



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:32 PM GMT

PDB ID : 1U1G  
Title : Structure of E. coli uridine phosphorylase complexed to 5-(m-(benzyloxy)benzyl)barbituric acid (BBBA)  
Authors : Bu, W.; Settembre, E.C.; Ealick, S.E.  
Deposited on : 2004-07-15  
Resolution : 1.95 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

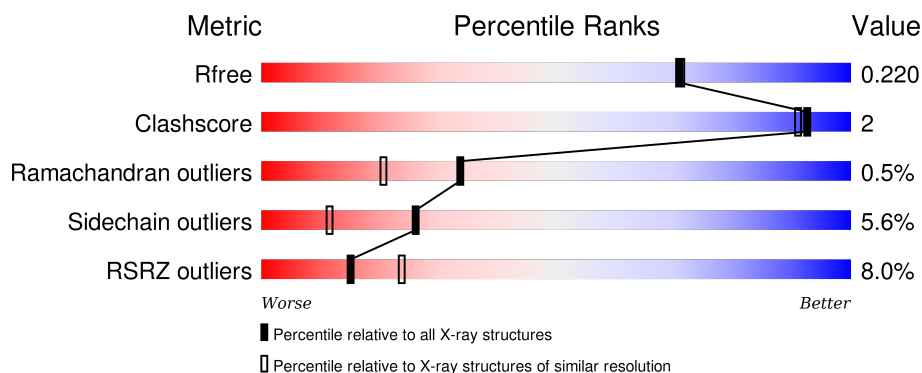
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.95 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))
$R_{free}$	91344	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	256	<div> <div>3%</div> <div>90%</div> <div>5%</div> <div>.</div> </div>
1	B	256	<div> <div>7%</div> <div>88%</div> <div>9%</div> <div>..</div> </div>
1	C	256	<div> <div>4%</div> <div>88%</div> <div>9%</div> <div>..</div> </div>
1	D	256	<div> <div>7%</div> <div>90%</div> <div>7%</div> <div>..</div> </div>
1	E	256	<div> <div>7%</div> <div>85%</div> <div>11%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	256	

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	K	A	1002	-	-	-	X
2	K	C	1001	-	-	-	X
2	K	E	1003	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12025 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 Uridine phosphorylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	245	Total	C	N	O	S	0	0	0
			1825	1144	316	354	11			
1	B	251	Total	C	N	O	S	0	0	0
			1879	1178	326	364	11			
1	C	250	Total	C	N	O	S	0	0	0
			1870	1172	324	363	11			
1	D	250	Total	C	N	O	S	0	0	0
			1870	1172	324	363	11			
1	E	247	Total	C	N	O	S	0	0	0
			1842	1154	320	357	11			
1	F	250	Total	C	N	O	S	0	0	0
			1870	1172	324	363	11			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	CLONING ARTIFACT	UNP P12758
A	-1	SER	-	CLONING ARTIFACT	UNP P12758
A	0	HIS	-	CLONING ARTIFACT	UNP P12758
A	1	MET	-	CLONING ARTIFACT	UNP P12758
B	-2	GLY	-	CLONING ARTIFACT	UNP P12758
B	-1	SER	-	CLONING ARTIFACT	UNP P12758
B	0	HIS	-	CLONING ARTIFACT	UNP P12758
B	1	MET	-	CLONING ARTIFACT	UNP P12758
C	-2	GLY	-	CLONING ARTIFACT	UNP P12758
C	-1	SER	-	CLONING ARTIFACT	UNP P12758
C	0	HIS	-	CLONING ARTIFACT	UNP P12758
C	1	MET	-	CLONING ARTIFACT	UNP P12758
D	-2	GLY	-	CLONING ARTIFACT	UNP P12758
D	-1	SER	-	CLONING ARTIFACT	UNP P12758
D	0	HIS	-	CLONING ARTIFACT	UNP P12758
D	1	MET	-	CLONING ARTIFACT	UNP P12758
E	-2	GLY	-	CLONING ARTIFACT	UNP P12758

