



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:27 PM UTC

PDB ID : 6RG0 / pdb_00006rg0
Title : Structure of pdxj
Authors : Rohweder, B.; Rajendran, C.; Sterner, R.
Deposited on : 2019-04-16
Resolution : 3.07 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

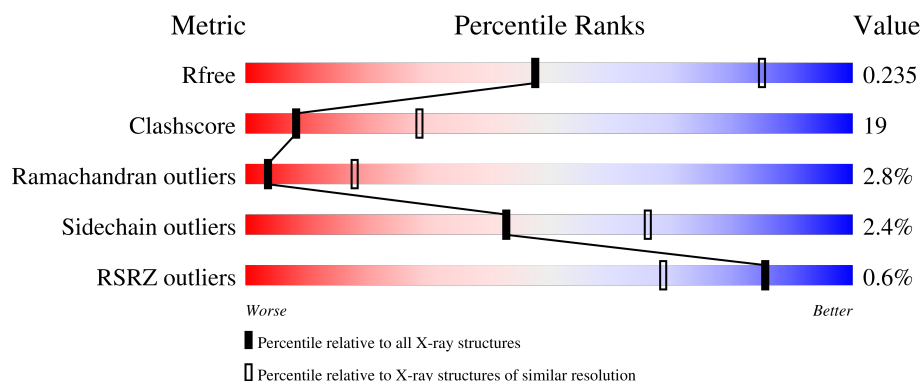
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.07 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	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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	268	 63% 26% • 10%
1	B	268	 56% 31% • 10%
1	C	268	 62% 27% • 10%
1	D	268	 50% 26% 5% 18%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 6975 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 Pyridoxine 5'-phosphate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	242	Total	C	N	O	S	0	0	0
			1814	1129	334	340	11			
1	B	242	Total	C	N	O	S	0	0	0
			1812	1128	331	342	11			
1	C	242	Total	C	N	O	S	0	0	0
			1789	1115	328	335	11			
1	D	220	Total	C	N	O	S	0	0	0
			1560	980	274	295	11			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP P0A794
A	2	HIS	-	expression tag	UNP P0A794
A	3	HIS	-	expression tag	UNP P0A794
A	4	HIS	-	expression tag	UNP P0A794
A	5	HIS	-	expression tag	UNP P0A794
A	6	HIS	-	expression tag	UNP P0A794
A	7	HIS	-	expression tag	UNP P0A794
A	8	THR	-	expression tag	UNP P0A794
A	9	ASP	-	expression tag	UNP P0A794
A	10	PRO	-	expression tag	UNP P0A794
A	11	ALA	-	expression tag	UNP P0A794
A	12	LEU	-	expression tag	UNP P0A794
A	13	ARG	-	expression tag	UNP P0A794
A	14	ALA	-	expression tag	UNP P0A794
A	159	LYS	GLU	conflict	UNP P0A794
A	211	ARG	HIS	conflict	UNP P0A794
A	237	LEU	MET	conflict	UNP P0A794
A	242	VAL	ASP	conflict	UNP P0A794
A	257	GLY	-	expression tag	UNP P0A794
A	258	LEU	-	expression tag	UNP P0A794
A	259	GLU	-	expression tag	UNP P0A794

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Chain	Residue	Modelled	Actual	Comment	Reference
A	260	PRO	-	expression tag	UNP P0A794
A	261	LEU	-	expression tag	UNP P0A794
A	262	ARG	-	expression tag	UNP P0A794
A	263	VAL	-	expression tag	UNP P0A794
A	264	VAL	-	expression tag	UNP P0A794
A	265	SER	-	expression tag	UNP P0A794
A	266	LEU	-	expression tag	UNP P0A794
A	267	ILE	-	expression tag	UNP P0A794
A	268	SER	-	expression tag	UNP P0A794
B	1	MET	-	initiating methionine	UNP P0A794
B	2	HIS	-	expression tag	UNP P0A794
B	3	HIS	-	expression tag	UNP P0A794
B	4	HIS	-	expression tag	UNP P0A794
B	5	HIS	-	expression tag	UNP P0A794
B	6	HIS	-	expression tag	UNP P0A794
B	7	HIS	-	expression tag	UNP P0A794
B	8	THR	-	expression tag	UNP P0A794
B	9	ASP	-	expression tag	UNP P0A794
B	10	PRO	-	expression tag	UNP P0A794
B	11	ALA	-	expression tag	UNP P0A794
B	12	LEU	-	expression tag	UNP P0A794
B	13	ARG	-	expression tag	UNP P0A794
B	14	ALA	-	expression tag	UNP P0A794
B	159	LYS	GLU	conflict	UNP P0A794
B	211	ARG	HIS	conflict	UNP P0A794
B	237	LEU	MET	conflict	UNP P0A794
B	242	VAL	ASP	conflict	UNP P0A794
B	257	GLY	-	expression tag	UNP P0A794
B	258	LEU	-	expression tag	UNP P0A794
B	259	GLU	-	expression tag	UNP P0A794
B	260	PRO	-	expression tag	UNP P0A794
B	261	LEU	-	expression tag	UNP P0A794
B	262	ARG	-	expression tag	UNP P0A794
B	263	VAL	-	expression tag	UNP P0A794
B	264	VAL	-	expression tag	UNP P0A794
B	265	SER	-	expression tag	UNP P0A794
B	266	LEU	-	expression tag	UNP P0A794
B	267	ILE	-	expression tag	UNP P0A794
B	268	SER	-	expression tag	UNP P0A794
C	1	MET	-	initiating methionine	UNP P0A794
C	2	HIS	-	expression tag	UNP P0A794
C	3	HIS	-	expression tag	UNP P0A794

