Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:06 pm BST

PDB ID	:	4IW4
Title	:	Crystal structure of the serine protease domain of MASP-3 in complex with ecotin
Authors	:	Gaboriaud, C.
Deposited on	:	2013-01-23
Resolution	:	3.20 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:

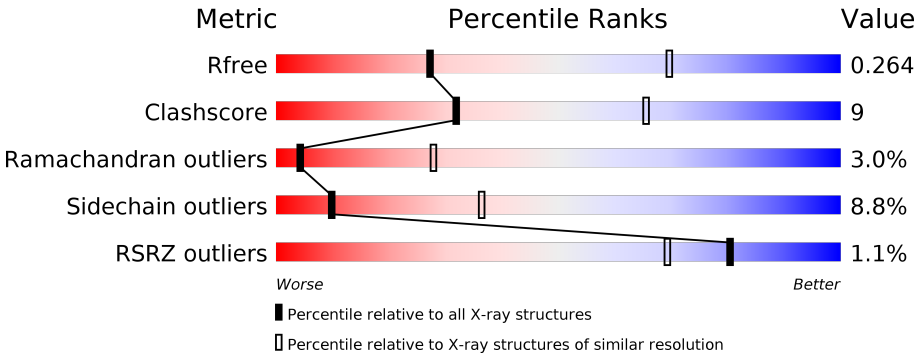
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	C	142	77% 18%
1	D	142	% 85% 8% 6%
2	E	279	% 67% 14% 5% 13%
2	F	279	% 65% 16% 14%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5735 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 Ecotin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	137	Total	C	N	O	S	0	0	0
			1063	679	176	202	6			
1	D	134	Total	C	N	O	S	0	0	0
			1023	656	170	191	6			

- Molecule 2 is a protein called Mannan-binding lectin serine protease 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	244	Total	C	N	O	S	0	0	0
			1850	1190	312	339	9			
2	F	240	Total	C	N	O	S	0	0	0
			1795	1156	298	332	9			

- Molecule 3 is water.

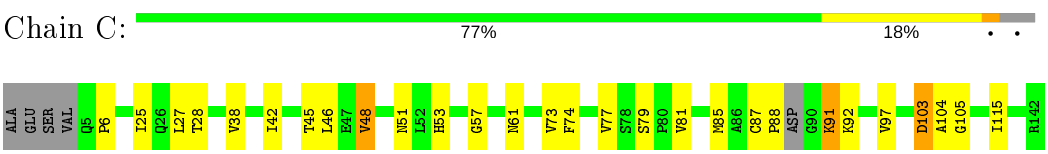
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	3	Total	O	0	0
			3	3		
3	F	1	Total	O	0	0
			1	1		

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.

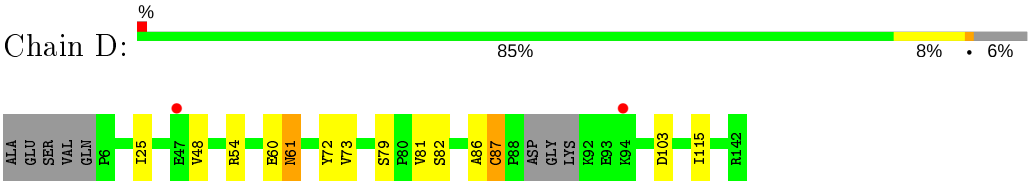
- Molecule 1: Ecotin

Chain C:



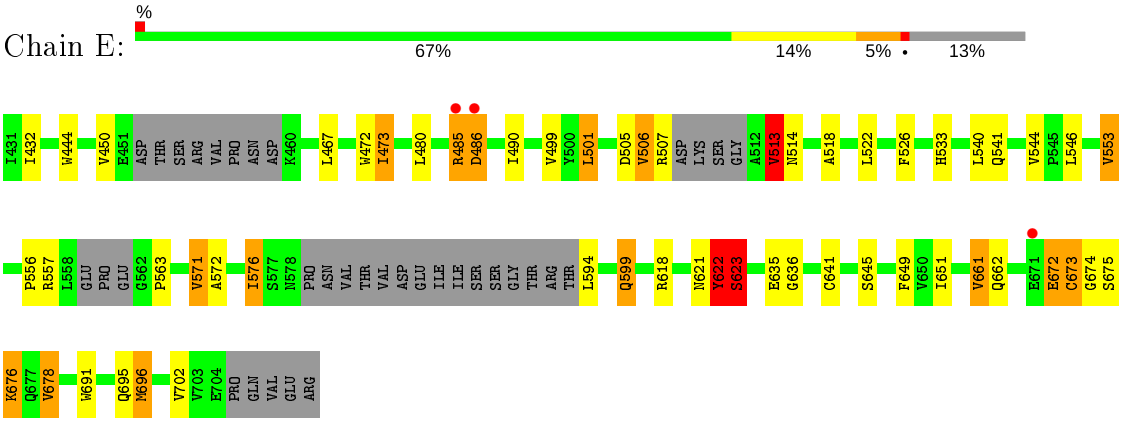
- Molecule 1: Ecotin

Chain D:



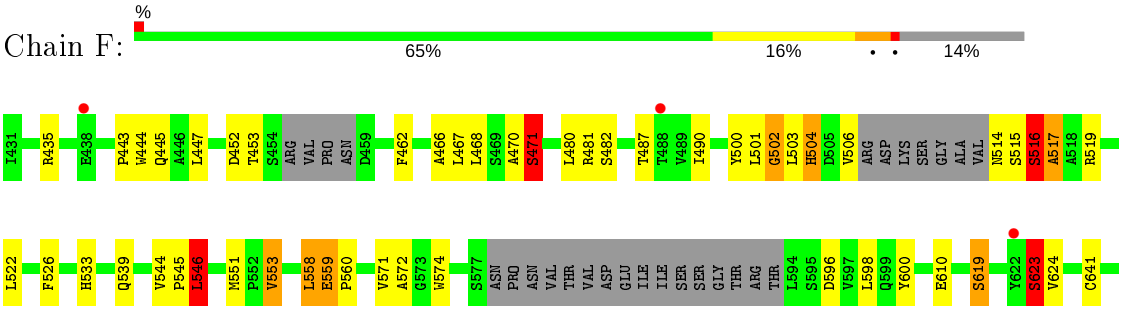
- Molecule 2: Mannan-binding lectin serine protease 3

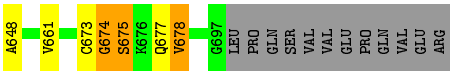
Chain E:



- Molecule 2: Mannan-binding lectin serine protease 3

Chain F:




A648
V661
C673
G674
S675
K676
Q677
V678
G697
LEU
PRO
GLN
SER
VAL
VAL
GLU
PRO
GLN
VAL
GLU
ARG

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	66.72Å 164.62Å 90.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 3.20 19.98 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.98-3.20) 100.0 (19.98-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.92 (at 3.22Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.208 , 0.269 0.208 , 0.264	Depositor DCC
R_{free} test set	852 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	80.0	Xtriage
Anisotropy	0.470	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 65.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	5735	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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	C	0.32	0/1084	0.57	0/1470
1	D	0.31	0/1044	0.54	0/1421
2	E	0.34	0/1900	0.56	0/2598
2	F	0.35	0/1846	0.59	0/2529
All	All	0.34	0/5874	0.56	0/8018

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
2	E	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	513	VAL	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	C	1063	0	1041	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1023	0	989	10	0
2	E	1850	0	1768	37	0
2	F	1795	0	1685	42	0
3	E	3	0	0	0	0
3	F	1	0	0	0	0
All	All	5735	0	5483	100	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 9.