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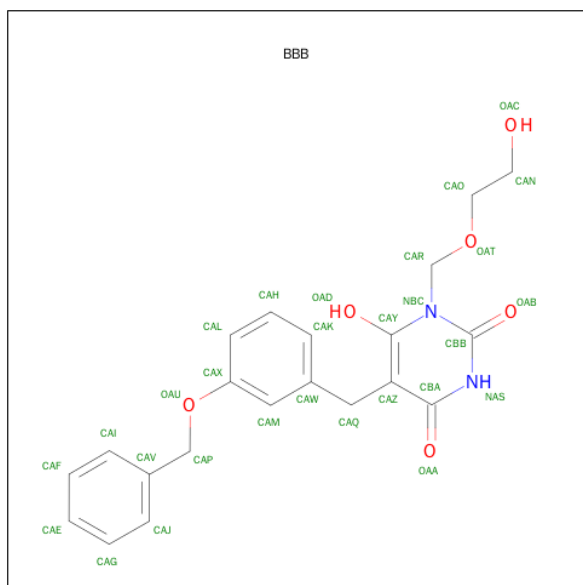
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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	SER	-	CLONING ARTIFACT	UNP P12758
E	0	HIS	-	CLONING ARTIFACT	UNP P12758
E	1	MET	-	CLONING ARTIFACT	UNP P12758
F	-2	GLY	-	CLONING ARTIFACT	UNP P12758
F	-1	SER	-	CLONING ARTIFACT	UNP P12758
F	0	HIS	-	CLONING ARTIFACT	UNP P12758
F	1	MET	-	CLONING ARTIFACT	UNP P12758

- Molecule 2 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total K 1 1	0	0
2	C	1	Total K 1 1	0	0
2	E	1	Total K 1 1	0	0

- Molecule 3 is 1-((2-HYDROXYETHOXY)METHYL)-5-(3-(BENZYLOXY)BENZYL)-6-HYDROXYPYRIMIDINE-2,4(1H,3H)-DIONE (three-letter code: BBB) (formula: C<sub>21</sub>H<sub>22</sub>N<sub>2</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 29 21 2 6	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			29	21	2	6		
3	C	1	Total	C	N	O	0	0
			29	21	2	6		
3	D	1	Total	C	N	O	0	0
			29	21	2	6		
3	E	1	Total	C	N	O	0	0
			29	21	2	6		
3	F	1	Total	C	N	O	0	0
			29	21	2	6		

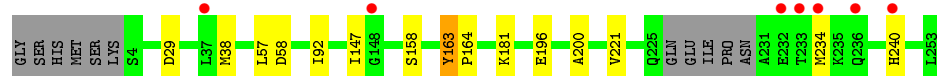
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	143	Total	O	0	0
			143	143		
4	B	106	Total	O	0	0
			106	106		
4	C	147	Total	O	0	0
			147	147		
4	D	130	Total	O	0	0
			130	130		
4	E	90	Total	O	0	0
			90	90		
4	F	76	Total	O	0	0
			76	76		

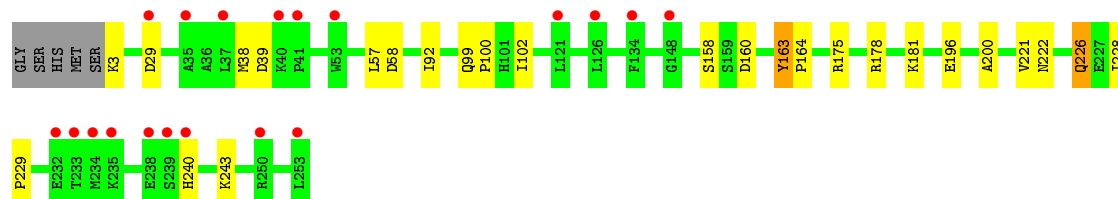
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

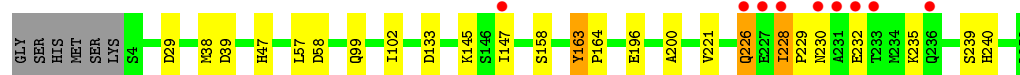
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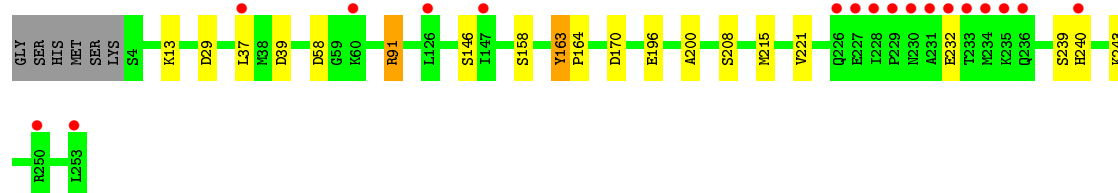
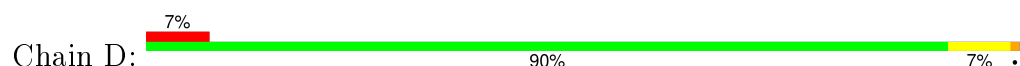
- Molecule 1: Uridine phosphorylase