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	HIS	-	expression tag	UNP P0A794
C	5	HIS	-	expression tag	UNP P0A794
C	6	HIS	-	expression tag	UNP P0A794
C	7	HIS	-	expression tag	UNP P0A794
C	8	THR	-	expression tag	UNP P0A794
C	9	ASP	-	expression tag	UNP P0A794
C	10	PRO	-	expression tag	UNP P0A794
C	11	ALA	-	expression tag	UNP P0A794
C	12	LEU	-	expression tag	UNP P0A794
C	13	ARG	-	expression tag	UNP P0A794
C	14	ALA	-	expression tag	UNP P0A794
C	159	LYS	GLU	conflict	UNP P0A794
C	211	ARG	HIS	conflict	UNP P0A794
C	237	LEU	MET	conflict	UNP P0A794
C	242	VAL	ASP	conflict	UNP P0A794
C	257	GLY	-	expression tag	UNP P0A794
C	258	LEU	-	expression tag	UNP P0A794
C	259	GLU	-	expression tag	UNP P0A794
C	260	PRO	-	expression tag	UNP P0A794
C	261	LEU	-	expression tag	UNP P0A794
C	262	ARG	-	expression tag	UNP P0A794
C	263	VAL	-	expression tag	UNP P0A794
C	264	VAL	-	expression tag	UNP P0A794
C	265	SER	-	expression tag	UNP P0A794
C	266	LEU	-	expression tag	UNP P0A794
C	267	ILE	-	expression tag	UNP P0A794
C	268	SER	-	expression tag	UNP P0A794
D	1	MET	-	initiating methionine	UNP P0A794
D	2	HIS	-	expression tag	UNP P0A794
D	3	HIS	-	expression tag	UNP P0A794
D	4	HIS	-	expression tag	UNP P0A794
D	5	HIS	-	expression tag	UNP P0A794
D	6	HIS	-	expression tag	UNP P0A794
D	7	HIS	-	expression tag	UNP P0A794
D	8	THR	-	expression tag	UNP P0A794
D	9	ASP	-	expression tag	UNP P0A794
D	10	PRO	-	expression tag	UNP P0A794
D	11	ALA	-	expression tag	UNP P0A794
D	12	LEU	-	expression tag	UNP P0A794
D	13	ARG	-	expression tag	UNP P0A794
D	14	ALA	-	expression tag	UNP P0A794
D	159	LYS	GLU	conflict	UNP P0A794

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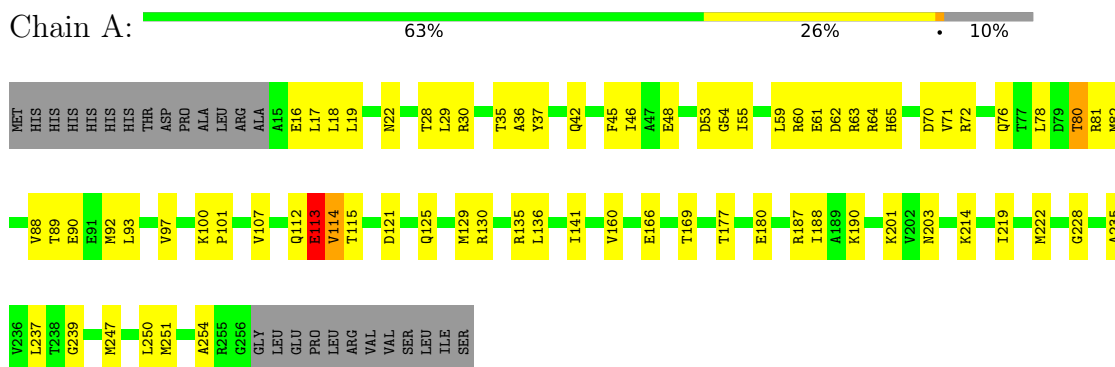
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Chain	Residue	Modelled	Actual	Comment	Reference
D	211	ARG	HIS	conflict	UNP P0A794
D	237	LEU	MET	conflict	UNP P0A794
D	242	VAL	ASP	conflict	UNP P0A794
D	257	GLY	-	expression tag	UNP P0A794
D	258	LEU	-	expression tag	UNP P0A794
D	259	GLU	-	expression tag	UNP P0A794
D	260	PRO	-	expression tag	UNP P0A794
D	261	LEU	-	expression tag	UNP P0A794
D	262	ARG	-	expression tag	UNP P0A794
D	263	VAL	-	expression tag	UNP P0A794
D	264	VAL	-	expression tag	UNP P0A794
D	265	SER	-	expression tag	UNP P0A794
D	266	LEU	-	expression tag	UNP P0A794
D	267	ILE	-	expression tag	UNP P0A794
D	268	SER	-	expression tag	UNP P0A794

