



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2026 – 01:18 pm BST

PDB ID : 9IC8 / pdb_00009ic8
Title : Structure of BstEII with DNA substrate
Authors : Rety, S.; Xi, X.G.
Deposited on : 2025-02-14
Resolution : 2.72 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

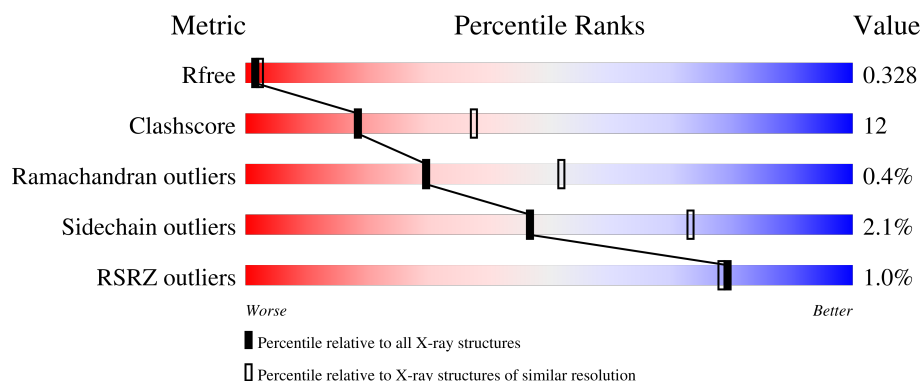
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	288	 68% 31% .
1	B	288	 71% 28% .
1	C	288	 71% 27% ..
1	D	288	 69% 27% ..

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9428 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 BstEII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	0	0
			2357	1515	398	437	7			
1	B	286	Total	C	N	O	S	0	0	0
			2357	1515	398	437	7			
1	C	286	Total	C	N	O	S	0	0	0
			2357	1515	398	437	7			
1	D	286	Total	C	N	O	S	0	0	0
			2357	1515	398	437	7			

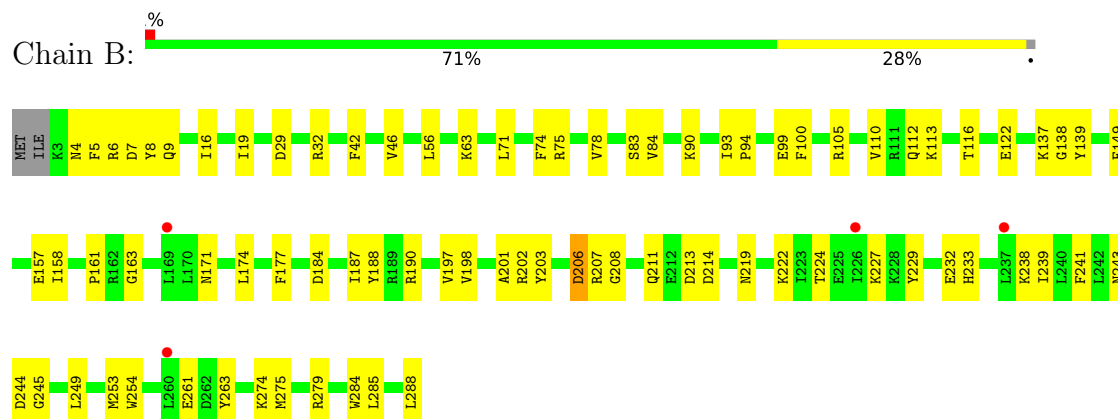
3 Residue-property plots [i](#)

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.

