Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2017 – 04:53 PM EDT

PDB ID	:	5DJS
Title	:	Thermobaculum terrenum O-GlcNAc transferase mutant - K341M
Authors	:	Ostrowski, A.; Gundogdu, M.; Ferenbach, A.T.; Lebedev, A.; van Aalten, D.M.F.
Deposited on	:	unknown
Resolution	:	2.80 Å(reported)

The following versions of software and data (see references (1)) were used in the production of this report:

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20029824

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 2.80 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	Percentile Ranks	Value
Rfree		0.216
Clashscore		3
Ramachandran outliers		0.6%
Sidechain outliers		8.4%
RSRZ outliers		2.1%

Worse   *Better*

∎ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
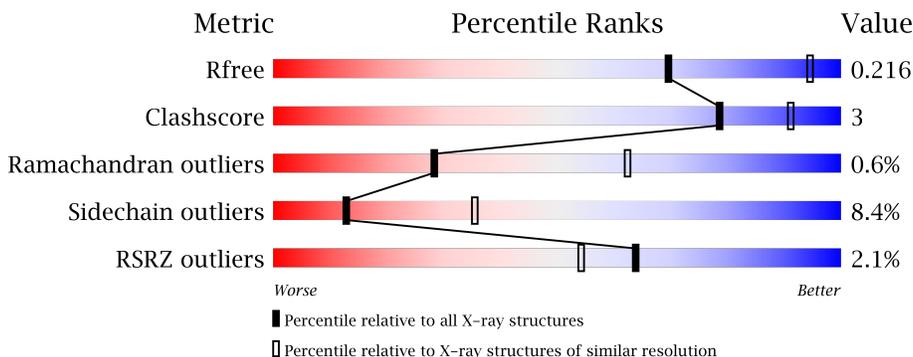
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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 >=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 <=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	529	2% 85% 13% •
1	B	529	2% 85% 13% •
1	C	529	2% 85% 13% ••
1	D	529	2% 85% 13% ••
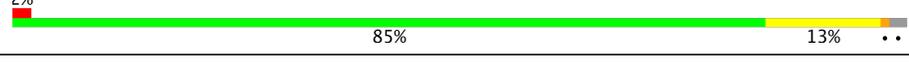
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	UDP	A	601	-	-	-	X
2	UDP	B	601	-	-	-	X
2	UDP	C	601	-	-	-	X
2	UDP	D	601	-	-	-	X

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 16645 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 Tetratricopeptide TPR_2 repeat protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	520	Total 4103	C 2586	N 752	O 744	S 21	0	1	0
1	B	520	Total 4103	C 2586	N 752	O 744	S 21	0	1	0
1	C	520	Total 4103	C 2586	N 752	O 744	S 21	0	1	0
1	D	520	Total 4103	C 2586	N 752	O 744	S 21	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	341	MET	LYS	engineered mutation	UNP D1CIY5
B	341	MET	LYS	engineered mutation	UNP D1CIY5
C	341	MET	LYS	engineered mutation	UNP D1CIY5
D	341	MET	LYS	engineered mutation	UNP D1CIY5

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$).
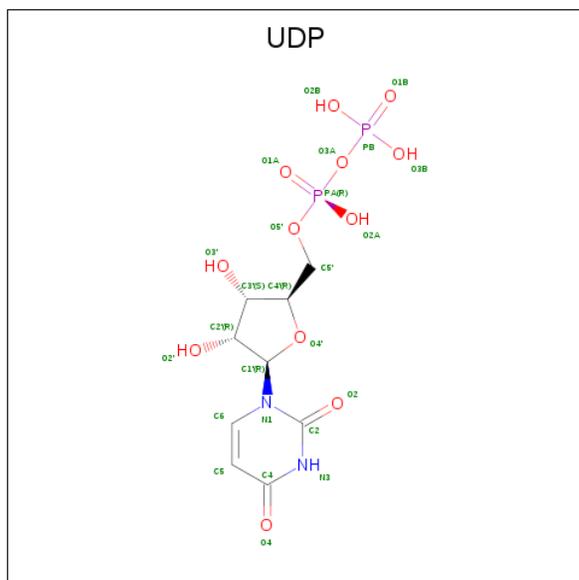
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	D	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	31	Total	O	0	0
			31	31		
3	B	34	Total	O	0	0
			34	34		
3	C	35	Total	O	0	0
			35	35		
3	D	33	Total	O	0	0
			33	33		