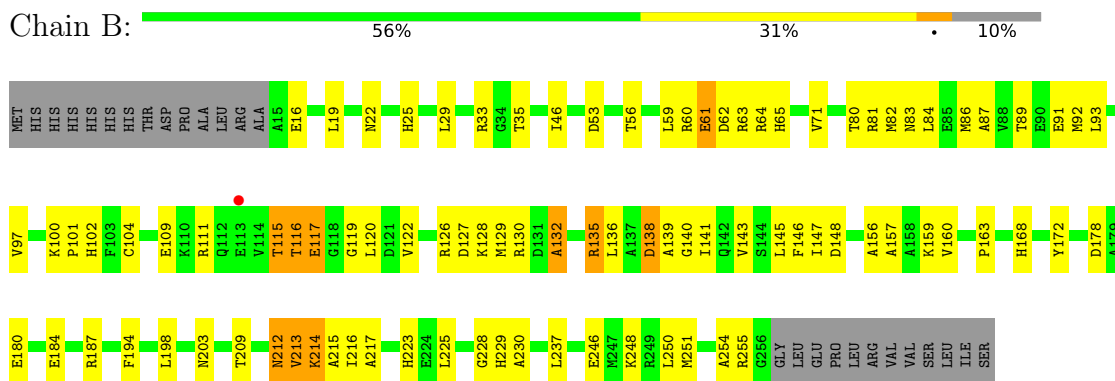
3 Residue-property plots

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.

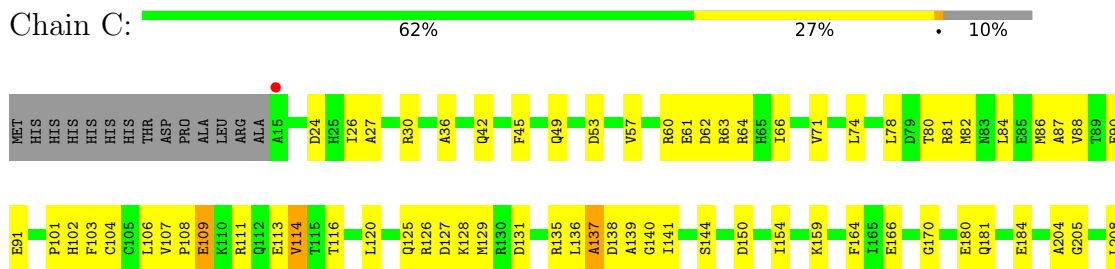
• Molecule 1: Pyridoxine 5'-phosphate synthase

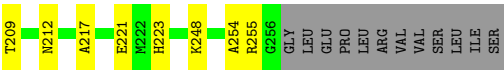


• Molecule 1: Pyridoxine 5'-phosphate synthase

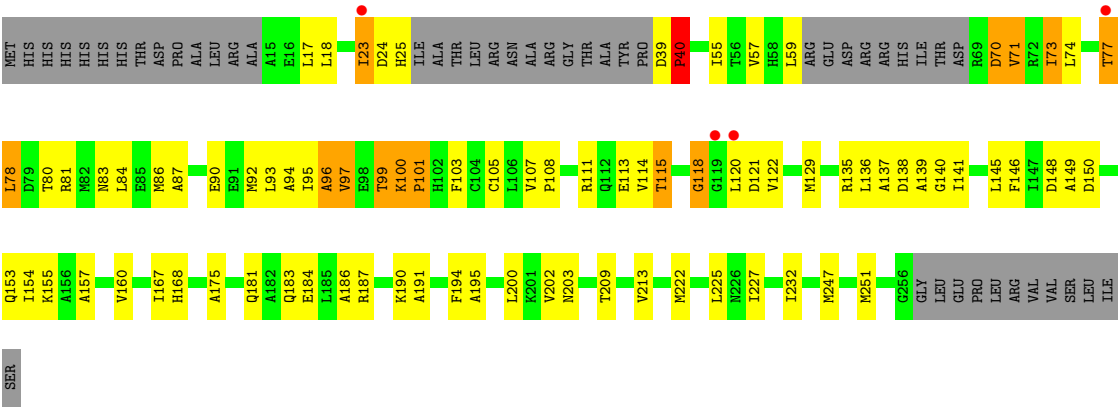


• Molecule 1: Pyridoxine 5'-phosphate synthase





● Molecule 1: Pyridoxine 5'-phosphate synthase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	80.05Å 188.12Å 192.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.44 – 3.07 48.44 – 3.07	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.44-3.07) 99.0 (48.44-3.07)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.24 (at 3.07Å)	Xtriage
Refinement program	PHENIX (1.14_3260: ???)	Depositor
R, R_{free}	0.182 , 0.248 (Not available) , 0.235	Depositor DCC
R_{free} test set	1368 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	85.5	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 79.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6975	wwPDB-VP
Average B, all atoms (Å ²)	96.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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	0.75	2/1835 (0.1%)	0.84	2/2481 (0.1%)
1	B	0.64	2/1833 (0.1%)	0.84	3/2479 (0.1%)
1	C	0.62	0/1810	0.74	0/2452
1	D	0.74	0/1575	0.92	4/2138 (0.2%)
All	All	0.69	4/7053 (0.1%)	0.84	9/9550 (0.1%)

