



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2024 – 09:57 AM EST

PDB ID : 3P8B  
Title : X-ray crystal structure of Pyrococcus furiosus transcription elongation factor Spt4/5  
Authors : Murakami, K.S.; Klein, B.J.  
Deposited on : 2010-10-13  
Resolution : 1.80 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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

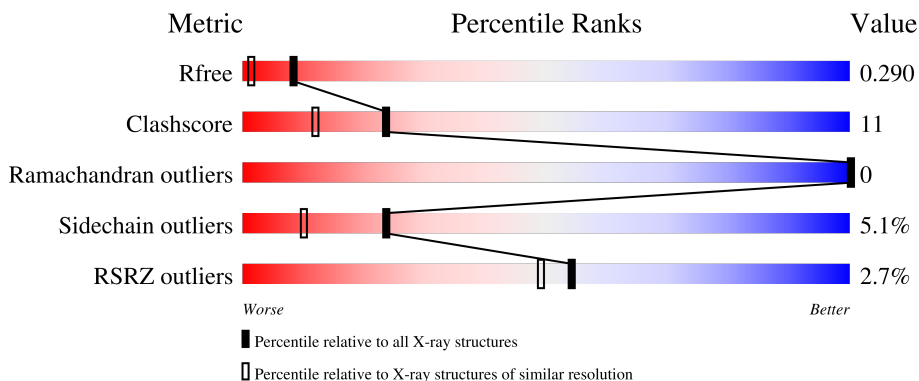
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	81	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 64%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 9%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 26%; height: 10px; background-color: grey; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">2%      64%      9%      •      26%</p>
1	C	81	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 53%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 20%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 26%; height: 10px; background-color: grey; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">2%      53%      20%      •      26%</p>
2	B	152	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 80%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 14%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 3%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">3%      80%      14%      • •</p>
2	D	152	<div style="display: flex; align-items: center;"> <div style="width: 2%; height: 10px; background-color: red; margin-right: 2px;"></div> <div style="width: 77%; height: 10px; background-color: green; margin-right: 2px;"></div> <div style="width: 17%; height: 10px; background-color: yellow; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: orange; margin-right: 2px;"></div> <div style="width: 2%; height: 10px; background-color: grey; margin-right: 2px;"></div> </div> <p style="margin-left: 20px;">2%      77%      17%      • •</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
4	BME	D	156	-	-	X	-

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 3405 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-directed RNA polymerase, subunit e”.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	60	477	297	86	90	4	0	0	0
1	C	60	477	297	86	90	4	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q8U440
A	-18	GLY	-	expression tag	UNP Q8U440
A	-17	SER	-	expression tag	UNP Q8U440
A	-16	SER	-	expression tag	UNP Q8U440
A	-15	HIS	-	expression tag	UNP Q8U440
A	-14	HIS	-	expression tag	UNP Q8U440
A	-13	HIS	-	expression tag	UNP Q8U440
A	-12	HIS	-	expression tag	UNP Q8U440
A	-11	HIS	-	expression tag	UNP Q8U440
A	-10	HIS	-	expression tag	UNP Q8U440
A	-9	SER	-	expression tag	UNP Q8U440
A	-8	SER	-	expression tag	UNP Q8U440
A	-7	GLY	-	expression tag	UNP Q8U440
A	-6	LEU	-	expression tag	UNP Q8U440
A	-5	VAL	-	expression tag	UNP Q8U440
A	-4	PRO	-	expression tag	UNP Q8U440
A	-3	ARG	-	expression tag	UNP Q8U440
A	-2	GLY	-	expression tag	UNP Q8U440
A	-1	SER	-	expression tag	UNP Q8U440
A	0	HIS	-	expression tag	UNP Q8U440
C	-19	MET	-	expression tag	UNP Q8U440
C	-18	GLY	-	expression tag	UNP Q8U440
C	-17	SER	-	expression tag	UNP Q8U440
C	-16	SER	-	expression tag	UNP Q8U440
C	-15	HIS	-	expression tag	UNP Q8U440

