



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:43 PM UTC

PDB ID : 1RHG / pdb_00001rhg
Title : THE STRUCTURE OF GRANULOCYTE-COLONY-STIMULATING
FACTOR AND ITS RELATIONSHIP TO THOSE OF OTHER GROWTH
FACTORS
Authors : Hill, C.P.; Osslund, T.D.; Eisenberg, D.
Deposited on : 1993-01-29
Resolution : 2.20 Å(reported)

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

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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

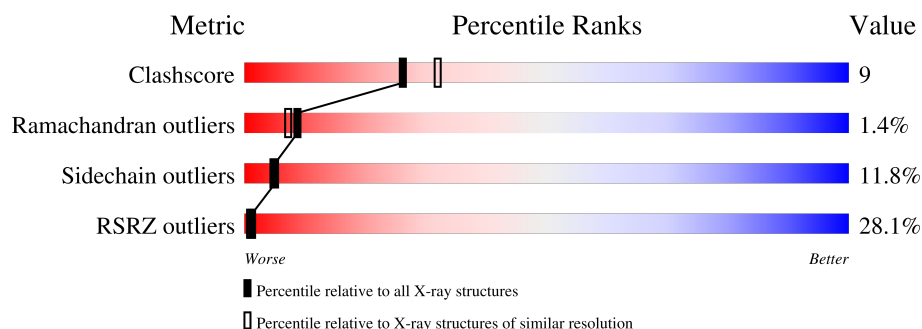
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	174	
1	B	174	
1	C	174	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4078 atoms, of which 735 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	145	Total	C	H	N	O	S	0	0	0
			1320	716	215	182	200	7			
1	B	144	Total	C	H	N	O	S	0	0	0
			1321	708	223	186	197	7			
1	C	145	Total	C	H	N	O	S	0	0	0
			1317	711	217	184	198	7			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	VAL	deletion	UNP P09919
A	?	-	SER	deletion	UNP P09919
A	?	-	GLU	deletion	UNP P09919
B	?	-	VAL	deletion	UNP P09919
B	?	-	SER	deletion	UNP P09919
B	?	-	GLU	deletion	UNP P09919
C	?	-	VAL	deletion	UNP P09919
C	?	-	SER	deletion	UNP P09919
C	?	-	GLU	deletion	UNP P09919

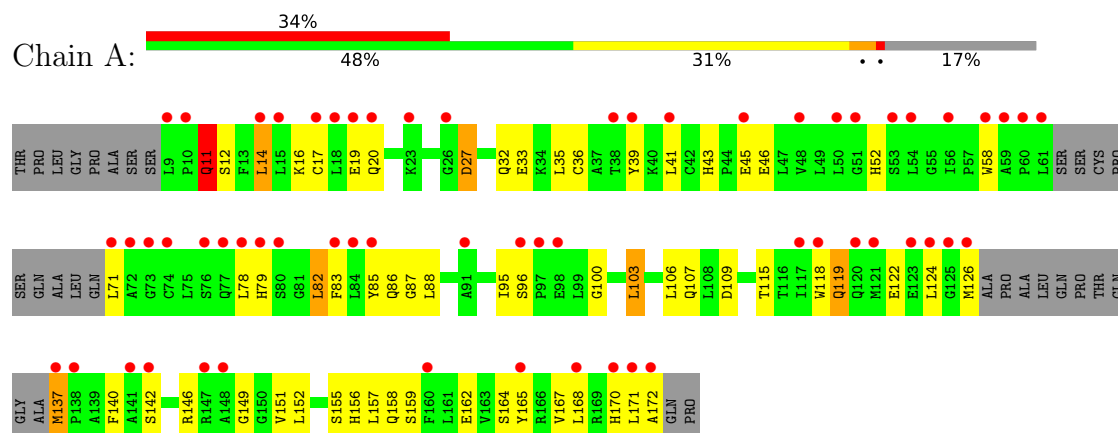
- Molecule 2 is water.

