Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 02:25 PM EDT

PDB ID	:	6D8G
Title	:	D341A D367A calcium binding mutant of Bacteroides uniformis beta-glucuronidase 2
Authors	:	Walton, W.G.; Pellock, S.J.; Redinbo, M.R.
Deposited on	:	2018-04-26
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*
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.

The following versions of software and data (see references ⓘ) were used in the production of this report:

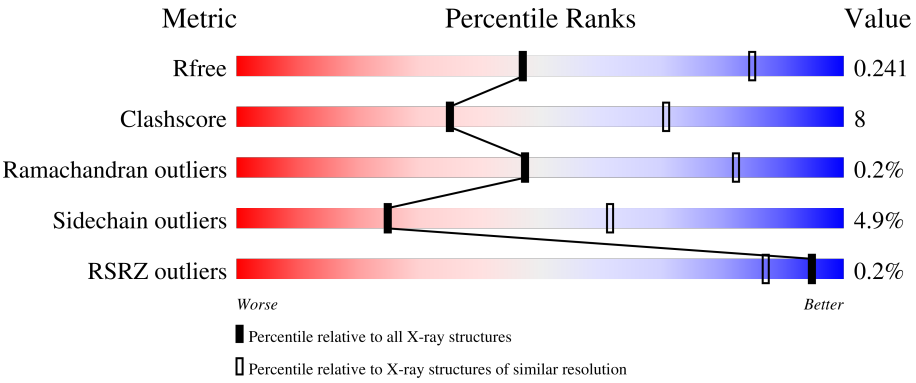
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	886	72% 20% • 6%
1	B	886	74% 18% • 6%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13437 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 Glycosyl hydrolases family 2, sugar binding domain protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	832	Total	C	N	O	S	0	0	0
			6723	4281	1157	1265	20			
1	B	831	Total	C	N	O	S	0	0	0
			6712	4275	1153	1264	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	341	ALA	ASP	engineered mutation	UNP A0A078SUX9
A	367	ALA	ASP	engineered mutation	UNP A0A078SUX9
B	341	ALA	ASP	engineered mutation	UNP A0A078SUX9
B	367	ALA	ASP	engineered mutation	UNP A0A078SUX9

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

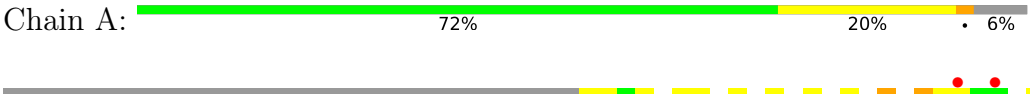
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		

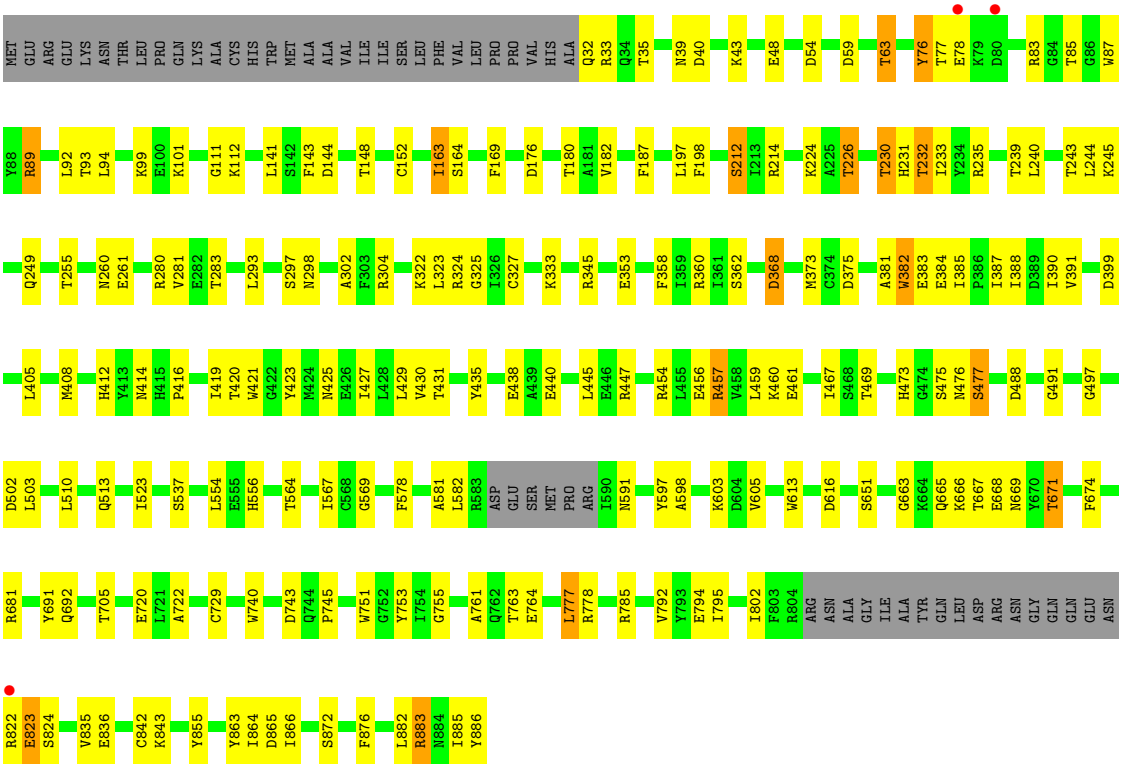
3 Residue-property plots (i)

