Full wwPDB X-ray Structure Validation Report ⓘ

Dec 9, 2023 – 08:16 am GMT

PDB ID	:	2VE8
Title	:	Xray structure of FtsK gamma domain (P. aeruginosa)
Authors	:	Lowe, J.; Allen, M.A.; Sherratt, D.J.
Deposited on	:	2007-10-17
Resolution	:	1.40 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:

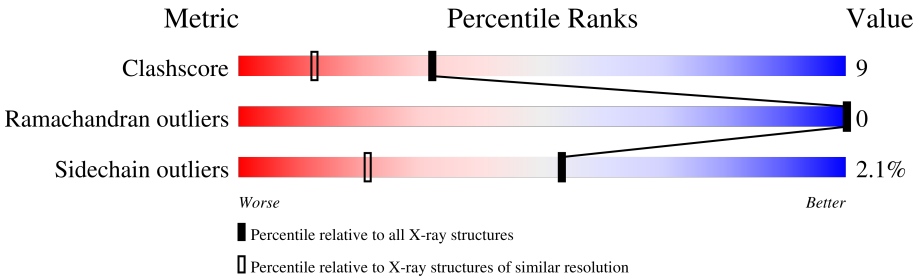
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 1.40 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))
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)

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%

Mol	Chain	Length	Quality of chain
1	A	73	77% 14% • 8%
1	B	73	74% 14% • 11%
1	C	73	71% 10% • • 14%
1	D	73	81% 8% • 7%
1	E	73	73% 16% • 8%
1	F	73	73% 15% • 10%
1	G	73	64% 15% • 16%
1	H	73	68% 12% 5% 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 4633 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 DNA TRANSLOCASE FTSK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	67	Total	C	N	O	S	0	0	0
			520	318	97	101	4			
1	B	65	Total	C	N	O	S	0	0	0
			500	308	92	96	4			
1	C	63	Total	C	N	O	S	0	0	1
			477	295	89	89	4			
1	D	68	Total	C	N	O	S	0	0	0
			526	321	98	103	4			
1	E	67	Total	C	N	O	S	0	0	1
			507	311	94	98	4			
1	F	66	Total	C	N	O	S	0	0	1
			500	306	93	97	4			
1	G	61	Total	C	N	O	S	0	0	1
			465	286	88	87	4			
1	H	63	Total	C	N	O	S	0	0	1
			477	294	90	89	4			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	94	Total	O	0	0
			94	94		
2	B	92	Total	O	0	0
			92	92		
2	C	89	Total	O	0	0
			89	89		
2	D	81	Total	O	0	0
			81	81		
2	E	67	Total	O	0	0
			67	67		
2	F	67	Total	O	0	0
			67	67		

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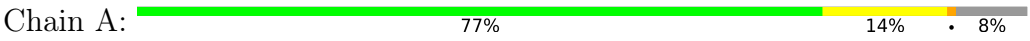
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	97	Total O 97 97	0	0
2	H	74	Total O 74 74	0	0

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. 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. 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: DNA TRANSLOCASE FTSK

Chain A:



• Molecule 1: DNA TRANSLOCASE FTSK

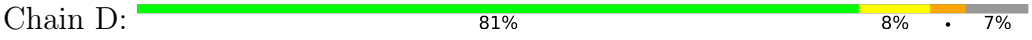
Chain B:

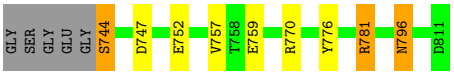
• Molecule 1: DNA TRANSLOCASE FTSK

Chain C:

• Molecule 1: DNA TRANSLOCASE FTSK

Chain D:





• Molecule 1: DNA TRANSLOCASE FTSK

Chain E:

• Molecule 1: DNA TRANSLOCASE FTSK

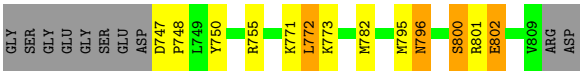
Chain F:

• Molecule 1: DNA TRANSLOCASE FTSK

Chain G:

• Molecule 1: DNA TRANSLOCASE FTSK

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.49Å 58.50Å 95.41Å 90.00° 92.51° 90.00°	Depositor
Resolution (Å)	95.35 – 1.40 40.98 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (95.35-1.40) 43.6 (40.98-1.40)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.90 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.3.0037	Depositor
R, R_{free}	0.144 , 0.192 0.144 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	13.0	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	2.91 , 99.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	None for h,-k,-l	Xtriage
F_o,F_c correlation	0.12	EDS
Total number of atoms	4633	wwPDB-VP
Average B, all atoms (Å^2)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.59% 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	1.41	3/526 (0.6%)	1.28	2/708 (0.3%)
1	B	1.41	3/506 (0.6%)	1.21	0/683
1	C	1.45	5/482 (1.0%)	1.15	1/649 (0.2%)
1	D	1.37	3/532 (0.6%)	1.17	3/716 (0.4%)
1	E	1.54	7/513 (1.4%)	1.28	6/693 (0.9%)
1	F	1.56	5/506 (1.0%)	1.51	5/683 (0.7%)
1	G	1.69	10/470 (2.1%)	1.44	8/633 (1.3%)
1	H	1.38	3/483 (0.6%)	1.29	6/652 (0.9%)
All	All	1.48	39/4018 (1.0%)	1.29	31/5417 (0.6%)

