



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:26 PM GMT

PDB ID : 4IC6  
Title : Crystal structure of Deg8  
Authors : Gong, W.; Sun, W.; Fan, H.; Gao, F.; Liu, L.  
Deposited on : 2012-12-10  
Resolution : 2.00 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

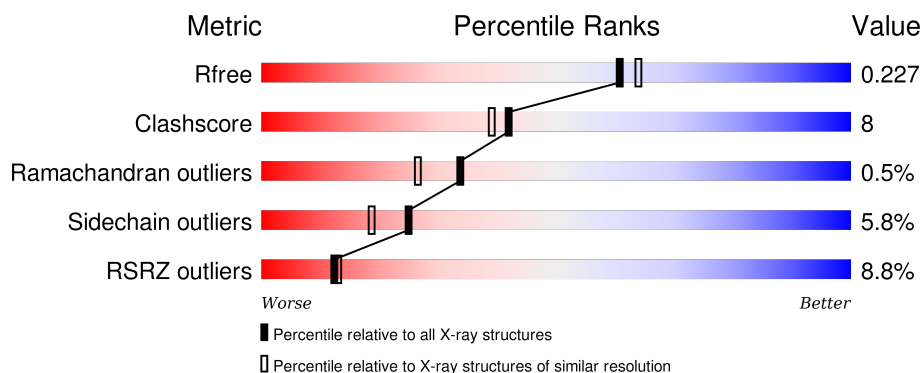
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	368	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>14%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	368	<div> <div>11%</div> <div> <div></div> <div>73%</div> <div>17%</div> <div>•</div> <div>8%</div> </div> </div>
1	C	368	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>14%</div> <div>•</div> <div>9%</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7728 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 Protease Do-like 8, chloroplastic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	0	0
			2445	1559	424	460	2			
1	B	339	Total	C	N	O	S	0	0	0
			2352	1500	410	440	2			
1	C	335	Total	C	N	O	S	0	2	0
			2447	1554	432	459	2			

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	MET	-	EXPRESSION TAG	UNP Q9LU10
A	90	GLY	-	EXPRESSION TAG	UNP Q9LU10
A	292	ALA	SER	ENGINEERED MUTATION	UNP Q9LU10
A	449	LEU	-	EXPRESSION TAG	UNP Q9LU10
A	450	GLU	-	EXPRESSION TAG	UNP Q9LU10
A	451	HIS	-	EXPRESSION TAG	UNP Q9LU10
A	452	HIS	-	EXPRESSION TAG	UNP Q9LU10
A	453	HIS	-	EXPRESSION TAG	UNP Q9LU10
A	454	HIS	-	EXPRESSION TAG	UNP Q9LU10
A	455	HIS	-	EXPRESSION TAG	UNP Q9LU10
A	456	HIS	-	EXPRESSION TAG	UNP Q9LU10
B	89	MET	-	EXPRESSION TAG	UNP Q9LU10
B	90	GLY	-	EXPRESSION TAG	UNP Q9LU10
B	292	ALA	SER	ENGINEERED MUTATION	UNP Q9LU10
B	449	LEU	-	EXPRESSION TAG	UNP Q9LU10
B	450	GLU	-	EXPRESSION TAG	UNP Q9LU10
B	451	HIS	-	EXPRESSION TAG	UNP Q9LU10
B	452	HIS	-	EXPRESSION TAG	UNP Q9LU10
B	453	HIS	-	EXPRESSION TAG	UNP Q9LU10
B	454	HIS	-	EXPRESSION TAG	UNP Q9LU10
B	455	HIS	-	EXPRESSION TAG	UNP Q9LU10
B	456	HIS	-	EXPRESSION TAG	UNP Q9LU10
C	89	MET	-	EXPRESSION TAG	UNP Q9LU10

