Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:18 am BST

PDB ID	:	3TC2
Title	:	Crystal structure of potato serine protease inhibitor.
Authors	:	Meulenbroek, E.M.; Thomassen, E.A.J.; Pannu, N.S.
Deposited on	:	2011-08-08
Resolution	:	1.60 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 following versions of software and data (see references ①) were used in the production of this report:

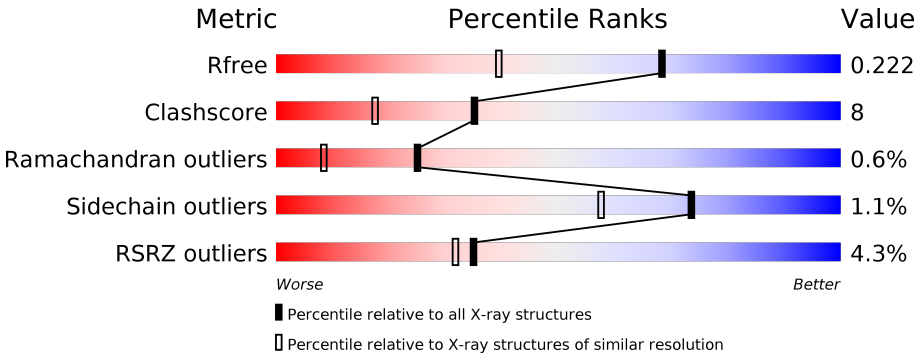
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 1.60 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}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 on 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	187	2% 77% 16%
1	B	187	5% 80% 12% 5%
1	C	187	5% 73% 19% 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4642 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 Kunitz-type proteinase inhibitor P1H5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	181	Total	C	N	O	S	0	1	0
			1394	890	231	267	6			
1	B	177	Total	C	N	O	S	0	2	0
			1368	875	226	261	6			
1	C	178	Total	C	N	O	S	0	2	0
			1379	882	230	261	6			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	THR	DELETION	UNP Q8S380
A	?	-	MET	DELETION	UNP Q8S380
A	?	-	THR	DELETION	UNP Q8S380
A	?	-	LEU	DELETION	UNP Q8S380
A	?	-	PRO	DELETION	UNP Q8S380
A	?	-	PHE	DELETION	UNP Q8S380
B	?	-	THR	DELETION	UNP Q8S380
B	?	-	MET	DELETION	UNP Q8S380
B	?	-	THR	DELETION	UNP Q8S380
B	?	-	LEU	DELETION	UNP Q8S380
B	?	-	PRO	DELETION	UNP Q8S380
B	?	-	PHE	DELETION	UNP Q8S380
C	?	-	THR	DELETION	UNP Q8S380
C	?	-	MET	DELETION	UNP Q8S380
C	?	-	THR	DELETION	UNP Q8S380
C	?	-	LEU	DELETION	UNP Q8S380
C	?	-	PRO	DELETION	UNP Q8S380
C	?	-	PHE	DELETION	UNP Q8S380

- Molecule 2 is water.

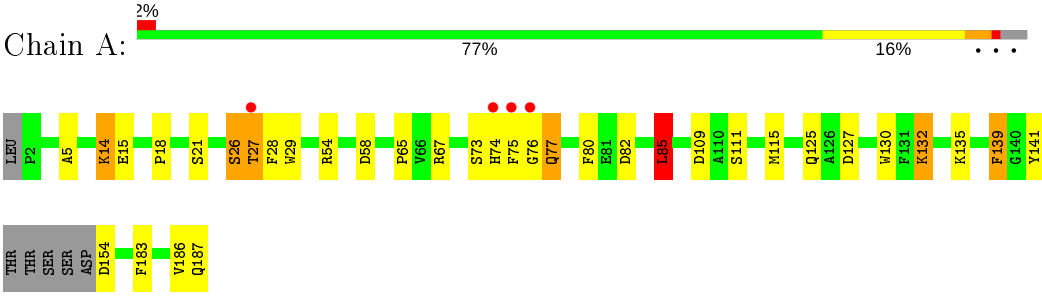
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	178	Total O 178 178	0	0
2	B	141	Total O 141 141	0	0
2	C	182	Total O 182 182	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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.

