Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:18 PM GMT

PDB ID	:	4L3F
Title	:	Crystal structure of Internalin K (InlK) from Listeria monocytogenes
Authors	:	Neves, D.
Deposited on	:	2013-06-05
Resolution	:	2.39 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

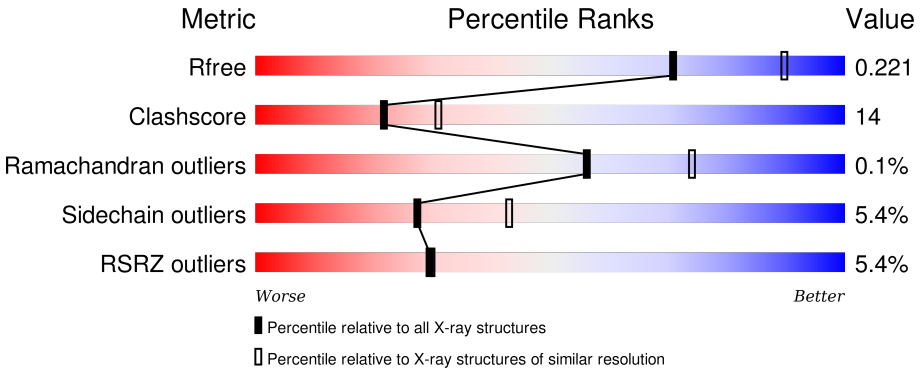
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.39 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}	91344	2919 (2.40-2.40)
Clashscore	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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. 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	347	2% 71% 16% • 10%
1	B	347	2% 63% 23% • 10%
1	C	347	5% 62% 26% • 10%
1	D	347	9% 62% 25% • 10%
1	E	347	12% 66% 22% • 10%

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Mol	Chain	Length	Quality of chain
1	F	347	3% 68% 20% • 10%
1	G	347	4% 65% 23% • 10%
1	H	347	% 63% 22% • 10%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20171 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 Internalin K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	0	0	0
			2436	1528	396	504	8			
1	B	311	Total	C	N	O	S	0	0	0
			2436	1528	396	504	8			
1	C	311	Total	C	N	O	S	0	0	0
			2436	1528	396	504	8			
1	D	311	Total	C	N	O	S	0	0	0
			2436	1528	396	504	8			
1	E	311	Total	C	N	O	S	0	0	0
			2436	1528	396	504	8			
1	F	311	Total	C	N	O	S	0	0	0
			2436	1528	396	504	8			
1	G	311	Total	C	N	O	S	0	0	0
			2436	1528	396	504	8			
1	H	311	Total	C	N	O	S	0	0	0
			2436	1528	396	504	8			

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	EXPRESSION TAG	UNP Q8Y7I7
A	24	GLY	-	EXPRESSION TAG	UNP Q8Y7I7
A	25	SER	-	EXPRESSION TAG	UNP Q8Y7I7
A	26	SER	-	EXPRESSION TAG	UNP Q8Y7I7
A	27	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
A	28	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
A	29	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
A	30	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
A	31	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
A	32	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
A	33	SER	-	EXPRESSION TAG	UNP Q8Y7I7
A	34	SER	-	EXPRESSION TAG	UNP Q8Y7I7
A	35	GLY	-	EXPRESSION TAG	UNP Q8Y7I7

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Chain	Residue	Modelled	Actual	Comment	Reference
A	36	LEU	-	EXPRESSION TAG	UNP Q8Y7I7
A	37	VAL	-	EXPRESSION TAG	UNP Q8Y7I7
A	38	PRO	-	EXPRESSION TAG	UNP Q8Y7I7
A	39	ARG	-	EXPRESSION TAG	UNP Q8Y7I7
A	40	GLY	-	EXPRESSION TAG	UNP Q8Y7I7
A	41	SER	-	EXPRESSION TAG	UNP Q8Y7I7
A	42	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
A	43	MET	-	EXPRESSION TAG	UNP Q8Y7I7
A	44	ALA	-	EXPRESSION TAG	UNP Q8Y7I7
B	23	MET	-	EXPRESSION TAG	UNP Q8Y7I7
B	24	GLY	-	EXPRESSION TAG	UNP Q8Y7I7
B	25	SER	-	EXPRESSION TAG	UNP Q8Y7I7
B	26	SER	-	EXPRESSION TAG	UNP Q8Y7I7
B	27	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
B	28	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
B	29	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
B	30	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
B	31	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
B	32	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
B	33	SER	-	EXPRESSION TAG	UNP Q8Y7I7
B	34	SER	-	EXPRESSION TAG	UNP Q8Y7I7
B	35	GLY	-	EXPRESSION TAG	UNP Q8Y7I7
B	36	LEU	-	EXPRESSION TAG	UNP Q8Y7I7
B	37	VAL	-	EXPRESSION TAG	UNP Q8Y7I7
B	38	PRO	-	EXPRESSION TAG	UNP Q8Y7I7
B	39	ARG	-	EXPRESSION TAG	UNP Q8Y7I7
B	40	GLY	-	EXPRESSION TAG	UNP Q8Y7I7
B	41	SER	-	EXPRESSION TAG	UNP Q8Y7I7
B	42	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
B	43	MET	-	EXPRESSION TAG	UNP Q8Y7I7
B	44	ALA	-	EXPRESSION TAG	UNP Q8Y7I7
C	23	MET	-	EXPRESSION TAG	UNP Q8Y7I7
C	24	GLY	-	EXPRESSION TAG	UNP Q8Y7I7
C	25	SER	-	EXPRESSION TAG	UNP Q8Y7I7
C	26	SER	-	EXPRESSION TAG	UNP Q8Y7I7
C	27	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
C	28	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
C	29	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
C	30	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
C	31	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
C	32	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
C	33	SER	-	EXPRESSION TAG	UNP Q8Y7I7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	34	SER	-	EXPRESSION TAG	UNP Q8Y7I7
C	35	GLY	-	EXPRESSION TAG	UNP Q8Y7I7
C	36	LEU	-	EXPRESSION TAG	UNP Q8Y7I7
C	37	VAL	-	EXPRESSION TAG	UNP Q8Y7I7
C	38	PRO	-	EXPRESSION TAG	UNP Q8Y7I7
C	39	ARG	-	EXPRESSION TAG	UNP Q8Y7I7
C	40	GLY	-	EXPRESSION TAG	UNP Q8Y7I7
C	41	SER	-	EXPRESSION TAG	UNP Q8Y7I7
C	42	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
C	43	MET	-	EXPRESSION TAG	UNP Q8Y7I7
C	44	ALA	-	EXPRESSION TAG	UNP Q8Y7I7
D	23	MET	-	EXPRESSION TAG	UNP Q8Y7I7
D	24	GLY	-	EXPRESSION TAG	UNP Q8Y7I7
D	25	SER	-	EXPRESSION TAG	UNP Q8Y7I7
D	26	SER	-	EXPRESSION TAG	UNP Q8Y7I7
D	27	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
D	28	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
D	29	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
D	30	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
D	31	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
D	32	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
D	33	SER	-	EXPRESSION TAG	UNP Q8Y7I7
D	34	SER	-	EXPRESSION TAG	UNP Q8Y7I7
D	35	GLY	-	EXPRESSION TAG	UNP Q8Y7I7
D	36	LEU	-	EXPRESSION TAG	UNP Q8Y7I7
D	37	VAL	-	EXPRESSION TAG	UNP Q8Y7I7
D	38	PRO	-	EXPRESSION TAG	UNP Q8Y7I7
D	39	ARG	-	EXPRESSION TAG	UNP Q8Y7I7
D	40	GLY	-	EXPRESSION TAG	UNP Q8Y7I7
D	41	SER	-	EXPRESSION TAG	UNP Q8Y7I7
D	42	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
D	43	MET	-	EXPRESSION TAG	UNP Q8Y7I7
D	44	ALA	-	EXPRESSION TAG	UNP Q8Y7I7
E	23	MET	-	EXPRESSION TAG	UNP Q8Y7I7
E	24	GLY	-	EXPRESSION TAG	UNP Q8Y7I7
E	25	SER	-	EXPRESSION TAG	UNP Q8Y7I7
E	26	SER	-	EXPRESSION TAG	UNP Q8Y7I7
E	27	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
E	28	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
E	29	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
E	30	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
E	31	HIS	-	EXPRESSION TAG	UNP Q8Y7I7

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Chain	Residue	Modelled	Actual	Comment	Reference
E	32	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
E	33	SER	-	EXPRESSION TAG	UNP Q8Y7I7
E	34	SER	-	EXPRESSION TAG	UNP Q8Y7I7
E	35	GLY	-	EXPRESSION TAG	UNP Q8Y7I7
E	36	LEU	-	EXPRESSION TAG	UNP Q8Y7I7
E	37	VAL	-	EXPRESSION TAG	UNP Q8Y7I7
E	38	PRO	-	EXPRESSION TAG	UNP Q8Y7I7
E	39	ARG	-	EXPRESSION TAG	UNP Q8Y7I7
E	40	GLY	-	EXPRESSION TAG	UNP Q8Y7I7
E	41	SER	-	EXPRESSION TAG	UNP Q8Y7I7
E	42	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
E	43	MET	-	EXPRESSION TAG	UNP Q8Y7I7
E	44	ALA	-	EXPRESSION TAG	UNP Q8Y7I7
F	23	MET	-	EXPRESSION TAG	UNP Q8Y7I7
F	24	GLY	-	EXPRESSION TAG	UNP Q8Y7I7
F	25	SER	-	EXPRESSION TAG	UNP Q8Y7I7
F	26	SER	-	EXPRESSION TAG	UNP Q8Y7I7
F	27	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
F	28	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
F	29	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
F	30	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
F	31	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
F	32	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
F	33	SER	-	EXPRESSION TAG	UNP Q8Y7I7
F	34	SER	-	EXPRESSION TAG	UNP Q8Y7I7
F	35	GLY	-	EXPRESSION TAG	UNP Q8Y7I7
F	36	LEU	-	EXPRESSION TAG	UNP Q8Y7I7
F	37	VAL	-	EXPRESSION TAG	UNP Q8Y7I7
F	38	PRO	-	EXPRESSION TAG	UNP Q8Y7I7
F	39	ARG	-	EXPRESSION TAG	UNP Q8Y7I7
F	40	GLY	-	EXPRESSION TAG	UNP Q8Y7I7
F	41	SER	-	EXPRESSION TAG	UNP Q8Y7I7
F	42	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
F	43	MET	-	EXPRESSION TAG	UNP Q8Y7I7
F	44	ALA	-	EXPRESSION TAG	UNP Q8Y7I7
G	23	MET	-	EXPRESSION TAG	UNP Q8Y7I7
G	24	GLY	-	EXPRESSION TAG	UNP Q8Y7I7
G	25	SER	-	EXPRESSION TAG	UNP Q8Y7I7
G	26	SER	-	EXPRESSION TAG	UNP Q8Y7I7
G	27	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
G	28	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
G	29	HIS	-	EXPRESSION TAG	UNP Q8Y7I7

