



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:35 AM GMT

PDB ID : 2AXV  
Title : Structure of PrgX Y153C mutant  
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Deposited on : 2005-09-06  
Resolution : 3.00 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

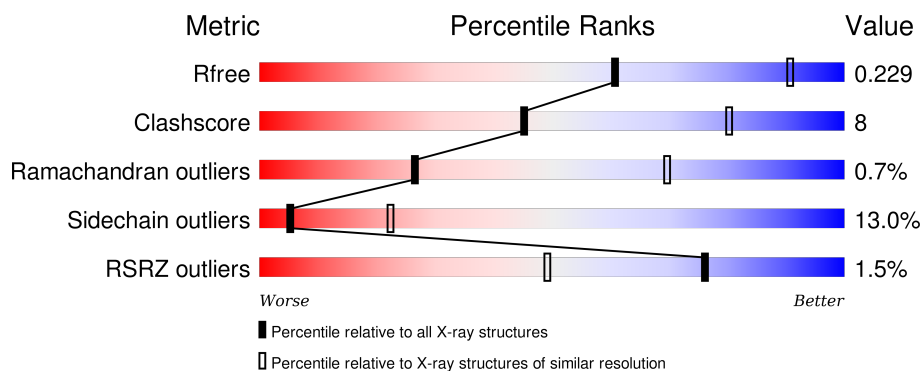
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	317	<div> <div>2%</div> <div>63% 27% 5%</div> </div>
1	B	317	<div> <div>72% 20%</div> </div>
1	C	317	<div> <div>2%</div> <div>69% 21% 5%</div> </div>
1	D	317	<div> <div>2%</div> <div>72% 21% 5%</div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10026 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 PrgX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2496	1620	402	468	6			
1	B	303	Total	C	N	O	S	0	0	0
			2501	1623	403	469	6			
1	C	302	Total	C	N	O	S	0	0	0
			2496	1620	402	468	6			
1	D	302	Total	C	N	O	S	0	0	0
			2496	1620	402	468	6			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	153	CYS	TYR	ENGINEERED	UNP Q04114
B	153	CYS	TYR	ENGINEERED	UNP Q04114
C	153	CYS	TYR	ENGINEERED	UNP Q04114
D	153	CYS	TYR	ENGINEERED	UNP Q04114

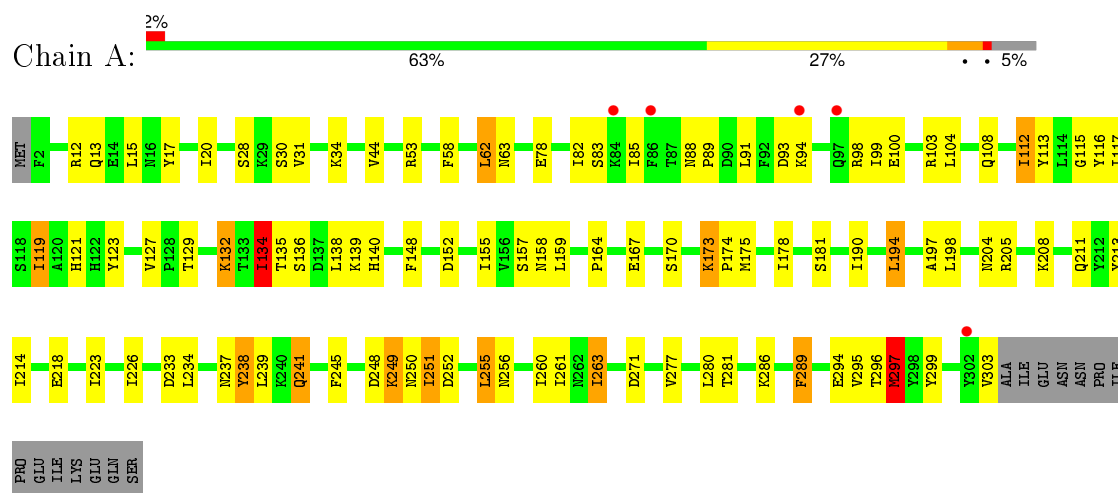
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	8	Total	O	0	0
			8	8		
2	B	5	Total	O	0	0
			5	5		
2	C	8	Total	O	0	0
			8	8		
2	D	16	Total	O	0	0
			16	16		

