



# Full wwPDB X-ray Structure Validation Report ⓘ

May 11, 2026 – 10:12 AM EDT

PDB ID : 9OBR / pdb\_00009obr  
Title : Dye-decolorizing peroxidase from Acinetobacter baumannii  
Authors : Smith, T.J.  
Deposited on : 2025-04-23  
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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 : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

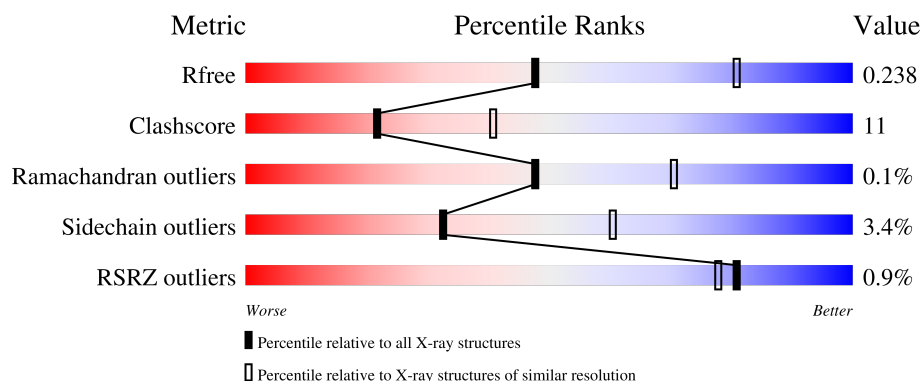
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	313	
1	B	313	
1	C	313	
1	D	313	
1	E	313	

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Mol	Chain	Length	Quality of chain
1	F	313	<div><div>%</div><div><div></div><div>81%</div><div>17%</div><div></div></div><div></div></div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 16195 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 Dye-decolorizing peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2481	1578	414	481	8			
1	B	313	Total	C	N	O	S	0	0	0
			2489	1583	415	482	9			
1	C	313	Total	C	N	O	S	0	0	0
			2489	1583	415	482	9			
1	D	313	Total	C	N	O	S	0	0	0
			2489	1583	415	482	9			
1	E	313	Total	C	N	O	S	0	0	0
			2489	1583	415	482	9			
1	F	313	Total	C	N	O	S	0	0	0
			2489	1583	415	482	9			

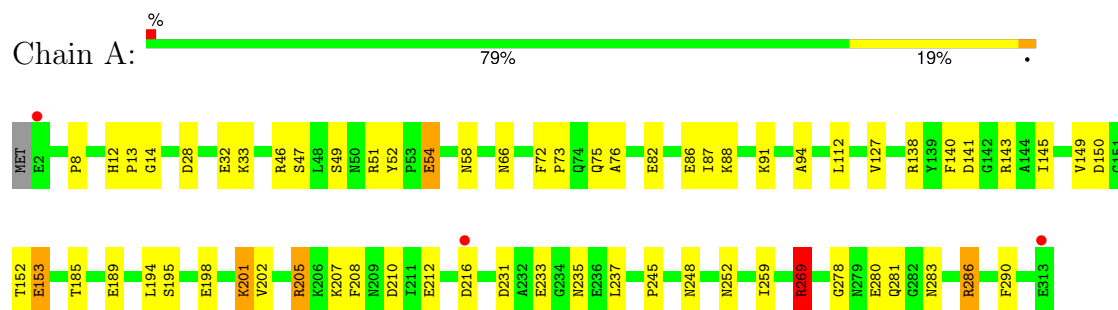
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	262	Total	O	0	0
			262	262		
2	B	153	Total	O	0	0
			153	153		
2	C	179	Total	O	0	0
			179	179		
2	D	200	Total	O	0	0
			200	200		
2	E	220	Total	O	0	0
			220	220		
2	F	255	Total	O	0	0
			255	255		

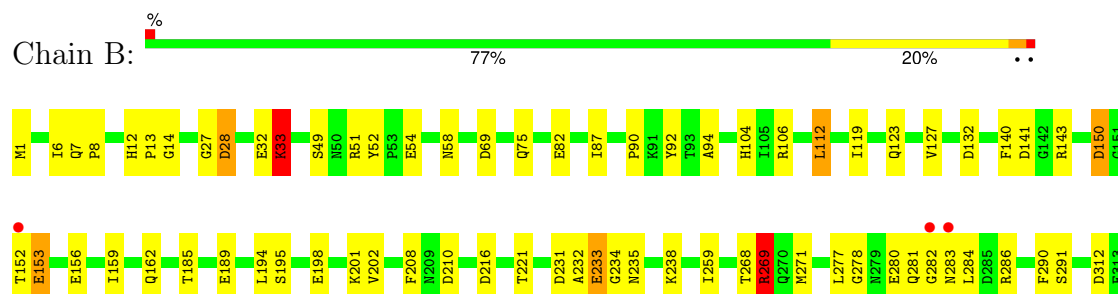
### 3 Residue-property plots

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.