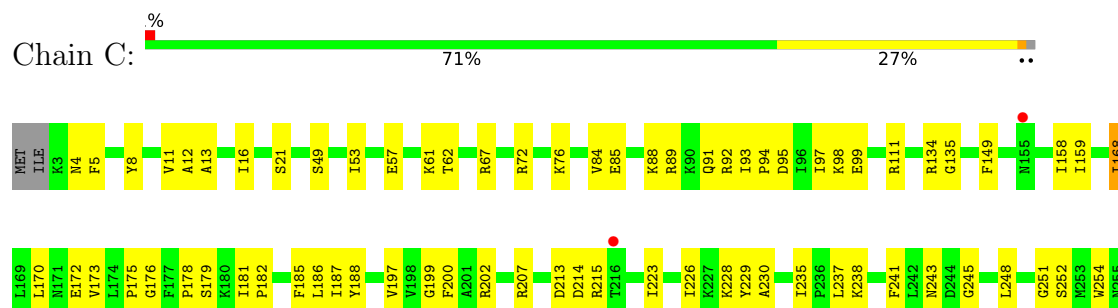
• Molecule 1: BstEII

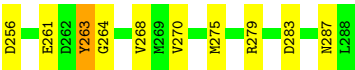


• Molecule 1: BstEII

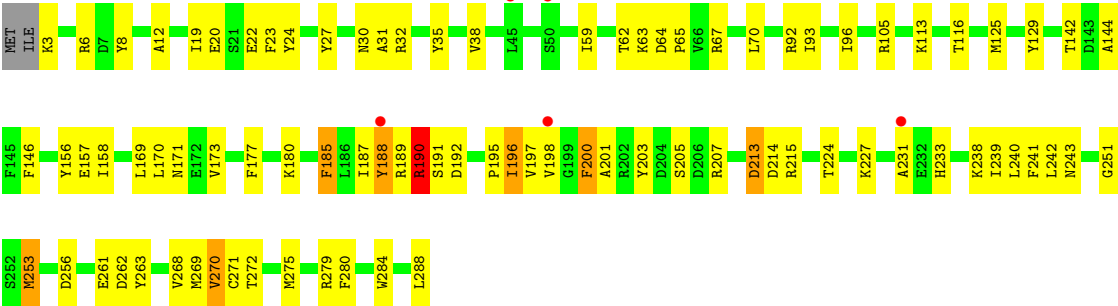


• Molecule 1: BstEII





● Molecule 1: BstEII



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	37.97 Å 203.99 Å 75.77 Å 90.00° 91.76° 90.00°	Depositor
Resolution (Å)	101.99 – 2.72 101.99 – 2.72	Depositor EDS
% Data completeness (in resolution range)	98.6 (101.99-2.72) 89.8 (101.99-2.72)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 2.73 Å)	Xtriage
Refinement program	PHENIX 1.21.2_5419	Depositor
R, R_{free}	0.275 , 0.325 0.278 , 0.328	Depositor DCC
R_{free} test set	1490 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 99.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.118 for h,-k,-l	Xtriage
Reported twinning fraction	0.210 for h,-k,-l	Depositor
Outliers	0 of 30279 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	9428	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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	0.12	0/2410	0.38	0/3249
1	B	0.13	0/2410	0.38	0/3249
1	C	0.12	0/2410	0.39	0/3249
1	D	0.15	0/2410	0.51	0/3249
All	All	0.13	0/9640	0.42	0/12996

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	D	0	4

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	185	PHE	Peptide
1	D	190	ARG	Peptide
1	D	24	TYR	Peptide
1	D	253	MET	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	2357	0	2349	60	3
1	B	2357	0	2349	55	2
1	C	2357	0	2349	55	1
1	D	2357	0	2349	59	0
All	All	9428	0	9396	225	3

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 12.