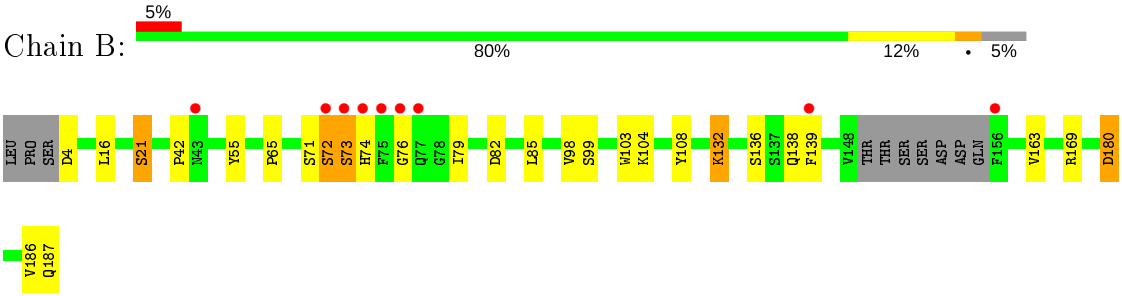
- Molecule 1: Kunitz-type proteinase inhibitor P1H5

Chain A:



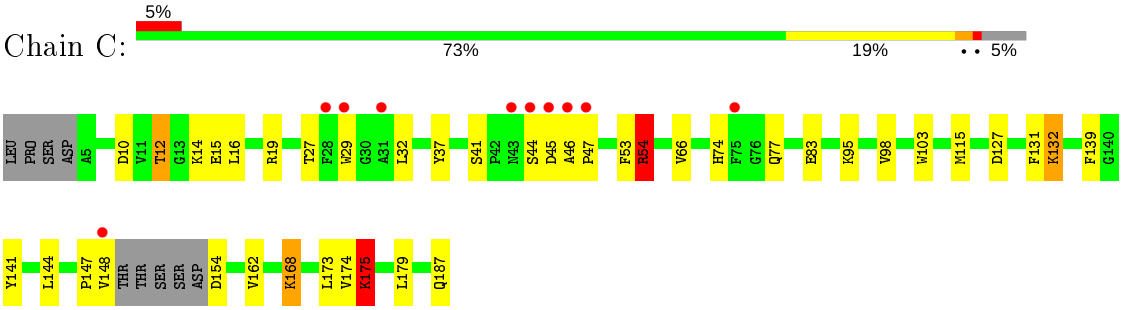
- Molecule 1: Kunitz-type proteinase inhibitor P1H5

Chain B:



- Molecule 1: Kunitz-type proteinase inhibitor P1H5

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.82Å 93.92Å 55.44Å 90.00° 100.69° 90.00°	Depositor
Resolution (Å)	54.23 – 1.60 53.87 – 1.60	Depositor EDS
% Data completeness (in resolution range)	69.9 (54.23-1.60) 69.9 (53.87-1.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	1.59 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.6.0116	Depositor
R, R_{free}	0.168 , 0.221 0.167 , 0.222	Depositor DCC
R_{free} test set	2533 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	17.5	Xtriage
Anisotropy	0.615	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.023 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4642	wwPDB-VP
Average B, all atoms (Å^2)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] 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

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	1.49	12/1429 (0.8%)	1.28	9/1936 (0.5%)
1	B	1.48	8/1405 (0.6%)	1.16	8/1904 (0.4%)
1	C	1.40	8/1413 (0.6%)	1.70	11/1913 (0.6%)
All	All	1.46	28/4247 (0.7%)	1.40	28/5753 (0.5%)

