



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:23 AM UTC

PDB ID : 1YF2 / pdb_00001yf2
Title : Three-dimensional structure of DNA sequence specificity (S) subunit of a type I restriction-modification enzyme and its functional implications
Authors : Kim, J.S.; Degiovanni, A.; Jancarik, J.; Adams, P.D.; Yokota, H.A.; Kim, R.; Kim, S.H.; Berkeley Structural Genomics Center (BSGC)
Deposited on : 2004-12-30
Resolution : 2.40 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

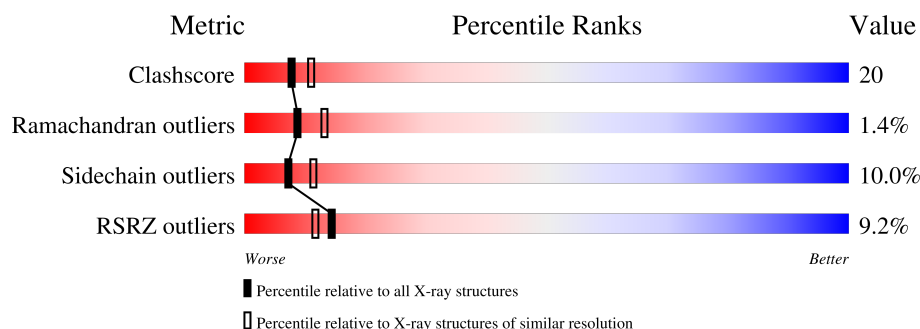
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	425	10% 58% 37% .
1	B	425	9% 59% 35% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7157 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 Type I restriction-modification enzyme, S subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	425	Total	C	N	O	S	0	0	0
			3412	2201	558	644	9			
1	B	425	Total	C	N	O	S	0	0	0
			3416	2204	559	644	9			

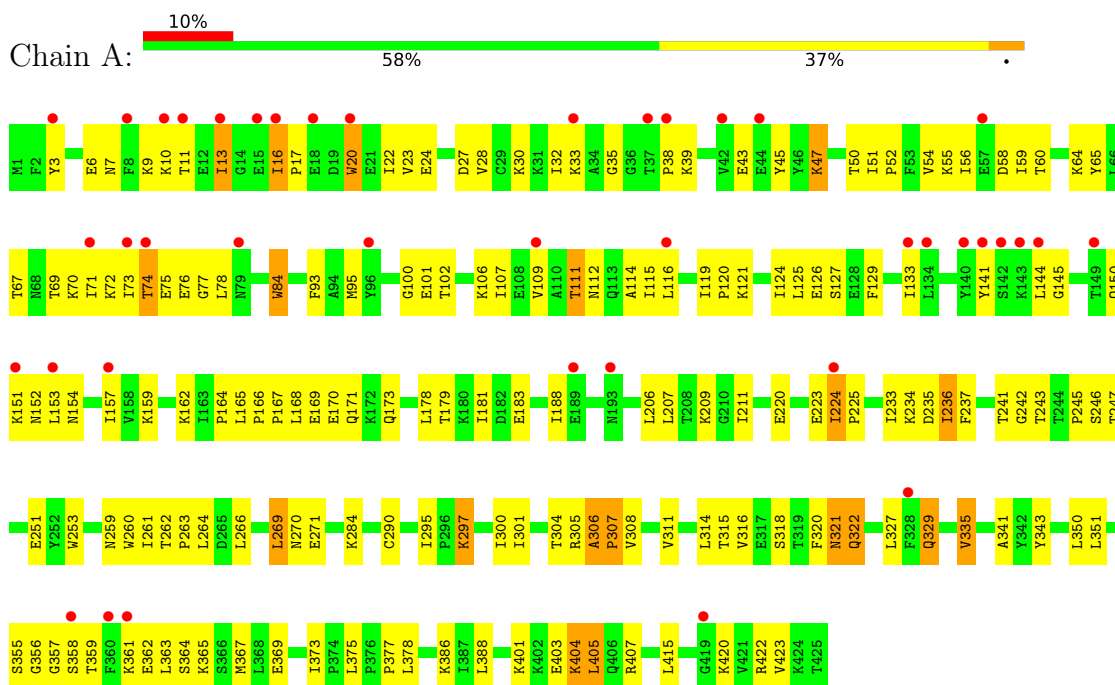
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	150	Total	O	0	0
			150	150		
2	B	179	Total	O	0	0
			179	179		

