



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:49 AM UTC

PDB ID : 5GW9 / pdb_00005gw9
Title : Crystal structure of C163, a backbone circularized G-CSF
Authors : Miyafusa, T.; Honda, S.
Deposited on : 2016-09-09
Resolution : 1.65 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

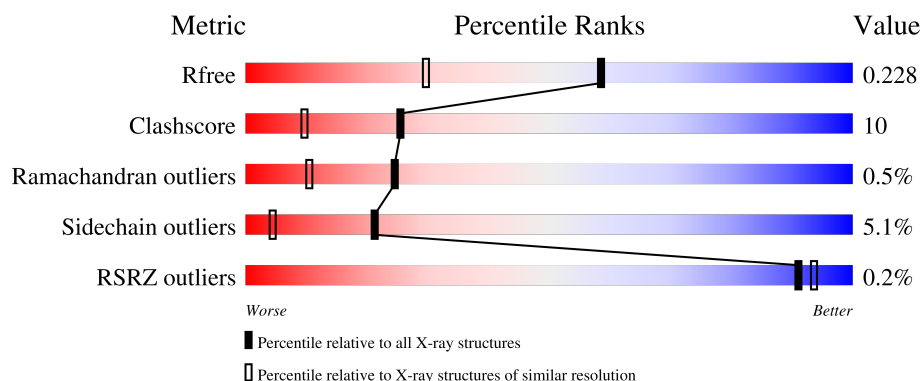
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	163	68% 25% 6% .
1	B	163	64% 27% 8% .
1	C	163	65% 26% 7% .
1	D	163	67% 26% 6% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5803 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 Granulocyte colony-stimulating factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	12	0
			1333	847	231	247	8			
1	B	163	Total	C	N	O	S	0	11	0
			1322	841	227	247	7			
1	C	163	Total	C	N	O	S	0	13	0
			1349	856	235	251	7			
1	D	163	Total	C	N	O	S	0	11	0
			1321	842	226	246	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	11	SER	PRO	engineered mutation	UNP P09919
A	18	SER	CYS	engineered mutation	UNP P09919
A	173	GLY	ALA	engineered mutation	UNP P09919
B	11	SER	PRO	engineered mutation	UNP P09919
B	18	SER	CYS	engineered mutation	UNP P09919
B	173	GLY	ALA	engineered mutation	UNP P09919
C	11	SER	PRO	engineered mutation	UNP P09919
C	18	SER	CYS	engineered mutation	UNP P09919
C	173	GLY	ALA	engineered mutation	UNP P09919
D	11	SER	PRO	engineered mutation	UNP P09919
D	18	SER	CYS	engineered mutation	UNP P09919
D	173	GLY	ALA	engineered mutation	UNP P09919

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	116	Total	O	0	0
			116	116		
2	B	126	Total	O	0	0
			126	126		

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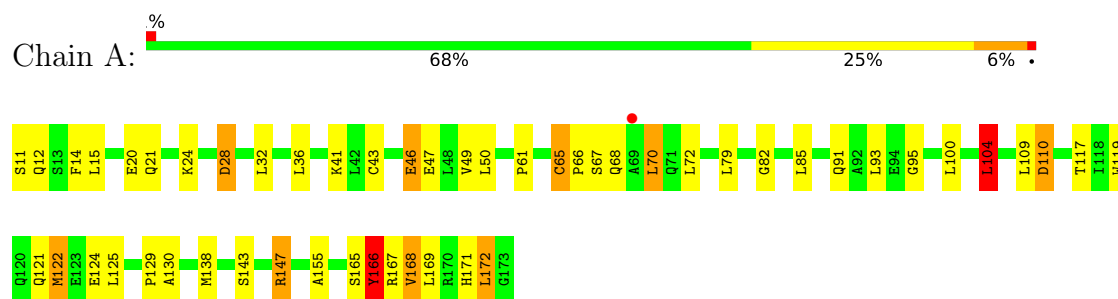
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	124	Total 124	O 124	0	0
2	D	112	Total 112	O 112	0	0