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Chain	Residue	Modelled	Actual	Comment	Reference
C	90	GLY	-	EXPRESSION TAG	UNP Q9LU10
C	292	ALA	SER	ENGINEERED MUTATION	UNP Q9LU10
C	449	LEU	-	EXPRESSION TAG	UNP Q9LU10
C	450	GLU	-	EXPRESSION TAG	UNP Q9LU10
C	451	HIS	-	EXPRESSION TAG	UNP Q9LU10
C	452	HIS	-	EXPRESSION TAG	UNP Q9LU10
C	453	HIS	-	EXPRESSION TAG	UNP Q9LU10
C	454	HIS	-	EXPRESSION TAG	UNP Q9LU10
C	455	HIS	-	EXPRESSION TAG	UNP Q9LU10
C	456	HIS	-	EXPRESSION TAG	UNP Q9LU10

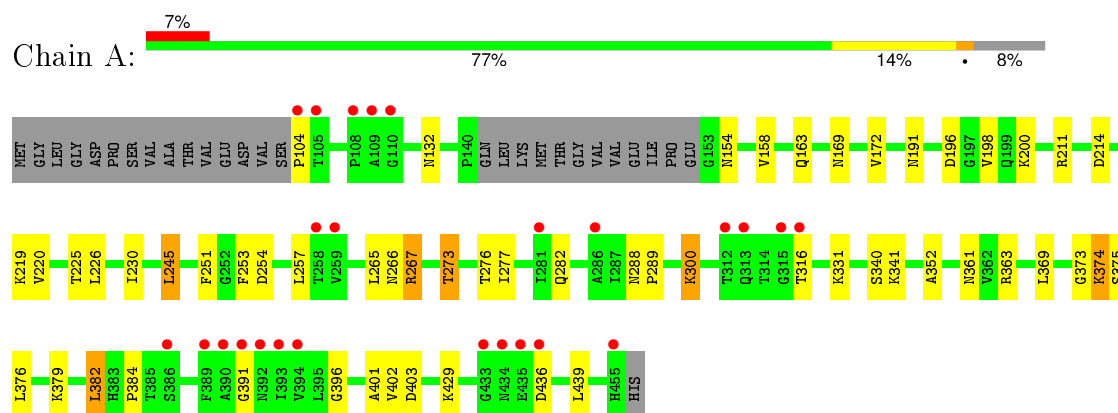
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	165	Total O 165 165	0	0
2	B	112	Total O 112 112	0	0
2	C	207	Total O 207 207	0	0

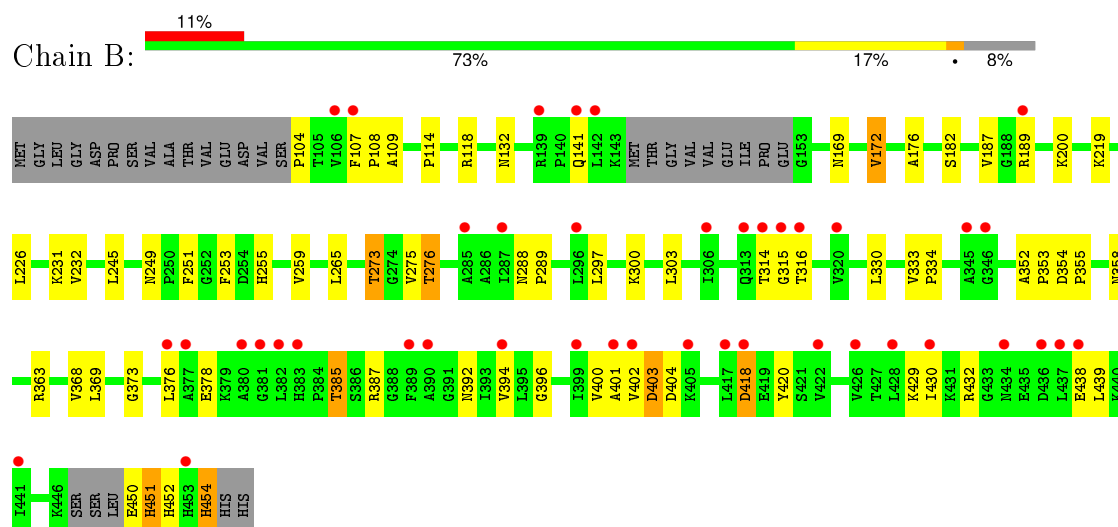
### 3 Residue-property plots

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.

