



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 16, 2024 – 10:32 AM EST

PDB ID : 3IC8  
Title : The Crystal Structure of a GST-like protein from Pseudomonas syringae to 2.4Å  
Authors : Stein, A.J.; Chhor, G.; Freeman, L.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2009-07-17  
Resolution : 2.40 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

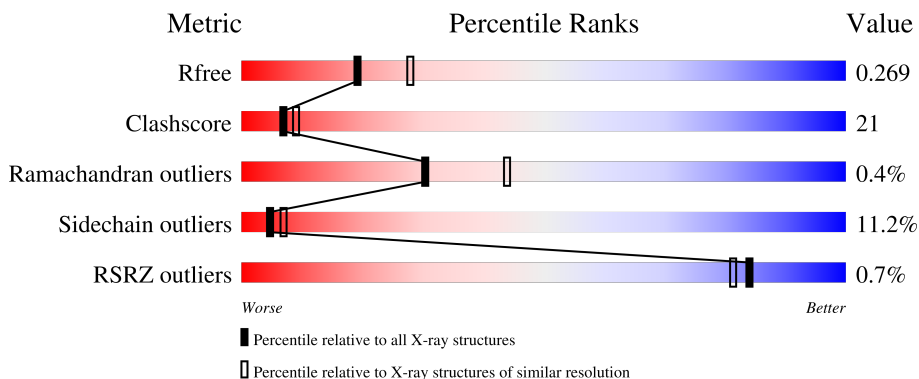
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$ . 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	310	<div> <div></div> <div>65% 23% 10%</div> </div>
1	B	310	<div> <div></div> <div>65% 20% 11%</div> </div>
1	C	310	<div> <div></div> <div>62% 23% 12%</div> </div>
1	D	310	<div> <div></div> <div>49% 32% 7% 12%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 8579 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 uncharacterized GST-like proteinprotein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	Se	0	0	0
			2131	1374	363	387	1	6			
1	B	275	Total	C	N	O	S	Se	0	0	0
			2118	1366	360	384	1	7			
1	C	272	Total	C	N	O	S	Se	0	0	0
			2083	1345	353	380	1	4			
1	D	273	Total	C	N	O	S	Se	0	0	0
			2069	1340	351	371	1	6			

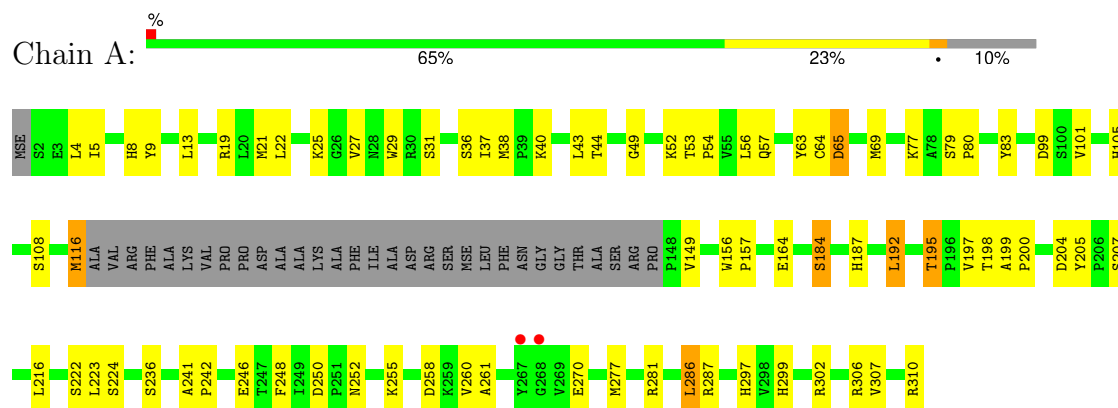
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	55	Total	O	0	0
			55	55		
2	B	52	Total	O	0	0
			52	52		
2	C	54	Total	O	0	0
			54	54		
2	D	17	Total	O	0	0
			17	17		

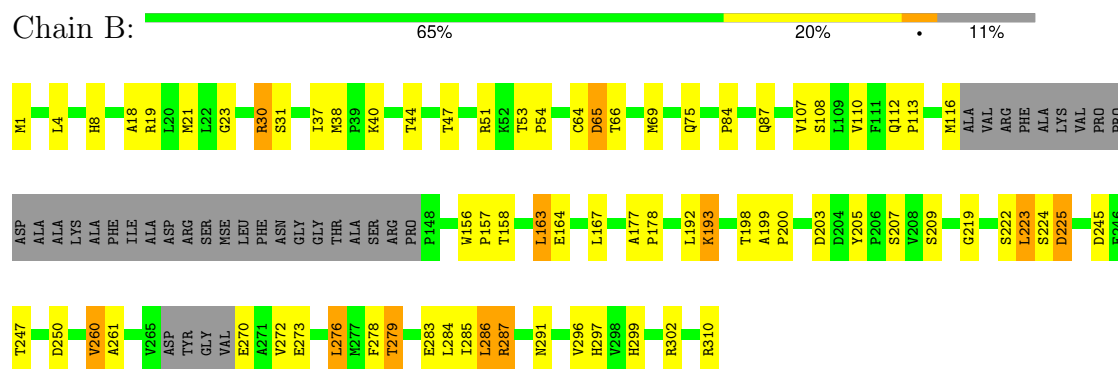
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

