



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:51 PM UTC

PDB ID : 1NKV / pdb_00001nkv
Title : X-RAY STRUCTURE OF YJHP FROM E.COLI NORTHEAST STRUCTURAL GENOMICS RESEARCH CONSORTIUM (NESG) TARGET ER13
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Deposited on : 2003-01-03
Resolution : 2.90 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
Mogul : 2022.3.0, CSD as543be (2022)
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

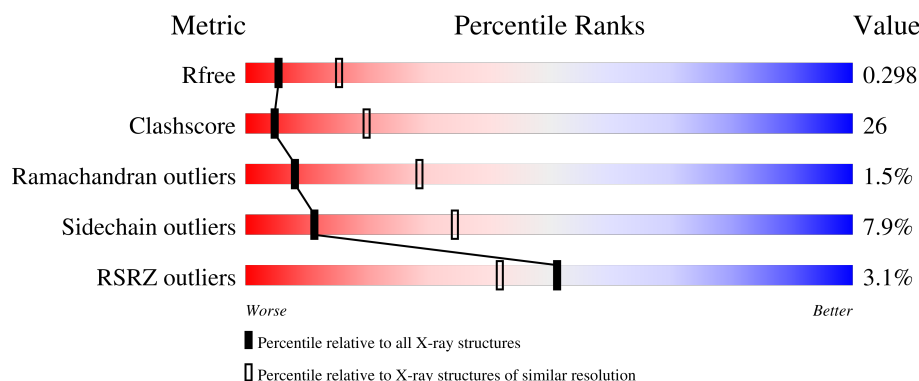
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	256	0% 55% 36% 5% .
1	B	256	5% 42% 43% 5% . 10%
1	C	256	2% 57% 36% 5% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 5760 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 HYPOTHETICAL PROTEIN yjhP.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	Se	0	0	0
			1899	1201	330	357	5	6			
1	B	231	Total	C	N	O	S	Se	0	0	0
			1805	1145	312	337	5	6			
1	C	249	Total	C	N	O	S	Se	0	0	0
			1945	1228	340	365	5	7			

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P39367
A	34	MSE	MET	modified residue	UNP P39367
A	50	MSE	MET	modified residue	UNP P39367
A	67	MSE	MET	modified residue	UNP P39367
A	136	MSE	MET	modified residue	UNP P39367
A	184	MSE	MET	modified residue	UNP P39367
A	203	MSE	MET	modified residue	UNP P39367
A	249	LEU	-	expression tag	UNP P39367
A	250	GLU	-	expression tag	UNP P39367
A	251	HIS	-	expression tag	UNP P39367
A	252	HIS	-	expression tag	UNP P39367
A	253	HIS	-	expression tag	UNP P39367
A	254	HIS	-	expression tag	UNP P39367
A	255	HIS	-	expression tag	UNP P39367
A	256	HIS	-	expression tag	UNP P39367
B	1	MSE	MET	modified residue	UNP P39367
B	34	MSE	MET	modified residue	UNP P39367
B	50	MSE	MET	modified residue	UNP P39367
B	67	MSE	MET	modified residue	UNP P39367
B	136	MSE	MET	modified residue	UNP P39367
B	184	MSE	MET	modified residue	UNP P39367
B	203	MSE	MET	modified residue	UNP P39367
B	249	LEU	-	expression tag	UNP P39367

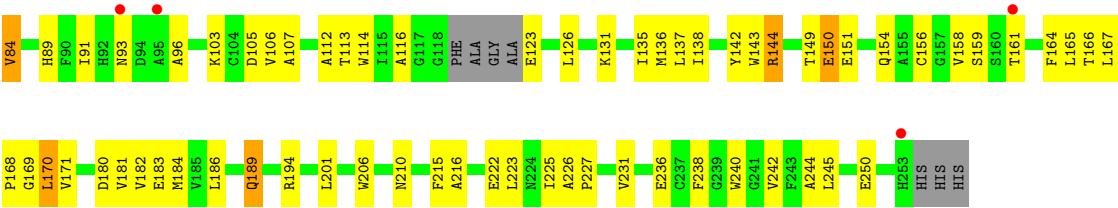
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Chain	Residue	Modelled	Actual	Comment	Reference
B	250	GLU	-	expression tag	UNP P39367
B	251	HIS	-	expression tag	UNP P39367
B	252	HIS	-	expression tag	UNP P39367
B	253	HIS	-	expression tag	UNP P39367
B	254	HIS	-	expression tag	UNP P39367
B	255	HIS	-	expression tag	UNP P39367
B	256	HIS	-	expression tag	UNP P39367
C	1	MSE	MET	modified residue	UNP P39367