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 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: Tetratricopeptide TPR_2 repeat protein

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- Molecule 1: Tetratricopeptide TPR_2 repeat protein

L485 L489 R490 L493 R494 S495 V496 S497 M498 S499 D500 Q501 T505 D510 Q521 T522 A523 A524 GLY ARG GLN GLY ALA

• Molecule 1: Tetratricopeptide TPR_2 repeat protein

Chain D:

2%

85%   13%

M1 T2 A19 S22 A27 R30 N42 L46 L49 L65 S99 L100 Y110 Y127 R161 R162 L163 R164 I165 E171 L172 R173 C174 H175 P176 V177 F180 I185 E186 A187 Y193 C197 Y198 T208 L211 L214 S215 W218 R219

D220 V221 R235 L244 S245 W246 H247 L248 R252 L268 N272 R306 F307 Y308 L309 P322 A323 D324 PRO LEU GLY ARG G329 E345 V346 L347 R363 T374 R377 L382 R391 L394 R400 L404 D415 T416 L417 P418 Y419 S420 G421 C422 T423

T424 S425 T437 A441 T448 L451 Q458 L482 L485 L489 R490 L493 V496 D500 Q501 T505 D510 T522 A523 A524 GLY ARG GLN GLY ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	70.19Å 216.36Å 216.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 2.80 49.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.00-2.80) 99.8 (49.00-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.218 , 0.246 0.186 , 0.216	Depositor DCC
R_{free} test set	4119 reflections (5.28%)	DCC
Wilson B-factor (Å²)	53.5	Xtriage
Anisotropy	0.217	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.33 , 38.8	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.216 for -h,l,k	Xtriage
Reported twinning fraction	0.506 for H, K, L 0.494 for -H, L, K	Depositor
Outliers	5 of 82181 reflections (0.006%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	16645	wwPDB-VP
Average B, all atoms (Å²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 21.45 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 7.0014e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[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 (i)

5.1 Standard geometry (i)

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

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	0/4203	0.75	0/5729
1	B	0.45	0/4203	0.75	0/5729
1	C	0.46	0/4203	0.76	1/5729 (0.0%)
1	D	0.45	0/4203	0.75	1/5729 (0.0%)
All	All	0.45	0/16812	0.75	2/22916 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	161	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	D	235	ARG	NE-CZ-NH1	5.09	122.84	120.30

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	4103	0	4060	27	0
1	B	4103	0	4060	28	0
1	C	4103	0	4060	26	0
1	D	4103	0	4060	29	0
2	A	25	0	11	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	25	0	11	1	0
2	C	25	0	11	0	0
2	D	25	0	11	1	0
3	A	31	0	0	0	0
3	B	34	0	0	3	0
3	C	35	0	0	1	0
3	D	33	0	0	4	0
All	All	16645	0	16284	108	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 3.