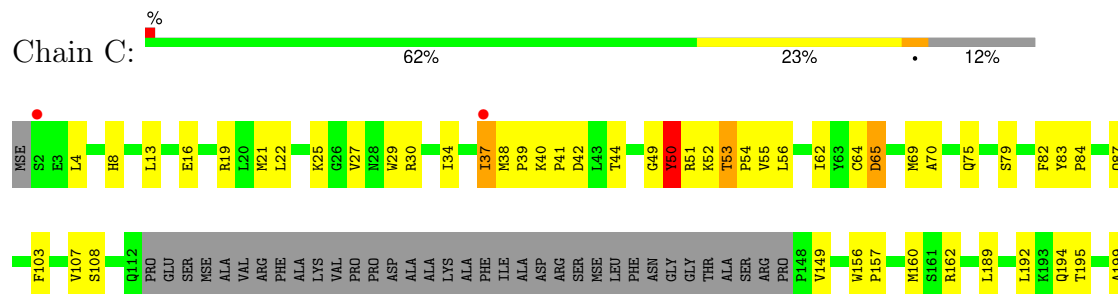
- Molecule 1: uncharacterized GST-like proteinprotein

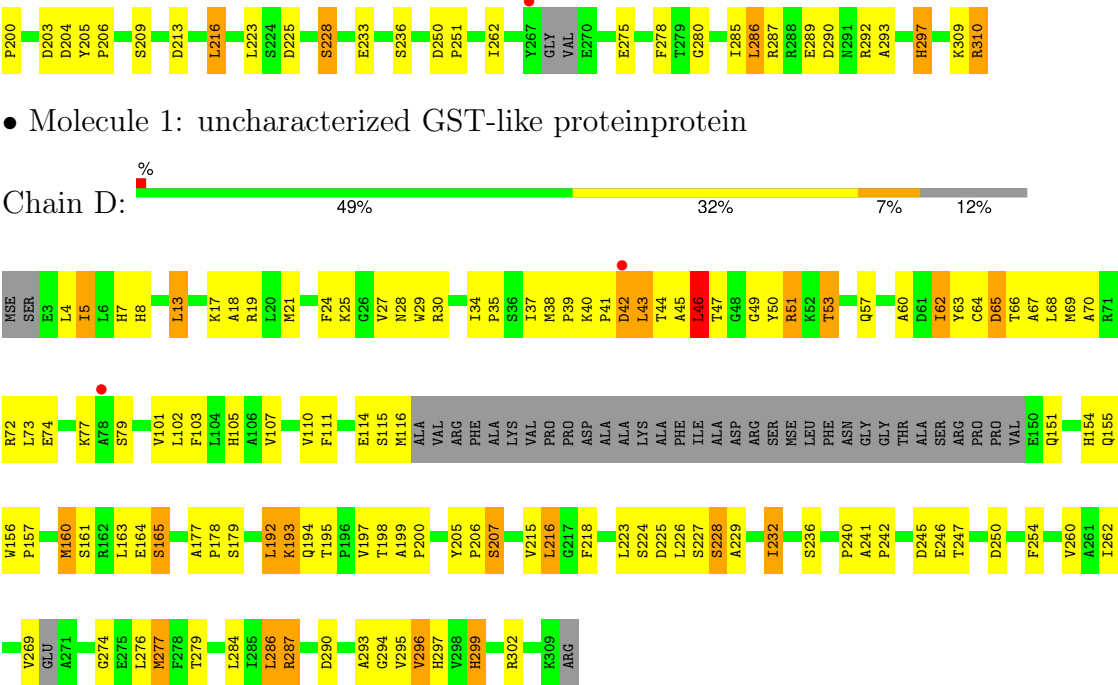


- Molecule 1: uncharacterized GST-like proteinprotein



- Molecule 1: uncharacterized GST-like proteinprotein





● Molecule 1: uncharacterized GST-like proteinprotein



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.67Å 102.27Å 148.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.34 – 2.40 48.34 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (48.34-2.40) 98.5 (48.34-2.40)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 2.39Å)	Xtriage
Refinement program	REFMAC refmac_5.5.0054	Depositor
R, $R_{free}$	0.192 , 0.246 0.226 , 0.269	Depositor DCC
$R_{free}$ test set	2560 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	47.4	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 50.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	8579	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.59% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.50	2/2184 (0.1%)	0.73	0/2966
1	B	1.47	1/2170 (0.0%)	0.71	0/2944
1	C	1.47	1/2135 (0.0%)	0.74	2/2902 (0.1%)
1	D	1.30	0/2120	0.77	1/2880 (0.0%)
All	All	1.44	4/8609 (0.0%)	0.74	3/11692 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	83	TYR	CD1-CE1	-5.56	1.31	1.39
1	C	83	TYR	CD2-CE2	-5.27	1.31	1.39
1	A	63	TYR	CD2-CE2	-5.21	1.31	1.39
1	B	1	MSE	CG-SE	-5.05	1.78	1.95

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	46	LEU	CB-CG-CD2	-5.72	101.27	111.00
1	C	50	TYR	N-CA-C	-5.66	95.72	111.00
1	C	162	ARG	NE-CZ-NH1	5.20	122.90	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	2131	0	2077	55	0
1	B	2118	0	2072	63	0
1	C	2083	0	2016	62	0
1	D	2069	0	2006	180	0
2	A	55	0	0	2	0
2	B	52	0	0	1	0
2	C	54	0	0	2	0
2	D	17	0	0	1	0
All	All	8579	0	8171	345	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 21.