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	802	GLU	CG-CD	11.83	1.69	1.51
1	G	802	GLU	CD-OE1	9.96	1.36	1.25
1	G	802	GLU	CG-CD	9.81	1.66	1.51
1	A	757	VAL	CB-CG2	-9.71	1.32	1.52
1	E	802	GLU	CG-CD	9.01	1.65	1.51
1	G	802	GLU	CD-OE2	8.25	1.34	1.25
1	G	762	ARG	CZ-NH1	7.69	1.43	1.33
1	C	746	ASP	CB-CG	7.40	1.67	1.51
1	F	802	GLU	CD-OE1	6.96	1.33	1.25
1	D	757	VAL	CB-CG1	-6.84	1.38	1.52
1	F	800	SER	CB-OG	-6.82	1.33	1.42
1	B	776	TYR	CD2-CE2	6.80	1.49	1.39
1	G	762	ARG	CZ-NH2	6.79	1.41	1.33
1	C	795	MET	CB-CG	6.69	1.72	1.51
1	B	752	GLU	CG-CD	6.61	1.61	1.51
1	B	757	VAL	CB-CG1	-6.24	1.39	1.52
1	G	801	ARG	CZ-NH1	6.23	1.41	1.33
1	D	759	GLU	CD-OE1	6.10	1.32	1.25
1	D	776	TYR	CD2-CE2	6.09	1.48	1.39
1	E	752	GLU	CG-CD	6.05	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	802	GLU	CD-OE2	5.97	1.32	1.25
1	E	800	SER	CA-CB	5.88	1.61	1.52
1	H	750	TYR	CE2-CZ	-5.85	1.30	1.38
1	C	776	TYR	CD2-CE2	5.80	1.48	1.39
1	F	751	ASP	CB-CG	5.68	1.63	1.51
1	G	760	SER	CB-OG	5.57	1.49	1.42
1	C	776	TYR	CE2-CZ	-5.49	1.31	1.38
1	G	802	GLU	CB-CG	5.49	1.62	1.52
1	C	799	GLY	N-CA	5.47	1.54	1.46
1	H	800	SER	CB-OG	-5.44	1.35	1.42
1	E	752	GLU	CD-OE1	5.41	1.31	1.25
1	G	759	GLU	CG-CD	5.34	1.59	1.51
1	H	802	GLU	CG-CD	-5.33	1.44	1.51
1	A	755	ARG	CG-CD	5.25	1.65	1.51
1	E	776	TYR	CD2-CE2	5.25	1.47	1.39
1	G	800	SER	CA-CB	5.23	1.60	1.52
1	E	802	GLU	CB-CG	5.22	1.62	1.52
1	F	802	GLU	CD-OE2	5.21	1.31	1.25
1	A	784	GLU	CD-OE1	5.10	1.31	1.25

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	751	ASP	CB-CG-OD2	14.74	131.57	118.30
1	F	770	ARG	NE-CZ-NH2	11.57	126.09	120.30
1	F	751	ASP	CB-CG-OD1	-9.85	109.44	118.30
1	H	801	ARG	NE-CZ-NH2	-8.61	116.00	120.30
1	F	770	ARG	NE-CZ-NH1	-8.57	116.02	120.30
1	G	751	ASP	CB-CG-OD2	8.48	125.93	118.30
1	G	762	ARG	NE-CZ-NH2	-8.45	116.08	120.30
1	E	751	ASP	CB-CG-OD2	8.45	125.90	118.30
1	G	801	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	E	751	ASP	CB-CG-OD1	-7.85	111.24	118.30
1	H	772	LEU	CB-CG-CD2	-7.39	98.43	111.00
1	C	757	VAL	CG1-CB-CG2	7.03	122.15	110.90
1	D	781	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	H	755	ARG	NE-CZ-NH1	-6.60	117.00	120.30
1	G	778	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	E	755	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	G	781	ARG	NE-CZ-NH2	6.39	123.49	120.30
1	E	788	MET	CG-SD-CE	6.25	110.19	100.20
1	A	755	ARG	CG-CD-NE	-6.00	99.21	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	802	GLU	OE1-CD-OE2	-5.90	116.22	123.30
1	G	761	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	H	773	LYS	CD-CE-NZ	5.75	124.93	111.70
1	H	782	MET	CG-SD-CE	5.74	109.38	100.20
1	A	781	ARG	NE-CZ-NH1	-5.54	117.53	120.30
1	G	762	ARG	NH1-CZ-NH2	5.52	125.47	119.40
1	E	802	GLU	CG-CD-OE2	5.42	129.14	118.30
1	G	801	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	D	747	ASP	CB-CG-OD2	5.38	123.14	118.30
1	H	772	LEU	CB-CG-CD1	5.29	120.00	111.00
1	F	761	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	D	770	ARG	NE-CZ-NH2	-5.07	117.77	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	520	0	522	9	0
1	B	500	0	505	9	0
1	C	477	0	485	15	1
1	D	526	0	527	7	0
1	E	507	0	510	8	0
1	F	500	0	501	10	0
1	G	465	0	474	8	0
1	H	477	0	486	12	1
2	A	94	0	0	4	0
2	B	92	0	0	5	0
2	C	89	0	0	9	0
2	D	81	0	0	5	0
2	E	67	0	0	3	0
2	F	67	0	0	3	0
2	G	97	0	0	4	0
2	H	74	0	0	5	0
All	All	4633	0	4010	71	1

