wwPDB X-ray Structure Validation Summary Report (i)

Nov 15, 2023 – 12:51 AM JST

PDB ID	:	6II2
Title	:	Crystal structure of alpha-beta hydrolase (ABH) and Makes Caterpillars Floppy (MCF)-Like effectors of Vibrio vulnificus MO6-24/O
Authors	:	Lee, Y.; Kim, B.S.; Choi, S.; Lee, E.Y.; Park, S.; Hwang, J.; Kwon, Y.; Hyung, J.; Lee, C.; Eom, S.H.; Kim, M.H.
Deposited on	:	2018-10-03
Resolution	:	3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (1)) were used in the production of this report:

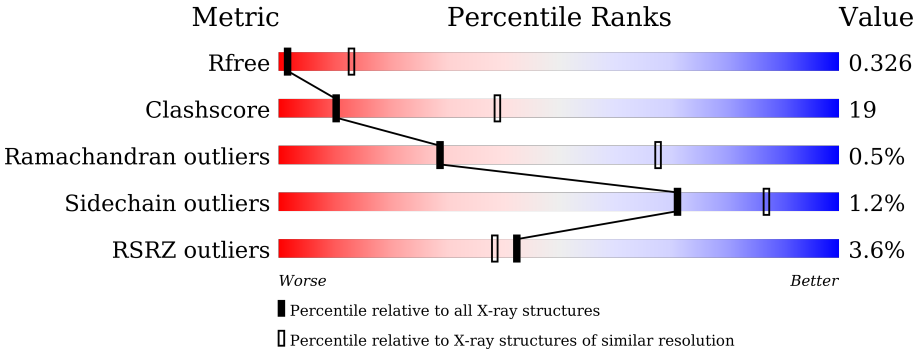
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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	694	.% 71% 16% • 12%
1	B	694	2% 71% 15% • 12%
1	C	694	5% 64% 16% • 18%
1	D	694	4% 53% 22% •• 22%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 17825 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 Putative RTX-toxin.

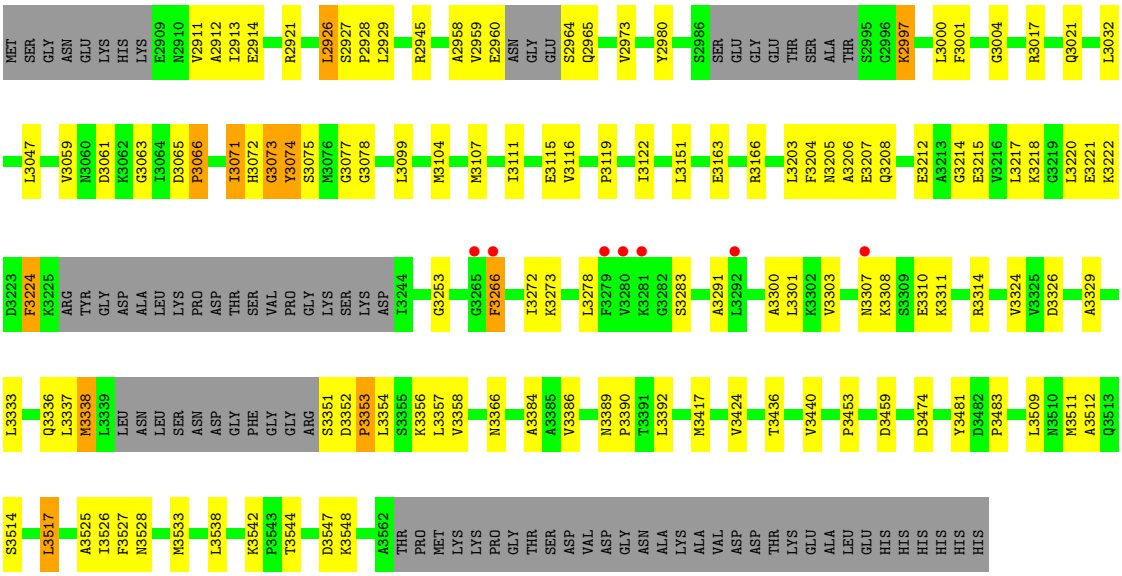
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	614	4681	2938	808	920	15	0	0	0
1	B	612	4673	2932	808	918	15	0	0	0
1	C	568	4338	2732	748	847	11	0	0	0
1	D	539	4133	2604	717	800	12	0	0	0

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.