All (225) 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:D:63:LYS:HB2	1:D:64:ASP:HA	1.56	0.87
1:C:11:VAL:O	1:C:13:ALA:N	2.14	0.81
1:A:238:LYS:NZ	1:A:284:TRP:O	2.22	0.73
1:C:264:GLY:HA3	1:C:268:VAL:HG12	1.71	0.73
1:B:174:LEU:HD11	1:B:229:TYR:CZ	2.25	0.71
1:D:188:TYR:HB3	1:D:196:ILE:H	1.55	0.70
1:D:188:TYR:HB2	1:D:195:PRO:HA	1.74	0.69
1:A:207:ARG:NH1	1:A:208:GLY:O	2.25	0.69
1:D:105:ARG:HH12	1:D:113:LYS:HG2	1.57	0.68
1:B:207:ARG:NH1	1:B:208:GLY:O	2.27	0.68
1:D:207:ARG:HH12	1:D:251:GLY:HA3	1.57	0.68
1:A:206:ASP:OD1	1:A:207:ARG:N	2.24	0.67
1:D:190:ARG:O	1:D:190:ARG:HG3	1.94	0.67
1:B:261:GLU:OE2	1:B:279:ARG:NH2	2.28	0.66
1:B:29:ASP:OD1	1:B:32:ARG:NH2	2.28	0.66
1:D:196:ILE:HG22	1:D:197:VAL:HG23	1.78	0.66
1:A:198:VAL:HB	1:A:239:ILE:HD13	1.79	0.65
1:A:224:THR:OG1	1:A:263:TYR:OH	2.15	0.64
1:D:190:ARG:NH1	1:D:191:SER:OG	2.30	0.64
1:D:238:LYS:NZ	1:D:284:TRP:O	2.30	0.64
1:C:283:ASP:OD1	1:C:287:ASN:ND2	2.30	0.64
1:A:269:MET:HG3	1:A:279:ARG:HH21	1.64	0.62
1:B:198:VAL:HB	1:B:239:ILE:HD13	1.82	0.62
1:A:16:ILE:HG21	1:A:249:LEU:HD11	1.82	0.62
1:B:187:ILE:HB	1:B:197:VAL:HB	1.83	0.61
1:D:213:ASP:OD1	1:D:215:ARG:N	2.31	0.61
1:B:238:LYS:NZ	1:B:284:TRP:O	2.26	0.60
1:B:19:ILE:O	1:B:137:LYS:NZ	2.30	0.60
1:B:16:ILE:HD13	1:B:249:LEU:HD11	1.83	0.60
1:D:59:ILE:HD12	1:D:70:LEU:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:261:GLU:OE2	1:A:279:ARG:NH2	2.35	0.59
1:A:271:CYS:HA	1:A:275:MET:HE2	1.85	0.59
1:B:16:ILE:HG21	1:B:249:LEU:HD11	1.85	0.58
1:C:202:ARG:HH22	1:C:241:PHE:HD1	1.52	0.58
1:C:72:ARG:HG2	1:C:84:VAL:HG21	1.85	0.57
1:D:224:THR:HG1	1:D:263:TYR:HH	1.50	0.57
1:D:240:LEU:HD13	1:D:269:MET:HE3	1.84	0.57
1:D:113:LYS:O	1:D:116:THR:HG22	2.05	0.57
1:B:206:ASP:OD1	1:B:207:ARG:N	2.30	0.57
1:A:206:ASP:CG	1:A:207:ARG:H	2.13	0.56
1:A:72:ARG:HG2	1:A:84:VAL:HG21	1.87	0.56
1:B:5:PHE:HD1	1:B:275:MET:HE1	1.71	0.56
1:A:139:TYR:CE1	1:A:163:GLY:HA2	2.40	0.56
1:C:187:ILE:HB	1:C:197:VAL:HB	1.88	0.56
1:B:5:PHE:CD1	1:B:275:MET:HE1	2.41	0.56
1:B:171:ASN:HA	1:B:177:PHE:HB3	1.88	0.56
1:B:174:LEU:HD12	1:B:177:PHE:HB2	1.87	0.56
1:B:224:THR:OG1	1:B:263:TYR:OH	2.24	0.56
1:D:272:THR:H	1:D:275:MET:HE2	1.71	0.56
1:B:219:ASN:HA	1:B:222:LYS:HE2	1.87	0.55
1:A:94:PRO:HG3	1:C:228:LYS:HB3	1.89	0.55
1:A:74:PHE:O	1:A:78:VAL:HG22	2.06	0.55
1:C:200:PHE:HB3	1:C:202:ARG:HH12	1.72	0.54
1:A:219:ASN:HA	1:A:222:LYS:HE2	1.89	0.54
1:D:213:ASP:HA	1:D:214:ASP:C	2.32	0.54
1:C:223:ILE:HG21	1:C:263:TYR:HB3	1.89	0.54