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

• Molecule 1: Glycosyl hydrolases family 2, sugar binding domain protein

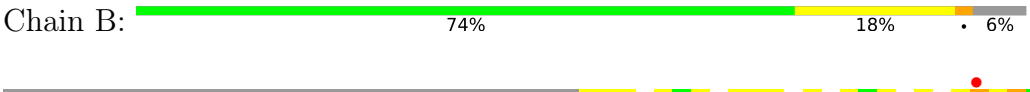
Chain A:

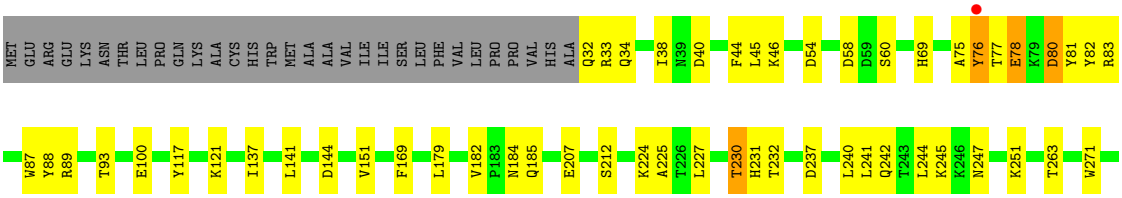


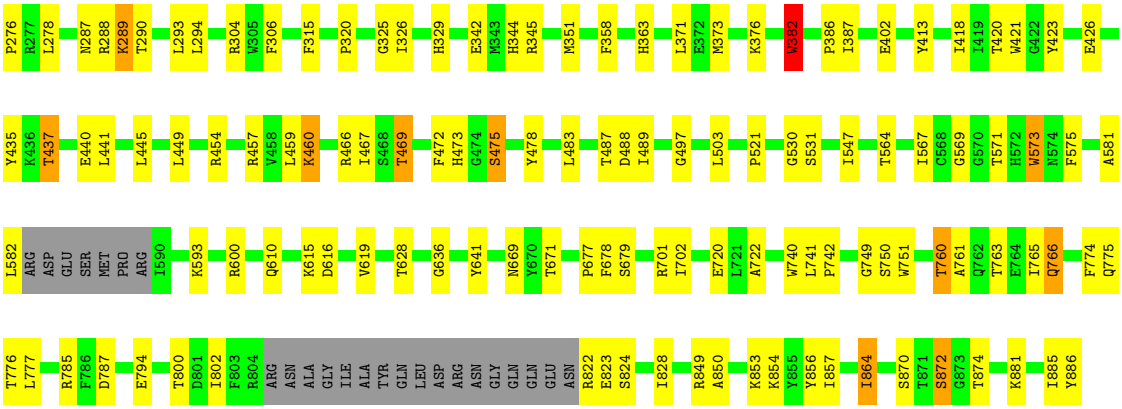


• Molecule 1: Glycosyl hydrolases family 2, sugar binding domain protein

Chain B:






P276 R277 L278 N287 R288 K289 T290 L293 L294 R304 W305 F306 F315 P320 G325 I326 H329 E342 M343 H344 R345 M351 F358 H363 L371 E372 M373 K376 W382 P386 I387 E402 Y413 I418 I419 T420 W421 G422 Y423 E426
Y435 K436 T437 E440 L441 L445 L449 R454 R457 V458 L459 K460 R466 I467 S468 T469 F472 H473 G474 S475 Y478 L483 T487 D488 I489 G497 L503 P521 G530 S531 I547 T564 I567 C568 G569 G570 T571 H572 W573 N574 F575 A581
L582 ARG ASP GLU SER MET PRO ARG I590 K593 R600 Q610 K615 D616 V619 T628 G636 Y641 N669 Y670 T671 P677 F678 S679 R701 I702 E720 L721 A722 W740 L741 P742 G749 S750 W751 T760 A761 Q762 T763 E764 I765 Q766 F774 Q775
T776 L777 R785 F786 D787 E794 T800 D801 I802 F803 R804 ARG ASN ALA GLY ILE ALA TYR GLN LEU ASP ARG ASN GLY GLN GLN GLU ASN R822 E823 S824 I828 R849 A850 K853 K854 Y855 Y856 I857 I864 S870 T871 S872 G873 T874 K881 I885 Y886

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	74.99Å 142.02Å 181.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.55 – 3.00 29.55 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.55-3.00) 100.0 (29.55-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.82 (at 3.00Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575)	Depositor
R, R_{free}	0.166 , 0.241 0.166 , 0.241	Depositor DCC
R_{free} test set	2000 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	67.7	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 34.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13437	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	0.45	0/6900	0.61	1/9366 (0.0%)
1	B	0.45	1/6889 (0.0%)	0.60	1/9352 (0.0%)
All	All	0.45	1/13789 (0.0%)	0.61	2/18718 (0.0%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	144	ASP	C-N	6.65	1.49	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	382	TRP	CA-CB-CG	8.12	129.13	113.70
1	B	382	TRP	CA-CB-CG	6.50	126.05	113.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	381	ALA	Peptide