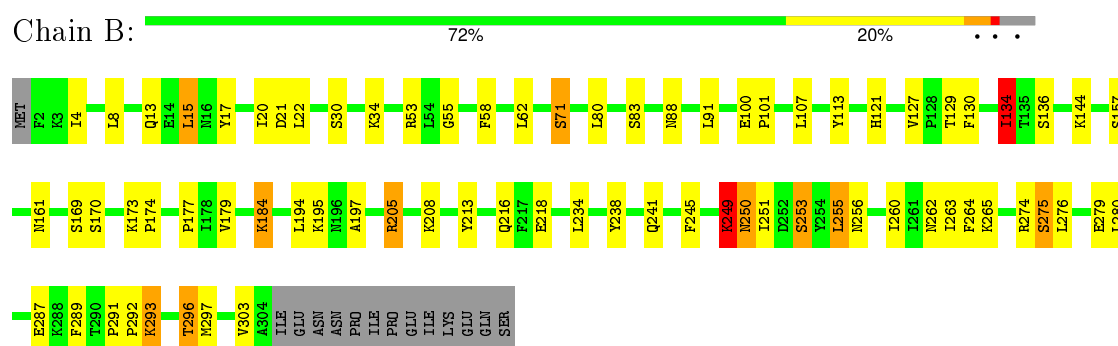
### 3 Residue-property plots [i](#)

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.

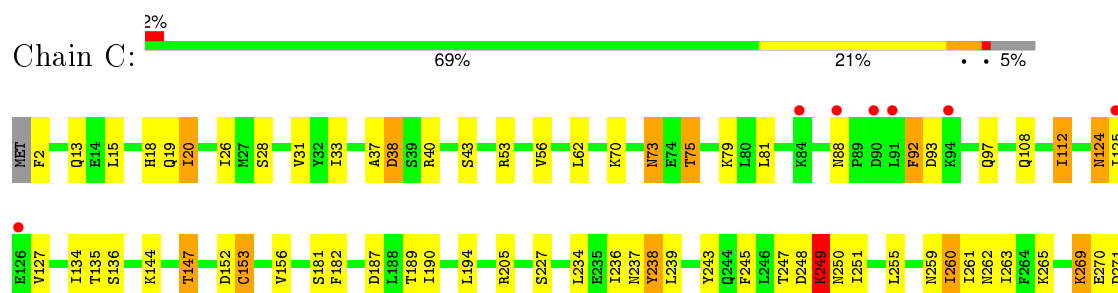
#### • Molecule 1: PrgX



#### • Molecule 1: PrgX

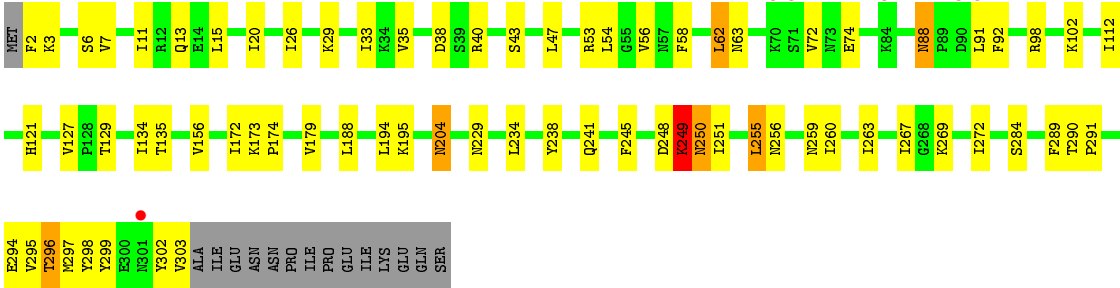


#### • Molecule 1: PrgX





● Molecule 1: PrgX



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.08 Å 82.08 Å 263.48 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 48.42 – 2.57	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.00) 88.8 (48.42-2.57)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.33 (at 2.58 Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.239 , 0.280 0.230 , 0.229	Depositor DCC
$R_{free}$ test set	1822 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	69.0	Xtriage
Anisotropy	0.654	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 52.5	EDS
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 51059 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	10026	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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	0.90	2/2547 (0.1%)	0.88	5/3440 (0.1%)
1	B	0.89	0/2552	0.90	3/3447 (0.1%)
1	C	0.94	3/2547 (0.1%)	0.91	2/3440 (0.1%)
1	D	0.95	0/2547	0.86	0/3440
All	All	0.92	5/10193 (0.0%)	0.89	10/13767 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	271	ASP	CB-CG	7.08	1.66	1.51
1	C	153	CYS	CB-SG	-6.46	1.71	1.82
1	C	271	ASP	CB-CG	5.50	1.63	1.51
1	A	100	GLU	CB-CG	5.38	1.62	1.52
1	C	289	PHE	CB-CG	-5.15	1.42	1.51