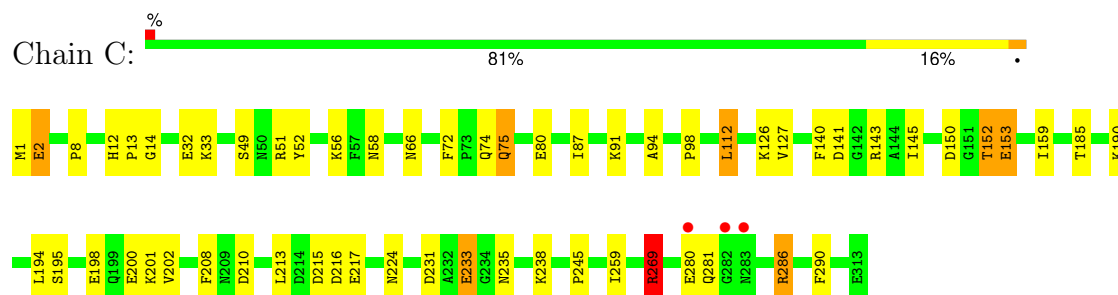
#### • Molecule 1: Dye-decolorizing peroxidase



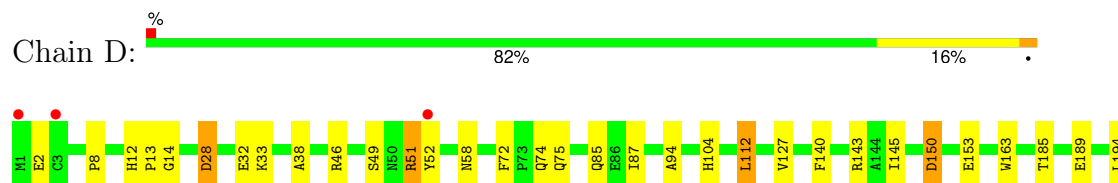
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#### • Molecule 1: Dye-decolorizing peroxidase

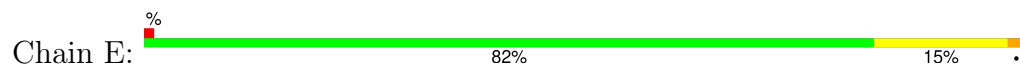


#### • Molecule 1: Dye-decolorizing peroxidase

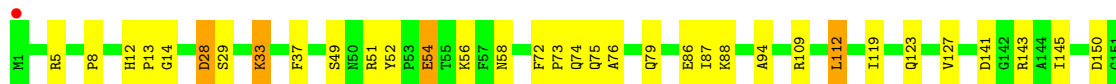
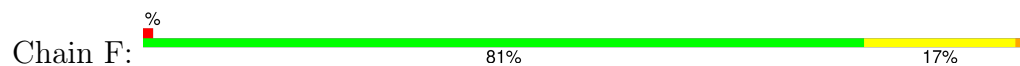




- Molecule 1: Dye-decolorizing peroxidase



- Molecule 1: Dye-decolorizing peroxidase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.26Å 141.25Å 86.99Å 90.00° 102.88° 90.00°	Depositor
Resolution (Å)	23.15 – 2.60 23.15 – 2.60	Depositor EDS
% Data completeness (in resolution range)	95.0 (23.15-2.60) 98.8 (23.15-2.60)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.87 (at 2.60Å)	Xtriage
Refinement program	PHENIX 1.21rc1_5134	Depositor
R, $R_{free}$	0.195 , 0.238 0.195 , 0.238	Depositor DCC
$R_{free}$ test set	1974 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.2	Xtriage
Anisotropy	0.882	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 48.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.001 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	16195	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.85% 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	0.52	3/2540 (0.1%)	0.62	5/3434 (0.1%)
1	B	0.55	5/2548 (0.2%)	0.64	5/3444 (0.1%)
1	C	0.52	4/2548 (0.2%)	0.63	3/3444 (0.1%)
1	D	0.47	2/2548 (0.1%)	0.59	2/3444 (0.1%)
1	E	0.59	9/2548 (0.4%)	0.65	5/3444 (0.1%)
1	F	0.48	2/2548 (0.1%)	0.61	2/3444 (0.1%)
All	All	0.52	25/15280 (0.2%)	0.63	22/20654 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	E	0	1
1	F	0	1
All	All	0	5

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	205	ARG	CZ-NH1	-9.00	1.20	1.32
1	B	189	GLU	CD-OE2	8.58	1.41	1.25
1	E	269	ARG	CD-NE	-7.96	1.35	1.46
1	B	189	GLU	CD-OE1	-7.65	1.10	1.25
1	C	269	ARG	CZ-NH1	7.62	1.43	1.32
1	E	269	ARG	CZ-NH1	7.05	1.42	1.32
1	E	54	GLU	CD-OE2	-6.56	1.12	1.25
1	C	75	GLN	CD-NE2	-6.46	1.19	1.33
1	B	54	GLU	CD-OE2	-6.43	1.13	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	75	GLN	CD-NE2	-6.17	1.20	1.33
1	B	150	ASP	CG-OD2	-6.11	1.13	1.25
1	B	54	GLU	CD-OE1	-5.97	1.14	1.25
1	D	150	ASP	CG-OD1	-5.91	1.14	1.25
1	E	54	GLU	CD-OE1	-5.82	1.14	1.25
1	E	150	ASP	CG-OD1	-5.80	1.14	1.25
1	F	54	GLU	CD-OE1	-5.73	1.14	1.25
1	C	150	ASP	CG-OD1	-5.67	1.14	1.25
1	A	150	ASP	CG-OD2	-5.66	1.14	1.25
1	F	150	ASP	CG-OD2	-5.59	1.14	1.25
1	E	269	ARG	CG-CD	-5.48	1.36	1.52
1	E	150	ASP	CG-OD2	-5.48	1.15	1.25
1	E	23	GLY	CA-C	-5.23	1.47	1.52
1	C	150	ASP	CG-OD2	-5.11	1.15	1.25
1	A	150	ASP	CG-OD1	-5.07	1.15	1.25
1	D	150	ASP	CG-OD2	-5.04	1.15	1.25