C	34	MSE	MET	modified residue	UNP P39367
C	50	MSE	MET	modified residue	UNP P39367
C	67	MSE	MET	modified residue	UNP P39367
C	136	MSE	MET	modified residue	UNP P39367
C	184	MSE	MET	modified residue	UNP P39367
C	203	MSE	MET	modified residue	UNP P39367
C	249	LEU	-	expression tag	UNP P39367
C	250	GLU	-	expression tag	UNP P39367
C	251	HIS	-	expression tag	UNP P39367
C	252	HIS	-	expression tag	UNP P39367
C	253	HIS	-	expression tag	UNP P39367
C	254	HIS	-	expression tag	UNP P39367
C	255	HIS	-	expression tag	UNP P39367
C	256	HIS	-	expression tag	UNP P39367

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	44	Total O 44 44	0	0
2	B	26	Total O 26 26	0	0
2	C	41	Total O 41 41	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.97Å 54.42Å 118.33Å 90.00° 99.83° 90.00°	Depositor
Resolution (Å)	19.99 – 2.90 19.99 – 2.90	Depositor EDS
% Data completeness (in resolution range)	93.9 (19.99-2.90) 97.2 (19.99-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.87 (at 2.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.220 , 0.290 0.235 , 0.298	Depositor DCC
R_{free} test set	1773 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	43.4	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 24.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5760	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% 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	0.54	0/1937	0.90	2/2616 (0.1%)
1	B	0.54	1/1836 (0.1%)	0.96	5/2474 (0.2%)
1	C	0.57	1/1984 (0.1%)	0.93	3/2679 (0.1%)
All	All	0.55	2/5757 (0.0%)	0.93	10/7769 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	250	GLU	C-N	8.51	1.47	1.33
1	B	248	ARG	C-N	-6.99	1.23	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	87	ARG	N-CA-C	-12.11	98.69	114.31
1	A	15	ARG	N-CA-C	-6.22	106.23	113.88
1	C	144	ARG	N-CA-C	-6.16	104.56	111.28
1	B	234	ALA	N-CA-C	6.09	117.92	111.28
1	C	73	ALA	N-CA-C	-6.03	105.91	113.20
1	B	217	ALA	N-CA-C	-6.00	106.05	113.19
1	C	225	ILE	CB-CA-C	-5.47	104.71	110.62
1	B	219	VAL	N-CA-C	-5.36	104.39	111.09
1	B	28	LEU	N-CA-C	-5.22	105.49	111.07
1	A	69	SER	N-CA-C	-5.11	106.21	112.90

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	1899	0	1839	92	0
1	B	1805	0	1764	111	0
1	C	1945	0	1880	93	0
2	A	44	0	0	2	0
2	B	26	0	0	4	0
2	C	41	0	0	2	0
All	All	5760	0	5483	284	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 26.