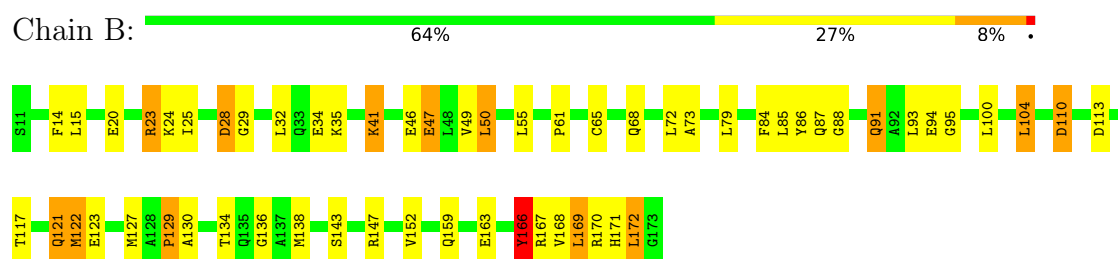
3 Residue-property plots [i](#)

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.

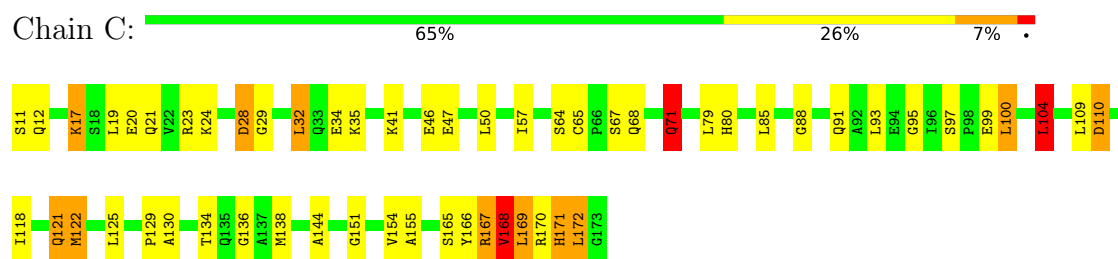
- Molecule 1: Granulocyte colony-stimulating factor



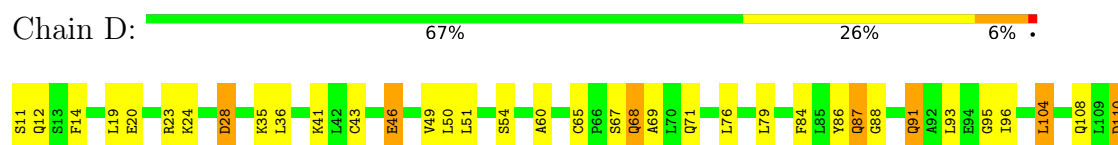
- Molecule 1: Granulocyte colony-stimulating factor



- Molecule 1: Granulocyte colony-stimulating factor



- Molecule 1: Granulocyte colony-stimulating factor





4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	60.94Å 60.94Å 178.51Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	34.08 – 1.65 34.08 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.08-1.65) 99.9 (34.08-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.36 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.177 , 0.218 0.190 , 0.228	Depositor DCC
R_{free} test set	4463 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	22.5	Xtriage
Anisotropy	0.035	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.486 for -h,-k,l 0.487 for h,-h-k,-l 0.487 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5803	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.33% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 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	2.03	36/1360 (2.6%)	1.59	9/1845 (0.5%)
1	B	2.08	41/1348 (3.0%)	1.62	11/1827 (0.6%)
1	C	1.99	36/1376 (2.6%)	1.61	13/1865 (0.7%)
1	D	2.01	39/1347 (2.9%)	1.61	19/1826 (1.0%)
All	All	2.03	152/5431 (2.8%)	1.61	52/7363 (0.7%)

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	B	0	1
1	C	0	1
1	D	0	1
All	All	0	3

