



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:30 AM UTC

PDB ID : 3E5M / pdb_00003e5m
Title : Crystal structure of the HSCARG Y81A mutant
Authors : Li, Y.; Meng, G.; Dai, X.; Luo, M.; Zheng, X.
Deposited on : 2008-08-14
Resolution : 2.70 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

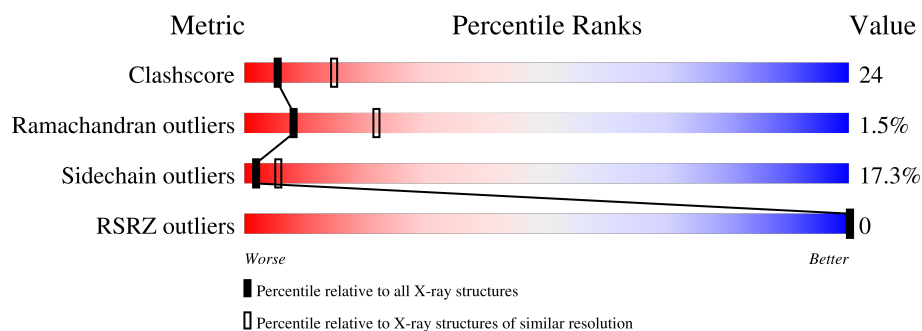
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	299	
1	B	299	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 4605 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 NmrA-like family domain-containing protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	294	Total	C	N	O	S	0	0	0
			2298	1459	402	427	10			
1	B	295	Total	C	N	O	S	0	0	0
			2307	1465	404	428	10			

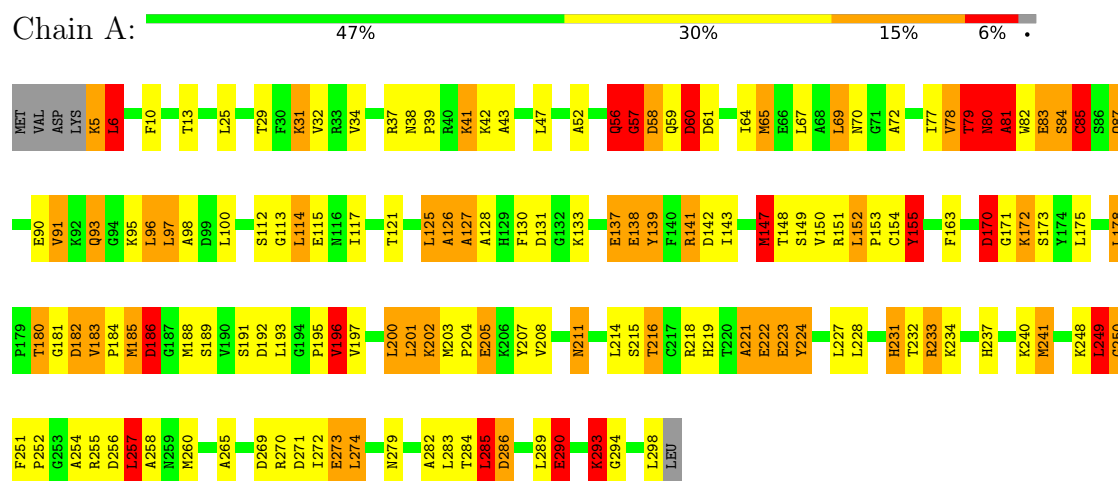
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	81	ALA	TYR	engineered mutation	UNP Q9HBL8
B	81	ALA	TYR	engineered mutation	UNP Q9HBL8

