wwPDB X-ray Structure Validation Summary Report (i)

Jun 17, 2024 – 11:59 PM EDT

PDB ID	:	3V8U
Title	:	The crystal structure of transferrin binding protein B (TbpB) from Neisseria meningitidis serogroup B
Authors	:	Noinaj, N.; Easley, N.; Buchanan, S.K.
Deposited on	:	2011-12-23
Resolution	:	2.40 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:

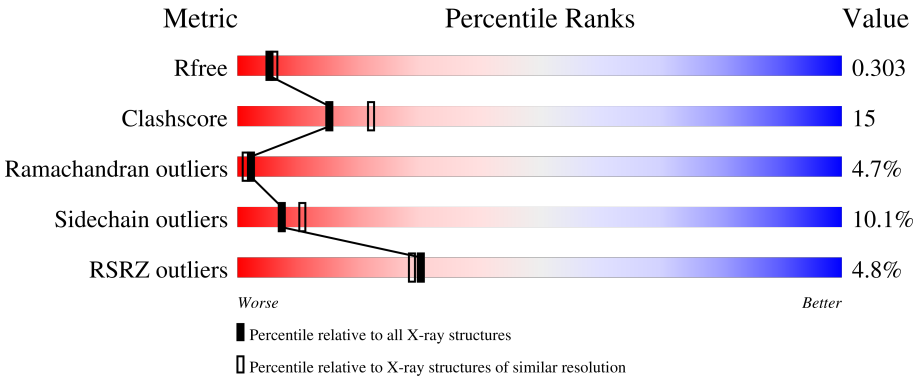
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	717	4% 44% 25% • • 26%
1	B	717	3% 45% 25% • • 26%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 8366 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 Transferrin binding-protein B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	532	Total	C	N	O	S	0	0	0
			4113	2586	707	814	6			
1	B	532	Total	C	N	O	S	0	0	0
			4106	2581	708	811	6			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-25	MET	-	EXPRESSION TAG	UNP Q9JPI9
A	-24	SER	-	EXPRESSION TAG	UNP Q9JPI9
A	-23	TYR	-	EXPRESSION TAG	UNP Q9JPI9
A	-22	TYR	-	EXPRESSION TAG	UNP Q9JPI9
A	-21	HIS	-	EXPRESSION TAG	UNP Q9JPI9
A	-20	HIS	-	EXPRESSION TAG	UNP Q9JPI9
A	-19	HIS	-	EXPRESSION TAG	UNP Q9JPI9
A	-18	HIS	-	EXPRESSION TAG	UNP Q9JPI9
A	-17	HIS	-	EXPRESSION TAG	UNP Q9JPI9
A	-16	HIS	-	EXPRESSION TAG	UNP Q9JPI9
A	-15	ASP	-	EXPRESSION TAG	UNP Q9JPI9
A	-14	TYR	-	EXPRESSION TAG	UNP Q9JPI9
A	-13	ASP	-	EXPRESSION TAG	UNP Q9JPI9
A	-12	ILE	-	EXPRESSION TAG	UNP Q9JPI9
A	-11	PRO	-	EXPRESSION TAG	UNP Q9JPI9
A	-10	THR	-	EXPRESSION TAG	UNP Q9JPI9
A	-9	THR	-	EXPRESSION TAG	UNP Q9JPI9
A	-8	GLU	-	EXPRESSION TAG	UNP Q9JPI9
A	-7	ASN	-	EXPRESSION TAG	UNP Q9JPI9
A	-6	LEU	-	EXPRESSION TAG	UNP Q9JPI9
A	-5	TYR	-	EXPRESSION TAG	UNP Q9JPI9
A	-4	PHE	-	EXPRESSION TAG	UNP Q9JPI9
A	-3	GLN	-	EXPRESSION TAG	UNP Q9JPI9
A	-2	GLY	-	EXPRESSION TAG	UNP Q9JPI9
A	-1	ALA	-	EXPRESSION TAG	UNP Q9JPI9