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	B	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	LEU	C-O	-6.77	1.15	1.23
1	B	214	LYS	C-O	-5.63	1.17	1.24
1	B	212	ASN	C-O	-5.50	1.17	1.24
1	A	17	LEU	CA-C	-5.07	1.46	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	24	ASP	N-CA-C	-9.70	100.67	111.14
1	D	100	LYS	CA-C-N	8.96	131.04	119.84
1	D	100	LYS	C-N-CA	8.96	131.04	119.84
1	B	213	VAL	N-CA-C	7.67	125.30	109.34
1	B	111	ARG	N-CA-C	6.99	120.34	108.67
1	A	107	VAL	CA-C-N	-5.46	113.01	119.84
1	A	107	VAL	C-N-CA	-5.46	113.01	119.84
1	B	111	ARG	CB-CA-C	-5.31	110.01	117.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	96	ALA	O-C-N	5.30	128.42	122.22

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	127	ASP	Peptide
1	B	135	ARG	Peptide
1	B	61	GLU	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	1814	0	1838	65	0
1	B	1812	0	1831	69	0
1	C	1789	0	1793	55	0
1	D	1560	0	1534	91	0
All	All	6975	0	6996	268	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 19.

All (268) 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:108:PRO:HB3	1:D:113:GLU:CB	1.42	1.45
1:D:93:LEU:O	1:D:97:VAL:CG2	1.73	1.37
1:D:94:ALA:C	1:D:97:VAL:HG23	1.51	1.35
1:D:94:ALA:O	1:D:97:VAL:HG23	1.16	1.27
1:D:114:VAL:O	1:D:115:THR:OG1	1.55	1.22
1:B:115:THR:HG22	1:B:119:GLY:O	1.41	1.17
1:B:115:THR:CG2	1:B:119:GLY:O	1.92	1.16
1:D:94:ALA:HA	1:D:97:VAL:HG21	1.19	1.16
1:D:94:ALA:C	1:D:97:VAL:CG2	2.31	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:PRO:CB	1:D:113:GLU:CB	2.36	1.02
1:D:94:ALA:CA	1:D:97:VAL:CG2	2.37	1.02
1:D:93:LEU:O	1:D:97:VAL:HG22	0.84	1.01
1:D:94:ALA:O	1:D:97:VAL:CG2	2.08	1.01
1:D:94:ALA:HA	1:D:97:VAL:CG2	1.90	1.01
1:D:94:ALA:CA	1:D:97:VAL:HG21	1.96	0.96
1:D:39:ASP:HB3	1:D:40:PRO:CD	2.01	0.91
1:D:39:ASP:CB	1:D:40:PRO:HD2	2.00	0.91
1:D:93:LEU:C	1:D:97:VAL:HG22	1.95	0.90
1:A:71:VAL:HG13	1:A:82:MET:HE1	1.53	0.90
1:D:90:GLU:HA	1:D:93:LEU:HB2	1.56	0.86
1:D:39:ASP:CB	1:D:40:PRO:CD	2.55	0.84
1:D:95:ILE:O	1:D:99:THR:HG22	1.76	0.84
1:A:136:LEU:HD22	1:A:141:ILE:HD11	1.58	0.84
1:C:71:VAL:HG13	1:C:82:MET:HE1	1.60	0.83
1:A:114:VAL:CG2	1:A:115:THR:N	2.44	0.81
1:D:101:PRO:HD2	1:D:141:ILE:HG12	1.63	0.79
1:D:114:VAL:O	1:D:115:THR:CB	2.29	0.78
1:B:225:LEU:HD12	1:B:251:MET:HE2	1.66	0.78
1:D:95:ILE:O	1:D:99:THR:CG2	2.33	0.76
1:B:71:VAL:HG13	1:B:82:MET:HE1	1.68	0.76
1:D:23:ILE:HD13	1:D:55:ILE:CG2	2.17	0.75
1:C:81:ARG:HD3	1:C:102:HIS:CG	2.22	0.74
1:D:39:ASP:HB2	1:D:40:PRO:HD2	1.71	0.73
1:D:175:ALA:HB3	1:D:181:GLN:HG3	1.70	0.73
1:B:16:GLU:OE1	1:B:16:GLU:N	2.21	0.72
1:A:62:ASP:OD2	1:A:64:ARG:NH1	2.22	0.71
1:D:23:ILE:CD1	1:D:55:ILE:CG2	2.68	0.71
1:D:93:LEU:C	1:D:97:VAL:CG2	2.58	0.71
1:C:60:ARG:NH2	1:C:62:ASP:OD2	2.23	0.71
1:C:113:GLU:CB	1:C:125:GLN:HE22	2.04	0.70
1:B:81:ARG:HH12	1:B:102:HIS:CE1	2.10	0.69
1:C:62:ASP:HB3	1:C:64:ARG:HG2	1.73	0.69
1:B:53:ASP:OD2	1:B:248:LYS:NZ	2.27	0.68
1:B:115:THR:CG2	1:B:119:GLY:C	2.66	0.68
1:C:137:ALA:O	1:C:139:ALA:N	2.26	0.68
1:B:115:THR:OG1	1:B:116:THR:N	2.26	0.67
1:A:37:TYR:HE2	1:B:230:ALA:HA	1.59	0.67
1:D:120:LEU:N	1:D:146:PHE:O	2.26	0.67
1:B:132:ALA:O	1:B:136:LEU:N	2.28	0.67
1:B:146:PHE:HZ	1:B:168:HIS:HD1	1.43	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:LYS:HG2	1:A:254:ALA:HB2	1.77	0.66