All (152) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	166	TYR	N-CA	11.16	1.60	1.46
1	C	122	MET	SD-CE	-10.83	1.52	1.79
1	B	166	TYR	N-CA	10.66	1.59	1.46
1	A	166	TYR	N-CA	10.60	1.59	1.46
1	B	122	MET	SD-CE	-10.10	1.54	1.79
1	D	166	TYR	N-CA	9.69	1.58	1.46
1	B	24	LYS	N-CA	-9.60	1.34	1.46
1	B	167	ARG	N-CA	-9.38	1.34	1.46
1	B	172	LEU	N-CA	-9.31	1.33	1.46
1	A	122	MET	SD-CE	-9.16	1.56	1.79
1	A	167	ARG	N-CA	-9.05	1.35	1.46
1	D	122	MET	SD-CE	-8.97	1.57	1.79
1	D	170	ARG	C-O	-8.84	1.12	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	24	LYS	N-CA	-8.69	1.36	1.46
1	A	166	TYR	CB-CG	8.19	1.69	1.51
1	B	65	CYS	CA-C	8.07	1.63	1.52
1	D	65	CYS	CA-C	7.88	1.62	1.52
1	C	130	ALA	C-O	7.70	1.33	1.23
1	C	28	ASP	CG-OD2	7.56	1.39	1.25
1	D	166	TYR	CB-CG	7.55	1.68	1.51
1	C	65	CYS	CA-C	7.55	1.62	1.52
1	C	169	LEU	N-CA	-7.52	1.37	1.46
1	D	28	ASP	CG-OD2	7.36	1.39	1.25
1	C	20	GLU	CA-C	7.30	1.62	1.52
1	A	20	GLU	CA-C	7.25	1.62	1.52
1	B	166	TYR	CB-CG	7.21	1.67	1.51
1	A	166	TYR	CZ-OH	7.15	1.53	1.38
1	C	166	TYR	CB-CG	7.11	1.67	1.51
1	D	167	ARG	N-CA	-7.11	1.37	1.46
1	B	147	ARG	N-CA	7.10	1.55	1.46
1	A	169	LEU	N-CA	-7.09	1.37	1.46
1	D	166	TYR	CZ-OH	7.02	1.52	1.38
1	B	110	ASP	CG-OD2	-7.01	1.12	1.25
1	A	130	ALA	CA-C	-6.99	1.43	1.52
1	A	130	ALA	N-CA	6.96	1.55	1.46
1	C	155	ALA	CA-CB	-6.93	1.42	1.53
1	B	143	SER	C-O	6.89	1.32	1.23
1	B	130	ALA	N-CA	6.84	1.54	1.46
1	D	20	GLU	CA-C	6.83	1.61	1.52
1	A	28	ASP	CG-OD2	6.82	1.38	1.25
1	C	24	LYS	N-CA	-6.75	1.38	1.46
1	D	130	ALA	N-CA	6.75	1.54	1.46
1	B	41	LYS	CA-CB	6.74	1.63	1.53
1	B	20	GLU	CA-C	6.71	1.61	1.52
1	D	41	LYS	CA-CB	6.70	1.64	1.53
1	B	28	ASP	CG-OD2	6.68	1.38	1.25
1	A	43	CYS	N-CA	-6.66	1.38	1.46
1	C	17	LYS	CA-C	6.65	1.61	1.52
1	C	21	GLN	CD-NE2	-6.60	1.19	1.33
1	B	117	THR	CB-OG1	-6.56	1.33	1.43
1	C	57	ILE	N-CA	6.56	1.54	1.46
1	B	130	ALA	C-O	6.53	1.31	1.23
1	C	110	ASP	CG-OD2	-6.52	1.12	1.25
1	D	130	ALA	CA-C	-6.52	1.44	1.52
1	B	167	ARG	C-N	-6.50	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	LEU	N-CA	-6.48	1.37	1.46
1	B	88	GLY	CA-C	6.46	1.59	1.52
1	B	170	ARG	C-O	-6.43	1.14	1.24
1	D	169	LEU	N-CA	-6.43	1.38	1.46
1	A	21	GLN	CD-NE2	-6.42	1.19	1.33
1	A	41	LYS	CA-CB	6.33	1.62	1.53
1	C	151	GLY	N-CA	6.30	1.53	1.45
1	D	110	ASP	CG-OD2	-6.26	1.13	1.25
1	B	15	LEU	C-O	6.22	1.31	1.24
1	B	169	LEU	N-CA	-6.22	1.38	1.46
1	D	24	LYS	N-CA	-6.20	1.39	1.46
1	A	130	ALA	C-O	6.16	1.31	1.23
1	C	28	ASP	CA-CB	6.15	1.63	1.53
1	B	61	PRO	N-CA	-6.13	1.39	1.46
1	D	88	GLY	CA-C	6.09	1.58	1.52
1	B	129	PRO	CA-CB	-6.09	1.46	1.53
1	D	110	ASP	CG-OD1	6.08	1.36	1.25
1	A	110	ASP	CG-OD2	-6.05	1.13	1.25
1	A	117	THR	CB-OG1	-6.04	1.34	1.43
