



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 28, 2019 – 07:06 PM EST

PDB ID : 5Q08  
Title : Human liver fructose-1,6-bisphosphatase 1 (fructose 1,6-bisphosphate 1-phosphatase, E.C.3.1.3.11) complexed with the allosteric inhibitor 1-(1-benzothiophen-3-ylsulfonyl)-3-(5-bromo-1,3-thiazol-2-yl)urea  
Authors : Ruf, A.; Joseph, C.; Alker, A.; Banner, D.; Tetaz, T.; Benz, J.; Kuhn, B.; Rudolph, M.G.; Yang, H.; Shao, C.; Burley, S.K.  
Deposited on : 2017-04-18  
Resolution : 2.20 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.

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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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031633  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031633

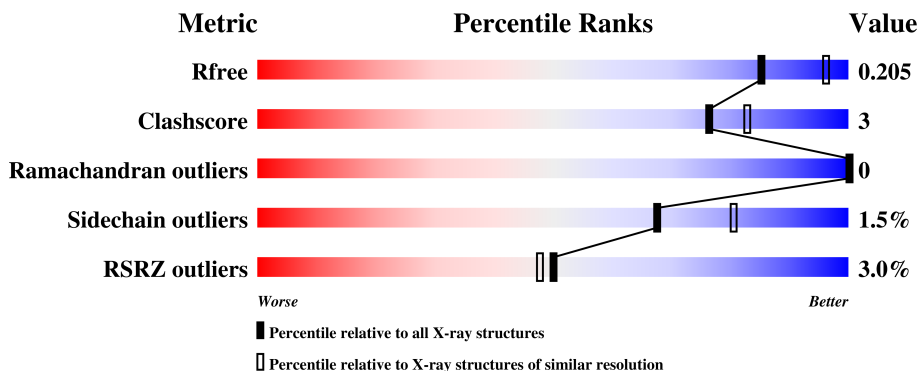
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
$R_{free}$	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (2.20-2.20)

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	338	 3% 86% 9% 6%
1	B	338	 3% 84% 9% 6%
1	C	338	 % 85% 9% 6%
1	D	338	 % 87% 7% 6%
1	E	338	 5% 87% 7% 6%

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Mol	Chain	Length	Quality of chain
1	F	338	 <p>6% 86% 7% • 6%</p>
1	G	338	 <p>% 85% 8% 6%</p>
1	H	338	 <p>2% 87% 6% • 6%</p>

## 2 Entry composition

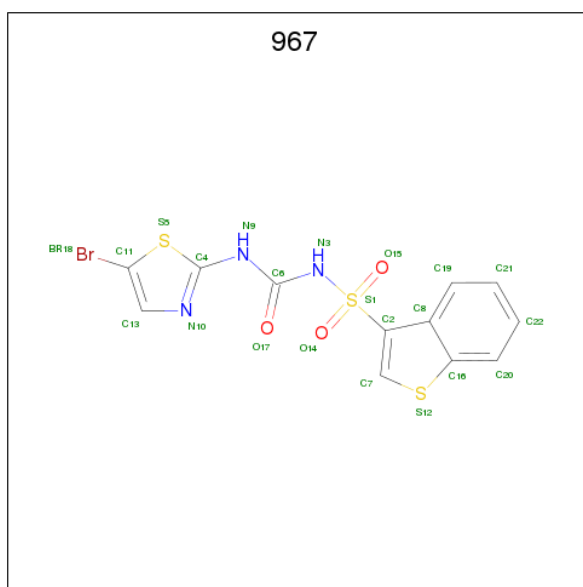
There are 3 unique types of molecules in this entry. The entry contains 21011 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fructose-1,6-bisphosphatase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	319	2446	1558	412	459	17	0	1	0
1	B	317	2437	1551	410	458	18	0	2	0
1	C	317	2431	1548	407	458	18	0	1	0
1	D	319	2447	1559	412	459	17	0	1	0
1	E	319	2447	1559	412	459	17	0	1	0
1	F	317	2442	1553	411	459	19	0	2	0
1	G	317	2430	1547	409	457	17	0	1	0
1	H	317	2434	1551	408	458	17	0	1	0

