Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 05:13 PM EDT

PDB ID	:	3RP2
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 (i) 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 (1)) were used in the production of this report:

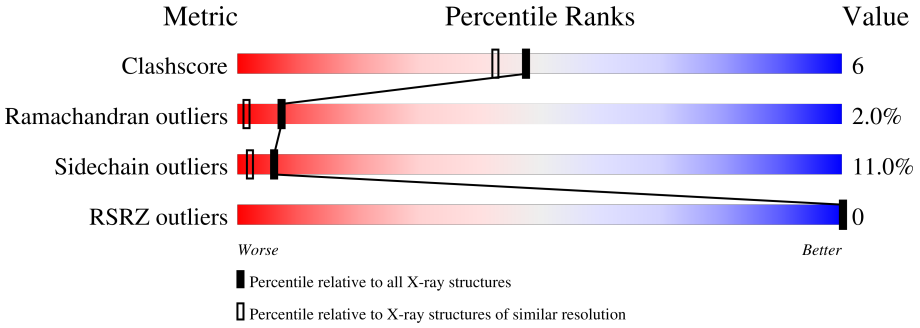
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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 <=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	71% 20% 7% •
1	B	224	64% 23% 9% •

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	224	1726	1106	298	311	11	98	0	0
1	B	224	1726	1106	298	311	11	88	0	0

- Molecule 2 is water.

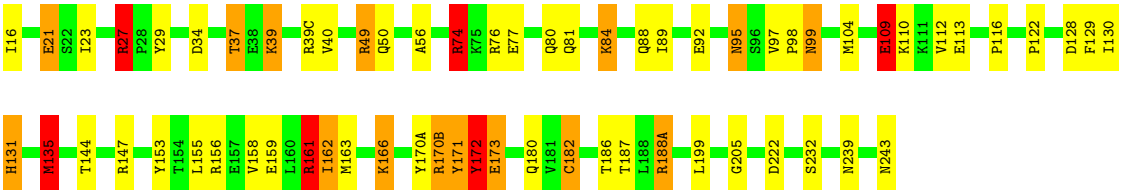
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
2	A	61	61	61	0	0
2	B	62	62	62	0	0

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.

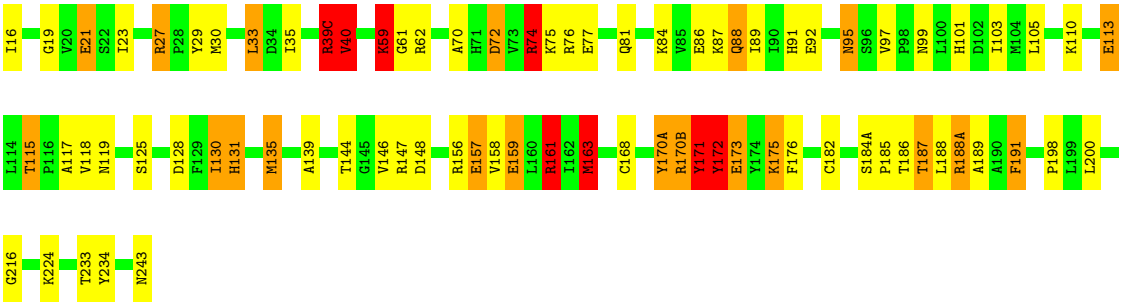
- Molecule 1: RAT MAST CELL PROTEASE II

Chain A:



- Molecule 1: RAT MAST CELL PROTEASE II

Chain B:



4 Data and refinement statistics (i)

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) 44.5 (5.00-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$	-	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)	0.74 , 131.5	EDS
L-test for twinning[1]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	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:

[1]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	0.86	0/1770	1.55	22/2406 (0.9%)
1	B	0.90	0/1770	1.63	33/2406 (1.4%)
All	All	0.88	0/3540	1.59	55/4812 (1.1%)

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	A	1	24
1	B	1	35
All	All	2	59

There are no bond length outliers.