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 9.

All (71) 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:D:744:SER:HB2	2:D:2001:HOH:O	1.15	1.29
1:B:809:VAL:C	2:B:2092:HOH:O	1.72	1.26
1:H:802:GLU:CD	2:H:2063:HOH:O	1.76	1.21
1:H:802:GLU:OE2	2:H:2062:HOH:O	1.60	1.18
1:H:802:GLU:OE1	2:H:2063:HOH:O	1.63	1.12
1:B:752:GLU:HB2	1:C:752:GLU:OE1	1.54	1.07
1:D:752:GLU:OE1	2:D:2021:HOH:O	1.73	1.07
1:H:802:GLU:OE2	2:H:2063:HOH:O	1.68	1.06
1:F:744:SER:N	2:F:2002:HOH:O	1.85	1.06
1:E:744:SER:N	2:E:2001:HOH:O	1.98	0.95
1:C:796:ASN:HB3	2:C:2064:HOH:O	1.65	0.94
1:C:746:ASP:N	2:C:2006:HOH:O	2.06	0.89
1:G:747:ASP:N	2:G:2005:HOH:O	2.06	0.87
1:C:800:SER:HB2	2:C:2070:HOH:O	1.81	0.79
1:H:747:ASP:N	2:H:2001:HOH:O	2.17	0.77
1:F:809:VAL:N	2:F:2066:HOH:O	2.18	0.76
1:C:796:ASN:C	1:C:796:ASN:HD22	1.88	0.75
1:A:770:ARG:NH2	2:A:2047:HOH:O	2.19	0.75
1:C:795:MET:SD	2:C:2089:HOH:O	2.45	0.74
1:D:781:ARG:HD2	2:D:2047:HOH:O	1.87	0.74
1:A:752:GLU:HB2	1:D:752:GLU:OE2	1.91	0.70
1:D:744:SER:CB	2:D:2001:HOH:O	1.96	0.68
1:A:773:LYS:NZ	2:A:2050:HOH:O	2.09	0.67
1:E:771:LYS:HG3	1:E:772:LEU:HD22	1.80	0.63
1:F:795:MET:HG2	1:F:799:GLY:HA2	1.81	0.62
1:F:795:MET:HE1	1:H:795:MET:HG2	1.82	0.61
1:B:773:LYS:NZ	2:B:2046:HOH:O	2.22	0.60
1:A:796:ASN:ND2	1:A:800:SER:H	1.98	0.60
1:H:796:ASN:C	1:H:796:ASN:HD22	2.05	0.60
1:B:762:ARG:HD3	2:B:2033:HOH:O	2.03	0.58
1:F:788:MET:SD	2:F:2016:HOH:O	2.57	0.58
1:E:796:ASN:C	1:E:796:ASN:HD22	2.05	0.57
1:C:795:MET:HE3	1:C:800:SER:HA	1.89	0.54
1:G:796:ASN:C	1:G:796:ASN:HD22	2.10	0.54
1:C:800:SER:CB	2:C:2070:HOH:O	2.49	0.54
1:A:811:ASP:OD1	1:A:811:ASP:C	2.47	0.53
1:C:795:MET:HE2	1:C:799:GLY:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:771:LYS:CG	1:E:772:LEU:HD22	2.40	0.52
1:F:771:LYS:HG3	1:F:772:LEU:HD22	1.91	0.52
1:D:796:ASN:C	1:D:796:ASN:HD22	2.14	0.51
1:F:796:ASN:HD22	1:F:796:ASN:C	2.12	0.51
1:G:781:ARG:NH1	2:G:2059:HOH:O	2.44	0.50
1:A:762:ARG:NE	2:A:2038:HOH:O	2.44	0.49
1:E:809:VAL:HG23	1:E:810:ARG:N	2.28	0.49
1:F:795:MET:HE3	1:H:795:MET:CE	2.43	0.49
1:D:781:ARG:NH2	2:D:2047:HOH:O	2.10	0.48
1:A:796:ASN:C	1:A:796:ASN:HD22	2.17	0.48
1:C:795:MET:CB	2:C:2089:HOH:O	2.61	0.48
1:A:811:ASP:OXT	1:C:755:ARG:NH1	2.38	0.48
1:B:745:GLU:CA	2:B:2005:HOH:O	2.62	0.47
1:C:795:MET:HB2	2:C:2089:HOH:O	2.14	0.47
1:C:770:ARG:NH2	2:C:2038:HOH:O	2.07	0.46
1:C:795:MET:CG	2:C:2089:HOH:O	2.64	0.46
1:G:796:ASN:ND2	1:G:800:SER:H	2.14	0.45
1:H:796:ASN:ND2	1:H:800:SER:H	2.15	0.45
1:E:784:GLU:HG3	2:E:2046:HOH:O	2.17	0.45
1:F:795:MET:HE3	1:H:795:MET:SD	2.57	0.45
1:H:771:LYS:HG3	1:H:772:LEU:HD12	1.99	0.45
1:G:747:ASP:N	2:G:2008:HOH:O	2.49	0.45
1:G:807:ALA:N	2:G:2090:HOH:O	2.49	0.44
1:B:746:ASP:OD2	1:H:771:LYS:NZ	2.49	0.43
1:B:795:MET:HB3	1:B:795:MET:HE3	1.71	0.43
1:C:795:MET:HE3	1:C:800:SER:CA	2.49	0.43
1:F:796:ASN:ND2	1:F:800:SER:H	2.17	0.42
1:B:745:GLU:N	2:B:2005:HOH:O	2.53	0.41
1:E:796:ASN:ND2	1:E:800:SER:H	2.18	0.41
1:B:755:ARG:O	1:B:759:GLU:HG3	2.21	0.41
1:E:744:SER:CA	2:E:2001:HOH:O	2.58	0.41
1:A:762:ARG:HB2	2:A:2038:HOH:O	2.21	0.41
1:G:796:ASN:C	1:G:796:ASN:ND2	2.74	0.40
1:G:796:ASN:ND2	1:G:798:ASN:H	2.19	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:802:GLU:OE1	1:H:748:PRO:CB[1_655]	2.03	0.17

