



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:21 PM UTC

PDB ID : 8GEX / pdb\_00008gex  
Title : Crystal structure of the ferric enterobactin transporter (XusB) from *Bacteroides thetaiotaomicron*  
Authors : Perera, Y.R.; Chazin, W.J.  
Deposited on : 2023-03-07  
Resolution : 2.55 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

<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>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

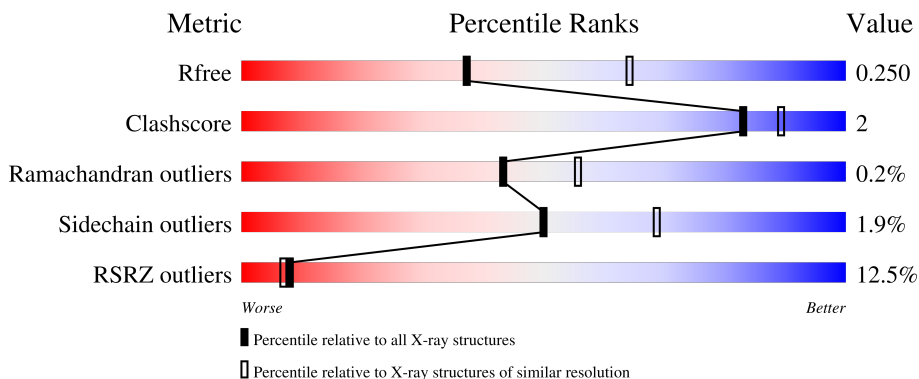
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.55 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.



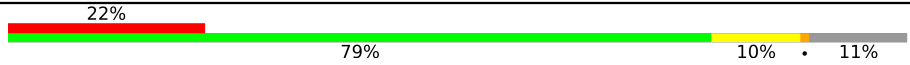
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	424	 10% 91% 6%
1	B	424	 9% 90% 6%
1	C	424	 7% 89% 7%
1	D	424	 8% 89% 7%
1	E	424	 15% 87% 8%

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Mol	Chain	Length	Quality of chain
1	F	424	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment on the left labeled '22%', a large green segment labeled '79%', a yellow segment labeled '10%', and a grey segment on the far right labeled '11%'.</p>

## 2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 19062 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 DUF4374 domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	411	3189	2024	524	631	10	0	0	0
1	B	408	3163	2006	521	626	10	0	0	0
1	C	406	3153	2001	519	623	10	0	0	0
1	D	410	3175	2012	523	630	10	0	0	0
1	E	406	3147	1998	517	622	10	0	0	0
1	F	378	2954	1888	475	581	10	0	0	0

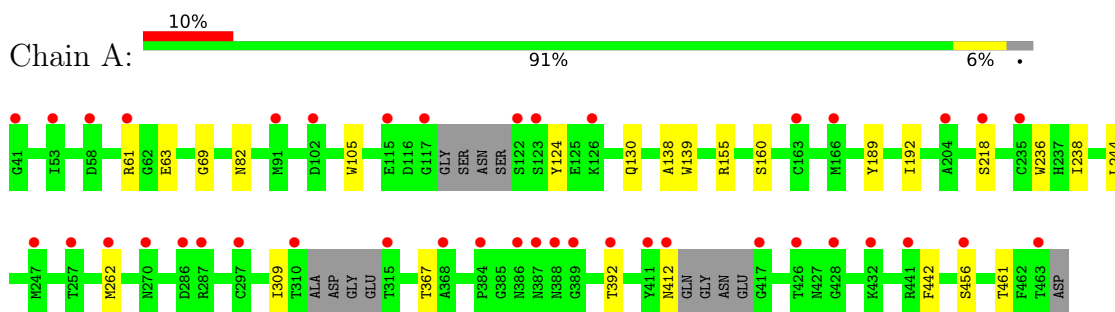
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	75	Total 75	O 75	0	0
2	B	77	Total 77	O 77	0	0
2	C	42	Total 42	O 42	0	0
2	D	42	Total 42	O 42	0	0
2	E	25	Total 25	O 25	0	0
2	F	20	Total 20	O 20	0	0