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	1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	108	TYR	CE1-CZ	16.56	1.60	1.38
1	B	108	TYR	CG-CD2	15.74	1.59	1.39
1	B	21	SER	CB-OG	-11.59	1.27	1.42
1	C	66	VAL	CB-CG2	-8.72	1.34	1.52
1	B	108	TYR	CG-CD1	7.74	1.49	1.39
1	A	130	TRP	CD2-CE2	7.56	1.50	1.41
1	A	139	PHE	CE1-CZ	6.92	1.50	1.37
1	A	148	VAL	CB-CG1	-6.72	1.38	1.52
1	A	132	LYS	CD-CE	-6.48	1.35	1.51
1	A	26	SER	C-O	6.38	1.35	1.23
1	A	141	TYR	CD1-CE1	6.30	1.48	1.39
1	B	163	VAL	CB-CG2	-6.21	1.39	1.52
1	C	54	ARG	CZ-NH1	6.04	1.40	1.33
1	C	131	PHE	CD1-CE1	5.82	1.50	1.39
1	A	183	PHE	CD2-CE2	5.78	1.50	1.39
1	A	29	TRP	CD2-CE2	5.64	1.48	1.41
1	C	29	TRP	CD2-CE2	5.54	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	141	TYR	CD1-CE1	5.46	1.47	1.39
1	C	175	LYS	CG-CD	5.41	1.70	1.52
1	A	27	THR	CA-CB	5.39	1.67	1.53
1	B	103	TRP	CD2-CE2	5.33	1.47	1.41
1	A	132	LYS	CE-NZ	5.18	1.62	1.49
1	B	55	TYR	CD1-CE1	5.17	1.47	1.39
1	B	136	SER	CB-OG	-5.16	1.35	1.42
1	C	103	TRP	CZ2-CH2	5.15	1.47	1.37
1	A	21	SER	CA-CB	5.14	1.60	1.52
1	A	135	LYS	CD-CE	5.13	1.64	1.51
1	C	12	THR	CB-CG2	-5.10	1.35	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	54	ARG	NE-CZ-NH2	-37.01	101.80	120.30
1	C	54	ARG	NE-CZ-NH1	35.25	137.93	120.30
1	A	54	ARG	NE-CZ-NH1	16.72	128.66	120.30
1	C	54	ARG	CD-NE-CZ	14.34	143.67	123.60
1	A	54	ARG	NE-CZ-NH2	-12.26	114.17	120.30
1	B	180[A]	ASP	CB-CG-OD1	8.34	125.81	118.30
1	B	180[B]	ASP	CB-CG-OD1	8.34	125.81	118.30
1	B	108	TYR	CZ-CE2-CD2	-7.88	112.70	119.80
1	A	85	LEU	CB-CG-CD1	-7.18	98.79	111.00
1	C	127	ASP	CB-CG-OD1	6.41	124.07	118.30
1	B	108	TYR	CE1-CZ-CE2	6.39	130.03	119.80
1	B	108	TYR	CB-CG-CD1	-6.31	117.21	121.00
1	A	127	ASP	CB-CG-OD1	6.26	123.93	118.30
1	A	58	ASP	CB-CG-OD2	-6.06	112.84	118.30
1	A	28	PHE	N-CA-C	-5.95	94.95	111.00
1	B	169	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	B	104	LYS	CD-CE-NZ	5.71	124.84	111.70
1	C	179	LEU	CB-CG-CD2	-5.65	101.39	111.00
1	C	132	LYS	CB-CA-C	-5.65	99.11	110.40
1	B	132	LYS	CA-CB-CG	5.29	125.03	113.40
1	A	14	LYS	CD-CE-NZ	-5.27	99.57	111.70
1	C	16	LEU	CB-CG-CD2	5.26	119.94	111.00
1	A	67	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	C	12	THR	CA-CB-CG2	5.16	119.63	112.40
1	C	141	TYR	CD1-CE1-CZ	-5.14	115.17	119.80
1	A	54	ARG	CD-NE-CZ	5.09	130.73	123.60
1	C	168[A]	LYS	CD-CE-NZ	5.06	123.34	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	168[B]	LYS	CD-CE-NZ	5.06	123.34	111.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	54	ARG	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	1394	0	1363	18	1
1	B	1368	0	1340	18	1
1	C	1379	0	1357	36	1
2	A	178	0	0	4	0
2	B	141	0	0	2	0
2	C	182	0	0	9	1
All	All	4642	0	4060	67	2

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 8.