1	B	166	TYR	CZ-OH	6.04	1.50	1.38
1	C	97	SER	CA-C	-6.03	1.45	1.52
1	B	93	LEU	CA-C	-6.03	1.44	1.52
1	B	100	LEU	N-CA	6.02	1.54	1.46
1	C	165	SER	CA-C	-6.01	1.44	1.52
1	D	147	ARG	N-CA	6.01	1.53	1.46
1	D	108	GLN	CD-NE2	-5.97	1.20	1.33
1	C	172	LEU	N-CA	-5.94	1.38	1.46
1	C	100	LEU	N-CA	5.93	1.53	1.46
1	D	166	TYR	CA-C	5.93	1.60	1.52
1	D	147	ARG	CD-NE	-5.91	1.38	1.46
1	D	36	LEU	C-O	5.91	1.31	1.24
1	B	55	LEU	C-N	-5.90	1.26	1.33
1	A	15	LEU	C-O	5.86	1.30	1.24
1	B	147	ARG	CZ-NH2	-5.86	1.25	1.33
1	C	71	GLN	N-CA	5.86	1.53	1.46
1	D	130	ALA	C-O	5.84	1.31	1.23
1	C	93	LEU	N-CA	5.83	1.54	1.46
1	C	130	ALA	N-CA	5.82	1.53	1.46
1	D	171	HIS	N-CA	5.80	1.54	1.46
1	A	147	ARG	N-CA	5.77	1.53	1.46
1	B	121	GLN	CA-C	-5.76	1.45	1.52
1	C	88	GLY	CA-C	5.74	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	147	ARG	CD-NE	-5.73	1.38	1.46
1	D	117	THR	CB-OG1	-5.73	1.34	1.43
1	B	73	ALA	C-O	-5.70	1.17	1.24
1	C	57	ILE	C-N	5.65	1.40	1.33
1	B	29	GLY	N-CA	-5.65	1.38	1.45
1	B	123	GLU	C-O	5.65	1.30	1.24
1	B	127	MET	C-O	-5.65	1.17	1.23
1	A	43	CYS	CA-CB	5.62	1.62	1.53
1	D	172	LEU	CA-C	-5.61	1.45	1.52
1	D	167	ARG	C-N	-5.58	1.26	1.33
1	B	32	LEU	CA-C	5.55	1.59	1.52
1	B	171	HIS	N-CA	5.55	1.53	1.46
1	C	41	LYS	CA-CB	5.51	1.61	1.53
1	C	24	LYS	CA-C	5.51	1.59	1.52
1	B	24	LYS	CA-C	5.46	1.59	1.52
1	C	172	LEU	CA-C	-5.43	1.45	1.52
1	A	12	GLN	C-O	5.40	1.30	1.24
1	A	167	ARG	C-N	-5.39	1.27	1.33
1	A	104	LEU	CB-CG	-5.39	1.42	1.53
1	C	154	VAL	N-CA	5.38	1.52	1.46
1	B	166	TYR	CA-C	5.36	1.59	1.52
1	B	84	PHE	C-O	-5.33	1.17	1.24
1	C	167	ARG	N-CA	-5.33	1.39	1.46
1	A	172	LEU	CA-C	-5.33	1.45	1.52
1	D	76	LEU	N-CA	5.32	1.52	1.46
1	A	110	ASP	CG-OD1	5.32	1.35	1.25
1	C	12	GLN	C-O	5.29	1.30	1.24
1	C	121	GLN	CD-OE1	5.28	1.33	1.23
1	D	169	LEU	C-N	5.28	1.41	1.33
1	A	143	SER	C-O	5.26	1.30	1.23
1	A	100	LEU	N-CA	5.26	1.53	1.46
1	C	165	SER	N-CA	5.25	1.52	1.46
1	B	152	VAL	CA-CB	5.25	1.60	1.54
1	A	155	ALA	CA-CB	-5.22	1.45	1.53
1	A	171	HIS	N-CA	5.22	1.53	1.46
1	D	12	GLN	C-O	5.20	1.30	1.24
1	D	28	ASP	CA-CB	5.19	1.61	1.53
1	A	61	PRO	CA-C	5.19	1.58	1.52
1	C	170	ARG	C-O	-5.19	1.17	1.24
1	D	172	LEU	N-CA	-5.18	1.39	1.46
1	B	163	GLU	CA-CB	5.17	1.61	1.53
1	D	157	HIS	N-CA	-5.15	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	25	ILE	C-O	-5.15	1.18	1.24
1	D	69	ALA	CA-C	5.12	1.59	1.53
1	C	144	ALA	CA-CB	-5.11	1.45	1.53
1	A	121	GLN	CD-OE1	5.11	1.33	1.23
1	C	99	GLU	CA-C	5.10	1.59	1.52
1	D	51	LEU	CA-C	-5.09	1.46	1.52
1	D	43	CYS	N-CA	-5.09	1.40	1.46
1	A	72	LEU	CA-CB	-5.07	1.45	1.53
1	A	93	LEU	CA-C	-5.05	1.45	1.52
1	D	93	LEU	CA-C	-5.05	1.45	1.52
1	A	32	LEU	CA-C	5.04	1.59	1.52
1	D	49	VAL	N-CA	5.02	1.52	1.46
1	D	117	THR	C-O	5.02	1.29	1.24