All (100) 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)
2:F:452:ASP:CB	2:F:453:THR:CB	2.27	1.11
1:D:86:ALA:HA	1:D:87:CYS:HB2	1.50	0.94
1:D:86:ALA:HA	1:D:87:CYS:CB	2.00	0.92
2:F:545:PRO:HA	2:F:546:LEU:HB2	1.71	0.73
2:E:672:GLU:HB3	2:E:678:VAL:HG11	1.73	0.70
2:F:545:PRO:CA	2:F:546:LEU:HB2	2.22	0.68
2:F:444:TRP:CD2	2:F:553:VAL:HG13	2.29	0.68
2:F:558:LEU:HA	2:F:559:GLU:CB	2.27	0.65
2:F:470:ALA:N	2:F:471:SER:HB2	2.13	0.64
2:E:563:PRO:HB3	2:E:662:GLN:HG2	1.80	0.63
2:F:558:LEU:CA	2:F:559:GLU:CB	2.77	0.62
2:E:485:ARG:O	2:E:486:ASP:CB	2.48	0.62
2:E:473:ILE:CD1	2:E:499:VAL:HG11	2.30	0.61
1:C:104:ALA:N	1:C:105:GLY:HA3	2.16	0.61
1:D:86:ALA:CA	1:D:87:CYS:HB2	2.29	0.59
2:E:675:SER:HB2	2:E:676:LYS:CB	2.34	0.57
2:F:445:GLN:HG2	2:F:598:LEU:HD11	1.85	0.57
1:C:48:VAL:HG22	1:C:53:HIS:CE1	2.39	0.57
2:E:444:TRP:CD2	2:E:553:VAL:HG13	2.41	0.56
2:E:467:LEU:HD13	2:E:501:LEU:HD21	1.88	0.55
2:E:675:SER:HB3	2:E:678:VAL:HG12	1.87	0.55
2:F:443:PRO:HB2	2:F:551:MET:H	1.70	0.55
2:F:467:LEU:HD13	2:F:501:LEU:HD21	1.86	0.55
2:F:470:ALA:HB3	2:F:471:SER:CB	2.36	0.55
1:D:54:ARG:NH2	2:F:619:SER:OG	2.38	0.55
2:F:470:ALA:HB3	2:F:471:SER:OG	2.07	0.55
2:F:502:GLY:HA3	2:F:503:LEU:HB2	1.87	0.54
2:F:545:PRO:HA	2:F:546:LEU:CB	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:473:ILE:HD13	2:E:499:VAL:HG11	1.90	0.53
2:F:574:TRP:CZ2	2:F:598:LEU:HD12	2.44	0.53
1:C:87:CYS:HB3	1:C:88:PRO:HD2	1.90	0.53
2:E:518:ALA:HB2	2:E:541:GLN:HA	1.91	0.53
2:E:622:TYR:HA	2:E:623:SER:CB	2.40	0.53
2:F:480:LEU:HB2	2:F:522:LEU:HD21	1.91	0.53
1:C:103:ASP:N	1:C:103:ASP:OD1	2.42	0.52
1:D:25:ILE:HB	1:D:115:ILE:HB	1.92	0.52
1:C:103:ASP:HB3	1:D:103:ASP:HB3	1.92	0.52
2:F:470:ALA:H	2:F:471:SER:HB2	1.74	0.52
2:F:504:HIS:C	2:F:504:HIS:CD2	2.84	0.52
2:E:651:ILE:HD12	2:E:662:GLN:HG2	1.91	0.51
1:D:86:ALA:HA	1:D:87:CYS:HB3	1.88	0.51
2:F:482:SER:HB3	2:F:490:ILE:HG13	1.93	0.51
2:E:506:VAL:HA	2:E:507:ARG:C	2.32	0.50
2:F:501:LEU:O	2:F:502:GLY:C	2.50	0.50
2:E:571:VAL:HG22	2:E:649:PHE:HD1	1.76	0.50
1:C:25:ILE:HB	1:C:115:ILE:HB	1.94	0.49
2:F:516:SER:HA	2:F:517:ALA:HB2	1.93	0.49
2:E:621:ASN:O	2:E:622:TYR:C	2.51	0.49
2:F:519:ARG:HB2	2:F:539:GLN:HB3	1.94	0.49
2:E:622:TYR:HA	2:E:623:SER:OG	2.12	0.49
2:F:574:TRP:CE2	2:F:598:LEU:HD12	2.48	0.49
2:E:702:VAL:O	2:E:702:VAL:HG12	2.13	0.48
1:C:79:SER:O	2:E:618:ARG:NH1	2.46	0.48
