



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:35 PM GMT

PDB ID : 4IRV  
Title : Structure of the Helicobacter pylori CagA Oncogene Bound to the Human  
Tumor Suppressor Apoptosis-stimulating Protein of p53-2  
Authors : Stebbins, C.E.; Nesic, D.  
Deposited on : 2013-01-15  
Resolution : 2.04 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

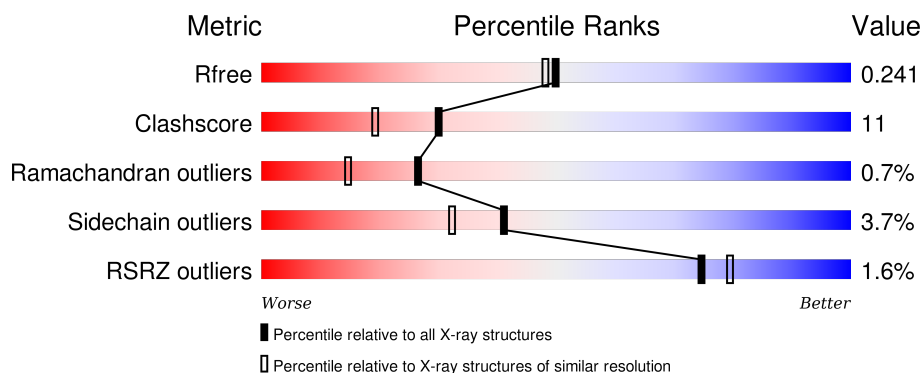
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.04 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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  $\geq 3$ , 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	221	<div> <div>68%</div> <div>17%</div> <div>•</div> <div>11%</div> </div>
1	B	221	<div> <div>68%</div> <div>17%</div> <div>•</div> <div>12%</div> </div>
1	C	221	<div> <div>68%</div> <div>18%</div> <div>•</div> <div>13%</div> </div>
1	D	221	<div> <div>75%</div> <div>12%</div> <div>•</div> <div>10%</div> </div>
2	E	62	<div> <div>23%</div> <div>10%</div> <div>68%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	62	<div><div><div></div><div></div><div></div><div></div></div><div><div>3%</div><div>24%</div><div>8%</div><div>68%</div></div></div>
2	G	62	<div><div><div></div><div></div><div></div><div></div></div><div><div>3%</div><div>19%</div><div>13%</div><div>68%</div></div></div>
2	H	62	<div><div><div></div><div></div><div></div><div></div></div><div><div>2%</div><div>26%</div><div>5%</div><div>68%</div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7530 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 Cytotoxicity-associated immunodominant antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	Se	0	0	0
			1609	1018	276	313	2			
1	B	194	Total	C	N	O	Se	0	0	0
			1592	1008	272	310	2			
1	C	192	Total	C	N	O	Se	0	0	0
			1572	994	270	306	2			
1	D	198	Total	C	N	O	Se	0	0	0
			1616	1023	277	314	2			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	GLY	-	EXPRESSION TAG	UNP P55980
A	16	PRO	-	EXPRESSION TAG	UNP P55980
A	17	VAL	-	EXPRESSION TAG	UNP P55980
A	18	ASP	-	EXPRESSION TAG	UNP P55980
B	15	GLY	-	EXPRESSION TAG	UNP P55980
B	16	PRO	-	EXPRESSION TAG	UNP P55980
B	17	VAL	-	EXPRESSION TAG	UNP P55980
B	18	ASP	-	EXPRESSION TAG	UNP P55980
C	15	GLY	-	EXPRESSION TAG	UNP P55980
C	16	PRO	-	EXPRESSION TAG	UNP P55980
C	17	VAL	-	EXPRESSION TAG	UNP P55980
C	18	ASP	-	EXPRESSION TAG	UNP P55980
D	15	GLY	-	EXPRESSION TAG	UNP P55980
D	16	PRO	-	EXPRESSION TAG	UNP P55980
D	17	VAL	-	EXPRESSION TAG	UNP P55980
D	18	ASP	-	EXPRESSION TAG	UNP P55980