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	13	Total	H	O	0	0
			39	26	13		
2	B	13	Total	H	O	0	0
			39	26	13		
2	C	14	Total	H	O	0	0
			42	28	14		

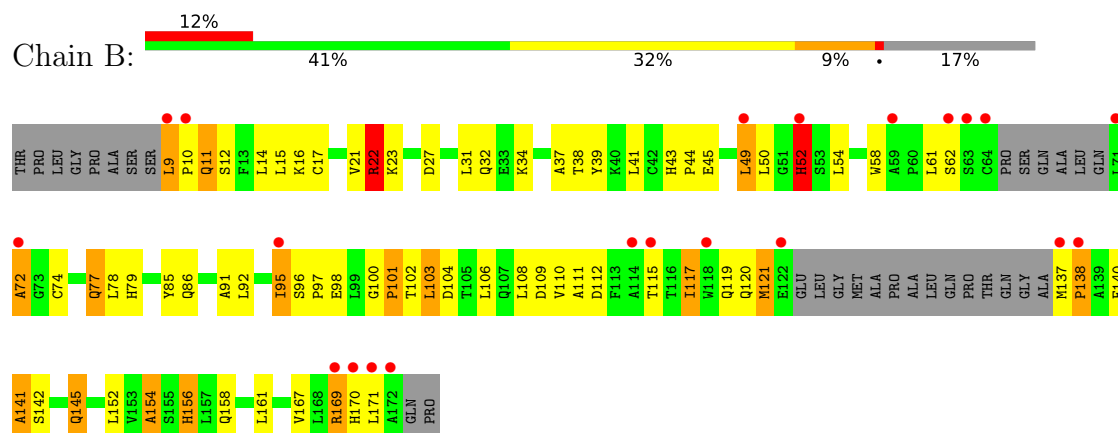
3 Residue-property plots

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.

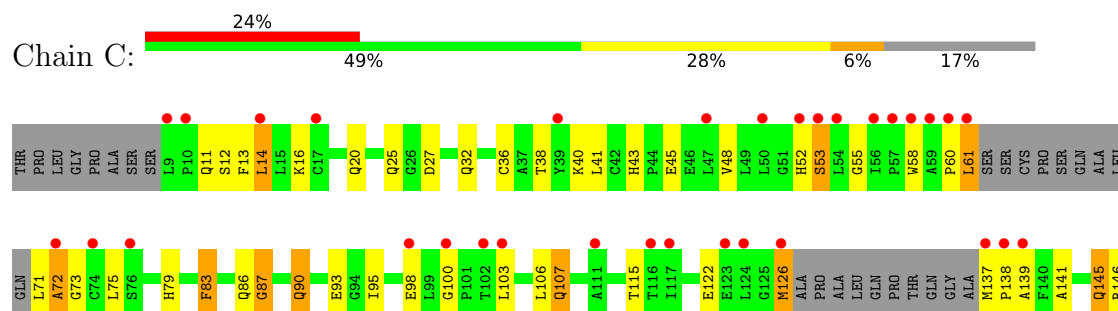
• Molecule 1: GRANULOCYTE COLONY-STIMULATING FACTOR



• Molecule 1: GRANULOCYTE COLONY-STIMULATING FACTOR



• Molecule 1: GRANULOCYTE COLONY-STIMULATING FACTOR





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.90Å 110.70Å 49.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.20 70.25 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) ((Not available)-2.20) 91.3 (70.25-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.66 (at 2.05Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.215 , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	36.9	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 78.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4078	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.76% 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	1.24	7/1127 (0.6%)	1.91	28/1528 (1.8%)
1	B	1.27	6/1120 (0.5%)	2.16	51/1518 (3.4%)
1	C	1.31	8/1122 (0.7%)	2.04	31/1522 (2.0%)
All	All	1.27	21/3369 (0.6%)	2.04	110/4568 (2.4%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	153	VAL	CA-CB	10.26	1.68	1.54
1	B	156	HIS	CD2-NE2	-7.14	1.29	1.37
1	B	79	HIS	CD2-NE2	-6.71	1.30	1.37
1	C	156	HIS	CD2-NE2	-6.63	1.30	1.37
1	C	43	HIS	CD2-NE2	-6.61	1.30	1.37
1	B	52	HIS	CD2-NE2	-6.42	1.30	1.37
1	B	43	HIS	CG-ND1	-6.12	1.31	1.38
1	A	52	HIS	CD2-NE2	-6.10	1.31	1.37
1	C	52	HIS	CD2-NE2	-6.04	1.31	1.37
1	A	156	HIS	CD2-NE2	-6.02	1.31	1.37
1	A	170	HIS	CD2-NE2	-5.79	1.31	1.37
1	A	79	HIS	CD2-NE2	-5.65	1.31	1.37
1	A	43	HIS	CD2-NE2	-5.62	1.31	1.37
1	C	36	CYS	CA-CB	-5.52	1.44	1.53
1	C	79	HIS	CD2-NE2	-5.49	1.31	1.37
1	B	117	ILE	CA-CB	5.40	1.60	1.54
1	A	79	HIS	CG-ND1	-5.38	1.32	1.38
1	C	156	HIS	CG-ND1	-5.29	1.32	1.38
1	B	170	HIS	CD2-NE2	-5.17	1.32	1.37
1	C	170	HIS	CD2-NE2	-5.15	1.32	1.37
1	A	156	HIS	CG-ND1	-5.02	1.32	1.38