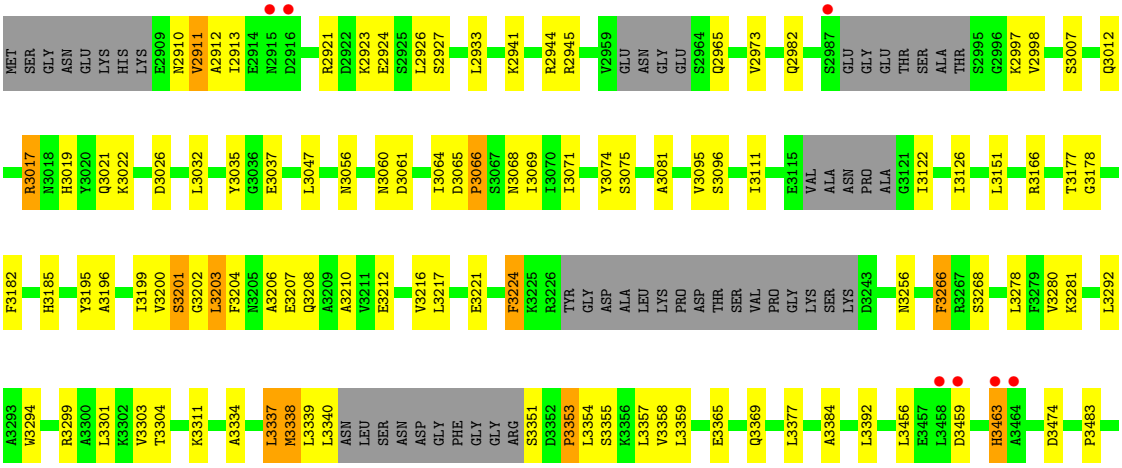
- Molecule 1: Putative RTX-toxin

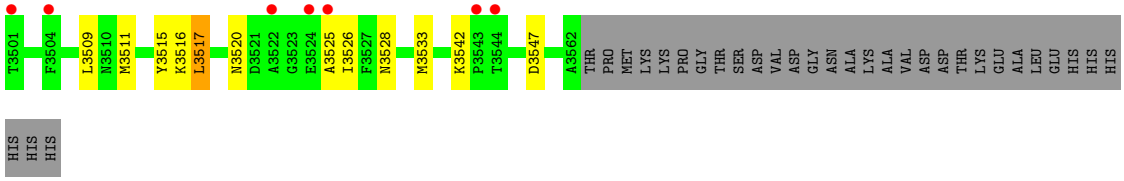
Chain A:



- Molecule 1: Putative RTX-toxin

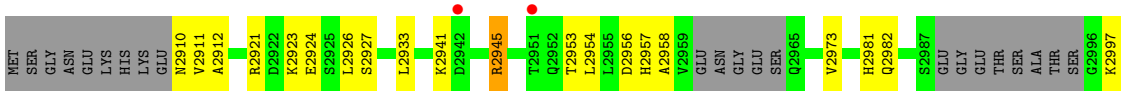
Chain B:

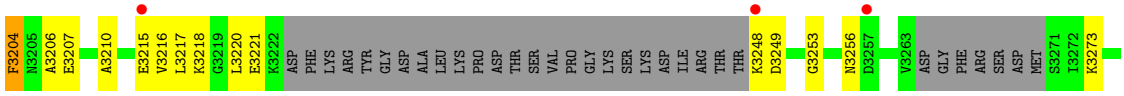


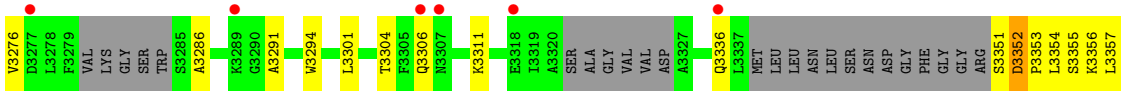


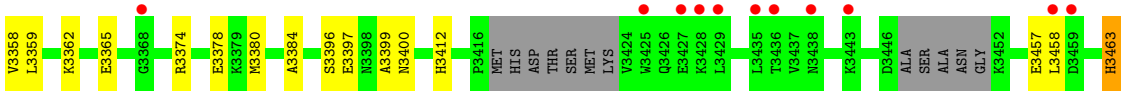
• Molecule 1: Putative RTX-toxin

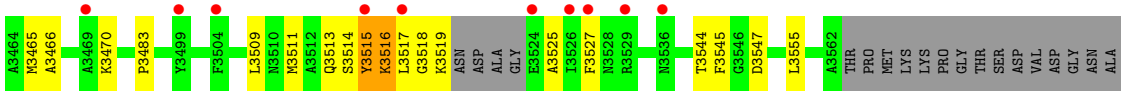
Chain C: 5% 64% 16% • 18%





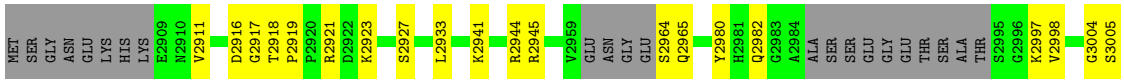


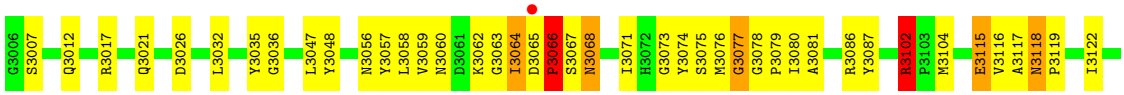


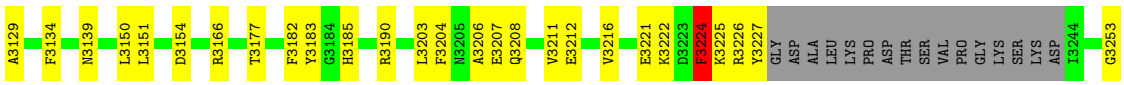


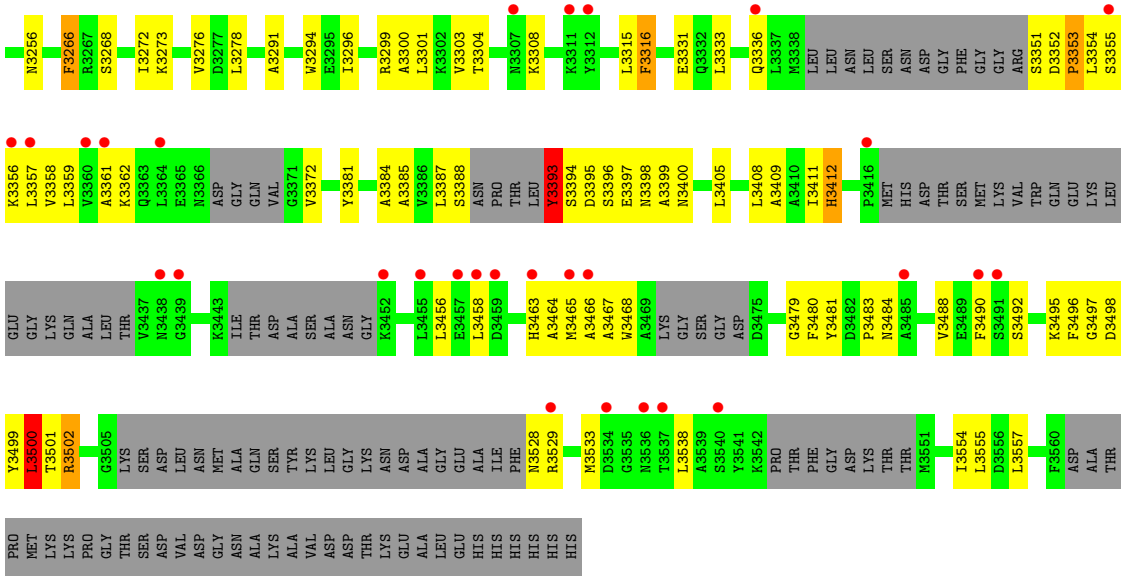
• Molecule 1: Putative RTX-toxin

Chain D: 4% 53% 22% •• 22%








Y3499 L3500 T3501 R3502 G3505 LYS SER ASP LEU ASN MET ALA GLN SER TYR LYS LEU GLY LYS ASN ASP ALA GLY GLU ALA ILE PHE N3528 R3529 M3533 D3534 G3535 N3536 T3537 L3538 A3539 S3540 Y3541 K3542 PRO THR PHE GLY ASP LYS THR THR M3551 I3554 L3555 D3556 L3557 F3560 ASP ALA THR
PRO MET LYS LYS PRO GLY THR SER ASP VAL ASP GLY ASN ALA LYS ALA VAL ASP ASP THR LYS GLU ALA LEU GLU HIS HIS HIS HIS HIS
GLU GLY LYS GLN ALA LEU THR V3437 N3438 G3439 K3443 ILE THR ASP ALA SER ALA ASN GLY K3452 L3455 L3456 E3457 L3458 D3459 H3463 A3464 M3465 A3466 A3467 W3468 A3469 LYS GLY SER GLY ASP D3475 G3479 F3480 Y3481 D3482 P3483 N3484 A3485 V3488 E3489 F3490 S3491 S3492 K3495 F3496 G3497 D3498
K3356 L3357 V3358 L3359 V3360 A3361 K3362 Q3363 L3364 E3365 N3366 ASP GLY GLN VAL G3371 V3372 Y3381 A3384 A3385 V3386 L3387 S3388 ASN PRO THR LEU Y3393 S3394 D3395 S3396 E3397 N3398 A3399 N3400 L3405 L3408 A3409 A3410 I3411 H3412 P3416 MET HIS ASP THR SER MET LYS VAL TRP GLN GLU LYS LEU
N3256 F3266 R3267 S3268 I3272 K3273 V3276 D3277 L3278 A3291 W3294 E3295 I3296 R3299 A3300 L3301 K3302 V3303 T3304 N3307 K3308 K3311 Y3312 L3315 F3316 E3331 Q3332 L3333 Q3336 L3337 M3338 LEU LEU ASN LEU SER ASN ASP GLY PHE GLY GLY ARG S3351 D3352 P3353 L3354 S3355

