Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2024 – 11:21 AM JST

PDB ID	:	5ZB8
Title	:	Crystal structure of the novel lesion-specific endonuclease PfuEndoQ from Pyrococcus furiosus
Authors	:	Miyazono, K.; Ito, T.; Tanokura, M.
Deposited on	:	2018-02-10
Resolution	:	2.50 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:

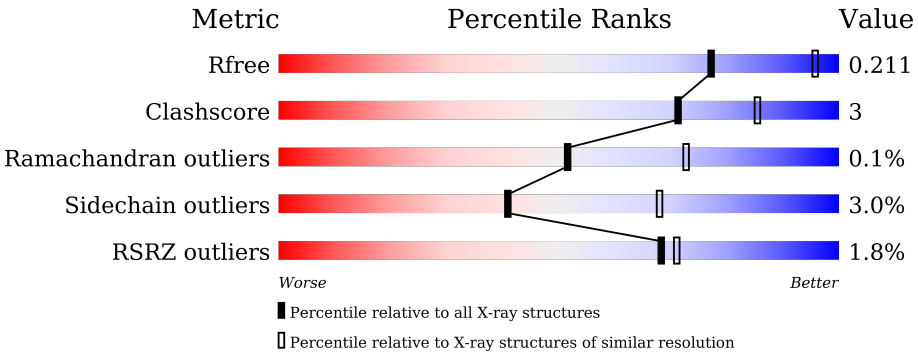
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.50 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	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	400	89% 11%
1	B	400	3% 86% 12%
1	C	400	86% 12%
1	D	400	4% 90% 9%
1	E	400	2% 89% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 16243 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 PfuEndoQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3163	2019	549	583	12			
1	B	398	Total	C	N	O	S	0	2	0
			3168	2021	552	583	12			
1	C	399	Total	C	N	O	S	0	0	0
			3156	2016	548	580	12			
1	D	399	Total	C	N	O	S	0	0	0
			3156	2016	548	580	12			
1	E	400	Total	C	N	O	S	0	0	0
			3163	2019	549	583	12			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	expression tag	UNP I6V2I0
A	2	VAL	-	expression tag	UNP I6V2I0
B	1	MET	-	expression tag	UNP I6V2I0
B	2	VAL	-	expression tag	UNP I6V2I0
C	1	MET	-	expression tag	UNP I6V2I0
C	2	VAL	-	expression tag	UNP I6V2I0
D	1	MET	-	expression tag	UNP I6V2I0
D	2	VAL	-	expression tag	UNP I6V2I0
E	1	MET	-	expression tag	UNP I6V2I0
E	2	VAL	-	expression tag	UNP I6V2I0

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	3	Total	Zn	0	0
			3	3		
2	B	3	Total	Zn	0	0
			3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	3	Total Zn 3 3	0	0
2	D	3	Total Zn 3 3	0	0
2	E	3	Total Zn 3 3	0	0

- Molecule 3 is SAMARIUM (III) ION (three-letter code: SM) (formula: Sm).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Sm 1 1	0	0
3	C	2	Total Sm 2 2	0	0
3	D	1	Total Sm 1 1	0	0
3	E	3	Total Sm 3 3	0	0

- Molecule 4 is water.

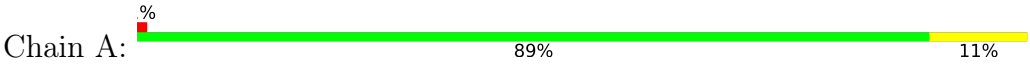
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	109	Total O 109 109	0	0
4	B	83	Total O 83 83	0	0
4	C	85	Total O 85 85	0	0
4	D	66	Total O 66 66	0	0
4	E	72	Total O 72 72	0	0