All (345) 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:D:37:ILE:CD1	1:D:39:PRO:HD2	1.22	1.61
1:D:5:ILE:HD11	1:D:57:GLN:NE2	1.37	1.35
1:D:37:ILE:HD13	1:D:39:PRO:CD	1.65	1.26
1:D:37:ILE:CD1	1:D:39:PRO:CD	2.13	1.24
1:D:287:ARG:HG3	1:D:297:HIS:CD2	1.76	1.21
1:D:164:GLU:OE2	1:D:206:PRO:HD2	1.43	1.19
1:D:46:LEU:HD23	1:D:46:LEU:N	1.50	1.15
1:D:43:LEU:O	1:D:43:LEU:HD22	1.46	1.15
1:D:228:SER:O	1:D:232:ILE:CD1	1.96	1.13
1:D:47:THR:CG2	1:D:50:TYR:H	1.64	1.11
1:C:310:ARG:HH11	1:C:310:ARG:HB2	1.10	1.10
1:D:63:TYR:CE1	1:D:299:HIS:CD2	2.39	1.10
1:D:287:ARG:HG3	1:D:297:HIS:NE2	1.68	1.08
1:D:72:ARG:HG3	1:D:72:ARG:HH11	1.11	1.07
1:D:232:ILE:N	1:D:232:ILE:HD12	1.68	1.05
1:D:216:LEU:H	1:D:216:LEU:CD2	1.69	1.04
1:D:274:GLY:HA3	1:D:286:LEU:CD1	1.87	1.04
1:D:5:ILE:CD1	1:D:57:GLN:NE2	2.22	1.03
1:D:30:ARG:HD2	1:D:224:SER:OG	1.60	1.01
1:D:37:ILE:HD12	1:D:39:PRO:HD2	1.41	0.99
1:D:232:ILE:CD1	1:D:232:ILE:H	1.73	0.98
1:D:77:LYS:HE3	1:D:79:SER:O	1.63	0.98
1:D:274:GLY:HA3	1:D:286:LEU:HD11	1.42	0.98
1:D:30:ARG:CD	1:D:224:SER:OG	2.13	0.97
1:D:216:LEU:HD22	1:D:216:LEU:N	1.81	0.96
1:D:287:ARG:CG	1:D:297:HIS:CD2	2.48	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ILE:CD1	1:C:37:ILE:N	2.30	0.95
1:B:250:ASP:OD2	1:B:279:THR:HG21	1.66	0.94
1:D:228:SER:O	1:D:232:ILE:HD13	1.66	0.94
1:D:35:PRO:O	1:D:40:LYS:NZ	1.98	0.94
1:D:5:ILE:HD11	1:D:57:GLN:HE21	1.12	0.93
1:B:286:LEU:HD12	1:B:286:LEU:O	1.68	0.93
1:C:203:ASP:HA	1:D:38:MSE:HG2	1.50	0.92
1:D:72:ARG:HG3	1:D:72:ARG:NH1	1.80	0.92
1:B:270:GLU:O	1:B:270:GLU:HG3	1.70	0.91
1:D:216:LEU:CD2	1:D:216:LEU:N	2.34	0.91
1:B:286:LEU:HD12	1:B:286:LEU:C	1.88	0.91
1:C:37:ILE:N	1:C:37:ILE:HD13	1.84	0.91
1:D:63:TYR:CE1	1:D:299:HIS:HD2	1.88	0.91
1:D:228:SER:O	1:D:232:ILE:HD11	1.72	0.88
1:D:43:LEU:HD22	1:D:43:LEU:C	1.90	0.88
1:D:232:ILE:CD1	1:D:232:ILE:N	2.30	0.88
1:B:286:LEU:C	1:B:286:LEU:CD1	2.42	0.87
1:D:5:ILE:CD1	1:D:57:GLN:HE21	1.86	0.87
1:C:37:ILE:HD13	1:C:37:ILE:H	1.40	0.86
1:A:204:ASP:OD2	1:B:37:ILE:CD1	2.23	0.86
1:D:37:ILE:HD12	1:D:39:PRO:CD	2.00	0.86
1:A:260:VAL:CG1	1:A:261:ALA:N	2.39	0.85
1:A:246:GLU:OE1	1:A:281:ARG:NH1	2.09	0.85
1:C:310:ARG:HH11	1:C:310:ARG:CB	1.89	0.85
1:A:195:THR:HG22	1:A:198:THR:H	1.41	0.85
1:D:250:ASP:OD1	1:D:279:THR:OG1	1.96	0.84
1:C:310:ARG:HB2	1:C:310:ARG:NH1	1.92	0.83
1:D:37:ILE:HD11	1:D:39:PRO:HD2	1.58	0.83
1:D:269:VAL:HG23	1:D:269:VAL:O	1.78	0.83
1:D:63:TYR:CZ	1:D:72:ARG:HD3	2.14	0.82
1:D:223:LEU:H	1:D:223:LEU:HD23	1.44	0.82
1:D:47:THR:CG2	1:D:50:TYR:N	2.42	0.82
1:A:286:LEU:C	1:A:286:LEU:HD23	2.01	0.82
1:D:37:ILE:HD13	1:D:39:PRO:HD2	0.84	0.82
1:D:290:ASP:O	1:D:294:GLY:N	2.12	0.82
1:B:223:LEU:HD12	1:B:223:LEU:C	1.99	0.81
1:D:232:ILE:HD12	1:D:232:ILE:H	1.34	0.81
1:D:63:TYR:HE1	1:D:299:HIS:HD2	1.25	0.81
1:D:35:PRO:HG2	1:D:40:LYS:HG3	1.62	0.81
1:D:223:LEU:HD23	1:D:223:LEU:N	1.96	0.81
1:B:273:GLU:OE2	1:B:310:ARG:NH1	2.15	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ASP:OD1	1:A:184:SER:OG	1.99	0.80
