Full wwPDB X-ray Structure Validation Report ⓘ

Jul 25, 2023 – 02:06 PM EDT

PDB ID	:	8GEX
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*
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:

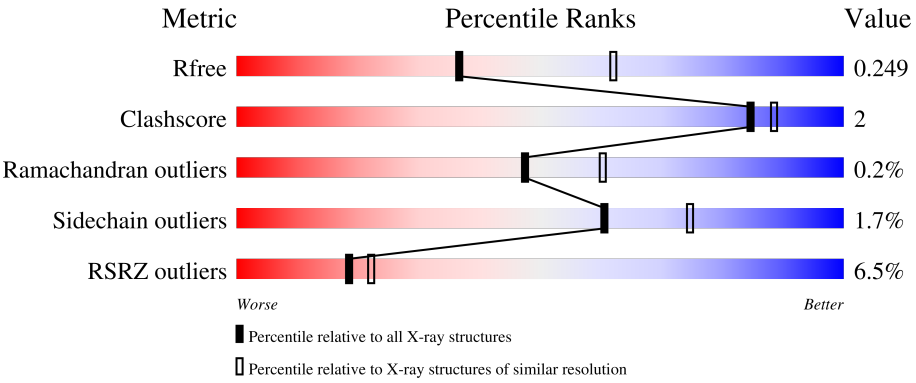
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.34
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

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 2.55 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}	130704	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

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	424	3% 92% 5% ·
1	B	424	4% 90% 6% ·
1	C	424	4% 90% 6% ·
1	D	424	4% 90% 7% ·
1	E	424	8% 88% 8% ·

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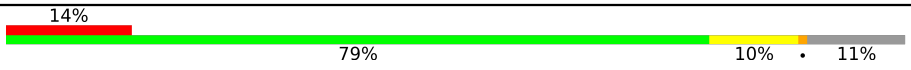
Mol	Chain	Length	Quality of chain
1	F	424	

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

- Molecule 2 is water.

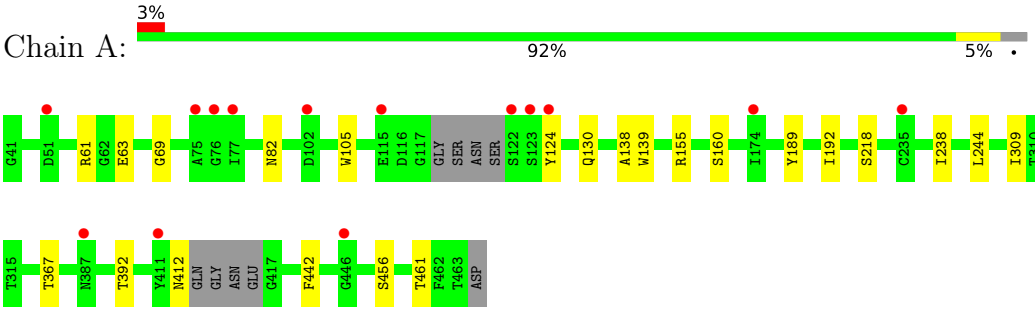
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	75	Total	O	0	0
			75	75		
2	B	77	Total	O	0	0
			77	77		
2	C	42	Total	O	0	0
			42	42		
2	D	42	Total	O	0	0
			42	42		
2	E	25	Total	O	0	0
			25	25		
2	F	20	Total	O	0	0
			20	20		

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.

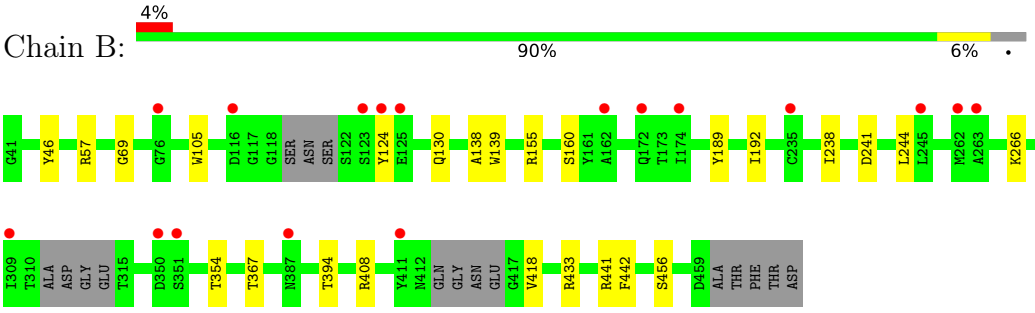
• Molecule 1: DUF4374 domain-containing protein

Chain A:



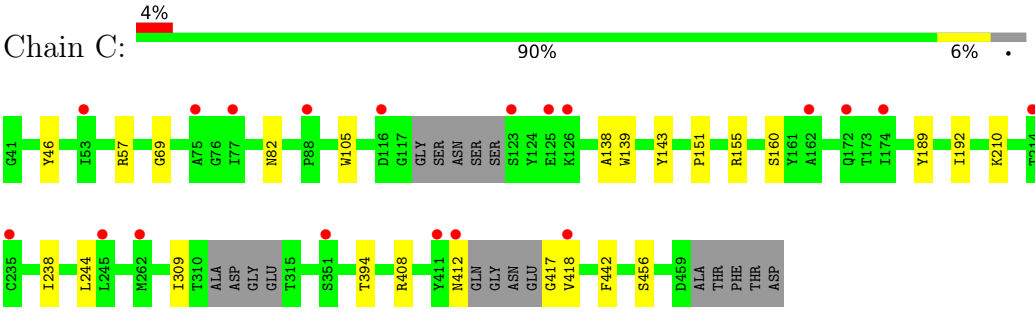
• Molecule 1: DUF4374 domain-containing protein

Chain B:



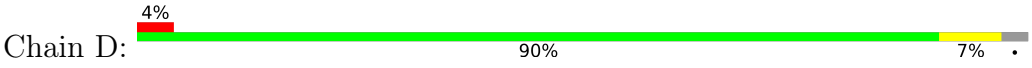
• Molecule 1: DUF4374 domain-containing protein

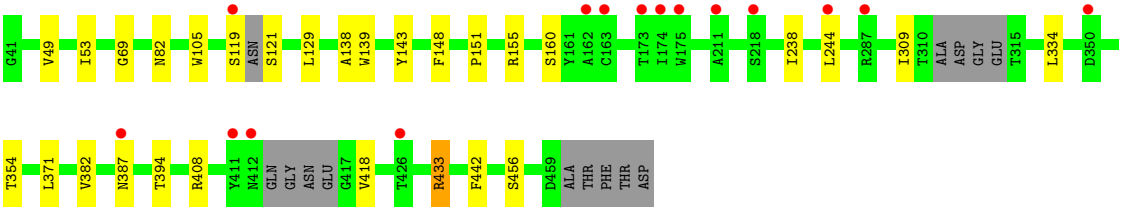
Chain C:



• Molecule 1: DUF4374 domain-containing protein

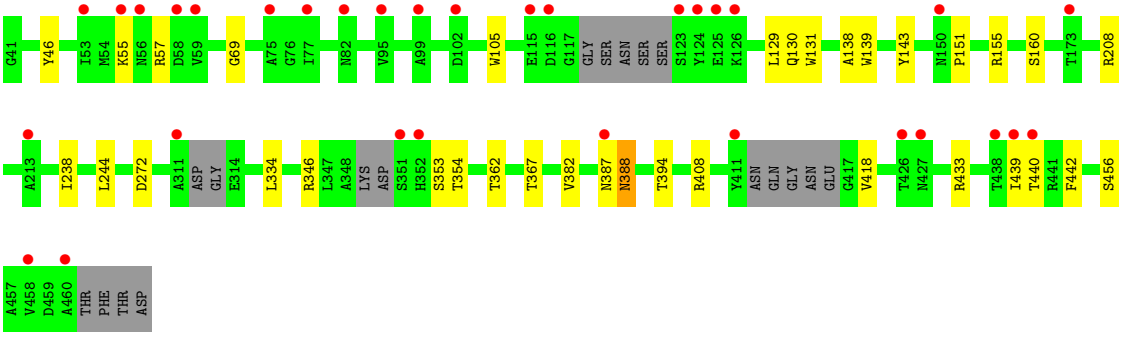
Chain D:





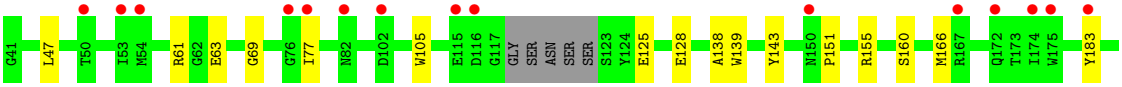
• Molecule 1: DUF4374 domain-containing protein

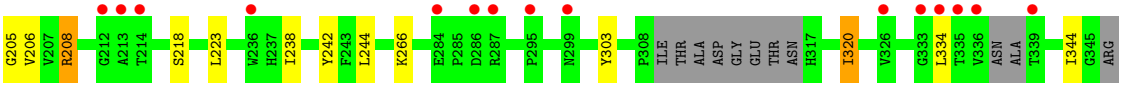
Chain E:

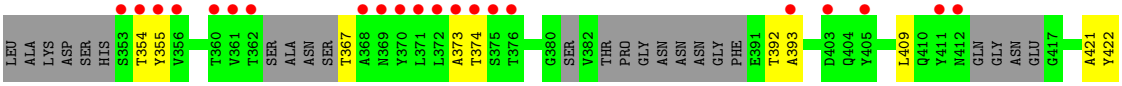


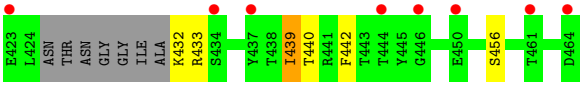
• Molecule 1: DUF4374 domain-containing protein

Chain F:









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	1.65 (at 2.54Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.224 , 0.247 0.233 , 0.249	Depositor DCC
R_{free} test set	8538 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	44.9	Xtriage
Anisotropy	1.100	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	19062	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage'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.*

[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	0.25	0/3262	0.50	0/4439
1	B	0.24	0/3235	0.50	0/4401
1	C	0.24	0/3225	0.49	0/4388
1	D	0.25	0/3247	0.50	0/4417
1	E	0.25	0/3218	0.50	0/4378
1	F	0.25	0/3017	0.50	0/4096
All	All	0.25	0/19204	0.50	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

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	8	0
1	B	3163	0	3030	11	0
1	C	3153	0	3022	13	0
1	D	3175	0	3040	13	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	84	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 (84) 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: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: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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	41	51
1	C	398/424 (94%)	384 (96%)	14 (4%)	0	100	100
1	D	402/424 (95%)	385 (96%)	16 (4%)	1 (0%)	47	60
1	E	396/424 (93%)	382 (96%)	12 (3%)	2 (0%)	29	40
1	F	359/424 (85%)	348 (97%)	11 (3%)	0	100	100
All	All	2358/2544 (93%)	2275 (96%)	79 (3%)	4 (0%)	47	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	433	ARG

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Mol	Chain	Res	Type
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%)	53	68
1	B	335/347 (96%)	332 (99%)	3 (1%)	78	86
1	C	334/347 (96%)	331 (99%)	3 (1%)	78	86
1	D	337/347 (97%)	330 (98%)	7 (2%)	53	68
1	E	332/347 (96%)	330 (99%)	2 (1%)	86	92
1	F	312/347 (90%)	300 (96%)	12 (4%)	33	45
All	All	1988/2082 (96%)	1954 (98%)	34 (2%)	60	75

All (34) 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	354	THR
1	B	367	THR
1	B	441	ARG
1	C	82	ASN
1	C	218	SER
1	C	309	ILE
1	D	53	ILE
1	D	82	ASN

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Mol	Chain	Res	Type
1	D	129	LEU
1	D	309	ILE
1	D	354	THR
1	D	371	LEU
1	D	387	ASN
1	E	129	LEU
1	E	354	THR
1	F	47	LEU
1	F	77	ILE
1	F	166	MET
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 (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	412	ASN