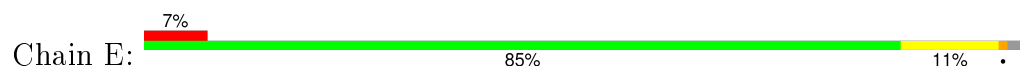
- Molecule 1: Uridine phosphorylase

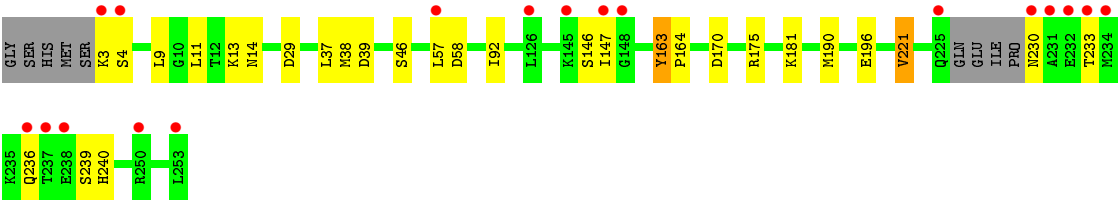


- Molecule 1: Uridine phosphorylase

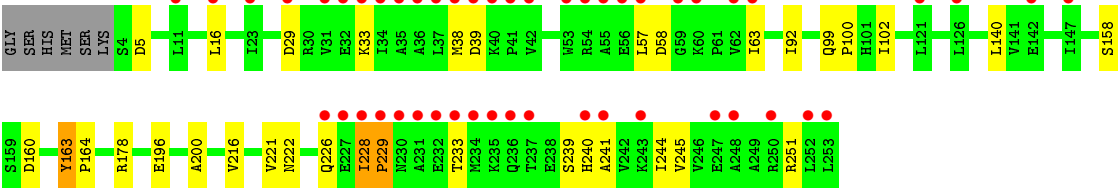
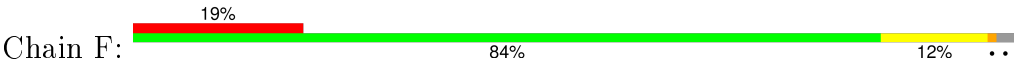


- Molecule 1: Uridine phosphorylase





• Molecule 1: Uridine phosphorylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.68Å 127.12Å 143.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 1.95 49.23 – 1.95	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.39-1.95) 93.6 (49.23-1.95)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.04 (at 1.95Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.200 , 0.221 0.199 , 0.220	Depositor DCC
$R_{free}$ test set	8280 reflections (7.69%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.1	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 117748 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12025	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: K, BBB

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	0.32	0/1855	0.66	2/2519 (0.1%)
1	B	0.32	0/1911	0.65	3/2595 (0.1%)
1	C	0.34	0/1902	0.66	4/2584 (0.2%)
1	D	0.33	0/1902	0.65	4/2584 (0.2%)
1	E	0.31	0/1872	0.65	4/2541 (0.2%)
1	F	0.31	0/1902	0.64	4/2584 (0.2%)
All	All	0.32	0/11344	0.65	21/15407 (0.1%)

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	58	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	58	ASP	CB-CG-OD2	5.80	123.53	118.30
1	E	58	ASP	CB-CG-OD2	5.74	123.47	118.30
1	C	58	ASP	CB-CG-OD2	5.67	123.40	118.30
1	D	58	ASP	CB-CG-OD2	5.61	123.35	118.30
1	F	58	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	29	ASP	CB-CG-OD2	5.48	123.24	118.30
1	E	29	ASP	CB-CG-OD2	5.35	123.12	118.30
1	F	29	ASP	CB-CG-OD2	5.21	122.99	118.30
1	D	29	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	29	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	29	ASP	CB-CG-OD2	5.16	122.95	118.30
1	B	39	ASP	CB-CG-OD2	5.16	122.94	118.30
1	E	39	ASP	CB-CG-OD2	5.15	122.94	118.30
1	E	170	ASP	CB-CG-OD2	5.12	122.91	118.30
1	D	170	ASP	CB-CG-OD2	5.10	122.89	118.30
1	F	39	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	39	ASP	CB-CG-OD2	5.06	122.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	39	ASP	CB-CG-OD2	5.02	122.82	118.30
1	F	5	ASP	CB-CG-OD2	5.01	122.81	118.30
1	C	133	ASP	CB-CG-OD2	5.01	122.81	118.30