1:D:47:THR:HG22	1:D:50:TYR:H	1.46	0.79
1:A:8:HIS:HD2	1:A:19:ARG:HH11	1.30	0.78
1:D:269:VAL:O	1:D:269:VAL:CG2	2.30	0.78
1:D:8:HIS:N	1:D:34:ILE:HD12	1.98	0.78
1:D:216:LEU:H	1:D:216:LEU:HD23	1.46	0.78
1:D:43:LEU:O	1:D:43:LEU:CD2	2.30	0.77
1:B:8:HIS:HD2	1:B:19:ARG:HH11	1.31	0.77
1:D:53:THR:OG1	2:D:312:HOH:O	2.00	0.77
1:D:277:MSE:HE3	1:D:277:MSE:HA	1.67	0.76
1:A:260:VAL:HG12	1:A:261:ALA:N	2.01	0.75
1:C:53:THR:HB	1:C:54:PRO:HA	1.69	0.74
1:A:204:ASP:OD2	1:B:37:ILE:HD11	1.86	0.74
1:A:204:ASP:OD2	1:B:37:ILE:HD12	1.86	0.73
1:D:241:ALA:HB1	1:D:242:PRO:HD2	1.69	0.73
1:D:30:ARG:HD3	1:D:224:SER:OG	1.88	0.72
1:D:60:ALA:O	1:D:296:VAL:HG12	1.89	0.72
1:A:101:VAL:O	1:A:105:HIS:HD2	1.72	0.72
1:A:21:MSE:HE2	1:A:69:MSE:HE2	1.72	0.72
1:D:274:GLY:CA	1:D:286:LEU:HD11	2.19	0.72
1:D:43:LEU:C	1:D:43:LEU:CD2	2.59	0.71
1:A:9:TYR:OH	1:B:193:LYS:HE2	1.90	0.71
1:D:287:ARG:CG	1:D:297:HIS:HD2	2.04	0.71
1:B:279:THR:HG22	1:B:302:ARG:HH12	1.56	0.71
1:B:21:MSE:HE2	1:B:69:MSE:HE2	1.73	0.71
1:D:227:SER:OG	1:D:229:ALA:HB3	1.91	0.70
1:D:241:ALA:HB1	1:D:242:PRO:CD	2.21	0.70
1:D:37:ILE:HD12	1:D:37:ILE:C	2.12	0.70
1:B:53:THR:HB	1:B:54:PRO:HA	1.74	0.69
1:D:25:LYS:NZ	1:D:74:GLU:OE2	2.25	0.69
1:B:30:ARG:NH2	1:C:213:ASP:OD2	2.24	0.69
1:B:270:GLU:O	1:B:270:GLU:CG	2.39	0.69
1:D:18:ALA:HB1	1:D:69:MSE:HE1	1.75	0.69
1:D:47:THR:HG22	1:D:49:GLY:H	1.57	0.69
1:C:309:LYS:O	1:C:310:ARG:C	2.29	0.69
1:D:27:VAL:HG22	1:D:28:ASN:H	1.58	0.68
1:A:255:LYS:N	1:A:258:ASP:OD2	2.21	0.68
1:D:199:ALA:N	1:D:200:PRO:CD	2.56	0.68
1:B:250:ASP:OD2	1:B:279:THR:CG2	2.39	0.68
1:C:49:GLY:O	1:C:50:TYR:C	2.29	0.68
1:D:227:SER:OG	1:D:229:ALA:N	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:THR:HG23	2:A:364:HOH:O	1.92	0.67
1:D:5:ILE:HD11	1:D:57:GLN:HB3	1.76	0.67
1:D:156:TRP:N	1:D:157:PRO:HD2	2.09	0.67
1:A:53:THR:HB	1:A:54:PRO:HA	1.77	0.67
1:D:5:ILE:CG1	1:D:57:GLN:HB3	2.25	0.67
1:C:64:CYS:O	1:C:65:ASP:HB3	1.95	0.66
1:B:37:ILE:HG22	1:B:38:MSE:O	1.95	0.66
1:C:64:CYS:O	1:C:65:ASP:CB	2.43	0.66
1:C:310:ARG:CB	1:C:310:ARG:NH1	2.56	0.66
1:D:279:THR:OG1	1:D:302:ARG:NH2	2.29	0.65
1:D:290:ASP:OD2	1:D:293:ALA:HB3	1.96	0.65
1:A:8:HIS:CD2	1:A:19:ARG:HH11	2.15	0.65
1:D:46:LEU:HD23	1:D:46:LEU:H	1.57	0.64
1:C:53:THR:HG22	1:C:55:VAL:HG23	1.80	0.64
1:D:5:ILE:HG12	1:D:57:GLN:HB3	1.80	0.64
1:B:156:TRP:N	1:B:157:PRO:HD2	2.12	0.63
1:D:8:HIS:CA	1:D:34:ILE:HD12	2.28	0.63
1:D:274:GLY:HA3	1:D:286:LEU:HD13	1.75	0.63
1:D:46:LEU:HB3	1:D:62:ILE:HD12	1.80	0.63
1:D:63:TYR:CZ	1:D:299:HIS:CD2	2.86	0.63
1:D:232:ILE:H	1:D:232:ILE:HD13	1.61	0.63
1:C:49:GLY:O	1:C:51:ARG:N	2.32	0.62
1:D:47:THR:HG21	1:D:50:TYR:N	2.14	0.62
1:C:103:PHE:O	1:C:107:VAL:HG13	2.00	0.62
1:A:260:VAL:HG13	1:A:261:ALA:N	2.15	0.61
1:B:40:LYS:H	1:B:51:ARG:NH1	1.98	0.61
1:D:5:ILE:CD1	1:D:57:GLN:HB3	2.30	0.61
1:D:114:GLU:OE1	1:D:114:GLU:N	2.32	0.60
1:D:13:LEU:N	1:D:13:LEU:HD23	2.15	0.60
1:A:44:THR:HG22	1:A:49:GLY:HA2	1.83	0.60
1:D:64:CYS:O	1:D:65:ASP:HB3	2.02	0.59
1:B:8:HIS:HD2	1:B:19:ARG:NH1	2.00	0.59