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	EXPRESSION TAG	UNP Q9JPI9
B	-25	MET	-	EXPRESSION TAG	UNP Q9JPI9
B	-24	SER	-	EXPRESSION TAG	UNP Q9JPI9
B	-23	TYR	-	EXPRESSION TAG	UNP Q9JPI9
B	-22	TYR	-	EXPRESSION TAG	UNP Q9JPI9
B	-21	HIS	-	EXPRESSION TAG	UNP Q9JPI9
B	-20	HIS	-	EXPRESSION TAG	UNP Q9JPI9
B	-19	HIS	-	EXPRESSION TAG	UNP Q9JPI9
B	-18	HIS	-	EXPRESSION TAG	UNP Q9JPI9
B	-17	HIS	-	EXPRESSION TAG	UNP Q9JPI9
B	-16	HIS	-	EXPRESSION TAG	UNP Q9JPI9
B	-15	ASP	-	EXPRESSION TAG	UNP Q9JPI9
B	-14	TYR	-	EXPRESSION TAG	UNP Q9JPI9
B	-13	ASP	-	EXPRESSION TAG	UNP Q9JPI9
B	-12	ILE	-	EXPRESSION TAG	UNP Q9JPI9
B	-11	PRO	-	EXPRESSION TAG	UNP Q9JPI9
B	-10	THR	-	EXPRESSION TAG	UNP Q9JPI9
B	-9	THR	-	EXPRESSION TAG	UNP Q9JPI9
B	-8	GLU	-	EXPRESSION TAG	UNP Q9JPI9
B	-7	ASN	-	EXPRESSION TAG	UNP Q9JPI9
B	-6	LEU	-	EXPRESSION TAG	UNP Q9JPI9
B	-5	TYR	-	EXPRESSION TAG	UNP Q9JPI9
B	-4	PHE	-	EXPRESSION TAG	UNP Q9JPI9
B	-3	GLN	-	EXPRESSION TAG	UNP Q9JPI9
B	-2	GLY	-	EXPRESSION TAG	UNP Q9JPI9
B	-1	ALA	-	EXPRESSION TAG	UNP Q9JPI9
B	0	MET	-	EXPRESSION TAG	UNP Q9JPI9

- Molecule 2 is water.

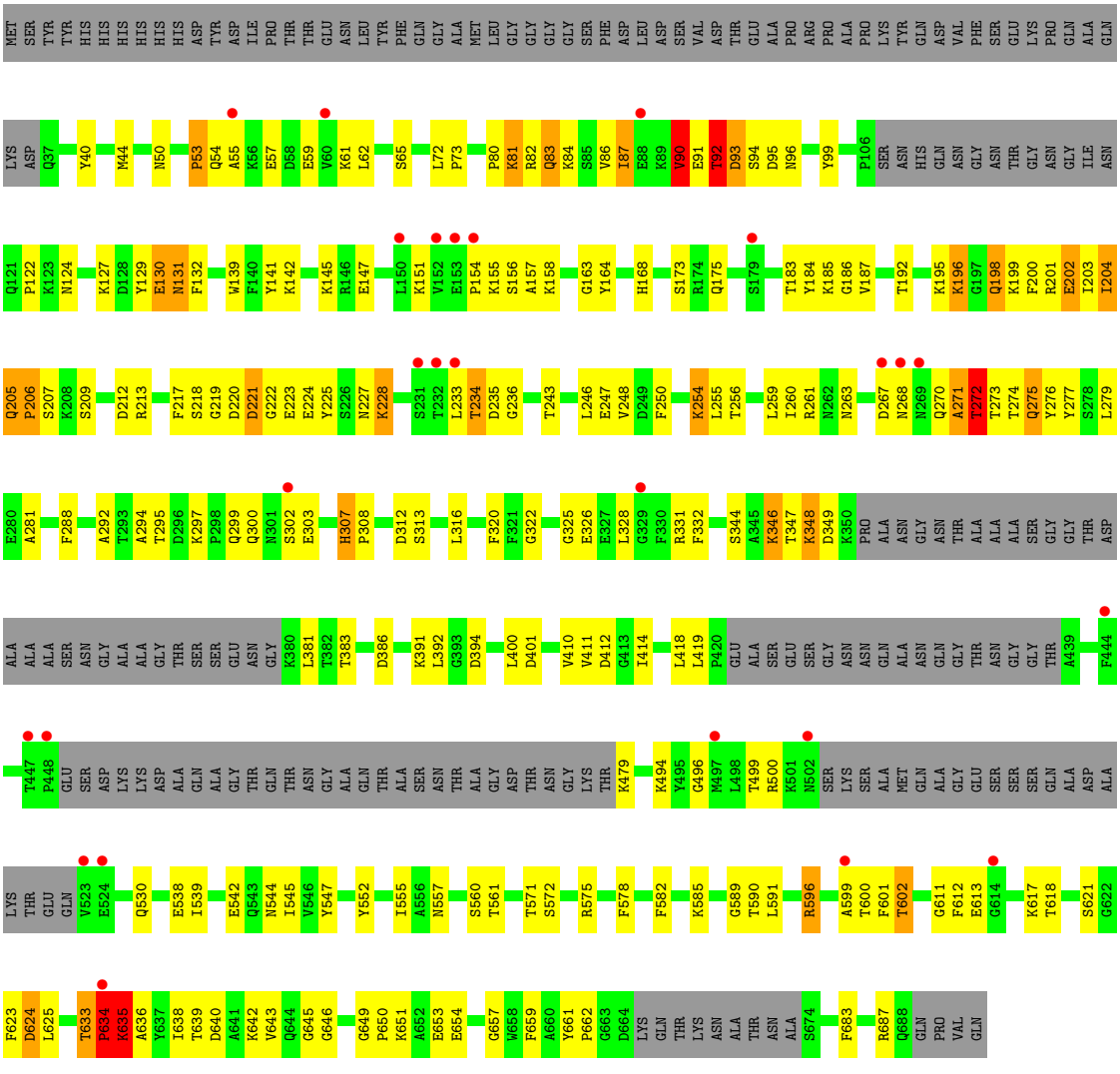
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	78	Total O 78 78	0	0
2	B	69	Total O 69 69	0	0

