



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:16 PM UTC

PDB ID : 3RP2 / pdb_00003rp2
Title : THE STRUCTURE OF RAT MAST CELL PROTEASE II AT 1.9-
ANGSTROMS RESOLUTION
Authors : Reynolds, R.; Remington, S.; Weaver, L.; Fischer, R.; Anderson, W.; Ammon,
H.; Matthews, B.
Deposited on : 1984-09-10
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
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

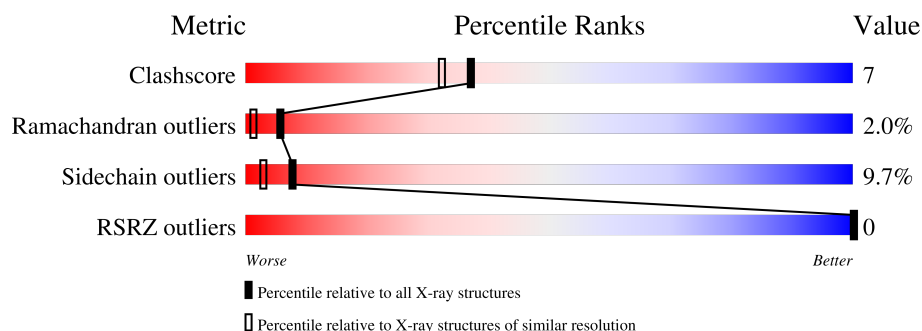
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)
RSRZ outliers	180081	7790 (1.90-1.90)

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

Mol	Chain	Length	Quality of chain
1	A	224	
1	B	224	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3575 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 RAT MAST CELL PROTEASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	224	Total	C	N	O	S	98	0	0
			1726	1106	298	311	11			
1	B	224	Total	C	N	O	S	88	0	0
			1726	1106	298	311	11			

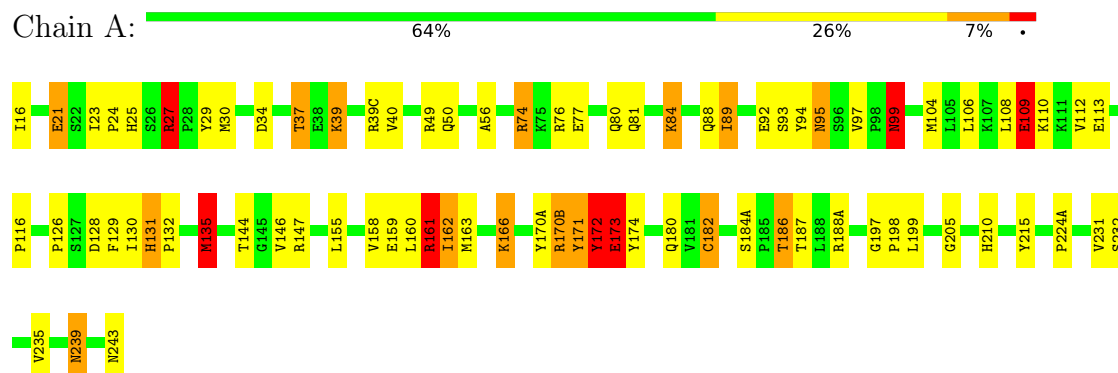
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	61	Total	O	0	0
			61	61		
2	B	62	Total	O	0	0
			62	62		