- Molecule 2 is a protein called Apoptosis-stimulating of p53 protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	20	Total 157	C 100	N 27	O 29	Se 1	0	0	0
2	F	20	Total 157	C 100	N 27	O 29	Se 1	0	0	0
2	G	20	Total 157	C 100	N 27	O 29	Se 1	0	0	0
2	H	20	Total 157	C 100	N 27	O 29	Se 1	0	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	721	GLY	-	EXPRESSION TAG	UNP Q13625
E	722	PRO	-	EXPRESSION TAG	UNP Q13625
E	723	LYS	-	EXPRESSION TAG	UNP Q13625
E	724	LEU	-	EXPRESSION TAG	UNP Q13625
E	725	ALA	-	EXPRESSION TAG	UNP Q13625
F	721	GLY	-	EXPRESSION TAG	UNP Q13625
F	722	PRO	-	EXPRESSION TAG	UNP Q13625
F	723	LYS	-	EXPRESSION TAG	UNP Q13625
F	724	LEU	-	EXPRESSION TAG	UNP Q13625
F	725	ALA	-	EXPRESSION TAG	UNP Q13625
G	721	GLY	-	EXPRESSION TAG	UNP Q13625
G	722	PRO	-	EXPRESSION TAG	UNP Q13625
G	723	LYS	-	EXPRESSION TAG	UNP Q13625
G	724	LEU	-	EXPRESSION TAG	UNP Q13625
G	725	ALA	-	EXPRESSION TAG	UNP Q13625
H	721	GLY	-	EXPRESSION TAG	UNP Q13625
H	722	PRO	-	EXPRESSION TAG	UNP Q13625
H	723	LYS	-	EXPRESSION TAG	UNP Q13625
H	724	LEU	-	EXPRESSION TAG	UNP Q13625
H	725	ALA	-	EXPRESSION TAG	UNP Q13625

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	124	Total 124	O 124	0	0
3	B	148	Total 148	O 148	0	0
3	C	92	Total 92	O 92	0	0
3	D	120	Total 120	O 120	0	0

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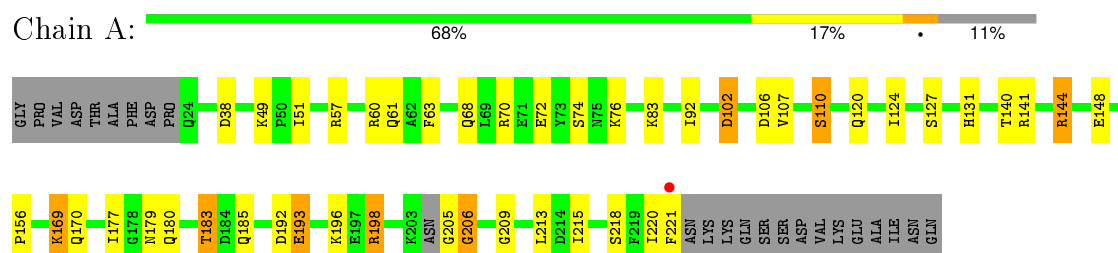
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	9	Total 9	O 9	0	0
3	F	10	Total 10	O 10	0	0
3	G	6	Total 6	O 6	0	0
3	H	4	Total 4	O 4	0	0

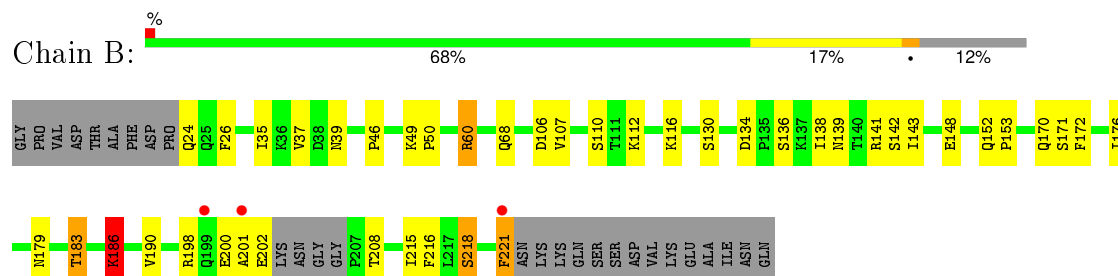
### 3 Residue-property plots [i](#)

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.