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	44	PRO	CA-C-N	8.53	132.05	120.54
1	B	44	PRO	C-N-CA	8.53	132.05	120.54
1	C	156	HIS	CA-CB-CG	-8.46	105.34	113.80
1	A	11	GLN	OE1-CD-NE2	-7.99	114.61	122.60
1	B	109	ASP	N-CA-C	7.80	120.47	111.11
1	A	27	ASP	CA-CB-CG	7.76	120.36	112.60
1	B	52	HIS	CB-CG-CD2	-7.73	121.15	131.20
1	A	85	TYR	CA-C-O	-7.69	112.40	120.55
1	B	79	HIS	CB-CG-CD2	-7.60	121.32	131.20
1	B	145	GLN	CA-CB-CG	-7.53	99.03	114.10
1	B	112	ASP	CB-CA-C	-7.50	99.10	110.88
1	A	140	PHE	N-CA-C	-7.50	94.67	108.24
1	C	25	GLN	OE1-CD-NE2	-7.47	115.13	122.60
1	A	79	HIS	CA-CB-CG	-7.35	106.45	113.80
1	C	20	GLN	OE1-CD-NE2	-7.31	115.29	122.60
1	C	145	GLN	CA-CB-CG	-7.22	99.65	114.10
1	B	52	HIS	CA-CB-CG	7.21	121.01	113.80
1	B	169	ARG	N-CA-C	-6.94	103.80	111.36
1	C	60	PRO	N-CA-C	6.91	122.04	111.19
1	C	32	GLN	OE1-CD-NE2	-6.80	115.80	122.60
1	A	19	GLU	CA-CB-CG	6.77	127.64	114.10
1	B	41	LEU	CD1-CG-CD2	-6.73	95.99	110.80
1	B	32	GLN	OE1-CD-NE2	-6.60	116.00	122.60
1	A	109	ASP	CA-C-O	-6.47	113.56	120.42
1	B	12	SER	O-C-N	6.46	129.52	122.15
1	C	38	THR	N-CA-C	6.46	119.13	111.71
1	A	11	GLN	CG-CD-NE2	6.42	126.03	116.40
1	B	37	ALA	CB-CA-C	-6.41	100.82	110.88
1	C	107	GLN	N-CA-C	6.29	117.80	111.07
1	B	22	ARG	NE-CZ-NH2	6.21	124.78	119.20
1	B	115	THR	CA-C-O	-6.20	113.36	120.24
1	B	77	GLN	OE1-CD-NE2	-6.14	116.46	122.60
1	C	41	LEU	N-CA-C	-6.06	95.81	107.57
1	C	166	ARG	N-CA-C	6.00	117.62	111.14
1	A	19	GLU	N-CA-CB	-5.99	101.00	110.22
1	A	52	HIS	CB-CG-CD2	-5.98	123.43	131.20
1	B	17	CYS	CA-CB-SG	-5.97	100.67	114.40
1	C	58	TRP	CG-CD2-CE3	5.94	139.84	133.90
1	C	155	SER	N-CA-CB	-5.93	101.38	110.16
1	C	115	THR	CA-CB-OG1	-5.93	100.70	109.60
1	C	12	SER	CA-C-O	-5.92	114.14	120.42
1	A	43	HIS	CB-CG-CD2	-5.90	123.53	131.20
1	B	34	LYS	CB-CA-C	-5.90	101.61	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	100	GLY	CA-C-N	5.85	125.32	119.24
1	A	100	GLY	C-N-CA	5.85	125.32	119.24
1	B	16	LYS	N-CA-C	-5.80	104.87	111.14
1	B	120	GLN	OE1-CD-NE2	-5.78	116.82	122.60
1	C	169	ARG	CB-CG-CD	5.75	124.54	111.30
1	A	122	GLU	CA-CB-CG	-5.75	102.61	114.10
1	B	52	HIS	CB-CG-ND1	5.74	131.30	122.70
1	B	61	LEU	CA-C-O	-5.67	112.40	120.51
1	C	139	ALA	N-CA-C	-5.66	100.66	109.72
1	A	118	TRP	CG-CD2-CE3	5.66	139.56	133.90
1	B	154	ALA	N-CA-C	-5.60	105.07	111.07