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	6723	0	6499	116	0
1	B	6712	0	6486	104	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
All	All	13437	0	12985	217	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 (217) 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:382:TRP:HB3	1:B:420:THR:HG23	1.42	0.99
1:B:54:ASP:O	1:B:89:ARG:NH2	1.98	0.95
1:A:382:TRP:HB3	1:A:420:THR:HG23	1.60	0.83
1:B:247:ASN:HB2	1:B:288:ARG:HH21	1.45	0.81
1:B:413:TYR:O	1:B:466:ARG:NH2	2.13	0.80
1:B:766:GLN:OE1	1:B:849:ARG:NH1	2.15	0.79
1:B:326:ILE:HD11	1:B:351:MET:SD	2.23	0.78
1:B:75:ALA:HB1	1:B:581:ALA:HB2	1.66	0.76
1:A:435:TYR:HB3	1:A:440:GLU:HG3	1.71	0.72
1:B:823:GLU:O	1:B:872:SER:HB3	1.89	0.72
1:B:326:ILE:HD13	1:B:575:PHE:HB2	1.71	0.71
1:A:388:ILE:HG22	1:A:425:ASN:HB3	1.73	0.71
1:B:77:THR:HA	1:B:581:ALA:HB1	1.72	0.71
1:A:35:THR:OG1	1:A:180:THR:HG23	1.91	0.69
1:A:32:GLN:HG3	1:A:293:LEU:HD22	1.77	0.67
1:B:76:TYR:CD1	1:B:80:ASP:HB3	2.29	0.67
1:B:426:GLU:HG2	1:B:473:HIS:HB3	1.76	0.67
1:B:230:THR:HG23	1:B:245:LYS:HG3	1.77	0.66
1:A:54:ASP:O	1:A:89:ARG:NH2	2.30	0.65
1:A:497:GLY:HA3	1:A:503:LEU:HD23	1.78	0.65
1:A:212:SER:OG	1:A:214:ARG:NH1	2.31	0.64
1:A:777:LEU:HD22	1:A:876:PHE:HB2	1.80	0.64
1:B:628:THR:HG22	1:B:702:ILE:HG22	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:231:HIS:HB2	1:B:244:LEU:HB2	1.81	0.62
1:A:280:ARG:NH1	1:A:298:ASN:OD1	2.33	0.62
1:B:678:PHE:HE2	1:B:702:ILE:HD11	1.65	0.61
1:A:460:LYS:NZ	1:A:488:ASP:OD2	2.33	0.61
1:B:765:ILE:HD12	1:B:800:THR:HG21	1.82	0.61
1:B:437:THR:HG23	1:B:440:GLU:HB2	1.82	0.61
1:B:720:GLU:HG2	1:B:881:LYS:HD2	1.82	0.61
1:A:78:GLU:HA	1:A:83:ARG:HH22	1.67	0.60
1:B:497:GLY:HA3	1:B:503:LEU:HD23	1.84	0.60
1:B:247:ASN:HB2	1:B:288:ARG:NH2	2.16	0.59
1:B:306:PHE:HE1	1:B:467:ILE:HD13	1.67	0.58
1:B:610:GLN:HG2	1:B:619:VAL:HG21	1.85	0.58
1:A:358:PHE:CZ	1:A:382:TRP:HD1	2.20	0.58
1:B:472:PHE:HB3	1:B:478:TYR:CD2	2.38	0.58
1:A:233:ILE:HG12	1:A:281:VAL:HG22	1.86	0.57
1:A:510:LEU:HD13	1:A:567:ILE:HD11	1.84	0.57
1:A:94:LEU:HD11	1:A:141:LEU:HD13	1.85	0.57
1:A:391:VAL:HG23	1:A:427:ILE:HD11	1.87	0.57
1:A:77:THR:HG23	1:A:582:LEU:HA	1.87	0.57
1:A:475:SER:OG	1:A:477:SER:OG	2.11	0.57
1:A:59:ASP:OD2	1:A:89:ARG:NH1	2.38	0.56
1:A:669:ASN:O	1:A:671:THR:HG22	2.06	0.56
1:A:794:GLU:OE2	1:A:883:ARG:NH1	2.39	0.56
1:A:795:ILE:HD13	1:A:866:ILE:HD11	1.88	0.56
1:B:32:GLN:HA	1:B:294:LEU:O	2.06	0.55
1:B:454:ARG:O	1:B:457:ARG:HG3	2.06	0.55
1:A:476:ASN:OD1	1:A:513:GLN:NE2	2.39	0.55