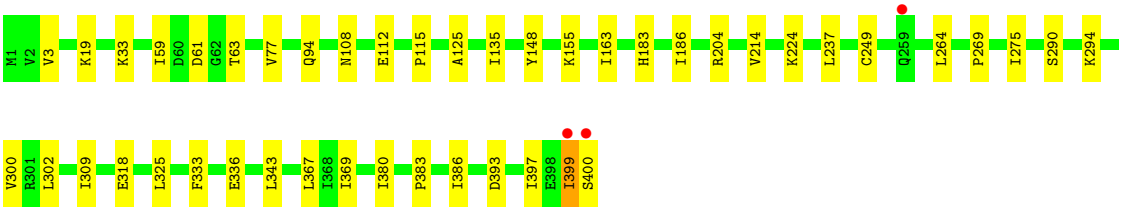
3 Residue-property plots

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: PfuEndoQ

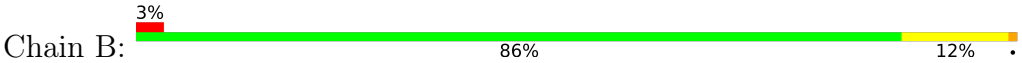
Chain A:

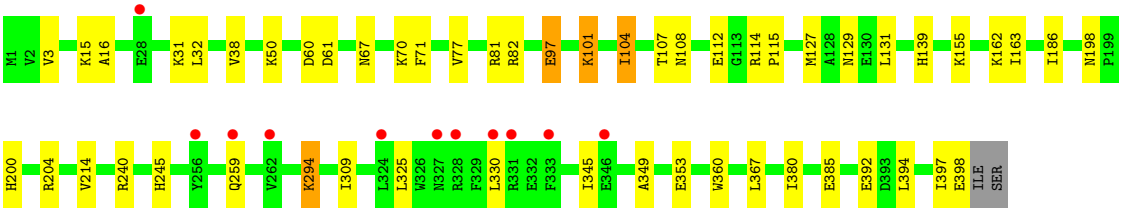




• Molecule 1: PfuEndoQ

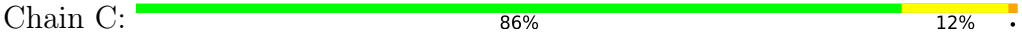
Chain B:

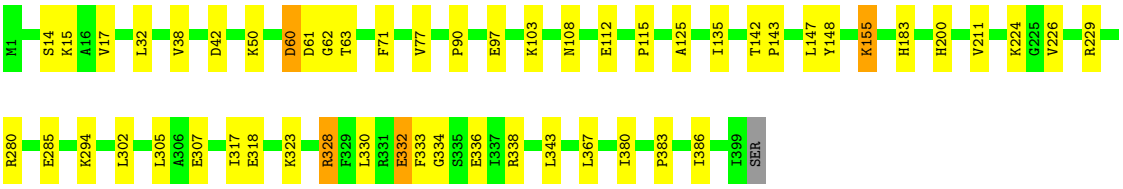




• Molecule 1: PfuEndoQ

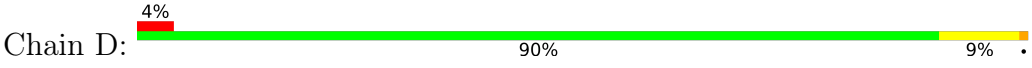
Chain C:

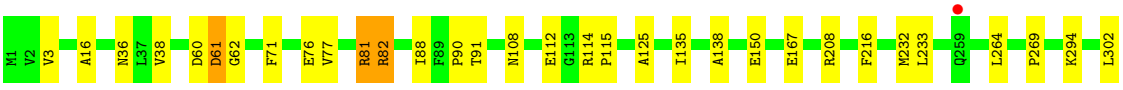


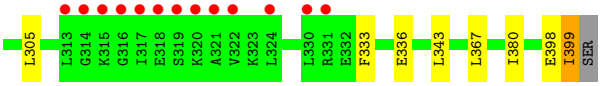


• Molecule 1: PfuEndoQ

Chain D:

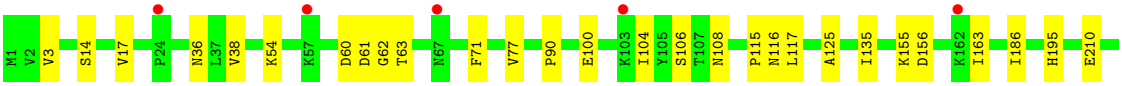


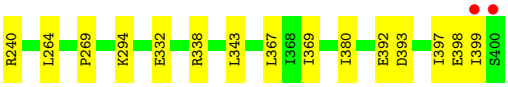




• Molecule 1: PfuEndoQ

Chain E:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	257.35Å 82.25Å 116.58Å 90.00° 109.13° 90.00°	Depositor
Resolution (Å)	41.12 – 2.50 42.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.1 (41.12-2.50) 98.1 (42.90-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.26 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.176 , 0.209 0.177 , 0.211	Depositor DCC
R_{free} test set	3871 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	38.4	Xtriage
Anisotropy	0.012	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 46.2	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	0.95	EDS
Total number of atoms	16243	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SM