1:C:53:ILE:HG23	1:C:97:ILE:HD13	1.90	0.54
1:D:170:LEU:HA	1:D:173:VAL:HG12	1.90	0.54
1:B:74:PHE:O	1:B:78:VAL:HG22	2.07	0.53
1:A:172:GLU:N	1:A:172:GLU:OE1	2.41	0.53
1:B:139:TYR:CE1	1:B:163:GLY:HA2	2.43	0.53
1:B:112:GLN:O	1:B:116:THR:HG23	2.09	0.53
1:D:23:PHE:O	1:D:27:TYR:HD2	1.91	0.53
1:C:241:PHE:HB2	1:C:270:VAL:HG22	1.91	0.53
1:C:243:ASN:HB3	1:C:248:LEU:HD21	1.91	0.53
1:D:203:TYR:HD2	1:D:205:SER:HB2	1.74	0.53
1:C:5:PHE:HD1	1:C:275:MET:HE1	1.74	0.53
1:A:5:PHE:HD1	1:A:275:MET:HE1	1.73	0.52
1:A:232:GLU:HG3	1:A:233:HIS:ND1	2.24	0.52
1:C:5:PHE:CD1	1:C:275:MET:HE1	2.45	0.52
1:C:207:ARG:HH22	1:C:251:GLY:HA3	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ASN:HA	1:A:177:PHE:HB3	1.92	0.52
1:D:207:ARG:HD2	1:D:253:MET:HE2	1.91	0.52
1:B:244:ASP:OD1	1:B:245:GLY:N	2.42	0.52
1:C:62:THR:O	1:C:67:ARG:NE	2.43	0.51
1:D:188:TYR:HB3	1:D:197:VAL:H	1.76	0.51
1:C:252:SER:O	1:C:256:ASP:N	2.36	0.51
1:C:261:GLU:HA	1:C:268:VAL:HG13	1.93	0.51
1:A:239:ILE:HB	1:A:268:VAL:HG22	1.93	0.51
1:B:78:VAL:HG12	1:B:110:VAL:HG21	1.93	0.51
1:C:168:ILE:O	1:C:182:PRO:HA	2.11	0.51
1:C:176:GLY:HA3	1:C:229:TYR:CE1	2.46	0.50
1:A:157:GLU:HG3	1:A:188:TYR:HB2	1.94	0.50
1:A:149:PHE:HB3	1:A:158:ILE:HD11	1.94	0.50
1:D:156:TYR:HE1	1:D:191:SER:HB3	1.77	0.50
1:B:174:LEU:HD12	1:B:177:PHE:HD2	1.77	0.50
1:A:113:LYS:O	1:A:116:THR:OG1	2.30	0.49
1:C:72:ARG:O	1:C:76:LYS:HD3	2.12	0.49
1:A:5:PHE:CD1	1:A:275:MET:HE1	2.47	0.49
1:A:78:VAL:HG12	1:A:110:VAL:HG21	1.94	0.49
1:A:16:ILE:HD13	1:A:249:LEU:HD11	1.94	0.49
1:C:4:ASN:C	1:C:279:ARG:HH12	2.20	0.49
1:A:49:SER:O	1:A:111:ARG:NH2	2.46	0.48
1:C:91:GLN:HE22	1:D:144:ALA:HB2	1.78	0.48
1:C:202:ARG:NH2	1:C:243:ASN:OD1	2.37	0.48
1:B:232:GLU:HG3	1:B:233:HIS:ND1	2.27	0.48
1:C:200:PHE:HB3	1:C:202:ARG:NH1	2.27	0.48
1:D:19:ILE:HG22	1:D:20:GLU:H	1.77	0.48
1:C:159:ILE:HG12	1:C:188:TYR:HE1	1.78	0.48
1:D:185:PHE:HA	1:D:187:ILE:HG13	1.95	0.48
1:A:157:GLU:HB3	1:A:190:ARG:HG2	1.95	0.48
1:B:4:ASN:C	1:B:279:ARG:HH12	2.22	0.48
1:D:156:TYR:HB3	1:D:189:ARG:O	2.12	0.48
1:C:158:ILE:HG12	1:C:187:ILE:HG12	1.94	0.48
1:D:64:ASP:HB2	1:D:65:PRO:HD3	1.96	0.48
1:C:176:GLY:C	1:C:178:PRO:HD2	2.38	0.48
1:A:91:GLN:H	1:A:91:GLN:CD	2.22	0.47
1:B:157:GLU:HG3	1:B:188:TYR:HB2	1.96	0.47
1:C:89:ARG:HA	1:C:89:ARG:HD3	1.57	0.47
1:D:169:LEU:HD23	1:D:180:LYS:HB3	1.96	0.47
1:B:149:PHE:CG	1:B:158:ILE:HD11	2.50	0.47
1:B:157:GLU:HB3	1:B:190:ARG:HG2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:ILE:HG23	1:C:237:LEU:HD23	1.97	0.47
