



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:30 AM GMT

PDB ID : 3M6D  
Title : The crystal structure of the d307a mutant of glycoside Hydrolase (family 31) from ruminococcus obeum atcc 29174  
Authors : Tan, K.; Tesar, C.; Freeman, L.; Babnigg, G.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)  
Deposited on : 2010-03-15  
Resolution : 2.90 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

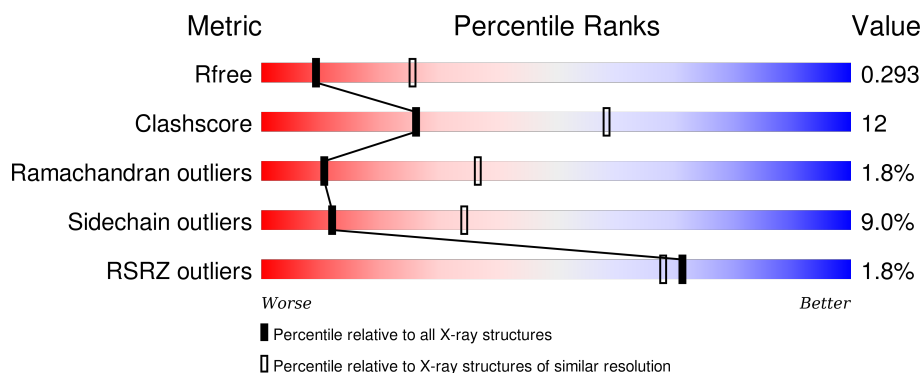
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

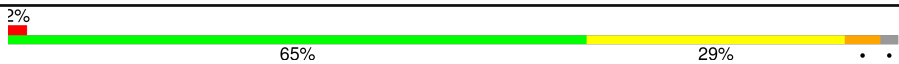

The reported resolution of this entry is 2.90 Å.

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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	666	
1	B	666	

## 2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 10735 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 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	655	Total	C	N	O	S	0	0	0
			5357	3442	878	1003	34			
1	B	658	Total	C	N	O	S	0	0	0
			5378	3453	881	1009	35			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP A5ZY13
A	-1	ASN	-	EXPRESSION TAG	UNP A5ZY13
A	0	ALA	-	EXPRESSION TAG	UNP A5ZY13
A	307	ALA	ASP	ENGINEERED	UNP A5ZY13
B	-2	SER	-	EXPRESSION TAG	UNP A5ZY13
B	-1	ASN	-	EXPRESSION TAG	UNP A5ZY13
B	0	ALA	-	EXPRESSION TAG	UNP A5ZY13
B	307	ALA	ASP	ENGINEERED	UNP A5ZY13

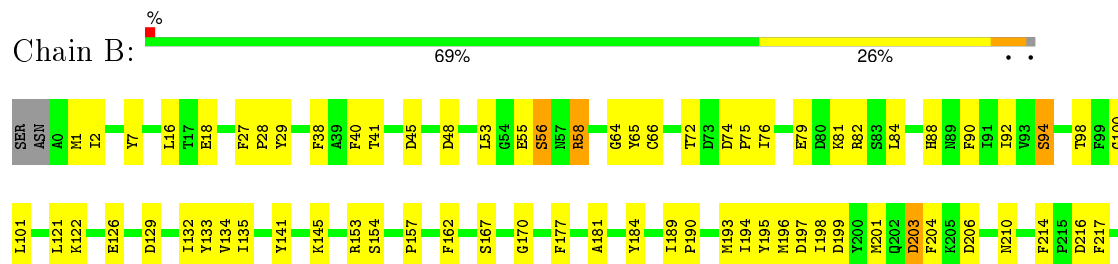
### 3 Residue-property plots [i](#)