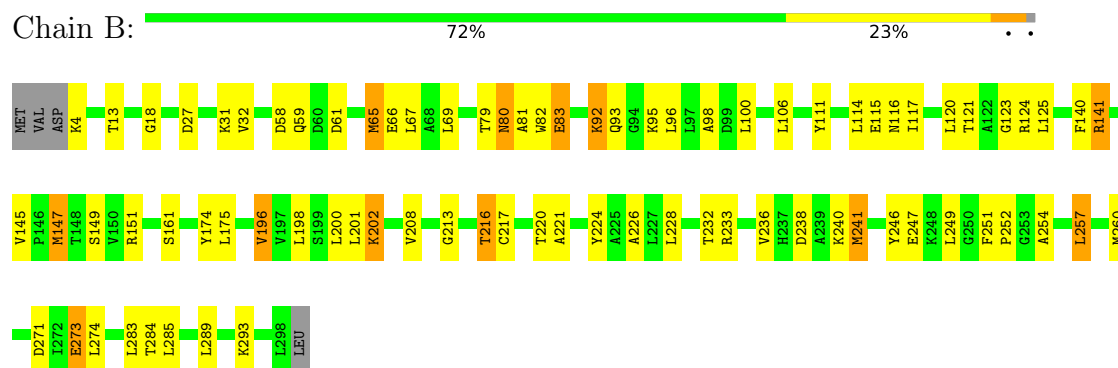
3 Residue-property plots

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: NmrA-like family domain-containing protein 1



- Molecule 1: NmrA-like family domain-containing protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	46.96Å 89.04Å 84.18Å 90.00° 88.23° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 20.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.1 (20.00-2.70) 89.5 (20.00-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.88 (at 2.71Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.260 , 0.273 0.264 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 10.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.34$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	0.308 for h,-k,-l	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	4605	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% 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	1.53	17/2342 (0.7%)	1.37	20/3165 (0.6%)
1	B	1.20	1/2351 (0.0%)	1.17	6/3176 (0.2%)
All	All	1.37	18/4693 (0.4%)	1.27	26/6341 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	10

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	CYS	C-O	-6.59	1.16	1.23
1	A	52	ALA	CA-CB	-6.44	1.43	1.53
1	A	254	ALA	CA-CB	-6.40	1.43	1.53
1	A	290	GLU	CA-C	6.26	1.61	1.52
1	A	221	ALA	C-O	-6.21	1.16	1.24
1	A	222	GLU	CA-C	-5.91	1.45	1.52
1	A	155	TYR	C-O	-5.70	1.17	1.23
1	B	98	ALA	CA-CB	-5.38	1.44	1.53
1	A	257	LEU	CA-C	-5.26	1.45	1.52
1	A	279	ASN	C-O	-5.24	1.20	1.24
1	A	196	VAL	CB-CG1	-5.23	1.35	1.52
1	A	286	ASP	C-O	-5.20	1.18	1.24
1	A	126	ALA	C-O	-5.17	1.17	1.23
1	A	216	THR	CA-C	-5.16	1.46	1.52
1	A	163	PHE	N-CA	-5.12	1.40	1.46
1	A	258	ALA	N-CA	-5.07	1.40	1.46
1	A	173	SER	C-O	5.06	1.29	1.23
1	A	57	GLY	N-CA	5.00	1.52	1.45

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	290	GLU	N-CA-C	7.03	119.84	111.33
1	A	96	LEU	CA-CB-CG	6.32	138.43	116.30
1	A	78	VAL	N-CA-C	-6.14	101.33	108.82
1	A	127	ALA	N-CA-C	5.91	117.39	108.46
1	A	224	TYR	N-CA-C	5.90	118.19	111.11
1	A	249	LEU	N-CA-C	5.80	119.61	112.54
1	A	282	ALA	CA-C-N	5.71	129.58	121.42
1	A	282	ALA	C-N-CA	5.71	129.58	121.42
1	A	211	ASN	N-CA-C	5.68	117.93	109.25
1	B	161	SER	O-C-N	5.58	124.96	120.83
1	A	285	LEU	N-CA-C	-5.49	105.68	112.38
1	A	293	LYS	N-CA-C	-5.46	102.54	110.24
1	A	257	LEU	N-CA-C	-5.46	104.98	111.69
1	A	282	ALA	N-CA-C	5.43	118.11	109.96
1	A	294	GLY	N-CA-C	-5.43	108.22	114.69
1	A	6	LEU	N-CA-C	5.39	118.38	110.30
1	B	226	ALA	N-CA-C	5.38	117.14	111.28
1	A	41	LYS	N-CA-C	5.32	117.15	110.24
1	A	231	HIS	N-CA-C	-5.23	107.44	113.88
1	A	283	LEU	N-CA-C	5.21	118.43	110.20
1	B	196	VAL	N-CA-C	5.12	115.89	110.72
1	B	147	MET	N-CA-C	5.09	116.99	108.99
1	B	18	GLY	N-CA-C	-5.09	106.33	112.49
1	B	66	GLU	N-CA-C	-5.08	106.34	112.54
1	A	147	MET	N-CA-C	5.07	117.42	108.75
1	A	60	ASP	N-CA-C	-5.07	107.05	113.18