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	0.24	0/3229	0.43	0/4358
1	B	0.24	0/3234	0.43	0/4365
1	C	0.24	0/3222	0.44	0/4350
1	D	0.24	0/3222	0.43	0/4350
1	E	0.24	0/3229	0.42	0/4358
All	All	0.24	0/16136	0.43	0/21781

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	3163	0	3221	22	0
1	B	3168	0	3222	31	0
1	C	3156	0	3216	25	0
1	D	3156	0	3216	21	0
1	E	3163	0	3221	19	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3	0	0	0	0
2	E	3	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
3	E	3	0	0	0	0
4	A	109	0	0	1	0
4	B	83	0	0	1	0
4	C	85	0	0	0	0
4	D	66	0	0	0	0
4	E	72	0	0	0	0
All	All	16243	0	16096	111	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 3.

All (111) 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:E:367:LEU:HD13	1:E:380:ILE:HD11	1.64	0.79
1:B:398:GLU:OE2	1:D:114:ARG:NH2	2.18	0.74
1:E:3:VAL:HG23	1:E:36:ASN:HB2	1.70	0.74
1:C:328:ARG:NH1	1:C:332:GLU:OE2	2.23	0.71
1:D:82:ARG:HB3	1:D:82:ARG:HH11	1.57	0.68
1:B:367:LEU:HD13	1:B:380:ILE:HD11	1.75	0.68
1:D:367:LEU:HD13	1:D:380:ILE:HD11	1.78	0.66
1:B:77:VAL:HG12	1:B:115:PRO:HG2	1.81	0.62
1:B:385:GLU:HG2	1:D:16:ALA:HB2	1.81	0.62
1:B:163:ILE:HD11	1:B:186:ILE:HD13	1.82	0.61
1:E:125:ALA:HA	1:E:135:ILE:HD13	1.81	0.61
1:A:3:VAL:HG11	1:A:214:VAL:HG22	1.83	0.59
1:B:60:ASP:OD2	1:B:61:ASP:N	2.37	0.58
1:C:125:ALA:HA	1:C:135:ILE:HD13	1.86	0.58
1:D:81:ARG:NH1	1:D:150:GLU:OE1	2.38	0.56
1:E:163:ILE:HD11	1:E:186:ILE:HD13	1.88	0.55
1:A:204:ARG:NH2	4:A:602:HOH:O	2.38	0.54
1:A:386:ILE:HD11	1:A:399:ILE:HD11	1.88	0.54
1:C:367:LEU:HD13	1:C:380:ILE:HD11	1.89	0.54
1:A:163:ILE:HD11	1:A:186:ILE:HD13	1.89	0.54
1:B:82:ARG:NH1	1:E:393:ASP:OD1	2.40	0.54
1:A:61:ASP:N	1:A:61:ASP:OD1	2.41	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:ASN:HD22	1:C:112:GLU:HG3	1.73	0.54
1:B:114:ARG:NH2	1:E:398:GLU:OE1	2.37	0.53
1:D:3:VAL:HG13	1:D:36:ASN:HB2	1.90	0.53
1:B:104:ILE:HG12	1:B:104:ILE:O	2.09	0.53
1:D:108:ASN:HD22	1:D:112:GLU:HG3	1.74	0.53
1:B:198:ASN:OD1	1:B:200:HIS:ND1	2.42	0.53
1:B:108:ASN:HD22	1:B:112:GLU:HG3	1.75	0.51
1:B:129:ASN:ND2	4:B:602:HOH:O	2.36	0.51
1:C:148:TYR:OH	1:C:183:HIS:NE2	2.36	0.51
1:D:61:ASP:HB3	1:D:91:THR:HG22	1.92	0.51
1:D:125:ALA:HA	1:D:135:ILE:HD13	1.92	0.51
1:B:3:VAL:HG11	1:B:214:VAL:HG22	1.93	0.51
1:E:14:SER:HB3	1:E:17:VAL:HG21	1.93	0.51
1:B:16:ALA:HB3	1:E:398:GLU:HB3	1.93	0.51
1:C:32:LEU:HD22	1:C:330:LEU:HD23	1.93	0.50
1:A:369:ILE:HG13	1:A:380:ILE:HD12	1.92	0.50
1:C:333:PHE:CD1	1:C:343:LEU:HD11	2.46	0.50
1:B:32:LEU:HD22	1:B:330:LEU:HD13	1.93	0.50
1:B:70:LYS:HD2	1:B:214:VAL:HB	1.93	0.50
1:A:333:PHE:CG	1:A:343:LEU:HD11	2.47	0.50
1:A:367:LEU:HD13	1:A:380:ILE:HD11	1.92	0.50
1:B:309:ILE:HG23	1:B:325:LEU:HD23	1.95	0.49
1:C:317:ILE:HG23	1:C:318:GLU:HG2	1.94	0.48
1:E:60:ASP:HB3	1:E:63:THR:HB	1.95	0.48
1:A:77:VAL:HG12	1:A:115:PRO:HG2	1.96	0.48
1:C:77:VAL:HG12	1:C:115:PRO:HG2	1.96	0.48
1:C:383:PRO:HG2	1:C:386:ILE:HG12	1.96	0.47
1:D:77:VAL:HG12	1:D:115:PRO:HG2	1.97	0.47
1:D:399:ILE:H	1:D:399:ILE:HD13	1.79	0.47