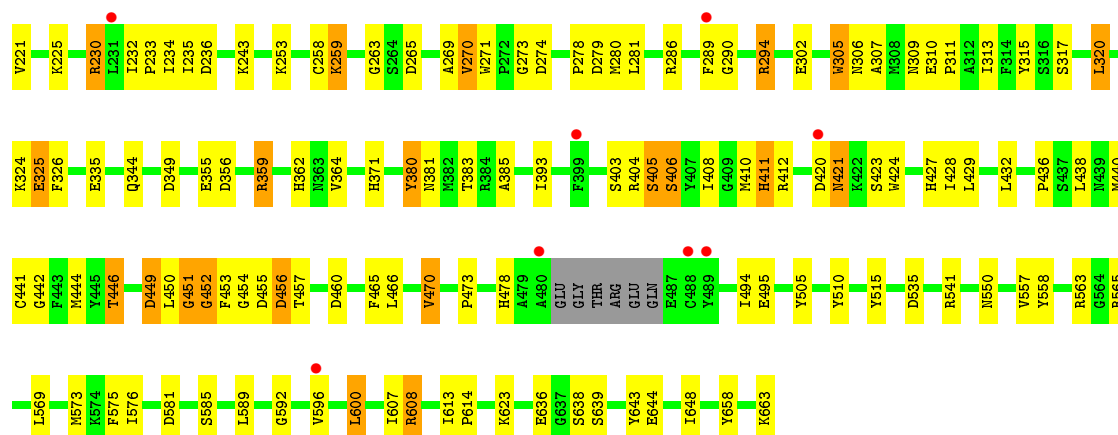
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: Uncharacterized protein



#### • Molecule 1: Uncharacterized protein





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.86 Å 124.03 Å 87.83 Å 90.00° 108.15° 90.00°	Depositor
Resolution (Å)	49.78 – 2.90 49.78 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.78-2.90) 98.8 (49.78-2.90)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.86 (at 2.91 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.218 , 0.297 0.208 , 0.293	Depositor DCC
$R_{free}$ test set	1481 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	54.9	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.22 , 5.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 29072 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10735	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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	0.67	0/5498	0.72	0/7412
1	B	0.66	0/5519	0.73	0/7441
All	All	0.66	0/11017	0.73	0/14853

There are no bond length outliers.

There are no bond angle outliers.

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	5357	0	5136	151	0
1	B	5378	0	5149	114	0
All	All	10735	0	10285	259	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 12.