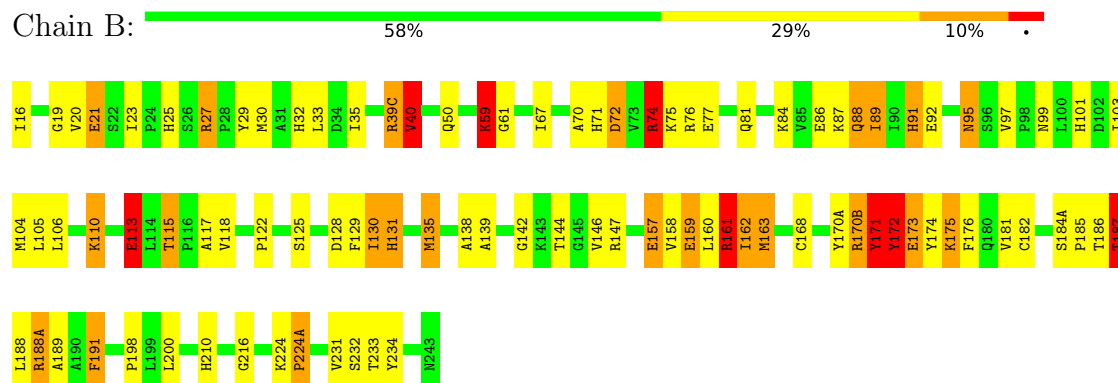
3 Residue-property plots

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: RAT MAST CELL PROTEASE II



• Molecule 1: RAT MAST CELL PROTEASE II



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	78.20Å 78.20Å 96.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	5.00 – 1.90 5.00 – 1.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (5.00-1.90) 42.1 (5.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$	-	Xtriage
Refinement program	EREF	Depositor
R, R_{free}	0.191 , (Not available) 0.183 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.70 , 125.0	EDS
L-test for twinning ¹	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l 0.084 for h,-h-k,-l 0.043 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3575	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows:

¹Theoretical 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	1.21	5/1770 (0.3%)	1.96	45/2406 (1.9%)
1	B	1.26	9/1770 (0.5%)	1.99	52/2406 (2.2%)
All	All	1.23	14/3540 (0.4%)	1.97	97/4812 (2.0%)

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	A	1	24
1	B	1	35
All	All	2	59

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	235	VAL	CA-CB	7.60	1.57	1.54
1	B	210	HIS	CD2-NE2	-6.16	1.31	1.37
1	A	39(C)	ARG	NE-CZ	-5.77	1.26	1.33
1	B	32	HIS	CD2-NE2	-5.67	1.31	1.37
1	B	187	THR	N-CA	5.62	1.52	1.46
1	A	210	HIS	CD2-NE2	-5.59	1.31	1.37
1	B	162	ILE	CA-CB	5.53	1.60	1.54
1	B	142	GLY	N-CA	5.46	1.51	1.45
1	A	131	HIS	CG-ND1	-5.30	1.32	1.38
1	B	172	TYR	C-N	5.26	1.41	1.33
1	B	173	GLU	N-CA	5.25	1.52	1.46
1	B	25	HIS	CG-ND1	-5.20	1.32	1.38
1	B	131	HIS	CG-ND1	-5.14	1.32	1.38
1	A	231	VAL	CA-CB	-5.08	1.48	1.54