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Chain	Residue	Modelled	Actual	Comment	Reference
G	30	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
G	31	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
G	32	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
G	33	SER	-	EXPRESSION TAG	UNP Q8Y7I7
G	34	SER	-	EXPRESSION TAG	UNP Q8Y7I7
G	35	GLY	-	EXPRESSION TAG	UNP Q8Y7I7
G	36	LEU	-	EXPRESSION TAG	UNP Q8Y7I7
G	37	VAL	-	EXPRESSION TAG	UNP Q8Y7I7
G	38	PRO	-	EXPRESSION TAG	UNP Q8Y7I7
G	39	ARG	-	EXPRESSION TAG	UNP Q8Y7I7
G	40	GLY	-	EXPRESSION TAG	UNP Q8Y7I7
G	41	SER	-	EXPRESSION TAG	UNP Q8Y7I7
G	42	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
G	43	MET	-	EXPRESSION TAG	UNP Q8Y7I7
G	44	ALA	-	EXPRESSION TAG	UNP Q8Y7I7
H	23	MET	-	EXPRESSION TAG	UNP Q8Y7I7
H	24	GLY	-	EXPRESSION TAG	UNP Q8Y7I7
H	25	SER	-	EXPRESSION TAG	UNP Q8Y7I7
H	26	SER	-	EXPRESSION TAG	UNP Q8Y7I7
H	27	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
H	28	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
H	29	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
H	30	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
H	31	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
H	32	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
H	33	SER	-	EXPRESSION TAG	UNP Q8Y7I7
H	34	SER	-	EXPRESSION TAG	UNP Q8Y7I7
H	35	GLY	-	EXPRESSION TAG	UNP Q8Y7I7
H	36	LEU	-	EXPRESSION TAG	UNP Q8Y7I7
H	37	VAL	-	EXPRESSION TAG	UNP Q8Y7I7
H	38	PRO	-	EXPRESSION TAG	UNP Q8Y7I7
H	39	ARG	-	EXPRESSION TAG	UNP Q8Y7I7
H	40	GLY	-	EXPRESSION TAG	UNP Q8Y7I7
H	41	SER	-	EXPRESSION TAG	UNP Q8Y7I7
H	42	HIS	-	EXPRESSION TAG	UNP Q8Y7I7
H	43	MET	-	EXPRESSION TAG	UNP Q8Y7I7
H	44	ALA	-	EXPRESSION TAG	UNP Q8Y7I7

- Molecule 2 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Ni 1 1	0	0
2	F	1	Total Ni 1 1	0	0

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	H	1	Total Na 1 1	0	0
3	G	1	Total Na 1 1	0	0

- Molecule 4 is water.

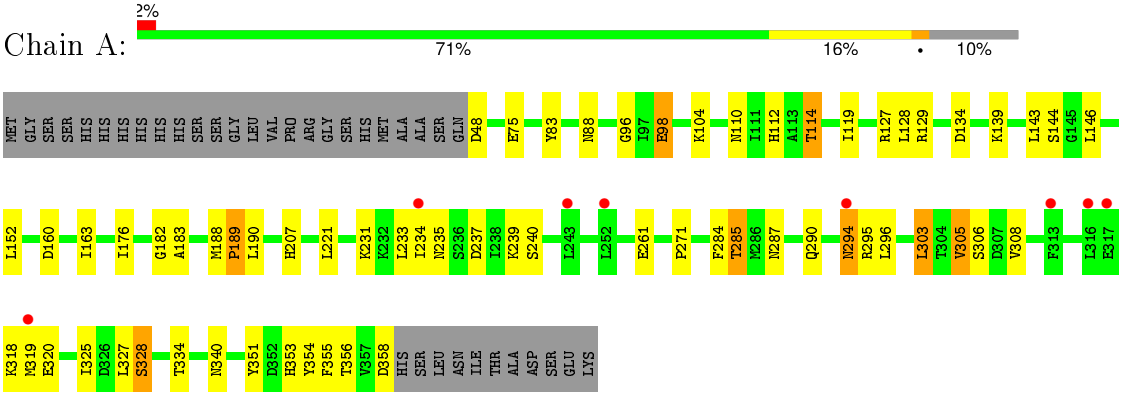
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	96	Total O 96 96	0	0
4	B	93	Total O 93 93	0	0
4	C	99	Total O 99 99	0	0
4	D	95	Total O 95 95	0	0
4	E	59	Total O 59 59	0	0
4	F	87	Total O 87 87	0	0
4	G	65	Total O 65 65	0	0
4	H	85	Total O 85 85	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

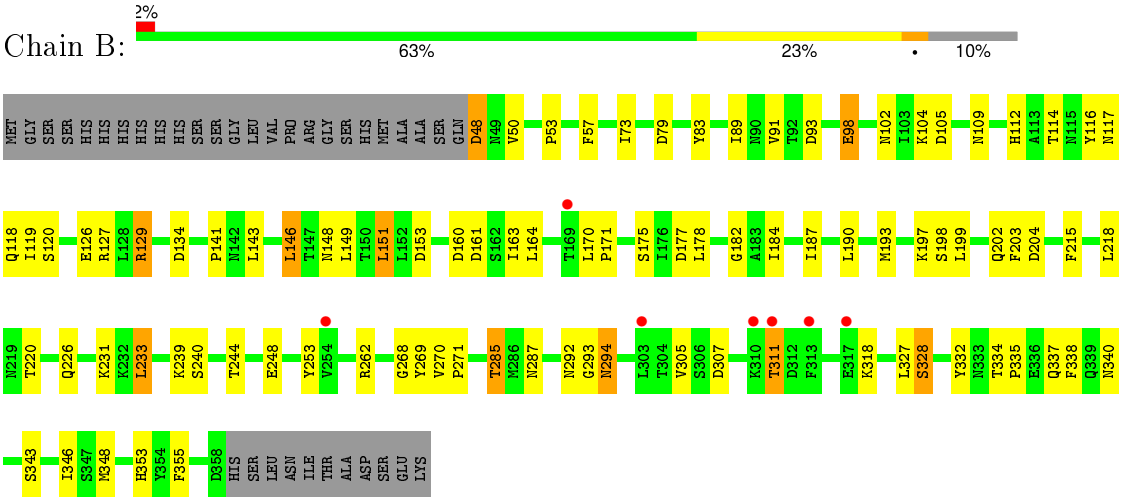
- Molecule 1: Internalin K

Chain A:



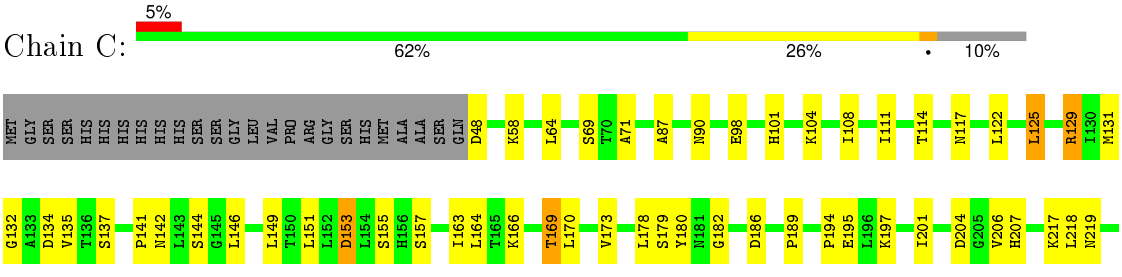
- Molecule 1: Internalin K

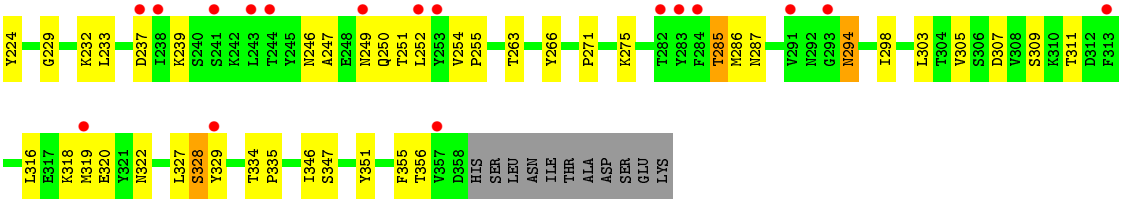
Chain B:



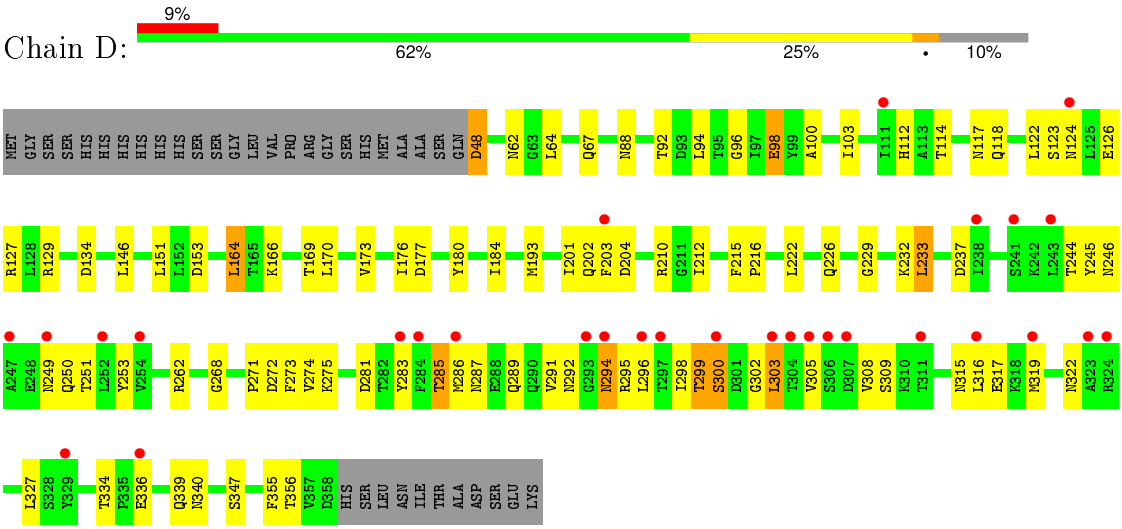
- Molecule 1: Internalin K

Chain C:

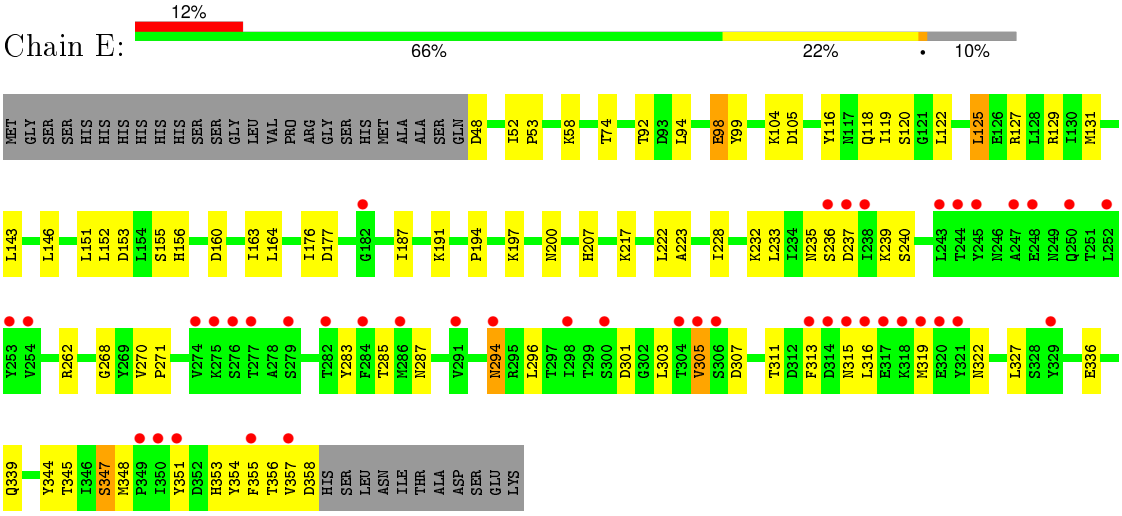




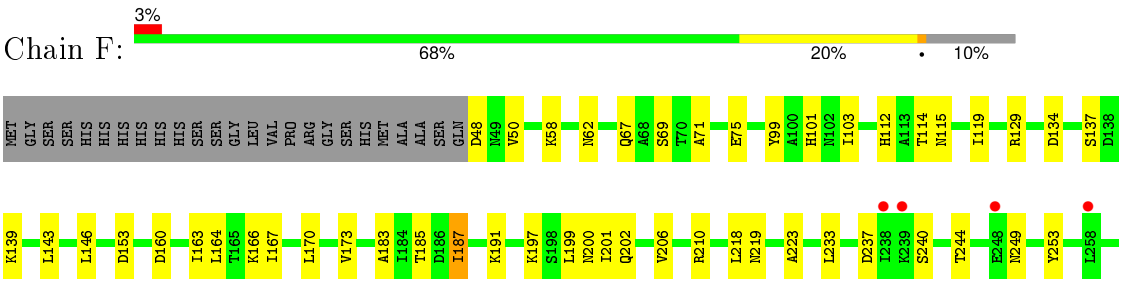
- Molecule 1: Internalin K

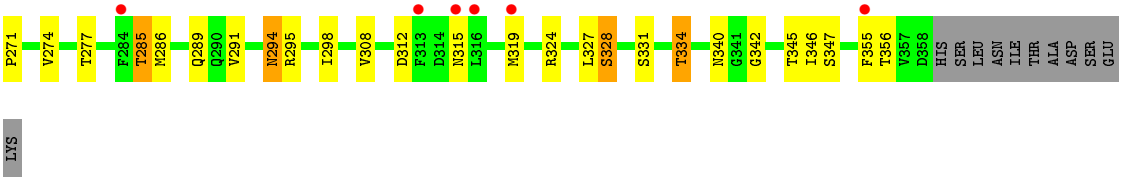


- Molecule 1: Internalin K



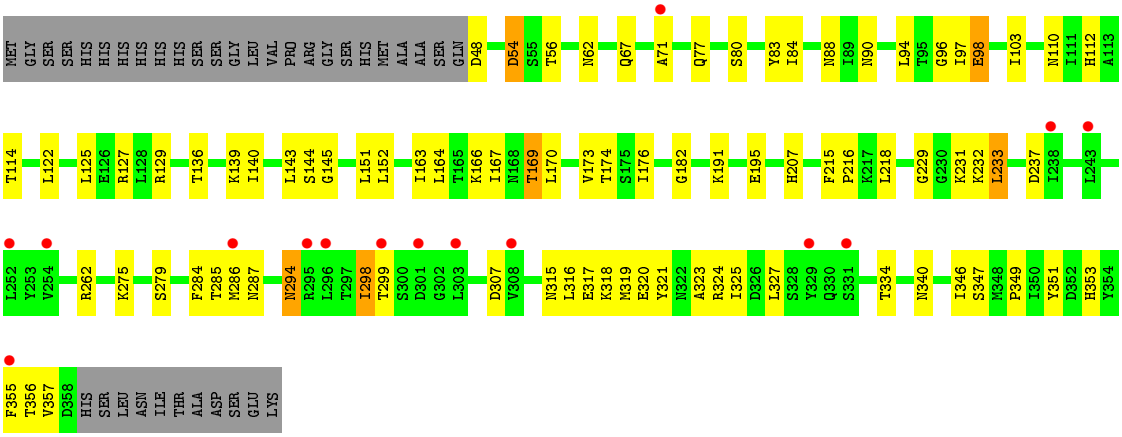
- Molecule 1: Internalin K





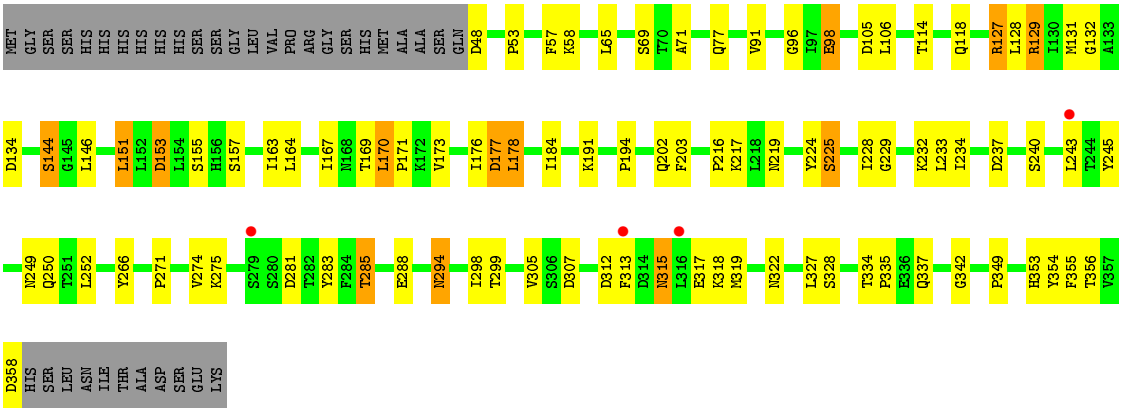
- Molecule 1: Internalin K

Chain G:



- Molecule 1: Internalin K

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	90.10Å 89.50Å 186.30Å 90.00° 103.50° 90.00°	Depositor
Resolution (Å)	47.90 – 2.39 47.90 – 2.40	Depositor EDS
% Data completeness (in resolution range)	80.7 (47.90-2.39) 80.8 (47.90-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.19 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.192 , 0.232 0.195 , 0.221	Depositor DCC
R_{free} test set	9215 reflections (11.10%)	DCC
Wilson B-factor (Å^2)	27.4	Xtriage
Anisotropy	1.120	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 9.9	EDS
Estimated twinning fraction	0.679 for H, K, L 0.321 for -H, -K, H+L 0.299 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.679 for H, K, L 0.321 for -H, -K, H+L	Depositor
L-test for twinning[2]	$< \|L\| > = 0.35$, $< L^2 > = 0.18$	Xtriage
Outliers	0 of 92214 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	20171	wwPDB-VP
Average B, all atoms (Å^2)	36.0	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 29.09 % 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 1.6461e-03.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NI, NA

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	0.74	0/2478	0.87	1/3373 (0.0%)
1	B	0.83	0/2478	0.90	1/3373 (0.0%)
1	C	0.77	0/2478	0.89	4/3373 (0.1%)
1	D	0.74	0/2478	0.87	3/3373 (0.1%)
1	E	0.64	0/2478	0.80	1/3373 (0.0%)
1	F	0.79	0/2478	0.89	0/3373
1	G	0.74	1/2478 (0.0%)	0.90	1/3373 (0.0%)
1	H	0.78	0/2478	0.94	4/3373 (0.1%)
All	All	0.75	1/19824 (0.0%)	0.88	15/26984 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	83	TYR	CB-CG	5.25	1.59	1.51

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	127	ARG	NE-CZ-NH2	-7.70	116.45	120.30
1	D	177	ASP	CB-CG-OD1	6.44	124.10	118.30
1	H	129	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	C	129	ARG	NE-CZ-NH1	-5.89	117.35	120.30
1	A	127	ARG	NE-CZ-NH1	-5.85	117.37	120.30
1	H	153	ASP	CB-CG-OD1	5.70	123.43	118.30
1	C	151	LEU	CA-CB-CG	5.61	128.21	115.30
1	H	177	ASP	CB-CG-OD1	5.61	123.34	118.30
1	D	164	LEU	CB-CG-CD1	5.52	120.39	111.00
1	C	64	LEU	CB-CG-CD1	-5.49	101.66	111.00
1	G	54	ASP	CB-CG-OD2	5.30	123.07	118.30
1	E	177	ASP	CB-CG-OD1	5.26	123.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	129	ARG	CG-CD-NE	-5.25	100.78	111.80
1	D	64	LEU	CB-CG-CD1	-5.17	102.21	111.00
1	C	153	ASP	CB-CG-OD1	5.09	122.88	118.30

There are no chirality outliers.

There are no planarity outliers.

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	2436	0	2375	48	0
1	B	2436	0	2375	81	0
1	C	2436	0	2375	82	0
1	D	2436	0	2375	90	0
1	E	2436	0	2375	62	0
1	F	2436	0	2375	59	0
1	G	2436	0	2375	62	1
1	H	2436	0	2375	66	0
2	B	1	0	0	0	0
2	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	96	0	0	15	0
4	B	93	0	0	29	0
4	C	99	0	0	27	0
4	D	95	0	0	38	0
4	E	59	0	0	17	0
4	F	87	0	0	15	0
4	G	65	0	0	15	0
4	H	85	0	0	19	1
All	All	20171	0	19000	537	1

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 14.