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	147	ARG	CG-CD-NE	-8.75	92.75	112.00
1	C	168	VAL	CB-CA-C	-7.84	99.38	112.16
1	D	171	HIS	N-CA-C	7.53	122.11	113.15
1	D	46	GLU	N-CA-C	7.36	120.17	111.71
1	A	147	ARG	CG-CD-NE	-7.21	96.13	112.00
1	D	138	MET	CG-SD-CE	-7.20	85.05	100.90
1	B	49	VAL	N-CA-C	6.90	117.04	110.42
1	B	28	ASP	CA-CB-CG	6.85	119.45	112.60
1	C	32	LEU	CD1-CG-CD2	6.80	125.75	110.80
1	B	86	TYR	O-C-N	-6.73	114.99	122.12
1	A	49	VAL	N-CA-C	6.29	116.46	110.42
1	D	49	VAL	N-CA-C	6.10	116.84	110.62
1	D	60	ALA	N-CA-C	6.06	118.21	109.48
1	D	86	TYR	O-C-N	-6.02	115.74	122.12
1	C	47	GLU	CA-C-O	6.01	126.82	119.44
1	B	172	LEU	CB-CA-C	5.96	120.03	110.09
1	C	47	GLU	CB-CG-CD	5.93	122.68	112.60
1	C	172	LEU	CA-CB-CG	-5.91	95.60	116.30
1	D	28	ASP	CA-CB-CG	5.88	118.48	112.60
1	A	36	LEU	N-CA-C	5.87	117.68	111.28
1	C	47	GLU	N-CA-C	5.85	119.59	112.46
1	A	47	GLU	CA-C-O	5.81	126.52	119.38
1	A	82	GLY	O-C-N	-5.79	116.58	122.19
1	A	168	VAL	N-CA-C	-5.78	103.69	111.44
1	B	171	HIS	N-CA-C	5.73	119.89	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	65	CYS	CA-C-N	5.70	125.70	119.89
1	A	65	CYS	C-N-CA	5.70	125.70	119.89
1	D	148	ARG	CA-C-O	5.59	126.45	120.70
1	D	147	ARG	NE-CZ-NH2	-5.54	114.21	119.20
1	B	93	LEU	N-CA-C	5.49	119.59	113.01
1	C	118	ILE	O-C-N	-5.45	116.57	121.91
1	D	65	CYS	CA-C-N	-5.42	114.39	120.14
1	D	65	CYS	C-N-CA	-5.42	114.39	120.14
1	C	104	LEU	N-CA-C	-5.34	105.53	111.36
1	D	113	ASP	O-C-N	-5.31	116.60	122.07
1	B	86	TYR	CA-C-O	5.30	126.17	120.55
1	C	29	GLY	O-C-N	5.29	127.27	122.19
1	C	166	TYR	N-CA-C	5.29	122.06	110.80
1	A	110	ASP	CA-CB-CG	-5.27	107.33	112.60
1	B	50	LEU	CD1-CG-CD2	5.25	122.35	110.80
1	D	68	GLN	N-CA-C	-5.22	101.76	110.17
1	B	47	GLU	CA-CB-CG	5.21	124.53	114.10
1	C	122	MET	CG-SD-CE	-5.21	89.44	100.90
1	D	54	SER	N-CA-C	5.19	117.68	111.71
1	B	113	ASP	O-C-N	-5.18	116.73	122.07
1	C	28	ASP	CA-CB-CG	5.17	117.78	112.60
1	D	84	PHE	O-C-N	5.11	127.54	122.12
1	D	87	GLN	CB-CG-CD	5.11	121.29	112.60
1	C	171	HIS	N-CA-C	5.10	119.22	113.15
1	D	147	ARG	CA-C-N	5.09	127.37	120.44
1	D	147	ARG	C-N-CA	5.09	127.37	120.44
1	B	88	GLY	O-C-N	5.03	127.02	122.19