1:A:578:PHE:O	1:A:591:ASN:HB3	2.06	0.55
1:A:176:ASP:OD2	1:B:854:LYS:NZ	2.37	0.55
1:B:418:ILE:O	1:B:466:ARG:NH1	2.38	0.55
1:B:885:ILE:HG22	1:B:886:TYR:CD2	2.41	0.55
1:A:382:TRP:CB	1:A:420:THR:HG23	2.35	0.55
1:A:99:LYS:HA	1:A:143:PHE:CE1	2.42	0.54
1:A:232:THR:HG23	1:A:243:THR:HG23	1.89	0.54
1:A:419:ILE:HG13	1:A:420:THR:HG22	1.88	0.54
1:B:435:TYR:HB2	1:B:441:LEU:HD23	1.90	0.54
1:A:597:TYR:CZ	1:A:603:LYS:HG2	2.43	0.54
1:A:43:LYS:HA	1:A:63:THR:O	2.08	0.53
1:A:226:THR:HG23	1:A:249:GLN:HG3	1.90	0.53
1:B:242:GLN:OE1	1:B:263:THR:N	2.41	0.53
1:A:76:TYR:CD1	1:A:76:TYR:N	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:PHE:HE2	1:B:320:PRO:HG3	1.74	0.53
1:B:750:SER:OG	1:B:751:TRP:N	2.41	0.53
1:B:489:ILE:HG22	1:B:521:PRO:HG2	1.92	0.52
1:B:760:THR:HG23	1:B:776:THR:HG22	1.91	0.52
1:B:435:TYR:HB3	1:B:440:GLU:HB3	1.92	0.52
1:A:421:TRP:HB2	1:A:459:LEU:HD11	1.92	0.51
1:B:87:TRP:HH2	1:B:117:TYR:CE1	2.28	0.51
1:A:101:LYS:HB3	1:A:182:VAL:O	2.10	0.51
1:A:836:GLU:HG2	1:A:855:TYR:OH	2.09	0.51
1:A:87:TRP:CH2	1:A:152:CYS:HB2	2.45	0.51
1:A:537:SER:HB2	1:A:729:CYS:SG	2.51	0.50
1:A:230:THR:HG23	1:A:245:LYS:HG2	1.93	0.50
1:B:315:PHE:CE2	1:B:320:PRO:HG3	2.47	0.50
1:A:231:HIS:CD2	1:A:260:ASN:HD22	2.28	0.50
1:A:345:ARG:HG2	1:A:373:MET:SD	2.52	0.50
1:A:795:ILE:HD11	1:A:864:ILE:HG21	1.93	0.50
1:B:678:PHE:CE2	1:B:702:ILE:HD11	2.45	0.50
1:A:39:ASN:ND2	1:A:176:ASP:OD1	2.40	0.50
1:B:185:GLN:HG2	1:B:227:LEU:HD21	1.94	0.50
1:A:48:GLU:HG2	1:A:85:THR:HB	1.94	0.49
1:A:399:ASP:HA	1:A:454:ARG:NH2	2.27	0.49
1:A:720:GLU:OE1	1:B:345:ARG:HD2	2.12	0.49
1:A:467:ILE:HG23	1:A:488:ASP:HB2	1.94	0.49
1:B:344:HIS:HD1	1:B:344:HIS:H	1.60	0.49
1:A:325:GLY:HA2	1:A:358:PHE:O	2.13	0.49
1:A:792:VAL:HB	1:A:886:TYR:HB2	1.94	0.49
1:A:375:ASP:CG	1:A:416:PRO:HD2	2.32	0.49
1:B:78:GLU:HG2	1:B:83:ARG:HH22	1.76	0.49
1:A:323:LEU:HB2	1:A:569:GLY:HA3	1.95	0.49
1:B:785:ARG:HA	1:B:864:ILE:O	2.12	0.49
1:B:325:GLY:HA2	1:B:358:PHE:O	2.13	0.49
1:A:324:ARG:HB3	1:A:613:TRP:CZ2	2.48	0.48
1:A:362:SER:HB3	1:A:384:GLU:HG3	1.95	0.48
1:A:581:ALA:C	1:A:582:LEU:HD12	2.34	0.48
1:B:185:GLN:HB2	1:B:294:LEU:HD13	1.96	0.48
1:B:304:ARG:NH1	1:B:306:PHE:HE2	2.11	0.48
1:B:325:GLY:HA3	1:B:571:THR:HG22	1.95	0.48
1:A:745:PRO:HB3	1:A:753:TYR:CZ	2.48	0.48
1:A:663:GLY:O	1:A:674:PHE:HE2	1.95	0.48
1:A:491:GLY:HA2	1:A:523:ILE:O	2.14	0.48
1:A:32:GLN:HG2	1:A:33:ARG:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:ALA:HB1	1:A:740:TRP:CD2	2.49	0.47
1:B:641:TYR:CE2	1:B:677:PRO:HB3	2.49	0.47