All (259) 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:B:450:LEU:O	1:B:451:GLY:O	1.64	1.16
1:A:514:GLU:OE2	1:A:517:LYS:HE3	1.59	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:VAL:HG12	1:A:271:TRP:H	1.29	0.94
1:B:429:LEU:HD22	1:B:558:TYR:CE1	2.11	0.86
1:B:230:ARG:HG3	1:B:230:ARG:HH11	1.40	0.85
1:A:420:ASP:O	1:A:451:GLY:HA3	1.76	0.85
1:B:270:VAL:HG12	1:B:271:TRP:H	1.39	0.85
1:A:75:PRO:O	1:A:420:ASP:HB2	1.78	0.84
1:B:455:ASP:C	1:B:457:THR:H	1.81	0.84
1:A:514:GLU:OE2	1:A:514:GLU:HA	1.84	0.77
1:B:234:ILE:HD11	1:B:307:ALA:CB	2.16	0.76
1:A:491:PHE:O	1:A:497:PHE:HE2	1.70	0.74
1:A:16:LEU:HD12	1:A:16:LEU:H	1.54	0.73
1:A:76:ILE:HG23	1:A:422:LYS:HZ2	1.54	0.71
1:A:510:TYR:CE1	1:A:514:GLU:HG2	2.26	0.70
1:A:362:HIS:NE2	1:A:371:HIS:HD2	1.89	0.70
1:A:459:ARG:HD2	1:A:492:GLU:HG3	1.74	0.70
1:A:436:PRO:HG3	1:A:546:LEU:HD22	1.76	0.68
1:A:296:LEU:CD1	1:A:304:PHE:HE1	2.08	0.67
1:B:2:ILE:HG23	1:B:135:ILE:HG12	1.75	0.67
1:A:296:LEU:HA	1:A:299:GLN:HG3	1.78	0.66
1:B:455:ASP:C	1:B:457:THR:N	2.46	0.65
1:A:545:GLN:NE2	1:A:553:MET:CE	2.58	0.65
1:B:575:PHE:HB2	1:B:589:LEU:HD12	1.78	0.65
1:B:270:VAL:HG12	1:B:271:TRP:N	2.12	0.65
1:A:447:GLY:HA3	1:A:474:LEU:HB3	1.78	0.65
1:B:16:LEU:HD22	1:B:133:TYR:CE1	2.32	0.65
1:B:201:MET:HB2	1:B:204:PHE:HA	1.78	0.65
1:B:455:ASP:O	1:B:457:THR:N	2.30	0.64
1:A:391:GLU:O	1:A:395:PRO:HG3	1.97	0.64
1:B:452:GLY:O	1:B:454:GLY:N	2.30	0.64
1:B:450:LEU:C	1:B:451:GLY:O	2.35	0.64
1:B:225:LYS:HE2	1:B:302:GLU:OE2	1.97	0.63
1:A:497:PHE:O	1:A:501:ILE:HG12	1.98	0.63
1:A:491:PHE:O	1:A:497:PHE:CE2	2.52	0.62
1:A:330:PHE:O	1:B:324:LYS:HE2	2.00	0.62
1:A:303:GLY:HA3	1:A:400:LEU:HB3	1.81	0.62
1:A:270:VAL:HG12	1:A:271:TRP:N	2.08	0.62
1:B:234:ILE:HD11	1:B:307:ALA:HB2	1.80	0.61
1:A:269:ALA:HA	1:A:273:GLY:O	1.99	0.61
1:A:494:ILE:HA	1:A:497:PHE:HD2	1.66	0.61
1:A:169:TRP:HD1	1:A:170:GLY:N	1.98	0.60
1:A:296:LEU:HD12	1:A:304:PHE:HE1	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:GLU:O	1:A:254:ASN:ND2	2.34	0.60
1:B:234:ILE:HD11	1:B:307:ALA:HB3	1.82	0.60
1:B:58:ARG:NH1	1:B:79:GLU:O	2.32	0.60
1:A:436:PRO:HG3	1:A:546:LEU:CD2	2.31	0.60
1:A:76:ILE:HG23	1:A:422:LYS:NZ	2.16	0.60
1:A:6:ARG:HG3	1:A:10:PRO:HG3	1.84	0.59
1:B:309:ASN:ND2	1:B:403:SER:OG	2.35	0.59
1:A:551:GLU:O	1:A:608:ARG:HG3	2.02	0.59