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	169	LEU	Mainchain
1	C	169	LEU	Mainchain
1	D	166	TYR	Sidechain

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	1333	0	1331	28	0
1	B	1322	0	1323	29	0
1	C	1349	0	1346	36	0
1	D	1321	0	1325	19	0
2	A	116	0	0	2	0
2	B	126	0	0	10	0
2	C	124	0	0	15	0
2	D	112	0	0	5	0
All	All	5803	0	5325	103	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 10.

All (103) 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:B:91[B]:GLN:OE1	2:B:201:HOH:O	1.68	1.11
1:C:91[B]:GLN:NE2	2:C:201:HOH:O	1.87	1.08
1:B:87:GLN:O	1:B:91[A]:GLN:HG2	1.70	0.91
1:D:91[B]:GLN:OE1	2:D:201:HOH:O	1.89	0.89
1:B:14:PHE:CE2	1:B:172:LEU:HD12	2.08	0.89
1:D:35[A]:LYS:HG3	2:D:234:HOH:O	1.73	0.86
1:B:35[A]:LYS:HG3	2:B:238:HOH:O	1.78	0.83
1:C:35[A]:LYS:HG3	2:C:225:HOH:O	1.80	0.82
1:C:79[B]:LEU:HD11	1:C:168:VAL:HG21	1.62	0.80
1:B:14:PHE:CZ	1:B:172:LEU:HD12	2.16	0.80
1:D:23[B]:ARG:NH2	2:D:202:HOH:O	2.05	0.80
1:D:79[B]:LEU:HD11	1:D:168:VAL:HG11	1.63	0.79
1:D:87:GLN:O	1:D:91[A]:GLN:HG3	1.84	0.77
1:B:23[A]:ARG:NH1	2:B:204:HOH:O	2.16	0.76
1:A:91[A]:GLN:OE1	2:A:201:HOH:O	2.04	0.75
1:C:134:THR:HG22	1:C:136:GLY:H	1.50	0.75
1:A:109[B]:LEU:HG	1:C:109[B]:LEU:HD21	1.68	0.75
1:C:19:LEU:O	1:C:23[B]:ARG:HG3	1.92	0.69
1:C:35[B]:LYS:HG2	1:C:100:LEU:CD1	2.23	0.69
1:C:35[B]:LYS:HG2	1:C:100:LEU:HD13	1.75	0.68
1:B:79[B]:LEU:HD11	1:B:168:VAL:HG11	1.76	0.68
1:B:35[A]:LYS:HE2	2:B:238:HOH:O	1.93	0.67
1:A:109[B]:LEU:HD21	1:C:109[B]:LEU:HG	1.76	0.65
1:C:28:ASP:OD1	2:C:203:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:ARG:HB2	2:C:208:HOH:O	1.97	0.64
1:A:79[B]:LEU:HD11	1:A:168:VAL:HG11	1.80	0.63
1:C:17:LYS:NZ	2:C:205:HOH:O	2.30	0.63
1:D:125:LEU:HD11	1:D:172:LEU:HD12	1.81	0.63
1:A:65:CYS:O	1:A:70:LEU:HD22	1.99	0.62
1:B:134:THR:HG22	1:B:136:GLY:H	1.64	0.62
1:C:28:ASP:OD2	1:C:110:ASP:OD2	2.19	0.60
1:A:95:GLY:HA2	1:A:104:LEU:HD12	1.84	0.59
1:B:121:GLN:NE2	2:B:202:HOH:O	2.08	0.59
1:A:46[B]:GLU:HA	1:A:46[B]:GLU:OE1	2.01	0.59
1:C:95:GLY:HA2	1:C:104:LEU:HD12	1.84	0.59
1:B:28:ASP:OD2	1:B:110:ASP:OD2	2.21	0.58
1:A:125:LEU:HD11	1:A:172:LEU:HD12	1.85	0.58
1:D:35[A]:LYS:HE2	2:D:234:HOH:O	2.01	0.58
1:C:171:HIS:CE1	2:C:265:HOH:O	2.58	0.57
1:A:28:ASP:OD2	1:A:110:ASP:OD2	2.22	0.57
1:D:79[B]:LEU:CD1	1:D:168:VAL:HG11	2.32	0.57
1:D:28:ASP:OD2	1:D:110:ASP:OD2	2.23	0.56
1:C:121:GLN:NE2	2:C:202:HOH:O	2.14	0.56
1:D:87:GLN:O	1:D:91[A]:GLN:CG	2.52	0.56
1:B:122:MET:HE1	1:B:129:PRO:HB3	1.88	0.55
1:D:122:MET:HE1	1:D:129:PRO:HB3	1.88	0.55
1:B:79[B]:LEU:CD1	1:B:168:VAL:HG11	2.38	0.54
1:B:87:GLN:HG2	2:B:203:HOH:O	2.06	0.54
1:A:122:MET:HE1	1:A:129:PRO:HB3	1.90	0.54