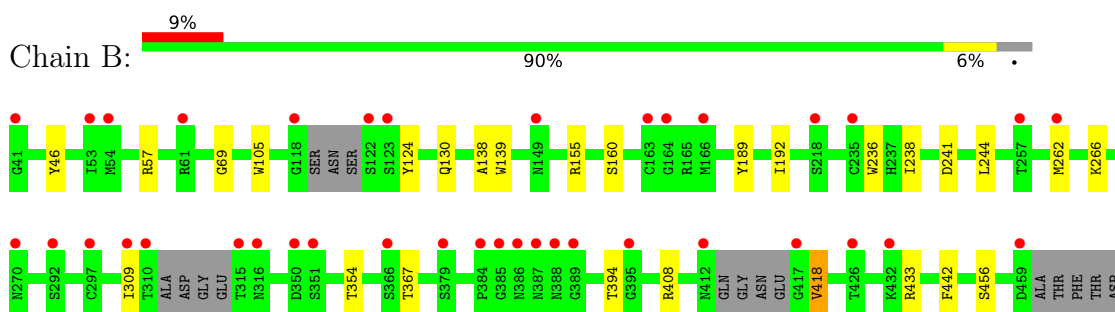
### 3 Residue-property plots [i](#)

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.

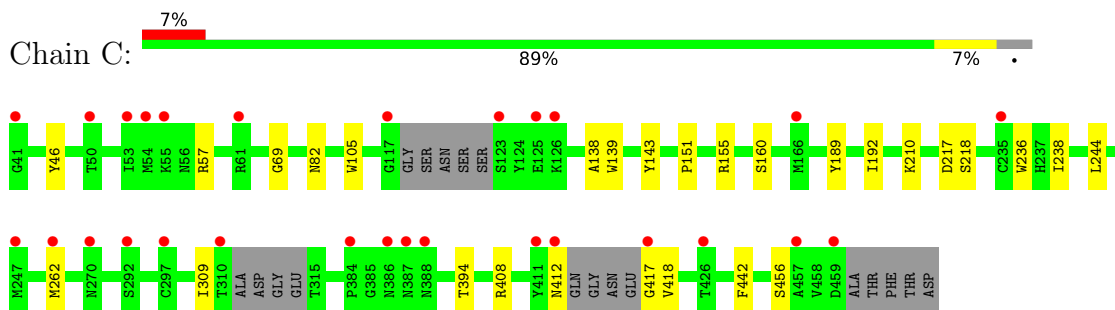
- Molecule 1: DUF4374 domain-containing protein



- Molecule 1: DUF4374 domain-containing protein



- Molecule 1: DUF4374 domain-containing protein



- Molecule 1: DUF4374 domain-containing protein





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	174.19Å 174.19Å 294.28Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.90 – 2.55 29.90 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.90-2.55) 99.8 (29.90-2.55)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.65 (at 2.54Å)	Xtrriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.224 , 0.247 0.232 , 0.250	Depositor DCC
$R_{free}$ test set	8538 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	44.9	Xtrriage
Anisotropy	1.100	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	19062	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.32% 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, 0.333 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	0.09	0/3262	0.28	0/4439
1	B	0.09	0/3235	0.28	0/4401
1	C	0.08	0/3225	0.27	0/4388
1	D	0.10	0/3247	0.29	0/4417
1	E	0.09	0/3218	0.28	0/4378
1	F	0.10	0/3017	0.30	0/4096
All	All	0.09	0/19204	0.28	0/26119

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 [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	3189	0	3055	9	0
1	B	3163	0	3030	12	0
1	C	3153	0	3022	14	0
1	D	3175	0	3040	14	0
1	E	3147	0	3014	19	0
1	F	2954	0	2829	20	0
2	A	75	0	0	0	0
2	B	77	0	0	0	0
2	C	42	0	0	0	0
2	D	42	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	25	0	0	0	0
2	F	20	0	0	0	0
All	All	19062	0	17990	88	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 2.