1:A:158:ILE:HG23	1:A:187:ILE:HG12	1.96	0.47
1:D:156:TYR:CD1	1:D:190:ARG:HA	2.49	0.47
1:D:171:ASN:HA	1:D:177:PHE:HB3	1.95	0.47
1:D:241:PHE:HB3	1:D:243:ASN:HD22	1.80	0.47
1:D:241:PHE:HB3	1:D:243:ASN:ND2	2.29	0.47
1:A:139:TYR:HE1	1:A:163:GLY:HA2	1.78	0.47
1:D:241:PHE:HB2	1:D:270:VAL:HA	1.96	0.47
1:C:179:SER:HB3	1:C:181:ILE:HD11	1.96	0.47
1:C:238:LYS:NZ	1:C:287:ASN:O	2.48	0.46
1:C:275:MET:HB3	1:C:279:ARG:HD3	1.96	0.46
1:B:138:GLY:HA2	1:B:203:TYR:HB3	1.96	0.46
1:A:4:ASN:C	1:A:279:ARG:HH12	2.24	0.46
1:B:7:ASP:OD2	1:D:233:HIS:NE2	2.49	0.46
1:B:207:ARG:NH1	1:B:211:GLN:H	2.14	0.46
1:C:8:TYR:HB2	1:C:254:TRP:HZ2	1.80	0.46
1:A:29:ASP:OD1	1:A:32:ARG:NH2	2.45	0.46
1:C:16:ILE:HD11	1:C:245:GLY:H	1.81	0.46
1:A:95:ASP:O	1:A:98:LYS:HG2	2.15	0.46
1:D:32:ARG:HA	1:D:125:MET:SD	2.56	0.46
1:A:207:ARG:NH1	1:A:211:GLN:H	2.15	0.45
1:B:32:ARG:NH1	1:B:122:GLU:OE2	2.49	0.45
1:A:161:PRO:HG3	1:A:167:ASP:HA	1.97	0.45
1:D:157:GLU:HG2	1:D:158:ILE:H	1.81	0.45
1:D:198:VAL:HB	1:D:239:ILE:HA	1.98	0.45
1:B:105:ARG:HH22	1:B:113:LYS:HE3	1.80	0.45
1:D:224:THR:OG1	1:D:263:TYR:OH	2.25	0.45
1:D:253:MET:HA	1:D:256:ASP:HB2	1.98	0.45
1:A:240:LEU:HD22	1:A:280:PHE:CE2	2.51	0.45
1:D:261:GLU:HA	1:D:268:VAL:HB	1.98	0.45
1:D:8:TYR:O	1:D:12:ALA:HB2	2.16	0.45
1:D:31:ALA:HB2	1:D:129:TYR:HD2	1.81	0.45
1:C:172:GLU:N	1:C:172:GLU:OE1	2.50	0.45
1:C:202:ARG:HE	1:C:243:ASN:HD21	1.64	0.45
1:A:187:ILE:HB	1:A:197:VAL:HB	1.99	0.45
1:B:4:ASN:N	1:B:7:ASP:OD2	2.49	0.45
1:B:213:ASP:HA	1:B:214:ASP:HA	1.59	0.45
1:B:9:GLN:HB2	1:B:254:TRP:NE1	2.33	0.44
1:B:63:LYS:HD2	1:B:63:LYS:N	2.31	0.44
1:D:6:ARG:NH1	1:D:262:ASP:OD2	2.50	0.44
1:A:9:GLN:HB2	1:A:254:TRP:NE1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:32:ARG:HD3	1:B:122:GLU:HG2	1.99	0.44
1:D:63:LYS:CB	1:D:64:ASP:HA	2.36	0.44
1:A:149:PHE:CG	1:A:158:ILE:HD11	2.53	0.43
1:B:274:LYS:HB3	1:C:175:PRO:O	2.18	0.43
1:C:185:PHE:CZ	1:C:199:GLY:HA3	2.53	0.43
1:A:75:ARG:HG2	1:A:80:PRO:HA	2.00	0.43
1:A:244:ASP:OD1	1:A:245:GLY:N	2.46	0.43
1:B:174:LEU:HD12	1:B:177:PHE:CD2	2.52	0.43
1:C:57:GLU:O	1:C:61:LYS:HG3	2.17	0.43
1:C:92:ARG:HD2	1:C:95:ASP:OD2	2.19	0.43
1:D:271:CYS:SG	1:D:279:ARG:HD3	2.58	0.43
1:A:129:TYR:O	1:A:132:LYS:HG2	2.18	0.43
1:C:8:TYR:HE2	1:C:279:ARG:HD2	1.83	0.43
1:A:13:ALA:HA	1:A:249:LEU:HD21	2.00	0.43
1:D:201:ALA:HA	1:D:242:LEU:O	2.18	0.43
1:A:63:LYS:H	1:A:63:LYS:HD2	1.83	0.43
1:A:214:ASP:O	1:A:218:GLY:N	2.52	0.43
1:B:71:LEU:HD11	1:B:90:LYS:NZ	2.33	0.43