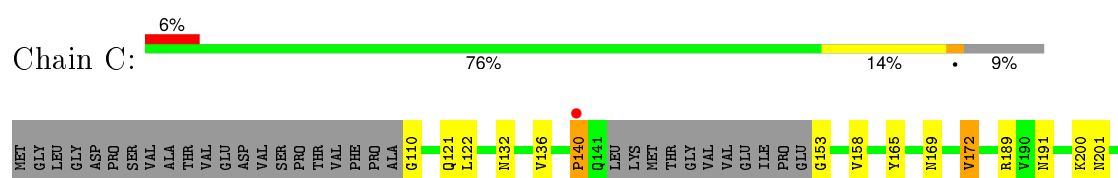
- Molecule 1: Protease Do-like 8, chloroplastic

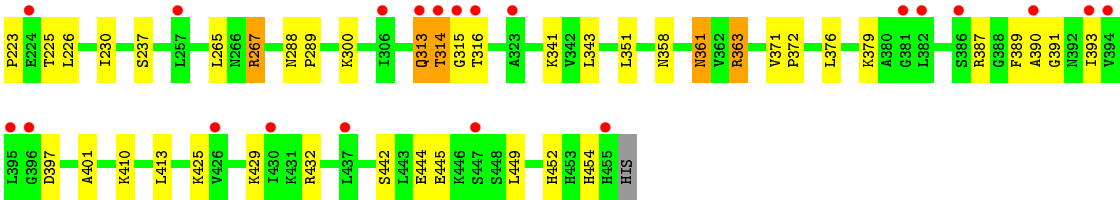


- Molecule 1: Protease Do-like 8, chloroplastic



- Molecule 1: Protease Do-like 8, chloroplastic





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	129.47Å 124.17Å 93.27Å 90.00° 132.41° 90.00°	Depositor
Resolution (Å)	29.59 – 2.00 37.24 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.3 (29.59-2.00) 92.2 (37.24-1.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.27 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, $R_{free}$	0.198 , 0.235 0.193 , 0.227	Depositor DCC
$R_{free}$ test set	3442 reflections (5.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	36.5	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 53.1	EDS
Estimated twinning fraction	0.008 for k,h,-1/2*k-h-1/2*k-l 0.000 for -k,-h,-1/2*h+1/2*k-l 0.005 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 73212 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7728	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% 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 [i](#)

### 5.1 Standard geometry [i](#)

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	0.37	0/2486	0.59	2/3386 (0.1%)
1	B	0.33	0/2389	0.53	1/3267 (0.0%)
1	C	0.40	0/2492	0.59	1/3388 (0.0%)
All	All	0.37	0/7367	0.57	4/10041 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	PRO	N-CA-CB	6.15	110.68	103.30
1	C	140	PRO	N-CA-CB	6.08	110.59	103.30
1	A	104	PRO	N-CA-CB	5.80	110.26	103.30
1	A	436	ASP	CB-CG-OD2	5.17	122.95	118.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2445	0	2455	41	0
1	B	2352	0	2284	43	0
1	C	2447	0	2470	38	0
2	A	165	0	0	12	1
2	B	112	0	0	7	0
2	C	207	0	0	7	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7728	0	7209	121	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 8.