All (284) 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:172:GLY:HA3	2:B:281:HOH:O	1.63	0.97
1:A:107:ALA:HB1	1:A:126:LEU:HD12	1.47	0.96
1:A:103:LYS:HE3	1:A:103:LYS:H	1.31	0.96
1:B:248:ARG:O	1:B:249:LEU:HB2	1.72	0.90
1:B:67:MSE:HB3	1:B:70:LEU:HD22	1.56	0.88
1:B:17:HIS:HE1	1:B:74:GLN:HE22	1.20	0.87
1:A:34:MSE:HE1	1:A:106:VAL:HG11	1.60	0.83
1:B:84:VAL:HG23	1:B:85:SER:H	1.43	0.83
1:C:18:ASN:ND2	1:C:20:PHE:HB2	1.94	0.82
1:C:166:THR:HG23	1:C:169:GLY:H	1.46	0.79
1:B:107:ALA:HB1	1:B:126:LEU:HD12	1.64	0.78
1:C:156:CYS:HB3	1:C:238:PHE:CZ	2.21	0.76
1:C:18:ASN:HD21	1:C:20:PHE:HB2	1.47	0.76
1:B:41:LEU:HB2	1:B:104:CYS:SG	2.27	0.75
1:B:40:ILE:HG12	1:B:106:VAL:HG13	1.68	0.75
1:C:78:ARG:HE	1:C:82:LEU:CD2	1.98	0.74
1:A:166:THR:HG23	1:A:169:GLY:H	1.51	0.74
1:A:50:MSE:HE1	1:A:110:VAL:HG21	1.70	0.74
1:A:40:ILE:HG12	1:A:106:VAL:CG1	2.18	0.73
1:A:156:CYS:SG	1:A:233:TYR:HB3	2.30	0.70
1:B:61:THR:HG22	1:B:62:GLY:H	1.56	0.70
1:B:72:THR:O	1:B:76:LYS:HG3	1.91	0.70
1:A:150:GLU:O	1:A:154:GLN:HG3	1.92	0.70
1:B:226:ALA:HB3	1:B:227:PRO:HD3	1.73	0.70
1:A:146:LEU:HD12	1:A:147:PRO:HD2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:18:ASN:HD22	1:C:20:PHE:H	1.40	0.69
1:B:56:ARG:HD3	1:B:82:LEU:HD12	1.75	0.68
1:B:72:THR:HG22	1:B:76:LYS:HE3	1.74	0.68
1:C:183:GLU:HB3	1:C:244:ALA:HB3	1.73	0.68
1:B:73:ALA:HA	1:B:76:LYS:HD2	1.76	0.68
1:B:126:LEU:HD22	1:B:126:LEU:H	1.59	0.67
1:A:18:ASN:ND2	1:A:20:PHE:HB2	2.09	0.67
1:B:23:GLU:HB2	2:B:268:HOH:O	1.95	0.66
1:C:136:MSE:HE3	1:C:138:ILE:HG21	1.76	0.66
1:B:136:MSE:HE2	1:B:245:LEU:HD12	1.78	0.66
1:C:78:ARG:HE	1:C:82:LEU:HD21	1.61	0.65
1:C:113:THR:HG23	1:C:116:ALA:H	1.61	0.65
1:A:136:MSE:HE3	1:A:138:ILE:HD11	1.79	0.65
1:A:25:TYR:HE1	1:A:50:MSE:HE3	1.60	0.64
1:B:35:LYS:HB2	1:B:36:PRO:HD2	1.79	0.64
1:B:194:ARG:HA	1:B:194:ARG:NE	2.13	0.64
1:C:5:ARG:HG3	1:C:9:ILE:HD13	1.80	0.64
1:A:74:GLN:HA	1:A:77:ARG:NH2	2.13	0.63
1:B:32:LEU:HD21	1:B:137:LEU:HD11	1.80	0.63
1:B:196:GLU:HG3	1:B:230:TYR:CD1	2.34	0.62
1:C:123:GLU:HG3	1:C:126:LEU:HD12	1.80	0.62
1:C:11:GLU:OE2	1:C:17:HIS:CD2	2.53	0.61
1:B:18:ASN:ND2	1:B:20:PHE:HB2	2.16	0.60
1:A:89:HIS:NE2	1:A:91:ILE:HG22	2.17	0.59
1:B:27:THR:O	1:B:31:VAL:HB	2.02	0.59
1:B:42:ASP:HB2	1:B:51:LEU:HD11	1.82	0.59
1:C:40:ILE:HG12	1:C:106:VAL:HB	1.84	0.59
1:C:5:ARG:HG2	1:C:215:PHE:CE2	2.38	0.59
1:A:63:THR:HA	1:A:89:HIS:O	2.03	0.59
1:A:194:ARG:HA	1:A:194:ARG:NE	2.18	0.59
1:C:6:ILE:HG13	1:C:7:PHE:H	1.68	0.58
1:A:171:VAL:HG21	1:C:231:VAL:HG21	1.85	0.58