1:B:161:PRO:HD2	1:B:184:ASP:O	2.18	0.43
1:B:224:THR:HA	1:B:227:LYS:HG2	2.00	0.43
1:B:275:MET:O	1:B:279:ARG:HB2	2.19	0.43
1:A:161:PRO:HD3	1:A:168:ILE:HG12	2.00	0.42
1:B:201:ALA:O	1:B:202:ARG:HD2	2.19	0.42
1:D:92:ARG:O	1:D:96:ILE:N	2.39	0.42
1:C:8:TYR:CE2	1:C:279:ARG:HD2	2.54	0.42
1:D:31:ALA:HB2	1:D:129:TYR:CD2	2.55	0.42
1:A:88:LYS:O	1:A:90:LYS:HE2	2.19	0.42
1:B:99:GLU:HB3	1:B:100:PHE:CD1	2.55	0.42
1:B:158:ILE:HG23	1:B:187:ILE:HG12	2.01	0.42
1:C:230:ALA:HB1	1:C:235:ILE:O	2.20	0.42
1:B:42:PHE:O	1:B:46:VAL:HG23	2.19	0.42
1:C:93:ILE:N	1:C:94:PRO:HD2	2.35	0.42
1:C:134:ARG:HA	1:C:135:GLY:HA2	1.60	0.42
1:D:207:ARG:NH1	1:D:251:GLY:HA3	2.32	0.42
1:C:186:LEU:HD23	1:C:188:TYR:OH	2.19	0.42
1:C:213:ASP:HA	1:C:214:ASP:HA	1.58	0.42
1:D:3:LYS:HD3	1:D:8:TYR:OH	2.20	0.42
1:C:94:PRO:O	1:C:98:LYS:HD3	2.20	0.42
1:A:74:PHE:CE2	1:A:78:VAL:HG21	2.55	0.42
1:B:139:TYR:HE1	1:B:163:GLY:HA2	1.84	0.42
1:D:35:TYR:O	1:D:38:VAL:HG22	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:TYR:HE1	1:B:279:ARG:HH11	1.68	0.41
1:C:49:SER:O	1:C:111:ARG:NH2	2.53	0.41
1:C:149:PHE:CD2	1:C:158:ILE:HD11	2.55	0.41
1:A:108:LYS:HE2	1:A:108:LYS:HB3	1.76	0.41
1:B:75:ARG:HD2	1:B:84:VAL:N	2.35	0.41
1:C:170:LEU:HD12	1:C:181:ILE:HB	2.01	0.41
1:A:138:GLY:HA2	1:A:203:TYR:HB3	2.02	0.41
1:A:213:ASP:HA	1:A:214:ASP:HA	1.61	0.41
1:B:56:LEU:HB2	1:B:74:PHE:CZ	2.55	0.41
1:D:227:LYS:O	1:D:231:ALA:N	2.44	0.41
1:A:202:ARG:NH1	1:A:211:GLN:OE1	2.51	0.41
1:B:206:ASP:CG	1:B:207:ARG:H	2.20	0.41
1:D:23:PHE:O	1:D:27:TYR:CD2	2.73	0.41
1:D:62:THR:O	1:D:67:ARG:HB2	2.21	0.41
1:A:262:ASP:OD1	1:A:263:TYR:N	2.54	0.41
1:A:32:ARG:HD3	1:A:122:GLU:HG2	2.03	0.41
1:A:133:ASP:HB3	1:A:136:LYS:HB2	2.03	0.41
1:A:161:PRO:HD2	1:A:184:ASP:O	2.20	0.41
1:B:93:ILE:N	1:B:94:PRO:HD2	2.36	0.41
1:B:241:PHE:HB3	1:B:243:ASN:HD22	1.86	0.40
1:C:85:GLU:O	1:C:88:LYS:HG2	2.21	0.40
1:C:168:ILE:HG23	1:C:173:VAL:HG21	2.02	0.40
1:D:146:PHE:CZ	1:D:185:PHE:HD1	2.39	0.40
1:A:22:GLU:HB3	1:A:27:TYR:HB3	2.03	0.40
1:A:119:HIS:HA	1:A:120:PRO:C	2.46	0.40
1:D:30:ASN:HB2	1:D:129:TYR:CE2	2.56	0.40
1:D:93:ILE:HD13	1:D:96:ILE:HD12	2.03	0.40
1:A:213:ASP:HB3	1:A:214:ASP:OD1	2.21	0.40
1:C:207:ARG:NH2	1:C:251:GLY:HA3	2.36	0.40
1:D:93:ILE:HA	1:D:96:ILE:HB	2.03	0.40
1:D:200:PHE:O	1:D:242:LEU:N	2.53	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ASP:OD2	1:B:83:SER:OG[1_655]	2.01	0.19
1:A:83:SER:OG	1:B:206:ASP:OD2[1_655]	2.13	0.07
1:A:14:LYS:NZ	1:C:99:GLU:O[2_555]	2.17	0.03