All (537) 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:H:217:LYS:HG3	4:H:579:HOH:O	1.35	1.26
1:C:328:SER:HB3	4:C:486:HOH:O	1.19	1.25
1:B:269:TYR:HA	4:B:574:HOH:O	1.32	1.23
1:B:239:LYS:NZ	4:B:539:HOH:O	1.71	1.22
1:D:298:ILE:HB	4:D:492:HOH:O	1.43	1.15
1:F:345:THR:HB	4:F:576:HOH:O	1.46	1.15
1:A:334:THR:HG23	4:A:422:HOH:O	1.43	1.15
1:B:338:PHE:CD2	4:B:581:HOH:O	2.00	1.14
1:B:285:THR:HG21	4:B:583:HOH:O	1.48	1.11
1:F:328:SER:O	1:F:331:SER:HB3	1.52	1.09
1:C:217:LYS:HE3	4:C:494:HOH:O	1.53	1.09
1:E:160:ASP:O	1:E:163:ILE:HG22	1.56	1.06
1:H:128:LEU:CD1	4:H:584:HOH:O	2.04	1.05
1:F:139:LYS:HD3	4:F:581:HOH:O	1.60	1.02
1:H:106:LEU:HG	4:H:584:HOH:O	1.60	1.00
1:C:166:LYS:HE2	4:C:487:HOH:O	1.61	1.00
1:A:104:LYS:HE3	4:A:479:HOH:O	1.64	0.97
1:C:104:LYS:NZ	4:C:457:HOH:O	1.98	0.96
1:E:345:THR:HG23	4:E:456:HOH:O	1.63	0.96
1:H:337:GLN:HG2	4:H:572:HOH:O	1.65	0.96
1:A:261:GLU:O	1:A:351:TYR:HE1	1.49	0.96
1:D:272:ASP:HA	4:D:451:HOH:O	1.65	0.96
1:D:319:MET:HG2	4:D:494:HOH:O	1.65	0.94
1:C:237:ASP:OD2	4:C:406:HOH:O	1.87	0.93
1:H:334:THR:HG23	4:H:567:HOH:O	1.70	0.91
1:C:129:ARG:HB3	4:C:484:HOH:O	1.69	0.91
1:B:340:ASN:ND2	4:B:543:HOH:O	2.03	0.91
1:G:207:HIS:HD2	4:G:555:HOH:O	1.51	0.91
1:F:137:SER:HB3	4:F:585:HOH:O	1.71	0.91
1:B:83:TYR:HE1	4:B:586:HOH:O	1.52	0.90
1:D:273:PHE:N	4:D:451:HOH:O	2.06	0.89
1:H:106:LEU:CG	4:H:584:HOH:O	2.19	0.89
1:E:336:GLU:O	4:E:442:HOH:O	1.91	0.88
1:B:73:ILE:HB	4:B:585:HOH:O	1.75	0.87
1:G:54:ASP:HA	4:G:565:HOH:O	1.73	0.86
1:B:93:ASP:OD2	4:B:538:HOH:O	1.94	0.84
1:E:239:LYS:HD3	1:E:358:ASP:HB3	1.59	0.84
1:E:99:TYR:OH	4:E:433:HOH:O	1.95	0.83
1:A:261:GLU:O	1:A:351:TYR:CE1	2.31	0.83
1:D:262:ARG:NH2	4:D:451:HOH:O	2.13	0.82
1:F:139:LYS:HB3	4:F:581:HOH:O	1.80	0.81
1:A:285:THR:CG2	4:A:492:HOH:O	2.28	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:334:THR:HG23	4:C:417:HOH:O	1.83	0.79
1:F:237:ASP:OD1	1:F:356:THR:OG1	2.01	0.79
1:B:48:ASP:O	1:B:48:ASP:OD1	2.01	0.79
1:B:117:ASN:HB3	4:C:480:HOH:O	1.83	0.78
1:C:311:THR:HB	4:C:492:HOH:O	1.85	0.77
1:C:329:TYR:HE1	4:C:477:HOH:O	1.66	0.77
1:F:163:ILE:HG23	1:F:164:LEU:HD12	1.67	0.77
1:C:217:LYS:HG2	4:C:476:HOH:O	1.83	0.77
1:H:216:PRO:HB2	4:H:579:HOH:O	1.85	0.76
1:F:115:ASN:HA	4:F:581:HOH:O	1.85	0.76
1:C:239:LYS:HG3	1:E:301:ASP:OD2	1.85	0.76
1:A:48:ASP:OD1	1:A:48:ASP:O	2.04	0.76
1:G:207:HIS:CD2	4:G:555:HOH:O	2.33	0.75
1:B:269:TYR:HD1	4:B:574:HOH:O	1.68	0.75
1:B:109:ASN:OD1	4:B:524:HOH:O	2.05	0.74
1:A:308:VAL:HB	4:A:495:HOH:O	1.86	0.74
1:B:175:SER:HB2	4:B:572:HOH:O	1.88	0.74
1:E:197:LYS:HE2	4:E:434:HOH:O	1.86	0.74
1:D:299:THR:OG1	1:D:300:SER:N	2.15	0.74
1:D:340:ASN:HB2	4:D:474:HOH:O	1.87	0.73
1:E:127:ARG:HG2	1:E:151:LEU:HD22	1.71	0.73
1:D:272:ASP:C	4:D:451:HOH:O	2.27	0.73
1:C:122:LEU:HB2	1:C:125:LEU:HD22	1.71	0.72
1:A:96:GLY:N	1:A:98:GLU:OE1	2.22	0.72
1:E:313:PHE:HZ	4:E:459:HOH:O	1.71	0.72
1:B:269:TYR:CD1	4:B:574:HOH:O	2.43	0.71
1:D:272:ASP:CA	4:D:451:HOH:O	2.30	0.71
1:C:58:LYS:HE2	1:C:71:ALA:O	1.89	0.71
1:D:124:ASN:HB2	4:D:408:HOH:O	1.91	0.71
1:B:98:GLU:HG3	1:B:118:GLN:HB3	1.73	0.70
1:D:340:ASN:CB	4:D:474:HOH:O	2.39	0.70
1:D:48:ASP:OD2	4:D:406:HOH:O	2.09	0.70
1:F:202:GLN:NE2	4:F:537:HOH:O	2.19	0.70
1:D:286:MET:HG2	4:D:494:HOH:O	1.90	0.69
1:H:312:ASP:OD2	4:H:532:HOH:O	2.08	0.69
1:F:185:THR:HG22	4:F:563:HOH:O	1.92	0.69
1:D:275:LYS:HA	4:D:492:HOH:O	1.93	0.69
1:B:53:PRO:HD2	4:B:532:HOH:O	1.91	0.69
1:F:69:SER:O	4:F:520:HOH:O	2.08	0.69
1:C:90:ASN:HB2	4:C:481:HOH:O	1.93	0.69
1:D:202:GLN:O	1:D:203:PHE:HB2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:TYR:CE1	4:C:477:HOH:O	2.42	0.69
1:E:339:GLN:O	4:E:401:HOH:O	2.11	0.68
1:B:220:THR:HG23	1:B:343:SER:HB2	1.74	0.68
1:C:101:HIS:HD2	4:C:485:HOH:O	1.75	0.68
1:G:340:ASN:HB2	4:G:557:HOH:O	1.94	0.68
1:E:120:SER:O	4:E:404:HOH:O	2.12	0.68
1:F:334:THR:HG23	4:F:568:HOH:O	1.93	0.67
1:F:200:ASN:OD1	1:F:202:GLN:HG3	1.94	0.67
1:B:204:ASP:O	1:B:226:GLN:OE1	2.13	0.67
1:D:336:GLU:HG2	4:D:486:HOH:O	1.93	0.67
1:E:207:HIS:CD2	4:E:453:HOH:O	2.48	0.66
1:D:262:ARG:NH2	1:D:271:PRO:O	2.28	0.66
1:A:285:THR:HG22	4:A:492:HOH:O	1.89	0.66
1:A:239:LYS:HD3	1:A:358:ASP:HB3	1.77	0.66
1:B:160:ASP:O	1:B:163:ILE:HG22	1.95	0.66
1:G:48:ASP:N	4:G:539:HOH:O	2.27	0.66
1:C:131:MET:CE	4:C:484:HOH:O	2.44	0.66
1:F:67:GLN:HG2	4:F:566:HOH:O	1.94	0.66
1:G:321:TYR:CE1	1:G:323:ALA:HB2	2.31	0.66
1:B:204:ASP:C	1:B:226:GLN:OE1	2.34	0.65
1:E:48:ASP:OD1	1:E:48:ASP:O	2.14	0.65
1:A:294:ASN:OD1	1:A:294:ASN:N	2.29	0.65
1:E:116:TYR:O	1:E:119:ILE:HG12	1.97	0.65
1:H:106:LEU:CB	4:H:584:HOH:O	2.44	0.65
1:C:271:PRO:HG3	1:C:327:LEU:HD13	1.77	0.65
1:H:294:ASN:N	1:H:294:ASN:OD1	2.27	0.65
1:F:328:SER:O	1:F:331:SER:CB	2.37	0.64
1:E:232:LYS:HA	4:E:457:HOH:O	1.97	0.64
1:A:160:ASP:O	1:A:163:ILE:HG22	1.98	0.64
1:E:287:ASN:HD21	1:E:316:LEU:HA	1.61	0.64
1:A:306:SER:HB3	4:A:493:HOH:O	1.97	0.64
1:E:347:SER:HB2	4:E:455:HOH:O	1.97	0.63
1:C:247:ALA:HB2	4:C:482:HOH:O	1.99	0.63
1:D:285:THR:HG22	4:D:491:HOH:O	1.98	0.63
1:G:340:ASN:CG	4:G:557:HOH:O	2.35	0.63
1:D:285:THR:CG2	4:D:491:HOH:O	2.46	0.63
1:G:110:ASN:OD1	1:G:112:HIS:CE1	2.51	0.63
1:G:340:ASN:CB	4:G:557:HOH:O	2.46	0.62
1:E:156:HIS:HE1	4:E:451:HOH:O	1.81	0.62
1:C:129:ARG:NH2	1:D:129:ARG:NE	2.48	0.62
1:E:236:SER:HB2	1:E:355:PHE:CD1	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:262:ARG:NH2	1:E:271:PRO:O	2.33	0.61
1:F:62:ASN:OD1	1:F:67:GLN:NE2	2.32	0.61
1:B:161:ASP:O	1:B:164:LEU:HB2	2.01	0.61
1:B:120:SER:OG	1:C:142:ASN:CB	2.49	0.61
1:B:334:THR:HG21	4:B:502:HOH:O	2.01	0.61
1:E:127:ARG:NH1	4:E:418:HOH:O	2.32	0.61
1:D:122:LEU:O	1:D:124:ASN:N	2.34	0.61
1:H:224:TYR:CD2	1:H:225:SER:HB2	2.36	0.60
1:G:122:LEU:O	1:G:125:LEU:HB2	2.01	0.60
1:C:179:SER:O	1:C:180:TYR:HB2	2.00	0.60
1:D:202:GLN:HE21	1:D:222:LEU:HB3	1.65	0.60
1:B:215:PHE:HB3	4:B:570:HOH:O	2.01	0.60