All (67) 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:138:GLN:NE2	1:B:180[A]:ASP:OD2	1.87	1.07
1:B:42:PRO:HG3	1:C:45:ASP:HB2	1.35	1.06
1:C:148:VAL:HG11	2:C:255:HOH:O	1.61	0.99
1:A:154:ASP:N	2:A:327:HOH:O	2.04	0.91
1:C:12:THR:HG22	1:C:14:LYS:HG2	1.64	0.80
1:C:175:LYS:CD	1:C:175:LYS:N	2.45	0.79
1:C:19:ARG:HD3	1:C:77:GLN:HE21	1.48	0.77
1:B:42:PRO:HA	1:C:45:ASP:O	1.88	0.74
1:C:47:PRO:HA	2:C:401:HOH:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:PRO:HG3	1:A:75:PHE:HE1	1.52	0.73
1:A:18:PRO:HG3	1:A:75:PHE:CE1	2.26	0.71
1:C:53:PHE:CD2	1:C:168[A]:LYS:HE2	2.27	0.70
1:B:76:GLY:HA2	2:B:503:HOH:O	1.91	0.69
1:C:175:LYS:HD2	1:C:175:LYS:N	2.06	0.68
1:B:42:PRO:HG3	1:C:45:ASP:CB	2.19	0.68
1:C:53:PHE:CE2	1:C:168[A]:LYS:HE2	2.29	0.67
1:C:37:TYR:OH	1:C:168[A]:LYS:HE3	1.96	0.66
1:C:187:GLN:CD	2:C:269:HOH:O	2.34	0.66
1:C:187:GLN:HG3	2:C:269:HOH:O	1.95	0.65
1:C:187:GLN:CG	2:C:269:HOH:O	2.45	0.64
1:B:42:PRO:CG	1:C:45:ASP:HB2	2.20	0.64
1:B:180[A]:ASP:OD1	2:B:220:HOH:O	2.16	0.64
1:C:46:ALA:O	2:C:401:HOH:O	2.15	0.62
1:A:132:LYS:HE3	1:A:146:CYS:SG	2.40	0.62
1:C:19:ARG:HH11	1:C:77:GLN:HG3	1.66	0.61
1:C:41:SER:O	1:C:44:SER:HB2	1.99	0.61
1:C:115:MET:CE	1:C:173:LEU:HD12	2.32	0.60
1:B:16:LEU:HB2	1:B:79:ILE:HB	1.82	0.59
1:A:76:GLY:O	1:A:77:GLN:HB2	2.03	0.58
1:A:27:THR:O	1:A:27:THR:HG22	2.05	0.56
1:A:73:SER:O	1:A:75:PHE:N	2.37	0.56
1:A:82:ASP:HA	1:A:132:LYS:HD3	1.88	0.55
1:C:175:LYS:N	1:C:175:LYS:HD3	2.20	0.55
1:A:14:LYS:HD2	2:A:235:HOH:O	2.08	0.54
1:C:115:MET:HE2	1:C:173:LEU:HD12	1.89	0.54
1:B:71:SER:O	1:B:72:SER:CB	2.57	0.53
1:A:77:GLN:HA	1:A:77:GLN:OE1	2.08	0.52
1:B:71:SER:O	1:B:72:SER:HB3	2.10	0.51
1:A:26:SER:HA	2:A:286:HOH:O	2.11	0.51
1:B:139:PHE:HB2	1:B:180[B]:ASP:OD2	2.10	0.50
1:C:95:LYS:O	1:C:98:VAL:HG12	2.12	0.50
1:A:65:PRO:HB3	1:A:186:VAL:HG21	1.95	0.48
1:B:82[B]:ASP:OD1	1:B:132:LYS:HE3	2.14	0.47
1:A:125:GLN:HG2	2:A:417:HOH:O	2.14	0.46
1:C:132:LYS:HE3	1:C:144:LEU:HD12	1.96	0.46
1:C:54:ARG:HD3	1:C:162:VAL:HG21	1.97	0.46
1:C:175:LYS:H	1:C:175:LYS:HD3	1.79	0.46
1:C:10:ASP:OD1	1:C:12:THR:HB	2.17	0.45
1:A:109:ASP:OD1	1:A:111:SER:HB2	2.16	0.45
1:C:32:LEU:O	1:C:54:ARG:NH2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:174:VAL:C	1:C:175:LYS:HD2	2.37	0.44
1:C:74:HIS:CE1	1:C:83:GLU:HB2	2.53	0.44
1:B:73:SER:OG	1:B:74:HIS:N	2.51	0.44
1:C:154:ASP:N	2:C:338:HOH:O	2.51	0.43
1:B:85:LEU:HD12	1:B:85:LEU:C	2.38	0.43
1:A:14:LYS:HG2	1:A:15:GLU:N	2.33	0.42
1:C:115:MET:HE1	1:C:173:LEU:HD12	2.01	0.42
1:C:19:ARG:HD3	1:C:77:GLN:NE2	2.26	0.42
1:C:147:PRO:HD2	2:C:289:HOH:O	2.19	0.42
1:B:21:SER:HB2	1:B:186:VAL:HB	2.01	0.42
1:C:148:VAL:HG22	2:C:254:HOH:O	2.18	0.42
1:B:65:PRO:HB3	1:B:186:VAL:HG21	2.02	0.41
1:B:98:VAL:HG23	1:B:99:SER:N	2.35	0.41
1:C:27:THR:HG21	1:C:139:PHE:HB2	2.02	0.41
1:A:5:ALA:HB1	1:A:80:PHE:CD1	2.56	0.41
1:A:85:LEU:C	1:A:85:LEU:HD12	2.41	0.40
1:A:187:GLN:HB2	1:B:187:GLN:NE2	2.37	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:GLN:NE2	1:C:15:GLU:OE2[1_655]	1.88	0.32
1:B:4:ASP:N	2:C:247:HOH:O[1_655]	2.05	0.15

