



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:58 AM UTC

PDB ID : 4ILS / pdb_00004ils
Title : Crystal structure of engineered protein. northeast structural genomics Consortium target or117
Authors : Seetharaman, J.; Lew, S.; Nivon, L.; Baker, D.; Bjelic, S.; Ciccocanti, C.; Sahdev, S.; Xiao, R.; Everett, J.K.; Acton, T.B.; Montelione, G.T.; Tong, L.; Hunt, J.F.; Northeast Structural Genomics Consortium (NESG)
Deposited on : 2012-12-31
Resolution : 2.50 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

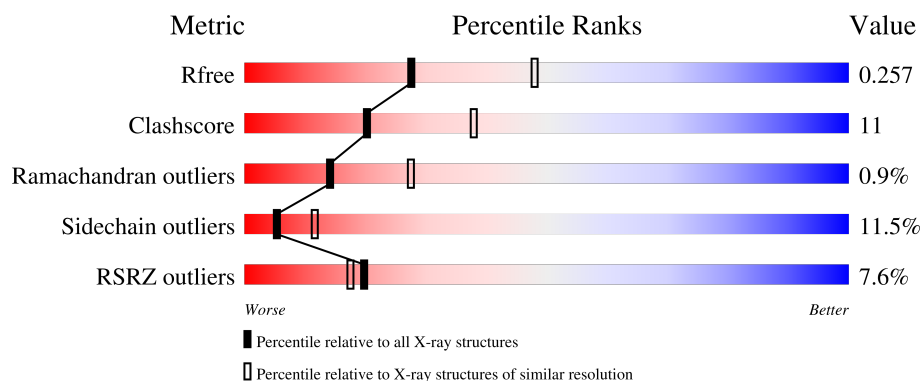
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	390	7% 68% 18% • 10%
1	B	390	6% 64% 18% 6% 12%
1	C	390	8% 63% 21% • 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8504 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 Engineered protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2786	1792	490	490	14			
1	B	344	Total	C	N	O	S	0	0	0
			2726	1749	481	481	15			
1	C	341	Total	C	N	O	S	0	0	0
			2721	1748	480	479	14			

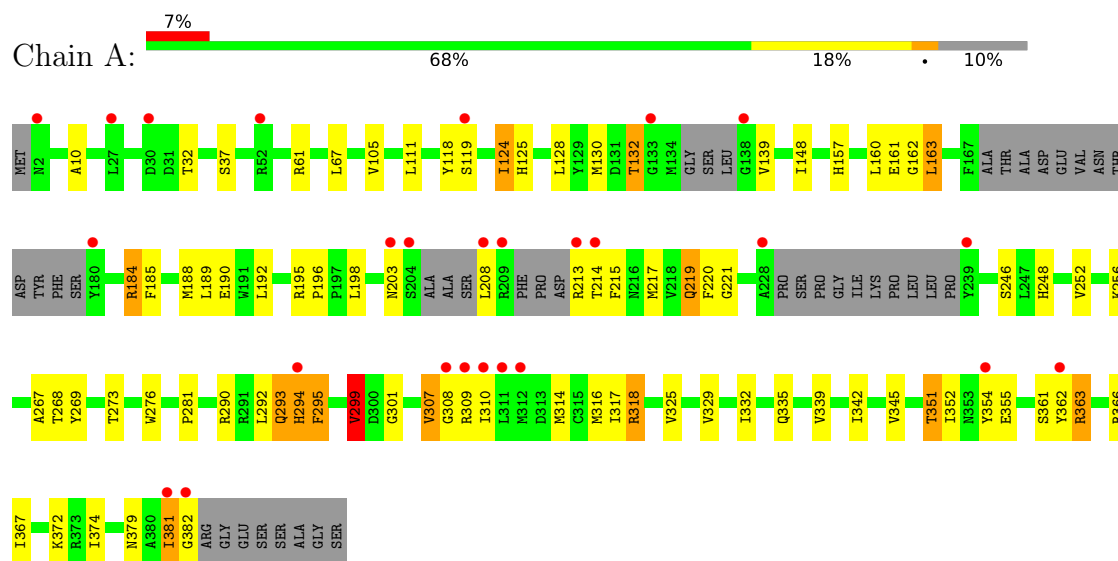
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	105	Total	O	0	0
			105	105		
2	B	88	Total	O	0	0
			88	88		
2	C	78	Total	O	0	0
			78	78		