All (121) 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:267:ARG:HH11	1:C:267:ARG:HG2	1.19	1.07
1:C:316:THR:O	2:C:686:HOH:O	1.83	0.96
1:A:267:ARG:HD2	2:A:621:HOH:O	1.67	0.94
1:A:316:THR:O	2:A:594:HOH:O	1.89	0.90
1:A:267:ARG:HG2	1:A:267:ARG:HH11	1.38	0.85
1:A:266:ASN:HB3	2:A:571:HOH:O	1.76	0.85
1:A:211:ARG:HE	1:A:273:THR:HG23	1.41	0.85
1:C:110:GLY:N	2:C:700:HOH:O	2.14	0.81
1:A:391:GLY:O	2:A:638:HOH:O	1.98	0.80
1:C:452:HIS:O	2:C:541:HOH:O	1.99	0.79
1:B:385:THR:HG22	1:B:396:GLY:H	1.47	0.77
1:C:267:ARG:NH1	1:C:267:ARG:HG2	1.98	0.77
1:C:267:ARG:HH11	1:C:267:ARG:CG	1.98	0.74
1:A:361:ASN:OD1	1:A:363:ARG:NH2	2.22	0.71
1:B:276:THR:HG22	1:B:452:HIS:ND1	2.05	0.71
1:A:196:ASP:OD2	1:A:200:LYS:NZ	2.23	0.71
1:A:300:LYS:HD3	2:A:602:HOH:O	1.90	0.70
1:B:438:GLU:O	2:B:609:HOH:O	2.11	0.68
1:A:282:GLN:OE1	2:A:621:HOH:O	2.13	0.67
1:A:391:GLY:C	2:A:638:HOH:O	2.34	0.64
1:B:378:GLU:OE2	2:B:598:HOH:O	2.15	0.64
1:A:267:ARG:CG	1:A:267:ARG:HH11	2.11	0.64
1:C:351:LEU:HD11	1:C:413:LEU:HD23	1.79	0.64
1:A:401:ALA:HB3	1:A:429:LYS:HB2	1.79	0.64
1:A:340:SER:O	2:A:580:HOH:O	2.15	0.63
1:C:358:ASN:OD1	1:C:363:ARG:NH1	2.32	0.62
1:B:245:LEU:HD22	1:B:259:VAL:HG22	1.81	0.62
1:A:300:LYS:NZ	2:A:602:HOH:O	1.88	0.61
1:B:273:THR:HG22	1:B:275:VAL:H	1.66	0.60
1:A:266:ASN:HB3	2:A:592:HOH:O	2.02	0.59
1:B:401:ALA:HB1	1:B:404:ASP:HA	1.85	0.59
1:B:451:HIS:N	1:B:451:HIS:ND1	2.50	0.59
1:A:267:ARG:HG2	1:A:267:ARG:NH1	2.13	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:GLY:HA2	2:B:598:HOH:O	2.02	0.59
1:B:403:ASP:OD2	1:B:420:TYR:OH	2.20	0.59
1:B:358:ASN:O	1:B:363:ARG:NH2	2.37	0.58
1:A:402:VAL:O	1:A:403:ASP:HB2	2.05	0.55
1:B:385:THR:HG22	1:B:396:GLY:N	2.20	0.54
1:B:450:GLU:N	2:B:608:HOH:O	2.40	0.54
2:B:547:HOH:O	1:C:300[A]:LYS:HD3	2.07	0.54
1:B:369:LEU:HA	1:B:385:THR:HG23	1.89	0.54
1:C:153:GLY:N	2:C:667:HOH:O	2.41	0.54
1:A:363:ARG:HH21	1:A:363:ARG:HG3	1.71	0.53
1:B:418:ASP:OD2	2:B:603:HOH:O	2.17	0.53
1:C:389:PHE:C	1:C:391:GLY:H	2.12	0.53
1:B:109:ALA:HB2	1:C:237[A]:SER:OG	2.07	0.53
1:C:158:VAL:CG2	1:C:230:ILE:HB	2.38	0.53
1:B:251:PHE:HB2	1:B:253:PHE:CE2	2.44	0.52
1:A:363:ARG:CG	1:A:363:ARG:HH21	2.23	0.52
1:A:288:ASN:HB2	1:A:289:PRO:CD	2.41	0.51
1:C:351:LEU:CD1	1:C:413:LEU:HD23	2.41	0.51
1:B:169:ASN:HB2	1:B:172:VAL:HG13	1.93	0.51
1:B:368:VAL:O	1:B:385:THR:HG23	2.11	0.50
1:A:288:ASN:HB2	1:A:289:PRO:HD2	1.93	0.50
1:C:361:ASN:HD22	1:C:363:ARG:HE	1.60	0.50
1:B:132:ASN:HB2	1:B:249:ASN:O	2.11	0.50
1:C:410:LYS:NZ	2:C:698:HOH:O	2.45	0.50
1:A:331:LYS:HD2	2:A:642:HOH:O	2.13	0.49
1:C:267:ARG:NH1	1:C:267:ARG:CG	2.63	0.49
1:A:169:ASN:HB2	1:A:172:VAL:HG13	1.94	0.49
1:B:232:VAL:HG11	1:B:330:LEU:HD21	1.94	0.49
1:C:223:PRO:HB2	1:C:225:THR:HG22	1.95	0.48