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	172	TYR	CA-C-N	14.08	148.44	121.54
1	B	172	TYR	C-N-CA	14.08	148.44	121.54
1	A	172	TYR	CA-C-N	11.54	143.59	121.54
1	A	172	TYR	C-N-CA	11.54	143.59	121.54
1	A	182	CYS	CB-CA-C	-11.54	90.88	109.80
1	B	157	GLU	N-CA-CB	-10.37	93.65	111.69
1	B	174	TYR	N-CA-C	9.72	121.87	111.28
1	A	95	ASN	CA-CB-CG	9.53	122.13	112.60
1	B	224(A)	PRO	N-CA-CB	9.49	108.50	103.19
1	B	161	ARG	NE-CZ-NH2	-8.39	111.65	119.20
1	A	21	GLU	CB-CA-C	-8.38	95.81	109.72
1	B	182	CYS	N-CA-CB	-8.17	96.89	110.37
1	A	99	ASN	CA-CB-CG	-7.79	104.81	112.60
1	B	27	ARG	CD-NE-CZ	7.69	135.17	124.40
1	B	59	LYS	CB-CA-C	-7.58	97.64	109.61
1	A	40	VAL	N-CA-CB	-7.54	99.80	112.47
1	B	115	THR	N-CA-CB	-7.48	97.06	110.37
1	B	172	TYR	O-C-N	7.19	132.15	122.59
1	A	171	TYR	CA-CB-CG	7.14	126.75	113.90
1	A	37	THR	N-CA-CB	-7.12	100.17	110.36
1	B	74	ARG	N-CA-CB	-7.02	99.69	110.44
1	B	231	VAL	N-CA-C	6.94	118.53	110.62
1	B	39(C)	ARG	CB-CA-C	-6.82	99.10	110.29
1	B	173	GLU	O-C-N	-6.80	113.55	122.59
1	A	231	VAL	N-CA-C	6.71	117.47	110.62
1	B	40	VAL	CA-CB-CG1	6.68	121.75	110.40
1	A	224(A)	PRO	N-CA-CB	6.67	106.92	103.19
1	A	174	TYR	N-CA-C	6.62	119.32	111.71
1	B	171	TYR	CA-CB-CG	6.61	125.79	113.90
1	A	108	LEU	CA-C-N	6.56	128.97	120.44
1	A	108	LEU	C-N-CA	6.56	128.97	120.44
1	B	131	HIS	CA-CB-CG	6.53	120.33	113.80
1	B	131	HIS	CB-CA-C	-6.50	99.36	109.11
1	A	235	VAL	N-CA-CB	6.43	114.83	110.52
1	A	94	TYR	CA-C-N	-6.42	111.28	122.64
1	A	94	TYR	C-N-CA	-6.42	111.28	122.64
1	A	224(A)	PRO	O-C-N	6.39	124.25	121.31
1	B	95	ASN	N-CA-C	-6.35	101.39	110.59
1	A	171	TYR	CB-CA-C	-6.32	107.31	116.54
1	A	232	SER	N-CA-CB	-6.29	99.52	109.78
1	B	95	ASN	CA-CB-CG	6.20	118.80	112.60
1	A	95	ASN	N-CA-CB	6.19	120.47	110.51
1	A	25	HIS	CA-CB-CG	-6.13	107.67	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	PRO	N-CA-CB	6.12	109.02	103.33
1	A	197	GLY	CA-C-N	6.10	126.02	119.85
1	A	197	GLY	C-N-CA	6.10	126.02	119.85
1	A	24	PRO	N-CA-CB	6.06	108.64	103.19
1	B	113	GLU	CB-CG-CD	-6.01	102.38	112.60
1	A	131	HIS	CB-CA-C	-5.94	99.71	109.27
1	B	175	LYS	CB-CA-C	-5.92	99.67	110.63
1	B	89	ILE	N-CA-C	5.90	115.82	106.32
1	B	115	THR	CA-CB-CG2	5.90	120.53	110.50
1	B	130	ILE	CB-CA-C	-5.87	103.63	110.91
1	B	91	HIS	CA-CB-CG	-5.81	107.99	113.80
1	B	175	LYS	N-CA-CB	5.80	119.15	110.22
1	B	157	GLU	CB-CG-CD	-5.79	102.75	112.60
1	B	130	ILE	N-CA-CB	5.79	117.03	110.72
1	B	161	ARG	N-CA-CB	-5.79	101.38	110.69
1	A	131	HIS	CA-CB-CG	5.78	119.58	113.80
1	A	171	TYR	O-C-N	5.74	126.22	122.03
1	B	40	VAL	N-CA-CB	-5.73	102.81	112.44
1	A	146	VAL	O-C-N	5.69	127.39	121.87
1	B	50	GLN	OE1-CD-NE2	5.68	128.28	122.60
1	A	99	ASN	N-CA-CB	-5.66	103.84	112.28
1	B	122	PRO	N-CA-CB	5.60	108.22	103.35
1	B	110	LYS	CA-C-O	-5.58	114.92	121.44
1	B	188(A)	ARG	NE-CZ-NH1	-5.54	115.96	121.50
1	A	173	GLU	CA-C-N	5.53	128.24	120.28
1	A	173	GLU	C-N-CA	5.53	128.24	120.28
1	B	187	THR	CB-CA-C	-5.51	98.78	109.68
1	A	239	ASN	CA-CB-CG	-5.49	107.11	112.60
1	B	173	GLU	N-CA-C	5.48	122.48	110.80
1	A	126	PRO	N-CA-CB	5.45	108.93	103.48
1	A	215	TYR	N-CA-C	5.44	117.07	108.96
1	B	188(A)	ARG	CD-NE-CZ	-5.41	116.83	124.40
1	A	89	ILE	N-CA-CB	-5.40	105.19	111.83
1	B	67	ILE	N-CA-C	5.34	115.27	107.37
1	B	50	GLN	N-CA-C	5.33	121.53	114.12
1	A	37	THR	CA-CB-CG2	5.32	119.54	110.50
1	B	71	HIS	CA-CB-CG	-5.31	108.49	113.80
1	B	138	ALA	CA-C-O	-5.30	115.09	120.71
1	B	210	HIS	CA-CB-CG	-5.28	108.53	113.80
1	B	129	PHE	CA-C-N	-5.25	115.60	122.37
1	B	129	PHE	C-N-CA	-5.25	115.60	122.37
1	A	27	ARG	CB-CA-C	-5.25	102.95	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	SER	CA-C-N	5.22	127.53	120.38
1	B	232	SER	C-N-CA	5.22	127.53	120.38
1	A	132	PRO	N-CA-CB	5.21	107.96	103.27
1	B	158	VAL	CA-CB-CG1	5.20	119.23	110.40
1	B	20	VAL	CA-C-O	-5.15	116.26	121.67
1	A	231	VAL	CA-C-N	5.14	128.53	120.82
1	A	231	VAL	C-N-CA	5.14	128.53	120.82
1	A	93	SER	O-C-N	5.12	128.87	122.22
1	B	74	ARG	NE-CZ-NH2	-5.12	114.60	119.20
1	A	161	ARG	N-CA-CB	-5.04	102.63	110.55
1	B	142	GLY	N-CA-C	5.03	120.31	112.31
1	A	161	ARG	NE-CZ-NH1	5.00	126.50	121.50