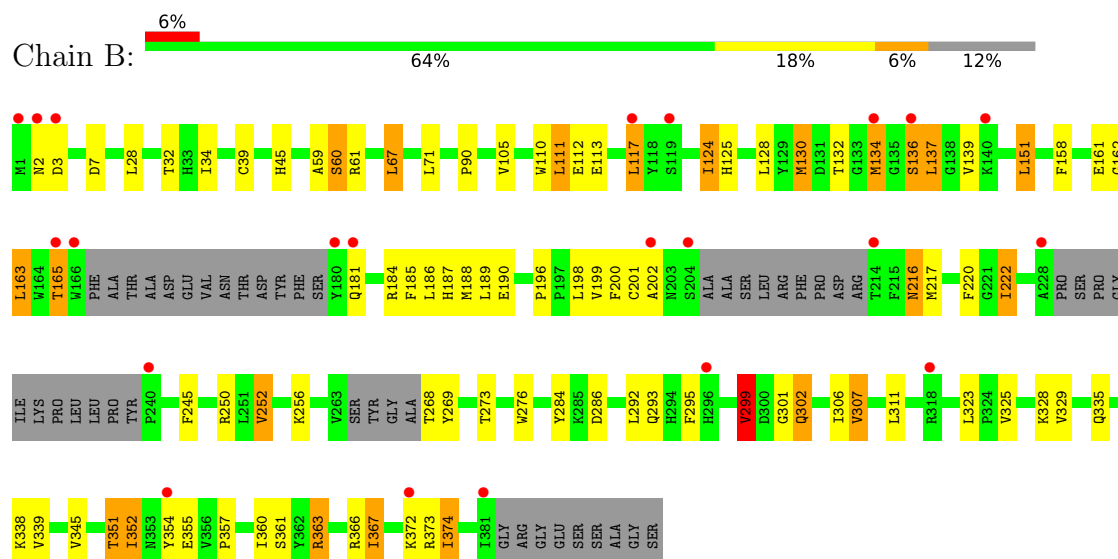
3 Residue-property plots [i](#)

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.

