



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:50 AM UTC

PDB ID : 3MJI / pdb_00003mji
Title : Activation of catalytic cysteine without a base in a Mutant Penicillin Acylase Precursor
Authors : Pathak, M.C.; Suresh, C.G.; Dodson, G.G.; Murshudov, G.N.
Deposited on : 2010-04-12
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

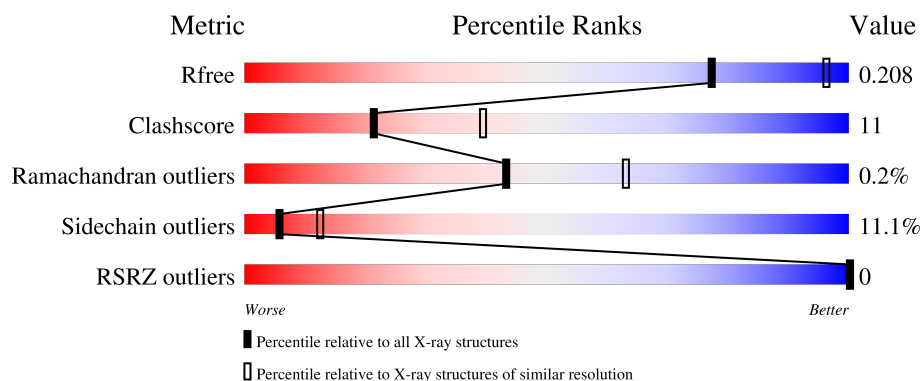
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	338	
1	B	338	
1	C	338	
1	D	338	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10729 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 Penicillin acylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	334	Total	C	N	O	S	0	0	0
			2606	1659	427	507	13			
1	B	334	Total	C	N	O	S	0	0	0
			2606	1659	427	507	13			
1	C	333	Total	C	N	O	S	0	0	0
			2599	1654	426	506	13			
1	D	333	Total	C	N	O	S	0	0	0
			2599	1654	426	506	13			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	SER	CYS	conflict	UNP P12256
A	101	ARG	THR	conflict	UNP P12256
B	4	SER	CYS	conflict	UNP P12256
B	101	ARG	THR	conflict	UNP P12256
C	4	SER	CYS	conflict	UNP P12256
C	101	ARG	THR	conflict	UNP P12256
D	4	SER	CYS	conflict	UNP P12256
D	101	ARG	THR	conflict	UNP P12256

- Molecule 2 is water.

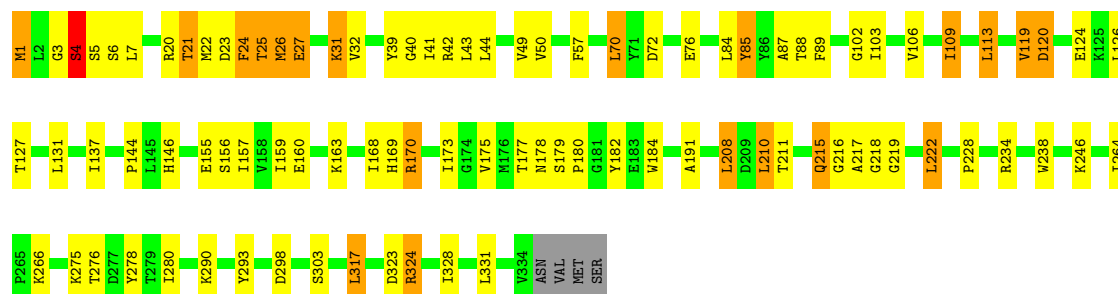
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	90	Total	O	0	0
			90	90		
2	B	69	Total	O	0	0
			69	69		
2	C	73	Total	O	0	0
			73	73		
2	D	87	Total	O	0	0
			87	87		

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.

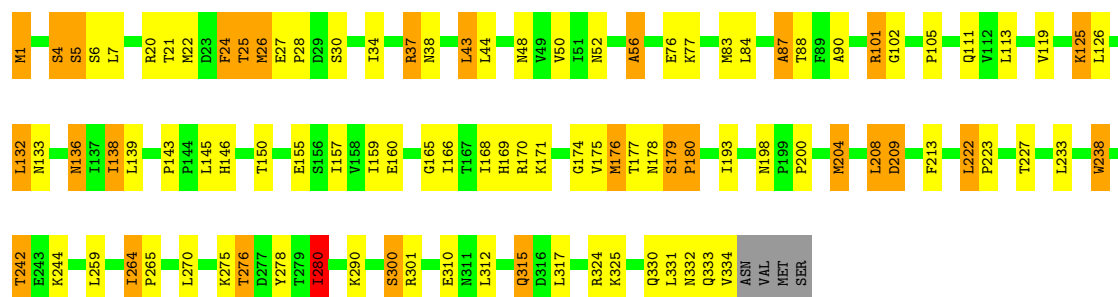
• Molecule 1: Penicillin acylase

Chain A: 