1:H:202:GLN:O	1:H:203:PHE:HB2	2.02	0.60
1:B:262:ARG:NH2	1:B:271:PRO:O	2.33	0.60
1:C:246:ASN:OD1	1:C:249:ASN:HB2	2.02	0.60
1:F:183:ALA:HA	4:F:507:HOH:O	2.02	0.59
1:B:328:SER:HA	1:B:348:MET:CE	2.33	0.59
1:F:319:MET:HB2	1:F:355:PHE:HB2	1.83	0.59
1:B:120:SER:OG	1:C:142:ASN:CG	2.41	0.59
1:A:183:ALA:HB2	1:A:231:LYS:HB2	1.83	0.59
1:G:325:ILE:HB	1:G:349:PRO:HG2	1.85	0.59
1:H:252:LEU:HB3	1:H:305:VAL:HB	1.84	0.59
1:A:328:SER:HB2	4:A:416:HOH:O	2.02	0.59
1:F:271:PRO:HG3	1:F:327:LEU:HD13	1.84	0.59
1:B:337:GLN:HG3	4:B:581:HOH:O	2.04	0.58
1:G:275:LYS:HD3	1:G:298:ILE:HG22	1.84	0.58
1:G:96:GLY:N	1:G:98:GLU:OE1	2.31	0.58
1:C:201:ILE:HD12	1:C:206:VAL:HG21	1.84	0.58
1:D:283:TYR:HB3	1:D:322:ASN:HB3	1.85	0.58
1:A:129:ARG:NH2	1:B:129:ARG:NH2	2.51	0.58
1:A:271:PRO:HG3	1:A:327:LEU:HD13	1.83	0.58
1:E:223:ALA:HB3	1:E:345:THR:O	2.03	0.58
1:A:104:LYS:HG3	4:A:490:HOH:O	2.03	0.58
1:F:129:ARG:HG2	1:F:153:ASP:HB3	1.85	0.58
1:C:153:ASP:OD1	1:C:155:SER:OG	2.15	0.57
1:C:129:ARG:NH2	1:D:129:ARG:HE	2.02	0.57
1:G:163:ILE:HG23	1:G:164:LEU:HD12	1.86	0.57
1:A:237:ASP:OD1	1:A:356:THR:OG1	2.20	0.57
1:F:48:ASP:N	4:F:549:HOH:O	2.38	0.57
1:G:315:ASN:HB3	4:G:556:HOH:O	2.05	0.56
1:G:77:GLN:O	1:G:80:SER:OG	2.16	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:TYR:CZ	1:D:203:PHE:CE2	2.93	0.56
1:E:98:GLU:CG	1:E:118:GLN:HB3	2.35	0.56
1:C:250:GLN:NE2	1:C:309:SER:HA	2.21	0.56
1:C:319:MET:HB2	1:C:355:PHE:HB2	1.86	0.56
1:C:287:ASN:HA	1:C:318:LYS:HB2	1.88	0.56
1:C:197:LYS:O	1:C:218:LEU:HD12	2.06	0.56
1:D:134:ASP:CA	4:D:479:HOH:O	2.54	0.56
1:C:48:ASP:HB3	4:C:474:HOH:O	2.05	0.56
1:G:287:ASN:ND2	1:G:315:ASN:O	2.39	0.55
1:E:104:LYS:NZ	4:E:426:HOH:O	2.37	0.55
1:G:317:GLU:O	1:G:356:THR:HA	2.06	0.55
1:G:77:GLN:HG2	4:G:527:HOH:O	2.07	0.55
1:C:287:ASN:HD21	1:C:316:LEU:HD12	1.71	0.55
1:D:134:ASP:HA	4:D:479:HOH:O	2.05	0.55
1:F:277:THR:HG22	1:F:298:ILE:HD12	1.87	0.55
1:B:269:TYR:CB	4:B:574:HOH:O	2.51	0.55
1:H:106:LEU:HB3	4:H:584:HOH:O	2.04	0.55
1:A:261:GLU:C	1:A:351:TYR:HE1	2.09	0.55
1:B:335:PRO:HB2	4:B:581:HOH:O	2.07	0.55
1:H:271:PRO:HG3	1:H:327:LEU:HD13	1.89	0.55
1:C:237:ASP:OD1	1:C:356:THR:OG1	2.14	0.54
1:H:48:ASP:N	4:H:507:HOH:O	2.39	0.54
1:G:285:THR:HG21	4:G:528:HOH:O	2.06	0.54
1:D:229:GLY:HA2	1:D:232:LYS:O	2.07	0.54
1:B:338:PHE:CE2	4:B:581:HOH:O	2.45	0.54
1:B:338:PHE:HD2	4:B:581:HOH:O	1.57	0.54
1:B:50:VAL:HB	4:B:585:HOH:O	2.06	0.54
1:F:295:ARG:NH2	1:F:308:VAL:HG23	2.23	0.54
1:H:128:LEU:HD12	4:H:584:HOH:O	1.85	0.54
1:G:127:ARG:HG2	1:G:151:LEU:HB3	1.88	0.54
1:F:187:ILE:HD13	1:F:199:LEU:HD23	1.90	0.54
1:E:283:TYR:HB3	1:E:322:ASN:HB3	1.90	0.54
1:C:201:ILE:CD1	1:C:206:VAL:HG21	2.38	0.54
1:E:98:GLU:HG3	1:E:118:GLN:HB3	1.88	0.54
1:C:48:ASP:N	4:C:443:HOH:O	2.40	0.54
1:G:62:ASN:OD1	1:G:67:GLN:NE2	2.40	0.54
1:B:146:LEU:HB3	1:B:149:LEU:HB2	1.90	0.54
1:D:98:GLU:HG3	1:D:118:GLN:HB3	1.89	0.54
1:D:134:ASP:CB	4:D:479:HOH:O	2.56	0.54
1:B:340:ASN:ND2	4:B:504:HOH:O	2.39	0.53
1:E:127:ARG:CZ	4:E:436:HOH:O	2.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:340:ASN:CG	4:D:474:HOH:O	2.46	0.53
1:C:246:ASN:ND2	4:C:452:HOH:O	2.40	0.53
1:F:112:HIS:HA	1:F:134:ASP:OD2	2.08	0.53
1:B:328:SER:HA	1:B:348:MET:HE2	1.90	0.53
1:F:210:ARG:HA	4:F:534:HOH:O	2.08	0.53
1:F:340:ASN:O	1:F:340:ASN:CG	2.46	0.53
1:B:153:ASP:HB2	4:B:591:HOH:O	2.08	0.53
1:E:351:TYR:CE2	1:E:353:HIS:HB2	2.44	0.53
1:F:163:ILE:O	1:F:166:LYS:HB2	2.09	0.53
1:F:271:PRO:HB3	1:F:327:LEU:HD13	1.89	0.53
1:F:308:VAL:HG13	1:F:312:ASP:HB2	1.91	0.53
1:D:134:ASP:HB3	4:D:479:HOH:O	2.09	0.53
1:H:58:LYS:HE2	1:H:71:ALA:O	2.08	0.53
1:A:152:LEU:O	1:A:176:ILE:HA	2.09	0.53
1:A:114:THR:O	1:A:139:LYS:HE2	2.08	0.53
1:A:75:GLU:O	4:A:445:HOH:O	2.19	0.52
1:H:98:GLU:HG3	1:H:118:GLN:HB3	1.92	0.52
1:E:311:THR:HG22	1:E:315:ASN:ND2	2.24	0.52
1:D:246:ASN:OD1	1:D:249:ASN:N	2.28	0.52
1:D:122:LEU:C	1:D:124:ASN:N	2.63	0.52
1:A:261:GLU:C	1:A:351:TYR:CE1	2.83	0.52
1:F:163:ILE:CG2	1:F:164:LEU:HD12	2.39	0.52
1:C:141:PRO:HA	4:C:487:HOH:O	2.09	0.52
1:G:229:GLY:O	1:G:233:LEU:HD12	2.10	0.52
1:A:351:TYR:CE2	1:A:353:HIS:HB2	2.45	0.52
1:E:207:HIS:HB3	1:E:228:ILE:HG12	1.91	0.52
1:F:170:LEU:HB3	1:F:173:VAL:CG2	2.40	0.52
1:E:319:MET:HB2	1:E:355:PHE:HB2	1.92	0.51
1:D:96:GLY:N	1:D:98:GLU:OE1	2.38	0.51
1:D:245:TYR:HD2	4:D:464:HOH:O	1.92	0.51
1:F:294:ASN:N	1:F:294:ASN:OD1	2.43	0.51
1:C:287:ASN:ND2	1:C:316:LEU:HD12	2.25	0.51
1:C:275:LYS:HD3	1:C:298:ILE:HG22	1.92	0.51
1:C:287:ASN:HD21	1:C:316:LEU:HA	1.75	0.51
1:F:201:ILE:HD13	1:F:206:VAL:HG21	1.92	0.51
1:E:92:THR:HG22	1:E:92:THR:O	2.11	0.51
1:G:294:ASN:OD1	1:G:294:ASN:N	2.44	0.51
1:D:122:LEU:C	1:D:124:ASN:H	2.12	0.51
1:F:160:ASP:O	1:F:163:ILE:HG22	2.10	0.51
1:H:48:ASP:OD1	1:H:48:ASP:O	2.29	0.51
1:F:170:LEU:HB3	1:F:173:VAL:HG23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:233:LEU:HB2	4:D:445:HOH:O	2.10	0.51
1:H:194:PRO:HD2	4:H:514:HOH:O	2.11	0.51
1:E:131:MET:HG2	1:E:155:SER:O	2.11	0.51
1:B:177:ASP:OD2	4:B:509:HOH:O	2.19	0.51
1:D:48:ASP:CB	4:D:406:HOH:O	2.58	0.51
1:D:216:PRO:HD3	4:D:418:HOH:O	2.11	0.51
1:H:170:LEU:HG	1:H:173:VAL:HG21	1.92	0.51
1:E:237:ASP:OD1	1:E:356:THR:OG1	2.27	0.51
1:C:247:ALA:CB	4:C:482:HOH:O	2.58	0.51
1:C:224:TYR:OH	4:C:414:HOH:O	2.20	0.51
1:G:351:TYR:CE2	1:G:353:HIS:HB2	2.46	0.50
1:E:311:THR:HG22	1:E:315:ASN:HD21	1.75	0.50
1:F:129:ARG:HH11	1:F:129:ARG:HG3	1.76	0.50
1:D:210:ARG:HD3	4:D:481:HOH:O	2.11	0.50
1:H:134:ASP:CG	4:H:520:HOH:O	2.49	0.50
1:D:286:MET:HG3	1:D:291:VAL:CG2	2.41	0.50
1:E:194:PRO:O	1:E:217:LYS:HD2	2.11	0.50
1:D:317:GLU:O	1:D:356:THR:HA	2.11	0.50
1:B:116:TYR:O	1:B:119:ILE:HG12	2.11	0.50
1:D:124:ASN:OD1	4:D:484:HOH:O	2.19	0.50
1:F:187:ILE:HG21	1:F:201:ILE:HG21	1.94	0.50
1:B:143:LEU:HB3	1:B:146:LEU:HD22	1.92	0.50
1:G:262:ARG:HB2	4:G:559:HOH:O	2.12	0.50