- Molecule 2 is N-[(5-bromo-1,3-thiazol-2-yl)carbamoyl]-1-benzothiophene-3-sulfonamide (three-letter code: 967) (formula: C<sub>12</sub>H<sub>8</sub>BrN<sub>3</sub>O<sub>3</sub>S<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	Br	C	N	O			S
2	A	1	Total 22	Br 1	C 12	N 3	O 3	S 3	0	0
2	B	1	Total 22	Br 1	C 12	N 3	O 3	S 3	0	0
2	C	1	Total 22	Br 1	C 12	N 3	O 3	S 3	0	0
2	D	1	Total 22	Br 1	C 12	N 3	O 3	S 3	0	0
2	E	1	Total 22	Br 1	C 12	N 3	O 3	S 3	0	0
2	F	1	Total 22	Br 1	C 12	N 3	O 3	S 3	0	0
2	G	1	Total 22	Br 1	C 12	N 3	O 3	S 3	0	0
2	H	1	Total 22	Br 1	C 12	N 3	O 3	S 3	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	156	Total 156	O 156	0	0
3	B	137	Total 137	O 137	0	0
3	C	201	Total 201	O 201	0	0
3	D	205	Total 205	O 205	0	0

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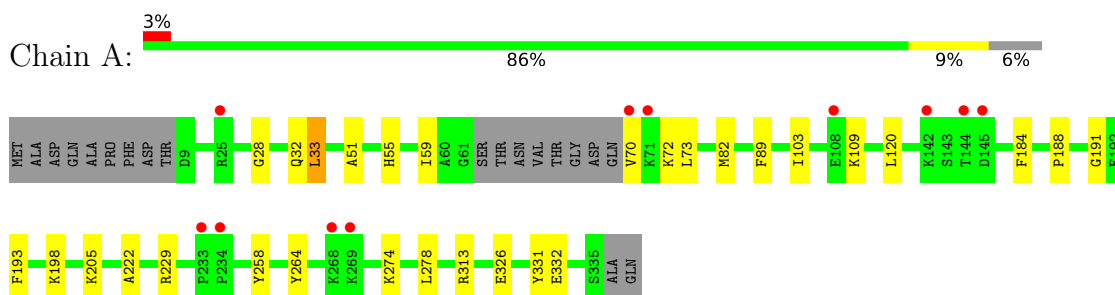
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<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	E	113	Total 113	O 113	0	0
3	F	120	Total 120	O 120	0	0
3	G	205	Total 205	O 205	0	0
3	H	184	Total 184	O 184	0	0

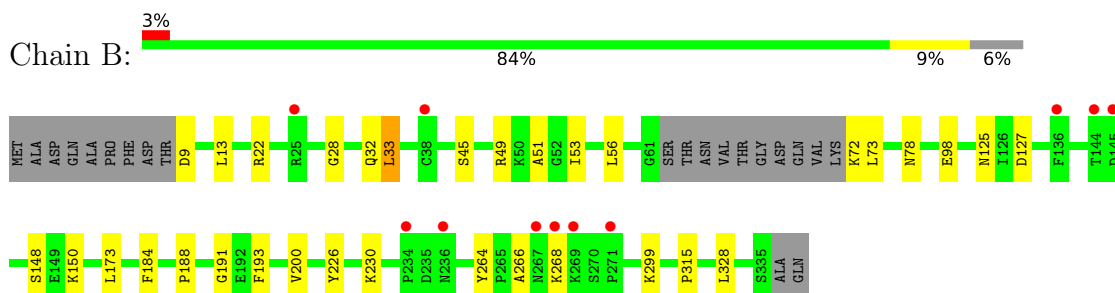
### 3 Residue-property plots [i](#)

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

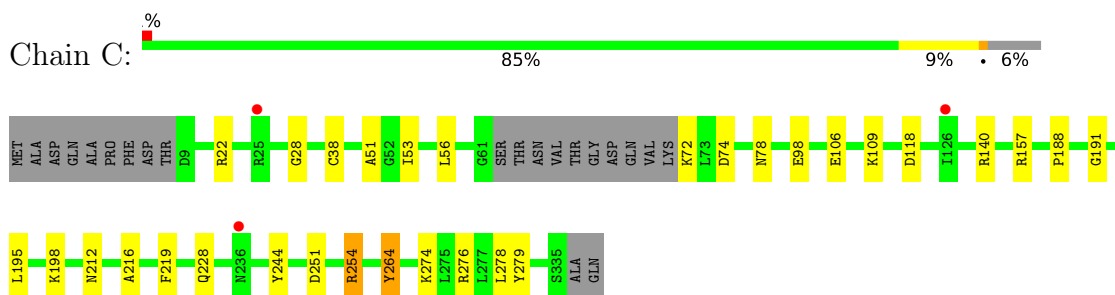
- Molecule 1: Fructose-1,6-bisphosphatase 1