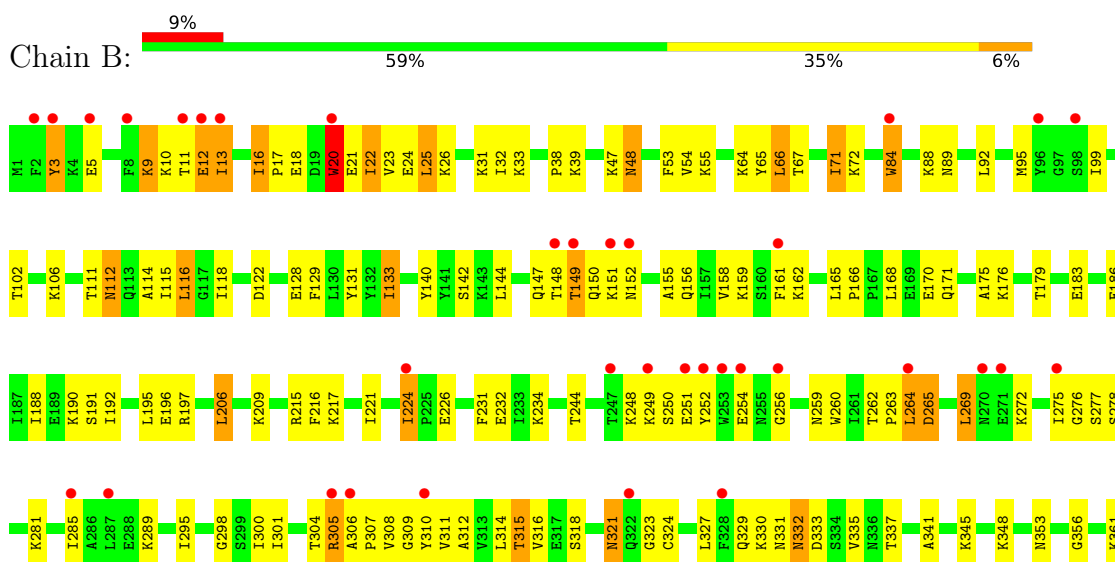
3 Residue-property plots

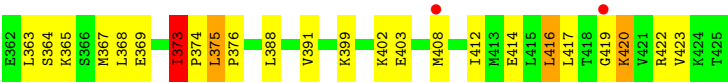
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Type I restriction-modification enzyme, S subunit



- Molecule 1: Type I restriction-modification enzyme, S subunit





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.97Å 94.22Å 103.52Å 90.00° 95.01° 90.00°	Depositor
Resolution (Å)	48.52 – 2.40 48.52 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.7 (48.52-2.40) 93.7 (48.52-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.65 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.279 0.234 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	57.3	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.3	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	0.94	EDS
Total number of atoms	7157	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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	0.71	1/3469 (0.0%)	0.90	3/4661 (0.1%)
1	B	0.75	0/3473	0.94	3/4665 (0.1%)
All	All	0.73	1/6942 (0.0%)	0.92	6/9326 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	236	ILE	CA-CB	5.86	1.61	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	341	ALA	N-CA-C	-6.72	103.89	111.14
1	A	341	ALA	N-CA-C	-6.42	104.20	111.07
1	A	261	ILE	N-CA-C	6.08	116.91	108.89
1	A	13	ILE	N-CA-C	-5.48	107.03	111.91
1	B	373	ILE	CA-C-N	5.17	125.07	119.85
1	B	373	ILE	C-N-CA	5.17	125.07	119.85

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	3412	0	3574	135	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3416	0	3585	144	0
2	A	150	0	0	3	0
2	B	179	0	0	2	0
All	All	7157	0	7159	278	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 20.