There are no chirality outliers.

All (10) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	139	TYR	Peptide
1	A	170	ASP	Peptide
1	A	180	THR	Peptide
1	A	186	ASP	Peptide
1	A	56	GLN	Peptide
1	A	79	THR	Peptide
1	A	81	ALA	Peptide
1	A	83	GLU	Peptide
1	A	84	SER	Peptide
1	A	85	CYS	Peptide

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	2298	0	2321	186	0
1	B	2307	0	2334	34	0
All	All	4605	0	4655	220	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 24.

All (220) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASN:CG	1:A:84:SER:HB3	1.51	1.35
1:A:65:MET:O	1:A:69:LEU:CD2	1.73	1.34
1:A:80:ASN:HA	1:A:81:ALA:CB	1.62	1.21
1:A:80:ASN:ND2	1:A:84:SER:HB3	1.54	1.20
1:A:80:ASN:CA	1:A:81:ALA:HB2	1.68	1.19
1:A:81:ALA:HB3	1:A:82:TRP:O	1.46	1.12
1:A:87:GLN:O	1:A:91:VAL:HG13	1.48	1.11
1:A:39:PRO:HG2	1:A:56:GLN:HB2	1.29	1.10
1:A:284:THR:HG22	1:A:286:ASP:H	1.13	1.09
1:A:148:THR:OG1	1:A:207:TYR:O	1.69	1.08
1:A:80:ASN:OD1	1:A:84:SER:HB3	1.52	1.08
1:A:65:MET:O	1:A:69:LEU:HD23	1.44	1.07
1:A:256:ASP:O	1:A:260:MET:HG3	1.55	1.06
1:A:141:ARG:NH1	1:A:147:MET:HE3	1.72	1.03
1:A:227:LEU:HD12	1:A:285:LEU:HD13	1.38	1.03
1:A:181:GLY:O	1:A:182:ASP:HB2	1.52	1.03
1:A:69:LEU:N	1:A:69:LEU:HD22	1.74	1.02
1:A:251:PHE:HB2	1:A:252:PRO:HD2	1.40	1.02
1:A:39:PRO:CG	1:A:56:GLN:HB2	1.89	1.01
1:A:141:ARG:NH2	1:A:211:ASN:OD1	1.94	0.99
1:A:139:TYR:HA	1:A:142:ASP:HB2	1.42	0.98
1:A:87:GLN:O	1:A:91:VAL:CG1	2.13	0.97
1:A:180:THR:HG21	1:A:221:ALA:H	1.30	0.96
1:A:232:THR:O	1:A:233:ARG:HG2	1.65	0.96
1:A:138:GLU:O	1:A:138:GLU:HG3	1.63	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:ASN:ND2	1:A:84:SER:CB	2.31	0.94
1:A:69:LEU:HD22	1:A:69:LEU:H	1.32	0.92
1:A:137:GLU:CD	1:A:151:ARG:HH21	1.79	0.91
1:A:227:LEU:HD12	1:A:285:LEU:CD1	2.01	0.90
1:A:141:ARG:CZ	1:A:147:MET:HE3	2.01	0.89
1:A:65:MET:HE3	1:A:65:MET:HA	1.53	0.88
1:A:39:PRO:HG2	1:A:56:GLN:CB	2.04	0.88
1:A:80:ASN:CA	1:A:81:ALA:CB	2.35	0.86
1:A:227:LEU:CD1	1:A:285:LEU:HD13	2.07	0.84
1:A:80:ASN:HD21	1:A:84:SER:HB3	1.44	0.83
1:A:69:LEU:CD2	1:A:69:LEU:H	1.91	0.82
1:A:80:ASN:CG	1:A:84:SER:CB	2.46	0.82
1:A:232:THR:O	1:A:233:ARG:CG	2.27	0.82
1:A:83:GLU:HG3	1:A:84:SER:H	1.42	0.82
1:B:82:TRP:N	1:B:83:GLU:HA	1.94	0.82
1:A:78:VAL:C	1:A:79:THR:CG2	2.54	0.81
1:B:65:MET:HE3	1:B:65:MET:HA	1.61	0.81
1:A:37:ARG:HG2	1:A:58:ASP:HA	1.62	0.80
1:A:151:ARG:NH2	1:A:211:ASN:ND2	2.29	0.80
1:A:251:PHE:HB2	1:A:252:PRO:CD	2.10	0.80
1:A:13:THR:CG2	1:A:41:LYS:HE2	2.11	0.80
1:A:80:ASN:OD1	1:A:84:SER:CB	2.30	0.80