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	1825	0	1813	4	0
1	B	1879	0	1876	9	0
1	C	1870	0	1863	8	0
1	D	1870	0	1862	5	0
1	E	1842	0	1832	8	0
1	F	1870	0	1863	11	0
2	A	1	0	0	0	0
2	C	1	0	0	0	0
2	E	1	0	0	0	0
3	A	29	0	21	0	0
3	B	29	0	21	0	0
3	C	29	0	21	0	0
3	D	29	0	21	0	0
3	E	29	0	21	1	0
3	F	29	0	21	0	0
4	A	143	0	0	0	0
4	B	106	0	0	1	0
4	C	147	0	0	1	0
4	D	130	0	0	0	0
4	E	90	0	0	1	0
4	F	76	0	0	0	0
All	All	12025	0	11235	44	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 (44) 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:B:222:ASN:H	1:B:226:GLN:HE21	1.45	0.64
1:B:38:MET:HG2	1:B:57:LEU:HD13	1.87	0.56
1:E:163:TYR:HB2	1:E:164:PRO:HD3	1.88	0.55
1:B:175:ARG:NH2	4:B:4318:HOH:O	2.39	0.54
1:E:38:MET:HG2	1:E:57:LEU:HD13	1.90	0.54
1:F:163:TYR:HB2	1:F:164:PRO:HD3	1.92	0.51
1:A:163:TYR:HB2	1:A:164:PRO:HD3	1.93	0.51
1:A:38:MET:HG2	1:A:57:LEU:HD13	1.94	0.50
1:F:38:MET:HG2	1:F:57:LEU:HD13	1.94	0.50
1:E:230:ASN:HD22	1:E:233:THR:H	1.61	0.49
1:D:158:SER:HB3	1:D:200:ALA:HB2	1.94	0.48
1:F:158:SER:HB3	1:F:200:ALA:HB2	1.96	0.48
1:B:158:SER:HB3	1:B:200:ALA:HB2	1.94	0.48
1:E:163:TYR:HB2	1:E:164:PRO:CD	2.44	0.48
1:C:158:SER:HB3	1:C:200:ALA:HB2	1.96	0.48
1:F:241:ALA:HA	1:F:244:ILE:HD12	1.96	0.47
1:C:47:HIS:HE1	4:C:5386:HOH:O	1.97	0.47
1:C:38:MET:HG2	1:C:57:LEU:HD13	1.96	0.47
1:B:99:GLN:HB2	1:B:102:ILE:HD12	1.99	0.45
1:B:163:TYR:HB2	1:B:164:PRO:HD3	1.99	0.45
1:D:163:TYR:HB2	1:D:164:PRO:HD3	1.99	0.45
1:C:99:GLN:HB2	1:C:102:ILE:HD12	1.98	0.45
1:F:163:TYR:HB2	1:F:164:PRO:CD	2.47	0.45
1:D:163:TYR:HB2	1:D:164:PRO:CD	2.46	0.45
1:F:228:ILE:HA	1:F:229:PRO:HD3	1.84	0.44
1:C:163:TYR:HB2	1:C:164:PRO:CD	2.48	0.43
1:D:91:ARG:HG2	1:D:215:MET:SD	2.59	0.43
1:C:163:TYR:HB2	1:C:164:PRO:HD3	2.00	0.43
1:A:163:TYR:HB2	1:A:164:PRO:CD	2.48	0.43
1:E:9:LEU:HB3	1:E:11:LEU:HD12	2.01	0.43
1:B:99:GLN:HA	1:B:100:PRO:HD3	1.91	0.42
1:C:228:ILE:HA	1:C:229:PRO:HD3	1.82	0.42
1:A:158:SER:HB3	1:A:200:ALA:HB2	2.01	0.42
1:B:163:TYR:HB2	1:B:164:PRO:CD	2.50	0.42
1:F:99:GLN:HB2	1:F:102:ILE:HD12	2.02	0.42
1:C:226:GLN:HB2	1:C:226:GLN:HE21	1.64	0.42
1:D:208:SER:HB2	1:E:190:MET:HG2	2.02	0.41
1:F:140:LEU:HD22	1:F:216:VAL:HB	2.02	0.41
1:F:102:ILE:O	1:F:222:ASN:ND2	2.54	0.41
1:B:228:ILE:HA	1:B:229:PRO:HD3	1.86	0.41
1:F:16:LEU:HD22	1:F:63:ILE:HG13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:175:ARG:NH1	4:E:7341:HOH:O	2.53	0.40
1:F:99:GLN:HA	1:F:100:PRO:HD3	1.91	0.40
1:E:221:VAL:HG11	3:E:7300:BBB:HAK	2.04	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	241/256 (94%)	237 (98%)	3 (1%)	1 (0%)	39	27
1	B	249/256 (97%)	246 (99%)	2 (1%)	1 (0%)	39	27
1	C	248/256 (97%)	245 (99%)	2 (1%)	1 (0%)	39	27
1	D	248/256 (97%)	245 (99%)	2 (1%)	1 (0%)	39	27
1	E	243/256 (95%)	238 (98%)	4 (2%)	1 (0%)	39	27
1	F	248/256 (97%)	238 (96%)	8 (3%)	2 (1%)	24	11
All	All	1477/1536 (96%)	1449 (98%)	21 (1%)	7 (0%)	34	21

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	TYR
1	B	163	TYR
1	C	163	TYR
1	D	163	TYR
1	E	163	TYR
1	F	163	TYR
1	F	229	PRO