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.

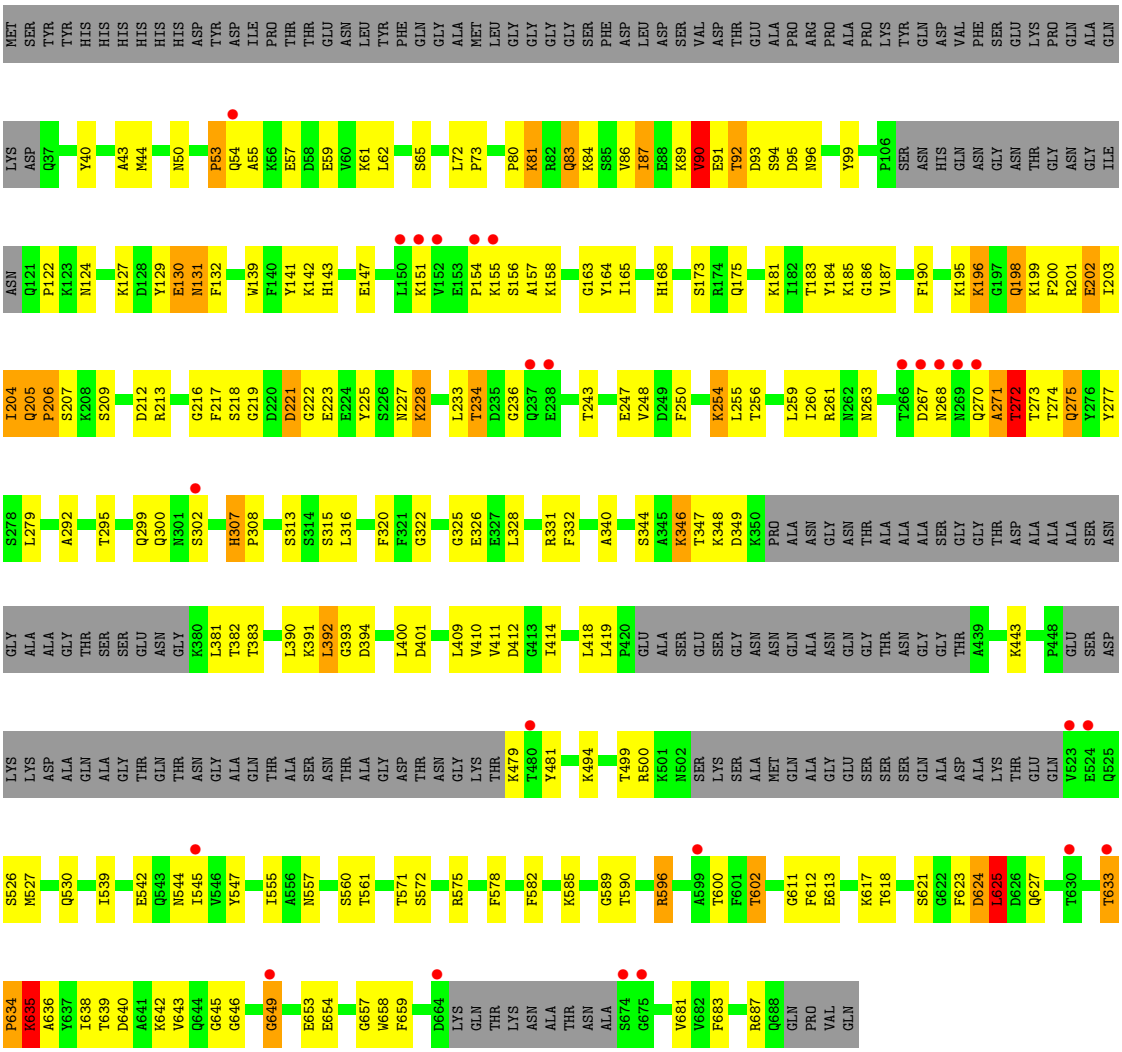
• Molecule 1: Transferrin binding-protein B