1:B:420:THR:OG1	1:B:469:THR:HG22	2.14	0.47
1:A:399:ASP:HA	1:A:454:ARG:HH22	1.79	0.47
1:A:722:ALA:HB1	1:A:740:TRP:CE3	2.49	0.47
1:A:554:LEU:HD12	1:A:605:VAL:HG21	1.97	0.47
1:B:345:ARG:HG3	1:B:373:MET:SD	2.54	0.47
1:B:761:ALA:HB2	1:B:802:ILE:HD12	1.95	0.47
1:A:503:LEU:HB3	1:A:556:HIS:CD2	2.50	0.47
1:B:83:ARG:HD3	1:B:169:PHE:CE2	2.50	0.47
1:A:665:GLN:HG3	1:A:674:PHE:CZ	2.50	0.46
1:B:76:TYR:CE1	1:B:80:ASP:HB3	2.50	0.46
1:A:390:ILE:HG13	1:A:431:THR:OG1	2.15	0.46
1:A:302:ALA:HB3	1:A:416:PRO:HB3	1.98	0.46
1:A:333:LYS:HD2	1:A:598:ALA:O	2.16	0.46
1:B:76:TYR:N	1:B:76:TYR:CD2	2.83	0.46
1:B:137:ILE:O	1:B:141:LEU:HG	2.15	0.46
1:B:669:ASN:O	1:B:671:THR:HG22	2.16	0.46
1:B:58:ASP:OD1	1:B:60:SER:OG	2.30	0.46
1:A:423:TYR:OH	1:A:456:GLU:HB2	2.15	0.46
1:A:324:ARG:HB3	1:A:613:TRP:CE2	2.51	0.45
1:A:244:LEU:HD21	1:A:261:GLU:O	2.16	0.45
1:A:390:ILE:HD12	1:A:430:VAL:HG12	1.98	0.45
1:B:460:LYS:NZ	1:B:488:ASP:OD2	2.49	0.45
1:A:235:ARG:HD2	1:A:239:THR:OG1	2.17	0.45
1:B:564:THR:HB	1:B:567:ILE:HD12	1.97	0.45
1:B:240:LEU:HD12	1:B:241:LEU:N	2.32	0.45
1:A:763:THR:HG22	1:A:764:GLU:O	2.17	0.45
1:A:83:ARG:HD3	1:A:169:PHE:CE2	2.52	0.45
1:B:741:LEU:HD22	1:B:742:PRO:HD2	1.99	0.45
1:B:774:PHE:CE1	1:B:850:ALA:HB1	2.51	0.45
1:A:226:THR:HG23	1:A:249:GLN:CG	2.47	0.44
1:A:761:ALA:HB2	1:A:802:ILE:HD12	1.98	0.44
1:B:387:ILE:HB	1:B:423:TYR:O	2.17	0.44
1:A:164:SER:O	1:A:388:ILE:HD11	2.17	0.44
1:A:92:LEU:HD23	1:A:92:LEU:HA	1.70	0.44
1:A:224:LYS:HB2	1:A:224:LYS:HE3	1.77	0.44
1:B:87:TRP:CH2	1:B:117:TYR:CE1	3.05	0.44
1:A:385:ILE:HD13	1:A:405:LEU:HB2	1.99	0.44
1:B:421:TRP:NE1	1:B:466:ARG:HD2	2.33	0.44
1:B:531:SER:HB2	1:B:547:ILE:HD13	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:749:GLY:N	1:B:787:ASP:OD2	2.50	0.44
1:A:666:LYS:NZ	1:A:668:GLU:OE2	2.36	0.44
1:A:231:HIS:CE1	1:A:283:THR:HG23	2.52	0.44
1:A:863:TYR:CD2	1:A:865:ASP:HB2	2.53	0.44
1:A:327:CYS:SG	1:A:360:ARG:HD3	2.58	0.44
1:A:502:ASP:N	1:A:502:ASP:OD1	2.51	0.44
1:B:530:GLY:HA2	1:B:593:LYS:HA	2.00	0.44
1:B:794:GLU:HB2	1:B:856:TYR:HE1	1.82	0.44
1:B:40:ASP:OD1	1:B:40:ASP:N	2.48	0.43
1:A:40:ASP:OD1	1:B:853:LYS:HE2	2.17	0.43
1:A:445:LEU:HD23	1:A:445:LEU:HA	1.85	0.43
1:B:371:LEU:HD13	1:B:418:ILE:HD11	1.99	0.43
1:B:38:ILE:HD13	1:B:179:LEU:HG	2.01	0.43
1:A:111:GLY:HA2	1:A:112:LYS:HA	1.63	0.43
1:A:391:VAL:HG12	1:A:447:ARG:HG2	1.99	0.43
1:A:835:VAL:HG23	1:A:836:GLU:H	1.84	0.43
1:B:46:LYS:HE3	1:B:82:TYR:CG	2.53	0.43
1:A:197:LEU:C	1:A:198:PHE:CD2	2.92	0.43