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	B	134	ILE	CB-CA-C	-6.99	97.62	111.60
1	A	233	ASP	CB-CG-OD1	6.42	124.08	118.30
1	A	134	ILE	CB-CA-C	-5.95	99.69	111.60
1	A	252	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	B	53	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	C	38	ASP	CB-CG-OD2	5.48	123.24	118.30
1	A	271	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	53	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	C	147	THR	CB-CA-C	-5.00	98.09	111.60

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	2496	0	2532	59	0
1	B	2501	0	2537	38	0
1	C	2496	0	2532	44	0
1	D	2496	0	2532	32	0
2	A	8	0	0	0	0
2	B	5	0	0	0	0
2	C	8	0	0	0	0
2	D	16	0	0	1	0
All	All	10026	0	10133	156	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 8.

All (156) 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:C:262:ASN:HD21	1:C:265:LYS:NZ	1.59	1.01
1:C:262:ASN:HD21	1:C:265:LYS:HZ3	1.12	0.90
1:D:29:LYS:O	1:D:33:ILE:HG13	1.80	0.80
1:D:88:ASN:OD1	1:D:91:LEU:HD13	1.88	0.74
1:C:262:ASN:ND2	1:C:265:LYS:HZ3	1.88	0.71
1:A:113:TYR:CE1	1:A:117:ILE:HD11	2.26	0.70
1:A:294:GLU:O	1:A:297:MET:HB3	1.91	0.69
1:A:263:ILE:CD1	1:B:263:ILE:HG13	2.22	0.69
1:C:182:PHE:C	1:D:63:ASN:HD22	1.97	0.68
1:A:197:ALA:HB1	1:A:213:TYR:CE2	2.29	0.67
1:D:3:LYS:HA	1:D:38:ASP:OD2	1.98	0.64
1:B:241:GLN:HG2	1:B:256:ASN:HB2	1.80	0.63
1:D:269:LYS:HG2	1:D:272:ILE:HD12	1.81	0.62
1:C:26:ILE:HD11	1:C:53:ARG:NH1	2.14	0.61
1:D:204:ASN:N	1:D:204:ASN:HD22	1.98	0.61
1:A:190:ILE:O	1:A:194:LEU:HD22	2.00	0.61
1:D:156:VAL:HG11	1:D:172:ILE:HG12	1.82	0.61
1:A:251:ILE:HB	1:C:290:THR:O	2.00	0.61
1:C:262:ASN:ND2	1:C:265:LYS:NZ	2.40	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:PHE:CG	1:A:175:MET:HG2	2.36	0.60
1:A:108:GLN:HG2	1:B:55:GLY:O	2.02	0.60
1:D:72:VAL:HG22	2:D:326:HOH:O	2.01	0.59
1:C:243:TYR:O	1:C:247:THR:HG23	2.03	0.59
1:B:130:PHE:O	1:B:134:ILE:HD13	2.02	0.58
1:A:250:ASN:HB2	1:C:290:THR:HB	1.86	0.57
1:C:124:ASN:N	1:C:124:ASN:HD22	2.02	0.57
1:C:19:GLN:HE22	1:C:33:ILE:HG12	1.68	0.57
1:C:43:SER:HA	1:D:43:SER:HA	1.87	0.56
1:C:28:SER:OG	1:C:31:VAL:HG23	2.05	0.56
1:A:299:TYR:O	1:A:303:VAL:HG22	2.06	0.56
1:B:71:SER:HB3	1:B:80:LEU:HD11	1.87	0.56
1:B:20:ILE:HD12	1:B:20:ILE:H	1.70	0.55
1:A:198:LEU:HG	1:A:239:LEU:HD13	1.89	0.55
1:D:188:LEU:HD13	1:D:229:ASN:HD22	1.72	0.55
1:C:262:ASN:HD21	1:C:265:LYS:HZ1	1.47	0.55
1:B:241:GLN:CG	1:B:256:ASN:HB2	2.37	0.55
1:A:248:ASP:HB2	1:A:250:ASN:HD22	1.72	0.55
1:B:173:LYS:N	1:B:174:PRO:HD2	2.22	0.54
1:A:20:ILE:HD12	1:A:20:ILE:H	1.73	0.54
1:B:275:SER:O	1:B:279:GLU:HG3	2.07	0.54
1:B:177:PRO:HA	1:B:216:GLN:NE2	2.22	0.54