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	GLU	OE1-CD-OE2	-8.96	101.40	122.90
1	A	32	GLU	CA-CB-CG	-7.45	99.21	114.10
1	E	280	GLU	CA-CB-CG	7.43	128.96	114.10
1	B	150	ASP	OD1-CG-OD2	-7.33	105.32	122.90
1	C	32	GLU	CA-CB-CG	-7.25	99.61	114.10
1	D	150	ASP	OD1-CG-OD2	-7.22	105.56	122.90
1	C	150	ASP	OD1-CG-OD2	-7.19	105.64	122.90
1	B	32	GLU	CA-CB-CG	-6.97	100.15	114.10
1	A	150	ASP	OD1-CG-OD2	-6.87	106.41	122.90
1	E	150	ASP	OD1-CG-OD2	-6.86	106.43	122.90
1	F	150	ASP	OD1-CG-OD2	-6.82	106.54	122.90
1	F	269	ARG	CG-CD-NE	-6.45	97.80	112.00
1	E	280	GLU	CB-CG-CD	6.34	123.38	112.60
1	A	54	GLU	OE1-CD-OE2	-5.67	109.29	122.90
1	E	54	GLU	OE1-CD-OE2	-5.60	109.45	122.90
1	C	269	ARG	NE-CZ-NH2	-5.46	114.29	119.20
1	D	32	GLU	CA-CB-CG	-5.45	103.20	114.10
1	A	205	ARG	NE-CZ-NH2	5.31	123.98	119.20
1	A	269	ARG	CG-CD-NE	-5.18	100.60	112.00
1	E	54	GLU	CG-CD-OE1	5.17	130.30	118.40
1	B	269	ARG	CG-CD-NE	-5.15	100.67	112.00
1	B	54	GLU	CG-CD-OE1	5.11	130.14	118.40

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	269	ARG	Sidechain
1	B	269	ARG	Sidechain
1	C	269	ARG	Sidechain
1	E	269	ARG	Sidechain
1	F	269	ARG	Sidechain

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2481	0	2383	64	0
1	B	2489	0	2395	67	0
1	C	2489	0	2395	57	0
1	D	2489	0	2395	50	0
1	E	2489	0	2395	48	0
1	F	2489	0	2395	58	0
2	A	262	0	0	24	0
2	B	153	0	0	27	0
2	C	179	0	0	18	0
2	D	200	0	0	16	0
2	E	220	0	0	19	0
2	F	255	0	0	26	0
All	All	16195	0	14358	316	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 11.