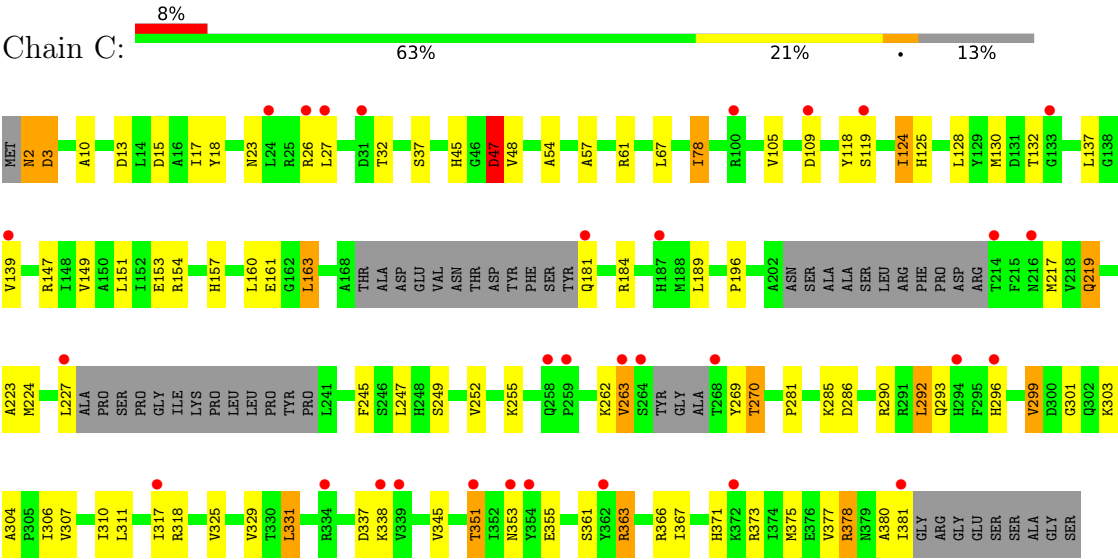
- Molecule 1: Engineered protein



- Molecule 1: Engineered protein



- Molecule 1: Engineered protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	112.85Å 112.85Å 232.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.37 – 2.50 49.37 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.37-2.50) 99.7 (49.37-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	8.75 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.218 , 0.265 (Not available) , 0.257	Depositor DCC
R_{free} test set	2689 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8504	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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 [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.62	0/2854	0.93	2/3871 (0.1%)
1	B	0.61	0/2791	0.90	3/3783 (0.1%)
1	C	0.52	0/2786	0.84	0/3777
All	All	0.58	0/8431	0.89	5/11431 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	GLN	N-CA-C	-10.68	94.47	110.28
1	B	299	VAL	CB-CA-C	-6.23	100.44	110.28
1	B	302	GLN	N-CA-C	5.74	118.13	109.23
1	B	252	VAL	CB-CA-C	5.65	116.19	110.65
1	A	299	VAL	CB-CA-C	-5.50	102.30	110.33

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2786	0	2756	64	0
1	B	2726	0	2716	74	0
1	C	2721	0	2720	54	0
2	A	105	0	0	8	0
2	B	88	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	78	0	0	6	0
All	All	8504	0	8192	185	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 11.