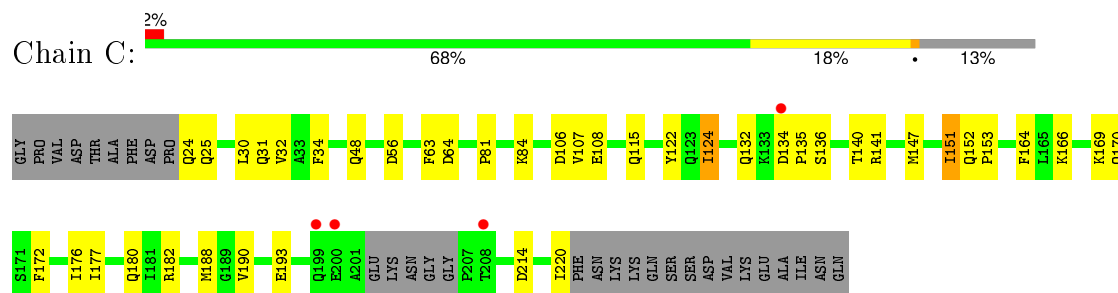
#### • Molecule 1: Cytotoxicity-associated immunodominant antigen



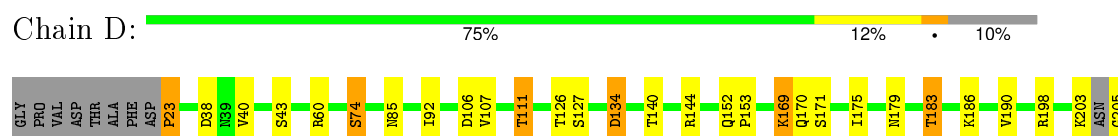
#### • Molecule 1: Cytotoxicity-associated immunodominant antigen

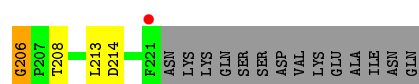


#### • Molecule 1: Cytotoxicity-associated immunodominant antigen

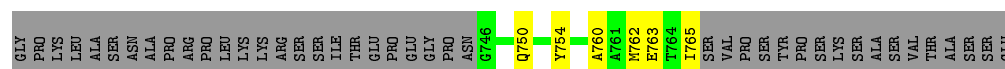


#### • Molecule 1: Cytotoxicity-associated immunodominant antigen

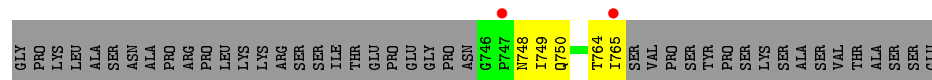




- Molecule 2: Apoptosis-stimulating of p53 protein 2



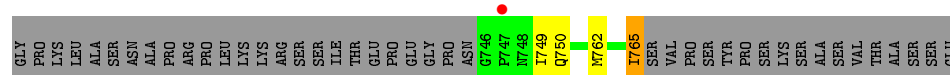
- Molecule 2: Apoptosis-stimulating of p53 protein 2



- Molecule 2: Apoptosis-stimulating of p53 protein 2



- Molecule 2: Apoptosis-stimulating of p53 protein 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	118.64Å 120.24Å 100.66Å 90.00° 115.64° 90.00°	Depositor
Resolution (Å)	90.75 – 2.04 90.75 – 2.04	Depositor EDS
% Data completeness (in resolution range)	96.7 (90.75-2.04) 96.7 (90.75-2.04)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.75 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, $R_{free}$	0.189 , 0.234 0.195 , 0.241	Depositor DCC
$R_{free}$ test set	4023 reflections (5.45%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.6	Xtriage
Anisotropy	0.629	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 80041 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7530	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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 ⓘ