All (316) 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:F:73:PRO:O	2:F:401:HOH:O	1.67	1.10
1:F:28:ASP:OD2	2:F:402:HOH:O	1.71	1.08
1:D:75:GLN:NE2	2:D:402:HOH:O	1.85	1.05
1:B:90:PRO:O	2:B:401:HOH:O	1.75	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:197:GLU:OE1	2:D:401:HOH:O	1.73	1.03
1:B:284:LEU:O	2:B:403:HOH:O	1.83	0.96
1:E:310:LEU:O	2:E:401:HOH:O	1.82	0.96
1:D:33:LYS:HG3	1:D:127:VAL:HG11	1.49	0.94
1:D:189:GLU:OE1	2:D:403:HOH:O	1.86	0.94
1:F:37:PHE:O	2:F:403:HOH:O	1.88	0.92
1:C:74:GLN:OE1	2:C:401:HOH:O	1.88	0.92
1:B:75:GLN:NE2	2:B:402:HOH:O	1.78	0.91
1:B:221:THR:O	2:B:403:HOH:O	1.90	0.90
1:A:28:ASP:O	2:A:402:HOH:O	1.89	0.89
1:B:232:ALA:O	2:B:404:HOH:O	1.91	0.89
1:F:216:ASP:OD2	2:F:404:HOH:O	1.91	0.88
1:E:33:LYS:HG3	1:E:127:VAL:HG11	1.53	0.87
1:D:248:ASN:ND2	2:D:407:HOH:O	2.07	0.87
1:F:74:GLN:NE2	2:F:408:HOH:O	2.08	0.87
1:E:72:PHE:HB3	1:E:75:GLN:HE21	1.38	0.85
1:A:33:LYS:HG3	1:A:127:VAL:HG11	1.58	0.84
1:F:29:SER:OG	2:F:405:HOH:O	1.95	0.83
1:E:72:PHE:HB3	1:E:75:GLN:NE2	1.93	0.82
1:C:33:LYS:HG3	1:C:127:VAL:HG11	1.62	0.81
1:D:52:TYR:HD2	1:D:112:LEU:HD21	1.47	0.80
1:A:212:GLU:OE1	2:A:404:HOH:O	1.99	0.80
1:F:269:ARG:NH2	2:F:406:HOH:O	2.05	0.79
1:E:153:GLU:OE1	1:E:153:GLU:HA	1.82	0.79
1:F:33:LYS:NZ	2:F:410:HOH:O	2.12	0.78
1:E:75:GLN:OE1	2:E:404:HOH:O	2.00	0.78
1:E:207:LYS:NZ	2:E:406:HOH:O	2.08	0.77
1:A:205:ARG:NH1	1:A:210:ASP:O	2.19	0.76
1:A:237:LEU:O	2:A:405:HOH:O	2.04	0.76
1:B:162:GLN:OE1	2:B:405:HOH:O	2.02	0.75
1:B:278:GLY:O	2:B:406:HOH:O	2.05	0.75
1:D:85:GLN:NE2	2:D:404:HOH:O	1.95	0.75
1:D:163:TRP:O	2:D:405:HOH:O	2.04	0.75
1:E:28:ASP:O	2:E:405:HOH:O	2.05	0.74
1:A:76:ALA:O	2:A:406:HOH:O	2.05	0.73
1:B:132:ASP:OD2	2:B:407:HOH:O	2.06	0.72
1:A:248:ASN:ND2	2:A:416:HOH:O	2.22	0.72
1:D:38:ALA:O	2:D:406:HOH:O	2.06	0.72
1:F:79:GLN:NE2	2:F:415:HOH:O	2.22	0.72
1:F:75:GLN:NE2	2:F:413:HOH:O	2.18	0.72
1:F:153:GLU:HA	1:F:153:GLU:OE1	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:154:ASN:OD1	2:F:407:HOH:O	2.07	0.72
1:C:200:GLU:OE1	2:C:402:HOH:O	2.07	0.71
1:C:238:LYS:NZ	2:C:408:HOH:O	2.20	0.71
1:D:283:ASN:OD1	2:D:408:HOH:O	2.09	0.70
1:C:66:ASN:ND2	2:C:410:HOH:O	2.21	0.70
1:C:280:GLU:OE1	2:C:403:HOH:O	2.09	0.70
1:E:150:ASP:OD1	2:E:407:HOH:O	2.09	0.70
1:A:91:LYS:O	2:A:407:HOH:O	2.09	0.69
1:B:277:LEU:HB2	2:B:406:HOH:O	1.91	0.69
1:A:153:GLU:HB2	2:A:567:HOH:O	1.91	0.69
1:F:75:GLN:OE1	2:F:409:HOH:O	2.09	0.69
1:E:12:HIS:CD2	1:E:14:GLY:H	2.11	0.69
1:C:80:GLU:OE2	2:C:404:HOH:O	2.11	0.68
1:E:97:THR:O	2:E:408:HOH:O	2.10	0.68
1:D:269:ARG:HG3	1:D:270:GLN:N	2.03	0.68
1:A:86:GLU:O	2:A:408:HOH:O	2.10	0.68
1:C:1:MET:O	1:C:2:GLU:HB3	1.93	0.68
1:F:12:HIS:CD2	1:F:14:GLY:H	2.12	0.68
1:D:28:ASP:OD2	1:D:28:ASP:N	2.26	0.67
1:B:69:ASP:OD1	2:B:408:HOH:O	2.13	0.66
1:B:12:HIS:CD2	1:B:14:GLY:H	2.13	0.66
1:C:12:HIS:CD2	1:C:14:GLY:H	2.13	0.66
1:D:276:PHE:O	2:D:409:HOH:O	2.13	0.66
1:A:66:ASN:C	1:A:66:ASN:HD22	2.02	0.66
1:A:88:LYS:NZ	2:A:423:HOH:O	2.28	0.66
1:A:140:PHE:CE1	1:D:52:TYR:HE2	2.14	0.66
1:E:2:GLU:OE1	2:E:409:HOH:O	2.12	0.66
1:B:234:GLY:O	2:B:409:HOH:O	2.14	0.66
1:E:73:PRO:O	2:E:410:HOH:O	2.13	0.66
1:F:233:GLU:N	1:F:233:GLU:OE1	2.28	0.66
1:B:233:GLU:OE1	1:B:233:GLU:N	2.28	0.65
1:C:56:LYS:HE2	1:F:54:GLU:OE2	1.95	0.65
1:B:156:GLU:OE2	1:D:46:ARG:NH1	2.30	0.65
1:A:140:PHE:CE1	1:D:52:TYR:CE2	2.85	0.65
1:E:312:ASP:O	2:E:411:HOH:O	2.14	0.65
1:D:233:GLU:OE1	1:D:233:GLU:N	2.29	0.64
1:B:51:ARG:HD2	1:E:149:VAL:HG21	1.79	0.64