### 5.3.2 Protein sidechains ⓘ

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	193/206 (94%)	186 (96%)	7 (4%)	42	28
1	B	200/206 (97%)	190 (95%)	10 (5%)	30	14
1	C	199/206 (97%)	188 (94%)	11 (6%)	27	12
1	D	199/206 (97%)	189 (95%)	10 (5%)	30	14
1	E	195/206 (95%)	180 (92%)	15 (8%)	16	5
1	F	199/206 (97%)	186 (94%)	13 (6%)	21	8
All	All	1185/1236 (96%)	1119 (94%)	66 (6%)	26	11

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	92	ILE
1	A	147	ILE
1	A	181	LYS
1	A	196	GLU
1	A	221	VAL
1	A	234	MET
1	A	240	HIS
1	B	3	LYS
1	B	92	ILE
1	B	160	ASP
1	B	178	ARG
1	B	181	LYS
1	B	196	GLU
1	B	221	VAL
1	B	226	GLN
1	B	240	HIS
1	B	243	LYS
1	C	145	LYS
1	C	147	ILE
1	C	196	GLU
1	C	221	VAL
1	C	226	GLN

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Mol	Chain	Res	Type
1	C	228	ILE
1	C	230	ASN
1	C	232	GLU
1	C	235	LYS
1	C	239	SER
1	C	240	HIS
1	D	13	LYS
1	D	37	LEU
1	D	91	ARG
1	D	146	SER
1	D	196	GLU
1	D	221	VAL
1	D	232	GLU
1	D	239	SER
1	D	240	HIS
1	D	243	LYS
1	E	3	LYS
1	E	4	SER
1	E	13	LYS
1	E	14	ASN
1	E	37	LEU
1	E	46	SER
1	E	92	ILE
1	E	146	SER
1	E	147	ILE
1	E	181	LYS
1	E	196	GLU
1	E	221	VAL
1	E	236	GLN
1	E	239	SER
1	E	240	HIS
1	F	33	LYS
1	F	92	ILE
1	F	160	ASP
1	F	178	ARG
1	F	196	GLU
1	F	221	VAL
1	F	226	GLN
1	F	228	ILE
1	F	233	THR
1	F	239	SER
1	F	240	HIS

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Mol	Chain	Res	Type
1	F	245	VAL
1	F	251	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	17	GLN
1	B	226	GLN
1	C	17	GLN
1	C	47	HIS
1	C	226	GLN
1	D	47	HIS
1	E	230	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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
3	BBB	A	3300	-	25,31,31	2.79	17 (68%)	27,41,41	2.73	3 (11%)
3	BBB	B	4300	-	25,31,31	2.78	17 (68%)	27,41,41	2.72	3 (11%)
3	BBB	C	5300	-	25,31,31	2.77	17 (68%)	27,41,41	2.76	3 (11%)
3	BBB	D	6300	-	25,31,31	2.78	17 (68%)	27,41,41	2.75	3 (11%)
3	BBB	E	7300	-	25,31,31	2.77	17 (68%)	27,41,41	2.80	4 (14%)
3	BBB	F	8300	-	25,31,31	2.77	17 (68%)	27,41,41	2.73	3 (11%)

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
3	BBB	A	3300	-	-	0/12/14/14	0/3/3/3
3	BBB	B	4300	-	-	0/12/14/14	0/3/3/3
3	BBB	C	5300	-	-	0/12/14/14	0/3/3/3
3	BBB	D	6300	-	-	0/12/14/14	0/3/3/3
3	BBB	E	7300	-	-	0/12/14/14	0/3/3/3
3	BBB	F	8300	-	-	0/12/14/14	0/3/3/3