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	HIS	-	expression tag	UNP Q8U440
C	-13	HIS	-	expression tag	UNP Q8U440
C	-12	HIS	-	expression tag	UNP Q8U440
C	-11	HIS	-	expression tag	UNP Q8U440
C	-10	HIS	-	expression tag	UNP Q8U440
C	-9	SER	-	expression tag	UNP Q8U440
C	-8	SER	-	expression tag	UNP Q8U440
C	-7	GLY	-	expression tag	UNP Q8U440
C	-6	LEU	-	expression tag	UNP Q8U440
C	-5	VAL	-	expression tag	UNP Q8U440
C	-4	PRO	-	expression tag	UNP Q8U440
C	-3	ARG	-	expression tag	UNP Q8U440
C	-2	GLY	-	expression tag	UNP Q8U440
C	-1	SER	-	expression tag	UNP Q8U440
C	0	HIS	-	expression tag	UNP Q8U440

- Molecule 2 is a protein called Transcription antitermination protein nusG.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	B	147	1142	744	193	205	0	0	0
2	D	147	1142	744	193	205	0	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	A	1	1	1	0	0
3	C	1	1	1	0	0

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C<sub>2</sub>H<sub>6</sub>OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	B	1	Total	C	O	S	0	0
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		
4	D	1	Total	C	O	S	0	0
			4	2	1	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0

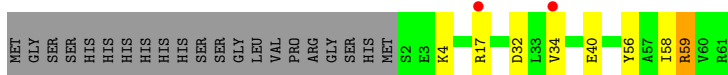
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	15	Total O 15 15	0	0
6	B	45	Total O 45 45	0	0
6	C	10	Total O 10 10	0	0
6	D	41	Total O 41 41	0	0

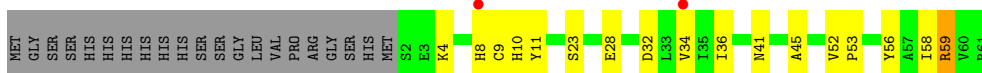
### 3 Residue-property plots [i](#)

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.

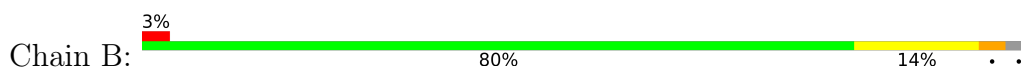
- Molecule 1: DNA-directed RNA polymerase, subunit e''



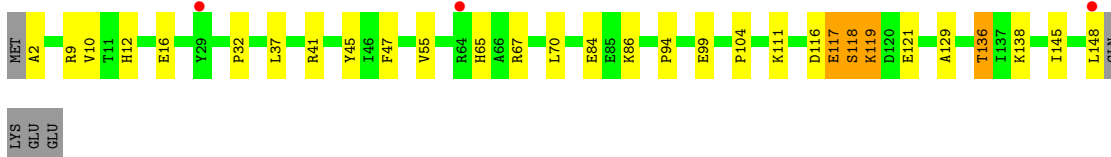
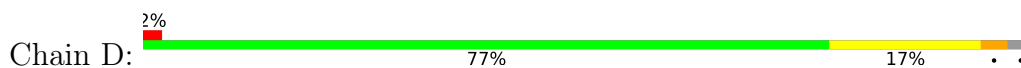
- Molecule 1: DNA-directed RNA polymerase, subunit e''



- Molecule 2: Transcription antitermination protein nusG



- Molecule 2: Transcription antitermination protein nusG





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	40.53Å 87.21Å 133.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 29.93 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.1 (30.00-1.80) 98.1 (29.93-1.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.52 (at 1.80Å)	Xtrriage
Refinement program	REFMAC 5.5.0072	Depositor
R, $R_{free}$	0.236 , 0.292 0.237 , 0.290	Depositor DCC
$R_{free}$ test set	2208 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	24.7	Xtrriage
Anisotropy	0.121	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 44.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	3405	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 31.73 % 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 1.0542e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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](#)

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

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	1.15	1/485 (0.2%)	1.25	2/651 (0.3%)
1	C	1.06	0/485	1.09	2/651 (0.3%)
2	B	1.13	2/1165 (0.2%)	0.96	1/1578 (0.1%)
2	D	1.07	0/1165	0.96	0/1578
All	All	1.10	3/3300 (0.1%)	1.03	5/4458 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	112	VAL	CB-CG1	5.77	1.65	1.52
1	A	58	ILE	CB-CG2	5.59	1.70	1.52
2	B	43	LYS	CB-CG	5.17	1.66	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	59	ARG	NE-CZ-NH1	14.55	127.57	120.30
1	A	59	ARG	NE-CZ-NH2	-11.42	114.59	120.30
1	C	59	ARG	NE-CZ-NH2	-9.64	115.48	120.30
1	C	59	ARG	NE-CZ-NH1	7.77	124.19	120.30
2	B	141	TYR	CA-CB-CG	5.38	123.62	113.40