1:A:189:PRO:HD3	4:A:474:HOH:O	2.11	0.50
1:B:244:THR:HB	1:B:253:TYR:HB3	1.92	0.50
1:B:294:ASN:OD1	1:B:294:ASN:N	2.45	0.50
1:E:235:ASN:HA	1:E:354:TYR:O	2.12	0.50
1:G:298:ILE:HB	4:G:521:HOH:O	2.12	0.49
1:H:170:LEU:HB3	1:H:173:VAL:HG23	1.94	0.49
1:D:117:ASN:HB3	4:D:462:HOH:O	2.12	0.49
1:D:233:LEU:O	4:D:469:HOH:O	2.20	0.49
1:D:268:GLY:HA2	4:D:481:HOH:O	2.11	0.49
1:E:163:ILE:HG23	1:E:164:LEU:HD12	1.94	0.49
1:H:128:LEU:HD13	4:H:584:HOH:O	1.91	0.49
1:D:286:MET:HA	4:D:494:HOH:O	2.12	0.49
1:B:175:SER:HB3	1:B:198:SER:HB3	1.94	0.49
1:D:210:ARG:CG	4:D:481:HOH:O	2.60	0.49
1:B:79:ASP:O	1:B:102:ASN:ND2	2.43	0.49
1:B:112:HIS:HA	1:B:134:ASP:OD2	2.13	0.49
1:H:127:ARG:HG2	1:H:151:LEU:CB	2.42	0.49
1:A:88:ASN:OD1	1:A:110:ASN:ND2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:126:GLU:HB3	4:D:415:HOH:O	2.12	0.49
1:G:163:ILE:CG2	1:G:164:LEU:HD12	2.42	0.49
1:H:127:ARG:HG2	1:H:151:LEU:HB3	1.94	0.49
1:C:87:ALA:HB3	1:D:88:ASN:HB2	1.95	0.49
1:A:295:ARG:O	1:A:305:VAL:HA	2.12	0.49
1:A:235:ASN:HA	1:A:354:TYR:O	2.12	0.48
1:F:143:LEU:HB3	1:F:146:LEU:HD22	1.94	0.48
1:B:148:ASN:ND2	4:B:565:HOH:O	2.46	0.48
1:G:327:LEU:HD23	1:G:346:ILE:O	2.13	0.48
1:E:143:LEU:HB3	1:E:146:LEU:HD22	1.95	0.48
1:H:202:GLN:HB3	1:H:203:PHE:CD2	2.48	0.48
1:A:182:GLY:HA3	1:A:231:LYS:HG3	1.95	0.48
1:A:128:LEU:HD23	1:A:152:LEU:HD13	1.94	0.48
1:C:194:PRO:HB2	1:C:195:GLU:HG2	1.93	0.48
1:D:296:LEU:HD22	1:D:303:LEU:HD11	1.95	0.48
1:G:182:GLY:HA3	1:G:231:LYS:HG3	1.96	0.48
1:G:140:ILE:O	1:G:166:LYS:NZ	2.39	0.48
1:H:129:ARG:HG2	1:H:153:ASP:HB3	1.94	0.48
1:C:207:HIS:O	1:C:263:THR:HA	2.13	0.48
1:E:271:PRO:HG3	1:E:327:LEU:HD13	1.95	0.48
1:D:170:LEU:HB3	1:D:173:VAL:HG23	1.95	0.48
1:B:98:GLU:HG2	1:C:144:SER:HB2	1.94	0.48
1:H:249:ASN:O	1:H:250:GLN:HB2	2.13	0.48
1:D:202:GLN:NE2	1:D:222:LEU:HB3	2.29	0.48
1:F:286:MET:O	1:F:289:GLN:HB2	2.14	0.48
1:B:178:LEU:HD13	1:B:184:ILE:HD13	1.95	0.48
1:C:129:ARG:NH2	1:D:129:ARG:NH2	2.62	0.47
1:A:285:THR:HB	1:A:320:GLU:HB3	1.96	0.47
1:B:204:ASP:O	1:B:226:GLN:HA	2.14	0.47
1:H:144:SER:O	4:H:558:HOH:O	2.20	0.47
1:D:62:ASN:OD1	1:D:67:GLN:NE2	2.47	0.47
1:H:176:ILE:HG22	1:H:177:ASP:N	2.29	0.47
1:D:339:GLN:O	4:D:403:HOH:O	2.20	0.47
1:H:245:TYR:HB2	1:H:313:PHE:CE1	2.49	0.47
1:G:353:HIS:CD2	1:G:355:PHE:CZ	3.03	0.47
1:E:296:LEU:HD23	1:E:305:VAL:HG13	1.97	0.47
1:A:188:MET:O	1:A:190:LEU:N	2.47	0.47
1:F:58:LYS:HE2	1:F:71:ALA:O	2.14	0.47
1:H:96:GLY:N	1:H:98:GLU:OE1	2.43	0.47
1:A:284:PHE:O	1:A:290:GLN:HA	2.15	0.47
1:A:143:LEU:HB3	1:A:146:LEU:HD22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:48:ASP:O	1:D:48:ASP:OD1	2.33	0.47
1:B:337:GLN:CG	4:B:581:HOH:O	2.63	0.47
1:D:103:ILE:O	1:D:124:ASN:O	2.32	0.47
1:F:143:LEU:HD12	1:F:167:ILE:HG22	1.95	0.47
1:B:105:ASP:OD1	1:B:127:ARG:CZ	2.63	0.47
1:D:244:THR:HB	1:D:253:TYR:HB3	1.97	0.47
1:E:236:SER:HB2	1:E:355:PHE:HD1	1.77	0.47
1:H:203:PHE:HA	1:H:225:SER:O	2.14	0.47
1:B:129:ARG:HG2	1:B:153:ASP:HB3	1.97	0.47
1:H:237:ASP:OD1	1:H:356:THR:OG1	2.26	0.47
1:H:315:ASN:OD1	1:H:315:ASN:N	2.47	0.47
1:G:94:LEU:O	1:G:97:ILE:HG22	2.13	0.47
1:C:129:ARG:NH2	1:D:129:ARG:CZ	2.77	0.46
1:E:105:ASP:OD1	1:E:127:ARG:HB2	2.15	0.46
1:E:125:LEU:HA	1:E:125:LEU:HD12	1.67	0.46
1:E:344:TYR:N	4:E:456:HOH:O	2.47	0.46
1:H:219:ASN:C	1:H:219:ASN:OD1	2.54	0.46
1:C:322:ASN:HA	1:C:351:TYR:O	2.15	0.46
1:D:253:TYR:CE1	1:D:302:GLY:HA3	2.51	0.46
1:B:89:ILE:HG13	1:B:91:VAL:HG23	1.97	0.46
1:C:132:GLY:O	1:C:157:SER:HA	2.15	0.46
1:G:174:THR:HA	1:G:195:GLU:O	2.16	0.46
1:C:134:ASP:OD1	1:C:134:ASP:N	2.49	0.46
1:G:84:ILE:HD12	1:G:103:ILE:HD13	1.97	0.46
1:B:118:GLN:HG3	1:C:169:THR:HG21	1.98	0.46
1:H:266:TYR:CD2	1:H:335:PRO:HG3	2.50	0.46
1:F:103:ILE:HG23	4:F:506:HOH:O	2.16	0.46
1:B:202:GLN:O	1:B:203:PHE:HB2	2.15	0.46
1:C:251:THR:HA	1:C:305:VAL:O	2.15	0.46
1:E:152:LEU:HD23	1:E:176:ILE:HG12	1.97	0.46
1:A:112:HIS:HA	1:A:134:ASP:OD2	2.16	0.46
1:D:274:VAL:HG21	1:D:281:ASP:HB3	1.97	0.46
1:C:137:SER:O	1:C:166:LYS:NZ	2.49	0.46
1:H:65:LEU:HD11	1:H:77:GLN:HB3	1.98	0.46
1:E:52:ILE:HB	1:E:58:LYS:HD2	1.98	0.45
1:D:92:THR:HG22	1:D:92:THR:O	2.16	0.45
1:B:311:THR:HG23	4:B:540:HOH:O	2.16	0.45
1:G:110:ASN:OD1	1:G:112:HIS:HE1	1.98	0.45
1:B:164:LEU:HD23	1:B:190:LEU:HG	1.97	0.45
1:B:126:GLU:O	1:B:149:LEU:HD12	2.17	0.45
1:H:129:ARG:HG3	1:H:129:ARG:HH11	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:266:TYR:CD2	1:C:335:PRO:HG3	2.51	0.45
1:D:127:ARG:HG2	1:D:151:LEU:HB3	1.99	0.45
1:D:166:LYS:HG2	4:D:463:HOH:O	2.16	0.45
1:C:294:ASN:OD1	1:C:294:ASN:N	2.49	0.45
1:D:251:THR:HA	1:D:305:VAL:O	2.16	0.45
1:B:353:HIS:CD2	1:B:355:PHE:CZ	3.05	0.45
1:B:268:GLY:O	1:B:270:VAL:HG23	2.16	0.45
1:F:295:ARG:HH22	1:F:308:VAL:CG2	2.29	0.45
1:G:136:THR:O	1:G:139:LYS:HB2	2.17	0.45
1:G:229:GLY:HA2	1:G:232:LYS:O	2.17	0.45
1:H:57:PHE:HB2	1:H:91:VAL:HG13	1.98	0.45
1:B:182:GLY:HA3	1:B:231:LYS:HG2	1.99	0.45
1:C:186:ASP:C	1:C:186:ASP:OD1	2.54	0.45
1:B:340:ASN:CG	4:B:543:HOH:O	2.45	0.45
1:F:219:ASN:O	1:F:342:GLY:HA3	2.17	0.45
1:C:178:LEU:HA	1:C:178:LEU:HD23	1.82	0.45
1:G:125:LEU:HA	1:G:125:LEU:HD12	1.77	0.45
1:D:153:ASP:C	1:D:153:ASP:OD1	2.54	0.45
1:D:275:LYS:CA	4:D:492:HOH:O	2.60	0.44
1:E:94:LEU:HD11	1:E:116:TYR:CD1	2.52	0.44
1:F:48:ASP:OD1	1:F:48:ASP:O	2.34	0.44
1:D:204:ASP:O	1:D:226:GLN:HA	2.17	0.44
1:H:234:ILE:HG21	1:H:353:HIS:CE1	2.52	0.44
1:B:187:ILE:HD12	1:B:199:LEU:CD2	2.47	0.44
1:B:127:ARG:HG2	1:B:151:LEU:HB3	1.99	0.44
1:F:50:VAL:HG22	1:F:75:GLU:HG2	1.98	0.44
1:G:284:PHE:HE2	1:G:286:MET:HG3	1.83	0.44
1:H:288:GLU:OE2	1:H:318:LYS:HE3	2.17	0.44
1:C:108:ILE:HG23	1:C:111:ILE:HG21	1.99	0.44
1:A:96:GLY:CA	1:A:98:GLU:OE1	2.65	0.44
1:H:170:LEU:HB3	1:H:173:VAL:CG2	2.48	0.44
1:H:283:TYR:HB3	1:H:322:ASN:HB3	1.99	0.44
1:F:223:ALA:HB3	1:F:346:ILE:HG22	2.00	0.44
1:B:292:ASN:OD1	1:B:293:GLY:N	2.50	0.44