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	242	ILE	CB
1	B	242	ILE	CB

All (59) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	GLU	Sidechain
1	A	110	LYS	Mainchain
1	A	112	VAL	Mainchain
1	A	116	PRO	Mainchain
1	A	128	ASP	Mainchain
1	A	131	HIS	Mainchain
1	A	135	MET	Mainchain
1	A	155	LEU	Mainchain
1	A	161	ARG	Sidechain
1	A	166	LYS	Mainchain
1	A	170(B)	ARG	Mainchain
1	A	180	GLN	Sidechain
1	A	205	GLY	Mainchain
1	A	21	GLU	Mainchain,Sidechain
1	A	239	ASN	Sidechain
1	A	27	ARG	Sidechain
1	A	39	LYS	Mainchain
1	A	49	ARG	Mainchain
1	A	50	GLN	Sidechain
1	A	74	ARG	Mainchain

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Mol	Chain	Res	Type	Group
1	A	76	ARG	Mainchain
1	A	92	GLU	Sidechain
1	A	99	ASN	Sidechain
1	B	110	LYS	Mainchain
1	B	113	GLU	Sidechain
1	B	118	VAL	Mainchain
1	B	128	ASP	Mainchain
1	B	131	HIS	Mainchain
1	B	139	ALA	Mainchain
1	B	157	GLU	Sidechain
1	B	159	GLU	Mainchain
1	B	161	ARG	Sidechain
1	B	163	MET	Mainchain
1	B	168	CYS	Mainchain
1	B	170(B)	ARG	Mainchain
1	B	171	TYR	Sidechain
1	B	175	LYS	Mainchain
1	B	188	LEU	Mainchain
1	B	189	ALA	Mainchain,Peptide
1	B	19	GLY	Mainchain
1	B	198	PRO	Mainchain
1	B	21	GLU	Sidechain
1	B	216	GLY	Mainchain
1	B	39(C)	ARG	Sidechain
1	B	59	LYS	Mainchain
1	B	61	GLY	Mainchain
1	B	70	ALA	Mainchain
1	B	72	ASP	Mainchain
1	B	74	ARG	Sidechain
1	B	75	LYS	Mainchain
1	B	76	ARG	Mainchain
1	B	77	GLU	Sidechain
1	B	86	GLU	Sidechain
1	B	87	LYS	Mainchain
1	B	88	GLN	Sidechain
1	B	95	ASN	Sidechain
1	B	99	ASN	Sidechain