1:A:60:ARG:NH1	1:A:65:HIS:HB2	2.11	0.66
1:B:115:THR:HG23	1:B:119:GLY:N	2.12	0.65
1:A:48:GLU:OE2	1:A:80:THR:OG1	2.13	0.64
1:B:122:VAL:HG13	1:B:129:MET:HG3	1.80	0.64
1:C:217:ALA:O	1:C:255:ARG:HD2	1.97	0.64
1:D:73:ILE:HG12	1:D:74:LEU:N	2.11	0.64
1:D:139:ALA:O	1:D:141:ILE:N	2.27	0.64
1:B:120:LEU:HD11	1:B:129:MET:HE1	1.80	0.63
1:B:64:ARG:O	1:B:65:HIS:ND1	2.30	0.63
1:B:115:THR:HG23	1:B:119:GLY:O	1.95	0.63
1:C:113:GLU:CB	1:C:125:GLN:NE2	2.61	0.63
1:A:114:VAL:HG23	1:A:115:THR:H	1.63	0.63
1:A:114:VAL:HG22	1:A:115:THR:N	2.13	0.63
1:B:115:THR:HG23	1:B:119:GLY:H	1.62	0.62
1:B:215:ALA:O	1:B:216:ILE:C	2.39	0.62
1:C:126:ARG:HH22	1:C:159:LYS:HE2	1.64	0.62
1:A:19:LEU:HD13	1:A:251:MET:HE1	1.81	0.62
1:D:23:ILE:HD13	1:D:55:ILE:HG23	1.81	0.62
1:D:114:VAL:C	1:D:115:THR:HG23	2.24	0.62
1:C:127:ASP:OD1	1:C:128:LYS:N	2.32	0.62
1:A:60:ARG:HH12	1:A:65:HIS:HB2	1.65	0.61
1:A:42:GLN:HG3	1:C:45:PHE:CG	2.35	0.61
1:B:87:ALA:CB	1:B:109:GLU:HB2	2.31	0.60
1:B:130:ARG:HH12	1:B:159:LYS:NZ	1.99	0.60
1:D:121:ASP:OD2	1:D:153:GLN:NE2	2.34	0.60
1:D:95:ILE:HG23	1:D:99:THR:HG21	1.81	0.60
1:D:73:ILE:HG12	1:D:74:LEU:H	1.66	0.60
1:D:183:GLN:O	1:D:186:ALA:N	2.33	0.60
1:A:114:VAL:HG23	1:A:115:THR:N	2.17	0.60
1:D:99:THR:O	1:D:99:THR:OG1	2.18	0.59
1:D:95:ILE:CG2	1:D:99:THR:HG21	2.31	0.59
1:D:71:VAL:O	1:D:74:LEU:N	2.35	0.59
1:B:117:GLU:OE1	1:B:187:ARG:NH1	2.32	0.59
1:D:23:ILE:CD1	1:D:55:ILE:HG21	2.32	0.59
1:B:217:ALA:O	1:B:255:ARG:HD2	2.03	0.59
1:D:59:LEU:HD22	1:D:86:MET:HA	1.85	0.59
1:D:154:ILE:HB	1:D:194:PHE:HE1	1.68	0.59
1:B:126:ARG:HE	1:B:159:LYS:HZ2	1.50	0.59
1:B:180:GLU:O	1:B:184:GLU:HG2	2.03	0.59
1:D:118:GLY:HA3	1:D:168:HIS:CD2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:ARG:C	1:A:65:HIS:HD2	2.11	0.58
1:A:53:ASP:C	1:A:80:THR:HG21	2.28	0.58
1:B:184:GLU:OE1	1:B:187:ARG:NH2	2.37	0.58
1:C:139:ALA:O	1:C:141:ILE:N	2.37	0.58
1:B:81:ARG:NH1	1:B:102:HIS:CE1	2.72	0.57
1:C:131:ASP:O	1:C:135:ARG:HG3	2.04	0.57
1:D:17:LEU:HD12	1:D:18:LEU:H	1.68	0.57
1:D:137:ALA:O	1:D:139:ALA:N	2.38	0.56
1:C:61:GLU:HA	1:C:63:ARG:HH21	1.69	0.56
1:C:221:GLU:OE1	1:C:221:GLU:N	2.37	0.56
1:A:59:LEU:HD22	1:A:71:VAL:HG21	1.88	0.56
1:C:87:ALA:CB	1:C:109:GLU:HG3	2.35	0.56
1:B:135:ARG:HA	1:B:138:ASP:OD1	2.05	0.56
1:B:117:GLU:HB3	1:B:148:ASP:OD2	2.06	0.55
1:D:59:LEU:HD12	1:D:92:MET:SD	2.47	0.55
1:D:118:GLY:HA3	1:D:168:HIS:HD2	1.71	0.55
1:D:122:VAL:HG13	1:D:129:MET:HG3	1.87	0.55
1:C:90:GLU:OE2	1:C:135:ARG:NH1	2.40	0.55
1:C:53:ASP:OD2	1:C:248:LYS:NZ	2.39	0.55
1:C:81:ARG:HD2	1:C:103:PHE:HE1	1.71	0.54
1:D:23:ILE:HD11	1:D:55:ILE:CG2	2.38	0.54
1:D:77:THR:HG23	1:D:78:LEU:H	1.73	0.54
1:B:203:ASN:OD1	1:B:223:HIS:HB3	2.07	0.54
1:D:150:ASP:O	1:D:154:ILE:HG13	2.07	0.54
1:D:39:ASP:HB3	1:D:40:PRO:HD3	1.86	0.54
1:D:59:LEU:HD13	1:D:87:ALA:H	1.73	0.54
1:A:29:LEU:O	1:B:229:HIS:HE1	1.91	0.54
1:D:154:ILE:HB	1:D:194:PHE:CE1	2.43	0.54
1:A:45:PHE:CD2	1:C:42:GLN:HG2	2.43	0.53
1:A:30:ARG:HH12	1:A:70:ASP:CG	2.16	0.53
1:C:61:GLU:HG3	1:C:91:GLU:OE1	2.08	0.53
1:C:136:LEU:O	1:C:141:ILE:HB	2.08	0.53
1:D:115:THR:OG1	1:D:148:ASP:OD2	2.27	0.53
1:C:101:PRO:HB2	1:C:103:PHE:O	2.09	0.53