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	65/73 (89%)	65 (100%)	0	0	100	100
1	B	63/73 (86%)	63 (100%)	0	0	100	100
1	C	59/73 (81%)	59 (100%)	0	0	100	100
1	D	66/73 (90%)	66 (100%)	0	0	100	100
1	E	65/73 (89%)	65 (100%)	0	0	100	100
1	F	64/73 (88%)	63 (98%)	1 (2%)	0	100	100
1	G	59/73 (81%)	59 (100%)	0	0	100	100
1	H	61/73 (84%)	60 (98%)	1 (2%)	0	100	100
All	All	502/584 (86%)	500 (100%)	2 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	55/58 (95%)	54 (98%)	1 (2%)	59	28
1	B	53/58 (91%)	53 (100%)	0	100	100
1	C	50/58 (86%)	48 (96%)	2 (4%)	31	5
1	D	56/58 (97%)	54 (96%)	2 (4%)	35	7
1	E	54/58 (93%)	53 (98%)	1 (2%)	57	25
1	F	53/58 (91%)	52 (98%)	1 (2%)	57	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	49/58 (84%)	48 (98%)	1 (2%)	55 23
1	H	50/58 (86%)	49 (98%)	1 (2%)	55 23
All	All	420/464 (90%)	411 (98%)	9 (2%)	53 21

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	796	ASN
1	C	795	MET
1	C	796	ASN
1	D	744	SER
1	D	796	ASN
1	E	796	ASN
1	F	796	ASN
1	G	796	ASN
1	H	796	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	777	ASN
1	A	796	ASN
1	C	777	ASN
1	C	796	ASN
1	D	777	ASN
1	D	796	ASN
1	E	777	ASN
1	E	796	ASN
1	F	777	ASN
1	F	796	ASN
1	G	777	ASN
1	G	796	ASN
1	H	777	ASN
1	H	796	ASN

5.3.3 RNA

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

6.1 Protein, DNA and RNA chains

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3 Carbohydrates

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4 Ligands

Unable to reproduce the depositors R factor - this section is therefore empty.

6.5 Other polymers

Unable to reproduce the depositors R factor - this section is therefore empty.