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	1726	0	1724	22	20
1	B	1726	0	1724	25	27
2	A	61	0	0	0	3
2	B	62	0	0	1	1
All	All	3575	0	3448	46	47

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 7.

All (46) 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:A:161:ARG:HG3	1:A:163:MET:CE	2.03	0.89
1:A:161:ARG:HG3	1:A:163:MET:HE2	1.62	0.82
1:B:161:ARG:HG3	1:B:163:MET:CE	2.08	0.82
1:B:135:MET:HE2	1:B:159:GLU:HG2	1.63	0.81
1:A:162:ILE:HD11	1:A:199:LEU:HD21	1.61	0.80
1:A:135:MET:HE2	1:A:159:GLU:HG2	1.64	0.77
1:B:81:GLN:HE22	1:B:113:GLU:H	1.34	0.74
1:B:115:THR:HG21	2:B:257:HOH:O	1.89	0.71
1:B:104:MET:HE3	1:B:106:LEU:HD21	1.82	0.60
1:A:81:GLN:HE22	1:A:113:GLU:H	1.51	0.56
1:B:135:MET:HE3	1:B:160:LEU:C	2.31	0.56
1:B:135:MET:CE	1:B:159:GLU:HG2	2.35	0.54
1:A:163:MET:HB2	1:A:182:CYS:HB3	1.89	0.53
1:B:35:ILE:HB	1:B:40:VAL:HG12	1.91	0.52
1:A:161:ARG:HG3	1:A:163:MET:HE1	1.88	0.52
1:A:163:MET:HB2	1:A:182:CYS:CB	2.40	0.51
1:B:176:PHE:CD1	1:B:233:THR:HG21	2.46	0.50
1:B:184(A):SER:C	1:B:186:THR:H	2.21	0.49
1:B:16:ILE:O	1:B:144:THR:HA	2.12	0.49
1:A:135:MET:HE3	1:A:160:LEU:O	2.13	0.49
1:B:72:ASP:OD2	1:B:74:ARG:HB3	2.13	0.48
1:B:91:HIS:HB2	1:B:103:ILE:HG23	1.94	0.48
1:A:27:ARG:HG3	1:A:29:TYR:OH	2.13	0.48
1:B:161:ARG:HG3	1:B:163:MET:HE1	1.92	0.48
1:B:115:THR:HG22	1:B:117:ALA:H	1.78	0.48
1:A:104:MET:HE3	1:A:106:LEU:HD21	1.98	0.46
1:A:135:MET:CE	1:A:159:GLU:HG2	2.39	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:THR:HG22	1:A:39:LYS:H	1.82	0.45
1:B:27:ARG:NH1	1:B:200:LEU:HD13	2.32	0.45
1:A:135:MET:HE2	1:A:135:MET:HB3	1.93	0.44
1:A:16:ILE:O	1:A:144:THR:HA	2.18	0.43
1:A:39:LYS:HA	1:B:147:ARG:HD2	2.00	0.43
1:B:27:ARG:HG2	1:B:29:TYR:OH	2.17	0.43
1:B:187:THR:HB	1:B:188(A):ARG:HG3	2.00	0.43
1:B:146:VAL:HA	1:B:191:PHE:CE2	2.53	0.42
1:A:135:MET:HE3	1:A:160:LEU:C	2.44	0.42
1:B:188(A):ARG:HH11	1:B:188(A):ARG:HD3	1.47	0.42
1:A:77:GLU:HB2	1:A:80:GLN:HG3	2.02	0.42
1:B:27:ARG:HB3	1:B:30:MET:HG2	2.01	0.41
1:A:56:ALA:HA	1:A:104:MET:HB2	2.03	0.41
1:A:184(A):SER:C	1:A:186:THR:H	2.29	0.41
1:B:23:ILE:HG21	1:B:23:ILE:HD13	1.80	0.41
1:A:84:LYS:O	1:A:109:GLU:HB2	2.20	0.41
1:B:74:ARG:HB3	1:B:74:ARG:HE	1.62	0.40
1:B:101:HIS:HD2	1:B:234:TYR:OH	2.04	0.40
1:A:158:VAL:CG2	1:A:188(A):ARG:HD2	2.52	0.40