1:A:509:PRO:HG2	1:A:630:MET:HE3	1.85	0.59
1:B:259:LYS:HG2	1:B:263:GLY:O	2.01	0.59
1:B:29:TYR:O	1:B:40:PHE:HE1	1.86	0.58
1:A:286:ARG:HG2	1:A:385:ALA:HB2	1.86	0.58
1:B:269:ALA:HA	1:B:273:GLY:O	2.03	0.58
1:A:148:ARG:HH21	1:A:148:ARG:HB3	1.68	0.58
1:A:398:ARG:NH1	1:A:645:ASP:OD2	2.37	0.57
1:A:29:TYR:O	1:A:40:PHE:HE1	1.87	0.57
1:A:545:GLN:NE2	1:A:553:MET:HE3	2.18	0.57
1:B:449:ASP:OD2	1:B:478:HIS:HB3	2.03	0.57
1:B:643:TYR:C	1:B:643:TYR:CD2	2.77	0.57
1:B:88:HIS:NE2	1:B:406:SER:HB2	2.20	0.57
1:A:494:ILE:HA	1:A:497:PHE:CD2	2.39	0.57
1:B:320:LEU:O	1:B:324:LYS:HG3	2.05	0.56
1:B:157:PRO:HG2	1:B:162:PHE:HE2	1.69	0.56
1:B:230:ARG:CG	1:B:230:ARG:HH11	2.15	0.56
1:B:309:ASN:HD21	1:B:404:ARG:H	1.53	0.56
1:A:310:GLU:N	1:A:311:PRO:HA	2.21	0.56
1:A:538:MET:HG2	1:A:568:TYR:CZ	2.41	0.55
1:A:169:TRP:HH2	1:A:271:TRP:CH2	2.25	0.55
1:A:48:ASP:OD1	1:A:95:GLY:HA3	2.07	0.55
1:A:217:PHE:HB3	1:A:218:PRO:HD3	1.90	0.54
1:B:45:ASP:HB3	1:B:48:ASP:OD1	2.07	0.54
1:A:424:TRP:HB3	1:B:79:GLU:OE2	2.08	0.54
1:A:396:GLU:O	1:A:649:HIS:HA	2.07	0.54
1:B:210:ASN:O	1:B:214:PHE:HB2	2.07	0.54
1:B:100:GLY:O	1:B:101:LEU:HD23	2.08	0.54
1:A:459:ARG:NH2	1:A:496:ASP:OD2	2.41	0.53
1:B:557:VAL:HG22	1:B:565:ARG:HG2	1.89	0.53
1:A:169:TRP:C	1:A:169:TRP:CD1	2.81	0.53
1:A:453:PHE:HB3	1:A:456:ASP:OD2	2.08	0.53
1:B:362:HIS:NE2	1:B:371:HIS:HD2	2.05	0.53
1:A:218:PRO:HG3	1:A:299:GLN:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:177:PHE:HD1	1:B:194:ILE:HG21	1.74	0.52
1:B:444:MET:O	1:B:473:PRO:HG2	2.09	0.52
1:B:573:MET:HG2	1:B:608:ARG:HA	1.90	0.52
1:A:651:ASP:OD1	1:A:654:LYS:HG3	2.09	0.52
1:A:293:TYR:CE1	1:A:386:ALA:HB2	2.45	0.52
1:A:505:TYR:HA	1:A:508:VAL:HG23	1.92	0.52
1:B:64:GLY:O	1:B:65:TYR:HB2	2.10	0.52
1:B:94:SER:HA	1:B:98:THR:HG23	1.91	0.51
1:A:88:HIS:HB3	1:A:408:ILE:HD11	1.92	0.51
1:B:356:ASP:OD1	1:B:359:ARG:NH2	2.44	0.51
1:B:38:PHE:CZ	1:B:132:ILE:HD11	2.45	0.51
1:A:76:ILE:HA	1:A:422:LYS:HZ1	1.75	0.51
1:A:271:TRP:HB2	1:A:272:PRO:HD3	1.92	0.51
1:B:411:HIS:HB2	1:B:442:GLY:O	2.11	0.51
1:A:117:ARG:NH1	1:A:119:ASP:OD2	2.44	0.51
1:B:309:ASN:OD1	1:B:405:SER:HB3	2.11	0.50
1:A:109:LEU:HD12	1:A:125:CYS:HB3	1.92	0.50
1:A:605:LEU:HD12	1:A:605:LEU:C	2.32	0.50
1:A:510:TYR:CE1	1:A:514:GLU:CG	2.94	0.50
1:B:286:ARG:HG2	1:B:385:ALA:HB2	1.94	0.50
1:B:259:LYS:HE2	1:B:265:ASP:OD1	2.11	0.50