All (108) 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:A:197:CYS:O	1:A:218:TRP:O	1.92	0.86
1:B:197:CYS:O	1:B:218:TRP:O	1.92	0.86
1:D:197:CYS:O	1:D:218:TRP:O	1.95	0.84
1:C:197:CYS:O	1:C:218:TRP:O	1.95	0.83
1:A:172:LEU:O	1:A:208:THR:HG22	1.81	0.80
1:D:172:LEU:O	1:D:208:THR:HG22	1.85	0.76
1:C:172:LEU:O	1:C:208:THR:HG22	1.85	0.76
1:B:172:LEU:O	1:B:208:THR:HG22	1.88	0.73
1:D:306:ARG:NH1	1:D:307:PHE:O	2.31	0.65
1:A:306:ARG:NH1	1:A:307:PHE:O	2.33	0.62
1:C:437:THR:HG21	1:C:448:THR:HB	1.83	0.61
1:B:437:THR:HG21	1:B:448:THR:HB	1.83	0.61
1:C:306:ARG:NH1	1:C:307:PHE:O	2.33	0.60
1:B:306:ARG:NH1	1:B:307:PHE:O	2.34	0.60
1:D:268:LEU:HD12	1:D:309:LEU:HD22	1.84	0.60
1:D:268:LEU:HD12	1:D:309:LEU:CD2	2.32	0.60
1:D:437:THR:HG21	1:D:448:THR:HB	1.83	0.59
1:A:268:LEU:HD12	1:A:309:LEU:CD2	2.33	0.58
1:A:268:LEU:HD12	1:A:309:LEU:HD22	1.85	0.58
1:B:268:LEU:HD12	1:B:309:LEU:CD2	2.32	0.58
1:C:268:LEU:HD12	1:C:309:LEU:CD2	2.33	0.58
1:A:437:THR:HG21	1:A:448:THR:HB	1.84	0.58
1:A:185:ILE:HG22	1:A:214:LEU:HB3	1.86	0.58
1:B:185:ILE:HG22	1:B:214:LEU:HB3	1.86	0.57
1:B:268:LEU:HD12	1:B:309:LEU:HD22	1.84	0.57
1:D:185:ILE:HG22	1:D:214:LEU:HB3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:PHE:HB2	1:D:268:LEU:HD11	1.87	0.57
1:D:501:GLN:O	1:D:505:THR:HG23	2.05	0.57
1:B:180:PHE:HB2	1:B:268:LEU:HD11	1.86	0.57
1:C:268:LEU:HD12	1:C:309:LEU:HD22	1.85	0.56
1:A:180:PHE:HB2	1:A:268:LEU:HD11	1.87	0.56
1:C:185:ILE:HG22	1:C:214:LEU:HB3	1.87	0.56
1:C:306:ARG:NH2	1:C:500:ASP:OD1	2.38	0.56
1:C:180:PHE:HB2	1:C:268:LEU:HD11	1.87	0.56
1:A:306:ARG:NH2	1:A:500:ASP:OD1	2.40	0.55
1:B:306:ARG:NH2	1:B:500:ASP:OD1	2.39	0.55
1:B:501:GLN:O	1:B:505:THR:HG23	2.07	0.55
1:C:501:GLN:O	1:C:505:THR:HG23	2.07	0.55
1:C:177:VAL:HA	1:C:268:LEU:HD21	1.89	0.54
1:D:177:VAL:HA	1:D:268:LEU:HD21	1.88	0.54
1:B:421:GLY:O	1:B:448:THR:HG23	2.07	0.53
1:D:306:ARG:NH2	1:D:500:ASP:OD1	2.42	0.53
1:B:177:VAL:HA	1:B:268:LEU:HD21	1.90	0.53
1:B:246:TRP:CE3	1:B:248:LEU:HG	2.43	0.53
1:B:408:ASN:HA	3:B:714:HOH:O	2.09	0.53
1:A:246:TRP:CE3	1:A:248:LEU:HG	2.44	0.53
1:C:421:GLY:O	1:C:448:THR:HG23	2.08	0.53
1:A:177:VAL:HA	1:A:268:LEU:HD21	1.90	0.52
1:C:246:TRP:CE3	1:C:248:LEU:HG	2.44	0.52
1:D:246:TRP:CE3	1:D:248:LEU:HG	2.45	0.52
1:A:501:GLN:O	1:A:505:THR:HG23	2.10	0.51
1:B:246:TRP:CZ3	1:B:248:LEU:HG	2.46	0.51
1:B:437:THR:HG21	1:B:448:THR:CB	2.41	0.50
1:D:421:GLY:O	1:D:448:THR:HG23	2.11	0.50
1:A:421:GLY:O	1:A:448:THR:HG23	2.12	0.50
1:A:246:TRP:CZ3	1:A:248:LEU:HG	2.47	0.49
1:A:49:LEU:HB3	1:A:65:LEU:HD13	1.95	0.49