1:A:12:HIS:CD2	1:A:14:GLY:H	2.15	0.64
1:A:235:ASN:ND2	2:A:425:HOH:O	2.30	0.64
1:F:13:PRO:HG2	2:F:479:HOH:O	1.99	0.62
1:A:82:GLU:OE2	2:A:409:HOH:O	2.16	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:202:VAL:HG13	1:B:286:ARG:HB3	1.80	0.62
1:C:215:ASP:O	2:C:406:HOH:O	2.16	0.61
1:D:12:HIS:CD2	1:D:14:GLY:H	2.19	0.61
1:E:233:GLU:N	1:E:233:GLU:OE1	2.33	0.61
1:F:269:ARG:O	1:F:269:ARG:HG2	1.96	0.61
1:B:82:GLU:HB3	2:B:416:HOH:O	2.00	0.61
1:A:233:GLU:N	1:A:233:GLU:OE1	2.34	0.61
1:D:33:LYS:CG	1:D:127:VAL:HG11	2.29	0.61
1:A:138:ARG:O	2:A:410:HOH:O	2.16	0.60
1:B:92:TYR:N	2:B:412:HOH:O	2.20	0.60
1:F:86:GLU:OE2	2:F:412:HOH:O	2.17	0.60
1:C:52:TYR:HD2	1:C:112:LEU:HD21	1.67	0.60
1:D:269:ARG:NH2	2:D:420:HOH:O	2.33	0.60
1:F:76:ALA:O	2:F:411:HOH:O	2.16	0.60
1:F:269:ARG:NH2	2:F:424:HOH:O	2.35	0.59
1:C:143:ARG:HG2	1:C:143:ARG:HH11	1.67	0.59
1:C:233:GLU:N	1:C:233:GLU:OE1	2.36	0.59
1:E:202:VAL:HG13	1:E:286:ARG:HB3	1.84	0.59
1:E:273:GLU:OE1	2:E:412:HOH:O	2.17	0.58
1:C:269:ARG:O	1:C:269:ARG:HG2	1.93	0.58
1:A:149:VAL:HG21	1:C:51:ARG:HD2	1.86	0.58
1:F:202:VAL:HG13	1:F:286:ARG:HB3	1.85	0.58
1:A:51:ARG:O	2:A:411:HOH:O	2.17	0.58
1:F:88:LYS:NZ	2:F:426:HOH:O	2.37	0.58
1:A:141:ASP:HB3	1:C:52:TYR:CE1	2.39	0.58
1:A:51:ARG:HB3	1:F:141:ASP:HB2	1.86	0.58
1:B:52:TYR:CE1	1:E:141:ASP:HB3	2.39	0.58
1:A:202:VAL:HG13	1:A:286:ARG:HB3	1.86	0.57
1:F:33:LYS:CG	1:F:127:VAL:HG11	2.34	0.57
1:A:208:PHE:O	1:C:51:ARG:NH1	2.38	0.57
1:B:33:LYS:CG	1:B:127:VAL:HG11	2.34	0.57
1:B:156:GLU:HG3	1:D:46:ARG:HD3	1.85	0.57
1:D:202:VAL:HG13	1:D:286:ARG:HB3	1.85	0.57
1:A:54:GLU:OE2	1:F:56:LYS:NZ	2.33	0.57
1:B:312:ASP:O	2:B:410:HOH:O	2.17	0.56
1:C:33:LYS:CG	1:C:127:VAL:HG11	2.32	0.56
1:D:52:TYR:CD2	1:D:112:LEU:HD21	2.35	0.56
1:B:198:GLU:HA	1:B:201:LYS:HG2	1.88	0.56
1:B:27:GLY:O	2:B:411:HOH:O	2.17	0.56
1:F:248:ASN:ND2	2:F:428:HOH:O	2.37	0.55
1:B:1:MET:HE3	1:B:6:ILE:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:109:ARG:NH1	2:F:414:HOH:O	2.21	0.55
1:D:198:GLU:HA	1:D:201:LYS:HG2	1.89	0.55
1:B:52:TYR:HD2	1:B:112:LEU:HD21	1.72	0.55
1:F:13:PRO:HD3	2:F:526:HOH:O	2.05	0.55
1:F:52:TYR:HD2	1:F:112:LEU:HD21	1.71	0.55
1:E:294:GLN:HG3	2:E:416:HOH:O	2.06	0.55
1:F:28:ASP:OD2	1:F:28:ASP:N	2.27	0.54
1:A:46:ARG:HG3	2:F:546:HOH:O	2.06	0.54
1:C:202:VAL:HG13	1:C:286:ARG:HB3	1.88	0.54
1:C:190:LYS:NZ	2:C:421:HOH:O	2.40	0.54
1:A:47:SER:O	1:A:51:ARG:HG3	2.08	0.54
1:A:33:LYS:CG	1:A:127:VAL:HG11	2.35	0.53
1:A:189:GLU:OE1	2:A:412:HOH:O	2.17	0.53
1:B:269:ARG:NH2	2:B:432:HOH:O	2.41	0.53
1:C:52:TYR:CD2	1:C:112:LEU:HD21	2.43	0.53
1:A:75:GLN:NE2	2:A:435:HOH:O	2.41	0.53
1:C:126:LYS:HB2	2:C:413:HOH:O	2.08	0.53
1:C:198:GLU:HA	1:C:201:LYS:HG2	1.90	0.53
1:E:33:LYS:CG	1:E:127:VAL:HG11	2.33	0.53
1:A:198:GLU:OE2	2:A:414:HOH:O	2.18	0.53
1:D:104:HIS:NE2	2:D:418:HOH:O	2.30	0.53
1:B:282:GLY:HA3	2:B:496:HOH:O	2.08	0.52
1:E:52:TYR:CD2	1:E:112:LEU:HD21	2.44	0.52
1:A:195:SER:OG	1:A:198:GLU:HG3	2.10	0.52
1:B:33:LYS:HG3	1:B:127:VAL:HG11	1.91	0.52
1:C:91:LYS:CE	2:C:411:HOH:O	2.57	0.52
1:C:216:ASP:OD1	1:C:216:ASP:N	2.42	0.52
1:F:52:TYR:CD2	1:F:112:LEU:HD21	2.45	0.52
1:B:52:TYR:CD2	1:B:112:LEU:HD21	2.45	0.51
1:E:269:ARG:O	1:E:269:ARG:HG2	2.01	0.51
1:E:251:LYS:HD2	2:E:560:HOH:O	2.10	0.51
1:F:193:ALA:HB3	2:F:423:HOH:O	2.11	0.51
1:D:311:GLY:O	2:D:411:HOH:O	2.19	0.50
1:B:28:ASP:OD2	1:B:28:ASP:N	2.37	0.50
2:B:405:HOH:O	1:D:2:GLU:O	2.19	0.50
1:C:126:LYS:N	2:C:413:HOH:O	2.31	0.50
1:B:51:ARG:HD2	1:E:149:VAL:CG2	2.42	0.50