All (88) 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:F:303:TYR:HB3	1:F:320:ILE:HD11	1.79	0.63
1:A:442:PHE:HA	1:A:456:SER:HB3	1.81	0.62
1:D:408:ARG:NH2	1:D:418:VAL:O	2.33	0.61
1:F:61:ARG:HE	1:F:63:GLU:HB2	1.66	0.60
1:F:205:GLY:HA2	1:F:223:LEU:HD23	1.83	0.60
1:C:210:LYS:NZ	1:C:217:ASP:OD2	2.33	0.59
1:D:442:PHE:HA	1:D:456:SER:HB2	1.86	0.57
1:F:354:THR:HG21	1:F:373:ALA:HB1	1.87	0.57
1:E:442:PHE:HA	1:E:456:SER:HB2	1.87	0.57
1:D:238:ILE:HD11	1:D:244:LEU:HB2	1.87	0.56
1:B:442:PHE:HA	1:B:456:SER:HB2	1.89	0.54
1:F:439:ILE:HD13	1:F:439:ILE:H	1.72	0.54
1:B:238:ILE:HD11	1:B:244:LEU:HB2	1.89	0.54
1:D:49:VAL:O	1:D:433:ARG:NH2	2.26	0.54
1:F:238:ILE:HD11	1:F:244:LEU:HB2	1.90	0.53
1:D:394:THR:O	1:D:408:ARG:NH1	2.41	0.53
1:A:61:ARG:HE	1:A:63:GLU:HB2	1.74	0.52
1:E:238:ILE:HD11	1:E:244:LEU:HB2	1.91	0.52
1:B:394:THR:O	1:B:408:ARG:NH1	2.42	0.52
1:E:394:THR:O	1:E:408:ARG:NH1	2.42	0.52
1:C:442:PHE:HA	1:C:456:SER:HB2	1.92	0.52
1:C:394:THR:O	1:C:408:ARG:NH1	2.43	0.52
1:E:69:GLY:HA3	1:E:105:TRP:CG	2.46	0.51
1:C:412:ASN:HA	1:C:417:GLY:HA3	1.92	0.51
1:F:421:ALA:HB3	1:F:433:ARG:HD3	1.93	0.51
1:E:46:TYR:HB2	1:E:55:LYS:HB2	1.92	0.50
1:E:46:TYR:HE2	1:E:57:ARG:HB2	1.77	0.50
1:B:408:ARG:NH2	1:B:418:VAL:O	2.46	0.48
1:B:139:TRP:CZ2	1:B:155:ARG:HD3	2.48	0.48
1:C:238:ILE:HD11	1:C:244:LEU:HB2	1.95	0.48
1:A:139:TRP:CZ2	1:A:155:ARG:HD3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:ILE:HD11	1:A:244:LEU:HB2	1.96	0.48
1:E:408:ARG:NH2	1:E:418:VAL:O	2.47	0.48
1:D:334:LEU:HD11	1:D:382:VAL:HG13	1.95	0.47
1:B:69:GLY:HA3	1:B:105:TRP:CG	2.49	0.47
1:F:442:PHE:HA	1:F:456:SER:HB2	1.96	0.47
1:D:236:TRP:HZ3	1:D:262:MET:HE1	1.78	0.47
1:E:346:ARG:HH12	1:E:353:SER:HB2	1.79	0.47
1:F:125:GLU:O	1:F:128:GLU:HG2	2.15	0.47
1:E:208:ARG:NH2	1:E:272:ASP:OD1	2.46	0.47
1:C:139:TRP:CZ2	1:C:155:ARG:HD3	2.50	0.46
1:D:119:SER:O	1:D:121:SER:N	2.48	0.46
1:F:183:TYR:CE2	1:F:208:ARG:HG3	2.49	0.46
1:B:189:TYR:CZ	1:B:192:ILE:HD11	2.51	0.46
1:C:69:GLY:HA3	1:C:105:TRP:CG	2.50	0.46
1:A:69:GLY:HA3	1:A:105:TRP:CG	2.52	0.46
1:E:362:THR:HG23	1:E:367:THR:HG22	1.97	0.46
1:F:206:VAL:HG12	1:F:223:LEU:HD21	1.98	0.46