1:D:20:ILE:H	1:D:20:ILE:HD12	1.72	0.53
1:A:251:ILE:O	1:A:255:LEU:HD22	2.08	0.53
1:A:134:ILE:HD12	1:A:135:THR:H	1.72	0.53
1:B:234:LEU:HD22	1:B:260:ILE:HG23	1.91	0.53
1:D:11:ILE:HG22	1:D:54:LEU:HD22	1.90	0.53
1:B:262:ASN:O	1:B:265:LYS:HB3	2.08	0.52
1:C:249:LYS:HZ1	1:C:287:GLU:HB3	1.72	0.52
1:C:234:LEU:HD23	1:D:267:ILE:HG21	1.91	0.52
1:A:173:LYS:N	1:A:174:PRO:HD2	2.25	0.51
1:C:269:LYS:HG2	1:C:272:ILE:HD12	1.92	0.51
1:A:181:SER:HB2	1:A:226:ILE:HD12	1.91	0.51
1:A:58:PHE:CE1	1:A:62:LEU:HD22	2.46	0.51
1:A:238:TYR:CE2	1:A:261:ILE:HD11	2.46	0.51
1:A:103:ARG:HD2	1:A:113:TYR:CE2	2.45	0.51
1:C:108:GLN:O	1:C:112:ILE:HG12	2.10	0.51
1:D:47:LEU:HD21	1:D:62:LEU:HD13	1.93	0.50
1:A:44:VAL:HG11	1:B:4:ILE:HD11	1.93	0.50
1:A:104:LEU:HD13	1:A:140:HIS:ND1	2.26	0.50
1:A:82:ILE:HD11	1:A:112:ILE:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:PHE:CZ	1:C:289:PHE:HZ	2.30	0.50
1:C:249:LYS:NZ	1:C:287:GLU:HB3	2.27	0.50
1:A:234:LEU:HD22	1:A:260:ILE:HG23	1.94	0.50
1:A:248:ASP:O	1:A:249:LYS:C	2.49	0.50
1:C:134:ILE:HD12	1:C:135:THR:N	2.28	0.49
1:A:263:ILE:HD13	1:B:263:ILE:HG13	1.94	0.49
1:D:3:LYS:O	1:D:7:VAL:HG23	2.13	0.49
1:A:152:ASP:HB3	1:A:175:MET:HE3	1.93	0.49
1:A:148:PHE:CD2	1:A:175:MET:HG2	2.47	0.49
1:D:291:PRO:HG2	1:D:296:THR:HG23	1.95	0.49
1:D:248:ASP:O	1:D:249:LYS:C	2.51	0.48
1:A:164:PRO:HG2	1:A:167:GLU:HB2	1.94	0.48
1:C:152:ASP:O	1:C:156:VAL:HG23	2.13	0.48
1:C:18:HIS:HB3	1:C:20:ILE:HD12	1.95	0.48
1:A:88:ASN:ND2	1:A:91:LEU:HD11	2.29	0.48
1:C:75:THR:HG21	1:C:108:GLN:HB3	1.95	0.48
1:C:88:ASN:O	1:C:88:ASN:OD1	2.32	0.48
1:A:197:ALA:HB1	1:A:213:TYR:CZ	2.49	0.47
1:B:251:ILE:O	1:B:255:LEU:HD22	2.13	0.47
1:A:289:PHE:CE2	1:C:251:ILE:HD11	2.49	0.47
1:A:28:SER:OG	1:A:31:VAL:HG23	2.13	0.47
1:C:79:LYS:NZ	1:C:108:GLN:HE22	2.11	0.47
1:B:88:ASN:OD1	1:B:91:LEU:HD12	2.15	0.47
1:A:277:VAL:O	1:A:281:THR:HG23	2.14	0.47
1:A:88:ASN:HD22	1:A:91:LEU:HD11	1.79	0.47
1:A:132:LYS:NZ	1:A:132:LYS:HA	2.29	0.47
1:C:124:ASN:N	1:C:124:ASN:ND2	2.63	0.46
1:D:269:LYS:CG	1:D:272:ILE:HD12	2.45	0.46
1:C:245:PHE:O	1:C:249:LYS:HA	2.15	0.46
1:A:113:TYR:HE1	1:A:117:ILE:HD11	1.79	0.46
1:B:276:LEU:HA	1:B:279:GLU:HG3	1.98	0.46
1:C:92:PHE:CE2	1:C:125:ILE:HG21	2.51	0.46
1:A:135:THR:O	1:A:139:LYS:HG2	2.15	0.46
1:B:100:GLU:HG2	1:B:113:TYR:HE1	1.80	0.46
1:C:37:ALA:O	1:C:38:ASP:HB2	2.17	0.45
1:B:205:ARG:HD2	1:B:287:GLU:OE2	2.17	0.45
1:B:177:PRO:HB3	1:B:216:GLN:HE22	1.81	0.45
1:B:100:GLU:HG2	1:B:113:TYR:CE1	2.51	0.45
1:C:263:ILE:HG13	1:D:263:ILE:HD13	1.98	0.45
1:B:197:ALA:HB1	1:B:213:TYR:CE2	2.51	0.45
1:A:82:ILE:HD11	1:A:112:ILE:CG2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:ASP:O	1:C:248:ASP:OD1	2.34	0.45