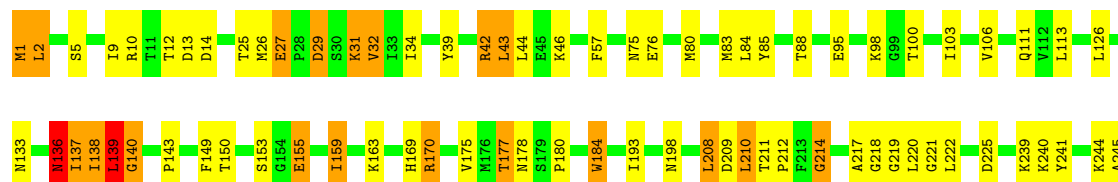
• Molecule 1: Penicillin acylase

Chain B: 



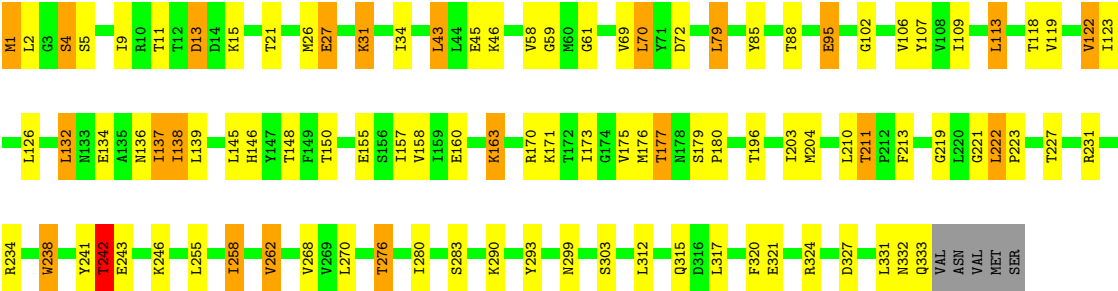
• Molecule 1: Penicillin acylase

Chain C: 





● Molecule 1: Penicillin acylase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.64Å 90.09Å 102.27Å 90.00° 102.13° 90.00°	Depositor
Resolution (Å)	19.95 – 2.50 19.95 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.95-2.50) 99.0 (19.95-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.69 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.6.0041	Depositor
R, R_{free}	0.166 , 0.211 0.172 , 0.208	Depositor DCC
R_{free} test set	3170 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	26.7	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 11.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.124 for l,-k,h	Xtriage
Reported twinning fraction	0.901 for H, K, L 0.099 for L, -K, H	Depositor
Outliers	2 of 62981 reflections (0.003%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	10729	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 22.84 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.2485e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	1.51	21/2661 (0.8%)	1.25	14/3616 (0.4%)
1	B	1.43	19/2661 (0.7%)	1.28	14/3616 (0.4%)
1	C	1.45	20/2654 (0.8%)	1.32	13/3606 (0.4%)
1	D	1.39	13/2654 (0.5%)	1.29	11/3606 (0.3%)
All	All	1.44	73/10630 (0.7%)	1.29	52/14444 (0.4%)