1:B:190:PRO:HB2	1:B:505:TYR:CE1	2.45	0.50
1:B:167:SER:O	1:B:478:HIS:HA	2.11	0.50
1:A:539:ALA:O	1:A:541:ARG:N	2.45	0.49
1:A:16:LEU:HA	1:A:151:ILE:HA	1.95	0.49
1:B:280:MET:O	1:B:381:ASN:HB3	2.13	0.49
1:A:371:HIS:HE1	1:A:375:HIS:ND1	2.10	0.49
1:B:55:GLU:HB2	1:B:438:LEU:HD21	1.95	0.49
1:A:227:GLN:O	1:A:229:LEU:HG	2.13	0.49
1:B:510:TYR:HB2	1:B:614:PRO:HD2	1.94	0.49
1:A:204:PHE:HB2	1:A:272:PRO:HG3	1.96	0.48
1:B:90:PHE:CZ	1:B:92:ILE:HD11	2.48	0.48
1:A:574:LYS:CE	1:A:586:GLU:OE2	2.61	0.48
1:B:636:GLU:CD	1:B:663:LYS:HE3	2.34	0.48
1:A:326:PHE:HD2	1:A:343:MET:HE3	1.77	0.48
1:B:75:PRO:O	1:B:421:ASN:HB3	2.13	0.48
1:A:536:ASP:HB3	1:A:539:ALA:HB3	1.95	0.48
1:A:545:GLN:NE2	1:A:553:MET:HE1	2.29	0.48
1:A:147:PHE:CE2	1:A:151:ILE:HG21	2.50	0.47
1:A:86:GLY:HA3	1:A:88:HIS:CE1	2.50	0.47
1:A:538:MET:HG2	1:A:568:TYR:CE1	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:ASP:OD1	1:A:646:ASP:C	2.52	0.47
1:A:654:LYS:O	1:A:657:ASN:HB2	2.14	0.47
1:B:141:TYR:CZ	1:B:145:LYS:HD3	2.49	0.47
1:A:247:VAL:HG22	1:A:292:LYS:HE2	1.97	0.47
1:B:380:TYR:C	1:B:380:TYR:CD1	2.88	0.47
1:A:278:PRO:O	1:A:280:MET:HG2	2.15	0.47
1:A:296:LEU:HD13	1:A:304:PHE:HE1	1.78	0.46
1:A:447:GLY:CA	1:A:474:LEU:HB3	2.45	0.46
1:B:423:SER:OG	1:B:452:GLY:HA2	2.14	0.46
1:A:148:ARG:NH1	1:A:444:MET:SD	2.88	0.46
1:B:410:MET:O	1:B:412:ARG:N	2.48	0.46
1:B:658:TYR:CD2	1:B:658:TYR:N	2.83	0.46
1:A:574:LYS:HB3	1:A:576:ILE:HD13	1.97	0.46
1:A:88:HIS:HA	1:A:408:ILE:HD12	1.98	0.46
1:A:78:THR:HB	1:B:424:TRP:CZ2	2.50	0.46
1:A:82:ARG:NH2	1:B:456:ASP:OD1	2.39	0.46
1:A:234:ILE:HD12	1:A:305:TRP:CZ2	2.50	0.46
1:A:510:TYR:HB2	1:A:614:PRO:HG2	1.98	0.46
1:A:189:ILE:HD11	1:A:494:ILE:HG12	1.96	0.46
1:A:568:TYR:O	1:A:570:PRO:HD3	2.16	0.46
1:B:235:ILE:HB	1:B:306:ASN:ND2	2.31	0.46
1:B:438:LEU:HD13	1:B:446:THR:HG21	1.98	0.46
1:B:196:MET:HB2	1:B:233:PRO:HA	1.98	0.46
1:A:92:ILE:HD11	1:A:144:VAL:HG22	1.97	0.46
1:B:428:ILE:HG22	1:B:558:TYR:HB3	1.97	0.45
1:A:196:MET:SD	1:A:231:LEU:HD13	2.57	0.45
1:A:422:LYS:HD2	1:A:424:TRP:CZ2	2.51	0.45
1:A:362:HIS:NE2	1:A:371:HIS:CD2	2.78	0.45
1:B:184:TYR:CD2	1:B:189:ILE:HB	2.50	0.45
1:B:162:PHE:HZ	1:B:515:TYR:CG	2.34	0.45
1:A:114:GLY:HA2	1:A:117:ARG:O	2.16	0.45
1:B:450:LEU:HD13	1:B:465:PHE:CE1	2.52	0.45
1:B:278:PRO:HB2	1:B:280:MET:CE	2.46	0.45