1	C	27	ASP	CA-CB-CG	5.60	118.20	112.60
1	B	141	ALA	O-C-N	-5.59	115.15	122.59
1	B	110	VAL	N-CA-C	-5.59	104.92	110.62
1	A	79	HIS	CB-CG-CD2	-5.58	123.94	131.20
1	B	58	TRP	CE2-CD2-CG	-5.54	100.55	107.20
1	B	158	GLN	CA-C-N	5.53	127.63	120.44
1	B	158	GLN	C-N-CA	5.53	127.63	120.44
1	C	11	GLN	OE1-CD-NE2	-5.53	117.07	122.60
1	C	122	GLU	CB-CA-C	-5.52	102.45	110.96
1	C	106	LEU	CA-C-O	-5.50	114.72	120.55
1	A	149	GLY	N-CA-C	-5.46	107.89	114.66
1	C	43	HIS	CB-CG-CD2	-5.44	124.12	131.20
1	B	91	ALA	N-CA-C	5.44	118.72	111.75
1	B	10	PRO	N-CA-C	5.42	119.99	111.38
1	B	52	HIS	CA-C-O	5.41	126.47	120.90
1	B	152	LEU	N-CA-C	5.40	117.16	111.28
1	B	102	THR	CA-C-O	5.37	126.43	120.63
1	C	156	HIS	CB-CG-CD2	-5.35	124.24	131.20
1	A	118	TRP	CB-CG-CD1	-5.35	118.87	126.90
1	C	20	GLN	CG-CD-NE2	5.34	124.41	116.40
1	C	13	PHE	CA-CB-CG	5.34	119.14	113.80
1	C	83	PHE	N-CA-C	-5.32	105.57	111.36
1	B	95	ILE	CA-C-O	-5.31	114.14	120.78
1	B	12	SER	CA-C-O	-5.28	114.82	120.42
1	B	58	TRP	CD1-CG-CD2	5.26	114.71	106.30
1	A	17	CYS	CA-C-O	-5.25	115.30	120.82
1	B	86	GLN	CA-C-N	5.25	125.77	119.94
1	B	86	GLN	C-N-CA	5.25	125.77	119.94
1	B	104	ASP	CA-CB-CG	5.24	117.84	112.60
1	A	146	ARG	N-CA-C	-5.21	105.51	111.14
1	A	96	SER	O-C-N	-5.21	115.33	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	112	ASP	CA-CB-CG	5.20	117.80	112.60
1	A	157	LEU	N-CA-C	-5.19	105.53	111.14
1	B	12	SER	N-CA-C	-5.18	105.71	111.36
1	A	83	PHE	CA-CB-CG	-5.16	108.64	113.80
1	A	20	GLN	CA-CB-CG	-5.13	103.84	114.10
1	B	167	VAL	CA-C-O	-5.13	115.80	121.29
1	B	119	GLN	OE1-CD-NE2	-5.12	117.48	122.60
1	C	58	TRP	CB-CG-CD1	-5.12	119.22	126.90
1	A	82	LEU	CA-C-O	5.10	125.83	119.97
1	A	16	LYS	N-CA-C	-5.09	105.81	111.36
1	B	72	ALA	N-CA-C	5.09	121.63	110.80
1	C	100	GLY	O-C-N	-5.08	116.69	121.77
1	C	87	GLY	O-C-N	5.08	127.06	122.19
1	C	166	ARG	O-C-N	-5.08	116.61	122.09
1	A	119	GLN	CG-CD-NE2	5.08	124.02	116.40
1	C	16	LYS	O-C-N	-5.07	116.75	122.12
1	C	53	SER	O-C-N	-5.07	116.75	122.12
1	B	121	MET	CA-CB-CG	-5.06	103.99	114.10
1	B	79	HIS	CB-CG-ND1	5.04	130.26	122.70
1	B	58	TRP	CG-CD1-NE1	-5.04	103.66	110.20
1	A	32	GLN	CG-CD-NE2	-5.03	108.86	116.40
1	B	101	PRO	CA-C-N	5.03	127.27	120.38
1	B	101	PRO	C-N-CA	5.03	127.27	120.38
1	B	23	LYS	CG-CD-CE	-5.02	99.75	111.30
1	B	119	GLN	CG-CD-NE2	5.01	123.92	116.40