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	C	0	2

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	175	VAL	C-O	-8.17	1.16	1.24
1	C	178	ASN	C-O	-7.77	1.14	1.24
1	D	177	THR	C-O	-7.67	1.17	1.23
1	A	168	ILE	C-O	-7.50	1.15	1.24
1	D	175	VAL	C-O	-7.44	1.16	1.24
1	C	143	PRO	CA-C	7.43	1.55	1.51
1	C	177	THR	C-O	-7.16	1.17	1.23
1	B	169	HIS	C-O	-6.82	1.16	1.24
1	D	211	THR	C-O	-6.77	1.15	1.24
1	C	175	VAL	C-O	-6.71	1.17	1.24
1	C	219	GLY	C-O	-6.66	1.16	1.24
1	A	177	THR	C-O	-6.64	1.18	1.23
1	B	178	ASN	C-O	-6.57	1.15	1.24
1	B	166	ILE	CA-CB	6.50	1.61	1.54
1	D	219	GLY	C-O	-6.45	1.15	1.24
1	A	169	HIS	C-O	-6.34	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	178	ASN	C-O	-6.33	1.16	1.24
1	B	176	MET	C-O	-6.28	1.16	1.23
1	B	175	VAL	C-O	-6.17	1.17	1.24
1	C	133	ASN	CA-C	-6.17	1.46	1.53
1	C	214	GLY	C-O	-6.12	1.15	1.23
1	A	173	ILE	C-O	-6.11	1.15	1.24
1	A	219	GLY	C-O	-6.06	1.17	1.24
1	C	159	ILE	CA-CB	6.05	1.61	1.54
1	A	4	SER	C-O	-6.03	1.16	1.23
1	B	56	ALA	CA-CB	-6.00	1.43	1.53
1	B	5	SER	C-O	-5.99	1.16	1.23
1	A	217	ALA	C-O	-5.96	1.16	1.24
1	A	211	THR	C-O	-5.84	1.16	1.24
1	A	24	PHE	C-O	-5.83	1.16	1.23
1	D	242	THR	CA-CB	5.82	1.62	1.53
1	A	216	GLY	C-O	-5.80	1.16	1.24
1	D	88	THR	CA-CB	5.78	1.63	1.53
1	C	217	ALA	C-O	-5.75	1.16	1.24
1	C	225	ASP	CA-C	5.71	1.61	1.53
1	A	177	THR	N-CA	-5.70	1.42	1.46
1	B	25	THR	CA-CB	-5.67	1.44	1.53
1	C	133	ASN	C-O	-5.64	1.17	1.23
1	D	158	VAL	CA-CB	5.59	1.61	1.54
1	D	210	LEU	C-O	-5.58	1.17	1.24
1	A	21	THR	C-O	-5.55	1.17	1.23
1	B	179	SER	C-O	-5.49	1.17	1.24
1	B	209	ASP	C-O	-5.48	1.17	1.24
1	A	7	LEU	C-O	-5.44	1.17	1.23
1	B	22	MET	C-O	-5.39	1.17	1.24
1	C	88	THR	CA-CB	5.39	1.62	1.53
1	B	177	THR	C-O	-5.37	1.19	1.23
1	A	22	MET	C-O	-5.36	1.18	1.24
1	B	6	SER	C-O	-5.36	1.17	1.23
1	C	276	THR	CA-CB	5.33	1.61	1.53
1	B	209	ASP	N-CA	-5.31	1.39	1.46
1	B	90	ALA	CA-CB	-5.26	1.46	1.53
1	A	215	GLN	C-O	-5.26	1.16	1.23
1	C	169	HIS	CA-C	-5.24	1.46	1.52
1	B	209	ASP	CA-CB	-5.23	1.45	1.53
1	D	173	ILE	C-O	-5.21	1.16	1.24
1	C	221	GLY	C-O	-5.20	1.16	1.24
1	D	221	GLY	C-O	-5.19	1.16	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	210	LEU	C-O	-5.14	1.18	1.24
1	C	184	TRP	CA-C	5.14	1.59	1.52
1	B	30	SER	C-O	-5.14	1.17	1.23
1	C	220	LEU	C-O	-5.14	1.17	1.23
1	C	218	GLY	C-O	-5.13	1.17	1.23
1	C	100	THR	CA-CB	5.13	1.63	1.53
1	A	218	GLY	C-O	-5.11	1.17	1.23
1	D	283	SER	N-CA	5.11	1.52	1.45
1	B	209	ASP	CB-CG	-5.09	1.39	1.52
1	D	196	THR	N-CA	5.07	1.49	1.46
1	C	245	ALA	CA-CB	-5.06	1.45	1.53
1	D	299	ASN	CA-C	-5.06	1.48	1.53
1	A	23	ASP	C-O	-5.02	1.18	1.24
1	B	24	PHE	C-O	-5.00	1.17	1.23
1	A	5	SER	C-O	-5.00	1.17	1.23

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	139	LEU	CA-C-N	11.14	132.26	120.00
1	C	139	LEU	C-N-CA	11.14	132.26	120.00
1	B	25	THR	N-CA-C	10.94	123.28	111.36
1	C	140	GLY	N-CA-C	9.39	124.79	112.77
1	D	13	ASP	N-CA-C	-8.94	101.35	112.88
1	C	136	ASN	CA-C-N	8.29	131.61	120.50
1	C	136	ASN	C-N-CA	8.29	131.61	120.50
1	A	25	THR	N-CA-C	8.06	119.84	111.14
1	C	219	GLY	N-CA-C	7.76	123.20	114.67
1	B	198	ASN	N-CA-C	7.66	119.30	109.72
1	B	227	THR	CA-C-N	7.05	126.87	119.05
1	B	227	THR	C-N-CA	7.05	126.87	119.05
1	A	120	ASP	N-CA-C	6.47	118.33	111.28
1	C	264	ILE	N-CA-C	6.42	113.91	107.55
1	A	109	ILE	N-CA-C	6.16	116.82	110.36
1	C	239	LYS	N-CA-C	-6.11	104.54	111.14
1	A	127	THR	N-CA-C	-6.02	105.91	113.20
1	C	138	ILE	N-CA-C	-5.96	96.94	109.34
1	A	264	ILE	N-CA-C	5.93	114.41	107.77
1	A	6	SER	N-CA-C	5.88	118.11	109.24
1	D	72	ASP	N-CA-C	-5.87	100.46	108.38
1	D	227	THR	CA-C-N	5.83	125.53	119.05
1	D	227	THR	C-N-CA	5.83	125.53	119.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	262	VAL	N-CA-C	5.78	117.75	112.43
1	B	280	ILE	CB-CA-C	-5.67	104.39	112.22
1	B	280	ILE	N-CA-C	5.66	116.43	110.72
1	B	264	ILE	N-CA-C	5.62	113.62	107.60
1	A	182	TYR	N-CA-C	5.53	117.30	111.28
1	A	211	THR	CB-CA-C	5.51	117.41	108.87
1	D	246	LYS	N-CA-C	5.45	118.14	111.82
1	C	248	GLU	N-CA-C	5.44	116.89	111.07
1	A	163	LYS	N-CA-C	-5.39	105.41	111.28
1	A	124	GLU	N-CA-C	5.39	117.58	111.11
1	B	139	LEU	N-CA-C	-5.35	106.63	114.39
1	B	168	ILE	CB-CA-C	-5.35	103.44	110.98
1	B	139	LEU	N-CA-CB	5.34	118.03	110.98
1	A	31	LYS	CA-C-N	-5.29	115.55	122.37
1	A	31	LYS	C-N-CA	-5.29	115.55	122.37
1	A	191	ALA	N-CA-C	-5.25	106.83	113.18
1	D	241	TYR	CA-C-N	-5.23	113.94	121.42
1	D	241	TYR	C-N-CA	-5.23	113.94	121.42
1	B	143	PRO	O-C-N	5.18	123.69	121.31
1	C	198	ASN	N-CA-C	5.18	116.19	109.72
1	D	242	THR	N-CA-CB	5.17	117.87	110.06
1	B	165	GLY	CA-C-N	5.15	127.99	120.98
1	B	165	GLY	C-N-CA	5.15	127.99	120.98
1	C	143	PRO	O-C-N	5.15	123.68	121.31
1	B	87	ALA	N-CA-C	5.14	117.67	109.96
1	A	102	GLY	N-CA-C	-5.12	105.21	112.37
1	D	13	ASP	N-CA-CB	-5.09	102.84	110.73
1	D	258	ILE	N-CA-C	-5.03	105.64	110.72
1	C	315	GLN	N-CA-C	-5.01	105.91	112.23