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	477	0	471	7	0
1	C	477	0	471	18	0
2	B	1142	0	1200	27	0
2	D	1142	0	1200	29	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	4	0	6	0	0
4	B	12	0	18	5	0
4	D	8	0	12	8	0
5	B	18	0	24	4	0
5	D	12	0	16	5	0
6	A	15	0	0	1	0
6	B	45	0	0	7	0
6	C	10	0	0	1	0
6	D	41	0	0	3	0
All	All	3405	0	3418	75	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 11.

All (75) 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)
2:B:138:LYS:H	4:D:156:BME:H22	1.12	1.10
5:B:154:GOL:H11	6:B:164:HOH:O	1.50	1.10
2:B:84:GLU:HG2	6:B:172:HOH:O	1.53	1.05
1:C:41:ASN:O	2:D:2:ALA:HB3	1.64	0.95
1:C:32:ASP:OD2	1:C:59:ARG:HD3	1.66	0.94
4:D:155:BME:O1	6:D:190:HOH:O	1.94	0.86
1:A:32:ASP:OD2	1:A:59:ARG:HD3	1.75	0.85
2:B:84:GLU:CG	6:B:172:HOH:O	2.12	0.85
2:D:41:ARG:HE	4:D:156:BME:H12	1.39	0.84
2:B:138:LYS:N	4:D:156:BME:H22	1.94	0.81
1:C:32:ASP:OD2	1:C:59:ARG:CD	2.30	0.80
2:B:16:GLU:OE1	5:B:153:GOL:H12	1.94	0.67
2:D:119:LYS:HB2	2:D:119:LYS:NZ	2.10	0.65
2:B:108:GLN:HB3	4:B:157:BME:H11	1.78	0.65
5:B:154:GOL:H2	2:D:104:PRO:HG3	1.79	0.64
2:D:116:ASP:OD1	2:D:119:LYS:NZ	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:VAL:HG12	2:B:37:LEU:HD13	1.81	0.63
2:B:133:ILE:HD13	2:D:47:PHE:CE1	2.34	0.63
2:B:137:ILE:HG23	4:D:156:BME:S2	2.39	0.63
2:D:116:ASP:OD2	2:D:118:SER:HB2	2.01	0.61
2:D:41:ARG:NE	4:D:156:BME:H12	2.13	0.61
2:D:138:LYS:HG2	6:D:162:HOH:O	2.03	0.57
1:C:36:ILE:HD12	1:C:45:ALA:HB2	1.87	0.57
2:B:123:VAL:HG22	2:B:136:THR:HB	1.88	0.56
2:B:31:LEU:O	4:B:156:BME:C1	2.54	0.55
2:D:119:LYS:HB2	2:D:119:LYS:HZ2	1.73	0.54
2:B:136:THR:HG22	6:B:169:HOH:O	2.07	0.54
2:B:113:VAL:CG2	2:B:125:GLN:HG3	2.38	0.54
2:D:12:HIS:HD2	5:D:154:GOL:O3	1.90	0.54
1:C:34:VAL:HG12	2:D:37:LEU:CD1	2.38	0.52
1:C:34:VAL:CG2	1:C:56:TYR:HB2	2.39	0.52
2:B:50:ALA:HB1	2:B:51:PRO:HD2	1.92	0.52
1:C:32:ASP:HB2	1:C:58:ILE:HB	1.90	0.51
2:B:7:ALA:HB3	2:B:70:LEU:HG	1.92	0.51
1:C:9:CYS:O	1:C:10:HIS:HB2	2.09	0.51
2:D:16:GLU:OE1	5:D:153:GOL:H31	2.12	0.50
1:A:32:ASP:OD2	1:A:59:ARG:CD	2.55	0.50
1:C:8:HIS:CD2	1:C:23:SER:CB	2.95	0.49