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	1105	215	1111	24	0
1	B	1098	223	1099	25	0
1	C	1100	217	1098	17	0
2	A	13	26	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	13	26	0	0	0
2	C	14	28	0	0	0
All	All	3343	735	3308	62	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 9.

All (62) 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:61:LEU:HD12	1:C:163:VAL:HG12	1.46	0.96
1:B:137:MET:HG3	1:B:138:PRO:HD2	1.57	0.85
1:A:14:LEU:HD22	1:A:172:ALA:HB3	1.68	0.76
1:C:71:LEU:HD12	1:C:126:MET:HE1	1.74	0.67
1:A:103:LEU:O	1:A:107:GLN:HG3	1.99	0.62
1:C:141:ALA:HB3	1:C:145:GLN:OE1	2.02	0.60
1:A:164:SER:HA	1:A:167:VAL:HG22	1.86	0.57
1:C:95:ILE:HG13	1:C:103:LEU:HD11	1.86	0.57
1:B:117:ILE:HG22	1:B:121:MET:HE2	1.86	0.57
1:C:61:LEU:HD12	1:C:163:VAL:CG1	2.29	0.56
1:A:162:GLU:O	1:A:165:TYR:HB3	2.07	0.54
1:B:31:LEU:HD11	1:B:103:LEU:HD12	1.92	0.52
1:B:49:LEU:O	1:B:52:HIS:HB3	2.10	0.51
1:A:95:ILE:HD12	1:A:103:LEU:HD11	1.91	0.51
1:C:86:GLN:HE22	1:C:107:GLN:HG2	1.75	0.51
1:B:54:LEU:HD21	1:B:145:GLN:HG2	1.92	0.50
1:B:100:GLY:N	1:B:101:PRO:HD2	2.26	0.50
1:A:36:CYS:HA	1:A:41:LEU:O	2.12	0.50
1:A:155:SER:O	1:A:158:GLN:HB3	2.12	0.49
1:B:85:TYR:OH	1:B:156:HIS:HB3	2.13	0.49
1:B:108:LEU:O	1:B:111:ALA:HB3	2.13	0.49
1:B:49:LEU:H	1:B:49:LEU:HD12	1.77	0.48
1:A:162:GLU:OE1	1:A:162:GLU:HA	2.12	0.48
1:B:22:ARG:NH2	1:C:83:PHE:CE2	2.81	0.48
1:C:14:LEU:HD11	1:C:172:ALA:HA	1.95	0.48
1:B:38:THR:HG22	1:B:39:TYR:CE1	2.49	0.47
1:A:87:GLY:HA3	1:A:137:MET:HE2	1.96	0.47
1:B:22:ARG:NH1	1:C:83:PHE:O	2.47	0.47
1:B:9:LEU:N	1:B:171:LEU:O	2.48	0.47
1:B:27:ASP:HB2	1:B:106:LEU:HD13	1.96	0.47
1:C:55:GLY:C	1:C:138:PRO:HG3	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:LEU:HD22	1:B:171:LEU:O	2.15	0.47
1:A:115:THR:O	1:A:119:GLN:HG3	2.14	0.46
1:A:167:VAL:O	1:A:171:LEU:HB2	2.14	0.46
1:B:22:ARG:NH1	1:C:87:GLY:N	2.62	0.46
1:A:71:LEU:HB3	1:A:126:MET:HE1	1.97	0.46
1:C:45:GLU:O	1:C:48:VAL:HG12	2.16	0.46
1:A:35:LEU:HD13	1:A:151:VAL:HG23	1.98	0.46
2:A:619:HOH:O	1:C:162:GLU:HG2	2.16	0.46
1:B:92:LEU:HD23	1:B:140:PHE:CD2	2.51	0.45
1:B:11:GLN:O	1:B:15:LEU:HD12	2.16	0.45
1:A:78:LEU:HD23	1:A:82:LEU:HD11	1.98	0.45
1:A:14:LEU:HD21	1:A:168:LEU:O	2.17	0.45
1:B:31:LEU:HD23	1:B:154:ALA:HB2	1.99	0.44
1:A:39:TYR:HB2	1:A:41:LEU:HD12	1.99	0.44
1:A:71:LEU:HA	1:A:71:LEU:HD12	1.76	0.43
1:B:137:MET:HE3	1:B:137:MET:HA	2.00	0.43
1:A:88:LEU:HG	1:A:137:MET:HE3	2.00	0.43
1:B:137:MET:CG	1:B:138:PRO:HD2	2.40	0.43
1:B:14:LEU:HD21	1:B:169:ARG:HD3	2.01	0.43
1:B:96:SER:HB2	1:B:97:PRO:HD2	2.01	0.43
1:B:22:ARG:NH1	1:C:87:GLY:CA	2.82	0.42
1:A:58:TRP:HA	1:A:58:TRP:CE3	2.54	0.42
1:A:71:LEU:HD23	1:A:124:LEU:HD21	2.02	0.41
1:C:72:ALA:HA	1:C:126:MET:SD	2.61	0.41
1:A:27:ASP:HB2	1:A:106:LEU:HD13	2.02	0.41
1:A:151:VAL:O	1:A:155:SER:HB3	2.20	0.41
1:C:90:GLN:HG3	1:C:107:GLN:NE2	2.36	0.41
1:A:88:LEU:HA	1:A:88:LEU:HD23	1.87	0.41
1:C:71:LEU:O	1:C:73:GLY:N	2.54	0.40
1:A:124:LEU:HG	1:A:126:MET:SD	2.60	0.40
1:B:21:VAL:HG13	1:B:161:LEU:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	139/174 (80%)	134 (96%)	4 (3%)	1 (1%)	18	19
1	B	138/174 (79%)	128 (93%)	6 (4%)	4 (3%)	3	2
1	C	139/174 (80%)	130 (94%)	8 (6%)	1 (1%)	18	19
All	All	416/522 (80%)	392 (94%)	18 (4%)	6 (1%)	9	7