1:C:149:LEU:HA	1:C:149:LEU:HD12	1.77	0.44
1:G:191:LYS:HA	1:G:215:PHE:CE1	2.52	0.44
1:B:120:SER:HB3	1:B:141:PRO:HG2	1.99	0.44
1:B:328:SER:HA	1:B:348:MET:HE1	1.99	0.44
1:D:287:ASN:HD21	1:D:316:LEU:HA	1.82	0.44
1:E:129:ARG:HA	1:E:153:ASP:HB3	2.00	0.44
1:G:319:MET:HB2	1:G:355:PHE:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:173:VAL:HG11	1:G:176:ILE:HG13	1.99	0.44
1:H:105:ASP:OD1	1:H:127:ARG:CZ	2.65	0.44
1:H:229:GLY:HA2	1:H:232:LYS:O	2.17	0.44
1:D:319:MET:HB2	1:D:355:PHE:HB2	1.99	0.44
1:D:245:TYR:OH	1:D:308:VAL:O	2.24	0.44
1:C:224:TYR:CZ	4:C:414:HOH:O	2.68	0.44
1:G:318:LYS:HA	1:G:355:PHE:O	2.18	0.44
1:C:170:LEU:HD13	1:C:173:VAL:HG21	2.00	0.44
1:H:285:THR:O	1:H:319:MET:HA	2.18	0.43
1:D:271:PRO:HB3	1:D:327:LEU:HD13	2.00	0.43
1:C:285:THR:HB	1:C:320:GLU:HB3	1.99	0.43
1:B:271:PRO:HB3	1:B:327:LEU:HD13	1.99	0.43
1:H:132:GLY:O	1:H:157:SER:HA	2.18	0.43
1:C:117:ASN:HA	1:C:141:PRO:HG3	2.00	0.43
1:H:170:LEU:HA	1:H:171:PRO:HD3	1.75	0.43
1:D:100:ALA:C	4:D:480:HOH:O	2.56	0.43
1:A:83:TYR:HE1	4:A:457:HOH:O	2.02	0.43
1:D:294:ASN:OD1	1:D:294:ASN:N	2.51	0.43
1:G:143:LEU:O	1:G:145:GLY:N	2.52	0.43
1:C:328:SER:CB	4:C:486:HOH:O	2.07	0.43
1:G:151:LEU:C	1:G:151:LEU:HD23	2.39	0.43
1:G:62:ASN:OD1	1:G:71:ALA:O	2.36	0.43
1:B:146:LEU:HD23	1:B:149:LEU:HD22	2.01	0.43
1:F:286:MET:HG3	1:F:291:VAL:CG2	2.48	0.43
1:F:274:VAL:HG22	1:F:324:ARG:O	2.19	0.43
1:E:191:LYS:HB3	1:E:191:LYS:HE2	1.79	0.43
1:H:129:ARG:NH1	1:H:129:ARG:HG3	2.33	0.43
1:E:122:LEU:O	1:E:125:LEU:HB2	2.19	0.43
1:H:353:HIS:CD2	1:H:355:PHE:CZ	3.06	0.43
1:G:170:LEU:HD13	1:G:173:VAL:HG21	2.00	0.43
1:D:292:ASN:HB3	1:D:295:ARG:HG3	2.00	0.43
1:D:250:GLN:NE2	1:D:309:SER:HA	2.33	0.43
1:E:200:ASN:HB2	1:E:222:LEU:HD12	2.01	0.43
1:C:69:SER:O	4:C:447:HOH:O	2.20	0.43
1:H:131:MET:HB3	1:H:155:SER:O	2.18	0.43
1:C:252:LEU:HB3	1:C:305:VAL:HB	1.99	0.43
1:H:228:ILE:HD11	4:H:581:HOH:O	2.19	0.43
1:C:131:MET:HE2	4:C:484:HOH:O	2.15	0.42
1:G:287:ASN:HD21	1:G:316:LEU:HA	1.82	0.42
1:H:317:GLU:O	1:H:356:THR:HA	2.19	0.42
1:C:219:ASN:C	1:C:219:ASN:OD1	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:ASN:HA	1:B:318:LYS:HB2	2.00	0.42
1:C:129:ARG:HH22	1:D:129:ARG:HH21	1.68	0.42
1:H:202:GLN:O	1:H:203:PHE:CB	2.67	0.42
1:D:237:ASP:OD1	1:D:356:THR:OG1	2.33	0.42
1:A:319:MET:HB2	1:A:355:PHE:HB2	2.01	0.42
1:G:316:LEU:HD23	1:G:357:VAL:HG21	2.01	0.42
1:D:129:ARG:HG3	1:D:129:ARG:HH11	1.84	0.42
1:F:334:THR:CG2	4:F:568:HOH:O	2.60	0.42
1:E:98:GLU:HG2	1:E:118:GLN:HB3	2.00	0.42
1:F:285:THR:HA	1:F:289:GLN:O	2.20	0.42
1:A:207:HIS:HD2	4:A:448:HOH:O	2.01	0.42
1:D:286:MET:O	1:D:289:GLN:HB2	2.18	0.42
1:F:197:LYS:C	1:F:218:LEU:HD12	2.40	0.42
1:H:163:ILE:HG23	1:H:164:LEU:HD12	2.00	0.42
1:A:334:THR:CG2	4:A:422:HOH:O	2.28	0.42
1:E:348:MET:HB2	4:E:455:HOH:O	2.19	0.42
1:F:129:ARG:HG3	1:F:129:ARG:NH1	2.35	0.42
1:C:229:GLY:HA2	1:C:232:LYS:O	2.20	0.42
1:B:170:LEU:HA	1:B:171:PRO:HD2	1.95	0.42
1:E:294:ASN:OD1	1:E:294:ASN:N	2.52	0.42
1:G:144:SER:HB3	1:G:169:THR:OG1	2.19	0.42
1:G:48:ASP:OD1	1:G:48:ASP:O	2.37	0.42
1:B:327:LEU:HA	1:B:327:LEU:HD12	1.62	0.42
1:F:295:ARG:NH2	1:F:308:VAL:CG2	2.83	0.42
1:H:275:LYS:HD3	1:H:298:ILE:HG22	2.00	0.42
1:G:152:LEU:HD12	1:G:152:LEU:HA	1.81	0.42
1:B:149:LEU:HA	1:B:149:LEU:HD12	1.81	0.42
1:D:176:ILE:HD11	1:D:193:MET:CE	2.50	0.42
1:E:336:GLU:O	1:E:339:GLN:HB2	2.20	0.42
1:G:285:THR:HB	1:G:320:GLU:HB3	2.01	0.42
1:A:221:LEU:HA	1:A:221:LEU:HD12	1.90	0.42
1:G:315:ASN:CB	4:G:556:HOH:O	2.67	0.42
1:D:210:ARG:CD	4:D:481:HOH:O	2.67	0.42
1:H:53:PRO:HG3	4:H:546:HOH:O	2.20	0.42
1:C:286:MET:HB2	1:C:286:MET:HE2	1.95	0.42
1:D:94:LEU:HD23	1:D:94:LEU:HA	1.79	0.42
1:E:236:SER:HB2	1:E:355:PHE:CE1	2.54	0.41
1:H:327:LEU:HB3	1:H:349:PRO:HD2	2.02	0.41
1:H:178:LEU:HA	1:H:178:LEU:HD12	1.97	0.41
1:F:99:TYR:HA	1:F:101:HIS:CE1	2.55	0.41
1:A:88:ASN:ND2	4:A:450:HOH:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:324:ARG:NH1	4:G:504:HOH:O	2.21	0.41
1:E:120:SER:HA	1:E:146:LEU:HD11	2.02	0.41
1:A:340:ASN:ND2	4:A:414:HOH:O	2.40	0.41
1:E:268:GLY:O	1:E:270:VAL:HG23	2.20	0.41
1:D:204:ASP:C	1:D:226:GLN:OE1	2.58	0.41
1:C:129:ARG:HH21	1:D:129:ARG:CZ	2.33	0.41
1:G:191:LYS:HA	1:G:215:PHE:CD1	2.56	0.41
1:C:170:LEU:HB3	1:C:173:VAL:HG23	2.01	0.41
1:G:94:LEU:HA	1:G:94:LEU:HD23	1.81	0.41
1:E:74:THR:CG2	4:E:435:HOH:O	2.68	0.41
1:H:274:VAL:HG21	1:H:281:ASP:HB3	2.03	0.41
1:F:271:PRO:CB	1:F:327:LEU:HD13	2.50	0.41
1:B:175:SER:CB	4:B:572:HOH:O	2.59	0.41
1:C:122:LEU:CB	1:C:125:LEU:HD22	2.47	0.41
1:B:197:LYS:HA	1:B:218:LEU:HA	2.02	0.41
1:E:164:LEU:HD21	1:E:187:ILE:HA	2.03	0.41
1:E:239:LYS:HA	1:E:239:LYS:HD3	1.88	0.41
1:B:117:ASN:HA	1:B:141:PRO:HG3	2.02	0.41
1:C:327:LEU:HD23	1:C:346:ILE:O	2.21	0.41
1:F:187:ILE:HD13	1:F:199:LEU:CD2	2.51	0.41
1:G:233:LEU:HD12	1:G:233:LEU:HA	1.84	0.41
1:D:170:LEU:HA	1:D:170:LEU:HD23	1.88	0.41
1:G:215:PHE:HA	1:G:216:PRO:HD2	1.94	0.41
1:H:354:TYR:HE1	4:H:583:HOH:O	2.03	0.41
1:C:201:ILE:HD12	1:C:206:VAL:CG2	2.51	0.40
1:G:163:ILE:HD12	1:G:163:ILE:HA	1.93	0.40
1:H:176:ILE:CG2	1:H:177:ASP:N	2.84	0.40
1:D:212:ILE:O	1:D:215:PHE:HB2	2.20	0.40
1:G:218:LEU:N	4:G:563:HOH:O	2.49	0.40
1:A:325:ILE:HD11	1:A:351:TYR:HB2	2.02	0.40
1:D:202:GLN:O	1:D:203:PHE:CB	2.64	0.40
1:A:296:LEU:HD22	1:A:303:LEU:HD11	2.03	0.40
1:B:332:TYR:CE1	1:B:346:ILE:HG12	2.57	0.40
1:C:163:ILE:HG23	1:C:164:LEU:HD12	2.03	0.40
1:B:233:LEU:HD12	1:B:233:LEU:HA	1.84	0.40
1:B:190:LEU:HD22	1:B:193:MET:SD	2.61	0.40
1:A:287:ASN:HA	1:A:318:LYS:HB2	2.03	0.40
1:F:244:THR:HB	1:F:253:TYR:HB3	2.04	0.40
1:C:182:GLY:HA2	1:C:204:ASP:HA	2.03	0.40
1:A:234:ILE:HD13	1:A:261:GLU:HG3	2.02	0.40
1:H:219:ASN:O	1:H:342:GLY:HA3	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:LYS:HD3	1:B:231:LYS:HA	1.91	0.40
1:C:135:VAL:HG22	4:C:432:HOH:O	2.21	0.40
1:C:254:VAL:HA	1:C:255:PRO:HD2	1.90	0.40