1:A:384:PRO:O	1:A:396:GLY:HA2	2.14	0.48
1:A:163:GLN:O	1:A:219:LYS:HE3	2.14	0.48
1:C:341:LYS:HE3	1:C:343:LEU:HD21	1.96	0.47
1:C:189:ARG:NH1	1:C:201:ASN:OD1	2.45	0.47
1:A:373:GLY:O	1:A:374:LYS:HG2	2.14	0.47
1:B:249:ASN:HB2	1:B:255:HIS:CD2	2.50	0.47
1:C:191:ASN:HD21	1:C:201:ASN:HD22	1.63	0.46
1:B:353:PRO:HB2	1:B:355:PRO:HD2	1.97	0.46
1:A:211:ARG:NE	1:A:273:THR:HG23	2.21	0.45
1:B:354:ASP:N	1:B:355:PRO:CD	2.79	0.45
1:B:400:VAL:HG22	1:B:429:LYS:O	2.16	0.45
1:A:341:LYS:HE2	2:A:632:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:ARG:HA	1:B:189:ARG:HD3	1.83	0.45
1:C:371:VAL:HA	1:C:372:PRO:HD3	1.86	0.45
1:A:374:LYS:HB3	1:A:374:LYS:HE3	1.69	0.44
1:C:401:ALA:HB3	1:C:429:LYS:CB	2.47	0.44
1:C:169:ASN:HB2	1:C:172:VAL:HG13	1.99	0.44
1:B:288:ASN:HB2	1:B:289:PRO:HD2	1.99	0.44
1:B:385:THR:HA	1:B:394:VAL:O	2.18	0.44
1:C:136:VAL:O	1:C:136:VAL:HG12	2.17	0.44
1:B:387:ARG:HA	1:B:392:ASN:O	2.18	0.44
1:B:300:LYS:HB2	1:B:300:LYS:HE2	1.77	0.44
1:A:267:ARG:CG	1:A:267:ARG:NH1	2.73	0.44
1:C:314:THR:HG23	1:C:315:GLY:H	1.83	0.44
1:B:454:HIS:N	1:B:454:HIS:ND1	2.66	0.44
1:C:358:ASN:O	1:C:363:ARG:NH2	2.49	0.44
1:A:245:LEU:HB3	1:A:257:LEU:HD11	2.00	0.44
1:B:288:ASN:HB2	1:B:289:PRO:CD	2.48	0.44
1:C:191:ASN:ND2	1:C:201:ASN:HD22	2.15	0.43
1:C:132:ASN:HB3	1:C:191:ASN:HB2	2.01	0.43
1:C:449:LEU:HA	1:C:449:LEU:HD23	1.81	0.43
1:B:314:THR:OG1	1:B:315:GLY:N	2.51	0.43
1:B:107:PHE:HA	1:B:108:PRO:HD3	1.81	0.43
1:C:121:GLN:HG3	2:C:565:HOH:O	2.18	0.43
1:B:432:ARG:HA	2:B:534:HOH:O	2.18	0.42
1:A:132:ASN:HB3	1:A:191:ASN:HB2	2.01	0.42
1:C:361:ASN:ND2	1:C:363:ARG:HE	2.18	0.42
1:C:397:ASP:OD2	1:C:432:ARG:NH1	2.52	0.42
1:A:251:PHE:HB2	1:A:253:PHE:CE2	2.53	0.42
1:C:288:ASN:HB2	1:C:289:PRO:CD	2.50	0.42
1:B:368:VAL:O	1:B:385:THR:CG2	2.67	0.42
1:A:363:ARG:CG	1:A:363:ARG:NH2	2.82	0.42
1:B:352:ALA:HB2	1:B:369:LEU:HG	2.02	0.42
1:A:382:LEU:HD12	1:A:439:LEU:HD12	2.01	0.42
1:B:114:PRO:O	1:B:118:ARG:HG3	2.21	0.41
1:B:333:VAL:HB	1:B:334:PRO:HD3	2.03	0.41
1:A:352:ALA:HB2	1:A:369:LEU:HD21	2.01	0.41
1:A:375:SER:O	1:A:379:LYS:HG3	2.21	0.41
1:B:297:LEU:HD23	1:B:303:LEU:HA	2.02	0.41
1:C:313:GLN:HG2	1:C:454:HIS:CD2	2.56	0.41
1:C:425:LYS:HE3	1:C:442:SER:OG	2.20	0.41
1:A:254:ASP:OD1	1:A:254:ASP:C	2.59	0.41
1:B:439:LEU:HA	1:B:439:LEU:HD23	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:158:VAL:HG13	1:A:230:ILE:HB	2.03	0.40
1:B:176:ALA:HB1	1:B:187:VAL:CG2	2.51	0.40
1:C:165:TYR:OH	2:C:707:HOH:O	2.21	0.40
1:C:444:GLU:HG3	1:C:445:GLU:O	2.22	0.40
1:B:402:VAL:O	1:B:404:ASP:N	2.54	0.40
1:A:214:ASP:HB2	1:A:277:ILE:HD11	2.04	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)
2:A:661:HOH:O	2:C:695:HOH:O[4_544]	1.64	0.56
2:C:694:HOH:O	2:C:694:HOH:O[2_553]	2.18	0.02