All (102) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	4300	BBB	CAP-CAV	-3.82	1.41	1.50
3	C	5300	BBB	CAP-CAV	-3.81	1.41	1.50
3	D	6300	BBB	CAP-CAV	-3.80	1.41	1.50
3	A	3300	BBB	CAP-CAV	-3.79	1.41	1.50
3	F	8300	BBB	CAP-CAV	-3.78	1.41	1.50
3	E	7300	BBB	CAP-CAV	-3.75	1.41	1.50
3	C	5300	BBB	CAH-CAL	2.38	1.43	1.38
3	D	6300	BBB	CAH-CAL	2.38	1.43	1.38
3	B	4300	BBB	CAH-CAL	2.41	1.43	1.38
3	A	3300	BBB	CAH-CAL	2.41	1.43	1.38
3	E	7300	BBB	CAH-CAL	2.41	1.43	1.38
3	F	8300	BBB	CAH-CAL	2.46	1.44	1.38
3	A	3300	BBB	CAF-CAE	2.65	1.44	1.38
3	E	7300	BBB	CAF-CAE	2.65	1.44	1.38
3	F	8300	BBB	CAF-CAE	2.65	1.44	1.38
3	C	5300	BBB	CAF-CAE	2.67	1.44	1.38
3	B	4300	BBB	CAF-CAE	2.71	1.45	1.38
3	D	6300	BBB	CAF-CAE	2.71	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5300	BBB	CAH-CAK	2.74	1.44	1.38
3	D	6300	BBB	OAU-CAP	2.74	1.52	1.43
3	F	8300	BBB	CAM-CAW	2.74	1.44	1.39
3	B	4300	BBB	CAM-CAW	2.76	1.44	1.39
3	C	5300	BBB	CAK-CAW	2.76	1.44	1.38
3	F	8300	BBB	CAG-CAJ	2.77	1.44	1.38
3	C	5300	BBB	OAU-CAP	2.77	1.52	1.43
3	B	4300	BBB	OAU-CAP	2.77	1.52	1.43
3	F	8300	BBB	CAH-CAK	2.78	1.44	1.38
3	F	8300	BBB	CAK-CAW	2.78	1.44	1.38
3	F	8300	BBB	OAU-CAP	2.78	1.52	1.43
3	A	3300	BBB	CAG-CAJ	2.79	1.44	1.38
3	E	7300	BBB	OAU-CAP	2.79	1.52	1.43
3	E	7300	BBB	CAH-CAK	2.79	1.44	1.38
3	D	6300	BBB	CAH-CAK	2.79	1.44	1.38
3	D	6300	BBB	CAK-CAW	2.80	1.44	1.38
3	A	3300	BBB	OAU-CAP	2.80	1.52	1.43
3	A	3300	BBB	CAK-CAW	2.81	1.44	1.38
3	E	7300	BBB	CAG-CAJ	2.81	1.44	1.38
3	B	4300	BBB	CAG-CAJ	2.81	1.44	1.38
3	B	4300	BBB	CAH-CAK	2.81	1.44	1.38
3	C	5300	BBB	CAM-CAW	2.81	1.44	1.39
3	B	4300	BBB	CAK-CAW	2.82	1.44	1.38
3	C	5300	BBB	CAG-CAJ	2.82	1.44	1.38
3	D	6300	BBB	CAM-CAW	2.83	1.44	1.39
3	A	3300	BBB	CAH-CAK	2.84	1.44	1.38
3	D	6300	BBB	CAG-CAJ	2.85	1.44	1.38
3	E	7300	BBB	CAM-CAW	2.85	1.44	1.39
3	F	8300	BBB	CAF-CAI	2.85	1.44	1.38
3	A	3300	BBB	CAM-CAW	2.86	1.44	1.39
3	E	7300	BBB	CAF-CAI	2.86	1.44	1.38
3	D	6300	BBB	CAF-CAI	2.87	1.44	1.38
3	E	7300	BBB	CAK-CAW	2.87	1.44	1.38
3	C	5300	BBB	CAF-CAI	2.87	1.44	1.38
3	B	4300	BBB	CAF-CAI	2.89	1.44	1.38
3	A	3300	BBB	CAF-CAI	2.89	1.44	1.38
3	C	5300	BBB	CAE-CAG	2.91	1.45	1.38
3	A	3300	BBB	CAE-CAG	2.94	1.45	1.38
3	E	7300	BBB	CAE-CAG	2.95	1.45	1.38
3	F	8300	BBB	CAE-CAG	2.97	1.45	1.38
3	B	4300	BBB	CAE-CAG	2.97	1.45	1.38
3	D	6300	BBB	CAE-CAG	2.98	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	5300	BBB	CAL-CAX	3.06	1.44	1.38
3	E	7300	BBB	CAJ-CAV	3.06	1.45	1.38
3	F	8300	BBB	CAJ-CAV	3.09	1.45	1.38
3	B	4300	BBB	CAJ-CAV	3.09	1.45	1.38
3	E	7300	BBB	CAL-CAX	3.11	1.44	1.38
3	B	4300	BBB	CAI-CAV	3.11	1.45	1.38
3	C	5300	BBB	CAJ-CAV	3.11	1.45	1.38
3	D	6300	BBB	CAI-CAV	3.11	1.45	1.38
3	F	8300	BBB	CAI-CAV	3.12	1.45	1.38
3	E	7300	BBB	CAI-CAV	3.13	1.45	1.38
3	A	3300	BBB	CAJ-CAV	3.13	1.45	1.38
3	C	5300	BBB	CAI-CAV	3.14	1.45	1.38
3	D	6300	BBB	CAJ-CAV	3.14	1.45	1.38
3	D	6300	BBB	CAL-CAX	3.15	1.45	1.38
3	B	4300	BBB	CAL-CAX	3.15	1.45	1.38
3	A	3300	BBB	CAL-CAX	3.16	1.45	1.38
3	A	3300	BBB	CAI-CAV	3.16	1.45	1.38
3	F	8300	BBB	CAL-CAX	3.17	1.45	1.38
3	E	7300	BBB	CAQ-CAZ	3.46	1.57	1.52
3	D	6300	BBB	CAQ-CAZ	3.47	1.57	1.52
3	A	3300	BBB	CAQ-CAZ	3.50	1.57	1.52
3	C	5300	BBB	CAQ-CAZ	3.50	1.57	1.52
3	F	8300	BBB	CAQ-CAZ	3.52	1.57	1.52
3	B	4300	BBB	CAQ-CAZ	3.58	1.57	1.52
3	B	4300	BBB	CAM-CAX	3.73	1.45	1.38
3	F	8300	BBB	CAM-CAX	3.78	1.45	1.38
3	A	3300	BBB	CAM-CAX	3.82	1.45	1.38
3	E	7300	BBB	CAM-CAX	3.85	1.45	1.38
3	D	6300	BBB	CAM-CAX	3.88	1.46	1.38
3	C	5300	BBB	CAM-CAX	3.92	1.46	1.38
3	D	6300	BBB	CAY-NBC	4.49	1.45	1.38
3	E	7300	BBB	CAY-NBC	4.50	1.45	1.38
3	B	4300	BBB	CAY-NBC	4.55	1.45	1.38
3	F	8300	BBB	CAY-NBC	4.56	1.45	1.38
3	C	5300	BBB	CAY-NBC	4.57	1.45	1.38
3	A	3300	BBB	CAY-NBC	4.58	1.45	1.38
3	C	5300	BBB	CBA-NAS	5.16	1.42	1.33
3	F	8300	BBB	CBA-NAS	5.18	1.42	1.33
3	E	7300	BBB	CBA-NAS	5.18	1.42	1.33
3	B	4300	BBB	CBA-NAS	5.19	1.42	1.33
3	D	6300	BBB	CBA-NAS	5.21	1.42	1.33
3	A	3300	BBB	CBA-NAS	5.29	1.42	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	7300	BBB	OAU-CAP-CAV	2.05	115.36	109.21
3	D	6300	BBB	CAQ-CAZ-CAY	3.11	122.70	119.61
3	C	5300	BBB	CAQ-CAZ-CAY	3.14	122.73	119.61
3	F	8300	BBB	CAQ-CAZ-CAY	3.21	122.79	119.61
3	E	7300	BBB	CAQ-CAZ-CAY	3.23	122.82	119.61
3	A	3300	BBB	CAQ-CAZ-CAY	3.26	122.84	119.61
3	B	4300	BBB	CAQ-CAZ-CAY	3.53	123.12	119.61
3	D	6300	BBB	CBA-NAS-CBB	6.88	121.19	115.25
3	A	3300	BBB	CBA-NAS-CBB	6.99	121.29	115.25
3	E	7300	BBB	CBA-NAS-CBB	7.06	121.35	115.25
3	F	8300	BBB	CBA-NAS-CBB	7.07	121.36	115.25
3	C	5300	BBB	CBA-NAS-CBB	7.19	121.47	115.25
3	B	4300	BBB	CBA-NAS-CBB	7.20	121.47	115.25
3	B	4300	BBB	CAP-OAU-CAX	11.11	147.53	117.70
3	F	8300	BBB	CAP-OAU-CAX	11.28	147.97	117.70
3	A	3300	BBB	CAP-OAU-CAX	11.35	148.16	117.70
3	C	5300	BBB	CAP-OAU-CAX	11.45	148.43	117.70
3	D	6300	BBB	CAP-OAU-CAX	11.54	148.68	117.70
3	E	7300	BBB	CAP-OAU-CAX	11.73	149.18	117.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	7300	BBB	1	0