1:A:368:ASP:OD1	1:A:412:HIS:NE2	2.49	0.43
1:B:287:ASN:HD21	1:B:289:LYS:HE3	1.84	0.43
1:A:163:ILE:H	1:A:163:ILE:HG13	1.62	0.42
1:A:681:ARG:NH1	1:A:705:THR:HG23	2.34	0.42
1:B:287:ASN:OD1	1:B:289:LYS:HG3	2.19	0.42
1:A:691:TYR:CD2	1:A:692:GLN:HG3	2.53	0.42
1:A:755:GLY:O	1:A:778:ARG:HD3	2.19	0.42
1:A:358:PHE:CZ	1:A:382:TRP:CD1	3.05	0.42
1:A:414:ASN:O	1:A:416:PRO:HD3	2.19	0.42
1:A:667:THR:C	1:A:668:GLU:HG2	2.40	0.42
1:B:722:ALA:HB1	1:B:740:TRP:CD2	2.54	0.42
1:B:326:ILE:C	1:B:326:ILE:HD12	2.40	0.42
1:B:179:LEU:HD23	1:B:179:LEU:HA	1.91	0.42
1:B:329:HIS:HB2	1:B:363:HIS:HB2	2.01	0.42
1:A:785:ARG:HD2	1:A:865:ASP:OD1	2.19	0.42
1:A:794:GLU:HB2	1:A:885:ILE:HD11	2.01	0.42
1:B:83:ARG:HD3	1:B:169:PHE:CZ	2.55	0.42
1:B:445:LEU:HD23	1:B:445:LEU:HA	1.74	0.42
1:B:44:PHE:CE2	1:B:69:HIS:HE1	2.38	0.42
1:B:271:TRP:CD1	1:B:276:PRO:HA	2.54	0.42
1:B:573:TRP:CD2	1:B:593:LYS:HB2	2.55	0.42
1:A:231:HIS:NE2	1:A:260:ASN:ND2	2.64	0.42
1:B:822:ARG:HD2	1:B:822:ARG:HA	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:ARG:HG2	1:B:34:GLN:N	2.34	0.41
1:B:304:ARG:HH12	1:B:306:PHE:HE2	1.69	0.41
1:A:429:LEU:HA	1:A:473:HIS:CE1	2.55	0.41
1:B:87:TRP:CH2	1:B:117:TYR:HE1	2.39	0.41
1:A:665:GLN:HG3	1:A:674:PHE:CE2	2.55	0.41
1:B:88:TYR:HB2	1:B:151:VAL:HB	2.01	0.41
1:B:567:ILE:HG22	1:B:569:GLY:H	1.85	0.41
1:B:77:THR:O	1:B:81:TYR:HB2	2.21	0.41
1:A:187:PHE:CZ	1:A:283:THR:HG22	2.55	0.41
1:A:421:TRP:O	1:A:469:THR:HG22	2.20	0.41
1:B:600:ARG:HA	1:B:600:ARG:HD2	1.80	0.41
1:A:457:ARG:NH1	1:A:461:GLU:OE1	2.54	0.41
1:A:751:TRP:HA	1:A:785:ARG:O	2.20	0.41
1:A:823:GLU:HG2	1:A:842:CYS:SG	2.61	0.41
1:B:75:ALA:CB	1:B:581:ALA:HB2	2.44	0.41
1:B:435:TYR:HB2	1:B:441:LEU:CD2	2.51	0.41
1:B:449:LEU:HD13	1:B:483:LEU:HD23	2.02	0.41
1:B:473:HIS:O	1:B:475:SER:N	2.51	0.41
1:B:763:THR:O	1:B:775:GLN:NE2	2.52	0.41
1:A:383:GLU:OE2	1:A:408:MET:SD	2.79	0.40
1:B:78:GLU:HG2	1:B:83:ARG:HH12	1.87	0.40
1:B:100:GLU:O	1:B:184:ASN:ND2	2.52	0.40
1:B:278:LEU:HD11	1:B:376:LYS:HA	2.04	0.40
1:A:822:ARG:HD2	1:A:822:ARG:HA	1.90	0.40
1:B:224:LYS:HG2	1:B:225:ALA:H	1.85	0.40
1:A:322:LYS:NZ	1:A:564:THR:O	2.54	0.40
1:A:597:TYR:CE2	1:A:603:LYS:HG2	2.57	0.40
1:B:582:LEU:H	1:B:582:LEU:HG	1.69	0.40
1:A:387:ILE:HB	1:A:423:TYR:O	2.21	0.40
1:A:510:LEU:HD13	1:A:567:ILE:CD1	2.49	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	826/886 (93%)	765 (93%)	61 (7%)	0	100 100
1	B	825/886 (93%)	769 (93%)	53 (6%)	3 (0%)	34 72
All	All	1651/1772 (93%)	1534 (93%)	114 (7%)	3 (0%)	47 82