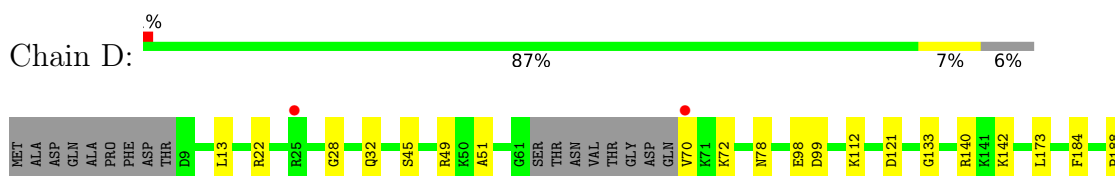
- Molecule 1: Fructose-1,6-bisphosphatase 1

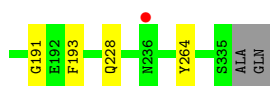


- Molecule 1: Fructose-1,6-bisphosphatase 1

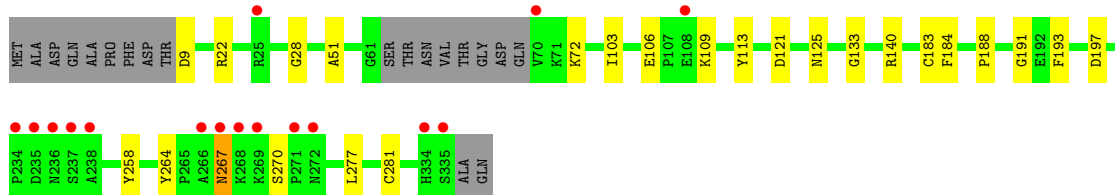
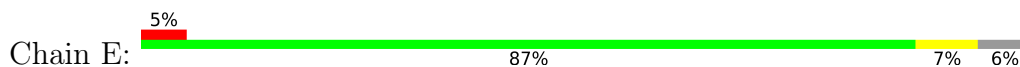


- Molecule 1: Fructose-1,6-bisphosphatase 1

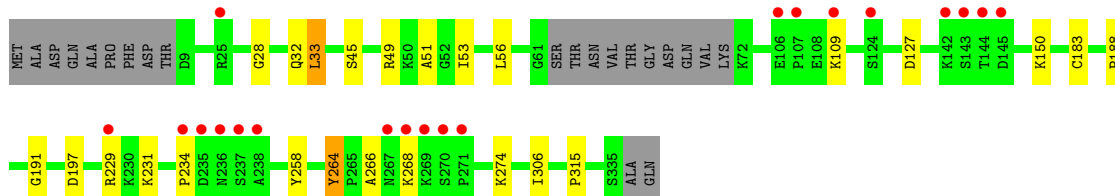
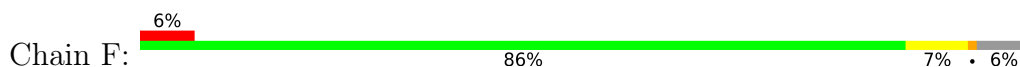




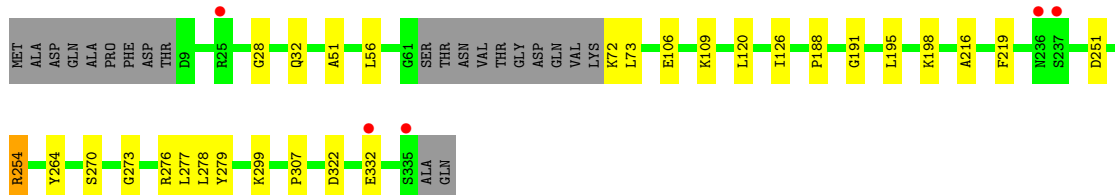
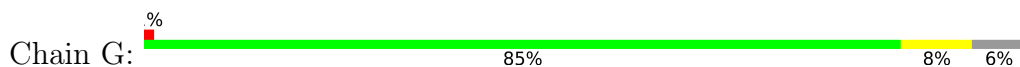
- Molecule 1: Fructose-1,6-bisphosphatase 1