2:D:45:TYR:CZ	5:D:154:GOL:H11	2.47	0.49
2:B:84:GLU:HG3	6:B:172:HOH:O	1.94	0.49
2:B:99:GLU:HB2	2:B:145:ILE:HD11	1.95	0.49
1:C:8:HIS:CD2	1:C:23:SER:OG	2.66	0.49
1:A:34:VAL:HG12	2:B:37:LEU:CD1	2.43	0.48
2:B:31:LEU:O	4:B:156:BME:H12	2.13	0.48
1:A:59:ARG:HD2	6:A:96:HOH:O	2.13	0.48
2:B:128:ASP:HB2	4:B:157:BME:H12	1.95	0.48
1:C:4:LYS:HE3	1:C:28:GLU:HG3	1.95	0.48
1:A:34:VAL:HG23	1:A:56:TYR:HB2	1.95	0.47
1:C:8:HIS:HD2	1:C:23:SER:OG	1.97	0.47
2:D:99:GLU:HB2	2:D:145:ILE:HD11	1.95	0.47
1:C:59:ARG:HD2	6:C:63:HOH:O	2.13	0.47
1:C:8:HIS:CD2	1:C:23:SER:HB2	2.51	0.45
1:A:34:VAL:CG2	1:A:56:TYR:HB2	2.47	0.45
2:D:9:ARG:HD3	5:D:154:GOL:O1	2.16	0.45
5:B:154:GOL:C1	6:B:164:HOH:O	2.29	0.45
2:B:31:LEU:O	4:B:156:BME:H11	2.17	0.45
2:D:119:LYS:HB3	2:D:121:GLU:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:16:GLU:OE2	5:D:153:GOL:H12	2.16	0.45
1:C:34:VAL:HG12	2:D:37:LEU:HD12	1.98	0.44
2:B:70:LEU:HD23	2:B:70:LEU:N	2.32	0.44
2:D:129:ALA:HB2	4:D:155:BME:H22	2.00	0.44
2:B:133:ILE:HD13	2:D:47:PHE:HE1	1.79	0.44
2:D:32:PRO:HG2	2:D:55:VAL:HG11	2.00	0.44
1:C:11:TYR:HD1	1:C:56:TYR:CZ	2.36	0.44
1:C:34:VAL:HG12	2:D:37:LEU:HD13	1.99	0.44
2:D:45:TYR:HE2	2:D:70:LEU:HD21	1.84	0.43
1:C:52:VAL:HA	1:C:53:PRO:HD2	1.81	0.43
2:D:10:VAL:HA	2:D:65:HIS:O	2.19	0.43
2:B:67:ARG:HD3	2:B:67:ARG:HA	1.59	0.42
2:D:117:GLU:HG2	6:D:186:HOH:O	2.19	0.42
6:B:160:HOH:O	2:D:136:THR:HG23	2.20	0.41
2:D:67:ARG:HD3	2:D:67:ARG:HA	1.86	0.41
2:B:133:ILE:HD13	2:D:47:PHE:CZ	2.56	0.41
2:B:113:VAL:CG2	2:B:125:GLN:CG	2.99	0.41
2:B:141:TYR:CE2	4:D:156:BME:S2	3.07	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	58/81 (72%)	57 (98%)	1 (2%)	0	100	100
1	C	58/81 (72%)	55 (95%)	3 (5%)	0	100	100
2	B	145/152 (95%)	144 (99%)	1 (1%)	0	100	100
2	D	145/152 (95%)	142 (98%)	3 (2%)	0	100	100
All	All	406/466 (87%)	398 (98%)	8 (2%)	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	53/71 (75%)	50 (94%)	3 (6%)	20	8
1	C	53/71 (75%)	53 (100%)	0	100	100
2	B	123/128 (96%)	117 (95%)	6 (5%)	25	11
2	D	123/128 (96%)	114 (93%)	9 (7%)	14	4
All	All	352/398 (88%)	334 (95%)	18 (5%)	24	10