All (47) 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:B:88:GLN:CA	1:B:170(A):TYR:CE1[2_545]	0.66	1.54
1:B:88:GLN:C	1:B:170(A):TYR:CZ[2_545]	0.77	1.43
1:A:88:GLN:C	1:A:170(A):TYR:CZ[3_664]	0.87	1.33
1:B:88:GLN:O	1:B:170(A):TYR:CD2[2_545]	0.89	1.31
1:A:88:GLN:O	1:A:170(A):TYR:CZ[3_664]	0.91	1.29
1:A:88:GLN:C	1:A:170(A):TYR:OH[3_664]	0.94	1.26
1:B:88:GLN:C	1:B:170(A):TYR:CE2[2_545]	0.96	1.24
1:B:89:ILE:N	1:B:170(A):TYR:CE2[2_545]	0.96	1.24
1:A:88:GLN:O	1:A:170(A):TYR:CE2[3_664]	0.98	1.22
1:B:88:GLN:CB	1:B:170(A):TYR:CE1[2_545]	1.01	1.19
1:B:88:GLN:O	1:B:170(A):TYR:CG[2_545]	1.07	1.13
1:A:23:ILE:CD1	2:B:248:HOH:O[2_555]	1.20	1.00
1:A:88:GLN:CA	1:A:170(A):TYR:OH[3_664]	1.23	0.97
1:B:89:ILE:N	1:B:170(A):TYR:CZ[2_545]	1.25	0.95
1:B:88:GLN:CA	1:B:170(A):TYR:CZ[2_545]	1.27	0.93
1:A:89:ILE:N	1:A:170(A):TYR:OH[3_664]	1.31	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:GLN:O	1:B:170(A):TYR:CE2[2_545]	1.41	0.79
1:B:88:GLN:C	1:B:170(A):TYR:CE1[2_545]	1.49	0.71
1:B:88:GLN:CB	1:B:170(A):TYR:CD1[2_545]	1.50	0.70
1:B:89:ILE:CA	1:B:170(A):TYR:CE2[2_545]	1.63	0.57
1:B:88:GLN:O	1:B:170(A):TYR:CD1[2_545]	1.64	0.56
1:B:23:ILE:CG1	2:A:248:HOH:O[3_554]	1.65	0.55
1:B:89:ILE:N	1:B:170(A):TYR:OH[2_545]	1.66	0.54
1:A:88:GLN:CA	1:A:170(A):TYR:CZ[3_664]	1.68	0.52
1:B:88:GLN:C	1:B:170(A):TYR:CD2[2_545]	1.69	0.51
1:A:88:GLN:O	1:A:170(A):TYR:CE1[3_664]	1.74	0.46
1:A:88:GLN:C	1:A:170(A):TYR:CE2[3_664]	1.75	0.45
1:A:88:GLN:N	1:A:170(A):TYR:CE1[3_664]	1.79	0.41
1:A:88:GLN:O	1:A:170(A):TYR:CD2[3_664]	1.81	0.39
1:B:88:GLN:N	1:B:170(A):TYR:CE1[2_545]	1.85	0.35
1:A:88:GLN:CA	1:A:170(A):TYR:CE1[3_664]	1.88	0.32
1:B:88:GLN:CA	1:B:170(A):TYR:CD1[2_545]	1.88	0.32
1:B:88:GLN:O	1:B:170(A):TYR:CZ[2_545]	1.88	0.32
1:B:105:LEU:O	1:B:170(A):TYR:OH[2_545]	1.91	0.29
1:B:23:ILE:CD1	2:A:248:HOH:O[3_554]	1.92	0.28
1:A:166:LYS:NZ	2:A:265:HOH:O[2_655]	1.94	0.26
1:A:89:ILE:N	1:A:170(A):TYR:CZ[3_664]	1.96	0.24
1:B:88:GLN:O	1:B:170(A):TYR:CE1[2_545]	1.98	0.22
1:A:88:GLN:C	1:A:170(A):TYR:CE1[3_664]	2.01	0.19
1:B:88:GLN:C	1:B:170(A):TYR:CD1[2_545]	2.04	0.16
1:A:88:GLN:N	1:A:170(A):TYR:OH[3_664]	2.06	0.14
1:B:88:GLN:CA	1:B:170(A):TYR:OH[2_545]	2.06	0.14
1:A:88:GLN:O	1:A:170(A):TYR:OH[3_664]	2.07	0.13
1:A:88:GLN:N	1:A:170(A):TYR:CZ[3_664]	2.09	0.11
1:B:88:GLN:C	1:B:170(A):TYR:OH[2_545]	2.09	0.11
1:B:88:GLN:C	1:B:170(A):TYR:CG[2_545]	2.12	0.08
1:A:88:GLN:CB	1:A:170(A):TYR:CE1[3_664]	2.16	0.04