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	1.03	6/1638 (0.4%)	1.06	13/2197 (0.6%)
1	B	1.03	3/1621 (0.2%)	1.02	6/2175 (0.3%)
1	C	0.88	0/1600	0.91	3/2147 (0.1%)
1	D	0.98	1/1646 (0.1%)	0.98	5/2208 (0.2%)
2	E	0.87	0/157	1.01	1/210 (0.5%)
2	F	0.95	0/157	0.92	0/210
2	G	0.73	0/157	0.87	0/210
2	H	0.81	0/157	0.81	0/210
All	All	0.97	10/7133 (0.1%)	0.99	28/9567 (0.3%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	193	GLU	CD-OE1	9.42	1.36	1.25
1	B	171	SER	CB-OG	-8.95	1.30	1.42
1	A	193	GLU	CD-OE2	8.28	1.34	1.25
1	D	74	SER	CB-OG	-7.24	1.32	1.42
1	A	102	ASP	CG-OD2	7.22	1.42	1.25
1	A	74	SER	CB-OG	-7.04	1.33	1.42
1	B	218	SER	CB-OG	-6.89	1.33	1.42
1	A	102	ASP	CB-CG	6.71	1.65	1.51
1	B	142	SER	CB-OG	-6.01	1.34	1.42
1	A	193	GLU	CG-CD	5.38	1.60	1.51

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	60	ARG	NE-CZ-NH2	-10.54	115.03	120.30
1	A	102	ASP	CB-CG-OD2	10.04	127.34	118.30
1	A	102	ASP	CB-CG-OD1	-9.23	109.99	118.30
1	A	169	LYS	CD-CE-NZ	-8.53	92.09	111.70
1	D	60	ARG	NE-CZ-NH1	8.35	124.47	120.30
1	B	60	ARG	NE-CZ-NH1	7.60	124.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	169	LYS	CD-CE-NZ	7.45	128.83	111.70
1	B	142	SER	CB-CA-C	-7.30	96.22	110.10
1	B	218	SER	CB-CA-C	-7.30	96.23	110.10
1	A	60	ARG	NE-CZ-NH2	-7.14	116.73	120.30
1	A	198	ARG	CB-CA-C	-6.55	97.29	110.40
2	E	762	MSE	CG-SE-CE	-6.13	85.42	98.90
1	A	60	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	B	186	LYS	CD-CE-NZ	-6.01	97.88	111.70
1	D	74	SER	CB-CA-C	-5.92	98.86	110.10
1	C	214	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	70	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	C	64	ASP	CB-CG-OD1	5.64	123.38	118.30
1	D	169	LYS	CG-CD-CE	-5.60	95.11	111.90
1	B	141	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	141	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	57	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	192	ASP	CB-CG-OD1	5.10	122.89	118.30
1	C	147	MSE	CG-SE-CE	-5.07	87.74	98.90
1	A	57	ARG	NE-CZ-NH2	-5.06	117.77	120.30
1	A	198	ARG	CG-CD-NE	5.03	122.36	111.80
1	A	198	ARG	N-CA-CB	5.02	119.64	110.60
1	D	60	ARG	NE-CZ-NH2	-5.01	117.79	120.30

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	1609	0	1570	38	0
1	B	1592	0	1552	34	0
1	C	1572	0	1537	39	0
1	D	1616	0	1578	32	0
2	E	157	0	167	4	0
2	F	157	0	167	5	0
2	G	157	0	167	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	157	0	167	6	0
3	A	124	0	0	12	0
3	B	148	0	0	20	0
3	C	92	0	0	11	0
3	D	120	0	0	12	2
3	E	9	0	0	1	0
3	F	10	0	0	0	0
3	G	6	0	0	2	0
3	H	4	0	0	1	0
All	All	7530	0	6905	155	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 11.