2:F:526:PHE:HA	2:F:533:HIS:HB2	1.95	0.48
2:F:470:ALA:HB3	2:F:471:SER:HB2	1.95	0.48
2:F:677:GLN:HA	2:F:678:VAL:CB	2.44	0.48
1:C:27:LEU:HD11	1:C:38:VAL:HG21	1.96	0.47
1:D:61:ASN:HB3	1:D:72:TYR:CE2	2.49	0.47
2:F:572:ALA:HB1	2:F:598:LEU:HD21	1.97	0.47
2:F:674:GLY:N	2:F:675:SER:HB2	2.30	0.47
1:C:42:ILE:HG21	1:C:74:PHE:CD2	2.49	0.47
2:F:452:ASP:N	2:F:453:THR:O	2.48	0.47
2:F:444:TRP:CE3	2:F:553:VAL:HG13	2.50	0.46
2:F:516:SER:CA	2:F:517:ALA:HB2	2.45	0.46
2:F:470:ALA:CA	2:F:471:SER:HB2	2.46	0.46
2:E:501:LEU:HD23	2:E:544:VAL:HG11	1.98	0.45
2:F:545:PRO:CB	2:F:546:LEU:HB2	2.46	0.45
2:F:553:VAL:HB	2:F:661:VAL:HG23	1.98	0.45
2:F:677:GLN:CB	2:F:678:VAL:C	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:675:SER:HB2	2:E:676:LYS:C	2.37	0.44
1:C:57:GLY:HA3	1:C:74:PHE:CZ	2.52	0.44
2:E:473:ILE:HD12	2:E:540:LEU:HD21	2.00	0.44
2:F:571:VAL:O	2:F:600:TYR:HA	2.17	0.43
1:D:60:GLU:HG2	1:D:73:VAL:HG22	2.00	0.43
2:E:505:ASP:O	2:E:506:VAL:HB	2.18	0.43
2:F:500:TYR:HB3	2:F:503:LEU:HD22	1.99	0.43
1:C:51:ASN:OD1	1:C:85:MET:HG2	2.18	0.43
2:E:480:LEU:HB2	2:E:522:LEU:HD21	2.01	0.43
2:E:444:TRP:CE3	2:E:553:VAL:HG13	2.54	0.43
1:C:103:ASP:CB	1:D:103:ASP:HB3	2.49	0.42
2:E:472:TRP:CZ2	2:E:696:MET:HA	2.55	0.42
2:E:553:VAL:HB	2:E:661:VAL:HG22	2.01	0.42
1:C:46:LEU:HD12	1:C:97:VAL:HG21	2.02	0.42
2:E:576:ILE:HD12	2:E:594:LEU:HD12	2.02	0.42
2:F:462:PHE:C	2:F:462:PHE:CD1	2.92	0.42
2:E:675:SER:CA	2:E:676:LYS:CB	2.98	0.41
2:F:466:ALA:HB2	2:F:648:ALA:HB2	2.02	0.41
2:E:572:ALA:HA	2:E:599:GLN:O	2.20	0.41
2:E:622:TYR:CA	2:E:623:SER:CB	2.99	0.41
2:E:636:GLY:HA3	2:E:674:GLY:O	2.20	0.41
2:E:526:PHE:HA	2:E:533:HIS:HB2	2.02	0.40
2:E:556:PRO:HG3	2:E:661:VAL:O	2.21	0.40
2:E:691:TRP:O	2:E:695:GLN:HG2	2.20	0.40
2:F:623:SER:OG	2:F:624:VAL:N	2.54	0.40
1:C:74:PHE:CE2	1:C:77:VAL:HG22	2.56	0.40
2:E:563:PRO:HB3	2:E:662:GLN:CG	2.48	0.40
2:E:432:ILE:CD1	2:E:673:CYS:HB3	2.50	0.40
2:F:447:LEU:HB2	2:F:574:TRP:CH2	2.57	0.40
2:E:506:VAL:HG13	2:E:506:VAL:O	2.20	0.40
1:C:91:LYS:C	1:C:92:LYS:HG2	2.42	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	C	133/142 (94%)	126 (95%)	6 (4%)	1 (1%)	19	58
1	D	130/142 (92%)	124 (95%)	5 (4%)	1 (1%)	19	58
2	E	234/279 (84%)	211 (90%)	14 (6%)	9 (4%)	3	22
2	F	232/279 (83%)	202 (87%)	19 (8%)	11 (5%)	2	17
All	All	729/842 (87%)	663 (91%)	44 (6%)	22 (3%)	4	28