1:D:143:TYR:CZ	1:D:151:PRO:HB3	2.52	0.45
1:F:242:TYR:CZ	1:F:266:LYS:HD2	2.52	0.45
1:C:189:TYR:CZ	1:C:192:ILE:HD11	2.52	0.45
1:E:130:GLN:HG2	1:E:131:TRP:CD1	2.52	0.45
1:E:387:ASN:O	1:E:388:ASN:ND2	2.50	0.44
1:F:139:TRP:CZ2	1:F:155:ARG:HD3	2.52	0.44
1:D:69:GLY:HA3	1:D:105:TRP:CG	2.52	0.44
1:E:139:TRP:CZ2	1:E:155:ARG:HD3	2.52	0.44
1:A:189:TYR:CZ	1:A:192:ILE:HD11	2.53	0.44
1:D:143:TYR:CE1	1:D:151:PRO:HB3	2.51	0.44
1:A:236:TRP:HZ3	1:A:262:MET:HE1	1.82	0.44
1:D:139:TRP:CZ2	1:D:155:ARG:HD3	2.53	0.44
1:E:46:TYR:CE2	1:E:57:ARG:HB2	2.53	0.44
1:E:334:LEU:HD11	1:E:382:VAL:HG13	2.00	0.44
1:F:392:THR:HG22	1:F:393:ALA:O	2.18	0.44
1:B:236:TRP:HZ3	1:B:262:MET:HE1	1.83	0.44
1:C:408:ARG:NH2	1:C:418:VAL:O	2.51	0.44
1:B:138:ALA:HB2	1:B:160:SER:O	2.18	0.43
1:E:143:TYR:CZ	1:E:151:PRO:HB3	2.53	0.43
1:C:236:TRP:HZ3	1:C:262:MET:HE1	1.83	0.42
1:F:303:TYR:CD1	1:F:320:ILE:HD11	2.54	0.42
1:A:124:TYR:HB3	1:A:130:GLN:NE2	2.35	0.42
1:B:46:TYR:CE2	1:B:57:ARG:HB2	2.55	0.42
1:D:143:TYR:CD1	1:D:148:PHE:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:TYR:CZ	1:C:151:PRO:HB3	2.56	0.41
1:E:138:ALA:HB2	1:E:160:SER:O	2.21	0.41
1:E:143:TYR:CE1	1:E:151:PRO:HB3	2.56	0.41
1:E:439:ILE:HD12	1:E:440:THR:O	2.20	0.41
1:C:46:TYR:HE2	1:C:57:ARG:HB2	1.85	0.41
1:C:138:ALA:HB2	1:C:160:SER:O	2.20	0.41
1:F:138:ALA:HB2	1:F:160:SER:O	2.21	0.41
1:C:143:TYR:CE1	1:C:151:PRO:HB3	2.56	0.41
1:F:69:GLY:HA3	1:F:105:TRP:CG	2.55	0.41
1:F:355:TYR:HB2	1:F:374:THR:HG23	2.03	0.41
1:B:241:ASP:OD1	1:B:266:LYS:NZ	2.50	0.41
1:F:143:TYR:CE1	1:F:151:PRO:HB3	2.55	0.40
1:D:138:ALA:HB2	1:D:160:SER:O	2.21	0.40
1:F:422:TYR:CD2	1:F:432:LYS:HA	2.56	0.40
1:A:138:ALA:HB2	1:A:160:SER:O	2.21	0.40
1:B:124:TYR:HB3	1:B:130:GLN:NE2	2.36	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	403/424 (95%)	390 (97%)	13 (3%)	0	100	100
1	B	400/424 (94%)	386 (96%)	13 (3%)	1 (0%)	36	45
1	C	398/424 (94%)	384 (96%)	14 (4%)	0	100	100
1	D	402/424 (95%)	385 (96%)	16 (4%)	1 (0%)	43	56
1	E	396/424 (93%)	382 (96%)	12 (3%)	2 (0%)	24	34
1	F	359/424 (85%)	348 (97%)	11 (3%)	0	100	100
All	All	2358/2544 (93%)	2275 (96%)	79 (3%)	4 (0%)	43	56