1:E:87:ILE:HB	1:E:94:ALA:HB3	1.94	0.50
1:A:207:LYS:NZ	2:A:437:HOH:O	2.44	0.50
1:D:194:LEU:HD23	2:D:540:HOH:O	2.11	0.50
1:B:216:ASP:OD1	1:B:216:ASP:N	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:72:PHE:CB	1:E:75:GLN:HE21	2.17	0.50
1:F:286:ARG:HG3	2:F:514:HOH:O	2.12	0.49
1:B:106:ARG:HD3	2:B:438:HOH:O	2.12	0.49
1:F:294:GLN:NE2	2:F:440:HOH:O	2.45	0.49
1:A:52:TYR:CD2	1:A:112:LEU:HD21	2.48	0.49
1:E:198:GLU:O	1:E:201:LYS:HB2	2.13	0.49
1:B:198:GLU:O	1:B:201:LYS:HB2	2.13	0.49
1:F:33:LYS:HG3	1:F:127:VAL:HG11	1.95	0.49
1:A:280:GLU:OE1	2:A:415:HOH:O	2.20	0.48
1:C:98:PRO:O	2:C:407:HOH:O	2.20	0.48
1:A:145:ILE:HB	1:A:245:PRO:HB3	1.95	0.48
1:B:221:THR:CA	2:B:403:HOH:O	2.61	0.48
1:D:281:GLN:OE1	1:D:281:GLN:N	2.47	0.48
1:B:119:ILE:HG23	1:B:123:GLN:HE21	1.77	0.48
1:B:143:ARG:HG2	1:B:143:ARG:HH11	1.77	0.48
1:B:51:ARG:NH1	1:E:208:PHE:O	2.46	0.48
1:D:145:ILE:HB	1:D:245:PRO:HB3	1.96	0.48
1:E:52:TYR:HD2	1:E:112:LEU:HD21	1.79	0.48
1:E:231:ASP:OD1	1:E:235:ASN:N	2.47	0.48
1:B:195:SER:OG	1:B:198:GLU:HG3	2.14	0.47
1:C:153:GLU:HA	1:C:153:GLU:OE1	2.14	0.47
1:B:140:PHE:CE1	1:C:52:TYR:CE2	3.02	0.47
1:B:156:GLU:CD	1:D:46:ARG:HD3	2.39	0.47
1:E:294:GLN:NE2	2:E:416:HOH:O	2.28	0.47
1:A:194:LEU:HD11	1:A:290:PHE:CZ	2.49	0.47
1:C:75:GLN:HB3	2:C:489:HOH:O	2.14	0.47
1:C:91:LYS:HE2	2:C:411:HOH:O	2.13	0.47
1:F:143:ARG:HH11	1:F:143:ARG:HG2	1.80	0.47
1:A:73:PRO:HD2	2:A:421:HOH:O	2.13	0.47
1:A:216:ASP:OD1	1:A:216:ASP:N	2.46	0.47
1:A:269:ARG:O	1:A:269:ARG:HG2	2.09	0.47
1:C:8:PRO:HG3	1:C:58:ASN:HB2	1.97	0.47
1:D:198:GLU:O	1:D:201:LYS:HB2	2.15	0.47
1:A:152:THR:HG21	1:A:210:ASP:OD2	2.15	0.47
1:B:281:GLN:OE1	1:B:281:GLN:N	2.48	0.46
1:F:8:PRO:HG3	1:F:58:ASN:HB2	1.97	0.46
1:B:221:THR:C	2:B:403:HOH:O	2.48	0.46
1:B:238:LYS:HA	2:B:430:HOH:O	2.14	0.46
1:D:143:ARG:HG2	1:D:143:ARG:HH11	1.79	0.46
1:F:194:LEU:HD11	1:F:290:PHE:CZ	2.49	0.46
1:D:33:LYS:HA	1:D:33:LYS:HD3	1.65	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:ASP:HB2	1:F:51:ARG:HB3	1.97	0.46
1:A:141:ASP:HB2	1:C:51:ARG:HB3	1.98	0.46
1:E:72:PHE:CB	1:E:75:GLN:NE2	2.72	0.46
1:A:12:HIS:CG	1:A:13:PRO:HD2	2.51	0.46
1:D:195:SER:OG	1:D:198:GLU:HG3	2.16	0.46
1:C:159:ILE:HD13	1:F:5:ARG:HD2	1.98	0.45
1:C:231:ASP:OD1	1:C:235:ASN:N	2.49	0.45
1:D:216:ASP:OD1	1:D:216:ASP:N	2.43	0.45
1:B:51:ARG:HD3	2:B:468:HOH:O	2.16	0.45
1:A:252:ASN:HB2	2:D:548:HOH:O	2.16	0.45
1:B:8:PRO:HG3	1:B:58:ASN:HB2	1.98	0.45
1:B:231:ASP:OD1	1:B:235:ASN:N	2.48	0.45
1:C:194:LEU:HD11	1:C:290:PHE:CZ	2.51	0.45
1:C:195:SER:OG	1:C:198:GLU:HG3	2.17	0.45
1:E:195:SER:OG	1:E:198:GLU:HG3	2.16	0.45
1:A:198:GLU:O	1:A:201:LYS:HB2	2.16	0.45
1:B:156:GLU:CD	1:D:46:ARG:HH11	2.24	0.45
1:E:284:LEU:HD13	2:E:569:HOH:O	2.16	0.45
1:A:281:GLN:N	1:A:281:GLN:OE1	2.50	0.45
1:D:280:GLU:HB2	1:D:281:GLN:OE1	2.16	0.45
1:B:12:HIS:CG	1:B:13:PRO:HD2	2.52	0.45
1:C:72:PHE:HA	1:C:75:GLN:NE2	2.32	0.45
1:A:149:VAL:CG2	1:C:51:ARG:HD2	2.46	0.45
1:A:8:PRO:HA	2:A:539:HOH:O	2.15	0.45
1:A:231:ASP:OD1	1:A:235:ASN:N	2.50	0.45
1:E:216:ASP:OD1	1:E:216:ASP:N	2.43	0.45
1:F:194:LEU:HA	2:F:474:HOH:O	2.17	0.45
1:A:143:ARG:HH11	1:A:143:ARG:HG2	1.82	0.45
1:D:8:PRO:HG3	1:D:58:ASN:HB2	2.00	0.44
1:D:231:ASP:OD1	1:D:235:ASN:N	2.49	0.44
1:C:198:GLU:O	1:C:201:LYS:HB2	2.17	0.44
1:C:213:LEU:O	2:C:409:HOH:O	2.21	0.44
1:C:12:HIS:CG	1:C:13:PRO:HD2	2.52	0.44
1:F:195:SER:OG	1:F:198:GLU:HG3	2.17	0.44
1:D:12:HIS:CG	1:D:13:PRO:HD2	2.52	0.44
1:B:156:GLU:CG	1:D:46:ARG:HD3	2.47	0.44