1:B:15:LYS:HD3	1:B:15:LYS:HA	1.68	0.47
1:A:383:PRO:HG2	1:A:386:ILE:HG12	1.96	0.47
1:D:208:ARG:HB3	1:D:233:LEU:HG	1.96	0.47
1:B:385:GLU:OE2	1:B:385:GLU:N	2.42	0.46
1:E:77:VAL:HG12	1:E:115:PRO:HG2	1.96	0.46
1:C:305:LEU:HB2	1:C:336:GLU:HG3	1.97	0.46
1:D:305:LEU:HB2	1:D:336:GLU:HG3	1.97	0.46
1:D:62:GLY:HA3	1:D:90:PRO:O	2.16	0.46
1:A:309:ILE:HG23	1:A:325:LEU:HD23	1.98	0.46
1:C:60:ASP:HB2	1:C:63:THR:HB	1.98	0.46
1:C:334:GLY:H	1:C:338:ARG:HH11	1.63	0.46
1:C:14:SER:OG	1:C:42:ASP:OD2	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:ALA:HB1	1:B:353:GLU:HG2	1.98	0.45
1:A:224:LYS:HD3	1:B:162:LYS:NZ	2.32	0.45
1:B:38:VAL:O	1:B:71:PHE:HA	2.17	0.44
1:B:97:GLU:HB3	1:B:131:LEU:HD13	1.99	0.44
1:C:200:HIS:NE2	1:C:307:GLU:OE1	2.48	0.44
1:C:15:LYS:HE2	1:C:112:GLU:OE2	2.17	0.44
1:B:345:ILE:HG13	1:B:360:TRP:HD1	1.82	0.43
1:B:394:LEU:HA	1:B:397:ILE:HG12	1.98	0.43
1:B:108:ASN:HB2	1:B:112:GLU:CG	2.49	0.43
1:A:59:ILE:HB	1:A:63:THR:HB	2.00	0.43
1:D:333:PHE:CD1	1:D:343:LEU:HD11	2.54	0.43
1:A:108:ASN:HD22	1:A:112:GLU:HG3	1.83	0.43
1:A:204:ARG:HD2	1:A:237:LEU:HD11	2.00	0.43
1:C:333:PHE:CG	1:C:343:LEU:HD11	2.53	0.43
1:D:264:LEU:HD13	1:D:269:PRO:HD3	1.99	0.43
1:D:208:ARG:HG2	1:D:232:MET:HB2	1.99	0.43
1:A:300:VAL:HG12	1:A:302:LEU:HG	2.01	0.43
1:C:62:GLY:HA3	1:C:90:PRO:O	2.18	0.43
1:E:38:VAL:O	1:E:71:PHE:HA	2.18	0.43
1:B:240:ARG:HA	1:B:245:HIS:CD2	2.54	0.43
1:D:138:ALA:HA	1:D:167:GLU:HB3	2.00	0.43
1:C:14:SER:HB2	1:C:17:VAL:HG21	2.01	0.42
1:E:108:ASN:ND2	1:E:116:ASN:OD1	2.51	0.42
1:B:101:LYS:HD2	1:B:127:MET:SD	2.59	0.42
1:A:249:CYS:HA	1:A:275:ILE:HA	2.01	0.42
1:A:393:ASP:O	1:A:397:ILE:HG12	2.19	0.42
1:C:211:VAL:HA	1:C:229:ARG:HG3	2.01	0.42
1:D:38:VAL:O	1:D:71:PHE:HA	2.20	0.42
1:D:88:ILE:HG22	1:D:216:PHE:HE1	1.83	0.42
1:D:76:GLU:O	1:D:114:ARG:HG3	2.19	0.42
1:B:294:LYS:H	1:B:294:LYS:CD	2.32	0.41
1:A:264:LEU:HD13	1:A:269:PRO:HD3	2.02	0.41
1:C:155:LYS:HE3	1:C:155:LYS:HB3	1.77	0.41
1:A:33:LYS:NZ	1:A:336:GLU:OE2	2.45	0.41
1:A:125:ALA:HA	1:A:135:ILE:HD13	2.02	0.41
1:E:264:LEU:HD13	1:E:269:PRO:HD3	2.03	0.41
1:B:82:ARG:HH22	1:E:392:GLU:HG3	1.85	0.41
1:A:148:TYR:HH	1:A:183:HIS:CE1	2.29	0.41
1:B:31:LYS:HE3	1:B:67:ASN:O	2.21	0.41
1:E:106:SER:HB2	1:E:117:LEU:HD23	2.03	0.41
1:E:240:ARG:NH2	1:E:369:ILE:HD12	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:103:LYS:HE3	1:C:103:LYS:HB2	1.86	0.40
1:C:323:LYS:HE3	1:C:323:LYS:HB2	1.92	0.40
1:E:397:ILE:HD12	1:E:397:ILE:HA	1.86	0.40
1:C:38:VAL:O	1:C:71:PHE:HA	2.21	0.40
1:C:142:THR:HA	1:C:143:PRO:HD3	1.97	0.40
1:E:338:ARG:CZ	1:E:343:LEU:HD21	2.51	0.40
1:E:62:GLY:HA3	1:E:90:PRO:O	2.22	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	398/400 (100%)	388 (98%)	10 (2%)	0	100	100
1	B	398/400 (100%)	392 (98%)	5 (1%)	1 (0%)	41	61
1	C	397/400 (99%)	391 (98%)	6 (2%)	0	100	100
1	D	397/400 (99%)	387 (98%)	10 (2%)	0	100	100
1	E	398/400 (100%)	391 (98%)	7 (2%)	0	100	100
All	All	1988/2000 (99%)	1949 (98%)	38 (2%)	1 (0%)	51	73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	139	HIS