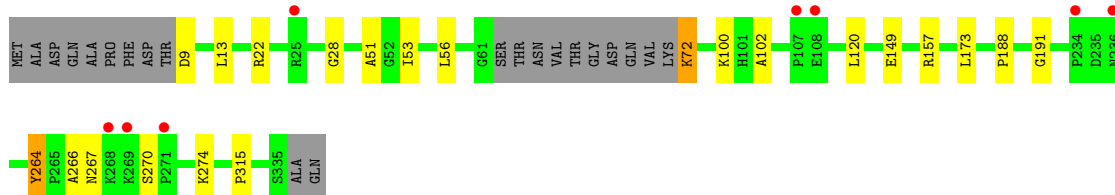
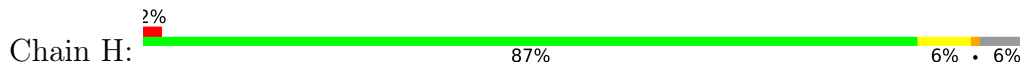
- Molecule 1: Fructose-1,6-bisphosphatase 1



- Molecule 1: Fructose-1,6-bisphosphatase 1



- Molecule 1: Fructose-1,6-bisphosphatase 1





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.22Å 285.13Å 83.36Å 90.00° 97.57° 90.00°	Depositor
Resolution (Å)	29.21 – 2.20 29.21 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.21-2.20) 99.8 (29.21-2.20)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.20Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.158 , 0.204 0.158 , 0.205	Depositor DCC
$R_{free}$ test set	7746 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.1	Xtrriage
Anisotropy	0.536	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 60.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	21011	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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, 0.333 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: 967

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	0.40	0/2495	0.59	1/3368 (0.0%)
1	B	0.37	0/2485	0.57	1/3355 (0.0%)
1	C	0.41	0/2474	0.59	1/3341 (0.0%)
1	D	0.43	0/2495	0.59	0/3368
1	E	0.36	0/2495	0.55	0/3368
1	F	0.36	0/2491	0.56	1/3363 (0.0%)
1	G	0.42	0/2479	0.60	1/3347 (0.0%)
1	H	0.43	0/2477	0.59	0/3344
All	All	0.40	0/19891	0.58	5/26854 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	LEU	CA-CB-CG	7.40	132.31	115.30
1	G	254	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	B	33	LEU	CA-CB-CG	5.71	128.43	115.30
1	F	33	LEU	CA-CB-CG	5.68	128.37	115.30
1	C	254	ARG	NE-CZ-NH2	-5.13	117.73	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	2446	0	2496	19	1
1	B	2437	0	2482	20	0
1	C	2431	0	2473	18	0
1	D	2447	0	2500	15	0
1	E	2447	0	2500	16	1
1	F	2442	0	2483	18	0
1	G	2430	0	2474	19	0
1	H	2434	0	2480	19	0
2	A	22	0	0	3	0
2	B	22	0	0	2	0
2	C	22	0	0	2	0
2	D	22	0	0	3	0
2	E	22	0	0	2	0
2	F	22	0	0	3	0
2	G	22	0	0	3	0
2	H	22	0	0	3	0
3	A	156	0	0	4	0
3	B	137	0	0	2	0
3	C	201	0	0	3	0
3	D	205	0	0	1	0
3	E	113	0	0	1	0
3	F	120	0	0	2	0
3	G	205	0	0	4	0
3	H	184	0	0	2	0
All	All	21011	0	19888	130	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 3.