1:B:201:LEU:O	1:B:205:ARG:HG2	2.04	0.58
1:A:34:MSE:CE	1:A:106:VAL:HG11	2.33	0.58
1:B:248:ARG:O	1:B:249:LEU:CB	2.45	0.58
1:A:25:TYR:CE1	1:A:50:MSE:HE3	2.38	0.58
1:A:67:MSE:O	1:A:92:HIS:NE2	2.38	0.57
1:B:40:ILE:HG22	1:B:41:LEU:N	2.20	0.57
1:A:136:MSE:HE3	1:A:138:ILE:CD1	2.35	0.57
1:B:6:ILE:HG21	1:B:222:GLU:HG3	1.88	0.56
1:B:40:ILE:HG23	1:B:106:VAL:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ILE:HD12	1:A:60:ILE:C	2.31	0.56
1:A:28:LEU:HD11	1:A:242:VAL:HG11	1.88	0.56
1:A:184:MSE:HE2	1:A:243:PHE:CE2	2.41	0.56
1:B:40:ILE:HG12	1:B:106:VAL:CG1	2.36	0.55
1:B:154:GLN:HA	1:B:158:VAL:O	2.06	0.55
1:B:64:GLY:O	1:B:65:ILE:HD13	2.05	0.55
1:C:144:ARG:HH12	1:C:236:GLU:HG3	1.71	0.55
1:A:50:MSE:CE	1:A:110:VAL:HG21	2.36	0.55
1:B:84:VAL:HG23	1:B:85:SER:N	2.18	0.55
1:C:56:ARG:HH11	1:C:56:ARG:HG2	1.72	0.55
1:A:40:ILE:HG12	1:A:106:VAL:HG13	1.87	0.54
1:C:156:CYS:HB3	1:C:238:PHE:CE1	2.42	0.54
1:C:31:VAL:O	1:C:33:ARG:HD3	2.07	0.54
1:A:199:LYS:O	1:A:203:MSE:HG3	2.07	0.54
1:A:23:GLU:CD	1:A:23:GLU:H	2.16	0.54
1:C:150:GLU:OE2	1:C:161:THR:HG22	2.08	0.54
1:B:156:CYS:HB3	1:B:238:PHE:CE1	2.43	0.54
1:B:78:ARG:O	1:B:82:LEU:HD23	2.07	0.54
1:B:131:LYS:HB2	1:B:132:PRO:HD2	1.89	0.54
1:C:77:ARG:O	1:C:77:ARG:HD3	2.08	0.54
1:A:231:VAL:HG21	1:B:171:VAL:HG21	1.89	0.53
1:B:40:ILE:HD11	1:B:60:ILE:CD1	2.39	0.53
1:C:206:TRP:HZ3	1:C:216:ALA:HA	1.72	0.53
1:C:25:TYR:CE1	1:C:50:MSE:HE2	2.43	0.53
1:C:32:LEU:HB3	1:C:34:MSE:HG3	1.91	0.53
1:B:28:LEU:HD22	1:B:32:LEU:HD22	1.88	0.53
1:C:55:ALA:O	1:C:59:GLY:HA2	2.09	0.53
1:A:40:ILE:HG22	1:A:41:LEU:N	2.24	0.53
1:A:65:ILE:N	1:A:65:ILE:HD12	2.23	0.53
1:A:109:CYS:HB2	1:A:126:LEU:HD21	1.90	0.53
1:A:21:THR:H	1:A:24:LYS:HB2	1.74	0.52
1:C:5:ARG:HG3	1:C:9:ILE:CD1	2.39	0.52
1:B:151:GLU:HG3	1:B:152:ILE:N	2.25	0.52
1:A:67:MSE:SE	1:A:94:ASP:HA	2.59	0.52
1:B:12:SER:HB3	1:B:202:THR:HG21	1.91	0.52
1:C:15:ARG:HG2	1:C:15:ARG:HH11	1.75	0.52
1:C:143:TRP:NE1	1:C:164:PHE:HB2	2.24	0.52
1:C:49:GLU:OE1	1:C:78:ARG:NH1	2.42	0.52
1:C:73:ALA:HA	1:C:76:LYS:HB2	1.92	0.52
1:C:38:THR:HG23	1:C:105:ASP:HB2	1.91	0.51
1:C:39:ARG:HG2	1:C:39:ARG:HH11	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ILE:O	1:C:91:ILE:HG13	2.10	0.51
1:B:151:GLU:HG3	1:B:152:ILE:H	1.76	0.51
1:C:63:THR:HA	1:C:89:HIS:O	2.10	0.51
1:C:166:THR:HG23	1:C:169:GLY:N	2.23	0.51
1:B:244:ALA:O	1:B:245:LEU:HD23	2.11	0.51
1:C:165:LEU:HD23	1:C:170:LEU:HA	1.93	0.51