1:A:78:VAL:O	1:A:79:THR:HG22	1.82	0.79
1:A:65:MET:O	1:A:69:LEU:HD21	1.80	0.79
1:A:79:THR:O	1:A:90:GLU:OE2	2.01	0.78
1:A:84:SER:HB2	1:A:85:CYS:O	1.84	0.78
1:A:65:MET:O	1:A:69:LEU:HD22	1.80	0.78
1:A:69:LEU:CD2	1:A:69:LEU:N	2.46	0.77
1:A:290:GLU:O	1:A:293:LYS:NZ	2.16	0.75
1:A:127:ALA:HB1	1:A:256:ASP:HB3	1.67	0.74
1:A:147:MET:HE1	1:A:149:SER:HB2	1.67	0.74
1:A:13:THR:HG21	1:A:41:LYS:HE2	1.68	0.74
1:A:170:ASP:OD1	1:A:170:ASP:C	2.31	0.74
1:B:59:GLN:NE2	1:B:80:ASN:O	2.20	0.73
1:B:251:PHE:HB2	1:B:252:PRO:HD2	1.71	0.72
1:A:137:GLU:OE1	1:A:151:ARG:NH2	2.22	0.72
1:A:181:GLY:O	1:A:182:ASP:CB	2.31	0.72
1:A:78:VAL:C	1:A:79:THR:HG23	2.13	0.71
1:A:79:THR:O	1:A:133:LYS:NZ	2.23	0.71
1:A:180:THR:HG23	1:A:181:GLY:HA2	1.73	0.71
1:A:203:MET:N	1:A:204:PRO:HD3	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:LEU:O	1:A:285:LEU:HD22	1.89	0.71
1:A:80:ASN:HA	1:A:81:ALA:HB2	0.78	0.70
1:A:138:GLU:O	1:A:142:ASP:CG	2.34	0.70
1:A:80:ASN:HD21	1:A:84:SER:CB	1.98	0.69
1:A:151:ARG:NH2	1:A:211:ASN:HD22	1.88	0.69
1:A:58:ASP:O	1:A:60:ASP:N	2.25	0.69
1:A:83:GLU:HG3	1:A:84:SER:N	2.06	0.69
1:A:83:GLU:CG	1:A:84:SER:H	2.06	0.69
1:A:78:VAL:HG12	1:A:112:SER:HB3	1.75	0.68
1:A:232:THR:O	1:A:233:ARG:NE	2.27	0.68
1:A:180:THR:CG2	1:A:221:ALA:CB	2.72	0.67
1:A:80:ASN:HB2	1:A:81:ALA:HB3	1.77	0.66
1:A:91:VAL:O	1:A:95:LYS:HG3	1.95	0.66
1:A:180:THR:HG22	1:A:221:ALA:HB2	1.76	0.66
1:A:126:ALA:O	1:A:127:ALA:HB2	1.96	0.66
1:A:137:GLU:O	1:A:139:TYR:N	2.30	0.64
1:A:78:VAL:O	1:A:79:THR:CG2	2.46	0.64
1:A:141:ARG:CZ	1:A:147:MET:CE	2.74	0.63
1:A:257:LEU:O	1:A:260:MET:HB2	1.97	0.63
1:A:180:THR:HG21	1:A:221:ALA:N	2.10	0.63
1:A:170:ASP:OD1	1:A:172:LYS:HB2	2.00	0.62
1:A:84:SER:OG	1:A:85:CYS:N	2.31	0.62
1:A:180:THR:HG22	1:A:221:ALA:CB	2.29	0.61
1:A:117:ILE:HG21	1:A:125:LEU:HD12	1.83	0.60
1:A:39:PRO:HG3	1:A:56:GLN:HB2	1.78	0.60
1:A:186:ASP:HB3	1:A:215:SER:OG	2.01	0.60
1:A:180:THR:CG2	1:A:221:ALA:HB2	2.31	0.60
1:A:251:PHE:O	1:A:255:ARG:NH2	2.34	0.59
1:B:228:LEU:O	1:B:232:THR:OG1	2.12	0.59
1:A:98:ALA:O	1:A:143:ILE:HD11	2.01	0.59
1:A:284:THR:HG22	1:A:286:ASP:N	1.99	0.59
1:A:34:VAL:HG11	1:A:47:LEU:HD13	1.85	0.59
1:A:284:THR:CG2	1:A:285:LEU:N	2.66	0.59
1:A:170:ASP:OD1	1:A:171:GLY:N	2.36	0.58
1:A:249:LEU:O	1:A:250:GLY:C	2.46	0.58
1:A:93:GLN:O	1:A:97:LEU:HD22	2.03	0.58
1:A:80:ASN:CB	1:A:81:ALA:CB	2.81	0.58
1:A:65:MET:HA	1:A:65:MET:CE	2.28	0.58
1:A:180:THR:HG21	1:A:221:ALA:CB	2.32	0.58
1:A:91:VAL:O	1:A:91:VAL:HG23	2.03	0.58