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	72	ALA
1	B	141	ALA
1	C	72	ALA
1	A	11	GLN
1	B	95	ILE
1	B	138	PRO

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	117/141 (83%)	105 (90%)	12 (10%)	7	7
1	B	116/141 (82%)	102 (88%)	14 (12%)	5	4
1	C	115/141 (82%)	100 (87%)	15 (13%)	4	3
All	All	348/423 (82%)	307 (88%)	41 (12%)	5	5

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	12	SER
1	A	14	LEU
1	A	33	GLU

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Mol	Chain	Res	Type
1	A	45	GLU
1	A	46	GLU
1	A	86	GLN
1	A	103	LEU
1	A	137	MET
1	A	142	SER
1	A	152	LEU
1	A	159	SER
1	B	9	LEU
1	B	11	GLN
1	B	22	ARG
1	B	45	GLU
1	B	49	LEU
1	B	50	LEU
1	B	52	HIS
1	B	62	SER
1	B	74	CYS
1	B	77	GLN
1	B	78	LEU
1	B	98	GLU
1	B	103	LEU
1	B	142	SER
1	C	14	LEU
1	C	40	LYS
1	C	53	SER
1	C	61	LEU
1	C	75	LEU
1	C	90	GLN
1	C	93	GLU
1	C	98	GLU
1	C	126	MET
1	C	137	MET
1	C	146	ARG
1	C	153	VAL
1	C	165	TYR
1	C	167	VAL
1	C	171	LEU

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

Mol	Chain	Res	Type
1	A	52	HIS

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Mol	Chain	Res	Type
1	A	120	GLN
1	A	158	GLN
1	B	11	GLN
1	B	20	GLN
1	B	77	GLN
1	B	79	HIS
1	C	52	HIS
1	C	86	GLN
1	C	107	GLN
1	C	170	HIS

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

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	145/174 (83%)	1.86	60 (41%) 0 0	15, 37, 64, 77	0
1	B	144/174 (82%)	1.00	21 (14%) 6 4	19, 32, 52, 77	0
1	C	145/174 (83%)	1.63	41 (28%) 1 1	17, 31, 71, 81	0
All	All	434/522 (83%)	1.50	122 (28%) 1 1	15, 33, 64, 81	0