1:C:269:ARG:NH2	2:C:422:HOH:O	2.41	0.44
1:D:72:PHE:HB3	1:D:75:GLN:NE2	2.33	0.44
1:A:278:GLY:HA2	1:A:283:ASN:O	2.18	0.44
1:C:224:ASN:HB2	2:C:466:HOH:O	2.17	0.44
1:F:281:GLN:N	1:F:281:GLN:OE1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:TYR:CE2	1:C:140:PHE:CE1	3.06	0.43
1:E:13:PRO:HD3	2:E:524:HOH:O	2.19	0.43
1:F:145:ILE:HB	1:F:245:PRO:HB3	2.00	0.43
1:B:208:PHE:CZ	2:D:413:HOH:O	2.71	0.43
1:A:33:LYS:HG3	1:A:127:VAL:CG1	2.39	0.43
1:E:198:GLU:O	1:E:202:VAL:HG23	2.19	0.43
1:A:47:SER:OG	2:A:401:HOH:O	1.83	0.43
1:A:52:TYR:CE2	1:D:140:PHE:CE1	3.05	0.43
1:F:278:GLY:HA2	1:F:283:ASN:O	2.17	0.43
1:A:13:PRO:HG2	2:A:495:HOH:O	2.19	0.43
1:E:194:LEU:HD11	1:E:290:PHE:CZ	2.54	0.43
1:A:52:TYR:HD2	1:A:112:LEU:HD21	1.84	0.43
1:A:205:ARG:NH2	2:A:447:HOH:O	2.50	0.43
1:F:33:LYS:HA	1:F:33:LYS:HD3	1.49	0.43
1:F:152:THR:HG21	1:F:210:ASP:OD2	2.19	0.43
1:B:104:HIS:O	2:B:414:HOH:O	2.21	0.42
1:B:159:ILE:HD12	2:B:497:HOH:O	2.18	0.42
1:D:33:LYS:HG3	1:D:127:VAL:CG1	2.34	0.42
1:F:87:ILE:HB	1:F:94:ALA:HB3	2.01	0.42
1:B:51:ARG:HB3	1:E:141:ASP:HB2	2.00	0.42
1:C:141:ASP:HB3	1:F:52:TYR:CE1	2.54	0.42
1:E:12:HIS:CG	1:E:13:PRO:HD2	2.55	0.42
1:A:143:ARG:NH1	1:A:149:VAL:HG23	2.34	0.42
1:B:87:ILE:HB	1:B:94:ALA:HB3	2.01	0.42
1:B:194:LEU:HD11	1:B:290:PHE:CZ	2.53	0.42
1:F:119:ILE:HG23	1:F:123:GLN:HE21	1.84	0.42
1:B:33:LYS:HA	1:B:33:LYS:HD3	1.45	0.42
1:C:208:PHE:HB2	2:E:592:HOH:O	2.20	0.42
1:E:206:LYS:HE3	1:E:206:LYS:HB3	1.85	0.42
1:C:281:GLN:N	1:C:281:GLN:OE1	2.53	0.42
1:D:87:ILE:HB	1:D:94:ALA:HB3	2.02	0.42
1:E:171:PRO:CD	2:E:459:HOH:O	2.68	0.42
1:A:8:PRO:HG3	1:A:58:ASN:HB2	2.01	0.42
1:B:269:ARG:O	1:B:269:ARG:HG2	2.07	0.42
1:F:198:GLU:HA	1:F:201:LYS:HG2	2.00	0.42
1:B:152:THR:HG21	1:B:210:ASP:OD2	2.19	0.42
1:C:87:ILE:HB	1:C:94:ALA:HB3	2.01	0.42
1:C:145:ILE:HB	1:C:245:PRO:HB3	2.02	0.42
1:C:159:ILE:HG21	1:F:5:ARG:HD2	2.01	0.42
1:A:87:ILE:HB	1:A:94:ALA:HB3	2.02	0.42
1:E:33:LYS:HD3	1:E:33:LYS:HA	1.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:216:ASP:OD1	1:F:216:ASP:N	2.48	0.42
1:B:278:GLY:HA2	1:B:283:ASN:O	2.20	0.41
1:C:72:PHE:HB3	1:C:75:GLN:NE2	2.35	0.41
1:B:268:THR:O	1:B:271:MET:HB2	2.20	0.41
1:E:152:THR:HG21	1:E:210:ASP:OD2	2.20	0.41
1:A:72:PHE:HB3	1:A:75:GLN:NE2	2.35	0.41
1:B:280:GLU:HG2	2:B:506:HOH:O	2.20	0.41
1:E:205:ARG:NH2	2:E:447:HOH:O	2.53	0.41
1:A:280:GLU:HA	2:A:415:HOH:O	2.21	0.41
1:F:72:PHE:HB3	1:F:75:GLN:NE2	2.35	0.41
1:B:141:ASP:HB2	1:D:51:ARG:HB3	2.02	0.41
1:C:152:THR:HG21	1:C:210:ASP:OD2	2.19	0.41
1:E:26:GLN:HA	2:E:403:HOH:O	2.19	0.41
1:C:33:LYS:HG3	1:C:127:VAL:CG1	2.43	0.41
1:F:12:HIS:CG	1:F:13:PRO:HD2	2.56	0.41
1:B:153:GLU:OE1	1:B:153:GLU:HA	2.21	0.41
1:D:74:GLN:OE1	1:D:74:GLN:HA	2.21	0.41
1:D:251:LYS:NZ	2:D:434:HOH:O	2.54	0.41
1:E:273:GLU:HG2	1:E:277:LEU:HD12	2.01	0.41
1:F:33:LYS:HE3	2:F:630:HOH:O	2.20	0.41
1:B:7:GLN:OE1	2:B:413:HOH:O	2.21	0.41
1:A:33:LYS:HB3	1:A:127:VAL:HG21	2.03	0.40
1:C:126:LYS:CB	2:C:413:HOH:O	2.69	0.40
1:D:194:LEU:HD11	1:D:290:PHE:CZ	2.55	0.40
1:F:231:ASP:OD1	1:F:235:ASN:N	2.53	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	310/313 (99%)	304 (98%)	6 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	311/313 (99%)	304 (98%)	6 (2%)	1 (0%)	36	58
1	C	311/313 (99%)	303 (97%)	7 (2%)	1 (0%)	36	58
1	D	311/313 (99%)	304 (98%)	7 (2%)	0	100	100
1	E	311/313 (99%)	303 (97%)	8 (3%)	0	100	100
1	F	311/313 (99%)	302 (97%)	9 (3%)	0	100	100
All	All	1865/1878 (99%)	1820 (98%)	43 (2%)	2 (0%)	48	70