1:A:64:CYS:O	1:A:65:ASP:CB	2.50	0.59
1:D:5:ILE:HD11	1:D:57:GLN:CD	2.16	0.59
1:D:38:MSE:O	1:D:40:LYS:HD2	2.02	0.59
1:A:8:HIS:HE1	1:A:31:SER:OG	1.86	0.59
1:A:164:GLU:OE1	1:A:207:SER:HB2	2.02	0.59
1:C:54:PRO:O	1:C:69:MSE:HE1	2.03	0.59
1:D:287:ARG:CG	1:D:297:HIS:NE2	2.54	0.59
1:D:160:MSE:CE	1:D:163:LEU:HD23	2.33	0.58
1:D:216:LEU:H	1:D:216:LEU:HD22	1.41	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:TYR:CE2	1:C:52:LYS:O	2.57	0.57
1:D:105:HIS:HE1	1:D:155:GLN:HE21	1.51	0.57
1:D:193:LYS:HE2	1:D:199:ALA:HB1	1.86	0.57
1:C:27:VAL:O	1:C:27:VAL:HG13	2.04	0.57
1:D:47:THR:HG22	1:D:49:GLY:N	2.19	0.57
1:D:72:ARG:NH1	1:D:72:ARG:CG	2.56	0.57
1:A:36:SER:OG	1:B:203:ASP:OD2	2.20	0.57
1:A:156:TRP:N	1:A:157:PRO:CD	2.67	0.57
1:D:64:CYS:O	1:D:65:ASP:CB	2.53	0.57
1:B:8:HIS:CD2	1:B:19:ARG:HH11	2.18	0.57
1:C:156:TRP:N	1:C:157:PRO:CD	2.67	0.57
1:A:25:LYS:O	1:A:77:LYS:HE3	2.05	0.57
1:D:63:TYR:CE1	1:D:72:ARG:HD3	2.40	0.57
1:C:209:SER:HB3	1:D:38:MSE:SE	2.55	0.57
1:D:30:ARG:CZ	1:D:226:LEU:HD13	2.35	0.56
1:A:108:SER:HA	1:B:116:MSE:HE2	1.87	0.56
1:C:8:HIS:HD2	1:C:19:ARG:HH11	1.54	0.56
1:A:8:HIS:HD2	1:A:19:ARG:NH1	2.03	0.55
1:D:27:VAL:HG22	1:D:28:ASN:N	2.21	0.55
1:D:30:ARG:CD	1:D:224:SER:HG	2.17	0.55
1:C:199:ALA:N	1:C:200:PRO:CD	2.70	0.54
1:C:262:ILE:HD12	1:C:286:LEU:HG	1.90	0.54
1:D:290:ASP:OD2	1:D:293:ALA:N	2.39	0.54
1:B:21:MSE:HE1	1:B:69:MSE:HG2	1.90	0.54
1:D:8:HIS:N	1:D:34:ILE:CD1	2.68	0.54
1:D:151:GLN:HB2	1:D:154:HIS:HB3	1.90	0.54
1:C:37:ILE:HG22	1:C:38:MSE:N	2.22	0.54
1:A:25:LYS:O	1:A:77:LYS:CE	2.55	0.54
1:B:164:GLU:OE1	1:B:207:SER:HB2	2.07	0.54
1:C:37:ILE:N	1:C:37:ILE:HD12	2.20	0.54
1:D:46:LEU:N	1:D:46:LEU:CD2	2.30	0.54
1:D:74:GLU:OE2	1:D:74:GLU:HA	2.07	0.54
1:D:114:GLU:CD	1:D:114:GLU:H	2.11	0.53
1:B:8:HIS:HE1	1:B:31:SER:OG	1.92	0.53
1:B:40:LYS:H	1:B:51:ARG:HH12	1.56	0.53
1:C:205:TYR:N	1:C:205:TYR:CD1	2.77	0.53
1:A:64:CYS:O	1:A:65:ASP:HB3	2.09	0.53
1:B:18:ALA:HB1	1:B:69:MSE:HE1	1.90	0.53
1:C:156:TRP:CZ2	1:C:160:MSE:HE3	2.43	0.53
1:D:47:THR:HG21	1:D:50:TYR:O	2.09	0.53
1:D:18:ALA:CB	1:D:69:MSE:HE1	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:ALA:HB1	1:B:178:PRO:HD2	1.91	0.53
1:B:272:VAL:HG12	1:B:286:LEU:HD21	1.90	0.52
1:D:287:ARG:HG2	1:D:297:HIS:CD2	2.39	0.52
1:B:113:PRO:HA	1:B:116:MSE:HE3	1.91	0.52
1:D:277:MSE:HA	1:D:277:MSE:CE	2.38	0.52
1:D:105:HIS:CE1	1:D:155:GLN:HE21	2.28	0.52
1:D:192:LEU:O	1:D:198:THR:OG1	2.24	0.52
1:C:203:ASP:CA	1:D:38:MSE:HG2	2.34	0.51
1:C:200:PRO:HA	1:C:203:ASP:HB2	1.91	0.51
1:D:227:SER:OG	1:D:229:ALA:CB	2.58	0.51
1:D:5:ILE:HG22	1:D:30:ARG:HB2	1.92	0.51
1:A:99:ASP:CG	1:A:184:SER:OG	2.49	0.51
1:C:42:ASP:HB3	1:C:228:SER:HB2	1.92	0.51
1:D:21:MSE:HE3	1:D:70:ALA:HB2	1.93	0.51
1:B:199:ALA:N	1:B:200:PRO:CD	2.74	0.51
1:C:290:ASP:HB3	1:C:293:ALA:HB3	1.91	0.51
1:D:223:LEU:N	1:D:223:LEU:CD2	2.69	0.51
1:C:309:LYS:O	1:C:310:ARG:O	2.30	0.50
1:A:199:ALA:N	1:A:200:PRO:CD	2.74	0.50
1:D:65:ASP:OD2	1:D:67:ALA:HB3	2.12	0.50
1:A:286:LEU:C	1:A:286:LEU:CD2	2.77	0.50