1:A:109[B]:LEU:CD2	1:C:109[B]:LEU:HG	2.37	0.54
1:C:23[B]:ARG:NH2	2:C:206:HOH:O	2.31	0.54
1:C:168:VAL:N	2:C:208:HOH:O	2.40	0.53
1:C:125:LEU:HD11	1:C:172:LEU:HD23	1.91	0.53
1:B:46[B]:GLU:HA	1:B:46[B]:GLU:OE1	2.09	0.53
1:A:166:TYR:CE2	1:B:166:TYR:CE2	2.97	0.53
1:A:79[B]:LEU:CD1	1:A:168:VAL:HG11	2.40	0.52
1:B:46[B]:GLU:OE1	1:B:46[B]:GLU:CA	2.57	0.51
1:A:109[B]:LEU:HG	1:C:109[B]:LEU:CD2	2.38	0.51
1:D:96:ILE:HG13	1:D:104[B]:LEU:HD11	1.92	0.51
1:C:64:SER:HB3	1:C:71:GLN:HG3	1.91	0.51
1:B:94:GLU:HG3	2:B:307:HOH:O	2.11	0.51
1:C:35[A]:LYS:HE2	2:C:225:HOH:O	2.11	0.50
1:C:138:MET:HA	1:C:138:MET:HE2	1.94	0.50
1:A:129:PRO:HG2	1:C:129:PRO:HG2	1.94	0.50
1:B:87:GLN:NE2	2:B:203:HOH:O	2.13	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:CYS:N	1:A:66:PRO:CD	2.75	0.49
1:C:122:MET:HE1	1:C:129:PRO:HB3	1.93	0.49
1:A:119:TRP:CZ3	1:C:80:HIS:HE1	2.30	0.49
1:A:91[A]:GLN:HE21	1:A:91[A]:GLN:HB2	1.48	0.48
1:C:35[B]:LYS:HG2	1:C:100:LEU:HD11	1.96	0.48
1:A:166:TYR:HE2	1:B:166:TYR:CE2	2.33	0.47
1:A:147:ARG:NH1	2:A:204:HOH:O	2.42	0.47
1:D:11:SER:HB3	1:D:14:PHE:HB3	1.97	0.46
1:B:91[A]:GLN:NE2	2:B:201:HOH:O	2.48	0.46
1:B:138:MET:HE2	1:B:138:MET:HA	1.97	0.46
1:C:171:HIS:HE1	2:C:265:HOH:O	1.97	0.46
1:C:23[A]:ARG:HG3	2:C:270:HOH:O	2.16	0.46
1:C:11:SER:HB2	2:C:202:HOH:O	2.16	0.46
1:D:96:ILE:CG1	1:D:104[B]:LEU:HD11	2.45	0.46
1:B:159[B]:GLN:HG2	2:B:237:HOH:O	2.16	0.46
1:C:23[B]:ARG:HG2	2:C:270:HOH:O	2.14	0.46
1:B:72:LEU:HD11	1:B:172:LEU:CD2	2.46	0.45
1:A:85:LEU:HD12	1:A:138[A]:MET:HE1	1.98	0.45
1:B:95:GLY:HA2	1:B:104:LEU:HD12	1.97	0.45
1:C:168:VAL:HG22	2:C:208:HOH:O	2.17	0.44
1:D:95:GLY:HA2	1:D:104[A]:LEU:HD12	1.98	0.44
1:B:72:LEU:HD11	1:B:172:LEU:HD21	1.99	0.44
1:A:138[B]:MET:HE3	1:A:138[B]:MET:HB3	1.90	0.43
1:D:46:GLU:HG2	2:D:227:HOH:O	2.18	0.42
1:A:125:LEU:HD11	1:A:172:LEU:CD1	2.49	0.42
1:D:50:LEU:HA	1:D:50:LEU:HD23	1.88	0.42
1:B:85:LEU:CD1	1:B:138:MET:HE1	2.50	0.42
1:C:32:LEU:CD1	1:C:100:LEU:HD12	2.50	0.42
1:C:85:LEU:CD1	1:C:138:MET:HE1	2.50	0.42
1:A:165[A]:SER:O	1:A:166:TYR:C	2.63	0.41
1:B:14:PHE:CZ	1:B:172:LEU:CD1	2.98	0.41
1:A:46[A]:GLU:CD	1:A:46[A]:GLU:H	2.28	0.41
1:D:172:LEU:HA	1:D:172:LEU:HD13	1.75	0.41
1:C:50:LEU:HD23	1:C:50:LEU:HA	1.86	0.41
1:A:46[B]:GLU:OE1	1:A:46[B]:GLU:CA	2.69	0.41
1:A:166:TYR:CE2	1:B:166:TYR:HE2	2.38	0.41
1:D:19:LEU:O	1:D:23[B]:ARG:HG3	2.21	0.41
1:A:11:SER:HB3	1:A:14:PHE:HB3	2.02	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	173/163 (106%)	167 (96%)	5 (3%)	1 (1%)	21	8
1	B	172/163 (106%)	168 (98%)	3 (2%)	1 (1%)	21	8
1	C	175/163 (107%)	170 (97%)	5 (3%)	0	100	100
1	D	172/163 (106%)	167 (97%)	4 (2%)	1 (1%)	21	8
All	All	692/652 (106%)	672 (97%)	17 (2%)	3 (0%)	24	15