All (1) 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:G:90:ASN:OD1	4:H:569:HOH:O[1_545]	2.19	0.01

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	309/347 (89%)	289 (94%)	18 (6%)	2 (1%)	30 43
1	B	309/347 (89%)	282 (91%)	27 (9%)	0	100 100
1	C	309/347 (89%)	287 (93%)	22 (7%)	0	100 100
1	D	309/347 (89%)	288 (93%)	20 (6%)	1 (0%)	46 63
1	E	309/347 (89%)	294 (95%)	15 (5%)	0	100 100
1	F	309/347 (89%)	283 (92%)	26 (8%)	0	100 100
1	G	309/347 (89%)	298 (96%)	11 (4%)	0	100 100
1	H	309/347 (89%)	279 (90%)	30 (10%)	0	100 100
All	All	2472/2776 (89%)	2300 (93%)	169 (7%)	3 (0%)	56 74

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	123	SER
1	A	144	SER

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Mol	Chain	Res	Type
1	A	189	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	281/311 (90%)	271 (96%)	10 (4%)	42	63
1	B	281/311 (90%)	265 (94%)	16 (6%)	25	40
1	C	281/311 (90%)	268 (95%)	13 (5%)	33	51
1	D	281/311 (90%)	263 (94%)	18 (6%)	22	34
1	E	281/311 (90%)	269 (96%)	12 (4%)	35	55
1	F	281/311 (90%)	268 (95%)	13 (5%)	33	51
1	G	281/311 (90%)	265 (94%)	16 (6%)	25	40
1	H	281/311 (90%)	258 (92%)	23 (8%)	14	21
All	All	2248/2488 (90%)	2127 (95%)	121 (5%)	27	43

All (121) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	GLU
1	A	114	THR
1	A	119	ILE
1	A	233	LEU
1	A	240	SER
1	A	285	THR
1	A	294	ASN
1	A	303	LEU
1	A	305	VAL
1	A	328	SER
1	B	48	ASP
1	B	57	PHE
1	B	98	GLU
1	B	104	LYS

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Mol	Chain	Res	Type
1	B	114	THR
1	B	146	LEU
1	B	151	LEU
1	B	233	LEU
1	B	240	SER
1	B	248	GLU
1	B	285	THR
1	B	294	ASN
1	B	305	VAL
1	B	307	ASP
1	B	311	THR
1	B	328	SER
1	C	98	GLU
1	C	114	THR
1	C	125	LEU
1	C	146	LEU
1	C	169	THR
1	C	189	PRO
1	C	233	LEU
1	C	285	THR
1	C	294	ASN
1	C	303	LEU
1	C	307	ASP
1	C	328	SER
1	C	347	SER
1	D	48	ASP
1	D	98	GLU
1	D	112	HIS
1	D	114	THR
1	D	146	LEU
1	D	164	LEU
1	D	169	THR
1	D	184	ILE
1	D	201	ILE
1	D	233	LEU
1	D	285	THR
1	D	294	ASN
1	D	299	THR
1	D	300	SER
1	D	303	LEU
1	D	315	ASN
1	D	334	THR

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Mol	Chain	Res	Type
1	D	347	SER
1	E	53	PRO
1	E	98	GLU
1	E	125	LEU
1	E	233	LEU
1	E	240	SER
1	E	285	THR
1	E	294	ASN
1	E	303	LEU
1	E	305	VAL
1	E	307	ASP
1	E	347	SER
1	E	357	VAL
1	F	114	THR
1	F	119	ILE
1	F	187	ILE
1	F	191	LYS
1	F	233	LEU
1	F	240	SER
1	F	249	ASN
1	F	285	THR
1	F	294	ASN
1	F	315	ASN
1	F	328	SER
1	F	334	THR
1	F	347	SER
1	G	56	THR
1	G	88	ASN
1	G	98	GLU
1	G	114	THR
1	G	129	ARG
1	G	167	ILE
1	G	169	THR
1	G	233	LEU
1	G	237	ASP
1	G	279	SER
1	G	294	ASN
1	G	298	ILE
1	G	299	THR
1	G	307	ASP
1	G	334	THR
1	G	347	SER

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Mol	Chain	Res	Type
1	H	69	SER
1	H	98	GLU
1	H	114	THR
1	H	144	SER
1	H	146	LEU
1	H	151	LEU
1	H	167	ILE
1	H	169	THR
1	H	170	LEU
1	H	178	LEU
1	H	184	ILE
1	H	191	LYS
1	H	225	SER
1	H	233	LEU
1	H	240	SER
1	H	243	LEU
1	H	285	THR
1	H	294	ASN
1	H	299	THR
1	H	307	ASP
1	H	315	ASN
1	H	328	SER
1	H	358	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	148	ASN
1	C	101	HIS
1	C	207	HIS
1	C	250	GLN
1	D	112	HIS
1	D	156	HIS
1	D	202	GLN
1	D	250	GLN
1	E	156	HIS
1	E	207	HIS
1	E	315	ASN
1	F	51	ASN
1	F	72	ASN
1	F	292	ASN
1	F	322	ASN

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Mol	Chain	Res	Type
1	G	88	ASN
1	G	90	ASN
1	G	112	HIS
1	G	117	ASN
1	G	207	HIS
1	H	72	ASN
1	H	90	ASN
1	H	250	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

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	311/347 (89%)	0.27	8 (2%) 59 58	16, 30, 65, 82	0
1	B	311/347 (89%)	0.25	7 (2%) 64 63	13, 27, 58, 83	0
1	C	311/347 (89%)	0.39	17 (5%) 29 29	15, 29, 81, 99	0
1	D	311/347 (89%)	0.54	30 (9%) 10 10	17, 32, 79, 94	0
1	E	311/347 (89%)	0.78	43 (13%) 4 4	14, 39, 87, 97	0
1	F	311/347 (89%)	0.21	10 (3%) 51 51	14, 28, 67, 91	0
1	G	311/347 (89%)	0.38	15 (4%) 34 35	15, 33, 68, 87	0
1	H	311/347 (89%)	0.15	4 (1%) 79 79	12, 29, 66, 85	0
All	All	2488/2776 (89%)	0.37	134 (5%) 29 30	12, 31, 75, 99	0

All (134) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	316	LEU	7.3
1	C	243	LEU	6.5
1	E	304	THR	5.6
1	C	329	TYR	5.5
1	G	329	TYR	5.4
1	D	252	LEU	5.2
1	E	284	PHE	5.0
1	C	244	THR	4.7
1	D	238	ILE	4.6
1	D	300	SER	4.5
1	D	293	GLY	4.5
1	E	243	LEU	4.4
1	E	357	VAL	4.4
1	A	316	LEU	4.4
1	E	355	PHE	4.3
1	D	294	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	306	SER	4.3
1	E	252	LEU	4.1
1	C	313	PHE	4.1
1	D	329	TYR	4.0
1	E	317	GLU	3.9
1	E	245	TYR	3.9
1	D	241	SER	3.8
1	G	254	VAL	3.8
1	C	284	PHE	3.8
1	E	291	VAL	3.6
1	D	297	THR	3.5
1	E	247	ALA	3.5
1	E	286	MET	3.5
1	E	329	TYR	3.4
1	A	313	PHE	3.4
1	E	319	MET	3.4
1	D	305	VAL	3.3
1	G	296	LEU	3.3
1	H	243	LEU	3.3
1	D	286	MET	3.3
1	E	254	VAL	3.3
1	E	274	VAL	3.2
1	C	252	LEU	3.2
1	D	304	THR	3.2
1	G	308	VAL	3.1
1	A	243	LEU	3.1
1	G	243	LEU	3.1
1	E	306	SER	3.1
1	D	203	PHE	3.1
1	D	243	LEU	3.0
1	G	252	LEU	3.0
1	C	357	VAL	2.9
1	D	283	TYR	2.9
1	D	311	THR	2.9
1	C	249	ASN	2.9
1	E	244	THR	2.9
1	E	236	SER	2.9
1	E	279	SER	2.9
1	C	253	TYR	2.9
1	F	316	LEU	2.9
1	B	310	LYS	2.8
1	F	239	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	300	SER	2.8
1	C	241	SER	2.8
1	G	331	SER	2.8
1	A	252	LEU	2.8
1	E	313	PHE	2.8
1	F	284	PHE	2.7
1	G	286	MET	2.7
1	E	351	TYR	2.7
1	E	305	VAL	2.7
1	G	238	ILE	2.6
1	E	275	LYS	2.6
1	D	111	ILE	2.6
1	E	237	ASP	2.6
1	D	249	ASN	2.6
1	F	315	ASN	2.6
1	B	313	PHE	2.6
1	E	282	THR	2.6
1	E	238	ILE	2.5
1	G	301	ASP	2.5
1	B	303	LEU	2.5
1	D	303	LEU	2.5
1	E	315	ASN	2.4
1	E	253	TYR	2.4
1	D	307	ASP	2.4
1	C	319	MET	2.4
1	E	314	ASP	2.4
1	E	248	GLU	2.4
1	F	313	PHE	2.4
1	D	319	MET	2.3
1	E	298	ILE	2.3
1	G	295	ARG	2.3
1	C	237	ASP	2.3
1	D	254	VAL	2.3
1	D	124	ASN	2.3
1	F	355	PHE	2.3
1	E	182	GLY	2.3
1	E	318	LYS	2.3
1	C	238	ILE	2.3
1	F	238	ILE	2.3
1	E	277	THR	2.3
1	H	316	LEU	2.3
1	A	294	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	E	349	PRO	2.3
1	C	291	VAL	2.3
1	G	303	LEU	2.3
1	G	355	PHE	2.2
1	E	294	ASN	2.2
1	F	248	GLU	2.2
1	B	311	THR	2.2
1	D	323	ALA	2.2
1	A	319	MET	2.2
1	D	324	ARG	2.2
1	E	276	SER	2.2
1	A	317	GLU	2.2
1	C	283	TYR	2.2
1	D	284	PHE	2.2
1	B	317	GLU	2.2
1	C	282	THR	2.1
1	D	336	GLU	2.1
1	E	350	ILE	2.1
1	E	320	GLU	2.1
1	H	313	PHE	2.1
1	E	321	TYR	2.1
1	D	316	LEU	2.1
1	F	319	MET	2.1
1	G	71	ALA	2.1
1	A	234	ILE	2.1
1	E	250	GLN	2.1
1	D	247	ALA	2.1
1	G	299	THR	2.0
1	F	258	LEU	2.0
1	B	254	VAL	2.0
1	C	293	GLY	2.0
1	D	296	LEU	2.0
1	H	279	SER	2.0
1	B	169	THR	2.0

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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NA	H	401	1/1	0.97	0.12	-1.79	29,29,29,29	0
2	NI	B	401	1/1	0.98	0.09	-2.55	36,36,36,36	0
2	NI	F	401	1/1	0.99	0.05	-3.28	40,40,40,40	0
3	NA	G	401	1/1	0.95	0.07	-	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.