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	86.22Å 108.59Å 334.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.60 – 3.50 49.62 – 3.50	Depositor EDS
% Data completeness (in resolution range)	77.5 (49.60-3.50) 77.6 (49.62-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.8.0158, REFMAC	Depositor
R, R_{free}	0.285 , 0.327 0.284 , 0.326	Depositor DCC
R_{free} test set	1514 reflections (4.81%)	wwPDB-VP
Wilson B-factor (Å^2)	44.1	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 33.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.79	EDS
Total number of atoms	17825	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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 (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	0.54	0/4756	0.66	8/6412 (0.1%)
1	B	0.50	0/4746	0.61	4/6394 (0.1%)
1	C	0.49	0/4402	0.66	6/5928 (0.1%)
1	D	0.55	0/4194	0.72	8/5643 (0.1%)
All	All	0.52	0/18098	0.66	26/24377 (0.1%)

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
1	B	0	4
1	C	0	3
1	D	0	6
All	All	0	14

There are no bond length outliers.

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	3102	ARG	NE-CZ-NH1	-9.04	115.78	120.30
1	C	3516	LYS	N-CA-C	-8.65	87.65	111.00
1	C	3065	ASP	N-CA-C	8.48	133.90	111.00
1	D	3102	ARG	NE-CZ-NH2	8.20	124.40	120.30
1	A	3073	GLY	N-CA-C	-7.49	94.36	113.10

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3283	SER	Peptide
1	B	2927	SER	Peptide
1	B	3201	SER	Peptide
1	B	3337	LEU	Peptide
1	B	3338	MET	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	4681	0	4639	143	0
1	B	4673	0	4633	148	0
1	C	4338	0	4314	143	0
1	D	4133	0	4104	249	0
All	All	17825	0	17690	666	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 19.

The worst 5 of 666 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:3304:THR:HG21	1:B:3337:LEU:HD23	1.31	1.13
1:C:2911:VAL:HA	1:C:3060:ASN:ND2	1.65	1.10
1:D:3315:LEU:HD21	1:D:3502:ARG:CB	1.82	1.09
1:A:3266:PHE:HB2	1:A:3278:LEU:CD2	1.84	1.06
1:A:3072:HIS:HD2	1:A:3099:LEU:HD23	1.18	1.06

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	604/694 (87%)	572 (95%)	29 (5%)	3 (0%)	29	68
1	B	600/694 (86%)	563 (94%)	34 (6%)	3 (0%)	29	68
1	C	546/694 (79%)	510 (93%)	34 (6%)	2 (0%)	34	72
1	D	515/694 (74%)	478 (93%)	34 (7%)	3 (1%)	25	64
All	All	2265/2776 (82%)	2123 (94%)	131 (6%)	11 (0%)	29	68

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	3066	PRO
1	D	3066	PRO
1	A	3353	PRO
1	C	3118	ASN
1	C	3352	ASP

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	490/555 (88%)	486 (99%)	4 (1%)	81	91
1	B	490/555 (88%)	485 (99%)	5 (1%)	76	88
1	C	453/555 (82%)	450 (99%)	3 (1%)	84	93
1	D	431/555 (78%)	421 (98%)	10 (2%)	50	77
All	All	1864/2220 (84%)	1842 (99%)	22 (1%)	71	87

5 of 22 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	3182	PHE
1	D	3316	PHE
1	D	3266	PHE

Continued on next page...

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Mol	Chain	Res	Type
1	D	3393	TYR
1	B	3266	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 (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 (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	614/694 (88%)	-0.29	7 (1%)	80	75	6, 33, 114, 159	0
1	B	612/694 (88%)	0.02	14 (2%)	60	54	22, 58, 99, 133	0
1	C	568/694 (81%)	0.40	34 (5%)	21	19	26, 74, 144, 172	0
1	D	539/694 (77%)	0.07	30 (5%)	24	22	17, 48, 145, 213	0
All	All	2333/2776 (84%)	0.04	85 (3%)	42	38	6, 54, 131, 213	0

The worst 5 of 85 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3527	PHE	6.2
1	D	3457	GLU	5.2
1	D	3065	ASP	4.8
1	D	3465	MET	4.6
1	C	3458	LEU	4.2

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 monosaccharides 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.