1:A:61:ASP:O	1:A:65:MET:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:LEU:CD2	1:A:289:LEU:HG	2.34	0.58
1:B:217:CYS:HB3	1:B:284:THR:HG23	1.85	0.57
1:A:203:MET:N	1:A:204:PRO:CD	2.67	0.57
1:A:231:HIS:O	1:A:293:LYS:HD3	2.04	0.57
1:A:223:GLU:O	1:A:227:LEU:HG	2.04	0.57
1:A:269:ASP:O	1:A:270:ARG:HD2	2.05	0.56
1:A:13:THR:HG21	1:A:41:LYS:CE	2.34	0.56
1:A:216:THR:HG22	1:A:216:THR:O	2.05	0.56
1:B:271:ASP:OD1	1:B:273:GLU:HG2	2.05	0.56
1:A:5:LYS:HB3	1:A:31:LYS:H	1.70	0.56
1:A:81:ALA:CB	1:A:82:TRP:O	2.38	0.56
1:A:137:GLU:C	1:A:139:TYR:H	2.14	0.55
1:A:185:MET:O	1:A:185:MET:HG3	2.02	0.55
1:A:58:ASP:C	1:A:60:ASP:H	2.12	0.55
1:B:58:ASP:HB3	1:B:61:ASP:HB2	1.89	0.55
1:A:80:ASN:HB2	1:A:81:ALA:CB	2.37	0.54
1:A:284:THR:HG22	1:A:285:LEU:N	2.22	0.54
1:B:65:MET:HA	1:B:65:MET:CE	2.35	0.54
1:A:138:GLU:O	1:A:142:ASP:OD1	2.25	0.54
1:A:117:ILE:N	1:A:131:ASP:OD1	2.41	0.54
1:A:196:VAL:HG21	1:A:214:LEU:HD21	1.89	0.54
1:B:174:TYR:HB2	1:B:236:VAL:HG22	1.90	0.54
1:A:117:ILE:CG2	1:A:125:LEU:HD12	2.39	0.53
1:A:180:THR:CG2	1:A:221:ALA:HB3	2.37	0.53
1:B:80:ASN:HA	1:B:82:TRP:HB3	1.90	0.53
1:B:81:ALA:HA	1:B:82:TRP:HB3	1.89	0.53
1:A:153:PRO:HG2	1:A:188:MET:HG2	1.90	0.53
1:A:241:MET:CE	1:A:241:MET:HA	2.39	0.53
1:B:121:THR:HG21	1:B:125:LEU:H	1.74	0.53
1:A:219:HIS:HB3	1:A:223:GLU:HB2	1.90	0.53
1:A:150:VAL:HB	1:A:214:LEU:HD11	1.90	0.52
1:A:214:LEU:O	1:A:215:SER:HB2	2.08	0.52
1:B:121:THR:HG23	1:B:123:GLY:H	1.74	0.52
1:A:180:THR:OG1	1:A:183:VAL:O	2.27	0.52
1:A:183:VAL:HG11	1:A:265:ALA:HA	1.91	0.52
1:A:83:GLU:CG	1:A:84:SER:N	2.70	0.51
1:A:184:PRO:HB3	1:A:218:ARG:O	2.11	0.51
1:B:238:ASP:HB3	1:B:240:LYS:HE2	1.93	0.51
1:A:192:ASP:O	1:A:195:PRO:HD2	2.10	0.51
1:A:222:GLU:OE2	1:A:240:LYS:NZ	2.38	0.50
1:A:139:TYR:CA	1:A:142:ASP:HB2	2.29	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:111:TYR:O	1:B:149:SER:HA	2.12	0.49
1:B:117:ILE:O	1:B:121:THR:HG22	2.12	0.49
1:A:80:ASN:HB2	1:A:83:GLU:HG3	1.93	0.49
1:A:80:ASN:CB	1:A:81:ALA:HB2	2.40	0.49
1:B:289:LEU:O	1:B:293:LYS:HB3	2.13	0.49
1:A:58:ASP:O	1:A:59:GLN:C	2.55	0.49
1:A:59:GLN:HA	1:A:65:MET:SD	2.53	0.49
1:B:79:THR:O	1:B:80:ASN:C	2.55	0.49
1:A:80:ASN:CB	1:A:81:ALA:HB3	2.43	0.49
1:A:87:GLN:CG	1:A:128:ALA:HB1	2.43	0.48
1:B:257:LEU:HD23	1:B:260:MET:HE3	1.95	0.48
1:A:113:GLY:HA2	1:A:133:LYS:HD2	1.94	0.48
1:A:180:THR:HG23	1:A:181:GLY:CA	2.42	0.48
1:A:87:GLN:HG3	1:A:128:ALA:HB1	1.94	0.48
1:A:189:SER:C	1:A:191:SER:N	2.69	0.48
1:A:178:LEU:HD21	1:A:185:MET:HE2	1.94	0.47
1:A:251:PHE:CB	1:A:252:PRO:CD	2.86	0.47