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	17	ARG
1	A	40	GLU
2	B	67	ARG
2	B	84	GLU
2	B	136	THR
2	B	143	ARG
2	B	146	SER
2	B	148	LEU
2	D	84	GLU
2	D	86	LYS
2	D	94	PRO
2	D	111	LYS
2	D	117	GLU
2	D	118	SER
2	D	119	LYS
2	D	136	THR
2	D	148	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	30	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	8	HIS
2	D	12	HIS
2	D	81	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 2 are monoatomic - leaving 11 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	BME	B	157	-	3,3,3	0.32	0	1,2,2	0.50	0
5	GOL	B	154	-	5,5,5	0.36	0	5,5,5	0.87	0
5	GOL	B	153	-	5,5,5	0.49	0	5,5,5	0.31	0
4	BME	D	156	-	3,3,3	0.27	0	1,2,2	0.09	0
4	BME	A	62	-	3,3,3	0.33	0	1,2,2	0.26	0
4	BME	D	155	-	3,3,3	0.79	0	1,2,2	0.09	0
5	GOL	D	154	-	5,5,5	0.28	0	5,5,5	0.48	0
5	GOL	B	155	-	5,5,5	0.38	0	5,5,5	0.79	0
4	BME	B	158	-	3,3,3	0.21	0	1,2,2	0.08	0
4	BME	B	156	-	3,3,3	0.19	0	1,2,2	0.48	0
5	GOL	D	153	-	5,5,5	0.37	0	5,5,5	0.29	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BME	B	157	-	-	1/1/1/1	-
5	GOL	B	154	-	-	2/4/4/4	-
5	GOL	B	153	-	-	2/4/4/4	-
4	BME	D	156	-	-	1/1/1/1	-
4	BME	A	62	-	-	0/1/1/1	-
4	BME	D	155	-	-	1/1/1/1	-
5	GOL	D	154	-	-	2/4/4/4	-
5	GOL	B	155	-	-	0/4/4/4	-
4	BME	B	158	-	-	0/1/1/1	-
4	BME	B	156	-	-	1/1/1/1	-
5	GOL	D	153	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	156	BME	O1-C1-C2-S2
4	D	155	BME	O1-C1-C2-S2
4	D	156	BME	O1-C1-C2-S2
5	D	153	GOL	C1-C2-C3-O3
5	D	154	GOL	O1-C1-C2-O2
5	D	154	GOL	O1-C1-C2-C3
5	B	154	GOL	O1-C1-C2-O2
5	B	153	GOL	C1-C2-C3-O3
5	B	154	GOL	O1-C1-C2-C3
5	D	153	GOL	O1-C1-C2-C3
5	B	153	GOL	O2-C2-C3-O3
5	D	153	GOL	O1-C1-C2-O2
5	D	153	GOL	O2-C2-C3-O3
4	B	157	BME	O1-C1-C2-S2

There are no ring outliers.

8 monomers are involved in 22 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	157	BME	2	0
5	B	154	GOL	3	0
5	B	153	GOL	1	0
4	D	156	BME	6	0
4	D	155	BME	2	0
5	D	154	GOL	3	0
4	B	156	BME	3	0
5	D	153	GOL	2	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	60/81 (74%)	0.22	2 (3%) 46 40	18, 29, 43, 49	0
1	C	60/81 (74%)	0.31	2 (3%) 46 40	19, 30, 44, 47	0
2	B	147/152 (96%)	0.04	4 (2%) 54 49	15, 29, 42, 52	0
2	D	147/152 (96%)	0.05	3 (2%) 65 61	19, 30, 41, 50	0
All	All	414/466 (88%)	0.11	11 (2%) 54 49	15, 30, 42, 52	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	ALA	5.3
2	B	148	LEU	3.8
2	D	64	ARG	3.4
1	A	17	ARG	2.9
2	D	148	LEU	2.9
1	C	34	VAL	2.7
1	C	8	HIS	2.6
1	A	34	VAL	2.6
2	B	37	LEU	2.5
2	B	128	ASP	2.3
2	D	29	TYR	2.2

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	BME	A	62	4/4	0.63	0.27	71,73,74,75	0
5	GOL	D	154	6/6	0.66	0.26	62,65,66,68	0
5	GOL	D	153	6/6	0.70	0.17	58,60,62,62	0
4	BME	B	156	4/4	0.75	0.17	44,48,50,57	0
5	GOL	B	154	6/6	0.80	0.24	59,62,64,64	0
5	GOL	B	153	6/6	0.86	0.14	49,50,52,54	0
4	BME	D	156	4/4	0.86	0.14	35,40,43,46	0
4	BME	B	158	4/4	0.87	0.12	41,47,49,58	0
4	BME	D	155	4/4	0.88	0.12	36,36,38,42	0
4	BME	B	157	4/4	0.92	0.21	60,61,62,62	0
5	GOL	B	155	6/6	0.93	0.11	39,46,48,52	0
3	ZN	C	101	1/1	0.99	0.04	21,21,21,21	0
3	ZN	A	101	1/1	0.99	0.03	21,21,21,21	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.