All (278) 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:269:LEU:HD21	1:B:275:ILE:HG22	1.45	0.96
1:A:329:GLN:OE1	1:A:329:GLN:N	1.99	0.95
1:A:70:LYS:HG3	1:A:71:ILE:HG13	1.53	0.90
1:B:275:ILE:HD11	1:B:314:LEU:HD12	1.56	0.88
1:A:329:GLN:H	1:A:329:GLN:CD	1.83	0.86
1:B:215:ARG:HD2	2:B:574:HOH:O	1.76	0.85
1:B:234:LYS:HB3	1:B:369:GLU:HB2	1.59	0.84
1:A:145:GLY:HA2	1:A:150:GLN:HA	1.60	0.83
1:B:12:GLU:HG2	1:B:22:ILE:HG21	1.61	0.82
1:B:269:LEU:HB2	1:B:272:LYS:HB2	1.61	0.82
1:A:16:ILE:HD11	1:A:164:PRO:HB3	1.63	0.80
1:A:306:ALA:HB1	1:A:307:PRO:CD	2.10	0.80
1:B:259:ASN:HB2	1:B:318:SER:CB	2.13	0.77
1:B:259:ASN:HB2	1:B:318:SER:HB2	1.64	0.77
1:B:112:ASN:C	1:B:112:ASN:HD22	1.93	0.77
1:A:154:ASN:H	1:A:157:ILE:HD12	1.51	0.76
1:A:129:PHE:O	1:A:133:ILE:HD13	1.87	0.75
1:B:10:LYS:HE2	1:B:18:GLU:HA	1.67	0.75
1:B:263:PRO:HG2	1:B:264:LEU:HD22	1.69	0.74
1:A:306:ALA:HB1	1:A:307:PRO:HD3	1.69	0.74
1:B:263:PRO:HG3	1:B:305:ARG:HD2	1.69	0.74
1:B:306:ALA:HB3	1:B:307:PRO:HD3	1.69	0.74
1:B:26:LYS:HB3	1:B:159:LYS:HB3	1.68	0.74
1:A:188:ILE:HD11	1:A:401:LYS:HE3	1.69	0.73
1:A:179:THR:O	1:A:183:GLU:HG3	1.89	0.72
1:A:30:LYS:HE2	1:A:119:ILE:HG21	1.70	0.72
1:A:9:LYS:HB2	1:A:16:ILE:O	1.90	0.71
1:B:365:LYS:O	1:B:369:GLU:HG2	1.91	0.71
1:A:55:LYS:HA	1:A:112:ASN:HD21	1.56	0.71
1:B:263:PRO:HG3	1:B:305:ARG:HH11	1.57	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:LYS:HA	1:A:112:ASN:ND2	2.08	0.69
1:B:304:THR:HG22	1:B:363:LEU:HB3	1.76	0.67
1:B:12:GLU:OE1	1:B:13:ILE:HG23	1.95	0.66
1:B:269:LEU:CD2	1:B:275:ILE:HG22	2.23	0.66
1:A:173:GLN:HB3	1:A:423:VAL:HG21	1.76	0.66
1:B:329:GLN:H	1:B:329:GLN:CD	2.04	0.65
1:B:234:LYS:O	1:B:330:LYS:HE3	1.97	0.64
1:A:266:LEU:O	1:A:269:LEU:HB2	1.97	0.64
1:A:22:ILE:HD12	1:A:22:ILE:H	1.63	0.64
1:A:121:LYS:HB2	1:A:124:ILE:HB	1.78	0.64
1:A:32:ILE:HD12	1:A:159:LYS:HG2	1.79	0.63
1:A:306:ALA:CB	1:A:307:PRO:CD	2.76	0.63
1:A:403:GLU:HB3	1:A:407:ARG:HH12	1.63	0.63
1:B:166:PRO:HG2	1:B:171:GLN:HG3	1.81	0.63
1:A:111:THR:HB	1:A:115:ILE:HB	1.81	0.63
1:B:231:PHE:CE1	1:B:375:LEU:HD12	2.34	0.63
1:A:13:ILE:HG21	1:A:162:LYS:HB3	1.81	0.63
1:A:59:ILE:HG22	1:A:101:GLU:HG3	1.81	0.63
1:B:16:ILE:HG23	1:B:20:TRP:HB2	1.80	0.62
1:A:236:ILE:CG2	1:A:335:VAL:HG21	2.29	0.62
1:B:259:ASN:ND2	1:B:277:SER:HA	2.14	0.62
1:B:221:ILE:HG13	1:B:224:ILE:HD13	1.82	0.62
1:B:231:PHE:HE1	1:B:375:LEU:HD12	1.65	0.61
1:A:404:LYS:HD2	1:A:405:LEU:N	2.16	0.61
1:A:236:ILE:HG21	1:A:335:VAL:HG21	1.83	0.61
1:B:306:ALA:HB3	1:B:307:PRO:CD	2.31	0.61
1:A:52:PRO:HG2	1:A:109:VAL:HG12	1.82	0.60
1:B:22:ILE:HD11	1:B:162:LYS:HD2	1.82	0.60
1:A:211:ILE:HD11	1:B:206:LEU:HD13	1.82	0.60
1:B:192:ILE:HD13	1:B:399:LYS:HG2	1.84	0.60
1:B:12:GLU:O	1:B:13:ILE:HG13	2.02	0.60
1:A:23:VAL:HG21	1:A:28:VAL:HG13	1.85	0.59
1:A:243:THR:HA	1:A:322:GLN:HG3	1.84	0.59
1:B:259:ASN:HB2	1:B:318:SER:HB3	1.84	0.59
1:B:20:TRP:CE2	1:B:166:PRO:HB3	2.37	0.59
1:B:20:TRP:CZ2	1:B:166:PRO:HB3	2.38	0.58
1:B:24:GLU:OE1	1:B:26:LYS:HE3	2.03	0.58
1:A:154:ASN:HB3	1:A:157:ILE:HG13	1.86	0.58
1:B:262:THR:HB	1:B:263:PRO:HD2	1.83	0.58
