 (3%) 42 37	18, 35, 60, 75	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	33	GLY	4.1
1	D	32	PHE	3.9
1	D	9	ASP	3.9
1	D	68	SER	3.7
1	D	67	GLY	3.7
1	A	190	GLN	3.7
1	B	131	LEU	3.1
1	D	190	GLN	3.0
1	A	132	GLN	3.0
1	C	132	GLN	3.0
1	D	132	GLN	2.8
1	A	10	SER	2.8
1	B	68	SER	2.8
1	D	128	MET	2.7
1	B	33	GLY	2.7
1	D	33	GLY	2.7
1	A	33	GLY	2.6
1	D	179	ASP	2.6
1	B	35	GLN	2.6
1	A	11	TYR	2.4
1	D	10	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	32	PHE	2.3
1	C	245	ILE	2.3
1	B	9	ASP	2.3
1	B	245	ILE	2.3
1	B	11	TYR	2.3
1	B	190	GLN	2.2
1	C	190	GLN	2.2
1	D	206	GLN	2.2
1	B	69	THR	2.2
1	C	11	TYR	2.2
1	B	132	GLN	2.1
1	A	130	GLY	2.1
1	D	245	ILE	2.1
1	D	11	TYR	2.1
1	C	130	GLY	2.1
1	C	9	ASP	2.0
1	A	66	LYS	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 oligosaccharides 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.