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	136	ASN	Peptide
1	C	139	LEU	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	2606	0	2587	48	0
1	B	2606	0	2587	57	0
1	C	2599	0	2578	59	0
1	D	2599	0	2578	70	0
2	A	90	0	0	2	0
2	B	69	0	0	1	0
2	C	73	0	0	1	0
2	D	87	0	0	3	0
All	All	10729	0	10330	225	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (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:C:137:ILE:O	1:C:140:GLY:HA2	1.34	1.27
1:A:24:PHE:HB3	1:A:280:ILE:CD1	1.66	1.26
1:C:136:ASN:HB3	1:C:137:ILE:C	1.73	1.14
1:C:137:ILE:HD12	1:C:137:ILE:H	1.07	1.13
1:C:137:ILE:H	1:C:137:ILE:CD1	1.63	1.11
1:A:24:PHE:CB	1:A:280:ILE:HD11	1.82	1.08
1:C:137:ILE:HD12	1:C:137:ILE:N	1.78	0.97
1:C:170:ARG:HH11	1:C:170:ARG:CG	1.80	0.94
1:D:95:GLU:OE1	1:D:95:GLU:HA	1.68	0.93
1:B:238:TRP:O	1:B:242:THR:HG23	1.67	0.93
1:D:27:GLU:OE1	1:D:324:ARG:HD3	1.70	0.92
1:A:24:PHE:HB3	1:A:280:ILE:HD11	0.92	0.92
1:D:238:TRP:O	1:D:242:THR:HG23	1.68	0.91
1:C:137:ILE:C	1:C:139:LEU:H	1.75	0.90
1:D:122:VAL:HG21	1:D:157:ILE:HD11	1.53	0.90
1:A:26:MET:O	1:A:26:MET:SD	2.30	0.90
1:B:238:TRP:O	1:B:242:THR:CG2	2.22	0.88
1:C:170:ARG:HH11	1:C:170:ARG:HG2	1.39	0.87
1:D:238:TRP:O	1:D:242:THR:CG2	2.25	0.84
1:C:170:ARG:HG2	1:C:170:ARG:NH1	1.93	0.82
1:D:59:GLY:HA3	1:D:70:LEU:HD23	1.58	0.82
1:C:170:ARG:HH11	1:C:170:ARG:CB	1.94	0.81
1:A:26:MET:SD	1:A:26:MET:C	2.64	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:136:ASN:HB3	1:C:137:ILE:O	1.81	0.80
1:A:89:PHE:CE2	1:A:180:PRO:HA	2.16	0.79
1:D:1:MET:HE1	1:D:4:SER:OG	1.82	0.78
1:C:136:ASN:HB3	1:C:138:ILE:N	2.02	0.75
1:C:1:MET:HE1	1:C:85:TYR:H	1.53	0.72
1:D:1:MET:HE1	1:D:4:SER:HG	1.52	0.71
1:A:24:PHE:CB	1:A:280:ILE:CD1	2.52	0.70
1:D:333:GLN:H	1:D:333:GLN:CD	1.99	0.69
1:B:25:THR:HG21	1:B:275:LYS:HD3	1.74	0.69
1:D:31:LYS:HB2	1:D:320:PHE:O	1.93	0.68
1:C:137:ILE:C	1:C:139:LEU:N	2.42	0.67
1:D:1:MET:CE	1:D:4:SER:OG	2.42	0.67
1:D:333:GLN:CD	1:D:333:GLN:N	2.53	0.66
1:C:32:VAL:HG13	1:C:320:PHE:HB2	1.77	0.66
1:C:136:ASN:CB	1:C:137:ILE:C	2.61	0.66
1:C:170:ARG:HH11	1:C:170:ARG:HB3	1.60	0.65
1:C:137:ILE:O	1:C:139:LEU:N	2.30	0.65
1:D:136:ASN:HA	1:D:137:ILE:HD13	1.80	0.63
1:A:1:MET:HE1	1:A:84:LEU:HA	1.81	0.62
1:D:138:ILE:HD13	2:D:4015:HOH:O	1.98	0.62
1:B:27:GLU:HG2	1:B:280:ILE:CG2	2.30	0.61
1:A:42:ARG:HG2	1:A:50:VAL:HG22	1.81	0.61
1:B:87:ALA:O	1:B:88:THR:OG1	2.14	0.61
1:D:4:SER:HB3	1:D:21:THR:O	2.01	0.60
1:A:89:PHE:CZ	1:A:180:PRO:HB3	2.35	0.60
1:B:270:LEU:HD23	1:B:276:THR:HA	1.83	0.59
2:A:1068:HOH:O	1:D:276:THR:HG21	2.03	0.59
1:D:1:MET:HE2	1:D:85:TYR:HB2	1.85	0.59
1:D:119:VAL:HA	1:D:122:VAL:HG13	1.84	0.59
1:D:95:GLU:OE1	1:D:95:GLU:CA	2.48	0.58
1:A:57:PHE:HE1	1:A:70:LEU:HD13	1.69	0.58
1:C:43:LEU:HD12	1:C:103:ILE:HG13	1.84	0.58
1:A:120:ASP:OD2	1:A:170:ARG:NH2	2.37	0.57
1:B:102:GLY:HA3	1:B:132:LEU:HD22	1.86	0.57
1:D:222:LEU:HD11	1:D:234:ARG:HG3	1.86	0.57
1:C:149:PHE:HE2	1:C:159:ILE:HD13	1.69	0.57
1:A:20:ARG:HD2	1:A:72:ASP:OD2	2.05	0.57
1:B:136:ASN:N	1:B:136:ASN:ND2	2.52	0.57
1:B:222:LEU:HD22	1:B:223:PRO:HD2	1.87	0.56
1:C:83:MET:C	1:C:84:LEU:HD12	2.30	0.56
1:D:118:THR:O	1:D:122:VAL:HG13	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:GLN:HE21	1:D:2:LEU:HD22	1.71	0.56
1:B:301:ARG:HB2	1:C:301:ARG:HG3	1.87	0.56
1:C:2:LEU:HD23	1:C:25:THR:HG23	1.88	0.56
1:B:179:SER:HB3	1:B:180:PRO:HA	1.88	0.56
1:D:122:VAL:HG21	1:D:157:ILE:CD1	2.31	0.55
1:B:25:THR:CG2	1:B:275:LYS:HD3	2.37	0.55
1:D:137:ILE:HD13	1:D:137:ILE:N	2.22	0.55
1:A:4:SER:HB3	1:A:21:THR:O	2.07	0.55
1:B:300:SER:OG	1:C:300:SER:O	2.25	0.55