1:A:223:GLU:O	1:A:224:ILE:HD12	2.03	0.58
1:A:305:ARG:HG2	1:A:362:GLU:HG3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:329:GLN:NE2	1:B:332:ASN:HD22	2.02	0.58
1:B:275:ILE:HD11	1:B:314:LEU:CD1	2.29	0.58
1:A:74:THR:HG22	1:A:75:GLU:H	1.69	0.58
1:A:359:THR:HG23	2:A:514:HOH:O	2.05	0.57
1:B:22:ILE:C	1:B:22:ILE:HD13	2.28	0.57
1:B:275:ILE:HG13	1:B:275:ILE:O	2.03	0.57
1:A:188:ILE:HD13	1:A:401:LYS:HG2	1.86	0.57
1:B:20:TRP:HH2	1:B:170:GLU:OE1	1.88	0.57
1:A:67:THR:HG22	1:A:106:LYS:HB2	1.87	0.56
1:A:356:GLY:HA2	1:A:361:LYS:HG2	1.85	0.56
1:A:150:GLN:O	1:A:151:LYS:HD2	2.05	0.56
1:B:158:VAL:HG13	1:B:161:PHE:CZ	2.40	0.56
1:A:23:VAL:HG11	1:A:28:VAL:HG11	1.86	0.56
1:B:3:TYR:HB3	1:B:423:VAL:HA	1.88	0.56
1:B:329:GLN:CD	1:B:329:GLN:N	2.60	0.56
1:A:112:ASN:OD1	1:A:114:ALA:HB3	2.05	0.56
1:B:140:TYR:CE2	1:B:144:LEU:HD11	2.40	0.56
1:B:311:VAL:O	1:B:345:LYS:HE3	2.06	0.56
1:A:64:LYS:HE2	1:A:65:TYR:CZ	2.41	0.56
1:A:209:LYS:NZ	1:A:223:GLU:HB3	2.20	0.56
1:B:305:ARG:O	1:B:308:VAL:HG23	2.06	0.56
1:A:35:GLY:HA3	1:A:111:THR:O	2.06	0.55
1:B:54:VAL:HB	1:B:111:THR:HG22	1.87	0.55
1:B:95:MET:O	1:B:99:ILE:HG12	2.06	0.55
1:B:133:ILE:HD12	1:B:417:LEU:HD22	1.88	0.55
1:A:16:ILE:HG23	1:A:20:TRP:HB2	1.87	0.55
1:A:93:PHE:HE2	1:A:153:LEU:HD13	1.72	0.55
1:A:260:TRP:CZ2	1:A:321:ASN:HB3	2.42	0.55
1:B:17:PRO:HD3	1:B:419:GLY:CA	2.36	0.54
1:A:107:ILE:O	1:A:109:VAL:HG13	2.07	0.54
1:B:95:MET:SD	1:B:116:LEU:HD22	2.47	0.54
1:A:52:PRO:CG	1:A:109:VAL:HG12	2.38	0.54
1:A:95:MET:SD	1:A:116:LEU:HD13	2.48	0.54
1:A:23:VAL:HG22	1:A:24:GLU:N	2.23	0.54
1:A:20:TRP:CE2	1:A:166:PRO:HB3	2.43	0.53
1:B:129:PHE:CG	1:B:171:GLN:HG2	2.44	0.53
1:A:115:ILE:N	1:A:115:ILE:HD12	2.24	0.53
1:A:356:GLY:C	1:A:358:SER:H	2.16	0.53
1:A:73:ILE:HD11	1:A:77:GLY:C	2.34	0.53
1:B:217:LYS:HD3	1:B:226:GLU:HA	1.90	0.53
1:B:48:ASN:H	1:B:48:ASN:ND2	2.06	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LYS:HG3	1:A:235:ASP:N	2.24	0.52
1:B:311:VAL:HB	1:B:345:LYS:HG3	1.91	0.52
1:B:262:THR:H	1:B:265:ASP:HB2	1.75	0.51
1:B:414:GLU:OE2	1:B:420:LYS:HE2	2.11	0.51
1:A:43:GLU:HG2	1:A:47:LYS:HB2	1.92	0.51
1:A:93:PHE:CD1	1:A:102:THR:HG22	2.45	0.51
1:A:38:PRO:HG3	1:A:73:ILE:HD12	1.92	0.51
1:B:88:LYS:O	1:B:89:ASN:HB2	2.11	0.51
1:A:120:PRO:HB2	1:A:125:LEU:O	2.09	0.51
1:A:245:PRO:HG2	1:A:253:TRP:CZ2	2.46	0.50
1:B:112:ASN:C	1:B:112:ASN:ND2	2.63	0.50
1:B:232:GLU:OE1	1:B:234:LYS:HE2	2.11	0.50
1:A:32:ILE:HB	1:A:159:LYS:HE3	1.93	0.50
1:A:126:GLU:H	1:A:171:GLN:NE2	2.09	0.50
1:A:304:THR:HG22	1:A:363:LEU:HB3	1.93	0.50
1:A:224:ILE:HD11	2:A:435:HOH:O	2.12	0.50
1:B:264:LEU:HD22	1:B:264:LEU:H	1.76	0.50
1:B:305:ARG:HB2	1:B:323:GLY:HA3	1.93	0.50
1:B:151:LYS:O	1:B:152:ASN:HB2	2.12	0.50
1:A:363:LEU:HD23	1:A:367:MET:HB2	1.93	0.50
1:A:28:VAL:HG11	1:A:165:LEU:HD22	1.94	0.50
1:A:304:THR:O	1:A:362:GLU:HA	2.12	0.50
1:B:92:LEU:O	1:B:102:THR:HA	2.12	0.50
1:A:270:ASN:O	1:A:271:GLU:HB2	2.12	0.49
1:A:20:TRP:N	1:A:20:TRP:HE3	2.09	0.49
1:A:93:PHE:HD1	1:A:102:THR:HG22	1.76	0.49
1:B:298:GLY:O	1:B:337:THR:HG21	2.13	0.49
1:A:415:LEU:HA	1:A:420:LYS:HG3	1.94	0.49