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	284/288 (99%)	282 (99%)	0	2 (1%)	18	39
1	B	284/288 (99%)	283 (100%)	0	1 (0%)	30	52
1	C	284/288 (99%)	281 (99%)	1 (0%)	2 (1%)	18	39
1	D	284/288 (99%)	282 (99%)	2 (1%)	0	100	100
All	All	1136/1152 (99%)	1128 (99%)	3 (0%)	5 (0%)	30	52

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	21	SER
1	A	206	ASP
1	B	206	ASP
1	C	12	ALA
1	C	21	SER

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	255/257 (99%)	252 (99%)	3 (1%)	63	82
1	B	255/257 (99%)	251 (98%)	4 (2%)	55	78
1	C	255/257 (99%)	252 (99%)	3 (1%)	63	82
1	D	255/257 (99%)	244 (96%)	11 (4%)	26	52
All	All	1020/1028 (99%)	999 (98%)	21 (2%)	47	73

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	142	THR
1	A	285	LEU
1	B	6	ARG
1	B	253	MET
1	B	285	LEU
1	B	288	LEU
1	C	168	ILE
1	C	215	ARG
1	C	263	TYR
1	D	22	GLU
1	D	142	THR
1	D	188	TYR
1	D	190	ARG
1	D	192	ASP
1	D	196	ILE
1	D	200	PHE
1	D	213	ASP
1	D	270	VAL
1	D	280	PHE
1	D	288	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	HIS
1	D	58	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	286/288 (99%)	-0.35	0 100 100	38, 68, 140, 212	0
1	B	286/288 (99%)	-0.03	4 (1%) 73 71	37, 93, 179, 249	0
1	C	286/288 (99%)	-0.26	2 (0%) 84 83	34, 81, 158, 231	0
1	D	286/288 (99%)	-0.09	5 (1%) 69 66	38, 95, 172, 381	0
All	All	1144/1152 (99%)	-0.18	11 (0%) 79 78	34, 81, 165, 381	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	231	ALA	3.6
1	D	50	SER	3.3
1	D	188	TYR	3.2
1	B	226	ILE	2.6
1	D	198	VAL	2.3
1	C	155	ASN	2.3
1	D	45	LEU	2.2
1	C	216	THR	2.1
1	B	169	LEU	2.0
1	B	237	LEU	2.0
1	B	260	LEU	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.