1:B:198:LEU:O	1:B:202:LYS:HG2	2.14	0.47
1:A:285:LEU:HD22	1:A:285:LEU:C	2.40	0.47
1:B:80:ASN:HA	1:B:82:TRP:CB	2.44	0.47
1:B:249:LEU:HB3	1:B:251:PHE:HD2	1.79	0.47
1:A:13:THR:HG23	1:A:43:ALA:HB3	1.95	0.47
1:A:79:THR:C	1:A:90:GLU:OE2	2.56	0.47
1:A:114:LEU:HB3	1:A:130:PHE:CD2	2.49	0.47
1:A:271:ASP:OD2	1:A:274:LEU:HB2	2.14	0.47
1:A:61:ASP:CG	1:A:64:ILE:HG12	2.40	0.46
1:A:65:MET:C	1:A:69:LEU:HD23	2.33	0.46
1:B:247:GLU:HA	1:B:254:ALA:HB1	1.97	0.46
1:B:92:LYS:HA	1:B:95:LYS:HB2	1.97	0.46
1:A:285:LEU:O	1:A:285:LEU:CD2	2.59	0.46
1:A:61:ASP:HB3	1:A:64:ILE:HB	1.98	0.46
1:A:25:LEU:HG	1:A:32:VAL:HG11	1.97	0.46
1:A:273:GLU:H	1:A:273:GLU:HG2	1.51	0.45
1:B:116:ASN:C	1:B:116:ASN:HD22	2.23	0.45
1:B:241:MET:HG2	1:B:246:TYR:HE1	1.82	0.45
1:A:152:LEU:HD22	1:A:214:LEU:HD12	1.98	0.45
1:A:139:TYR:O	1:A:143:ILE:HG12	2.17	0.45
1:A:203:MET:HA	1:A:205:GLU:OE2	2.17	0.45
1:A:117:ILE:O	1:A:121:THR:HG22	2.16	0.45
1:A:10:PHE:HB2	1:A:77:ILE:HA	2.00	0.44
1:A:203:MET:C	1:A:205:GLU:OE2	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:228:LEU:O	1:A:232:THR:HB	2.18	0.44
1:A:139:TYR:O	1:A:143:ILE:HG23	2.17	0.44
1:A:186:ASP:OD1	1:A:218:ARG:HG3	2.17	0.44
1:A:65:MET:C	1:A:69:LEU:CD2	2.76	0.44
1:A:221:ALA:HA	1:A:224:TYR:HB2	2.00	0.44
1:A:285:LEU:HD22	1:A:289:LEU:HG	2.00	0.44
1:B:121:THR:HG23	1:B:124:ARG:H	1.83	0.44
1:A:126:ALA:O	1:A:127:ALA:CB	2.60	0.43
1:A:79:THR:O	1:A:80:ASN:O	2.36	0.43
1:B:151:ARG:HB2	1:B:213:GLY:HA2	1.99	0.43
1:A:216:THR:HA	1:A:272:ILE:HG23	1.99	0.43
1:A:284:THR:C	1:A:286:ASP:N	2.75	0.43
1:A:151:ARG:CZ	1:A:211:ASN:HD22	2.32	0.42
1:A:193:LEU:O	1:A:197:VAL:HG23	2.19	0.42
1:B:140:PHE:HD1	1:B:145:VAL:HB	1.84	0.42
1:B:216:THR:HG21	1:B:283:LEU:C	2.44	0.42
1:A:200:LEU:O	1:A:202:LYS:N	2.51	0.42
1:B:220:THR:HG22	1:B:221:ALA:N	2.34	0.42
1:A:189:SER:C	1:A:191:SER:H	2.27	0.42
1:A:6:LEU:HB3	1:A:72:ALA:HA	2.00	0.42
1:A:80:ASN:HD21	1:A:84:SER:HB2	1.78	0.42
1:B:221:ALA:HA	1:B:224:TYR:HB2	2.02	0.42
1:A:70:ASN:OD1	1:A:70:ASN:C	2.63	0.42
1:A:202:LYS:C	1:A:204:PRO:HD3	2.45	0.41
1:A:251:PHE:CD2	1:A:251:PHE:N	2.88	0.41
1:A:290:GLU:HA	1:A:293:LYS:HE3	2.03	0.41
1:B:141:ARG:CZ	1:B:147:MET:HE3	2.50	0.41
1:A:38:ASN:HA	1:A:39:PRO:HD3	1.51	0.41
1:A:84:SER:CB	1:A:85:CYS:O	2.63	0.41
1:A:155:TYR:CD2	1:A:155:TYR:N	2.89	0.40
1:A:56:GLN:HG2	1:A:57:GLY:N	2.33	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	292/299 (98%)	261 (89%)	23 (8%)	8 (3%)	4	10
1	B	293/299 (98%)	272 (93%)	20 (7%)	1 (0%)	36	60
All	All	585/598 (98%)	533 (91%)	43 (7%)	9 (2%)	8	22