1:C:70:LYS:NZ	1:C:79:LYS:HE2	2.33	0.44
1:A:78:GLU:OE1	1:A:99:ILE:HD11	2.16	0.44
1:A:241:GLN:HG3	1:A:256:ASN:HB2	1.99	0.44
1:A:249:LYS:O	1:C:289:PHE:HA	2.17	0.44
1:C:73:ASN:HD22	1:C:73:ASN:H	1.65	0.43
1:A:155:ILE:O	1:A:158:ASN:HB2	2.18	0.43
1:A:152:ASP:HB3	1:A:175:MET:CE	2.48	0.43
1:B:234:LEU:HB3	1:B:264:PHE:CZ	2.54	0.43
1:A:103:ARG:HG3	1:A:104:LEU:N	2.34	0.43
1:B:292:PRO:HD3	1:D:251:ILE:HG21	2.01	0.43
1:B:255:LEU:HD11	1:D:255:LEU:CD2	2.48	0.43
1:A:115:GLY:O	1:A:119:ILE:HG13	2.17	0.43
1:A:245:PHE:O	1:A:249:LYS:HA	2.18	0.43
1:B:250:ASN:ND2	1:B:253:SER:HB2	2.34	0.43
1:A:108:GLN:O	1:A:112:ILE:HG13	2.19	0.43
1:C:236:ILE:HA	1:C:239:LEU:HD12	2.01	0.43
1:C:153:CYS:HB2	1:C:189:THR:HG22	2.00	0.43
1:B:8:LEU:HA	1:B:8:LEU:HD23	1.85	0.42
1:A:108:GLN:HG2	1:B:55:GLY:CA	2.49	0.42
1:A:138:LEU:HD21	1:A:159:LEU:HD21	2.02	0.42
1:B:197:ALA:HB1	1:B:213:TYR:CZ	2.54	0.42
1:C:278:GLU:O	1:C:282:LYS:HG3	2.18	0.42
1:D:298:TYR:O	1:D:302:TYR:CD1	2.73	0.42
1:D:241:GLN:NE2	1:D:256:ASN:HD22	2.18	0.42
1:C:238:TYR:CE2	1:C:261:ILE:HD11	2.55	0.42
1:A:85:ILE:HD13	1:A:116:TYR:HE1	1.85	0.42
1:B:58:PHE:CE1	1:B:62:LEU:HD11	2.55	0.42
1:A:214:ILE:O	1:A:218:GLU:HG2	2.19	0.42
1:B:15:LEU:HB3	1:B:17:TYR:CE1	2.55	0.42
1:A:89:PRO:HB3	1:A:123:TYR:CD2	2.54	0.42
1:D:58:PHE:CE1	1:D:62:LEU:HD22	2.55	0.42
1:D:234:LEU:HD21	1:D:263:ILE:CG2	2.50	0.41
1:D:35:VAL:HG22	1:D:40:ARG:HH21	1.85	0.41
1:D:204:ASN:ND2	1:D:204:ASN:N	2.67	0.41
1:D:26:ILE:HD11	1:D:53:ARG:NH1	2.36	0.41
1:A:148:PHE:CD1	1:A:148:PHE:N	2.88	0.41
1:A:12:ARG:HG2	1:A:17:TYR:HB2	2.01	0.41
1:B:291:PRO:HG2	1:B:296:THR:HG23	2.02	0.41
1:C:248:ASP:O	1:C:249:LYS:C	2.59	0.41
1:C:234:LEU:HD22	1:C:260:ILE:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:LYS:O	1:B:297:MET:HB2	2.20	0.41
1:D:299:TYR:CD1	1:D:299:TYR:C	2.94	0.41
1:B:100:GLU:N	1:B:101:PRO:CD	2.83	0.41
1:D:173:LYS:HB2	1:D:174:PRO:HD3	2.02	0.41
1:A:178:ILE:O	1:A:223:ILE:HD11	2.20	0.41
1:C:187:ASP:O	1:C:190:ILE:HG12	2.21	0.41
1:A:289:PHE:CZ	1:C:289:PHE:CZ	3.08	0.41
1:B:177:PRO:HA	1:B:216:GLN:HE22	1.84	0.41
1:D:245:PHE:HD1	1:D:250:ASN:O	2.04	0.41
1:B:245:PHE:O	1:B:249:LYS:HA	2.21	0.41
1:B:130:PHE:CZ	1:B:134:ILE:HD12	2.56	0.40
1:A:152:ASP:CB	1:A:175:MET:CE	2.99	0.40
1:D:245:PHE:O	1:D:249:LYS:HA	2.22	0.40
1:B:184:LYS:HG3	1:B:184:LYS:HZ2	1.82	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	300/317 (95%)	283 (94%)	15 (5%)	2 (1%)	26	70
1	B	301/317 (95%)	287 (95%)	12 (4%)	2 (1%)	26	70
1	C	300/317 (95%)	285 (95%)	13 (4%)	2 (1%)	26	70
1	D	300/317 (95%)	287 (96%)	11 (4%)	2 (1%)	26	70
All	All	1201/1268 (95%)	1142 (95%)	51 (4%)	8 (1%)	26	70