1:D:11:THR:OG1	1:D:13:ASP:HB3	2.06	0.55
1:C:27:GLU:HB3	1:C:324:ARG:HH11	1.72	0.55
1:C:149:PHE:CE2	1:C:159:ILE:HD13	2.41	0.55
1:C:240:LYS:HD3	1:C:241:TYR:CZ	2.42	0.54
1:A:24:PHE:CD2	1:A:26:MET:O	2.60	0.54
1:A:126:LEU:HD12	1:A:159:ILE:CD1	2.37	0.54
1:C:150:THR:HA	1:C:155:GLU:O	2.07	0.54
1:A:119:VAL:HG13	1:A:157:ILE:HG21	1.90	0.54
1:C:29:ASP:OD1	1:C:29:ASP:N	2.35	0.54
1:C:39:TYR:CE1	1:C:317:LEU:HD13	2.42	0.54
1:D:5:SER:HA	1:D:177:THR:HG22	1.90	0.54
1:D:119:VAL:O	1:D:122:VAL:HG22	2.08	0.53
1:C:25:THR:HA	1:C:276:THR:O	2.07	0.53
1:D:119:VAL:HA	1:D:122:VAL:CG1	2.39	0.53
1:B:83:MET:C	1:B:84:LEU:HD12	2.33	0.53
1:C:31:LYS:HB2	1:C:320:PHE:O	2.09	0.53
1:B:24:PHE:HD2	1:B:26:MET:O	1.90	0.53
1:D:122:VAL:CG2	1:D:123:ILE:N	2.72	0.53
1:A:109:ILE:HG22	1:A:113:LEU:HD22	1.89	0.53
1:B:34:ILE:HD13	1:B:310:GLU:HG3	1.90	0.53
1:A:184:TRP:CD1	1:C:184:TRP:CD1	2.97	0.52
1:A:103:ILE:CG2	1:A:131:LEU:HD12	2.40	0.52
1:B:136:ASN:N	1:B:136:ASN:HD22	2.08	0.52
1:C:208:LEU:HD13	1:C:210:LEU:HD13	1.91	0.52
1:B:204:MET:HA	1:B:208:LEU:O	2.10	0.51
1:C:136:ASN:CB	1:C:137:ILE:O	2.56	0.51
1:D:222:LEU:HD22	1:D:223:PRO:HD2	1.92	0.51
1:B:1:MET:N	1:B:24:PHE:CE1	2.75	0.51
1:B:332:ASN:O	1:B:334:VAL:HG23	2.10	0.51
1:A:27:GLU:O	1:A:27:GLU:HG2	2.09	0.51
1:A:126:LEU:HD12	1:A:159:ILE:HD13	1.92	0.51
1:C:10:ARG:O	1:C:244:LYS:HE3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:122:VAL:HG22	1:D:123:ILE:N	2.27	0.50
1:D:148:THR:HB	1:D:176:MET:CE	2.40	0.50
1:A:39:TYR:CE1	1:A:317:LEU:HD13	2.47	0.50
1:C:13:ASP:OD2	1:C:247:ASN:HA	2.11	0.50
1:D:238:TRP:O	1:D:242:THR:HG22	2.06	0.50
1:D:238:TRP:HA	1:D:238:TRP:CE3	2.46	0.50
1:D:242:THR:HG21	1:D:258:ILE:CG1	2.41	0.50
1:B:27:GLU:HG3	1:B:278:TYR:OH	2.12	0.49
1:A:3:GLY:C	1:A:4:SER:OG	2.54	0.49
1:C:57:PHE:HB3	1:C:75:ASN:HA	1.92	0.49
1:A:3:GLY:O	1:A:4:SER:OG	2.29	0.49
1:A:208:LEU:HD13	1:A:210:LEU:HD21	1.95	0.49
1:C:27:GLU:OE2	1:C:278:TYR:OH	2.22	0.49
1:C:80:MET:HE2	1:C:287:ALA:HB2	1.94	0.49
1:C:240:LYS:NZ	1:D:204:MET:O	2.45	0.49
1:D:102:GLY:HA3	1:D:132:LEU:HD22	1.95	0.49
1:C:27:GLU:HB3	1:C:324:ARG:NH1	2.28	0.49
1:D:109:ILE:HG22	1:D:113:LEU:HD22	1.95	0.49
1:D:146:HIS:HB2	1:D:160:GLU:HG2	1.93	0.49
1:D:43:LEU:HD12	1:D:43:LEU:HA	1.54	0.49
1:B:330:GLN:HB3	1:B:334:VAL:HG23	1.95	0.48
1:D:231:ARG:HG2	1:D:262:VAL:CG1	2.43	0.48
1:A:180:PRO:HG3	1:D:213:PHE:CE1	2.48	0.48
1:B:157:ILE:HD12	1:B:159:ILE:HD11	1.95	0.48
1:C:136:ASN:HB3	1:C:138:ILE:CA	2.44	0.48
1:B:125:LYS:HA	1:B:125:LYS:HD3	1.62	0.48
1:C:43:LEU:HD13	1:C:111:GLN:NE2	2.29	0.48
1:B:200:PRO:HG3	2:B:2049:HOH:O	2.14	0.48
1:D:79:LEU:HD13	1:D:113:LEU:HD12	1.96	0.47
1:B:146:HIS:HB2	1:B:160:GLU:HG2	1.95	0.47
1:A:234:ARG:HG3	1:A:234:ARG:NH1	2.29	0.47
1:A:76:GLU:O	1:A:290:LYS:HE2	2.14	0.47
1:C:138:ILE:HG13	1:C:138:ILE:O	2.14	0.47
1:C:193:ILE:HB	1:D:203:ILE:HG12	1.97	0.47
1:B:238:TRP:O	1:B:242:THR:HG22	2.07	0.47
1:D:320:PHE:N	1:D:320:PHE:CD1	2.83	0.47
1:B:324:ARG:HE	1:B:324:ARG:HB2	1.58	0.47
1:C:159:ILE:HD12	1:C:159:ILE:N	2.30	0.46
1:A:85:TYR:CZ	1:A:144:PRO:HD2	2.50	0.46
1:B:315:GLN:H	1:B:315:GLN:HG2	1.35	0.46
1:C:13:ASP:O	1:C:14:ASP:HB2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ARG:HG3	1:A:234:ARG:HH11	1.80	0.46
1:D:179:SER:HB3	1:D:180:PRO:HA	1.98	0.46
1:A:126:LEU:HD23	1:A:126:LEU:HA	1.76	0.46
1:D:46:LYS:HB2	1:D:134:GLU:OE2	2.16	0.46
1:B:43:LEU:HD13	1:B:111:GLN:NE2	2.30	0.45
1:B:300:SER:O	1:C:300:SER:OG	2.32	0.45
1:D:61:GLY:HA3	1:D:69:VAL:O	2.16	0.45
1:D:136:ASN:CA	1:D:137:ILE:HD13	2.46	0.45
1:D:238:TRP:HA	1:D:238:TRP:HE3	1.80	0.45
1:A:87:ALA:C	1:A:88:THR:HG23	2.42	0.45