1:A:55:LYS:HG2	1:A:112:ASN:HD22	1.76	0.49
1:B:155:ALA:O	1:B:159:LYS:HG3	2.13	0.49
1:A:259:ASN:HB2	1:A:318:SER:HB2	1.94	0.49
1:A:351:LEU:HD22	1:A:363:LEU:HD11	1.95	0.49
1:B:263:PRO:CG	1:B:305:ARG:HD2	2.41	0.49
1:A:6:GLU:OE2	1:A:420:LYS:HA	2.12	0.48
1:B:364:SER:OG	1:B:367:MET:HE3	2.14	0.48
1:A:52:PRO:HB3	1:A:69:THR:HG21	1.95	0.48
1:A:297:LYS:HB2	1:A:297:LYS:NZ	2.29	0.48
1:B:48:ASN:H	1:B:48:ASN:HD22	1.62	0.48
1:B:197:ARG:HG3	2:B:572:HOH:O	2.13	0.48
1:B:221:ILE:HD12	1:B:374:PRO:HG3	1.94	0.48
1:B:38:PRO:O	1:B:39:LYS:C	2.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ILE:N	1:A:115:ILE:HD11	2.29	0.47
1:A:356:GLY:HA3	1:A:361:LYS:HE2	1.95	0.47
1:B:149:THR:HB	1:B:151:LYS:HG3	1.96	0.47
1:B:186:GLU:HG3	1:B:190:LYS:NZ	2.29	0.47
1:A:45:TYR:CE1	1:A:76:GLU:HG2	2.49	0.47
1:B:256:GLY:HA3	1:B:281:LYS:HB2	1.95	0.47
1:B:300:ILE:HB	1:B:327:LEU:HB2	1.97	0.47
1:A:401:LYS:O	1:A:404:LYS:HG3	2.14	0.47
1:B:301:ILE:HD11	1:B:324:CYS:HB3	1.95	0.47
1:A:24:GLU:HB2	1:A:27:ASP:OD2	2.15	0.47
1:A:364:SER:HB3	1:A:367:MET:HE3	1.97	0.47
1:B:17:PRO:HD3	1:B:419:GLY:HA2	1.95	0.47
1:B:158:VAL:HA	1:B:161:PHE:CE2	2.50	0.47
1:A:126:GLU:H	1:A:171:GLN:HE22	1.61	0.47
1:B:263:PRO:HG3	1:B:305:ARG:NH1	2.28	0.46
1:A:60:THR:HA	1:A:101:GLU:OE1	2.15	0.46
1:B:23:VAL:O	1:B:162:LYS:HA	2.14	0.46
1:B:25:LEU:HD22	1:B:161:PHE:CE1	2.50	0.46
1:B:275:ILE:HG23	1:B:312:ALA:HB1	1.97	0.46
1:B:20:TRP:CH2	1:B:170:GLU:OE1	2.67	0.46
1:B:64:LYS:HD3	1:B:65:TYR:CE1	2.51	0.46
1:A:245:PRO:HB3	1:A:290:CYS:SG	2.56	0.46
1:B:129:PHE:CZ	1:B:133:ILE:HD13	2.50	0.46
1:B:331:ASN:HD21	1:B:333:ASP:HB2	1.80	0.46
1:B:64:LYS:HG3	1:B:131:TYR:CZ	2.51	0.46
1:B:250:SER:C	1:B:252:TYR:H	2.23	0.46
1:A:262:THR:HB	1:A:263:PRO:HD2	1.98	0.46
1:B:3:TYR:CB	1:B:422:ARG:O	2.64	0.46
1:A:58:ASP:OD2	1:A:69:THR:HA	2.16	0.46
1:B:158:VAL:HG13	1:B:161:PHE:HZ	1.79	0.46
1:B:264:LEU:HD22	1:B:264:LEU:N	2.30	0.46
1:B:252:TYR:OH	1:B:289:LYS:HD3	2.16	0.46
1:B:276:GLY:O	1:B:316:VAL:HG12	2.16	0.46
1:B:179:THR:O	1:B:183:GLU:HG3	2.16	0.45
1:B:112:ASN:ND2	1:B:114:ALA:H	2.14	0.45
1:B:251:GLU:O	1:B:285:ILE:HD12	2.16	0.45
1:A:38:PRO:HG3	1:A:73:ILE:CD1	2.46	0.45
1:A:51:ILE:HD13	1:A:78:LEU:HD22	1.98	0.45
1:A:365:LYS:HE2	1:A:369:GLU:OE2	2.16	0.45
1:B:305:ARG:HB2	1:B:323:GLY:CA	2.47	0.45
1:A:24:GLU:O	1:A:28:VAL:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:ALA:O	1:A:308:VAL:N	2.50	0.45
1:B:9:LYS:HA	1:B:17:PRO:HA	1.98	0.45
1:B:66:LEU:C	1:B:66:LEU:HD13	2.41	0.45
1:A:245:PRO:O	1:A:246:SER:C	2.60	0.45
1:A:17:PRO:HG2	1:A:20:TRP:CD2	2.51	0.45
1:A:71:ILE:HG22	1:A:72:LYS:N	2.32	0.45
1:A:125:LEU:HA	1:A:171:GLN:HE22	1.81	0.45
1:B:54:VAL:HG12	1:B:115:ILE:HD13	1.99	0.45
1:A:33:LYS:O	1:A:84:TRP:CH2	2.70	0.44
1:B:412:ILE:HG23	1:B:416:LEU:CD2	2.47	0.44
1:A:300:ILE:HB	1:A:327:LEU:HB2	1.99	0.44
1:B:129:PHE:CD2	1:B:171:GLN:HG2	2.53	0.44
1:B:248:LYS:O	1:B:250:SER:N	2.49	0.44
1:B:188:ILE:HG21	1:B:402:LYS:HB2	1.99	0.44
1:A:295:ILE:HG13	1:A:314:LEU:CD2	2.48	0.44
1:A:52:PRO:CB	1:A:69:THR:HG21	2.47	0.44
1:B:151:LYS:O	1:B:152:ASN:CB	2.66	0.44