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	336/368 (91%)	319 (95%)	16 (5%)	1 (0%)	46	41
1	B	333/368 (90%)	320 (96%)	11 (3%)	2 (1%)	30	22
1	C	333/368 (90%)	320 (96%)	11 (3%)	2 (1%)	30	22
All	All	1002/1104 (91%)	959 (96%)	38 (4%)	5 (0%)	34	26

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	403	ASP
1	C	390	ALA
1	B	418	ASP
1	C	140	PRO
1	A	154	ASN

### 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	255/301 (85%)	242 (95%)	13 (5%)	29	23
1	B	229/301 (76%)	213 (93%)	16 (7%)	19	12
1	C	258/301 (86%)	244 (95%)	14 (5%)	27	21
All	All	742/903 (82%)	699 (94%)	43 (6%)	25	19

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	VAL
1	A	220	VAL
1	A	225	THR
1	A	226	LEU
1	A	245	LEU
1	A	265	LEU
1	A	267	ARG
1	A	273	THR
1	A	276	THR
1	A	300	LYS
1	A	374	LYS
1	A	376	LEU
1	A	382	LEU
1	B	141	GLN
1	B	172	VAL
1	B	182	SER
1	B	200	LYS
1	B	219	LYS
1	B	226	LEU
1	B	231	LYS
1	B	265	LEU
1	B	273	THR
1	B	276	THR
1	B	316	THR
1	B	376	LEU
1	B	385	THR