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	249	LYS

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Mol	Chain	Res	Type
1	D	249	LYS
1	B	249	LYS
1	C	249	LYS
1	C	92	PHE
1	A	297	MET
1	D	92	PHE
1	B	303	VAL

### 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	285/299 (95%)	247 (87%)	38 (13%)	5	21
1	B	285/299 (95%)	249 (87%)	36 (13%)	5	24
1	C	285/299 (95%)	245 (86%)	40 (14%)	4	19
1	D	285/299 (95%)	251 (88%)	34 (12%)	6	26
All	All	1140/1196 (95%)	992 (87%)	148 (13%)	5	22

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLN
1	A	15	LEU
1	A	30	SER
1	A	34	LYS
1	A	62	LEU
1	A	63	ASN
1	A	83	SER
1	A	93	ASP
1	A	94	LYS
1	A	98	ARG
1	A	112	ILE
1	A	119	ILE
1	A	121	HIS
1	A	127	VAL

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Mol	Chain	Res	Type
1	A	129	THR
1	A	132	LYS
1	A	134	ILE
1	A	136	SER
1	A	157	SER
1	A	170	SER
1	A	173	LYS
1	A	194	LEU
1	A	204	ASN
1	A	205	ARG
1	A	208	LYS
1	A	211	GLN
1	A	237	ASN
1	A	238	TYR
1	A	241	GLN
1	A	251	ILE
1	A	255	LEU
1	A	263	ILE
1	A	280	LEU
1	A	286	LYS
1	A	289	PHE
1	A	295	VAL
1	A	296	THR
1	A	297	MET
1	B	13	GLN
1	B	15	LEU
1	B	21	ASP
1	B	22	LEU
1	B	30	SER
1	B	34	LYS
1	B	71	SER
1	B	83	SER
1	B	107	LEU
1	B	121	HIS
1	B	127	VAL
1	B	129	THR
1	B	134	ILE
1	B	136	SER
1	B	144	LYS
1	B	157	SER
1	B	161	ASN
1	B	169	SER