All (185) 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:130:MET:O	1:B:165:THR:HG22	1.42	1.16
1:B:134:MET:HB2	1:B:181:GLN:NE2	1.64	1.09
1:A:381:ILE:HD11	2:A:439:HOH:O	1.58	1.03
1:B:128:LEU:HB3	1:B:130:MET:HE1	1.44	0.97
1:B:134:MET:CB	1:B:181:GLN:NE2	2.26	0.97
1:C:147:ARG:HG2	2:C:470:HOH:O	1.68	0.93
1:B:134:MET:HB2	1:B:181:GLN:HE22	1.31	0.92
1:A:132:THR:HG22	2:A:404:HOH:O	1.72	0.89
1:A:128:LEU:HB3	1:A:130:MET:CE	2.03	0.88
1:C:361:SER:OG	1:C:363:ARG:HG3	1.75	0.86
1:B:130:MET:O	1:B:165:THR:CG2	2.24	0.85
1:B:299:VAL:HG13	1:B:329:VAL:HG22	1.58	0.85
1:A:351:THR:HG21	1:A:355:GLU:OE2	1.79	0.83
1:B:374:ILE:HG22	2:B:429:HOH:O	1.78	0.82
1:B:351:THR:HG22	1:C:290:ARG:HH11	1.44	0.79
1:A:190:GLU:OE2	1:B:187:HIS:CE1	2.36	0.79
1:B:124:ILE:CD1	1:B:158:PHE:CD1	2.67	0.77
1:B:130:MET:HB2	1:B:165:THR:HG23	1.68	0.75
1:A:190:GLU:OE2	1:B:187:HIS:HE1	1.70	0.74
1:B:199:VAL:H	1:B:216:ASN:HD21	1.37	0.73
1:A:379:ASN:OD1	1:A:381:ILE:HG13	1.88	0.73
1:C:351:THR:HG21	1:C:355:GLU:OE2	1.88	0.73
1:A:293:GLN:O	1:A:294:HIS:HB2	1.89	0.72
1:B:199:VAL:H	1:B:216:ASN:ND2	1.88	0.72
1:B:132:THR:HG23	1:B:165:THR:HG21	1.73	0.71
1:A:128:LEU:HB3	1:A:130:MET:HE2	1.73	0.71
1:B:286:ASP:OD1	1:B:363:ARG:HD2	1.90	0.71
1:C:48:VAL:HG23	1:C:78:ILE:CD1	2.21	0.70
1:A:361:SER:OG	1:A:363:ARG:HG3	1.91	0.70
1:C:48:VAL:HG23	1:C:78:ILE:HD13	1.73	0.69
1:C:3:ASP:HB3	2:C:420:HOH:O	1.93	0.68
1:B:134:MET:HA	1:B:181:GLN:HE21	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:ASN:HB2	1:C:377:VAL:O	1.94	0.68
1:B:301:GLY:H	1:B:335:GLN:HE21	1.44	0.66
1:C:286:ASP:OD1	1:C:363:ARG:HD3	1.97	0.64
1:A:125:HIS:HD2	1:A:161:GLU:OE2	1.79	0.64
1:A:299:VAL:HG13	1:A:329:VAL:HG22	1.80	0.64
1:A:125:HIS:CD2	1:A:161:GLU:OE2	2.51	0.64
1:C:54:ALA:HB2	1:C:224:MET:CE	2.29	0.63
1:A:290:ARG:HA	1:A:310:ILE:HB	1.81	0.63
1:B:351:THR:HG21	1:B:355:GLU:OE2	1.99	0.63
1:C:363:ARG:HB3	1:C:381:ILE:HD11	1.81	0.62
1:B:136:SER:HB2	1:B:137:LEU:HD13	1.81	0.61
1:C:132:THR:O	1:C:181:GLN:HG2	2.01	0.61
1:B:124:ILE:HD11	1:B:158:PHE:CD1	2.36	0.61
1:C:125:HIS:HD2	1:C:161:GLU:OE2	1.83	0.60
1:A:163:LEU:HD13	1:A:192:LEU:HD11	1.83	0.60
1:A:37:SER:HB2	1:A:219:GLN:HE22	1.66	0.60
1:A:130:MET:HE3	1:A:163:LEU:HD11	1.82	0.60
1:A:301:GLY:H	1:A:335:GLN:HE21	1.49	0.59
1:A:61:ARG:NH2	1:A:161:GLU:OE1	2.35	0.59
1:B:3:ASP:HB3	2:B:486:HOH:O	2.03	0.59
1:B:130:MET:CB	1:B:165:THR:HG23	2.33	0.59
1:A:128:LEU:HD21	1:A:148:ILE:HG21	1.85	0.58
1:B:134:MET:CA	1:B:181:GLN:HE21	2.16	0.58
1:A:352:ILE:HD13	1:A:354:TYR:HB2	1.84	0.58
1:A:381:ILE:O	1:A:382:GLY:C	2.45	0.58
1:C:361:SER:HG	1:C:363:ARG:HG3	1.70	0.57
1:A:292:LEU:HD21	1:A:345:VAL:HG13	1.85	0.57
1:B:128:LEU:HB3	1:B:130:MET:CE	2.26	0.57
1:A:214:THR:HG22	2:A:412:HOH:O	2.04	0.57
1:B:201:CYS:O	1:B:202:ALA:HB3	2.04	0.57