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	411/424 (96%)	0.26	14 (3%)	45	52	44, 62, 91, 149	0
1	B	408/424 (96%)	0.29	19 (4%)	31	38	44, 60, 86, 126	0
1	C	406/424 (95%)	0.34	19 (4%)	31	38	52, 69, 96, 128	0
1	D	410/424 (96%)	0.36	15 (3%)	41	48	54, 72, 94, 131	0
1	E	406/424 (95%)	0.48	32 (7%)	12	16	61, 81, 114, 144	0
1	F	378/424 (89%)	0.89	59 (15%)	2	2	63, 94, 127, 149	0
All	All	2419/2544 (95%)	0.43	158 (6%)	18	22	44, 71, 112, 149	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	353	SER	6.3
1	F	361	VAL	5.5
1	F	299	ASN	5.1
1	F	362	THR	5.0
1	F	434	SER	4.6
1	E	411	TYR	4.3
1	F	376	THR	4.2
1	F	116	ASP	4.1
1	F	373	ALA	4.1
1	F	374	THR	4.1
1	E	427	ASN	4.0
1	F	286	ASP	3.7
1	E	58	ASP	3.7
1	E	387	ASN	3.6
1	F	412	ASN	3.6
1	F	370	TYR	3.6
1	F	53	ILE	3.6
1	F	287	ARG	3.5
1	F	371	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	E	116	ASP	3.4
1	E	438	THR	3.4
1	F	372	LEU	3.4
1	C	123	SER	3.4
1	E	125	GLU	3.4
1	E	115	GLU	3.4
1	F	360	THR	3.3
1	E	102	ASP	3.3
1	A	122	SER	3.2
1	D	411	TYR	3.1
1	C	351	SER	3.1
1	F	411	TYR	3.1
1	F	115	GLU	3.0
1	E	311	ALA	3.0
1	E	426	THR	3.0
1	B	411	TYR	3.0
1	E	460	ALA	2.9
1	F	354	THR	2.9
1	F	450	GLU	2.9
1	C	418	VAL	2.9
1	C	53	ILE	2.9
1	F	212	GLY	2.9
1	A	411	TYR	2.9
1	B	123	SER	2.9
1	F	339	THR	2.9
1	F	50	THR	2.8
1	F	403	ASP	2.8
1	B	387	ASN	2.8
1	E	53	ILE	2.8
1	F	183	TYR	2.8
1	F	77	ILE	2.8
1	F	423	GLU	2.8
1	C	411	TYR	2.8
1	F	150	ASN	2.8
1	F	356	VAL	2.8
1	D	174	ILE	2.7
1	E	439	ILE	2.7
1	F	334	LEU	2.7
1	A	123	SER	2.7
1	D	218	SER	2.7
1	F	284	GLU	2.7
1	A	102	ASP	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	174	ILE	2.7
1	E	99	ALA	2.7
1	A	77	ILE	2.7
1	F	167	ARG	2.7
1	A	75	ALA	2.6
1	D	119	SER	2.6
1	D	287	ARG	2.6
1	E	55	LYS	2.6
1	C	125	GLU	2.6
1	C	412	ASN	2.5
1	F	336	VAL	2.5
1	E	352	HIS	2.5
1	F	355	TYR	2.5
1	B	262	MET	2.5
1	C	126	LYS	2.5
1	D	387	ASN	2.5
1	F	82	ASN	2.5
1	A	387	ASN	2.5
1	B	162	ALA	2.5
1	B	116	ASP	2.4
1	F	54	MET	2.4
1	E	440	THR	2.4
1	B	351	SER	2.4
1	C	235	CYS	2.4
1	E	59	VAL	2.4
1	F	375	SER	2.4
1	C	77	ILE	2.4
1	F	326	VAL	2.4
1	D	173	THR	2.4
1	C	174	ILE	2.4
1	E	77	ILE	2.4
1	E	126	LYS	2.4
1	F	214	THR	2.4
1	F	393	ALA	2.4
1	B	286	ASP	2.4
1	A	174	ILE	2.4
1	B	235	CYS	2.4
1	C	172	GLN	2.4
1	C	214	THR	2.4
1	F	236	TRP	2.4
1	F	76	GLY	2.3
1	B	174	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	162	ALA	2.3
1	D	412	ASN	2.3
1	F	369	ASN	2.3
1	B	245	LEU	2.3
1	A	115	GLU	2.3
1	F	175	TRP	2.3
1	F	295	PRO	2.3
1	C	88	PRO	2.3
1	B	309	ILE	2.3
1	E	123	SER	2.3
1	F	405	TYR	2.3
1	F	213	ALA	2.3
1	D	175	TRP	2.2
1	D	350	ASP	2.2
1	C	162	ALA	2.2
1	F	333	GLY	2.2
1	F	464	ASP	2.2
1	A	235	CYS	2.2
1	C	75	ALA	2.2
1	C	245	LEU	2.2
1	E	124	TYR	2.2
1	F	102	ASP	2.2
1	E	95	VAL	2.2
1	F	335	THR	2.2
1	B	125	GLU	2.2
1	E	458	VAL	2.1
1	F	446	GLY	2.1
1	A	446	GLY	2.1
1	D	426	THR	2.1
1	B	299	ASN	2.1
1	A	76	GLY	2.1
1	A	124	TYR	2.1
1	E	75	ALA	2.1
1	E	213	ALA	2.1
1	F	172	GLN	2.1
1	C	116	ASP	2.1
1	E	56	ASN	2.1
1	B	172	GLN	2.1
1	F	368	ALA	2.1
1	B	350	ASP	2.1
1	E	82	ASN	2.1
1	E	150	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	444	THR	2.1
1	A	51	ASP	2.1
1	B	76	GLY	2.1
1	C	262	MET	2.0
1	E	173	THR	2.0
1	B	263	ALA	2.0
1	F	461	THR	2.0
1	D	244	LEU	2.0
1	F	437	TYR	2.0
1	D	163	CYS	2.0
1	D	211	ALA	2.0
1	E	351	SER	2.0
1	B	124	TYR	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 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.