1:D:51:ARG:NE	1:D:51:ARG:CA	2.73	0.50
1:D:290:ASP:OD2	1:D:293:ALA:CB	2.59	0.50
1:C:204:ASP:O	1:C:206:PRO:HD2	2.11	0.50
1:A:116:MSE:HE1	1:B:108:SER:HA	1.93	0.50
1:D:160:MSE:HG2	1:D:205:TYR:CE1	2.47	0.50
1:B:223:LEU:HD12	1:B:223:LEU:O	2.12	0.49
1:A:44:THR:CG2	1:A:49:GLY:HA2	2.43	0.49
1:D:47:THR:HG23	1:D:50:TYR:HB3	1.95	0.49
1:B:286:LEU:C	1:B:286:LEU:HD13	2.31	0.49
1:C:297:HIS:HD2	2:C:316:HOH:O	1.96	0.49
1:A:156:TRP:HB3	1:A:157:PRO:HD3	1.94	0.49
1:D:290:ASP:O	1:D:294:GLY:CA	2.61	0.48
1:A:197:VAL:HG23	2:A:364:HOH:O	2.13	0.48
1:C:37:ILE:O	1:C:40:LYS:NZ	2.36	0.48
1:D:44:THR:O	1:D:44:THR:CG2	2.59	0.48
1:D:72:ARG:HH11	1:D:72:ARG:CG	1.96	0.48
1:B:64:CYS:O	1:B:65:ASP:CB	2.62	0.48
1:B:205:TYR:N	1:B:205:TYR:CD1	2.81	0.48
1:C:16:GLU:HG3	1:C:16:GLU:O	2.14	0.48
1:D:286:LEU:O	1:D:297:HIS:HA	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:42:ASP:OD1	1:C:292:ARG:NH2	2.38	0.48
1:D:241:ALA:CB	1:D:242:PRO:CD	2.89	0.48
1:B:223:LEU:C	1:B:223:LEU:CD1	2.73	0.48
1:C:34:ILE:CD1	1:C:53:THR:HG21	2.44	0.48
1:D:156:TRP:N	1:D:157:PRO:CD	2.76	0.48
1:D:25:LYS:O	1:D:77:LYS:HE2	2.14	0.48
1:D:30:ARG:HD2	1:D:224:SER:HG	1.69	0.48
1:D:250:ASP:HB3	1:D:254:PHE:H	1.79	0.48
1:D:51:ARG:HE	1:D:51:ARG:HA	1.79	0.47
1:D:161:SER:O	1:D:165:SER:OG	2.32	0.47
1:D:193:LYS:CE	1:D:199:ALA:HB1	2.44	0.47
1:D:160:MSE:HE2	1:D:163:LEU:HD23	1.95	0.47
1:D:110:VAL:HG12	1:D:111:PHE:CD1	2.50	0.47
1:A:205:TYR:CD1	1:A:205:TYR:N	2.82	0.47
1:B:64:CYS:O	1:B:65:ASP:HB3	2.15	0.47
1:D:29:TRP:O	1:D:223:LEU:HA	2.14	0.47
1:A:22:LEU:HD13	1:A:29:TRP:CD2	2.50	0.47
1:A:116:MSE:HE2	1:B:107:VAL:O	2.15	0.47
1:D:7:HIS:CD2	1:D:7:HIS:N	2.83	0.47
1:A:38:MSE:HE1	1:A:40:LYS:HE3	1.96	0.47
1:A:250:ASP:OD1	1:A:252:ASN:N	2.42	0.47
1:B:260:VAL:HG13	1:B:261:ALA:N	2.30	0.47
1:C:160:MSE:HE1	1:C:189:LEU:HD21	1.98	0.46
1:D:45:ALA:C	1:D:46:LEU:HD23	2.27	0.46
1:D:77:LYS:CE	1:D:79:SER:O	2.50	0.46
1:C:278:PHE:CE2	1:C:280:GLY:HA3	2.51	0.46
1:D:8:HIS:C	1:D:34:ILE:HD12	2.36	0.46
1:C:22:LEU:HD13	1:C:29:TRP:CD2	2.51	0.46
1:C:297:HIS:CD2	2:C:316:HOH:O	2.68	0.46
1:A:192:LEU:HD12	1:A:198:THR:HB	1.96	0.46
1:D:51:ARG:CA	1:D:51:ARG:HE	2.28	0.46
1:C:203:ASP:OD1	1:D:38:MSE:HG2	2.15	0.46
1:C:53:THR:CB	1:C:54:PRO:HA	2.40	0.45
1:D:37:ILE:HD12	1:D:39:PRO:N	2.30	0.45
1:C:236:SER:HA	1:C:293:ALA:O	2.16	0.45
1:C:199:ALA:N	1:C:200:PRO:HD2	2.30	0.45
1:D:160:MSE:HE3	1:D:160:MSE:HA	1.99	0.45
1:B:30:ARG:NH1	1:B:225:ASP:O	2.48	0.45
1:D:206:PRO:HG2	1:D:207:SER:H	1.82	0.45
1:B:299:HIS:CD2	1:B:299:HIS:N	2.85	0.45
1:D:8:HIS:CA	1:D:34:ILE:CD1	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:LEU:HD22	1:C:194:GLN:HG3	1.98	0.45
1:D:8:HIS:O	1:D:34:ILE:HD12	2.17	0.45
1:D:38:MSE:O	1:D:40:LYS:CD	2.66	0.44
1:B:287:ARG:HG2	1:B:297:HIS:CD2	2.52	0.44
1:D:103:PHE:O	1:D:107:VAL:HG13	2.17	0.44
1:A:5:ILE:HB	1:A:57:GLN:HB3	2.00	0.44
1:B:21:MSE:HE2	1:B:69:MSE:CE	2.45	0.44
1:C:39:PRO:HB2	1:C:41:PRO:HD3	1.99	0.44
1:D:199:ALA:HB3	1:D:200:PRO:HD3	1.98	0.44
1:C:203:ASP:OD1	1:D:38:MSE:CG	2.66	0.44