1:C:138:ILE:HD11	1:C:245:LEU:HD11	1.93	0.51
1:B:54:TRP:O	1:B:58:HIS:HB2	2.10	0.51
1:C:78:ARG:HE	1:C:82:LEU:HD23	1.73	0.51
1:C:78:ARG:HH21	1:C:82:LEU:HD21	1.75	0.51
1:A:183:GLU:HB3	1:A:244:ALA:HB3	1.93	0.50
1:B:58:HIS:O	1:B:59:GLY:C	2.54	0.50
1:B:28:LEU:O	1:B:31:VAL:HG12	2.11	0.50
1:B:110:VAL:HG13	1:B:240:TRP:HH2	1.75	0.50
1:C:75:ALA:O	1:C:78:ARG:HB3	2.12	0.50
1:B:10:SER:O	1:B:199:LYS:HG2	2.12	0.50
1:B:175:ASP:C	1:B:177:LEU:H	2.20	0.50
1:B:40:ILE:HG22	1:B:41:LEU:H	1.75	0.50
1:B:140:GLU:CD	1:B:141:PRO:HD2	2.36	0.49
1:A:14:HIS:HA	2:A:298:HOH:O	2.12	0.49
1:A:183:GLU:HB3	1:A:244:ALA:CB	2.42	0.49
1:A:184:MSE:HE2	1:A:243:PHE:HE2	1.75	0.49
1:A:158:VAL:HG22	1:A:159:SER:H	1.78	0.49
1:A:89:HIS:CE1	1:A:91:ILE:HG22	2.48	0.49
1:A:60:ILE:O	1:A:87:ARG:HD2	2.13	0.49
1:A:106:VAL:HA	1:A:135:ILE:O	2.13	0.49
1:B:43:LEU:HD11	1:B:98:TYR:HD2	1.78	0.49
1:C:18:ASN:HD22	1:C:20:PHE:N	2.09	0.49
1:C:184:MSE:HE3	1:C:186:LEU:HD11	1.95	0.49
1:A:124:GLU:O	1:A:128:GLN:HG3	2.13	0.49
1:B:156:CYS:SG	1:B:233:TYR:HB3	2.52	0.49
1:C:39:ARG:HH12	1:C:61:THR:HG21	1.78	0.49
1:B:99:VAL:HG13	1:B:128:GLN:O	2.13	0.48
1:B:189:GLN:HE22	1:B:236:GLU:HG3	1.78	0.48
1:B:201:LEU:HB2	1:C:182:VAL:O	2.13	0.48
1:A:70:LEU:O	1:A:74:GLN:HG3	2.14	0.48
1:A:141:PRO:HB3	1:A:240:TRP:HD1	1.78	0.48
1:B:17:HIS:CE1	1:B:74:GLN:HE22	2.13	0.48
1:C:6:ILE:HG13	1:C:7:PHE:N	2.28	0.48
1:B:147:PRO:HG3	1:B:153:ALA:HB2	1.96	0.48
1:C:114:TRP:HA	2:C:258:HOH:O	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:THR:OG1	1:C:168:PRO:HD2	2.14	0.48
1:A:28:LEU:O	1:A:31:VAL:HG12	2.14	0.48
1:A:168:PRO:HA	1:A:171:VAL:HG22	1.95	0.48
1:B:173:ALA:O	1:B:177:LEU:HD23	2.14	0.48
1:A:5:ARG:HG2	1:A:5:ARG:O	2.14	0.47
1:C:65:ILE:HG23	1:C:93:ASN:HB3	1.96	0.47
1:B:203:MSE:SE	1:B:222:GLU:HB3	2.65	0.47
1:B:221:ALA:O	1:B:225:ILE:HG12	2.14	0.47
1:B:41:LEU:HG	1:B:43:LEU:CD2	2.44	0.47
1:A:200:TRP:CZ2	1:A:227:PRO:HA	2.50	0.47
1:B:167:LEU:N	1:B:168:PRO:HD2	2.30	0.47
1:A:144:ARG:N	1:A:237:CYS:O	2.48	0.47
1:C:189:GLN:HE21	1:C:189:GLN:HA	1.80	0.47
1:C:13:GLU:HB2	2:C:262:HOH:O	2.14	0.46
1:B:107:ALA:H	1:B:130:LEU:HD13	1.79	0.46
1:C:114:TRP:HB2	1:C:240:TRP:CD1	2.50	0.46
1:A:147:PRO:HG2	1:A:161:THR:HG22	1.96	0.46
1:B:3:ILE:HG23	1:B:3:ILE:O	2.15	0.46
1:B:143:TRP:NE1	1:B:164:PHE:HB2	2.30	0.46
1:A:10:SER:HB2	1:A:199:LYS:HB3	1.98	0.46
1:A:15:ARG:HG2	1:A:15:ARG:HH11	1.81	0.46
1:A:23:GLU:CD	1:A:23:GLU:N	2.74	0.46
1:B:150:GLU:O	1:B:154:GLN:HG3	2.15	0.46