1:B:399:LYS:O	1:B:403:GLU:HG3	2.17	0.44
1:B:305:ARG:CG	1:B:306:ALA:H	2.31	0.44
1:A:403:GLU:HB3	1:A:407:ARG:NH1	2.30	0.44
1:B:374:PRO:C	1:B:376:PRO:HD3	2.43	0.44
1:B:305:ARG:O	1:B:306:ALA:C	2.61	0.43
1:B:321:ASN:C	1:B:321:ASN:ND2	2.76	0.43
1:A:242:GLY:O	1:A:243:THR:HG23	2.18	0.43
1:A:75:GLU:O	1:A:78:LEU:HB3	2.18	0.43
1:B:140:TYR:O	1:B:144:LEU:HG	2.18	0.43
1:A:166:PRO:HG2	1:A:171:GLN:CG	2.48	0.43
1:A:6:GLU:HB3	1:A:9:LYS:NZ	2.33	0.43
1:B:419:GLY:O	1:B:420:LYS:C	2.62	0.43
1:B:186:GLU:HG3	1:B:190:LYS:HZ2	1.82	0.43
1:A:167:PRO:HD2	1:A:170:GLU:OE1	2.19	0.42
1:B:209:LYS:HG3	1:B:216:PHE:CE2	2.54	0.42
1:A:233:ILE:HD13	1:A:373:ILE:HD13	2.00	0.42
1:B:95:MET:CE	1:B:116:LEU:HD13	2.49	0.42
1:B:188:ILE:O	1:B:191:SER:HB3	2.19	0.42
1:B:295:ILE:HG13	1:B:314:LEU:HD22	2.00	0.42
1:B:373:ILE:HA	1:B:374:PRO:HD3	1.84	0.42
1:B:353:ASN:O	1:B:356:GLY:N	2.51	0.42
1:A:377:PRO:O	1:A:378:LEU:C	2.63	0.42
1:B:53:PHE:HB3	1:B:71:ILE:HG22	2.01	0.42
1:A:166:PRO:HG2	1:A:171:GLN:HG3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ILE:HD11	1:B:162:LYS:HB3	2.01	0.42
1:B:128:GLU:HB3	1:B:175:ALA:HB1	2.00	0.42
1:B:55:LYS:C	1:B:115:ILE:HD11	2.44	0.42
1:B:309:GLY:HA3	1:B:348:LYS:HG3	2.01	0.42
1:B:329:GLN:HE21	1:B:332:ASN:HD22	1.66	0.42
1:B:32:ILE:O	1:B:32:ILE:HG22	2.19	0.42
1:B:106:LYS:HE3	1:B:106:LYS:HB3	1.84	0.42
1:A:207:LEU:HD13	1:A:343:TYR:HA	2.02	0.41
1:B:33:LYS:HB3	1:B:84:TRP:CZ3	2.54	0.41
1:B:361:LYS:HD2	1:B:361:LYS:N	2.35	0.41
1:A:242:GLY:HA3	1:A:320:PHE:O	2.20	0.41
1:A:355:SER:C	1:A:357:GLY:H	2.28	0.41
1:B:32:ILE:HG12	1:B:118:ILE:HG23	2.02	0.41
1:B:259:ASN:HD22	1:B:278:SER:H	1.68	0.41
1:B:148:THR:C	1:B:150:GLN:H	2.28	0.41
1:A:45:TYR:HE1	1:A:76:GLU:HG2	1.85	0.41
1:A:50:THR:HG23	1:A:51:ILE:HG13	2.01	0.41
1:B:12:GLU:O	1:B:13:ILE:C	2.63	0.41
1:B:251:GLU:HA	1:B:254:GLU:CG	2.51	0.41
1:B:304:THR:CG2	1:B:363:LEU:HB3	2.47	0.41
1:B:21:GLU:O	1:B:165:LEU:HB3	2.20	0.41
1:A:30:LYS:HE2	1:A:119:ILE:CG2	2.45	0.41
1:A:95:MET:HB3	1:A:153:LEU:O	2.20	0.41
1:A:350:LEU:HD23	1:A:350:LEU:O	2.20	0.41
1:B:244:THR:HG23	1:B:260:TRP:CZ2	2.55	0.41
1:A:178:LEU:HD23	1:A:181:ILE:HD12	2.03	0.41
1:B:16:ILE:HG23	1:B:20:TRP:CB	2.48	0.41
1:A:51:ILE:HB	1:A:73:ILE:HG23	2.03	0.41
1:A:100:GLY:O	1:A:102:THR:HG23	2.21	0.41
1:A:111:THR:CB	1:A:115:ILE:HB	2.48	0.41
1:A:141:TYR:O	1:A:144:LEU:HG	2.21	0.41
1:B:275:ILE:HD13	1:B:301:ILE:HG21	2.03	0.41
1:A:51:ILE:O	1:A:73:ILE:HG22	2.21	0.41
1:A:224:ILE:HG23	1:A:225:PRO:N	2.35	0.41
1:A:3:TYR:CB	1:A:422:ARG:HB2	2.51	0.40
1:A:173:GLN:NE2	1:A:423:VAL:HG11	2.37	0.40
1:A:54:VAL:HG21	1:A:109:VAL:HG21	2.03	0.40
1:A:356:GLY:C	1:A:358:SER:N	2.79	0.40
1:A:290:CYS:SG	2:A:432:HOH:O	2.63	0.40
1:B:275:ILE:O	1:B:315:THR:HB	2.20	0.40
1:A:13:ILE:HG23	1:A:22:ILE:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:PHE:CE2	1:A:329:GLN:HG3	2.56	0.40
1:B:307:PRO:HB2	1:B:310:TYR:HE1	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	423/425 (100%)	378 (89%)	38 (9%)	7 (2%)	7	10
1	B	423/425 (100%)	379 (90%)	39 (9%)	5 (1%)	10	16
All	All	846/850 (100%)	757 (90%)	77 (9%)	12 (1%)	9	13