1:A:116:MSE:CE	1:B:108:SER:HA	2.48	0.44
1:B:21:MSE:CE	1:B:69:MSE:HG2	2.47	0.44
1:D:29:TRP:CE2	1:D:223:LEU:HB3	2.53	0.44
1:D:30:ARG:NH1	1:D:226:LEU:HD13	2.33	0.44
1:D:66:THR:HA	1:D:69:MSE:HB3	1.98	0.44
1:D:73:LEU:HD23	1:D:73:LEU:HA	1.83	0.44
1:B:69:MSE:HB2	2:B:331:HOH:O	2.17	0.44
1:C:149:VAL:H	1:C:149:VAL:HG23	1.55	0.44
1:D:41:PRO:HD2	1:D:42:ASP:H	1.83	0.44
1:C:25:LYS:HE2	1:C:82:PHE:CE2	2.52	0.44
1:C:203:ASP:O	1:C:206:PRO:HD3	2.18	0.44
1:B:84:PRO:HB2	1:B:87:GLN:HE21	1.82	0.43
1:C:275:GLU:O	1:C:286:LEU:HD23	2.17	0.43
1:D:199:ALA:N	1:D:200:PRO:HD3	2.33	0.43
1:D:8:HIS:HD2	1:D:19:ARG:HH11	1.65	0.43
1:D:262:ILE:HD12	1:D:286:LEU:HD23	1.99	0.43
1:D:215:VAL:HB	1:D:216:LEU:HD22	1.99	0.43
1:A:299:HIS:CD2	1:A:299:HIS:N	2.86	0.43
1:A:13:LEU:O	1:A:187:HIS:HE1	2.01	0.43
1:C:278:PHE:HB3	1:C:285:ILE:HD12	2.01	0.43
1:A:277:MSE:HG3	1:A:287:ARG:HB2	2.00	0.43
1:B:163:LEU:HD22	1:B:167:LEU:CD1	2.49	0.43
1:B:156:TRP:N	1:B:157:PRO:CD	2.80	0.43
1:C:205:TYR:HA	1:C:206:PRO:HD2	1.77	0.43
1:D:160:MSE:HG2	1:D:205:TYR:CD1	2.53	0.43
1:D:295:VAL:O	1:D:295:VAL:HG12	2.19	0.43
1:B:223:LEU:HD12	1:B:224:SER:N	2.31	0.42
1:D:5:ILE:HA	1:D:30:ARG:O	2.19	0.42
1:A:223:LEU:C	1:A:223:LEU:HD12	2.39	0.42
1:B:278:PHE:HB3	1:B:285:ILE:HD12	2.01	0.42
1:A:241:ALA:HB1	1:A:242:PRO:HD2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:SER:HA	1:A:80:PRO:C	2.39	0.42
1:A:248:PHE:HE2	1:A:302:ARG:HH21	1.66	0.42
1:D:44:THR:O	1:D:44:THR:HG22	2.18	0.42
1:B:21:MSE:CE	1:B:69:MSE:HE2	2.47	0.42
1:D:177:ALA:HB1	1:D:178:PRO:HD2	2.02	0.42
1:D:29:TRP:CH2	1:D:223:LEU:HD13	2.55	0.41
1:D:197:VAL:HG23	1:D:198:THR:HG23	2.02	0.41
1:B:276:LEU:HD22	1:B:285:ILE:O	2.20	0.41
1:D:24:PHE:HD1	1:D:218:PHE:CE1	2.38	0.41
1:D:260:VAL:HG23	1:D:286:LEU:HD21	2.03	0.41
1:B:44:THR:HA	1:B:47:THR:OG1	2.21	0.41
1:B:112:GLN:HA	1:B:113:PRO:HD3	1.91	0.41
1:C:84:PRO:HB2	1:C:87:GLN:HE21	1.85	0.41
1:D:102:LEU:HD12	1:D:102:LEU:HA	1.88	0.41
1:D:30:ARG:NH1	1:D:226:LEU:CD1	2.83	0.41
1:A:116:MSE:HE3	1:A:116:MSE:HB3	1.98	0.41
1:B:260:VAL:CG1	1:B:261:ALA:N	2.83	0.41
1:C:21:MSE:HE3	1:C:70:ALA:HB2	2.03	0.41
1:C:250:ASP:HA	1:C:251:PRO:HD3	1.83	0.41
1:A:49:GLY:O	1:A:270:GLU:HB3	2.21	0.41
1:A:306:ARG:HG2	1:A:307:VAL:N	2.36	0.41
1:B:110:VAL:HA	1:B:198:THR:HG21	2.03	0.41
1:B:66:THR:HA	1:B:69:MSE:HB3	2.02	0.40
1:D:37:ILE:HD11	1:D:39:PRO:O	2.21	0.40
1:D:240:PRO:HB3	1:D:297:HIS:ND1	2.35	0.40
1:B:23:GLY:HA3	1:B:219:GLY:O	2.20	0.40
1:A:25:LYS:O	1:A:77:LYS:HE2	2.21	0.40
1:D:299:HIS:ND1	1:D:299:HIS:N	2.70	0.40
1:C:30:ARG:NH2	1:C:225:ASP:O	2.52	0.40
1:C:216:LEU:HD12	1:C:216:LEU:HA	1.82	0.40
1:D:37:ILE:HD12	1:D:38:MSE:N	2.37	0.40
1:D:101:VAL:O	1:D:105:HIS:HD2	2.05	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	A	274/310 (88%)	270 (98%)	3 (1%)	1 (0%)	30	44
1	B	269/310 (87%)	266 (99%)	2 (1%)	1 (0%)	30	44
1	C	266/310 (86%)	261 (98%)	4 (2%)	1 (0%)	30	44
1	D	267/310 (86%)	263 (98%)	3 (1%)	1 (0%)	30	44
All	All	1076/1240 (87%)	1060 (98%)	12 (1%)	4 (0%)	30	44