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	81	ALA
1	A	182	ASP
1	A	201	LEU
1	A	250	GLY
1	B	80	ASN
1	A	137	GLU
1	A	138	GLU
1	A	80	ASN
1	A	57	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	245/250 (98%)	191 (78%)	54 (22%)	1	3
1	B	246/250 (98%)	215 (87%)	31 (13%)	4	11
All	All	491/500 (98%)	406 (83%)	85 (17%)	2	5

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LYS
1	A	6	LEU
1	A	29	THR
1	A	31	LYS

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Mol	Chain	Res	Type
1	A	42	LYS
1	A	56	GLN
1	A	58	ASP
1	A	60	ASP
1	A	65	MET
1	A	67	LEU
1	A	69	LEU
1	A	79	THR
1	A	80	ASN
1	A	85	CYS
1	A	87	GLN
1	A	91	VAL
1	A	93	GLN
1	A	96	LEU
1	A	97	LEU
1	A	100	LEU
1	A	114	LEU
1	A	115	GLU
1	A	125	LEU
1	A	141	ARG
1	A	147	MET
1	A	152	LEU
1	A	155	TYR
1	A	170	ASP
1	A	172	LYS
1	A	175	LEU
1	A	178	LEU
1	A	183	VAL
1	A	185	MET
1	A	186	ASP
1	A	196	VAL
1	A	200	LEU
1	A	201	LEU
1	A	202	LYS
1	A	205	GLU
1	A	208	VAL
1	A	223	GLU
1	A	233	ARG
1	A	234	LYS
1	A	237	HIS
1	A	241	MET
1	A	248	LYS