1:D:119:VAL:CA	1:D:122:VAL:HG13	2.46	0.45
1:B:56:ALA:CB	1:B:312:LEU:HD22	2.46	0.45
1:B:213:PHE:CE1	1:C:180:PRO:HG3	2.52	0.45
1:C:5:SER:HA	1:C:177:THR:HG22	1.99	0.45
1:D:170:ARG:HB2	1:D:170:ARG:NH1	2.32	0.45
1:B:7:LEU:HA	1:B:174:GLY:O	2.17	0.45
1:C:333:GLN:H	1:C:333:GLN:HG3	1.52	0.44
1:C:42:ARG:O	1:C:111:GLN:NE2	2.50	0.44
1:A:266:LYS:HE3	1:A:278:TYR:CE2	2.53	0.44
1:A:146:HIS:ND1	1:A:160:GLU:OE2	2.48	0.44
1:B:136:ASN:HB2	1:B:138:ILE:HG13	1.99	0.44
1:D:119:VAL:C	1:D:122:VAL:HG13	2.43	0.44
1:B:27:GLU:OE1	1:B:324:ARG:HD3	2.18	0.44
1:B:38:ASN:HA	1:B:52:ASN:OD1	2.17	0.44
1:C:170:ARG:NH1	1:C:170:ARG:HB3	2.28	0.44
1:A:293:TYR:HA	1:A:303:SER:O	2.17	0.44
1:A:146:HIS:HB2	1:A:160:GLU:HG2	2.00	0.44
1:B:259:LEU:HD23	1:B:259:LEU:HA	1.82	0.44
1:C:12:THR:OG1	1:C:246:LYS:HA	2.17	0.44
1:D:138:ILE:H	1:D:138:ILE:HG13	1.63	0.44
1:A:40:GLY:O	1:A:41:ILE:HD13	2.18	0.44
1:B:238:TRP:HA	1:B:238:TRP:CE3	2.53	0.43
1:B:84:LEU:HD13	1:B:176:MET:CE	2.48	0.43
1:B:27:GLU:HG2	1:B:280:ILE:HG22	2.00	0.43
1:A:155:GLU:HG2	1:A:156:SER:N	2.33	0.43
1:D:148:THR:HB	1:D:176:MET:HE2	2.00	0.43
1:C:211:THR:OG1	1:C:212:PRO:HD2	2.19	0.43
1:D:222:LEU:CD1	1:D:234:ARG:HG3	2.47	0.43
1:A:179:SER:O	1:A:228:PRO:HB2	2.19	0.43
1:B:4:SER:CB	1:B:21:THR:O	2.67	0.43
1:B:208:LEU:HA	1:B:208:LEU:HD23	1.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LEU:HD12	1:A:317:LEU:HA	1.86	0.43
1:B:27:GLU:HA	1:B:28:PRO:HD3	1.77	0.43
1:C:214:GLY:C	2:C:3047:HOH:O	2.62	0.43
1:D:293:TYR:HA	1:D:303:SER:O	2.19	0.43
1:D:211:THR:HG22	2:D:4049:HOH:O	2.19	0.43
1:A:323:ASP:OD1	1:A:323:ASP:C	2.61	0.43
1:D:59:GLY:HA3	1:D:70:LEU:CD2	2.38	0.43
1:D:118:THR:O	1:D:122:VAL:CG1	2.67	0.43
1:B:76:GLU:O	1:B:290:LYS:HE2	2.19	0.42
1:A:298:ASP:OD2	1:A:324:ARG:HG2	2.19	0.42
1:D:34:ILE:HG12	1:D:58:VAL:HG23	2.02	0.42
1:B:101:ARG:HE	1:B:101:ARG:HB3	1.23	0.42
1:D:327:ASP:HB2	2:D:4086:HOH:O	2.19	0.42
1:B:264:ILE:HA	1:B:265:PRO:HD3	1.91	0.42
1:B:24:PHE:CD2	1:B:26:MET:O	2.72	0.42
1:B:238:TRP:HA	1:B:238:TRP:HE3	1.85	0.42
1:D:122:VAL:CG2	1:D:157:ILE:HD11	2.38	0.42
1:B:150:THR:HA	1:B:155:GLU:O	2.20	0.42
1:D:11:THR:HG1	1:D:15:LYS:H	1.68	0.42
1:D:332:ASN:O	1:D:333:GLN:C	2.58	0.42
1:B:119:VAL:HG21	1:B:155:GLU:HG2	2.00	0.41
1:A:87:ALA:O	1:A:88:THR:OG1	2.16	0.41
1:A:222:LEU:HD12	1:A:238:TRP:CZ2	2.56	0.41
1:C:9:ILE:HG23	1:C:255:LEU:HD21	2.02	0.41
1:A:25:THR:HG23	1:A:275:LYS:HB3	2.01	0.41
1:B:84:LEU:HD13	1:B:176:MET:HE2	2.01	0.41
1:D:150:THR:HA	1:D:155:GLU:O	2.21	0.41
1:B:5:SER:O	1:B:20:ARG:HA	2.21	0.41
1:B:27:GLU:HG2	1:B:280:ILE:HG21	2.02	0.41
2:A:1068:HOH:O	1:D:276:THR:CG2	2.66	0.41
1:B:4:SER:HB3	1:B:21:THR:O	2.19	0.41
1:B:77:LYS:HD2	1:B:77:LYS:HA	1.91	0.41
1:C:76:GLU:O	1:C:290:LYS:HE2	2.21	0.41
1:D:45:GLU:OE1	1:D:107:TYR:OH	2.36	0.41
1:D:9:ILE:HG12	1:D:255:LEU:HD21	2.03	0.41
1:D:270:LEU:HD23	1:D:276:THR:HA	2.02	0.41
1:A:89:PHE:CE2	1:A:180:PRO:CA	2.97	0.40
1:B:37:ARG:HH21	1:B:312:LEU:HD12	1.86	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	332/338 (98%)	316 (95%)	15 (4%)	1 (0%)	36	55
1	B	332/338 (98%)	309 (93%)	22 (7%)	1 (0%)	36	55
1	C	331/338 (98%)	311 (94%)	20 (6%)	0	100	100
1	D	331/338 (98%)	313 (95%)	17 (5%)	1 (0%)	36	55
All	All	1326/1352 (98%)	1249 (94%)	74 (6%)	3 (0%)	43	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	163	LYS
1	A	119	VAL
1	B	180	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	290/294 (99%)	267 (92%)	23 (8%)	11	24
1	B	290/294 (99%)	253 (87%)	37 (13%)	4	9
1	C	289/294 (98%)	253 (88%)	36 (12%)	4	9
1	D	289/294 (98%)	256 (89%)	33 (11%)	5	12
All	All	1158/1176 (98%)	1029 (89%)	129 (11%)	6	12