1:A:390:PHE:CE2	1:A:399:PHE:HB2	2.51	0.45
1:A:232:ILE:HD12	1:A:400:LEU:HD23	1.99	0.45
1:A:196:MET:HB2	1:A:233:PRO:HA	1.99	0.45
1:B:7:TYR:O	1:B:129:ASP:HA	2.17	0.45
1:B:121:LEU:HD12	1:B:122:LYS:N	2.31	0.45
1:B:230:ARG:HG3	1:B:230:ARG:NH1	2.19	0.45
1:A:644:GLU:OE2	1:A:659:ARG:NH2	2.49	0.45
1:A:16:LEU:HB3	1:A:150:VAL:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:ARG:NH1	1:A:523:ASP:O	2.49	0.45
1:A:166:GLN:NE2	1:A:477:ASP:OD2	2.50	0.45
1:A:85:TYR:CE1	1:A:404:ARG:HD2	2.51	0.45
1:B:436:PRO:O	1:B:440:MET:HG3	2.17	0.45
1:A:169:TRP:CD1	1:A:170:GLY:N	2.84	0.44
1:A:291:ASP:O	1:A:294:ARG:HB2	2.16	0.44
1:B:466:LEU:O	1:B:470:VAL:HG23	2.16	0.44
1:B:197:ASP:O	1:B:199:ASP:N	2.50	0.44
1:A:423:SER:HB3	1:A:461:LEU:HD21	2.00	0.44
1:B:281:LEU:HB3	1:B:364:VAL:HG22	1.98	0.44
1:A:577:LYS:HB2	1:A:585:SER:OG	2.18	0.44
1:A:537:LYS:HD2	1:A:537:LYS:HA	1.53	0.44
1:A:289:PHE:O	1:A:292:LYS:HB2	2.18	0.44
1:A:62:LYS:CE	1:A:62:LYS:HA	2.48	0.43
1:A:361:TYR:CE1	1:A:370:ARG:HG3	2.53	0.43
1:A:154:SER:OG	1:A:442:GLY:O	2.31	0.43
1:B:429:LEU:HD12	1:B:432:LEU:HD23	1.99	0.43
1:A:421:ASN:O	1:A:422:LYS:HG3	2.17	0.43
1:A:348:LYS:HD2	1:B:344:GLN:NE2	2.33	0.43
1:A:281:LEU:CD1	1:A:374:VAL:HG21	2.49	0.43
1:B:53:LEU:HA	1:B:88:HIS:O	2.17	0.43
1:A:176:ASP:O	1:A:180:VAL:HG23	2.18	0.43
1:A:517:LYS:O	1:A:521:ASN:HB2	2.18	0.43
1:B:575:PHE:HB2	1:B:589:LEU:CD1	2.47	0.43
1:A:260:ARG:NH1	1:A:264:SER:OG	2.51	0.43
1:B:217:PHE:O	1:B:221:VAL:HG23	2.19	0.43
1:B:195:TYR:CD2	1:B:232:ILE:HB	2.53	0.43
1:A:444:MET:HB3	1:A:444:MET:HE2	1.82	0.43
1:A:390:PHE:CD2	1:A:399:PHE:HB2	2.54	0.43
1:B:294:ARG:NH2	1:B:393:ILE:HG12	2.33	0.43
1:B:428:ILE:CG2	1:B:558:TYR:HB3	2.49	0.43
1:B:230:ARG:CG	1:B:230:ARG:NH1	2.79	0.43
1:A:417:TRP:NE1	1:A:476:ARG:NH2	2.65	0.43
1:B:310:GLU:N	1:B:311:PRO:HA	2.34	0.43
1:A:204:PHE:CB	1:A:272:PRO:HG3	2.49	0.43
1:A:296:LEU:HD13	1:A:304:PHE:CE1	2.53	0.43
1:A:439:ASN:HB3	1:A:524:MET:HE2	2.01	0.43
1:A:130:LEU:N	1:A:130:LEU:HD23	2.34	0.43
1:A:169:TRP:CH2	1:A:271:TRP:CH2	3.06	0.42
1:A:447:GLY:HA3	1:A:474:LEU:HD23	2.00	0.42
1:B:280:MET:O	1:B:281:LEU:HD12	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:ILE:HG22	1:B:315:TYR:N	2.33	0.42
1:B:92:ILE:HD12	1:B:92:ILE:N	2.33	0.42
1:A:433:LYS:O	1:A:436:PRO:HD2	2.19	0.42