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	344/344 (100%)	336 (98%)	8 (2%)	50	76
1	B	344/344 (100%)	331 (96%)	13 (4%)	33	58
1	C	343/344 (100%)	329 (96%)	14 (4%)	30	55
1	D	343/344 (100%)	335 (98%)	8 (2%)	50	76
1	E	344/344 (100%)	333 (97%)	11 (3%)	39	65
All	All	1718/1720 (100%)	1664 (97%)	54 (3%)	41	67

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	LYS
1	A	94	GLN
1	A	155	LYS
1	A	290	SER
1	A	294	LYS
1	A	318	GLU
1	A	399	ILE
1	A	400	SER
1	B	50	LYS
1	B	81	ARG
1	B	97	GLU
1	B	101	LYS
1	B	104	ILE
1	B	107	THR
1	B	155	LYS
1	B	204[A]	ARG
1	B	204[B]	ARG
1	B	259	GLN
1	B	294	LYS
1	B	392[A]	GLU
1	B	392[B]	GLU
1	C	50	LYS
1	C	60	ASP
1	C	61	ASP
1	C	97	GLU
1	C	147	LEU
1	C	155	LYS
1	C	224	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	226	VAL
1	C	280	ARG
1	C	285	GLU
1	C	294	LYS
1	C	302	LEU
1	C	328	ARG
1	C	332	GLU
1	D	60	ASP
1	D	61	ASP
1	D	81	ARG
1	D	82	ARG
1	D	294	LYS
1	D	302	LEU
1	D	398	GLU
1	D	399	ILE
1	E	54	LYS
1	E	61	ASP
1	E	100	GLU
1	E	104	ILE
1	E	155	LYS
1	E	156	ASP
1	E	195	HIS
1	E	210	GLU
1	E	294	LYS
1	E	332	GLU
1	E	399	ILE