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	SER
1	A	26	MET
1	A	27	GLU
1	A	31	LYS
1	A	32	VAL
1	A	43	LEU
1	A	44	LEU
1	A	49	VAL
1	A	70	LEU
1	A	85	TYR
1	A	106	VAL
1	A	113	LEU
1	A	137	ILE
1	A	170	ARG
1	A	208	LEU
1	A	222	LEU
1	A	246	LYS
1	A	276	THR
1	A	317	LEU
1	A	324	ARG
1	A	328	ILE
1	A	331	LEU
1	B	1	MET
1	B	4	SER
1	B	26	MET
1	B	37	ARG
1	B	43	LEU
1	B	44	LEU
1	B	48	ASN
1	B	50	VAL
1	B	101	ARG
1	B	105	PRO
1	B	113	LEU
1	B	125	LYS
1	B	126	LEU
1	B	132	LEU
1	B	133	ASN
1	B	136	ASN
1	B	138	ILE
1	B	145	LEU
1	B	170	ARG
1	B	171	LYS

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Mol	Chain	Res	Type
1	B	193	ILE
1	B	204	MET
1	B	208	LEU
1	B	209	ASP
1	B	222	LEU
1	B	233	LEU
1	B	238	TRP
1	B	242	THR
1	B	244	LYS
1	B	276	THR
1	B	280	ILE
1	B	300	SER
1	B	315	GLN
1	B	317	LEU
1	B	325	LYS
1	B	331	LEU
1	B	333	GLN
1	C	1	MET
1	C	2	LEU
1	C	26	MET
1	C	27	GLU
1	C	29	ASP
1	C	31	LYS
1	C	32	VAL
1	C	34	ILE
1	C	42	ARG
1	C	43	LEU
1	C	44	LEU
1	C	46	LYS
1	C	95	GLU
1	C	98	LYS
1	C	106	VAL
1	C	113	LEU
1	C	126	LEU
1	C	137	ILE
1	C	139	LEU
1	C	153	SER
1	C	155	GLU
1	C	163	LYS
1	C	170	ARG
1	C	208	LEU
1	C	209	ASP