1:C:246:TRP:CZ3	1:C:248:LEU:HG	2.47	0.49
1:D:246:TRP:CZ3	1:D:248:LEU:HG	2.47	0.48
1:D:437:THR:HG21	1:D:448:THR:CB	2.43	0.48
1:C:437:THR:HG21	1:C:448:THR:CB	2.44	0.48
1:D:49:LEU:HB3	1:D:65:LEU:HD13	1.96	0.48
1:A:437:THR:HG21	1:A:448:THR:CB	2.44	0.47
1:B:180:PHE:CB	1:B:268:LEU:HD11	2.43	0.47
1:D:180:PHE:CB	1:D:268:LEU:HD11	2.44	0.47
1:B:49:LEU:HB3	1:B:65:LEU:HD13	1.96	0.47
1:D:423:THR:HG23	2:D:601:UDP:O2B	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:PHE:CB	1:C:268:LEU:HD11	2.45	0.46
1:C:49:LEU:HB3	1:C:65:LEU:HD13	1.97	0.46
1:C:1:MET:HB3	1:D:127:TYR:CE1	2.51	0.46
1:A:180:PHE:CB	1:A:268:LEU:HD11	2.45	0.45
1:C:187:ALA:HB3	1:C:505:THR:HG21	1.98	0.45
1:C:165:ILE:HD11	1:C:193:TYR:CD1	2.51	0.44
1:A:373:VAL:HG22	3:B:730:HOH:O	2.16	0.44
1:A:425:SER:CB	1:A:448:THR:HG22	2.48	0.44
1:D:165:ILE:HD11	1:D:193:TYR:CD1	2.52	0.44
1:A:370:GLN:N	1:A:370:GLN:OE1	2.48	0.44
1:B:427:GLU:OE2	2:B:601:UDP:O2'	2.35	0.44
1:D:374:THR:HG21	3:D:701:HOH:O	2.17	0.44
1:D:187:ALA:HB3	1:D:505:THR:HG21	1.99	0.43
1:B:171:GLU:HG3	1:B:175:HIS:CD2	2.54	0.43
1:C:370:GLN:OE1	1:C:370:GLN:N	2.46	0.43
1:B:415:ASP:CB	1:B:437:THR:HG22	2.48	0.43
1:A:415:ASP:CB	1:A:437:THR:HG22	2.48	0.43
1:C:415:ASP:CB	1:C:437:THR:HG22	2.49	0.43
1:D:425:SER:CB	1:D:448:THR:HG22	2.49	0.43
1:A:425:SER:OG	1:A:448:THR:CG2	2.67	0.42
1:A:198:TYR:HB3	1:A:221:VAL:HG21	2.01	0.42
1:A:375:SER:OG	1:B:142:ARG:NH2	2.53	0.42
1:D:171:GLU:HG3	1:D:175:HIS:CD2	2.54	0.42
1:D:415:ASP:CB	1:D:437:THR:HG22	2.49	0.42
1:B:187:ALA:HB3	1:B:505:THR:HG21	2.00	0.42
1:C:171:GLU:HG3	1:C:175:HIS:CD2	2.55	0.42
1:D:441:ALA:HB1	3:D:730:HOH:O	2.19	0.42
1:D:374:THR:HG22	3:D:704:HOH:O	2.19	0.42
1:B:425:SER:CB	1:B:448:THR:HG22	2.49	0.42
1:C:425:SER:CB	1:C:448:THR:HG22	2.49	0.41
1:D:198:TYR:HB3	1:D:221:VAL:HG21	2.03	0.41
1:D:377:ARG:NH1	3:D:704:HOH:O	2.47	0.41
1:B:481:THR:HG22	3:B:732:HOH:O	2.20	0.41
1:B:198:TYR:HB3	1:B:221:VAL:HG21	2.02	0.41
1:A:187:ALA:HB3	1:A:505:THR:HG21	2.01	0.41
1:B:425:SER:OG	1:B:448:THR:CG2	2.69	0.41
1:B:370:GLN:OE1	1:B:370:GLN:N	2.50	0.40
1:A:165:ILE:HD11	1:A:193:TYR:CD1	2.56	0.40
1:C:425:SER:OG	1:C:448:THR:CG2	2.70	0.40
1:C:494:ARG:HG3	3:C:728:HOH:O	2.22	0.40
1:A:171:GLU:HG3	1:A:175:HIS:CD2	2.57	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	517/529 (98%)	491 (95%)	23 (4%)	3 (1%)	28	62
1	B	517/529 (98%)	491 (95%)	23 (4%)	3 (1%)	28	62
1	C	517/529 (98%)	491 (95%)	23 (4%)	3 (1%)	28	62
1	D	517/529 (98%)	491 (95%)	23 (4%)	3 (1%)	28	62
All	All	2068/2116 (98%)	1964 (95%)	92 (4%)	12 (1%)	28	62