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	433	ARG
1	D	433	ARG
1	E	388	ASN
1	E	433	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	338/347 (97%)	331 (98%)	7 (2%)	47 66
1	B	335/347 (96%)	331 (99%)	4 (1%)	63 78
1	C	334/347 (96%)	331 (99%)	3 (1%)	70 82
1	D	337/347 (97%)	330 (98%)	7 (2%)	47 66
1	E	332/347 (96%)	327 (98%)	5 (2%)	57 74
1	F	312/347 (90%)	301 (96%)	11 (4%)	32 48
All	All	1988/2082 (96%)	1951 (98%)	37 (2%)	50 69

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ASN
1	A	218	SER
1	A	309	ILE
1	A	367	THR
1	A	392	THR
1	A	412	ASN
1	A	461	THR
1	B	309	ILE
1	B	354	THR
1	B	367	THR
1	B	418	VAL
1	C	82	ASN
1	C	218	SER

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Mol	Chain	Res	Type
1	C	309	ILE
1	D	53	ILE
1	D	82	ASN
1	D	129	LEU
1	D	309	ILE
1	D	354	THR
1	D	371	LEU
1	D	387	ASN
1	E	82	ASN
1	E	129	LEU
1	E	309	ILE
1	E	354	THR
1	E	439	ILE
1	F	47	LEU
1	F	77	ILE
1	F	208	ARG
1	F	218	SER
1	F	320	ILE
1	F	334	LEU
1	F	344	ILE
1	F	367	THR
1	F	409	LEU
1	F	439	ILE
1	F	440	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	GLN
1	B	52	GLN
1	B	56	ASN
1	B	328	HIS
1	B	337	ASN
1	B	404	GLN
1	B	451	ASN
1	C	52	GLN
1	C	337	ASN
1	C	451	ASN
1	D	56	ASN
1	D	337	ASN
1	D	387	ASN
1	E	337	ASN

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Mol	Chain	Res	Type
1	E	388	ASN
1	F	52	GLN
1	F	130	GLN
1	F	198	GLN
1	F	328	HIS

### 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 oligosaccharides 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	411/424 (96%)	0.86	41 (9%) 12 12	44, 62, 91, 149	0
1	B	408/424 (96%)	0.81	38 (9%) 14 13	44, 60, 86, 126	0
1	C	406/424 (95%)	0.81	28 (6%) 23 22	52, 69, 96, 128	0
1	D	410/424 (96%)	0.96	35 (8%) 16 16	54, 72, 94, 131	0
1	E	406/424 (95%)	1.17	65 (16%) 5 4	61, 81, 114, 144	0
1	F	378/424 (89%)	1.55	95 (25%) 1 1	63, 94, 127, 149	0
All	All	2419/2544 (95%)	1.02	302 (12%) 8 7	44, 71, 112, 149	0

All (302) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	424	LEU	9.5
1	F	382	VAL	8.0
1	E	311	ALA	6.9
1	F	367	THR	6.8
1	D	121	SER	6.2
1	E	460	ALA	5.7
1	F	362	THR	5.5
1	B	118	GLY	5.5
1	E	55	LYS	5.2
1	B	388	ASN	5.2
1	A	388	ASN	5.1
1	E	130	GLN	5.1
1	C	310	THR	5.0
1	B	122	SER	5.0
1	F	117	GLY	5.0
1	E	388	ASN	5.0
1	C	388	ASN	4.9
1	E	387	ASN	4.8
1	F	460	ALA	4.8