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

Of 22 ligands modelled in this entry, 22 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	400/400 (100%)	-0.24	3 (0%) 86 87	21, 37, 58, 94	0
1	B	398/400 (99%)	0.00	11 (2%) 53 56	23, 44, 75, 95	0
1	C	399/400 (99%)	-0.24	0 100 100	23, 40, 64, 81	0
1	D	399/400 (99%)	-0.09	14 (3%) 44 47	25, 46, 71, 92	0
1	E	400/400 (100%)	-0.08	7 (1%) 68 71	25, 46, 74, 108	0
All	All	1996/2000 (99%)	-0.13	35 (1%) 68 71	21, 42, 70, 108	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	262	VAL	3.7
1	B	324	LEU	3.6
1	D	315	LYS	3.6
1	D	320	LYS	3.6
1	D	318	GLU	3.6
1	B	331	ARG	3.5
1	D	321	ALA	3.4
1	B	333	PHE	3.3
1	B	259	GLN	3.0
1	D	319	SER	3.0
1	B	327	ASN	2.8
1	D	322	VAL	2.7
1	D	313	LEU	2.7
1	D	324	LEU	2.6
1	A	400	SER	2.6
1	E	67	ASN	2.6
1	B	256	TYR	2.6
1	A	259	GLN	2.6
1	B	330	LEU	2.6
1	B	328	ARG	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	330	LEU	2.4
1	E	400	SER	2.3
1	E	24	PRO	2.3
1	D	314	GLY	2.3
1	D	316	GLY	2.2
1	D	331	ARG	2.2
1	B	346	GLU	2.2
1	D	259	GLN	2.2
1	B	28	GLU	2.1
1	A	399	ILE	2.1
1	E	162	LYS	2.1
1	E	57	LYS	2.1
1	E	399	ILE	2.1
1	D	317	ILE	2.1
1	E	103	LYS	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SM	E	505	1/1	0.53	0.14	176,176,176,176	0
3	SM	E	506	1/1	0.83	0.13	161,161,161,161	1
2	ZN	E	501	1/1	0.94	0.14	42,42,42,42	0
3	SM	B	504	1/1	0.95	0.06	103,103,103,103	1
3	SM	C	505	1/1	0.96	0.09	81,81,81,81	1
2	ZN	E	502	1/1	0.96	0.14	44,44,44,44	0
3	SM	C	504	1/1	0.96	0.10	97,97,97,97	1
2	ZN	B	501	1/1	0.97	0.12	34,34,34,34	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SM	E	504	1/1	0.97	0.13	84,84,84,84	0
2	ZN	D	502	1/1	0.98	0.14	35,35,35,35	0
2	ZN	A	502	1/1	0.98	0.12	26,26,26,26	0
2	ZN	B	502	1/1	0.98	0.14	33,33,33,33	0
2	ZN	E	503	1/1	0.99	0.09	43,43,43,43	0
2	ZN	C	501	1/1	0.99	0.15	34,34,34,34	0
2	ZN	C	502	1/1	0.99	0.12	27,27,27,27	0
2	ZN	D	501	1/1	0.99	0.13	40,40,40,40	0
3	SM	D	504	1/1	0.99	0.10	64,64,64,64	0
2	ZN	A	501	1/1	0.99	0.14	32,32,32,32	0
2	ZN	A	503	1/1	0.99	0.09	39,39,39,39	0
2	ZN	B	503	1/1	0.99	0.14	40,40,40,40	0
2	ZN	C	503	1/1	1.00	0.10	31,31,31,31	0
2	ZN	D	503	1/1	1.00	0.09	39,39,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.