1:A:293:GLN:HG3	1:A:308:GLY:O	2.04	0.57
1:C:10:ALA:HB3	1:C:366:ARG:HD2	1.85	0.57
1:C:61:ARG:HD2	2:C:462:HOH:O	2.04	0.57
1:B:39:CYS:SG	1:C:285:LYS:NZ	2.78	0.57
1:C:54:ALA:HB2	1:C:224:MET:HE1	1.87	0.56
1:B:222:ILE:HG12	1:B:354:TYR:CZ	2.40	0.56
1:A:293:GLN:O	1:A:294:HIS:CB	2.54	0.56
1:B:90:PRO:HD3	1:B:110:TRP:NE1	2.21	0.55
1:B:256:LYS:HD3	1:B:276:TRP:CH2	2.41	0.55
1:A:374:ILE:HG22	2:A:465:HOH:O	2.05	0.55
1:B:269:TYR:CE1	1:B:307:VAL:HG22	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLY:N	2:A:444:HOH:O	2.39	0.54
1:B:134:MET:CB	1:B:181:GLN:HE21	2.14	0.54
1:B:124:ILE:HD13	1:B:158:PHE:CD1	2.40	0.54
1:A:318:ARG:HD2	2:A:496:HOH:O	2.07	0.54
1:C:227:LEU:HD23	1:C:353:ASN:HD21	1.71	0.54
1:A:290:ARG:NH2	1:A:309:ARG:HD2	2.22	0.54
1:A:362:TYR:HD2	1:A:362:TYR:H	1.54	0.54
1:B:301:GLY:H	1:B:335:GLN:NE2	2.06	0.54
1:B:367:ILE:N	1:B:367:ILE:HD13	2.23	0.54
1:B:216:ASN:HD22	1:B:216:ASN:H	1.56	0.54
1:A:128:LEU:HD13	1:A:160:LEU:HD13	1.89	0.54
1:A:281:PRO:HA	1:A:314:MET:HG2	1.90	0.54
1:B:130:MET:CB	1:B:165:THR:CG2	2.86	0.54
1:C:304:ALA:HB1	1:C:318:ARG:O	2.08	0.53
1:B:351:THR:HG22	1:C:290:ARG:NH1	2.19	0.53
1:B:61:ARG:HD3	1:B:217:MET:SD	2.49	0.53
1:B:163:LEU:HB2	1:B:196:PRO:HG2	1.90	0.53
1:A:269:TYR:CD1	1:A:307:VAL:HG13	2.44	0.53
1:B:34:ILE:HB	1:B:59:ALA:HA	1.91	0.52
1:C:125:HIS:CD2	1:C:161:GLU:OE2	2.63	0.52
1:C:128:LEU:HB3	1:C:130:MET:CE	2.39	0.52
1:A:128:LEU:HD23	1:A:130:MET:HE1	1.92	0.52
1:B:128:LEU:CB	1:B:130:MET:HE1	2.29	0.52
1:C:154:ARG:HD2	2:C:416:HOH:O	2.10	0.52
1:C:292:LEU:HD21	1:C:345:VAL:HG13	1.90	0.52
1:C:375:MET:HE1	2:C:422:HOH:O	2.10	0.51
1:B:130:MET:HE3	1:B:163:LEU:CD2	2.41	0.51
1:C:303:LYS:HG3	1:C:338:LYS:HE3	1.93	0.51
1:A:190:GLU:CD	1:B:187:HIS:CE1	2.89	0.51
1:B:295:PHE:HB3	1:B:306:ILE:HD12	1.92	0.51
1:B:198:LEU:HA	1:B:216:ASN:HD21	1.77	0.50
1:A:381:ILE:CD1	2:A:439:HOH:O	2.37	0.50
1:C:54:ALA:HB2	1:C:224:MET:HE3	1.93	0.50
1:A:316:MET:HB3	2:A:464:HOH:O	2.11	0.50
1:B:184:ARG:O	1:B:188:MET:HG3	2.11	0.49
1:C:371:HIS:C	1:C:373:ARG:H	2.19	0.49
1:C:249:SER:OG	1:C:281:PRO:HD2	2.13	0.49
1:C:247:LEU:HG	1:C:331:LEU:HD23	1.94	0.49
1:A:213:ARG:C	1:A:214:THR:HG23	2.37	0.49
1:A:214:THR:HA	1:A:215:PHE:HB2	1.95	0.48
1:A:379:ASN:OD1	1:A:381:ILE:CG1	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:HIS:NE2	1:B:245:PHE:HB2	2.29	0.48
1:B:165:THR:OG1	1:B:185:PHE:CE1	2.65	0.48
1:B:124:ILE:HD11	1:B:158:PHE:CE1	2.48	0.48
1:A:362:TYR:CD2	1:A:362:TYR:N	2.80	0.47
1:C:47:ASP:HB3	1:C:48:VAL:H	1.41	0.47
1:C:2:ASN:HB3	1:C:3:ASP:H	1.53	0.47
1:B:60:SER:HB2	1:B:61:ARG:HG3	1.96	0.46
1:B:7:ASP:HB3	1:B:250:ARG:HB2	1.97	0.46
1:C:119:SER:O	1:C:157:HIS:CD2	2.68	0.46
1:A:61:ARG:HD3	1:A:217:MET:SD	2.55	0.46
1:A:119:SER:O	1:A:157:HIS:HD2	1.98	0.46
1:C:18:TYR:CD2	1:C:57:ALA:HB2	2.50	0.46
1:C:13:ASP:OD1	1:C:15:ASP:HB2	2.15	0.46