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	87	CYS
2	E	506	VAL
2	E	514	ASN
2	F	502	GLY
2	F	546	LEU
2	E	486	ASP
2	E	622	TYR
2	E	673	CYS
2	E	676	LYS
2	F	471	SER
2	F	516	SER
2	F	517	ALA
2	F	623	SER
2	F	674	GLY
2	E	623	SER
2	F	675	SER
1	C	6	PRO
2	F	559	GLU
2	F	560	PRO
2	E	513	VAL
2	E	450	VAL
2	F	678	VAL

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	C	113/125 (90%)	105 (93%)	8 (7%)	14 47
1	D	106/125 (85%)	101 (95%)	5 (5%)	26 62
2	E	196/238 (82%)	176 (90%)	20 (10%)	7 29
2	F	187/238 (79%)	167 (89%)	20 (11%)	6 27
All	All	602/726 (83%)	549 (91%)	53 (9%)	10 36

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	28	THR
1	C	45	THR
1	C	48	VAL
1	C	61	ASN
1	C	73	VAL
1	C	81	VAL
1	C	91	LYS
1	C	103	ASP
1	D	48	VAL
1	D	61	ASN
1	D	79	SER
1	D	81	VAL
1	D	82	SER
2	E	473	ILE
2	E	485	ARG
2	E	490	ILE
2	E	501	LEU
2	E	513	VAL
2	E	546	LEU
2	E	553	VAL
2	E	557	ARG
2	E	571	VAL
2	E	576	ILE
2	E	599	GLN
2	E	622	TYR
2	E	623	SER
2	E	635	GLU
2	E	641	CYS
2	E	645	SER
2	E	661	VAL
2	E	672	GLU

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Mol	Chain	Res	Type
2	E	678	VAL
2	E	696	MET
2	F	435	ARG
2	F	468	LEU
2	F	471	SER
2	F	481	ARG
2	F	487	THR
2	F	504	HIS
2	F	506	VAL
2	F	514	ASN
2	F	515	SER
2	F	516	SER
2	F	544	VAL
2	F	546	LEU
2	F	553	VAL
2	F	558	LEU
2	F	596	ASP
2	F	610	GLU
2	F	619	SER
2	F	623	SER
2	F	641	CYS
2	F	673	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	61	ASN
2	F	504	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 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	C	137/142 (96%)	-0.23	0	100	100	56, 74, 104, 125	0
1	D	134/142 (94%)	-0.27	2 (1%)	73	61	55, 72, 95, 124	0
2	E	244/279 (87%)	-0.25	3 (1%)	79	67	42, 71, 107, 121	10 (4%)
2	F	240/279 (86%)	-0.08	3 (1%)	77	65	57, 90, 120, 132	10 (4%)
All	All	755/842 (89%)	-0.20	8 (1%)	80	69	42, 76, 112, 132	20 (2%)

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	488	THR	3.9
2	F	622	TYR	3.3
2	E	486	ASP	2.6
2	E	485	ARG	2.5
2	F	438	GLU	2.4
1	D	94	LYS	2.3
2	E	671	GLU	2.1
1	D	47	GLU	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.