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Mol	Chain	Res	Type
1	A	249	LEU
1	A	257	LEU
1	A	273	GLU
1	A	274	LEU
1	A	285	LEU
1	A	290	GLU
1	A	293	LYS
1	A	298	LEU
1	B	4	LYS
1	B	13	THR
1	B	27	ASP
1	B	31	LYS
1	B	32	VAL
1	B	65	MET
1	B	67	LEU
1	B	69	LEU
1	B	83	GLU
1	B	92	LYS
1	B	93	GLN
1	B	96	LEU
1	B	100	LEU
1	B	106	LEU
1	B	114	LEU
1	B	115	GLU
1	B	120	LEU
1	B	141	ARG
1	B	175	LEU
1	B	196	VAL
1	B	200	LEU
1	B	201	LEU
1	B	202	LYS
1	B	208	VAL
1	B	216	THR
1	B	233	ARG
1	B	241	MET
1	B	257	LEU
1	B	273	GLU
1	B	274	LEU
1	B	285	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	GLN
1	A	59	GLN
1	A	87	GLN
1	A	93	GLN
1	A	116	ASN
1	A	259	ASN
1	B	59	GLN
1	B	87	GLN
1	B	93	GLN
1	B	107	HIS
1	B	116	ASN
1	B	158	ASN
1	B	210	GLN
1	B	259	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 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	294/299 (98%)	-1.22	0 100 100	2, 15, 31, 40	0
1	B	295/299 (98%)	-1.16	0 100 100	2, 17, 37, 45	0
All	All	589/598 (98%)	-1.19	0 100 100	2, 16, 34, 45	0

There are no RSRZ outliers to report.

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.