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	178/187 (95%)	168 (94%)	9 (5%)	1 (1%)	25 8
1	B	175/187 (94%)	164 (94%)	9 (5%)	2 (1%)	14 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	C	176/187 (94%)	171 (97%)	5 (3%)	0	100 100
All	All	529/561 (94%)	503 (95%)	23 (4%)	3 (1%)	25 8

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	72	SER
1	B	73	SER
1	A	74	HIS

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	155/160 (97%)	151 (97%)	4 (3%)	46 21
1	B	152/160 (95%)	152 (100%)	0	100 100
1	C	153/160 (96%)	152 (99%)	1 (1%)	84 73
All	All	460/480 (96%)	455 (99%)	5 (1%)	73 57

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	85	LEU
1	A	115	MET
1	A	139	PHE
1	C	175	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	166	ASN
1	B	138	GLN

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Mol	Chain	Res	Type
1	C	77	GLN

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 carbohydrates 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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	181/187 (96%)	-0.32	4 (2%)	62	60	10, 18, 41, 114	0
1	B	177/187 (94%)	-0.11	9 (5%)	28	26	12, 24, 60, 151	0
1	C	178/187 (95%)	-0.18	10 (5%)	24	22	10, 19, 52, 115	0
All	All	536/561 (95%)	-0.20	23 (4%)	35	32	10, 20, 52, 151	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	73	SER	13.4
1	C	45	ASP	12.3
1	A	75	PHE	10.5
1	B	74	HIS	8.2
1	B	75	PHE	7.5
1	C	29	TRP	6.8
1	C	75	PHE	5.1
1	C	46	ALA	4.9
1	C	44	SER	4.4
1	C	148	VAL	4.1
1	B	43	ASN	3.9
1	B	76	GLY	3.9
1	C	28	PHE	3.5
1	A	27	THR	3.4
1	B	139	PHE	3.2
1	A	74	HIS	3.0
1	A	76	GLY	3.0
1	B	156	PHE	2.7
1	C	43	ASN	2.7
1	B	72	SER	2.6
1	C	31	ALA	2.2
1	C	47	PRO	2.2
1	B	77	GLN	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.