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Mol	Chain	Res	Type
1	C	210	LEU
1	C	222	LEU
1	C	246	LYS
1	C	260	SER
1	C	268	VAL
1	C	273	GLU
1	C	276	THR
1	C	317	LEU
1	C	319	THR
1	C	325	LYS
1	C	333	GLN
1	D	1	MET
1	D	4	SER
1	D	26	MET
1	D	27	GLU
1	D	31	LYS
1	D	43	LEU
1	D	70	LEU
1	D	79	LEU
1	D	95	GLU
1	D	106	VAL
1	D	113	LEU
1	D	122	VAL
1	D	126	LEU
1	D	132	LEU
1	D	137	ILE
1	D	138	ILE
1	D	139	LEU
1	D	145	LEU
1	D	163	LYS
1	D	171	LYS
1	D	222	LEU
1	D	238	TRP
1	D	242	THR
1	D	243	GLU
1	D	268	VAL
1	D	276	THR
1	D	280	ILE
1	D	290	LYS
1	D	312	LEU
1	D	315	GLN
1	D	317	LEU

Continued on next page...

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Mol	Chain	Res	Type
1	D	321	GLU
1	D	331	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	169	HIS
1	A	188	ASN
1	A	201	GLN
1	A	263	ASN
1	A	272	ASN
1	A	291	ASN
1	A	315	GLN
1	B	169	HIS
1	B	188	ASN
1	B	263	ASN
1	C	136	ASN
1	C	263	ASN
1	D	185	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 [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	334/338 (98%)	-1.70	0 100 100	15, 24, 42, 71	0
1	B	334/338 (98%)	-1.66	0 100 100	16, 26, 48, 67	0
1	C	333/338 (98%)	-1.67	0 100 100	15, 26, 44, 66	0
1	D	333/338 (98%)	-1.67	0 100 100	15, 26, 49, 62	0
All	All	1334/1352 (98%)	-1.67	0 100 100	15, 25, 46, 71	0

There are no RSRZ outliers to report.

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.