All (155) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:PHE:HD1	1:A:177:ILE:HD11	1.11	1.13
1:C:63:PHE:HD1	1:C:177:ILE:HD11	1.10	1.11
1:C:122:TYR:CE2	3:C:332:HOH:O	2.03	1.09
1:A:63:PHE:CD1	1:A:177:ILE:HD11	1.96	1.00
1:C:122:TYR:CD2	3:C:332:HOH:O	2.14	0.97
1:C:63:PHE:CD1	1:C:177:ILE:HD11	2.01	0.94
1:B:24:GLN:N	3:B:425:HOH:O	2.01	0.94
1:A:196:LYS:HG2	3:A:403:HOH:O	1.72	0.90
1:B:35:ILE:CD1	3:B:429:HOH:O	2.19	0.90
1:B:24:GLN:HA	3:B:428:HOH:O	1.70	0.89
1:D:205:GLY:O	1:D:206:GLY:O	1.92	0.87
1:A:38:ASP:OD1	1:A:169:LYS:HE3	1.76	0.86
1:B:35:ILE:HD13	3:B:429:HOH:O	1.74	0.85
1:C:182:ARG:HA	1:C:188:MSE:HE2	1.58	0.85
1:B:208:THR:HA	3:B:399:HOH:O	1.77	0.84
1:C:164:PHE:HE1	3:C:332:HOH:O	1.61	0.82
1:A:140:THR:O	1:A:144:ARG:HG3	1.79	0.82
1:A:148:GLU:HG3	3:A:377:HOH:O	1.81	0.81
1:C:84:LYS:NZ	1:C:190:VAL:O	2.14	0.80
1:D:85:ASN:HB3	3:D:407:HOH:O	1.83	0.77
1:C:134:ASP:OD2	1:C:136:SER:HB3	1.85	0.76
1:D:107:VAL:CG1	2:H:750:GLN:HB3	2.15	0.76
2:G:752:LEU:HD11	2:G:756:ARG:CZ	2.16	0.75
1:C:63:PHE:HD1	1:C:177:ILE:CD1	1.94	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ASN:O	1:A:183:THR:HB	1.86	0.75
1:A:183:THR:HG22	3:A:323:HOH:O	1.87	0.73
1:C:25:GLN:NE2	1:C:132:GLN:O	2.23	0.72
1:D:140:THR:O	1:D:144:ARG:HG2	1.89	0.72
1:D:179:ASN:O	1:D:183:THR:HB	1.90	0.72
2:G:752:LEU:HD13	2:G:752:LEU:C	2.10	0.71
1:D:203:LYS:HB3	3:D:403:HOH:O	1.89	0.71
1:C:151:ILE:O	3:C:303:HOH:O	2.08	0.70
1:B:202:GLU:OE2	3:B:320:HOH:O	2.09	0.69
1:C:122:TYR:CZ	3:C:332:HOH:O	2.32	0.69
1:B:216:PHE:CD1	3:B:426:HOH:O	2.45	0.69
1:D:106:ASP:H	1:D:170:GLN:HE21	1.41	0.68
1:A:205:GLY:O	1:A:206:GLY:O	2.11	0.68
1:B:106:ASP:H	1:B:170:GLN:HE21	1.44	0.66
1:A:107:VAL:HG12	2:E:750:GLN:HB3	1.77	0.66
1:A:209:GLY:HA2	1:A:215:ILE:HD11	1.77	0.66
1:B:208:THR:HG22	3:B:399:HOH:O	1.94	0.66
1:A:193:GLU:CG	3:A:321:HOH:O	2.44	0.66
1:A:61:GLN:HG3	3:A:417:HOH:O	1.97	0.65
1:A:68:GLN:NE2	3:A:306:HOH:O	2.23	0.64
1:C:107:VAL:HG12	2:G:750:GLN:HB3	1.80	0.63
1:B:179:ASN:O	1:B:183:THR:HB	1.98	0.63
2:E:765:ILE:C	3:E:805:HOH:O	2.37	0.63
1:C:164:PHE:CE1	3:C:332:HOH:O	2.43	0.62
1:A:83:LYS:HD3	1:B:46:PRO:HG2	1.80	0.62
1:B:24:GLN:CB	3:B:428:HOH:O	2.48	0.62
1:C:220:ILE:C	3:C:321:HOH:O	2.38	0.61
2:G:760:ALA:O	2:G:763:GLU:HG3	2.01	0.60