1:C:128:LEU:HB3	1:C:130:MET:HE2	1.97	0.46
1:C:263:VAL:HG22	1:C:269:TYR:HB3	1.97	0.46
1:A:246:SER:HB3	1:A:248:HIS:NE2	2.32	0.45
1:C:223:ALA:HA	1:C:227:LEU:HD12	1.98	0.45
1:A:301:GLY:H	1:A:335:GLN:NE2	2.14	0.45
1:B:128:LEU:HB2	1:B:163:LEU:HD22	1.98	0.45
1:C:163:LEU:HB2	1:C:196:PRO:HG3	1.98	0.45
1:A:128:LEU:HB3	1:A:130:MET:HE3	1.91	0.45
1:A:267:ALA:HB2	1:A:309:ARG:HG2	1.98	0.45
1:B:130:MET:HE3	1:B:163:LEU:CD1	2.46	0.45
1:A:130:MET:HE3	1:A:163:LEU:CD1	2.46	0.44
1:B:113:GLU:O	1:B:117:LEU:HG	2.18	0.44
1:B:124:ILE:CD1	1:B:158:PHE:HD1	2.23	0.44
1:B:352:ILE:H	1:B:352:ILE:HG13	1.43	0.44
1:A:332:ILE:HG21	1:A:342:ILE:HD13	1.99	0.44
1:B:162:GLY:HA2	1:B:198:LEU:O	2.17	0.44
1:C:61:ARG:HD3	1:C:217:MET:SD	2.58	0.44
1:C:378:ARG:HH11	1:C:380:ALA:HA	1.82	0.44
1:A:162:GLY:HA2	1:A:198:LEU:O	2.18	0.44
1:B:130:MET:HE3	1:B:163:LEU:HD21	1.99	0.44
1:A:10:ALA:HB3	1:A:366:ARG:HD2	2.00	0.43
1:C:23:ASN:O	1:C:26:ARG:HB3	2.18	0.43
1:C:45:HIS:NE2	1:C:245:PHE:HB2	2.33	0.43
1:B:28:LEU:HD12	1:B:34:ILE:HD11	2.00	0.43
1:A:267:ALA:HB2	1:A:309:ARG:CG	2.48	0.43
1:C:296:HIS:HB3	2:C:464:HOH:O	2.18	0.43
1:B:125:HIS:HD2	1:B:161:GLU:OE2	2.01	0.43
1:B:67:LEU:HD22	1:B:71:LEU:HG	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:222:ILE:H	1:B:222:ILE:HG13	1.64	0.43
1:A:290:ARG:HH21	1:A:309:ARG:HD2	1.83	0.43
1:C:262:LYS:HG2	1:C:270:THR:HG23	2.00	0.43
1:A:203:ASN:O	1:A:208:LEU:N	2.52	0.42
1:A:267:ALA:CB	1:A:309:ARG:HG2	2.49	0.42
1:B:111:LEU:HD23	1:B:111:LEU:HA	1.94	0.42
1:A:163:LEU:HD23	1:A:185:PHE:CZ	2.54	0.42
1:A:294:HIS:O	1:A:295:PHE:C	2.63	0.42
1:B:124:ILE:CD1	1:B:158:PHE:CE1	3.02	0.42
1:A:256:LYS:HD3	1:A:276:TRP:CZ2	2.55	0.42
1:C:378:ARG:NH1	1:C:380:ALA:HA	2.34	0.42
1:B:134:MET:CA	1:B:181:GLN:NE2	2.77	0.41
1:B:293:GLN:HB3	2:B:409:HOH:O	2.19	0.41
1:A:195:ARG:HA	1:A:196:PRO:HD3	1.93	0.41
1:B:292:LEU:HD21	1:B:345:VAL:HG13	2.02	0.41
1:C:128:LEU:HD13	1:C:160:LEU:CD1	2.50	0.41
1:C:306:ILE:HA	1:C:317:ILE:HG22	2.02	0.41
1:A:213:ARG:C	1:A:214:THR:CG2	2.93	0.41
1:C:299:VAL:HG13	1:C:329:VAL:HG22	2.02	0.41
1:B:200:PHE:HB3	1:B:217:MET:HB3	2.03	0.41
1:A:118:TYR:CD2	1:A:124:ILE:HD11	2.56	0.40
1:A:184:ARG:O	1:A:188:MET:HG3	2.20	0.40
1:C:118:TYR:CD2	1:C:124:ILE:HD11	2.56	0.40
1:B:28:LEU:HD12	1:B:34:ILE:CD1	2.51	0.40
1:C:37:SER:HB2	1:C:219:GLN:OE1	2.21	0.40
1:A:294:HIS:O	1:A:295:PHE:O	2.39	0.40
1:B:112:GLU:HG3	1:B:151:LEU:HD21	2.02	0.40
1:B:284:TYR:CD2	1:C:355:GLU:HG3	2.56	0.40
1:B:357:PRO:HA	1:B:360:ILE:HD12	2.02	0.40
1:C:149:VAL:O	1:C:153:GLU:HG3	2.21	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	338/390 (87%)	327 (97%)	7 (2%)	4 (1%)	10	20
1	B	334/390 (86%)	318 (95%)	16 (5%)	0	100	100
1	C	331/390 (85%)	313 (95%)	13 (4%)	5 (2%)	8	16
All	All	1003/1170 (86%)	958 (96%)	36 (4%)	9 (1%)	14	27