1:D:190:LYS:HG3	1:D:191:ALA:N	2.23	0.53
1:B:60:ARG:NH2	1:B:62:ASP:OD2	2.41	0.53
1:B:82:MET:HE2	1:B:84:LEU:HB2	1.91	0.53
1:C:150:ASP:O	1:C:154:ILE:HG13	2.09	0.52
1:A:114:VAL:HG22	1:A:115:THR:O	2.09	0.52
1:C:61:GLU:HA	1:C:63:ARG:NH2	2.25	0.52
1:D:225:LEU:HD12	1:D:251:MET:HE2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:PHE:CZ	1:B:198:LEU:HD11	2.44	0.52
1:D:83:ASN:HB3	1:D:103:PHE:HB2	1.91	0.52
1:A:90:GLU:CD	1:A:135:ARG:HH12	2.17	0.52
1:C:80:THR:OG1	1:C:81:ARG:N	2.40	0.52
1:C:81:ARG:HD3	1:C:102:HIS:CD2	2.44	0.52
1:A:42:GLN:NE2	1:C:49:GLN:OE1	2.36	0.52
1:A:28:THR:OG1	1:A:65:HIS:ND1	2.39	0.51
1:D:95:ILE:CG2	1:D:99:THR:CG2	2.89	0.51
1:D:73:ILE:CG1	1:D:74:LEU:N	2.73	0.51
1:D:122:VAL:N	1:D:153:GLN:OE1	2.44	0.51
1:D:80:THR:OG1	1:D:81:ARG:N	2.43	0.51
1:D:90:GLU:OE1	1:D:135:ARG:NH1	2.30	0.51
1:B:33:ARG:HB3	1:B:35:THR:HG23	1.92	0.51
1:A:29:LEU:HG	1:B:29:LEU:HD21	1.92	0.51
1:A:48:GLU:OE2	1:A:78:LEU:HD23	2.11	0.50
1:B:22:ASN:HB3	1:B:228:GLY:HA3	1.92	0.50
1:B:97:VAL:O	1:B:100:LYS:HE3	2.11	0.50
1:B:178:ASP:OD1	1:C:81:ARG:NH2	2.44	0.50
1:B:117:GLU:HG2	1:B:168:HIS:CD2	2.47	0.50
1:D:59:LEU:CD1	1:D:87:ALA:H	2.25	0.50
1:A:42:GLN:HG3	1:C:45:PHE:CD2	2.47	0.50
1:D:95:ILE:HG23	1:D:99:THR:CG2	2.41	0.50
1:D:155:LYS:HZ1	1:D:194:PHE:HZ	1.58	0.50
1:A:37:TYR:CE2	1:B:230:ALA:HA	2.44	0.50
1:C:60:ARG:HH21	1:C:64:ARG:HB2	1.77	0.50
1:A:89:THR:HG22	1:A:92:MET:HG2	1.93	0.50
1:C:109:GLU:CD	1:C:109:GLU:N	2.70	0.49
1:A:42:GLN:OE1	1:B:237:LEU:HD13	2.13	0.49
1:D:95:ILE:O	1:D:99:THR:HG23	2.12	0.49
1:B:89:THR:O	1:B:93:LEU:HD12	2.12	0.49
1:A:64:ARG:C	1:A:65:HIS:CD2	2.91	0.48
1:A:169:THR:HG22	1:A:188:ILE:HD13	1.95	0.48
1:C:57:VAL:HB	1:C:66:ILE:HG13	1.95	0.48
1:B:87:ALA:HB2	1:B:109:GLU:HB2	1.96	0.48
1:B:139:ALA:O	1:B:141:ILE:N	2.46	0.48
1:B:143:VAL:H	1:B:163:PRO:HG2	1.79	0.48
1:B:156:ALA:O	1:B:160:VAL:HG22	2.14	0.48
1:A:88:VAL:HG11	1:A:129:MET:HE1	1.95	0.48
1:C:104:CYS:HB2	1:C:141:ILE:CG2	2.43	0.48
1:C:57:VAL:CG2	1:C:82:MET:HE3	2.43	0.48
1:B:19:LEU:HD13	1:B:251:MET:HE1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:MET:SD	1:D:96:ALA:HB2	2.53	0.47
1:C:78:LEU:CD1	1:C:82:MET:HB2	2.43	0.47
1:D:23:ILE:HD11	1:D:55:ILE:HG21	1.97	0.47
1:A:60:ARG:HD3	1:A:64:ARG:NH2	2.29	0.47
1:A:93:LEU:O	1:A:97:VAL:HG23	2.14	0.47
1:A:187:ARG:HA	1:A:190:LYS:HE3	1.96	0.47
1:A:46:ILE:HD12	1:B:237:LEU:HD22	1.95	0.47
1:C:180:GLU:O	1:C:184:GLU:HG2	2.15	0.47
1:A:130:ARG:HA	1:A:160:VAL:HG13	1.97	0.47
1:C:88:VAL:HG11	1:C:129:MET:HE1	1.96	0.46
1:A:113:GLU:O	1:A:113:GLU:HG3	2.15	0.46
1:B:209:THR:H	1:B:212:ASN:HB2	1.80	0.46
1:B:87:ALA:HB3	1:B:109:GLU:HB2	1.97	0.46
1:B:89:THR:HG22	1:B:91:GLU:H	1.81	0.46
1:C:87:ALA:HB2	1:C:109:GLU:HG3	1.96	0.46
1:C:107:VAL:HB	1:C:108:PRO:HD2	1.98	0.46
1:A:235:ALA:O	1:A:239:GLY:N	2.43	0.46
1:C:120:LEU:HD12	1:C:120:LEU:HA	1.65	0.46
1:A:59:LEU:HB3	1:A:92:MET:HE1	1.97	0.45
1:B:194:PHE:CE1	1:B:198:LEU:HD21	2.51	0.45
1:D:167:ILE:HG12	1:D:203:ASN:O	2.16	0.45
1:A:136:LEU:HB3	1:A:141:ILE:CG1	2.47	0.45
1:A:177:THR:OG1	1:A:180:GLU:HG3	2.16	0.45
1:A:35:THR:HG22	1:A:36:ALA:H	1.82	0.45
1:B:84:LEU:HD23	1:B:101:PRO:HG3	1.97	0.45
1:C:24:ASP:C	1:C:26:ILE:H	2.25	0.45
1:C:111:ARG:HA	1:C:114:VAL:CG1	2.47	0.45