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	152	ASN
1	B	47	LYS
1	B	420	LYS
1	A	11	THR
1	A	39	LYS
1	A	306	ALA
1	B	12	GLU
1	B	249	LYS
1	A	10	LYS
1	B	20	TRP
1	A	47	LYS
1	A	307	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	385/387 (100%)	353 (92%)	32 (8%)	10	17
1	B	386/387 (100%)	341 (88%)	45 (12%)	5	7
All	All	771/774 (100%)	694 (90%)	77 (10%)	7	11

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	16	ILE
1	A	20	TRP
1	A	74	THR
1	A	84	TRP
1	A	111	THR
1	A	127	SER
1	A	168	LEU
1	A	169	GLU
1	A	206	LEU
1	A	220	GLU
1	A	224	ILE
1	A	241	THR
1	A	247	THR
1	A	251	GLU
1	A	264	LEU
1	A	269	LEU
1	A	284	LYS
1	A	297	LYS
1	A	301	ILE
1	A	311	VAL
1	A	315	THR
1	A	316	VAL
1	A	321	ASN
1	A	322	GLN
1	A	329	GLN
1	A	335	VAL

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Mol	Chain	Res	Type
1	A	375	LEU
1	A	386	LYS
1	A	388	LEU
1	A	404	LYS
1	A	405	LEU
1	B	3	TYR
1	B	5	GLU
1	B	9	LYS
1	B	11	THR
1	B	13	ILE
1	B	16	ILE
1	B	20	TRP
1	B	22	ILE
1	B	25	LEU
1	B	31	LYS
1	B	48	ASN
1	B	66	LEU
1	B	67	THR
1	B	71	ILE
1	B	72	LYS
1	B	84	TRP
1	B	112	ASN
1	B	116	LEU
1	B	122	ASP
1	B	133	ILE
1	B	142	SER
1	B	147	GLN
1	B	149	THR
1	B	156	GLN
1	B	168	LEU
1	B	176	LYS
1	B	195	LEU
1	B	196	GLU
1	B	206	LEU
1	B	224	ILE
1	B	264	LEU
1	B	265	ASP
1	B	269	LEU
1	B	305	ARG
1	B	315	THR
1	B	321	ASN
1	B	332	ASN