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	47	ASP
1	A	294	HIS
1	A	268	THR
1	C	263	VAL
1	C	301	GLY
1	C	293	GLN
1	A	295	PHE
1	A	372	LYS
1	C	3	ASP

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	289/325 (89%)	265 (92%)	24 (8%)	10	22
1	B	286/325 (88%)	243 (85%)	43 (15%)	3	6
1	C	287/325 (88%)	255 (89%)	32 (11%)	6	12
All	All	862/975 (88%)	763 (88%)	99 (12%)	5	11

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	THR

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Mol	Chain	Res	Type
1	A	67	LEU
1	A	105	VAL
1	A	111	LEU
1	A	124	ILE
1	A	132	THR
1	A	139	VAL
1	A	163	LEU
1	A	184	ARG
1	A	189	LEU
1	A	219	GLN
1	A	220	PHE
1	A	252	VAL
1	A	273	THR
1	A	299	VAL
1	A	307	VAL
1	A	317	ILE
1	A	318	ARG
1	A	325	VAL
1	A	339	VAL
1	A	351	THR
1	A	363	ARG
1	A	367	ILE
1	A	381	ILE
1	B	2	ASN
1	B	32	THR
1	B	60	SER
1	B	67	LEU
1	B	105	VAL
1	B	111	LEU
1	B	117	LEU
1	B	124	ILE
1	B	130	MET
1	B	134	MET
1	B	136	SER
1	B	137	LEU
1	B	139	VAL
1	B	151	LEU
1	B	163	LEU
1	B	165	THR
1	B	186	LEU
1	B	189	LEU
1	B	190	GLU

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Mol	Chain	Res	Type
1	B	216	ASN
1	B	220	PHE
1	B	222	ILE
1	B	252	VAL
1	B	268	THR
1	B	273	THR
1	B	299	VAL
1	B	302	GLN
1	B	307	VAL
1	B	311	LEU
1	B	323	LEU
1	B	325	VAL
1	B	328	LYS
1	B	338	LYS
1	B	339	VAL
1	B	351	THR
1	B	352	ILE
1	B	361	SER
1	B	363	ARG
1	B	366	ARG
1	B	367	ILE
1	B	372	LYS
1	B	373	ARG
1	B	374	ILE
1	C	2	ASN
1	C	17	ILE
1	C	27	LEU
1	C	32	THR
1	C	47	ASP
1	C	67	LEU
1	C	78	ILE
1	C	105	VAL
1	C	109	ASP
1	C	124	ILE
1	C	137	LEU
1	C	139	VAL
1	C	151	LEU
1	C	163	LEU
1	C	184	ARG
1	C	189	LEU
1	C	219	GLN
1	C	252	VAL