1:C:180:ASP:O	1:C:182:VAL:HG13	2.15	0.46
1:A:215:PHE:O	1:A:219:VAL:HG23	2.16	0.46
1:C:66:ASP:HB3	1:C:72:THR:HG21	1.97	0.46
1:B:40:ILE:HD11	1:B:60:ILE:HD13	1.97	0.46
1:A:42:ASP:HB3	1:A:45:SER:HB3	1.98	0.46
1:A:166:THR:OG1	1:A:168:PRO:HD2	2.16	0.46
1:A:182:VAL:HB	1:C:201:LEU:HA	1.97	0.46
1:A:153:ALA:O	1:A:158:VAL:HG12	2.16	0.45
1:A:175:ASP:OD1	1:A:248:ARG:NH2	2.49	0.45
1:B:104:CYS:O	1:B:130:LEU:HD12	2.16	0.45
1:C:226:ALA:HB3	1:C:227:PRO:HD3	1.96	0.45
1:B:126:LEU:H	1:B:126:LEU:CD2	2.28	0.45
1:B:213:ASP:CG	1:B:214:ASP:N	2.74	0.45
1:C:84:VAL:HG22	1:C:84:VAL:O	2.16	0.45
1:A:167:LEU:N	1:A:168:PRO:HD2	2.31	0.45
1:B:38:THR:HB	1:B:60:ILE:CD1	2.46	0.45
1:B:126:LEU:HD22	1:B:126:LEU:N	2.30	0.45
1:C:103:LYS:HB2	1:C:131:LYS:HG2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:ILE:HG12	1:A:222:GLU:HG3	1.98	0.45
1:A:22:GLU:HB2	1:A:23:GLU:OE2	2.16	0.45
1:B:5:ARG:O	1:B:9:ILE:HG12	2.16	0.45
1:A:140:GLU:OE1	1:A:141:PRO:HD2	2.17	0.45
1:B:149:THR:OG1	1:B:152:ILE:HG12	2.16	0.45
1:A:15:ARG:NE	2:A:293:HOH:O	2.50	0.45
1:B:43:LEU:HD23	1:B:126:LEU:CD1	2.47	0.45
1:B:220:ARG:O	1:B:224:ASN:OD1	2.35	0.45
1:B:192:TRP:O	1:B:193:ASP:C	2.60	0.44
1:B:110:VAL:HG13	1:B:240:TRP:CH2	2.53	0.44
1:C:32:LEU:HD21	1:C:137:LEU:HD21	2.00	0.44
1:C:143:TRP:CE2	1:C:164:PHE:HB2	2.52	0.44
1:A:158:VAL:HG22	1:A:159:SER:N	2.32	0.44
1:C:107:ALA:HB1	1:C:126:LEU:HD22	1.98	0.44
1:C:15:ARG:HG2	1:C:15:ARG:NH1	2.33	0.44
1:A:18:ASN:HD22	1:A:20:PHE:HB2	1.79	0.44
1:C:123:GLU:CB	1:C:126:LEU:HD12	2.48	0.44
1:C:123:GLU:CG	1:C:126:LEU:HD12	2.47	0.44
1:A:108:ALA:HB2	1:A:137:LEU:HB2	2.00	0.44
1:B:194:ARG:NE	1:B:194:ARG:CA	2.80	0.44
1:B:17:HIS:HE1	1:B:74:GLN:NE2	2.02	0.44
1:C:194:ARG:HA	1:C:194:ARG:NE	2.33	0.44
1:B:231:VAL:HG21	1:C:171:VAL:HG21	2.00	0.44
1:C:53:THR:HG23	1:C:54:TRP:N	2.30	0.44
1:C:106:VAL:HG13	1:C:137:LEU:HD13	1.99	0.43
1:A:156:CYS:HB3	1:A:238:PHE:CE2	2.52	0.43
1:A:136:MSE:HE2	1:A:245:LEU:HD12	2.00	0.43
1:A:181:VAL:O	1:A:181:VAL:HG22	2.17	0.43
1:B:140:GLU:OE1	1:B:141:PRO:HD2	2.18	0.43
1:B:231:VAL:HG23	1:C:168:PRO:HA	2.00	0.43
1:C:38:THR:CG2	1:C:105:ASP:HB2	2.49	0.43
1:C:144:ARG:NH1	1:C:236:GLU:HG3	2.33	0.43
1:C:142:TYR:OH	1:C:186:LEU:HD22	2.17	0.43
1:A:89:HIS:NE2	1:A:91:ILE:CG2	2.81	0.43
1:B:192:TRP:CZ2	1:B:238:PHE:HB3	2.54	0.43
1:B:201:LEU:HA	1:C:182:VAL:HB	2.00	0.43
1:A:15:ARG:HG2	1:A:15:ARG:NH1	2.34	0.43
1:B:193:ASP:O	1:B:194:ARG:C	2.62	0.43
1:A:38:THR:HG23	1:A:105:ASP:CB	2.48	0.43