1:B:25:HIS:CE1	1:B:229:HIS:HD1	2.34	0.45
1:A:247:MET:HG3	1:A:251:MET:HE3	1.98	0.45
1:D:23:ILE:H	1:D:23:ILE:HG12	1.56	0.45
1:D:145:LEU:HD12	1:D:157:ALA:HB1	1.98	0.45
1:A:80:THR:HB	1:A:81:ARG:H	1.23	0.44
1:D:136:LEU:O	1:D:141:ILE:HB	2.17	0.44
1:A:121:ASP:O	1:A:125:GLN:HG3	2.17	0.44
1:A:166:GLU:HA	1:A:203:ASN:O	2.17	0.44
1:A:250:LEU:HD23	1:A:250:LEU:HA	1.79	0.44
1:B:214:LYS:HG2	1:B:254:ALA:HB2	1.99	0.44
1:C:144:SER:HB2	1:C:164:PHE:HB2	2.00	0.44
1:A:89:THR:CG2	1:A:92:MET:HG2	2.47	0.44
1:A:114:VAL:CG2	1:A:115:THR:O	2.66	0.44
1:D:114:VAL:HA	1:D:121:ASP:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:LEU:HD12	1:A:59:LEU:HA	1.67	0.44
1:C:205:GLY:HA2	1:C:208:LEU:HD12	2.00	0.44
1:A:100:LYS:N	1:A:101:PRO:HD3	2.33	0.43
1:B:59:LEU:HD12	1:B:59:LEU:HA	1.75	0.43
1:C:86:MET:HE2	1:C:106:LEU:HD21	2.00	0.43
1:D:149:ALA:HA	1:D:154:ILE:HD11	1.99	0.43
1:D:195:ALA:O	1:D:200:LEU:HB2	2.19	0.43
1:B:86:MET:SD	1:B:92:MET:HB3	2.59	0.43
1:C:135:ARG:HE	1:C:135:ARG:HB3	1.70	0.43
1:D:23:ILE:HD13	1:D:55:ILE:HG21	1.93	0.43
1:D:105:CYS:O	1:D:107:VAL:HG13	2.19	0.43
1:A:54:GLY:O	1:A:55:ILE:HD13	2.19	0.43
1:C:166:GLU:HG2	1:C:204:ALA:HA	2.00	0.43
1:D:59:LEU:HD12	1:D:92:MET:CG	2.49	0.43
1:D:227:ILE:HG21	1:D:247:MET:HE3	2.01	0.42
1:B:115:THR:HG23	1:B:119:GLY:CA	2.49	0.42
1:D:184:GLU:HG2	1:D:187:ARG:HD3	2.00	0.42
1:A:90:GLU:OE1	1:A:135:ARG:NH1	2.52	0.42
1:D:120:LEU:HD12	1:D:120:LEU:HA	1.87	0.42
1:A:22:ASN:HB3	1:A:228:GLY:HA3	2.01	0.42
1:A:61:GLU:HA	1:A:63:ARG:NH2	2.34	0.42
1:B:147:ILE:HD12	1:B:148:ASP:O	2.19	0.42
1:A:62:ASP:HB2	1:A:64:ARG:HG2	2.01	0.42
1:B:61:GLU:C	1:B:63:ARG:N	2.78	0.42
1:A:219:ILE:HG22	1:A:222:MET:HG2	2.01	0.42
1:C:164:PHE:HE2	1:C:223:HIS:ND1	2.18	0.42
1:A:72:ARG:O	1:A:76:GLN:HG3	2.20	0.42
1:A:201:LYS:HE2	1:A:201:LYS:HB3	1.85	0.42
1:B:128:LYS:HE2	1:B:128:LYS:HB3	1.91	0.42
1:A:60:ARG:H	1:A:60:ARG:HG3	1.55	0.41
1:A:101:PRO:HD2	1:A:141:ILE:HG21	2.01	0.41
1:C:74:LEU:O	1:C:78:LEU:HG	2.20	0.41
1:C:84:LEU:O	1:C:104:CYS:HA	2.21	0.41
1:C:254:ALA:O	1:C:255:ARG:HG3	2.20	0.41
1:B:97:VAL:O	1:B:100:LYS:HG3	2.21	0.41
1:C:209:THR:H	1:C:212:ASN:HB2	1.85	0.41
1:C:27:ALA:HB2	1:C:66:ILE:HD13	2.03	0.41
1:D:209:THR:O	1:D:213:VAL:HB	2.20	0.41
1:B:56:THR:HA	1:B:83:ASN:O	2.21	0.41
1:D:71:VAL:O	1:D:74:LEU:HB2	2.20	0.41
1:D:57:VAL:HG23	1:D:84:LEU:HD12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:THR:C	1:B:117:GLU:H	2.28	0.41
1:D:23:ILE:O	1:D:23:ILE:HG13	2.21	0.41
1:D:95:ILE:HG22	1:D:99:THR:CG2	2.50	0.41
1:A:48:GLU:CD	1:A:80:THR:HG1	2.21	0.41
1:D:232:ILE:H	1:D:232:ILE:HG12	1.60	0.41
1:A:237:LEU:HD22	1:B:46:ILE:HD13	2.03	0.41
1:C:30:ARG:HG3	1:C:36:ALA:C	2.46	0.40
1:D:202:VAL:HG12	1:D:222:MET:SD	2.61	0.40
1:B:145:LEU:HD12	1:B:157:ALA:HB1	2.03	0.40
1:B:246:GLU:O	1:B:250:LEU:HD13	2.22	0.40
1:D:59:LEU:HD12	1:D:92:MET:HG3	2.02	0.40
1:D:157:ALA:HA	1:D:160:VAL:HB	2.02	0.40
1:B:172:TYR:CE2	1:B:216:ILE:HG12	2.56	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	240/268 (90%)	224 (93%)	13 (5%)	3 (1%)	9	33
1	B	240/268 (90%)	206 (86%)	26 (11%)	8 (3%)	3	15
1	C	240/268 (90%)	212 (88%)	24 (10%)	4 (2%)	7	27
1	D	214/268 (80%)	174 (81%)	29 (14%)	11 (5%)	1	8
All	All	934/1072 (87%)	816 (87%)	92 (10%)	26 (3%)	4	18