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	380	GLY	4.8
1	F	308	PRO	4.8
1	F	317	HIS	4.8
1	D	417	GLY	4.7
1	F	432	LYS	4.6
1	A	122	SER	4.6
1	A	102	ASP	4.6
1	F	53	ILE	4.6
1	E	417	GLY	4.5
1	A	412	ASN	4.5
1	F	183	TYR	4.4
1	A	117	GLY	4.4
1	E	117	GLY	4.3
1	E	351	SER	4.2
1	F	123	SER	4.2
1	A	387	ASN	4.2
1	D	412	ASN	4.2
1	B	386	ASN	4.2
1	E	123	SER	4.1
1	F	412	ASN	4.1
1	D	387	ASN	4.1
1	A	417	GLY	4.1
1	F	336	VAL	4.1
1	C	412	ASN	4.1
1	F	299	ASN	4.0
1	F	339	THR	4.0
1	B	459	ASP	4.0
1	F	417	GLY	4.0
1	D	41	GLY	3.9
1	A	386	ASN	3.9
1	B	412	ASN	3.9
1	F	353	SER	3.9
1	C	387	ASN	3.8
1	A	463	THR	3.8
1	B	310	THR	3.8
1	F	287	ARG	3.8
1	F	370	TYR	3.8
1	B	387	ASN	3.7
1	F	345	GLY	3.7
1	B	53	ILE	3.7
1	A	411	TYR	3.7
1	E	352	HIS	3.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	315	THR	3.6
1	E	458	VAL	3.6
1	E	53	ILE	3.6
1	F	371	LEU	3.6
1	A	310	THR	3.6
1	F	354	THR	3.6
1	F	434	SER	3.6
1	B	417	GLY	3.6
1	C	117	GLY	3.5
1	F	286	ASP	3.5
1	E	292	SER	3.5
1	E	348	ALA	3.5
1	E	386	ASN	3.5
1	E	125	GLU	3.4
1	F	361	VAL	3.4
1	B	41	GLY	3.4
1	E	41	GLY	3.4
1	F	167	ARG	3.4
1	C	41	GLY	3.4
1	F	423	GLU	3.4
1	F	102	ASP	3.4
1	F	82	ASN	3.4
1	C	417	GLY	3.4
1	F	166	MET	3.3
1	E	102	ASP	3.3
1	F	333	GLY	3.3
1	D	119	SER	3.3
1	E	411	TYR	3.3
1	D	310	THR	3.3
1	E	435	ASN	3.2
1	F	377	LEU	3.2
1	D	309	ILE	3.2
1	D	386	ASN	3.2
1	F	334	LEU	3.2
1	F	403	ASP	3.2
1	C	386	ASN	3.2
1	E	403	ASP	3.2
1	E	459	ASP	3.2
1	F	450	GLU	3.2
1	F	55	LYS	3.1
1	A	126	LYS	3.1
1	A	166	MET	3.1

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	440	THR	3.1
1	B	262	MET	3.0
1	D	459	ASP	3.0
1	E	163	CYS	3.0
1	D	411	TYR	3.0
1	F	411	TYR	3.0
1	C	123	SER	3.0
1	D	149	ASN	3.0
1	E	315	THR	2.9
1	F	376	THR	2.9
1	E	95	VAL	2.9
1	F	459	ASP	2.9
1	D	122	SER	2.9
1	E	434	SER	2.9
1	B	315	THR	2.9
1	E	310	THR	2.9
1	D	218	SER	2.8
1	D	270	ASN	2.8
1	A	262	MET	2.8
1	B	149	ASN	2.8
1	C	53	ILE	2.8
1	E	426	THR	2.8
1	D	166	MET	2.8
1	B	270	ASN	2.8
1	B	379	SER	2.8
1	C	54	MET	2.8
1	E	432	LYS	2.8
1	F	297	CYS	2.8
1	B	61	ARG	2.8
1	F	375	SER	2.7
1	F	456	SER	2.7
1	F	284	GLU	2.7
1	B	164	GLY	2.7
1	E	99	ALA	2.7
1	A	286	ASP	2.7
1	F	356	VAL	2.7
1	F	331	THR	2.7
1	A	392	THR	2.7
1	F	360	THR	2.7
1	F	464	ASP	2.6
1	B	385	GLY	2.6
1	D	118	GLY	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	247	MET	2.6
1	B	54	MET	2.6
1	D	287	ARG	2.6
1	F	247	MET	2.6
1	C	459	ASP	2.6
1	A	235	CYS	2.6
1	D	163	CYS	2.6
1	B	257	THR	2.6
1	E	392	THR	2.6
1	A	41	GLY	2.6
1	A	441	ARG	2.6
1	F	212	GLY	2.6
1	F	372	LEU	2.6
1	F	163	CYS	2.6
1	F	50	THR	2.5
1	F	292	SER	2.5
1	A	287	ARG	2.5
1	D	316	ASN	2.5
1	A	218	SER	2.5
1	C	235	CYS	2.5
1	D	367	THR	2.5
1	F	405	TYR	2.5
1	F	320	ILE	2.5
1	F	335	THR	2.5
1	E	127	GLY	2.5
1	E	271	GLY	2.5
1	F	391	GLU	2.5
1	F	49	VAL	2.5
1	F	326	VAL	2.5
1	A	123	SER	2.5
1	B	292	SER	2.5
1	D	315	THR	2.5
1	D	61	ARG	2.4
1	E	166	MET	2.4
1	A	257	THR	2.4
1	C	426	THR	2.4
1	E	214	THR	2.4
1	E	367	THR	2.4
1	B	235	CYS	2.4
1	A	91	MET	2.4
1	C	166	MET	2.4
1	E	56	ASN	2.4