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Mol	Chain	Res	Type
1	B	430	ILE
1	B	451	HIS
1	B	454	HIS
1	C	122	LEU
1	C	172	VAL
1	C	200	LYS
1	C	226	LEU
1	C	265	LEU
1	C	267	ARG
1	C	313	GLN
1	C	314	THR
1	C	361	ASN
1	C	363	ARG
1	C	376	LEU
1	C	379	LYS
1	C	387	ARG
1	C	393	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	132	ASN
1	C	191	ASN
1	C	361	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	340/368 (92%)	0.23	25 (7%) 17 18	25, 48, 82, 97	1 (0%)
1	B	339/368 (92%)	0.54	42 (12%) 5 6	27, 57, 93, 107	0
1	C	335/368 (91%)	0.24	22 (6%) 22 22	23, 40, 89, 96	0
All	All	1014/1104 (91%)	0.34	89 (8%) 12 13	23, 49, 89, 107	1 (0%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	417	LEU	6.9
1	A	394	VAL	5.5
1	B	313	GLN	5.3
1	A	434	ASN	5.2
1	B	315	GLY	5.0
1	B	380	ALA	4.6
1	A	315	GLY	4.4
1	C	437	LEU	4.3
1	C	394	VAL	4.2
1	A	436	ASP	4.1
1	B	428	LEU	4.1
1	B	422	VAL	4.1
1	B	437	LEU	4.1
1	B	390	ALA	4.0
1	B	346	GLY	3.8
1	A	393	ILE	3.8
1	B	381	GLY	3.7
1	A	386	SER	3.7
1	B	434	ASN	3.7
1	B	345	ALA	3.7
1	B	106	VAL	3.7
1	B	438	GLU	3.6
1	C	455	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	441	ILE	3.6
1	B	453	HIS	3.6
1	B	402	VAL	3.5
1	A	390	ALA	3.5
1	A	433	GLY	3.5
1	C	316	THR	3.4
1	C	393	ILE	3.4
1	B	426	VAL	3.4
1	C	426	VAL	3.3
1	A	455	HIS	3.1
1	A	108	PRO	3.0
1	C	386	SER	2.9
1	C	447	SER	2.9
1	A	389	PHE	2.9
1	B	401	ALA	2.9
1	B	107	PHE	2.8
1	B	377	ALA	2.8
1	C	396	GLY	2.7
1	C	381	GLY	2.7
1	C	382	LEU	2.7
1	A	104	PRO	2.7
1	B	389	PHE	2.7
1	B	383	HIS	2.6
1	A	435	GLU	2.6
1	A	316	THR	2.6
1	A	259	VAL	2.5
1	A	391	GLY	2.5
1	B	382	LEU	2.5
1	B	141	GLN	2.5
1	B	376	LEU	2.5
1	B	399	ILE	2.5
1	C	430	ILE	2.5
1	B	394	VAL	2.4
1	B	142	LEU	2.4
1	B	316	THR	2.4
1	A	110	GLY	2.4
1	B	436	ASP	2.4
1	C	315	GLY	2.4
1	C	140	PRO	2.4
1	C	395	LEU	2.4
1	B	287	ILE	2.3
1	A	286	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	313	GLN	2.3
1	B	139	ARG	2.2
1	B	314	THR	2.2
1	C	314	THR	2.2
1	B	306	ILE	2.2
1	A	258	THR	2.2
1	C	224	GLU	2.2
1	A	281	ILE	2.2
1	A	392	ASN	2.2
1	B	296	LEU	2.1
1	A	312	THR	2.1
1	C	323	ALA	2.1
1	C	390	ALA	2.1
1	A	105	THR	2.1
1	C	313	GLN	2.1
1	B	405	LYS	2.1
1	B	189	ARG	2.1
1	B	320	VAL	2.1
1	A	109	ALA	2.0
1	B	285	ALA	2.0
1	C	306	ILE	2.0
1	C	257	LEU	2.0
1	B	418	ASP	2.0
1	B	430	ILE	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.