1:D:106:ASP:H	1:D:170:GLN:NE2	1.98	0.60
1:B:60:ARG:NH2	3:B:409:HOH:O	2.35	0.60
1:D:203:LYS:HA	3:D:369:HOH:O	2.01	0.59
1:D:127:SER:OG	3:D:350:HOH:O	2.16	0.59
3:B:397:HOH:O	2:F:765:ILE:HA	2.01	0.59
1:A:140:THR:O	1:A:144:ARG:CG	2.50	0.59
1:C:172:PHE:O	1:C:176:ILE:HG12	2.02	0.58
1:D:134:ASP:HA	3:D:363:HOH:O	2.02	0.58
1:B:107:VAL:HG12	2:F:750:GLN:HB3	1.85	0.58
1:A:63:PHE:CD1	1:A:177:ILE:CD1	2.80	0.58
1:A:193:GLU:HG2	3:A:321:HOH:O	2.01	0.58
1:B:215:ILE:HG22	3:B:426:HOH:O	2.06	0.56
1:A:106:ASP:H	1:A:170:GLN:HE21	1.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:175:ILE:HD13	2:H:762:MSE:SE	2.55	0.56
1:C:48:GLN:HE21	1:C:166:LYS:HE2	1.71	0.56
1:B:24:GLN:CA	3:B:428:HOH:O	2.40	0.55
1:B:106:ASP:H	1:B:170:GLN:NE2	2.04	0.55
1:D:43:SER:HB3	3:D:376:HOH:O	2.06	0.54
1:B:26:PHE:CD2	2:F:765:ILE:CG2	2.91	0.54
1:C:152:GLN:HA	1:C:153:PRO:C	2.28	0.54
1:D:107:VAL:HG13	2:H:750:GLN:HB3	1.90	0.53
1:B:186:LYS:O	1:B:190:VAL:HG23	2.08	0.53
1:D:171:SER:O	1:D:175:ILE:HG13	2.08	0.53
1:A:180:GLN:NE2	3:A:418:HOH:O	2.40	0.53
1:D:144:ARG:CZ	3:D:376:HOH:O	2.56	0.53
1:D:107:VAL:HG12	2:H:750:GLN:HB3	1.90	0.53
1:A:179:ASN:OD1	1:A:221:PHE:HZ	1.92	0.53
1:C:124:ILE:N	1:C:124:ILE:HD13	2.24	0.53
1:D:183:THR:HG22	3:D:321:HOH:O	2.09	0.53
1:A:193:GLU:HG3	3:A:321:HOH:O	2.06	0.52
1:B:172:PHE:O	1:B:176:ILE:HG12	2.09	0.52
1:A:106:ASP:H	1:A:170:GLN:NE2	2.07	0.52
2:F:749:ILE:HD12	2:F:749:ILE:H	1.75	0.52
1:A:120:GLN:O	1:A:124:ILE:HG12	2.09	0.52
1:C:63:PHE:CD1	1:C:177:ILE:CD1	2.78	0.51
1:A:72:GLU:O	1:A:76:LYS:HG2	2.10	0.51
1:B:208:THR:CA	3:B:399:HOH:O	2.48	0.50
2:G:763:GLU:HG2	3:G:802:HOH:O	2.10	0.50
1:C:106:ASP:H	1:C:170:GLN:NE2	2.08	0.50
1:D:126:THR:HG22	2:H:765:ILE:HD11	1.93	0.50
1:C:24:GLN:OE1	1:C:24:GLN:HA	2.11	0.50
1:C:107:VAL:CG1	2:G:750:GLN:HB3	2.41	0.50
1:A:156:PRO:HD2	3:A:382:HOH:O	2.12	0.50
1:B:148:GLU:HG3	3:B:421:HOH:O	2.11	0.50
2:G:752:LEU:HD11	2:G:756:ARG:NE	2.26	0.50
1:B:139:ASN:O	1:B:143:ILE:HG12	2.11	0.50
1:C:56:ASP:HB2	1:C:169:LYS:NZ	2.27	0.50
2:H:749:ILE:HD12	3:H:802:HOH:O	2.11	0.50
1:B:68:GLN:NE2	3:B:342:HOH:O	2.45	0.49
1:A:107:VAL:HG13	2:E:754:TYR:HB2	1.94	0.49
1:D:107:VAL:O	1:D:111:THR:HB	2.13	0.49
1:B:26:PHE:CD1	1:B:130:SER:HB3	2.46	0.48
1:C:134:ASP:O	1:C:136:SER:N	2.46	0.48