1:A:53:LEU:HA	1:A:88:HIS:O	2.19	0.42
1:A:70:ASN:O	1:A:71:CYS:C	2.58	0.42
1:B:607:ILE:HD12	1:B:613:ILE:HG12	2.01	0.42
1:A:574:LYS:HE2	1:A:586:GLU:OE2	2.18	0.42
1:B:383:THR:HG21	1:B:410:MET:HE3	2.01	0.42
1:B:232:ILE:O	1:B:305:TRP:NE1	2.52	0.42
1:A:422:LYS:HD2	1:A:424:TRP:HZ2	1.84	0.42
1:B:193:MET:HG2	1:B:232:ILE:HD11	2.00	0.42
1:A:13:THR:O	1:A:380:TYR:HE2	2.03	0.42
1:A:256:TYR:CD2	1:A:288:TRP:CD2	3.08	0.42
1:B:643:TYR:CD2	1:B:644:GLU:N	2.88	0.42
1:B:101:LEU:HD22	1:B:134:VAL:HG22	2.02	0.42
1:A:617:GLU:OE1	1:A:617:GLU:HA	2.20	0.42
1:B:325:GLU:HG3	1:B:326:PHE:N	2.34	0.42
1:B:270:VAL:CG1	1:B:271:TRP:N	2.82	0.41
1:B:289:PHE:O	1:B:290:GLY:C	2.57	0.41
1:B:569:LEU:O	1:B:592:GLY:N	2.52	0.41
1:A:139:ASN:OD1	1:A:141:TYR:HB3	2.19	0.41
1:A:315:TYR:CE1	1:A:320:LEU:HD22	2.55	0.41
1:B:206:ASP:OD2	1:B:236:ASP:O	2.38	0.41
1:A:436:PRO:HB3	1:A:528:PRO:HG3	2.01	0.41
1:A:53:LEU:O	1:A:54:GLY:C	2.58	0.41
1:A:260:ARG:HB2	1:A:262:ASP:OD1	2.21	0.41
1:A:376:ASN:O	1:A:407:TYR:HB2	2.20	0.41
1:A:523:ASP:OD1	1:A:524:MET:N	2.51	0.41
1:A:563:ARG:HD2	1:B:541:ARG:HD2	2.01	0.41
1:A:514:GLU:OE2	1:A:517:LYS:CE	2.49	0.41
1:B:278:PRO:HB2	1:B:280:MET:HE2	2.03	0.41
1:A:421:ASN:OD1	1:A:421:ASN:N	2.53	0.41
1:B:189:ILE:HA	1:B:190:PRO:HD3	1.98	0.41
1:A:418:MET:HG2	1:A:418:MET:H	1.74	0.41
1:B:460:ASP:HB2	1:B:600:LEU:HD21	2.03	0.41
1:B:27:PHE:HA	1:B:28:PRO:HD3	1.94	0.41
1:B:306:ASN:HB3	1:B:309:ASN:HD22	1.86	0.41
1:B:153:ARG:O	1:B:412:ARG:HG2	2.20	0.41
1:B:380:TYR:HA	1:B:410:MET:SD	2.61	0.41
1:A:348:LYS:HE2	1:A:348:LYS:HB3	1.82	0.41
1:A:55:GLU:HB2	1:A:438:LEU:HD21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:TYR:CZ	1:A:233:PRO:HB2	2.56	0.40
1:A:417:TRP:CD1	1:A:476:ARG:NH2	2.89	0.40
1:B:56:SER:CA	1:B:84:LEU:HD12	2.51	0.40
1:A:598:VAL:HG11	1:A:604:PRO:HG3	2.03	0.40
1:A:527:LYS:NZ	1:A:550:ASN:OD1	2.54	0.40
1:A:343:MET:CE	1:A:347:MET:HE2	2.50	0.40
1:B:596:VAL:O	1:B:596:VAL:HG23	2.21	0.40
1:B:408:ILE:HD11	1:B:441:CYS:HB3	2.04	0.40
1:B:258:CYS:SG	1:B:279:ASP:HA	2.61	0.40
1:A:579:MET:HB3	1:A:581:ASP:OD1	2.21	0.40
1:A:22:THR:HG22	1:A:24:GLU:OE2	2.22	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	651/666 (98%)	591 (91%)	49 (8%)	11 (2%)	11	38
1	B	654/666 (98%)	588 (90%)	53 (8%)	13 (2%)	9	33
All	All	1305/1332 (98%)	1179 (90%)	102 (8%)	24 (2%)	11	37