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	573	TRP
1	B	636	GLY
1	B	386	PRO

5.3.2 Protein sidechains (i)

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	719/765 (94%)	688 (96%)	31 (4%)	29 66
1	B	718/765 (94%)	679 (95%)	39 (5%)	22 57
All	All	1437/1530 (94%)	1367 (95%)	70 (5%)	25 61

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	THR
1	A	76	TYR
1	A	89	ARG
1	A	93	THR
1	A	144	ASP
1	A	148	THR
1	A	163	ILE
1	A	212	SER
1	A	226	THR
1	A	230	THR

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Mol	Chain	Res	Type
1	A	232	THR
1	A	240	LEU
1	A	255	THR
1	A	297	SER
1	A	304	ARG
1	A	353	GLU
1	A	368	ASP
1	A	438	GLU
1	A	457	ARG
1	A	477	SER
1	A	616	ASP
1	A	651	SER
1	A	671	THR
1	A	743	ASP
1	A	777	LEU
1	A	823	GLU
1	A	824	SER
1	A	843	LYS
1	A	872	SER
1	A	882	LEU
1	A	883	ARG
1	B	45	LEU
1	B	76	TYR
1	B	78	GLU
1	B	80	ASP
1	B	93	THR
1	B	121	LYS
1	B	182	VAL
1	B	207	GLU
1	B	212	SER
1	B	230	THR
1	B	232	THR
1	B	237	ASP
1	B	251	LYS
1	B	289	LYS
1	B	290	THR
1	B	293	LEU
1	B	342	GLU
1	B	382	TRP
1	B	402	GLU
1	B	437	THR
1	B	459	LEU

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Mol	Chain	Res	Type
1	B	460	LYS
1	B	469	THR
1	B	475	SER
1	B	487	THR
1	B	615	LYS
1	B	616	ASP
1	B	679	SER
1	B	701	ARG
1	B	760	THR
1	B	766	GLN
1	B	777	LEU
1	B	824	SER
1	B	828	ILE
1	B	857	ILE
1	B	864	ILE
1	B	870	SER
1	B	872	SER
1	B	874	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	432	GLN
1	B	479	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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^{th} 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^2)	Q<0.9
1	A	832/886 (93%)	-0.54	3 (0%)	92	79	34, 54, 78, 117	0
1	B	831/886 (93%)	-0.47	1 (0%)	95	89	41, 58, 83, 108	0
All	All	1663/1772 (93%)	-0.51	4 (0%)	95	87	34, 56, 81, 117	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	822	ARG	2.5
1	A	78	GLU	2.4
1	B	76	TYR	2.3
1	A	80	ASP	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NA	A	901	1/1	0.94	0.28	39,39,39,39	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	NA	B	901	1/1	0.99	0.35	39,39,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.