Chain A:



• Molecule 1: Transferrin binding-protein B

Chain B:


MET SER TYR TYR HIS HIS HIS HIS HIS ASP TYR ASP ILE PRO THR THR GLU ASN LEU TYR PHE GLN GLY ALA MET LEU GLY GLY GLY GLY SER PHE ASP LEU ASP SER VAL ASP THR GLU ALA PRO ARG PRO ALA PRO LYS TYR GLN ASP VAL PHE SER GLU LYS PRO GLN ALA GLN
LYS ASP Q37 Y40 A43 M44 N50 P53 Q54 A55 K56 E57 D58 E59 V60 K61 L62 S65 L72 P73 P80 K81 R82 Q83 K84 S85 V86 I87 E88 K89 V90 E91 T92 D93 S94 D95 N96 Y99 P106 SER ASN HIS GLN ASN GLY ASN THR GLY ASN GLY ILE
ASN Q121 P122 K123 N124 K127 D128 Y129 E130 N131 F132 W139 F140 Y141 K142 H143 E147 L150 K151 V152 E153 P154 K155 S156 A157 K158 G163 Y164 I165 H168 S173 R174 Q175 K181 I182 T183 Y184 K185 G186 V187 F190 K195 K196 G197 Q198 K199 F200 R201 E202 I203
I204 Q205 P206 S207 K208 S209 D212 R213 G216 F217 S218 G219 D220 D221 G222 E223 E224 Y225 S226 N227 K228 L233 T234 D235 G236 Q237 E238 T243 E247 V248 D249 F250 K254 L255 T256 L259 I260 R261 N262 N263 T266 D267 N268 N269 Q270 A271 T272 T273 T274 Q275 Y276 Y277
S278 L279 A292 T295 Q299 Q300 N301 S302 H307 P308 S313 S314 S315 L316 F320 F321 G322 G325 E326 E327 L328 R331 F332 A340 S344 A345 K346 T347 K348 D349 K350 PRO ALA ASN GLY ASN THR ALA ALA ALA SER GLY GLY THR ASP ALA ALA ALA SER ASN
GLY ALA ALA GLY THR SER SER GLU ASN GLY K380 L381 T382 T383 L390 K391 L392 G393 D394 L400 D401 L409 V410 V411 D412 G413 I414 L418 L419 P420 GLU ALA SER GLU SER GLY ASN ASN GLN ALA ASN GLN GLY THR ASN GLY GLY THR A439 K443 P448 GLU SER ASP
LYS LYS ASP ALA GLN ALA GLY THR GLN THR ASN GLY ALA GLN THR ALA SER ASN THR ALA GLY ASP THR ASN GLY LYS THR K479 T480 Y481 K494 T499 R500 K501 N502 SER LYS SER ALA MET GLN ALA GLY GLU SER SER SER GLN ALA ASP ALA LYS THR GLU GLN V523 E524 Q525
S526 M527 Q530 I539 E542 Q543 N544 I545 V546 Y547 I555 A556 N557 S560 T561 T571 S572 R575 F578 F582 K585 G589 T590 R596 A599 T600 F601 T602 G611 F612 E613 K617 T618 S621 G622 F623 D624 L625 D626 Q627 T630 T633
P634 K635 A636 Y637 I638 T639 D640 A641 K642 V643 D644 G645 G646 G649 E653 E654 G657 W658 F659 D664 LYS GLN THR LYS ASN ALA THR ASN ALA S674 G675 V681 V682 F683 R687 D688 GLN PRO VAL GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.03Å 82.13Å 111.31Å 90.00° 106.07° 90.00°	Depositor
Resolution (Å)	29.50 – 2.40 38.19 – 2.38	Depositor EDS
% Data completeness (in resolution range)	95.1 (29.50-2.40) 94.4 (38.19-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	1.99 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.253 , 0.308 0.247 , 0.303	Depositor DCC
R_{free} test set	2001 reflections (4.04%)	wwPDB-VP
Wilson B-factor (Å^2)	35.6	Xtriage
Anisotropy	0.679	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8366	wwPDB-VP
Average B, all atoms (Å^2)	65.0	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 28.49 % 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 1.8259e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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