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	CYS
1	A	268	LEU
1	B	174	CYS
1	B	268	LEU
1	C	174	CYS
1	C	268	LEU
1	D	174	CYS
1	D	268	LEU
1	C	219	ARG
1	D	219	ARG
1	A	219	ARG
1	B	219	ARG

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	429/433 (99%)	394 (92%)	35 (8%)	13	37
1	B	429/433 (99%)	393 (92%)	36 (8%)	13	35
1	C	429/433 (99%)	392 (91%)	37 (9%)	12	34
1	D	429/433 (99%)	394 (92%)	35 (8%)	13	37
All	All	1716/1732 (99%)	1573 (92%)	143 (8%)	13	36

All (143) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	46	LEU
1	A	99	SER
1	A	100	LEU
1	A	110	TYR
1	A	161	ARG
1	A	162	ARG
1	A	163	LEU
1	A	211	LEU
1	A	215	SER
1	A	244	LEU
1	A	252	ARG
1	A	272	ASN
1	A	345	GLU
1	A	346	VAL
1	A	347	LEU
1	A	363	ARG
1	A	378	LEU
1	A	382	LEU
1	A	394	LEU
1	A	400	ARG
1	A	404	LEU
1	A	417	LEU
1	A	419	TYR
1	A	423	THR
1	A	451	LEU
1	A	458	GLN
1	A	482	LEU
1	A	485	LEU
1	A	489	LEU
1	A	490	ARG

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Mol	Chain	Res	Type
1	A	493	LEU
1	A	496	VAL
1	A	505	THR
1	A	510	ASP
1	B	42	ASN
1	B	46	LEU
1	B	99	SER
1	B	100	LEU
1	B	110	TYR
1	B	161	ARG
1	B	162	ARG
1	B	163	LEU
1	B	176	PRO
1	B	211	LEU
1	B	215	SER
1	B	244	LEU
1	B	252	ARG
1	B	272	ASN
1	B	340	SER
1	B	345	GLU
1	B	346	VAL
1	B	347	LEU
1	B	363	ARG
1	B	382	LEU
1	B	394	LEU
1	B	400	ARG
1	B	404	LEU
1	B	417	LEU
1	B	419	TYR
1	B	423	THR
1	B	451	LEU
1	B	458	GLN
1	B	482	LEU
1	B	485	LEU
1	B	489	LEU
1	B	490	ARG
1	B	493	LEU
1	B	496	VAL
1	B	505	THR
1	B	510	ASP
1	C	42	ASN
1	C	46	LEU

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Mol	Chain	Res	Type
1	C	99	SER
1	C	100	LEU
1	C	110	TYR
1	C	161	ARG
1	C	162	ARG
1	C	163	LEU
1	C	176	PRO
1	C	211	LEU
1	C	215	SER
1	C	244	LEU
1	C	252	ARG
1	C	272	ASN
1	C	340	SER
1	C	345	GLU
1	C	346	VAL
1	C	347	LEU
1	C	363	ARG
1	C	378	LEU
1	C	382	LEU
1	C	394	LEU
1	C	400	ARG
1	C	404	LEU
1	C	417	LEU
1	C	419	TYR
1	C	423	THR
1	C	451	LEU
1	C	458	GLN
1	C	482	LEU
1	C	485	LEU
1	C	489	LEU
1	C	490	ARG
1	C	493	LEU
1	C	496	VAL
1	C	505	THR
1	C	510	ASP
1	D	42	ASN
1	D	46	LEU
1	D	99	SER
1	D	100	LEU
1	D	110	TYR
1	D	161	ARG
1	D	162	ARG

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Mol	Chain	Res	Type
1	D	163	LEU
1	D	211	LEU
1	D	215	SER
1	D	244	LEU
1	D	252	ARG
1	D	272	ASN
1	D	345	GLU
1	D	346	VAL
1	D	347	LEU
1	D	363	ARG
1	D	382	LEU
1	D	391	ARG
1	D	394	LEU
1	D	400	ARG
1	D	404	LEU
1	D	417	LEU
1	D	419	TYR
1	D	423	THR
1	D	451	LEU
1	D	458	GLN
1	D	482	LEU
1	D	485	LEU
1	D	489	LEU
1	D	490	ARG
1	D	493	LEU
1	D	496	VAL
1	D	505	THR
1	D	510	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (42) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	85	ASN
1	A	111	HIS
1	A	122	HIS
1	A	200	ASN
1	A	247	HIS
1	A	251	HIS
1	A	272	ASN
1	A	287	HIS
1	A	458	GLN