All (122) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	126	MET	6.6
1	C	61	LEU	6.0
1	A	61	LEU	5.6
1	C	165	TYR	5.5
1	A	124	LEU	5.4
1	B	71	LEU	5.3
1	C	171	LEU	5.1
1	B	172	ALA	4.8
1	C	56	ILE	4.4
1	C	137	MET	4.4
1	B	9	LEU	4.4
1	C	59	ALA	4.3
1	C	172	ALA	4.3
1	A	172	ALA	4.1
1	A	141	ALA	4.0
1	C	126	MET	4.0
1	B	64	CYS	3.9
1	C	58	TRP	3.9
1	C	54	LEU	3.9
1	C	60	PRO	3.8
1	B	72	ALA	3.7
1	B	118	TRP	3.7
1	A	118	TRP	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	142	SER	3.6
1	A	51	GLY	3.6
1	C	52	HIS	3.5
1	C	57	PRO	3.5
1	B	170	HIS	3.5
1	A	78	LEU	3.4
1	C	116	THR	3.4
1	C	167	VAL	3.3
1	A	83	PHE	3.3
1	A	121	MET	3.3
1	A	96	SER	3.3
1	A	138	PRO	3.2
1	A	137	MET	3.1
1	A	98	GLU	3.1
1	C	123	GLU	3.1
1	C	74	CYS	3.1
1	A	9	LEU	3.0
1	A	168	LEU	3.0
1	C	168	LEU	3.0
1	A	120	GLN	3.0
1	C	111	ALA	3.0
1	C	14	LEU	3.0
1	C	72	ALA	2.9
1	B	63	SER	2.9
1	A	170	HIS	2.9
1	A	39	TYR	2.9
1	A	15	LEU	2.9
1	A	117	ILE	2.9
1	C	169	ARG	2.8
1	C	139	ALA	2.8
1	A	58	TRP	2.8
1	A	97	PRO	2.7
1	A	50	LEU	2.7
1	B	171	LEU	2.7
1	C	124	LEU	2.7
1	C	170	HIS	2.7
1	B	115	THR	2.7
1	A	17	CYS	2.7
1	A	18	LEU	2.7
1	C	50	LEU	2.7
1	C	9	LEU	2.7
1	A	53	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	14	LEU	2.5
1	A	71	LEU	2.5
1	C	100	GLY	2.5
1	A	60	PRO	2.5
1	C	164	SER	2.5
1	A	165	TYR	2.5
1	C	103	LEU	2.4
1	A	125	GLY	2.4
1	A	54	LEU	2.4
1	A	73	GLY	2.4
1	B	95	ILE	2.4
1	B	138	PRO	2.4
1	A	26	GLY	2.4
1	A	72	ALA	2.4
1	A	123	GLU	2.4
1	C	10	PRO	2.3
1	B	114	ALA	2.3
1	B	52	HIS	2.3
1	A	20	GLN	2.3
1	C	76	SER	2.3
1	A	171	LEU	2.3
1	B	137	MET	2.3
1	A	38	THR	2.3
1	A	80	SER	2.3
1	A	23	LYS	2.3
1	C	17	CYS	2.3
1	B	59	ALA	2.3
1	C	154	ALA	2.3
1	C	53	SER	2.3
1	A	79	HIS	2.2
1	A	148	ALA	2.2
1	B	10	PRO	2.2
1	A	59	ALA	2.2
1	A	76	SER	2.2
1	A	85	TYR	2.2
1	A	56	ILE	2.2
1	A	84	LEU	2.2
1	A	10	PRO	2.2
1	C	102	THR	2.2
1	A	19	GLU	2.2
1	C	98	GLU	2.2
1	C	39	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	41	LEU	2.1
1	C	47	LEU	2.1
1	C	117	ILE	2.1
1	A	74	CYS	2.1
1	B	62	SER	2.1
1	A	48	VAL	2.1
1	A	160	PHE	2.1
1	A	77	GLN	2.1
1	C	138	PRO	2.1
1	A	91	ALA	2.0
1	B	49	LEU	2.0
1	B	169	ARG	2.0
1	A	45	GLU	2.0
1	B	122	GLU	2.0
1	A	147	ARG	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.