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Mol	Chain	Res	Type
1	B	170	SER
1	B	179	VAL
1	B	184	LYS
1	B	194	LEU
1	B	195	LYS
1	B	208	LYS
1	B	218	GLU
1	B	238	TYR
1	B	249	LYS
1	B	250	ASN
1	B	253	SER
1	B	255	LEU
1	B	274	ARG
1	B	275	SER
1	B	280	LEU
1	B	289	PHE
1	B	293	LYS
1	B	296	THR
1	C	2	PHE
1	C	13	GLN
1	C	15	LEU
1	C	20	ILE
1	C	40	ARG
1	C	56	VAL
1	C	62	LEU
1	C	73	ASN
1	C	75	THR
1	C	81	LEU
1	C	93	ASP
1	C	97	GLN
1	C	112	ILE
1	C	124	ASN
1	C	127	VAL
1	C	136	SER
1	C	144	LYS
1	C	147	THR
1	C	181	SER
1	C	194	LEU
1	C	205	ARG
1	C	227	SER
1	C	237	ASN
1	C	238	TYR

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Mol	Chain	Res	Type
1	C	249	LYS
1	C	250	ASN
1	C	255	LEU
1	C	259	ASN
1	C	260	ILE
1	C	269	LYS
1	C	270	GLU
1	C	280	LEU
1	C	281	THR
1	C	289	PHE
1	C	290	THR
1	C	294	GLU
1	C	295	VAL
1	C	296	THR
1	C	297	MET
1	C	301	ASN
1	D	2	PHE
1	D	6	SER
1	D	13	GLN
1	D	15	LEU
1	D	56	VAL
1	D	62	LEU
1	D	74	GLU
1	D	88	ASN
1	D	98	ARG
1	D	102	LYS
1	D	112	ILE
1	D	121	HIS
1	D	127	VAL
1	D	129	THR
1	D	134	ILE
1	D	135	THR
1	D	179	VAL
1	D	194	LEU
1	D	195	LYS
1	D	204	ASN
1	D	238	TYR
1	D	249	LYS
1	D	250	ASN
1	D	255	LEU
1	D	259	ASN
1	D	260	ILE

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Mol	Chain	Res	Type
1	D	284	SER
1	D	289	PHE
1	D	290	THR
1	D	294	GLU
1	D	295	VAL
1	D	296	THR
1	D	297	MET
1	D	303	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	161	ASN
1	A	196	ASN
1	A	204	ASN
1	A	216	GLN
1	A	250	ASN
1	A	301	ASN
1	B	63	ASN
1	B	108	GLN
1	B	211	GLN
1	B	216	GLN
1	B	244	GLN
1	B	250	ASN
1	B	256	ASN
1	B	262	ASN
1	C	13	GLN
1	C	19	GLN
1	C	108	GLN
1	C	124	ASN
1	C	216	GLN
1	C	262	ASN
1	C	301	ASN
1	D	10	GLN
1	D	63	ASN
1	D	108	GLN
1	D	122	HIS
1	D	158	ASN
1	D	196	ASN
1	D	204	ASN
1	D	211	GLN

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Mol	Chain	Res	Type
1	D	216	GLN
1	D	225	ASN
1	D	241	GLN
1	D	244	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	302/317 (95%)	-0.16	5 (1%) 73 45	54, 75, 108, 119	0
1	B	303/317 (95%)	-0.25	0 100 100	54, 75, 106, 114	0
1	C	302/317 (95%)	-0.11	7 (2%) 64 33	53, 75, 106, 114	0
1	D	302/317 (95%)	-0.10	6 (1%) 68 39	53, 75, 108, 114	0
All	All	1209/1268 (95%)	-0.16	18 (1%) 76 49	53, 75, 107, 119	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	91	LEU	3.4
1	C	125	ILE	3.3
1	C	88	ASN	3.2
1	D	301	ASN	2.9
1	C	94	LYS	2.8
1	D	90	ASP	2.7
1	A	97	GLN	2.7
1	C	84	LYS	2.7
1	A	86	PHE	2.7
1	A	84	LYS	2.6
1	D	84	LYS	2.5
1	C	126	GLU	2.4
1	D	91	LEU	2.3
1	D	70	LYS	2.3
1	A	302	TYR	2.2
1	D	71	SER	2.2
1	C	90	ASP	2.2
1	A	94	LYS	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](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.