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	E	427	ASN	2.4
1	F	368	ALA	2.4
1	B	366	SER	2.4
1	F	322	LYS	2.4
1	B	389	GLY	2.4
1	D	235	CYS	2.4
1	E	430	ILE	2.4
1	F	433	ARG	2.4
1	F	418	VAL	2.4
1	F	240	GLY	2.3
1	E	390	PHE	2.3
1	E	457	ALA	2.3
1	D	354	THR	2.3
1	E	441	ARG	2.3
1	F	395	GLY	2.3
1	B	166	MET	2.3
1	F	270	ASN	2.3
1	B	384	PRO	2.3
1	F	283	PRO	2.3
1	A	456	SER	2.3
1	B	123	SER	2.3
1	D	385	GLY	2.3
1	F	344	ILE	2.3
1	E	91	MET	2.3
1	C	55	LYS	2.3
1	A	163	CYS	2.3
1	D	292	SER	2.3
1	E	98	SER	2.3
1	D	126	LYS	2.3
1	E	314	GLU	2.3
1	B	163	CYS	2.3
1	B	316	ASN	2.2
1	C	61	ARG	2.3
1	C	297	CYS	2.3
1	C	384	PRO	2.3
1	C	411	TYR	2.3
1	D	297	CYS	2.3
1	F	421	ALA	2.2
1	B	395	GLY	2.2
1	D	262	MET	2.2
1	E	126	LYS	2.2
1	F	210	LYS	2.2

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	F	262	MET	2.2
1	A	58	ASP	2.2
1	B	426	THR	2.2
1	F	48	HIS	2.2
1	A	432	LYS	2.2
1	C	247	MET	2.2
1	C	262	MET	2.2
1	E	309	ILE	2.2
1	F	298	GLU	2.2
1	A	270	ASN	2.2
1	F	191	LYS	2.2
1	F	379	SER	2.2
1	A	61	ARG	2.2
1	E	384	PRO	2.2
1	F	458	VAL	2.2
1	A	204	ALA	2.2
1	F	435	ASN	2.2
1	C	50	THR	2.2
1	E	438	THR	2.2
1	F	461	THR	2.2
1	A	428	GLY	2.2
1	C	292	SER	2.2
1	E	353	SER	2.2
1	D	102	ASP	2.2
1	E	61	ARG	2.2
1	E	155	ARG	2.2
1	B	432	LYS	2.2
1	F	273	LYS	2.2
1	E	59	VAL	2.1
1	A	368	ALA	2.1
1	A	389	GLY	2.1
1	E	212	GLY	2.1
1	F	73	THR	2.1
1	F	257	THR	2.1
1	B	297	CYS	2.1
1	B	218	SER	2.1
1	A	384	PRO	2.1
1	D	326	VAL	2.1
1	F	252	ILE	2.1
1	C	125	GLU	2.1
1	F	303	TYR	2.1
1	E	297	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	178	ASP	2.1
1	D	52	GLN	2.1
1	E	131	TRP	2.1
1	E	213	ALA	2.1
1	E	67	GLY	2.1
1	B	309	ILE	2.1
1	F	341	ILE	2.1
1	B	350	ASP	2.1
1	E	54	MET	2.1
1	E	270	ASN	2.1
1	E	424	LEU	2.1
1	A	115	GLU	2.1
1	D	443	THR	2.1
1	C	126	LYS	2.1
1	D	191	LYS	2.1
1	F	285	PRO	2.1
1	F	54	MET	2.1
1	C	457	ALA	2.0
1	F	99	ALA	2.0
1	C	270	ASN	2.0
1	F	139	TRP	2.0
1	F	271	GLY	2.0
1	F	340	GLY	2.0
1	E	194	ASP	2.0
1	B	351	SER	2.0
1	A	297	CYS	2.0
1	E	400	PHE	2.0
1	E	225	GLU	2.0
1	A	53	ILE	2.0
1	A	426	THR	2.0
1	F	105	TRP	2.0

## 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 oligosaccharides 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.