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	161	ARG	NE-CZ-NH2	-17.30	111.65	120.30
1	A	161	ARG	NE-CZ-NH1	12.41	126.50	120.30
1	B	74	ARG	NE-CZ-NH2	-11.41	114.60	120.30
1	B	172	TYR	C-N-CA	10.70	148.44	121.70
1	A	182	CYS	CB-CA-C	-9.76	90.88	110.40
1	B	157	GLU	N-CA-CB	-9.41	93.65	110.60
1	A	27	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	A	172	TYR	C-N-CA	8.76	143.59	121.70
1	B	188(A)	ARG	NE-CZ-NH1	-8.68	115.96	120.30
1	B	171	TYR	CB-CG-CD1	8.47	126.08	121.00
1	B	27	ARG	CD-NE-CZ	8.27	135.17	123.60
1	B	171	TYR	CB-CG-CD2	-8.22	116.07	121.00
1	A	171	TYR	CB-CG-CD1	7.99	125.79	121.00
1	B	182	CYS	N-CA-CB	-7.61	96.89	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	232	SER	N-CA-CB	-7.32	99.52	110.50
1	A	21	GLU	CB-CA-C	-7.29	95.81	110.40
1	B	33	LEU	CB-CG-CD1	7.26	123.34	111.00
1	B	40	VAL	CA-CB-CG1	7.23	121.75	110.90
1	A	188(A)	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	171	TYR	CA-CB-CG	7.03	126.75	113.40
1	B	115	THR	N-CA-CB	-6.97	97.06	110.30
1	A	171	TYR	CB-CG-CD2	-6.94	116.83	121.00
1	B	161	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	39(C)	ARG	NE-CZ-NH1	-6.83	116.88	120.30
1	B	171	TYR	CA-CB-CG	6.52	125.79	113.40
1	A	49	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	A	222	ASP	CB-CG-OD1	6.39	124.05	118.30
1	B	59	LYS	CB-CA-C	-6.38	97.64	110.40
1	B	27	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	B	130	ILE	CG1-CB-CG2	6.21	125.05	111.40
1	B	172	TYR	CB-CG-CD1	-6.14	117.32	121.00
1	B	74	ARG	N-CA-CB	-6.06	99.69	110.60
1	A	161	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	B	172	TYR	O-C-N	5.91	132.15	122.70
1	B	115	THR	CA-CB-CG2	5.81	120.53	112.40
1	B	163	MET	CG-SD-CE	-5.79	90.94	100.20
1	A	156	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	B	173	GLU	O-C-N	-5.72	113.55	122.70
1	B	39(C)	ARG	CB-CA-C	-5.65	99.10	110.40
1	B	156	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	B	158	VAL	CA-CB-CG1	5.56	119.23	110.90
1	B	131	HIS	CB-CA-C	-5.52	99.36	110.40
1	A	95	ASN	N-CA-CB	5.48	120.47	110.60
1	B	175	LYS	CB-CA-C	-5.37	99.67	110.40
1	A	131	HIS	CB-CA-C	-5.34	99.71	110.40
1	A	37	THR	N-CA-CB	-5.33	100.17	110.30
1	A	40	VAL	N-CA-CB	-5.32	99.80	111.50
1	A	153	TYR	CB-CG-CD1	-5.30	117.82	121.00
1	A	74	ARG	NE-CZ-NH1	-5.22	117.69	120.30
1	B	62	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	B	161	ARG	N-CA-CB	-5.12	101.38	110.60
1	A	37	THR	CA-CB-CG2	5.10	119.54	112.40
1	B	39(C)	ARG	NE-CZ-NH2	5.04	122.82	120.30
1	B	157	GLU	OE1-CD-OE2	-5.04	117.25	123.30
1	B	40	VAL	CG1-CB-CG2	5.04	118.96	110.90

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
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

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Mol	Chain	Res	Type	Group
1	B	188	LEU	Mainchain
1	B	189	ALA	Peptide,Mainchain
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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1726	0	1724	17	20
1	B	1726	0	1724	24	27
2	A	61	0	0	0	3
2	B	62	0	0	1	1
All	All	3575	0	3448	40	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 6.

All (40) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:MET:HE2	1:B:159:GLU:HG2	1.54	0.90
1:A:161:ARG:HG3	1:A:163:MET:CE	2.03	0.89
1:B:161:ARG:HG3	1:B:163:MET:CE	2.08	0.82
1:A:162:ILE:HD11	1:A:199:LEU:HD21	1.61	0.80
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:A:161:ARG:HG3	1:A:163:MET:HE2	1.70	0.71
1:A:161:ARG:HG3	1:A:163:MET:HE1	1.79	0.60
1:A:81:GLN:HE22	1:A:113:GLU:H	1.51	0.56
1:A:163:MET:HB2	1:A:182:CYS:HB3	1.89	0.53
1:A:135:MET:CE	1:A:159:GLU:HG2	2.39	0.53
1:A:135:MET:HE1	1:A:159:GLU:HG2	1.90	0.53
1:B:35:ILE:HB	1:B:40:VAL:HG12	1.91	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:135:MET:CE	1:B:159:GLU:HG2	2.35	0.49
1:B:16:ILE:O	1:B:144:THR:HA	2.12	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:115:THR:HG22	1:B:117:ALA:H	1.78	0.48
1:B:161:ARG:HG3	1:B:163:MET:HE3	1.97	0.46
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:B:184(A):SER:C	1:B:186:THR:H	2.21	0.45
1:B:161:ARG:HG3	1:B:163:MET:HE1	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 (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	222/224 (99%)	204 (92%)	14 (6%)	4 (2%)	8 2
1	B	222/224 (99%)	199 (90%)	18 (8%)	5 (2%)	6 1
All	All	444/448 (99%)	403 (91%)	32 (7%)	9 (2%)	7 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 (i)

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%)	166 (89%)	20 (11%)	6 2
1	B	186/190 (98%)	165 (89%)	21 (11%)	6 2
All	All	372/380 (98%)	331 (89%)	41 (11%)	6 2

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	ARG
1	A	34	ASP
1	A	74	ARG
1	A	84	LYS
1	A	95	ASN
1	A	98	PRO
1	A	99	ASN
1	A	109	GLU
1	A	122	PRO
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	39(C)	ARG
1	B	40	VAL
1	B	59	LYS
1	B	84	LYS
1	B	92	GLU
1	B	95	ASN
1	B	119	ASN
1	B	125	SER
1	B	130	ILE
1	B	135	MET
1	B	148	ASP

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Mol	Chain	Res	Type
1	B	161	ARG
1	B	170(A)	TYR
1	B	171	TYR
1	B	172	TYR
1	B	187	THR
1	B	191	PHE
1	B	224	LYS
1	B	243	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) 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	25	HIS
1	B	32	HIS
1	B	81	GLN
1	B	101	HIS
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 monosaccharides 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%)	-1.07	0	100	100	8, 21, 35, 44	19 (8%)
1	B	219/224 (97%)	-1.16	0	100	100	8, 18, 33, 42	19 (8%)
All	All	438/448 (97%)	-1.12	0	100	100	8, 20, 35, 44	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 monosaccharides 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.