## 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<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	245/256 (95%)	0.24	7 (2%) 55 65	13, 14, 18, 24	0
1	B	251/256 (98%)	0.57	19 (7%) 17 26	12, 14, 17, 21	0
1	C	250/256 (97%)	0.16	9 (3%) 46 57	12, 14, 21, 24	0
1	D	250/256 (97%)	0.36	18 (7%) 18 28	12, 14, 21, 24	0
1	E	247/256 (96%)	0.44	18 (7%) 18 28	13, 15, 17, 21	0
1	F	250/256 (97%)	1.00	49 (19%) 1 2	13, 15, 18, 20	0
All	All	1493/1536 (97%)	0.46	120 (8%) 15 24	12, 14, 18, 24	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	228	ILE	7.8
1	F	228	ILE	5.8
1	D	229	PRO	5.7
1	F	236	GLN	5.3
1	F	34	ILE	5.2
1	F	229	PRO	5.2
1	F	42	VAL	5.2
1	F	57	LEU	5.1
1	F	38	MET	4.9
1	F	36	ALA	4.6
1	F	37	LEU	4.5
1	E	234	MET	4.3
1	F	35	ALA	4.2
1	F	237	THR	4.1
1	F	227	GLU	4.1
1	F	243	LYS	4.1
1	D	227	GLU	4.1
1	D	147	ILE	3.9
1	D	234	MET	3.9