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	0.50	0/4200	0.70	0/5667
1	B	0.50	0/4192	0.70	1/5655 (0.0%)
All	All	0.50	0/8392	0.70	1/11322 (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	6
1	B	0	6
All	All	0	12

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	625	LEU	N-CA-C	-7.55	90.61	111.00

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	624	ASP	Peptide
1	A	633	THR	Peptide
1	A	634	PRO	Peptide
1	A	90	VAL	Peptide
1	A	92	THR	Peptide

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	4113	0	3871	122	0
1	B	4106	0	3871	117	0
2	A	78	0	0	4	0
2	B	69	0	0	4	0
All	All	8366	0	7742	239	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 15.

The worst 5 of 239 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:261:ARG:NH1	1:A:263:ASN:OD1	2.11	0.84
1:B:611:GLY:HA2	1:B:646:GLY:HA2	1.58	0.83
1:B:202:GLU:HB3	1:B:261:ARG:HH21	1.44	0.83
1:A:611:GLY:HA2	1:A:646:GLY:HA2	1.60	0.82
1:A:87:ILE:HD11	1:A:163:GLY:HA2	1.62	0.81

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	518/717 (72%)	446 (86%)	47 (9%)	25 (5%)	2 1
1	B	518/717 (72%)	449 (87%)	45 (9%)	24 (5%)	2 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1036/1434 (72%)	895 (86%)	92 (9%)	49 (5%)	2 1

5 of 49 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	A	93	ASP
1	A	94	SER
1	A	130	GLU
1	A	155	LYS

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	423/586 (72%)	381 (90%)	42 (10%)	8 11
1	B	422/586 (72%)	379 (90%)	43 (10%)	7 10
All	All	845/1172 (72%)	760 (90%)	85 (10%)	7 11

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	204	ILE
1	B	383	THR
1	B	228	LYS
1	B	299	GLN
1	B	499	THR

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

Mol	Chain	Res	Type
1	A	307	HIS
1	B	124	ASN
1	B	307	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	532/717 (74%)	0.28	26 (4%)	29	28	28, 62, 101, 140	0
1	B	532/717 (74%)	0.24	25 (4%)	31	30	30, 61, 101, 141	0
All	All	1064/1434 (74%)	0.26	51 (4%)	30	29	28, 62, 101, 141	0

The worst 5 of 51 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	269	ASN	6.3
1	A	232	THR	5.0
1	B	302	SER	4.9
1	B	674	SER	4.8
1	B	154	PRO	4.3

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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.