1:C:34:PHE:CE1	1:C:169:LYS:HE2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:92:ILE:HD11	1:A:213:LEU:HD23	1.95	0.47
1:C:48:GLN:NE2	1:C:166:LYS:HE2	2.29	0.47
1:D:152:GLN:HA	1:D:153:PRO:C	2.35	0.47
1:C:122:TYR:CE1	3:C:332:HOH:O	2.64	0.47
1:B:152:GLN:HA	1:B:153:PRO:C	2.35	0.47
2:G:752:LEU:HD13	2:G:752:LEU:O	2.14	0.47
1:D:198:ARG:HD3	1:D:214:ASP:OD1	2.14	0.47
2:G:755:GLN:O	2:G:759:ILE:HG13	2.15	0.47
2:E:760:ALA:O	2:E:763:GLU:HG2	2.15	0.47
1:C:31:GLN:HG2	1:C:176:ILE:HD12	1.96	0.46
1:D:23:PRO:HB3	3:D:391:HOH:O	2.14	0.46
1:A:198:ARG:HD2	3:A:364:HOH:O	2.16	0.46
1:D:40:VAL:HG13	1:D:144:ARG:HD2	1.98	0.46
1:A:51:ILE:HD12	1:A:51:ILE:N	2.31	0.46
1:B:221:PHE:HE2	3:B:395:HOH:O	1.99	0.46
1:C:122:TYR:CG	3:C:332:HOH:O	2.52	0.45
1:A:49:LYS:HD3	3:A:407:HOH:O	2.16	0.45
1:A:185:GLN:CD	1:C:24:GLN:HE21	2.20	0.45
1:B:49:LYS:HB3	1:B:50:PRO:HD3	1.98	0.45
1:D:92:ILE:HD11	1:D:213:LEU:HD23	1.99	0.45
1:B:107:VAL:CG1	2:F:750:GLN:HB3	2.47	0.44
1:A:63:PHE:HA	1:A:177:ILE:CD1	2.47	0.44
1:C:32:VAL:HG21	1:C:135:PRO:HB3	2.00	0.44
1:D:205:GLY:O	1:D:206:GLY:C	2.53	0.44
1:A:106:ASP:O	1:A:110:SER:HB2	2.18	0.44
1:A:63:PHE:HA	1:A:177:ILE:HD11	2.00	0.43
1:D:85:ASN:CB	3:D:407:HOH:O	2.53	0.43
2:G:752:LEU:CD1	2:G:752:LEU:C	2.83	0.43
1:B:39:ASN:HA	1:B:39:ASN:HD22	1.64	0.43
1:C:134:ASP:OD2	1:C:136:SER:CB	2.62	0.43
1:B:116:LYS:NZ	3:B:410:HOH:O	2.50	0.42
1:A:51:ILE:HD12	1:A:51:ILE:H	1.84	0.42
1:A:127:SER:O	1:A:131:HIS:HD2	2.02	0.42
1:C:134:ASP:O	1:C:135:PRO:C	2.55	0.42
1:D:144:ARG:NH2	3:D:376:HOH:O	2.52	0.42
1:C:122:TYR:CD1	3:C:332:HOH:O	2.73	0.42
1:C:176:ILE:O	1:C:180:GLN:HG2	2.20	0.42
1:B:216:PHE:N	3:B:426:HOH:O	2.53	0.42
1:D:38:ASP:OD1	1:D:169:LYS:HE3	2.20	0.42
1:B:60:ARG:HD2	3:B:429:HOH:O	2.20	0.41
1:C:193:GLU:HB3	3:C:384:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:85:ASN:CG	3:D:407:HOH:O	2.59	0.41
1:C:81:PRO:O	1:C:84:LYS:HB2	2.20	0.41
1:A:220:ILE:HG22	1:A:221:PHE:N	2.35	0.41
1:D:186:LYS:O	1:D:190:VAL:HG23	2.20	0.41
1:D:203:LYS:O	1:D:205:GLY:N	2.53	0.41
2:G:763:GLU:CG	3:G:802:HOH:O	2.69	0.40
1:C:108:GLU:HG3	2:G:750:GLN:HE22	1.86	0.40
1:B:138:ILE:HG23	1:B:143:ILE:HD11	2.03	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)
3:D:355:HOH:O	3:D:377:HOH:O[2_554]	1.98	0.22
3:D:355:HOH:O	3:D:404:HOH:O[2_554]	2.01	0.19