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	2	GLU
1	B	33	LYS

### 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	266/267 (100%)	260 (98%)	6 (2%)	44	71
1	B	267/267 (100%)	257 (96%)	10 (4%)	30	57
1	C	267/267 (100%)	258 (97%)	9 (3%)	32	60
1	D	267/267 (100%)	256 (96%)	11 (4%)	27	54
1	E	267/267 (100%)	257 (96%)	10 (4%)	30	57
1	F	267/267 (100%)	258 (97%)	9 (3%)	32	60
All	All	1601/1602 (100%)	1546 (97%)	55 (3%)	32	60

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	SER
1	A	153	GLU
1	A	185	THR
1	A	201	LYS

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Mol	Chain	Res	Type
1	A	259	ILE
1	A	286	ARG
1	B	28	ASP
1	B	33	LYS
1	B	49	SER
1	B	112	LEU
1	B	150	ASP
1	B	153	GLU
1	B	185	THR
1	B	233	GLU
1	B	259	ILE
1	B	291	SER
1	C	49	SER
1	C	112	LEU
1	C	152	THR
1	C	153	GLU
1	C	185	THR
1	C	217	GLU
1	C	233	GLU
1	C	259	ILE
1	C	286	ARG
1	D	28	ASP
1	D	49	SER
1	D	51	ARG
1	D	112	LEU
1	D	150	ASP
1	D	153	GLU
1	D	185	THR
1	D	217	GLU
1	D	233	GLU
1	D	259	ILE
1	D	286	ARG
1	E	28	ASP
1	E	49	SER
1	E	51	ARG
1	E	153	GLU
1	E	185	THR
1	E	196	ASP
1	E	201	LYS
1	E	259	ILE
1	E	286	ARG
1	E	291	SER

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Mol	Chain	Res	Type
1	F	28	ASP
1	F	33	LYS
1	F	49	SER
1	F	112	LEU
1	F	185	THR
1	F	233	GLU
1	F	259	ILE
1	F	286	ARG
1	F	291	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	66	ASN
1	A	75	GLN
1	A	110	GLN
1	A	162	GLN
1	A	294	GLN
1	B	12	HIS
1	B	66	ASN
1	B	85	GLN
1	B	123	GLN
1	B	294	GLN
1	C	12	HIS
1	C	66	ASN
1	C	74	GLN
1	C	162	GLN
1	D	12	HIS
1	D	75	GLN
1	D	162	GLN
1	D	283	ASN
1	E	12	HIS
1	E	66	ASN
1	E	75	GLN
1	E	121	ASN
1	E	162	GLN
1	E	252	ASN
1	F	12	HIS
1	F	66	ASN
1	F	75	GLN
1	F	121	ASN

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Mol	Chain	Res	Type
1	F	123	GLN
1	F	252	ASN
1	F	294	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 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

### 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	312/313 (99%)	-0.15	3 (0%) 79 76	12, 26, 61, 125	0
1	B	313/313 (100%)	-0.02	3 (0%) 79 76	14, 29, 67, 125	0
1	C	313/313 (100%)	-0.10	3 (0%) 79 76	12, 28, 66, 126	0
1	D	313/313 (100%)	-0.11	4 (1%) 75 71	13, 27, 64, 127	0
1	E	313/313 (100%)	-0.20	2 (0%) 85 83	13, 27, 64, 126	0
1	F	313/313 (100%)	-0.18	2 (0%) 85 83	12, 27, 63, 128	0
All	All	1877/1878 (99%)	-0.13	17 (0%) 81 78	12, 27, 65, 128	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	208	PHE	3.1
1	E	282	GLY	3.0
1	C	282	GLY	3.0
1	D	208	PHE	3.0
1	E	153	GLU	2.7
1	A	216	ASP	2.4
1	B	283	ASN	2.3
1	D	3	CYS	2.3
1	C	283	ASN	2.3
1	C	280	GLU	2.2
1	A	2	GLU	2.2
1	D	52	TYR	2.1
1	F	1	MET	2.1
1	B	152	THR	2.1
1	D	1	MET	2.1
1	B	282	GLY	2.0
1	A	313	GLU	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 oligosaccharides 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.