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Mol	Chain	Res	Type	RSRZ
1	F	41	PRO	3.8
1	D	230	ASN	3.7
1	D	232	GLU	3.7
1	E	4	SER	3.7
1	C	226	GLN	3.6
1	F	62	VAL	3.6
1	F	230	ASN	3.6
1	F	59	GLY	3.5
1	A	232	GLU	3.5
1	E	57	LEU	3.4
1	E	230	ASN	3.4
1	B	37	LEU	3.4
1	D	240	HIS	3.3
1	E	232	GLU	3.2
1	A	234	MET	3.2
1	B	29	ASP	3.2
1	F	235	LYS	3.2
1	C	228	ILE	3.2
1	F	253	LEU	3.2
1	C	227	GLU	3.1
1	D	253	LEU	3.1
1	F	250	ARG	3.1
1	E	231	ALA	3.1
1	B	234	MET	3.1
1	F	240	HIS	3.0
1	D	37	LEU	3.0
1	F	241	ALA	3.0
1	F	147	ILE	3.0
1	B	40	LYS	3.0
1	F	33	LYS	3.0
1	B	134	PHE	2.9
1	A	233	THR	2.9
1	F	252	LEU	2.8
1	D	226	GLN	2.8
1	E	233	THR	2.8
1	F	231	ALA	2.7
1	D	231	ALA	2.7
1	E	148	GLY	2.7
1	F	29	ASP	2.7
1	F	53	TRP	2.7
1	F	233	THR	2.6
1	A	240	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	F	16	LEU	2.6
1	C	233	THR	2.6
1	D	236	GLN	2.6
1	B	250	ARG	2.6
1	E	3	LYS	2.6
1	C	231	ALA	2.6
1	F	126	LEU	2.6
1	D	235	LYS	2.6
1	F	60	LYS	2.6
1	E	236	GLN	2.5
1	C	232	GLU	2.5
1	C	147	ILE	2.5
1	B	126	LEU	2.5
1	E	147	ILE	2.5
1	F	226	GLN	2.5
1	F	63	ILE	2.4
1	B	35	ALA	2.4
1	E	238	GLU	2.4
1	F	23	ILE	2.4
1	B	235	LYS	2.4
1	B	233	THR	2.4
1	F	234	MET	2.4
1	B	238	GLU	2.3
1	B	41	PRO	2.3
1	A	37	LEU	2.3
1	A	236	GLN	2.3
1	D	126	LEU	2.3
1	D	250	ARG	2.3
1	F	11	LEU	2.3
1	B	239	SER	2.3
1	F	232	GLU	2.3
1	E	237	THR	2.3
1	F	121	LEU	2.3
1	C	230	ASN	2.3
1	B	53	TRP	2.2
1	D	60	LYS	2.2
1	B	232	GLU	2.2
1	F	40	LYS	2.2
1	F	32	GLU	2.2
1	F	248	ALA	2.2
1	A	148	GLY	2.2
1	B	253	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	54	ARG	2.2
1	F	55	ALA	2.2
1	B	240	HIS	2.2
1	C	236	GLN	2.2
1	E	145	LYS	2.2
1	E	126	LEU	2.1
1	F	31	VAL	2.1
1	D	233	THR	2.1
1	B	121	LEU	2.1
1	F	56	GLU	2.1
1	E	225	GLN	2.1
1	B	148	GLY	2.1
1	F	247	GLU	2.1
1	F	39	ASP	2.1
1	E	250	ARG	2.1
1	E	253	LEU	2.1
1	F	142	GLU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	K	A	1002	1/1	0.74	0.32	12.21	62,62,62,62	0
2	K	E	1003	1/1	0.89	0.38	11.40	63,63,63,63	0
2	K	C	1001	1/1	0.98	0.14	3.04	49,49,49,49	0
3	BBB	B	4300	29/29	0.81	0.19	1.63	36,37,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BBB	A	3300	29/29	0.86	0.17	1.25	33,36,44,44	0
3	BBB	E	7300	29/29	0.85	0.18	1.13	36,37,45,45	0
3	BBB	F	8300	29/29	0.75	0.24	0.85	42,43,46,46	0
3	BBB	C	5300	29/29	0.90	0.15	0.37	27,30,40,40	0
3	BBB	D	6300	29/29	0.89	0.17	0.25	29,32,40,41	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.