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	112	GLN
1	B	140	GLY

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Mol	Chain	Res	Type
1	B	213	VAL
1	D	40	PRO
1	B	138	ASP
1	C	138	ASP
1	D	138	ASP
1	D	140	GLY
1	C	137	ALA
1	C	140	GLY
1	D	78	LEU
1	D	115	THR
1	A	113	GLU
1	B	104	CYS
1	B	116	THR
1	B	117	GLU
1	B	132	ALA
1	D	111	ARG
1	D	118	GLY
1	B	80	THR
1	D	77	THR
1	A	16	GLU
1	D	70	ASP
1	D	100	LYS
1	C	170	GLY
1	D	101	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	180/208 (86%)	177 (98%)	3 (2%)	53	71
1	B	180/208 (86%)	179 (99%)	1 (1%)	78	81
1	C	174/208 (84%)	170 (98%)	4 (2%)	44	67
1	D	146/208 (70%)	138 (94%)	8 (6%)	19	47
All	All	680/832 (82%)	664 (98%)	16 (2%)	43	66

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	THR
1	A	113	GLU
1	A	114	VAL
1	B	115	THR
1	C	109	GLU
1	C	114	VAL
1	C	116	THR
1	C	181	GLN
1	D	23	ILE
1	D	25	HIS
1	D	40	PRO
1	D	70	ASP
1	D	71	VAL
1	D	73	ILE
1	D	97	VAL
1	D	99	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	83	ASN
1	B	83	ASN
1	B	102	HIS
1	B	223	HIS
1	C	25	HIS
1	C	125	GLN
1	D	203	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	242/268 (90%)	-0.56	0 100 100	40, 64, 118, 196	0
1	B	242/268 (90%)	-0.46	1 (0%) 88 75	42, 86, 152, 213	0
1	C	242/268 (90%)	-0.32	1 (0%) 88 75	55, 91, 157, 196	0
1	D	220/268 (82%)	0.02	4 (1%) 67 45	60, 130, 192, 225	0
All	All	946/1072 (88%)	-0.34	6 (0%) 85 69	40, 89, 171, 225	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	120	LEU	3.2
1	C	15	ALA	2.7
1	D	119	GLY	2.7
1	D	77	THR	2.1
1	D	23	ILE	2.1
1	B	113	GLU	2.1

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.