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	222/224 (99%)	204 (92%)	14 (6%)	4 (2%)	6	1
1	B	222/224 (99%)	199 (90%)	18 (8%)	5 (2%)	5	1
All	All	444/448 (99%)	403 (91%)	32 (7%)	9 (2%)	6	1

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	170(B)	ARG
1	A	173	GLU
1	B	170(B)	ARG
1	B	173	GLU
1	A	172	TYR
1	A	97	VAL
1	B	97	VAL
1	B	172	TYR
1	B	185	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	186/190 (98%)	168 (90%)	18 (10%)	8	3
1	B	186/190 (98%)	168 (90%)	18 (10%)	8	3
All	All	372/380 (98%)	336 (90%)	36 (10%)	8	3

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	MET
1	A	34	ASP
1	A	74	ARG
1	A	84	LYS
1	A	95	ASN
1	A	99	ASN
1	A	109	GLU

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Mol	Chain	Res	Type
1	A	129	PHE
1	A	130	ILE
1	A	135	MET
1	A	147	ARG
1	A	162	ILE
1	A	171	TYR
1	A	172	TYR
1	A	173	GLU
1	A	186	THR
1	A	187	THR
1	A	243	ASN
1	B	21	GLU
1	B	33	LEU
1	B	40	VAL
1	B	59	LYS
1	B	84	LYS
1	B	92	GLU
1	B	125	SER
1	B	130	ILE
1	B	135	MET
1	B	161	ARG
1	B	162	ILE
1	B	171	TYR
1	B	172	TYR
1	B	181	VAL
1	B	187	THR
1	B	191	PHE
1	B	224	LYS
1	B	224(A)	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	HIS
1	A	81	GLN
1	A	101	HIS
1	A	180	GLN
1	A	221	HIS
1	A	239	ASN
1	B	81	GLN
1	B	180	GLN
1	B	239	ASN

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	219/224 (97%)	-0.84	0 100 100	5, 21, 33, 40	19 (8%)
1	B	219/224 (97%)	-0.93	0 100 100	6, 17, 31, 40	19 (8%)
All	All	438/448 (97%)	-0.88	0 100 100	5, 19, 33, 40	38 (8%)

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.