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Mol	Chain	Res	Type
1	C	255	LYS
1	C	270	THR
1	C	292	LEU
1	C	299	VAL
1	C	307	VAL
1	C	310	ILE
1	C	311	LEU
1	C	325	VAL
1	C	331	LEU
1	C	337	ASP
1	C	351	THR
1	C	363	ARG
1	C	367	ILE
1	C	378	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	125	HIS
1	A	157	HIS
1	A	187	HIS
1	A	203	ASN
1	A	219	GLN
1	A	258	GLN
1	A	335	GLN
1	B	98	GLN
1	B	99	GLN
1	B	125	HIS
1	B	157	HIS
1	B	181	GLN
1	B	187	HIS
1	B	216	ASN
1	B	258	GLN
1	B	293	GLN
1	B	335	GLN
1	B	348	HIS
1	C	5	HIS
1	C	125	HIS
1	C	157	HIS
1	C	258	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

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	350/390 (89%)	0.30	26 (7%)	20 18	20, 36, 62, 75	0
1	B	344/390 (88%)	0.30	22 (6%)	25 22	22, 38, 63, 107	0
1	C	341/390 (87%)	0.48	31 (9%)	15 13	25, 46, 74, 94	0
All	All	1035/1170 (88%)	0.36	79 (7%)	20 17	20, 40, 68, 107	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	180	TYR	5.3
1	A	382	GLY	5.1
1	C	263	VAL	5.1
1	A	228	ALA	5.0
1	B	214	THR	4.8
1	B	1	MET	4.7
1	A	239	TYR	4.6
1	A	209	ARG	4.5
1	B	134	MET	4.5
1	B	136	SER	4.4
1	C	214	THR	4.4
1	B	228	ALA	4.4
1	B	296	HIS	4.3
1	A	204	SER	4.3
1	A	213	ARG	4.2
1	B	166	TRP	4.1
1	A	294	HIS	4.1
1	A	311	LEU	4.0
1	B	240	PRO	4.0
1	A	312	MET	3.8
1	A	203	ASN	3.7
1	A	362	TYR	3.7
1	C	26	ARG	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	381	ILE	3.5
1	B	165	THR	3.5
1	C	227	LEU	3.5
1	C	264	SER	3.3
1	A	208	LEU	3.2
1	B	202	ALA	3.2
1	C	109	ASP	3.2
1	A	214	THR	3.1
1	A	52	ARG	3.1
1	B	117	LEU	3.0
1	A	180	TYR	3.0
1	C	362	TYR	3.0
1	B	3	ASP	2.9
1	B	318	ARG	2.8
1	C	133	GLY	2.8
1	A	138	GLY	2.7
1	C	296	HIS	2.7
1	C	259	PRO	2.7
1	C	294	HIS	2.7
1	C	31	ASP	2.7
1	B	372	LYS	2.7
1	C	339	VAL	2.7
1	A	2	ASN	2.6
1	B	181	GLN	2.6
1	A	30	ASP	2.6
1	A	27	LEU	2.6
1	C	119	SER	2.6
1	A	133	GLY	2.5
1	C	258	GLN	2.5
1	C	381	ILE	2.5
1	A	309	ARG	2.5
1	A	308	GLY	2.5
1	C	354	TYR	2.4
1	C	181	GLN	2.4
1	C	268	THR	2.4
1	C	338	LYS	2.4
1	C	139	VAL	2.3
1	A	119	SER	2.3
1	B	381	ILE	2.3
1	B	140	LYS	2.3
1	C	100	ARG	2.2
1	A	310	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	204	SER	2.2
1	C	372	LYS	2.2
1	C	351	THR	2.2
1	C	27	LEU	2.2
1	B	2	ASN	2.1
1	C	334	ARG	2.1
1	C	353	ASN	2.1
1	C	187	HIS	2.1
1	C	24	LEU	2.1
1	A	354	TYR	2.1
1	B	119	SER	2.1
1	C	216	ASN	2.0
1	C	317	ILE	2.0
1	B	354	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.