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	451	GLY
1	B	453	PHE
1	B	638	SER
1	A	54	GLY
1	A	540	ILE
1	B	198	ILE
1	B	456	ASP

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Mol	Chain	Res	Type
1	A	138	GLU
1	A	253	LYS
1	B	411	HIS
1	A	71	CYS
1	A	262	ASP
1	A	335	GLU
1	A	653	ASP
1	B	600	LEU
1	A	452	GLY
1	B	181	ALA
1	B	203	ASP
1	B	170	GLY
1	B	270	VAL
1	A	604	PRO
1	B	470	VAL
1	A	270	VAL
1	B	452	GLY

### 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	563/574 (98%)	511 (91%)	52 (9%)	11	33
1	B	565/574 (98%)	515 (91%)	50 (9%)	12	35
All	All	1128/1148 (98%)	1026 (91%)	102 (9%)	12	34

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	14	GLU
1	A	16	LEU
1	A	34	GLN
1	A	36	GLU
1	A	62	LYS

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Mol	Chain	Res	Type
1	A	74	ASP
1	A	76	ILE
1	A	115	TYR
1	A	118	MET
1	A	127	ASN
1	A	148	ARG
1	A	166	GLN
1	A	169	TRP
1	A	173	THR
1	A	192	ASP
1	A	240	LYS
1	A	243	LYS
1	A	246	GLU
1	A	254	ASN
1	A	280	MET
1	A	286	ARG
1	A	299	GLN
1	A	305	TRP
1	A	308	MET
1	A	334	THR
1	A	335	GLU
1	A	355	GLU
1	A	367	LYS
1	A	369	ILE
1	A	373	LYS
1	A	401	MET
1	A	403	SER
1	A	417	TRP
1	A	418	MET
1	A	422	LYS
1	A	430	LEU
1	A	432	LEU
1	A	433	LYS
1	A	434	MET
1	A	453	PHE
1	A	459	ARG
1	A	495	GLU
1	A	514	GLU
1	A	550	ASN
1	A	576	ILE
1	A	602	GLU
1	A	609	SER

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Mol	Chain	Res	Type
1	A	628	GLU
1	A	646	ASP
1	A	651	ASP
1	A	655	LYS
1	B	1	MET
1	B	18	GLU
1	B	41	THR
1	B	56	SER
1	B	58	ARG
1	B	66	CYS
1	B	72	THR
1	B	74	ASP
1	B	76	ILE
1	B	81	LYS
1	B	82	ARG
1	B	94	SER
1	B	126	GLU
1	B	154	SER
1	B	203	ASP
1	B	216	ASP
1	B	230	ARG
1	B	243	LYS
1	B	253	LYS
1	B	259	LYS
1	B	274	ASP
1	B	294	ARG
1	B	305	TRP
1	B	317	SER
1	B	320	LEU
1	B	325	GLU
1	B	335	GLU
1	B	349	ASP
1	B	355	GLU
1	B	359	ARG
1	B	380	TYR
1	B	405	SER
1	B	406	SER
1	B	420	ASP
1	B	421	ASN
1	B	427	HIS
1	B	446	THR
1	B	449	ASP

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Mol	Chain	Res	Type
1	B	494	ILE
1	B	495	GLU
1	B	535	ASP
1	B	550	ASN
1	B	563	ARG
1	B	576	ILE
1	B	581	ASP
1	B	585	SER
1	B	608	ARG
1	B	623	LYS
1	B	639	SER
1	B	648	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	89	ASN
1	A	166	GLN
1	A	187	ASN
1	A	254	ASN
1	A	306	ASN
1	A	344	GLN
1	A	371	HIS
1	A	493	ASN
1	A	502	ASN
1	A	545	GLN
1	B	70	ASN
1	B	77	HIS
1	B	146	GLN
1	B	187	ASN
1	B	306	ASN
1	B	344	GLN
1	B	371	HIS
1	B	431	ASN
1	B	478	HIS
1	B	493	ASN

### 5.3.3 RNA ⓘ

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	655/666 (98%)	-0.29	15 (2%) 64 59	42, 54, 69, 104	4 (0%)
1	B	658/666 (98%)	-0.29	8 (1%) 81 78	39, 53, 70, 92	1 (0%)
All	All	1313/1332 (98%)	-0.29	23 (1%) 71 68	39, 54, 69, 104	5 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	488	CYS	8.1
1	B	489	TYR	5.7
1	A	46	GLU	3.8
1	A	362	HIS	3.8
1	A	629	ASN	3.6
1	A	628	GLU	3.5
1	A	369	ILE	3.4
1	A	402	PHE	3.2
1	A	159	LYS	3.1
1	A	453	PHE	3.0
1	B	231	LEU	2.7
1	A	289	PHE	2.7
1	A	314	PHE	2.6
1	B	596	VAL	2.6
1	B	289	PHE	2.4
1	B	480	ALA	2.4
1	A	171	TYR	2.3
1	A	480	ALA	2.3
1	B	420	ASP	2.1
1	A	493	ASN	2.1
1	A	633	ILE	2.1
1	A	239	VAL	2.1
1	B	399	PHE	2.1

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.