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	65	ASP
1	A	65	ASP
1	B	65	ASP
1	C	65	ASP

### 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	221/243 (91%)	203 (92%)	18 (8%)	9	15
1	B	221/243 (91%)	199 (90%)	22 (10%)	6	9
1	C	214/243 (88%)	193 (90%)	21 (10%)	6	10
1	D	211/243 (87%)	175 (83%)	36 (17%)	1	2
All	All	867/972 (89%)	770 (89%)	97 (11%)	5	7

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
1	A	27	VAL

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Mol	Chain	Res	Type
1	A	37	ILE
1	A	43	LEU
1	A	52	LYS
1	A	56	LEU
1	A	116	MSE
1	A	149	VAL
1	A	184	SER
1	A	192	LEU
1	A	195	THR
1	A	216	LEU
1	A	222	SER
1	A	224	SER
1	A	236	SER
1	A	286	LEU
1	A	297	HIS
1	A	310	ARG
1	B	4	LEU
1	B	30	ARG
1	B	75	GLN
1	B	158	THR
1	B	163	LEU
1	B	192	LEU
1	B	193	LYS
1	B	209	SER
1	B	222	SER
1	B	223	LEU
1	B	225	ASP
1	B	245	ASP
1	B	247	THR
1	B	260	VAL
1	B	276	LEU
1	B	279	THR
1	B	283	GLU
1	B	284	LEU
1	B	286	LEU
1	B	287	ARG
1	B	291	ASN
1	B	296	VAL
1	C	4	LEU
1	C	37	ILE
1	C	44	THR
1	C	50	TYR

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Mol	Chain	Res	Type
1	C	53	THR
1	C	56	LEU
1	C	62	ILE
1	C	75	GLN
1	C	79	SER
1	C	108	SER
1	C	192	LEU
1	C	195	THR
1	C	216	LEU
1	C	223	LEU
1	C	228	SER
1	C	233	GLU
1	C	286	LEU
1	C	287	ARG
1	C	289	GLU
1	C	297	HIS
1	C	310	ARG
1	D	4	LEU
1	D	5	ILE
1	D	13	LEU
1	D	17	LYS
1	D	42	ASP
1	D	43	LEU
1	D	46	LEU
1	D	51	ARG
1	D	53	THR
1	D	62	ILE
1	D	68	LEU
1	D	115	SER
1	D	116	MSE
1	D	160	MSE
1	D	165	SER
1	D	179	SER
1	D	192	LEU
1	D	193	LYS
1	D	194	GLN
1	D	195	THR
1	D	207	SER
1	D	216	LEU
1	D	225	ASP
1	D	228	SER
1	D	232	ILE

*Continued on next page...*

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Mol	Chain	Res	Type
1	D	236	SER
1	D	245	ASP
1	D	246	GLU
1	D	247	THR
1	D	276	LEU
1	D	277	MSE
1	D	284	LEU
1	D	286	LEU
1	D	287	ARG
1	D	296	VAL
1	D	299	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	75	GLN
1	A	87	GLN
1	A	105	HIS
1	A	112	GLN
1	A	151	GLN
1	A	166	GLN
1	A	187	HIS
1	B	8	HIS
1	B	57	GLN
1	B	75	GLN
1	B	87	GLN
1	B	151	GLN
1	B	155	GLN
1	B	297	HIS
1	C	8	HIS
1	C	75	GLN
1	C	87	GLN
1	C	154	HIS
1	C	187	HIS
1	C	297	HIS
1	D	8	HIS
1	D	57	GLN
1	D	105	HIS
1	D	166	GLN
1	D	299	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	272/310 (87%)	-0.43	2 (0%) 84 81	4, 24, 30, 33	0
1	B	268/310 (86%)	-0.37	0 100 100	20, 26, 32, 38	0
1	C	267/310 (86%)	-0.28	3 (1%) 77 75	8, 25, 33, 37	0
1	D	267/310 (86%)	0.05	2 (0%) 84 81	18, 28, 36, 39	0
All	All	1074/1240 (86%)	-0.26	7 (0%) 84 81	4, 26, 34, 39	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	268	GLY	2.7
1	C	267	TYR	2.5
1	D	78	ALA	2.5
1	C	37	ILE	2.2
1	A	267	TYR	2.1
1	D	42	ASP	2.0
1	C	2	SER	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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.