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	166	TYR
1	D	166	TYR
1	B	166	TYR

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	144/132 (109%)	136 (94%)	8 (6%)	19	3
1	B	143/132 (108%)	133 (93%)	10 (7%)	14	2
1	C	146/132 (111%)	138 (94%)	8 (6%)	19	4
1	D	143/132 (108%)	136 (95%)	7 (5%)	22	5
All	All	576/528 (109%)	543 (94%)	33 (6%)	21	3

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46[A]	GLU
1	A	46[B]	GLU
1	A	50	LEU
1	A	67	SER
1	A	68	GLN
1	A	70	LEU
1	A	104	LEU
1	A	124	GLU
1	B	23[A]	ARG
1	B	23[B]	ARG
1	B	34	GLU
1	B	41	LYS
1	B	47	GLU
1	B	50	LEU
1	B	68	GLN
1	B	91[A]	GLN
1	B	91[B]	GLN
1	B	104	LEU
1	C	34	GLU
1	C	46[A]	GLU
1	C	46[B]	GLU
1	C	67	SER
1	C	68	GLN
1	C	71	GLN
1	C	104	LEU
1	C	168	VAL
1	D	67	SER
1	D	68	GLN
1	D	71	GLN
1	D	91[A]	GLN
1	D	91[B]	GLN
1	D	104[A]	LEU
1	D	104[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	26	GLN
1	A	135	GLN
1	A	171	HIS
1	B	12	GLN
1	B	21	GLN

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Mol	Chain	Res	Type
1	B	26	GLN
1	B	87	GLN
1	B	108	GLN
1	B	135	GLN
1	C	12	GLN
1	C	21	GLN
1	C	26	GLN
1	C	108	GLN
1	C	135	GLN
1	C	157	HIS
1	D	12	GLN
1	D	21	GLN
1	D	26	GLN
1	D	44	HIS
1	D	135	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	163/163 (100%)	-0.80	1 (0%) 85 90	11, 28, 49, 89	12 (7%)
1	B	163/163 (100%)	-0.83	0 100 100	11, 29, 50, 80	11 (6%)
1	C	163/163 (100%)	-0.80	0 100 100	9, 29, 48, 82	13 (7%)
1	D	163/163 (100%)	-0.83	0 100 100	11, 29, 50, 86	11 (6%)
All	All	652/652 (100%)	-0.82	1 (0%) 91 93	9, 29, 50, 89	47 (7%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	69	ALA	2.9

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.