1:A:149:THR:OG1	1:A:152:ILE:HG13	2.18	0.43
1:B:43:LEU:H	1:B:43:LEU:HD22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ALA:C	1:B:157:GLY:N	2.75	0.43
1:A:126:LEU:C	1:A:128:GLN:N	2.77	0.43
1:A:38:THR:HG23	1:A:105:ASP:HB2	2.01	0.42
1:A:40:ILE:HG23	1:A:106:VAL:HG13	2.01	0.42
1:A:103:LYS:H	1:A:103:LYS:CE	2.16	0.42
1:A:231:VAL:HG21	1:B:171:VAL:CG2	2.49	0.42
1:C:136:MSE:HE2	1:C:138:ILE:HD13	2.00	0.42
1:A:61:THR:HG22	1:A:62:GLY:N	2.33	0.42
1:A:136:MSE:CE	1:A:245:LEU:HD12	2.49	0.42
1:B:47:SER:HA	1:B:74:GLN:HE21	1.84	0.42
1:A:32:LEU:HD23	1:A:34:MSE:SE	2.69	0.42
1:A:207:LEU:HD12	1:A:207:LEU:HA	1.89	0.42
1:A:232:THR:HA	1:B:168:PRO:HB3	2.02	0.42
1:C:5:ARG:O	1:C:9:ILE:HD13	2.20	0.42
1:B:41:LEU:HG	1:B:43:LEU:HD22	2.01	0.42
1:B:51:LEU:HD13	2:B:277:HOH:O	2.20	0.42
1:B:207:LEU:HD21	1:B:220:ARG:HA	2.01	0.42
1:C:50:MSE:O	1:C:53:THR:HG22	2.19	0.42
1:A:231:VAL:HG21	1:B:171:VAL:HG11	2.00	0.42
1:B:28:LEU:CD1	1:B:242:VAL:HG11	2.50	0.42
1:C:135:ILE:HG22	1:C:137:LEU:HD12	2.01	0.42
1:C:39:ARG:HG2	1:C:39:ARG:NH1	2.34	0.42
1:B:21:THR:H	1:B:24:LYS:HB2	1.85	0.42
1:C:65:ILE:HG22	1:C:93:ASN:O	2.20	0.42
1:A:31:VAL:HG22	1:A:183:GLU:OE2	2.20	0.42
1:C:154:GLN:HA	1:C:158:VAL:O	2.20	0.42
1:B:38:THR:HB	1:B:60:ILE:HG13	2.01	0.41
1:B:220:ARG:NE	1:B:224:ASN:OD1	2.48	0.41
1:C:77:ARG:HD3	1:C:77:ARG:C	2.45	0.41
1:A:125:LEU:O	1:A:128:GLN:HB2	2.20	0.41
1:C:226:ALA:HB3	1:C:227:PRO:CD	2.50	0.41
1:A:183:GLU:OE1	1:A:184:MSE:N	2.43	0.41
1:B:229:ARG:NH1	2:B:280:HOH:O	2.53	0.41
1:A:231:VAL:CG2	1:B:171:VAL:HG21	2.51	0.41
1:B:28:LEU:HD13	1:B:54:TRP:CZ2	2.55	0.41
1:B:200:TRP:CZ2	1:B:227:PRO:HA	2.56	0.41
1:C:28:LEU:HD11	1:C:242:VAL:HG11	2.02	0.41
1:C:56:ARG:HG2	1:C:56:ARG:NH1	2.34	0.41
1:C:56:ARG:NH1	1:C:57:ASP:OD1	2.53	0.41
1:B:108:ALA:HA	1:B:137:LEU:O	2.20	0.41
1:C:39:ARG:NH1	1:C:61:THR:HG21	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:ASP:C	1:A:177:LEU:H	2.29	0.41
1:B:147:PRO:CG	1:B:153:ALA:HB2	2.51	0.41
1:C:123:GLU:HB2	1:C:126:LEU:HB2	2.03	0.41
1:B:30:ARG:HG3	1:B:31:VAL:N	2.36	0.41
1:B:216:ALA:C	1:B:218:GLU:H	2.28	0.41
1:A:126:LEU:C	1:A:128:GLN:H	2.28	0.40
1:C:138:ILE:HD11	1:C:245:LEU:CD1	2.51	0.40
1:C:25:TYR:HE1	1:C:50:MSE:HE2	1.85	0.40
1:B:32:LEU:HD12	1:B:32:LEU:HA	1.90	0.40
1:B:213:ASP:CG	1:B:214:ASP:H	2.29	0.40
1:B:231:VAL:CG2	1:C:168:PRO:HA	2.51	0.40
1:C:149:THR:HG23	1:C:151:GLU:HB2	2.03	0.40