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Mol	Chain	Res	Type
1	B	335	VAL
1	B	368	LEU
1	B	373	ILE
1	B	375	LEU
1	B	388	LEU
1	B	391	VAL
1	B	408	MET
1	B	416	LEU

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	80	ASN
1	A	89	ASN
1	A	139	ASN
1	A	171	GLN
1	A	255	ASN
1	A	270	ASN
1	A	321	ASN
1	A	400	GLN
1	A	406	GLN
1	B	48	ASN
1	B	68	ASN
1	B	112	ASN
1	B	147	GLN
1	B	152	ASN
1	B	173	GLN
1	B	204	HIS
1	B	255	ASN
1	B	259	ASN
1	B	331	ASN
1	B	332	ASN
1	B	353	ASN
1	B	400	GLN

5.3.3 RNA ⓘ

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	425/425 (100%)	0.70	41 (9%)	13 10	37, 73, 144, 187	0
1	B	425/425 (100%)	0.55	37 (8%)	16 13	38, 62, 114, 154	0
All	All	850/850 (100%)	0.63	78 (9%)	14 12	37, 66, 128, 187	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	419	GLY	5.3
1	A	361	LYS	4.6
1	B	328	PHE	4.5
1	B	149	THR	4.4
1	A	8	PHE	4.4
1	B	98	SER	4.3
1	A	3	TYR	4.0
1	A	328	PHE	3.9
1	B	2	PHE	3.9
1	B	152	ASN	3.8
1	B	161	PHE	3.7
1	A	18	GLU	3.7
1	A	360	PHE	3.7
1	A	74	THR	3.6
1	B	264	LEU	3.5
1	B	322	GLN	3.5
1	A	11	THR	3.3
1	B	11	THR	3.3
1	B	12	GLU	3.2
1	B	419	GLY	3.2
1	B	151	LYS	3.2
1	B	305	ARG	3.1
1	A	13	ILE	3.0
1	B	20	TRP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	109	VAL	3.0
1	A	144	LEU	3.0
1	A	71	ILE	2.9
1	B	13	ILE	2.9
1	B	285	ILE	2.8
1	A	42	VAL	2.8
1	A	153	LEU	2.7
1	A	96	TYR	2.7
1	A	37	THR	2.7
1	B	306	ALA	2.7
1	B	253	TRP	2.7
1	A	193	ASN	2.6
1	B	96	TYR	2.6
1	B	249	LYS	2.6
1	B	8	PHE	2.6
1	B	3	TYR	2.6
1	A	16	ILE	2.5
1	A	38	PRO	2.5
1	A	133	ILE	2.5
1	B	148	THR	2.4
1	B	254	GLU	2.4
1	A	189	GLU	2.4
1	A	149	THR	2.3
1	A	44	GLU	2.3
1	A	134	LEU	2.3
1	A	157	ILE	2.3
1	B	408	MET	2.3
1	A	140	TYR	2.3
1	A	141	TYR	2.3
1	A	143	LYS	2.3
1	B	251	GLU	2.3
1	B	5	GLU	2.3
1	B	256	GLY	2.2
1	A	33	LYS	2.2
1	B	275	ILE	2.2
1	A	57	GLU	2.2
1	A	10	LYS	2.2
1	A	151	LYS	2.2
1	A	73	ILE	2.1
1	B	252	TYR	2.1
1	B	84	TRP	2.1
1	A	79	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	271	GLU	2.1
1	A	116	LEU	2.1
1	B	247	THR	2.1
1	B	310	TYR	2.1
1	A	142	SER	2.1
1	B	270	ASN	2.0
1	A	15	GLU	2.0
1	B	287	LEU	2.0
1	A	224	ILE	2.0
1	B	224	ILE	2.0
1	A	20	TRP	2.0
1	A	358	SER	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.