## 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	193/221 (87%)	191 (99%)	1 (0%)	1 (0%)	34	22
1	B	190/221 (86%)	188 (99%)	0	2 (1%)	17	7
1	C	188/221 (85%)	181 (96%)	5 (3%)	2 (1%)	17	7
1	D	194/221 (88%)	190 (98%)	3 (2%)	1 (0%)	34	22
2	E	18/62 (29%)	18 (100%)	0	0	100	100
2	F	18/62 (29%)	18 (100%)	0	0	100	100
2	G	18/62 (29%)	17 (94%)	1 (6%)	0	100	100
2	H	18/62 (29%)	18 (100%)	0	0	100	100
All	All	837/1132 (74%)	821 (98%)	10 (1%)	6 (1%)	26	15



All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	206	GLY
1	D	206	GLY
1	C	140	THR
1	C	141	ARG
1	B	200	GLU
1	B	201	ALA

### 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	180/199 (90%)	175 (97%)	5 (3%)	51	44
1	B	179/199 (90%)	169 (94%)	10 (6%)	26	16
1	C	177/199 (89%)	173 (98%)	4 (2%)	58	51
1	D	181/199 (91%)	175 (97%)	6 (3%)	45	37
2	E	17/52 (33%)	17 (100%)	0	100	100
2	F	17/52 (33%)	15 (88%)	2 (12%)	6	2
2	G	17/52 (33%)	16 (94%)	1 (6%)	24	14
2	H	17/52 (33%)	16 (94%)	1 (6%)	24	14
All	All	785/1004 (78%)	756 (96%)	29 (4%)	41	32

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	102	ASP
1	A	110	SER
1	A	144	ARG
1	A	183	THR
1	A	218	SER
1	B	37	VAL
1	B	110	SER
1	B	112	LYS

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Mol	Chain	Res	Type
1	B	134	ASP
1	B	136	SER
1	B	183	THR
1	B	186	LYS
1	B	198	ARG
1	B	218	SER
1	B	221	PHE
1	C	30	LEU
1	C	115	GLN
1	C	124	ILE
1	C	151	ILE
1	D	23	PRO
1	D	74	SER
1	D	111	THR
1	D	134	ASP
1	D	183	THR
1	D	208	THR
2	F	748	ASN
2	F	764	THR
2	G	748	ASN
2	H	765	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	ASN
1	A	48	GLN
1	A	59	ASN
1	A	131	HIS
1	A	132	GLN
1	A	149	ASN
1	A	170	GLN
1	A	185	GLN
1	B	39	ASN
1	B	48	GLN
1	B	59	ASN
1	B	131	HIS
1	B	132	GLN
1	B	170	GLN
1	C	24	GLN
1	C	39	ASN
1	C	48	GLN

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Mol	Chain	Res	Type
1	C	59	ASN
1	C	131	HIS
1	C	132	GLN
1	C	145	ASN
1	C	170	GLN
1	D	48	GLN
1	D	59	ASN
1	D	131	HIS
1	D	132	GLN
1	D	170	GLN
2	G	750	GLN

### 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 [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

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	195/221 (88%)	-0.30	1 (0%) 91 93	18, 29, 56, 84	0
1	B	192/221 (86%)	-0.30	3 (1%) 74 79	16, 26, 49, 85	0
1	C	190/221 (85%)	-0.15	4 (2%) 67 72	23, 35, 64, 94	0
1	D	196/221 (88%)	-0.31	1 (0%) 91 93	19, 29, 58, 82	0
2	E	19/62 (30%)	-0.18	0 100 100	20, 31, 59, 62	0
2	F	19/62 (30%)	0.25	2 (10%) 8 9	21, 31, 71, 82	0
2	G	19/62 (30%)	0.65	2 (10%) 8 9	29, 42, 90, 90	0
2	H	19/62 (30%)	-0.17	1 (5%) 30 34	25, 32, 60, 61	0
All	All	849/1132 (75%)	-0.23	14 (1%) 74 79	16, 30, 61, 94	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	746	GLY	6.4
2	F	747	PRO	4.9
1	B	221	PHE	4.6
2	G	747	PRO	3.3
1	C	199	GLN	3.0
2	H	747	PRO	2.8
2	F	765	ILE	2.7
1	D	221	PHE	2.7
1	C	200	GLU	2.6
1	B	199	GLN	2.3
1	A	221	PHE	2.2
1	C	208	THR	2.2
1	B	201	ALA	2.1
1	C	134	ASP	2.1

## 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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.