1:C:167:LEU:N	1:C:168:PRO:HD2	2.36	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	243/256 (95%)	213 (88%)	26 (11%)	4 (2%)	7	27
1	B	223/256 (87%)	187 (84%)	33 (15%)	3 (1%)	9	32
1	C	245/256 (96%)	219 (89%)	22 (9%)	4 (2%)	7	27
All	All	711/768 (93%)	619 (87%)	81 (11%)	11 (2%)	8	28

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	234	ALA
1	A	118	GLY
1	B	66	ASP
1	B	85	SER

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Mol	Chain	Res	Type
1	C	112	ALA
1	A	119	PHE
1	B	106	VAL
1	C	96	ALA
1	C	159	SER
1	A	112	ALA
1	C	84	VAL

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	191/195 (98%)	177 (93%)	14 (7%)	13	38
1	B	184/195 (94%)	168 (91%)	16 (9%)	9	30
1	C	198/195 (102%)	183 (92%)	15 (8%)	12	36
All	All	573/585 (98%)	528 (92%)	45 (8%)	11	34

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	PHE
1	A	25	TYR
1	A	28	LEU
1	A	63	THR
1	A	70	LEU
1	A	103	LYS
1	A	125	LEU
1	A	137	LEU
1	A	145	GLN
1	A	181	VAL
1	A	205	ARG
1	A	207	LEU
1	A	222	GLU
1	A	223	LEU
1	B	5	ARG

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Mol	Chain	Res	Type
1	B	28	LEU
1	B	31	VAL
1	B	32	LEU
1	B	63	THR
1	B	67	MSE
1	B	70	LEU
1	B	77	ARG
1	B	84	VAL
1	B	91	ILE
1	B	106	VAL
1	B	137	LEU
1	B	171	VAL
1	B	177	LEU
1	B	207	LEU
1	B	222	GLU
1	C	1	MSE
1	C	5	ARG
1	C	18	ASN
1	C	20	PHE
1	C	28	LEU
1	C	32	LEU
1	C	56	ARG
1	C	63	THR
1	C	150	GLU
1	C	170	LEU
1	C	181	VAL
1	C	189	GLN
1	C	210	ASN
1	C	222	GLU
1	C	223	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	HIS
1	A	18	ASN
1	A	154	GLN
1	A	189	GLN
1	A	224	ASN
1	B	17	HIS
1	B	74	GLN
1	B	154	GLN

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Mol	Chain	Res	Type
1	C	17	HIS
1	C	18	ASN
1	C	89	HIS
1	C	101	ASN
1	C	145	GLN
1	C	154	GLN
1	C	189	GLN
1	C	210	ASN
1	C	253	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	239/256 (93%)	0.08	2 (0%) 82 77	13, 30, 68, 72	0
1	B	225/256 (87%)	0.49	14 (6%) 26 21	14, 44, 89, 101	0
1	C	242/256 (94%)	0.28	6 (2%) 58 48	13, 37, 69, 82	0
All	All	706/768 (91%)	0.28	22 (3%) 51 42	13, 38, 79, 101	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	46	GLY	3.7
1	C	93	ASN	3.5
1	A	126	LEU	3.3
1	B	88	VAL	2.6
1	C	253	HIS	2.6
1	B	60	ILE	2.6
1	B	65	ILE	2.6
1	B	47	SER	2.5
1	B	99	VAL	2.5
1	C	95	ALA	2.5
1	C	72	THR	2.4
1	B	41	LEU	2.4
1	A	119	PHE	2.3
1	B	40	ILE	2.3
1	C	66	ASP	2.2
1	B	90	PHE	2.2
1	B	70	LEU	2.2
1	B	98	TYR	2.2
1	B	79	ALA	2.1
1	B	120	ALA	2.1
1	B	87	ARG	2.0
1	C	161	THR	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.