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Mol	Chain	Res	Type
1	B	47	HIS
1	B	85	ASN
1	B	101	HIS
1	B	111	HIS
1	B	122	HIS
1	B	175	HIS
1	B	200	ASN
1	B	247	HIS
1	B	251	HIS
1	B	272	ASN
1	B	286	GLN
1	B	287	HIS
1	B	458	GLN
1	C	47	HIS
1	C	85	ASN
1	C	122	HIS
1	C	200	ASN
1	C	247	HIS
1	C	251	HIS
1	C	272	ASN
1	C	458	GLN
1	D	47	HIS
1	D	85	ASN
1	D	111	HIS
1	D	122	HIS
1	D	175	HIS
1	D	200	ASN
1	D	247	HIS
1	D	251	HIS
1	D	272	ASN
1	D	287	HIS
1	D	458	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)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	UDP	A	601	-	21,26,26	0.85	1 (4%)	22,40,40	2.08	3 (13%)
2	UDP	B	601	-	21,26,26	0.85	1 (4%)	22,40,40	2.03	2 (9%)
2	UDP	C	601	-	21,26,26	0.86	1 (4%)	22,40,40	2.25	2 (9%)
2	UDP	D	601	-	21,26,26	0.87	1 (4%)	22,40,40	1.97	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UDP	A	601	-	-	0/12/32/32	0/2/2/2
2	UDP	B	601	-	-	0/12/32/32	0/2/2/2
2	UDP	C	601	-	-	0/12/32/32	0/2/2/2
2	UDP	D	601	-	-	0/12/32/32	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	601	UDP	O4'-C1'	2.13	1.44	1.41
2	A	601	UDP	O4'-C1'	2.15	1.44	1.41
2	B	601	UDP	O4'-C1'	2.19	1.44	1.41
2	C	601	UDP	O4'-C1'	2.25	1.44	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	601	UDP	C4'-O4'-C1'	2.13	112.03	109.77
2	B	601	UDP	O4'-C1'-N1	2.46	113.00	108.08
2	A	601	UDP	O4'-C1'-N1	2.70	113.49	108.08
2	C	601	UDP	O4'-C1'-N1	3.03	114.15	108.08
2	A	601	UDP	C4-N3-C2	8.07	121.06	114.13
2	D	601	UDP	C4-N3-C2	8.12	121.11	114.13
2	B	601	UDP	C4-N3-C2	8.32	121.28	114.13
2	C	601	UDP	C4-N3-C2	9.17	122.01	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	UDP	1	0
2	D	601	UDP	1	0

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 (i)

6.1 Protein, DNA and RNA chains (i)

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, 95th 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	520/529 (98%)	-0.22	13 (2%)	58	47	35, 51, 83, 138	0
1	B	520/529 (98%)	-0.24	8 (1%)	74	67	33, 51, 79, 155	0
1	C	520/529 (98%)	-0.23	12 (2%)	61	51	34, 50, 78, 162	0
1	D	520/529 (98%)	-0.19	11 (2%)	64	54	34, 51, 79, 137	0
All	All	2080/2116 (98%)	-0.22	44 (2%)	64	54	33, 51, 80, 162	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	323	ALA	8.5
1	B	322	PRO	7.4
1	B	323	ALA	6.4
1	C	522	THR	5.9
1	D	322	PRO	5.8
1	A	323	ALA	5.7
1	B	324	ASP	4.5
1	C	324	ASP	4.4
1	C	521	GLN	3.9
1	D	324	ASP	3.9
1	D	323	ALA	3.8
1	D	522	THR	3.7
1	B	329	GLY	3.4
1	A	27	ALA	3.3
1	B	522	THR	3.3
1	C	322	PRO	3.3
1	A	4	ARG	3.2
1	A	322	PRO	3.1
1	A	523	ALA	3.0
1	C	498	MET	3.0
1	C	523	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	D	329	GLY	3.0
1	A	30	ARG	2.9
1	D	2	THR	2.9
1	A	521	GLN	2.9
1	A	2	THR	2.8
1	B	28	SER	2.8
1	A	26	LEU	2.8
1	D	30	ARG	2.7
1	D	22	SER	2.6
1	C	329	GLY	2.5
1	A	22	SER	2.4
1	D	523	ALA	2.4
1	A	524	ALA	2.4
1	A	24	ASP	2.4
1	C	34	ARG	2.3
1	D	19	ALA	2.3
1	B	321	ALA	2.2
1	B	34	ARG	2.2
1	C	524	ALA	2.2
1	C	31	ALA	2.1
1	C	1	MET	2.1
1	D	27	ALA	2.1
1	A	21	ARG	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)

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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	LLDF	B-factors(Å^2)	Q<0.9
2	UDP	A	601	25/25	0.88	0.27	4.91	64,73,78,81	25
2	UDP	B	601	25/25	0.88	0.27	3.71	67,75,81,83	25
2	UDP	C	601	25/25	0.89	0.27	2.83	64,86,91,91	25
2	UDP	D	601	25/25	0.91	0.25	2.54	56,66,82,87	25

6.5 Other polymers (i)

There are no such residues in this entry.