All (130) 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:G:72:LYS:N	3:G:501:HOH:O	2.09	0.85
1:E:9:ASP:N	3:E:501:HOH:O	2.23	0.72
1:G:251:ASP:OD1	1:G:254:ARG:NH2	2.23	0.71
1:B:22:ARG:NH1	1:D:32:GLN:OE1	2.22	0.70
1:A:326:GLU:OE1	3:A:501:HOH:O	2.11	0.68
1:A:274:LYS:HA	1:A:313:ARG:HD3	1.77	0.67
1:F:191:GLY:HA3	1:H:191:GLY:HA3	1.77	0.66
1:F:231:LYS:O	3:F:501:HOH:O	2.14	0.65
1:A:51:ALA:HA	1:B:188:PRO:HD2	1.80	0.63
1:G:299:LYS:NZ	3:G:505:HOH:O	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:GLN:OE1	1:C:22:ARG:NH1	2.30	0.62
1:B:191:GLY:HA3	1:D:191:GLY:HA3	1.82	0.62
1:C:251:ASP:OD1	1:C:254:ARG:NH2	2.30	0.62
1:C:188:PRO:HD2	1:D:51:ALA:HA	1.82	0.62
1:E:191:GLY:HA3	1:G:191:GLY:HA3	1.81	0.61
1:F:53:ILE:HD12	1:F:56:LEU:HD12	1.82	0.61
1:A:191:GLY:HA3	1:C:191:GLY:HA3	1.82	0.60
1:B:148:SER:OG	1:B:150:LYS:HG2	2.02	0.60
1:F:229:ARG:NH1	1:F:234:PRO:HG3	2.17	0.59
1:C:51:ALA:HA	1:D:188:PRO:HD2	1.84	0.59
1:H:53:ILE:HD12	1:H:56:LEU:HD12	1.84	0.59
1:B:53:ILE:HD12	1:B:56:LEU:HD12	1.84	0.58
1:H:102:ALA:HB3	1:H:149:GLU:HG2	1.84	0.58
1:F:32:GLN:OE1	1:H:22:ARG:NH1	2.32	0.56
1:F:229:ARG:HH12	1:F:234:PRO:HG3	1.71	0.55
1:F:266:ALA:HB2	1:F:315:PRO:HG3	1.88	0.55
1:A:205:LYS:NZ	3:A:504:HOH:O	2.39	0.55
1:H:267:ASN:OD1	1:H:270:SER:N	2.37	0.55
1:E:184:PHE:HB3	1:E:193:PHE:HB3	1.88	0.55
1:E:22:ARG:NH1	1:G:32:GLN:OE1	2.36	0.53
1:A:28:GLY:HA2	2:A:401:967:O17	2.08	0.52
1:B:9:ASP:N	3:B:509:HOH:O	2.43	0.52
1:B:28:GLY:HA2	2:B:401:967:O17	2.10	0.51
1:F:264:TYR:CZ	1:F:274:LYS:HD3	2.45	0.51
1:H:28:GLY:HA2	2:H:401:967:C6	2.40	0.51
1:D:28:GLY:HA2	2:D:401:967:O17	2.11	0.50
1:H:264:TYR:CZ	1:H:274:LYS:HD3	2.46	0.50
1:C:28:GLY:HA2	2:C:401:967:C6	2.42	0.50
1:H:28:GLY:HA2	2:H:401:967:O17	2.12	0.50
1:B:125:ASN:ND2	3:B:511:HOH:O	2.44	0.49
1:E:113:TYR:CE1	1:E:140[A]:ARG:HD2	2.47	0.49
1:G:216:ALA:HA	1:G:219:PHE:CD2	2.48	0.49
1:E:267:ASN:HD21	1:E:270:SER:HB2	1.77	0.48
1:A:184:PHE:HB3	1:A:193:PHE:HB3	1.96	0.48
1:H:102:ALA:CB	1:H:149:GLU:HG2	2.44	0.47
1:C:276:ARG:HG3	1:C:279:TYR:CE1	2.50	0.47
1:D:99:ASP:OD1	3:D:501:HOH:O	2.20	0.47
1:F:183:CYS:HB2	1:F:197:ASP:HB2	1.95	0.47
1:C:195:LEU:HD21	1:C:198:LYS:HG2	1.97	0.47
1:E:188:PRO:HD2	1:F:51:ALA:HA	1.96	0.47
1:B:78:ASN:HB2	1:B:98:GLU:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:PRO:HD2	1:B:51:ALA:HA	1.98	0.46
1:A:229:ARG:HD2	3:A:510:HOH:O	2.14	0.46
1:D:78:ASN:HB2	1:D:98:GLU:HG3	1.97	0.46
1:G:51:ALA:HA	1:H:188:PRO:HD2	1.97	0.46
1:B:28:GLY:HA2	2:B:401:967:C6	2.45	0.46
1:F:109:LYS:HE3	1:H:9:ASP:OD2	2.16	0.46
1:H:266:ALA:HB2	1:H:315:PRO:HG3	1.96	0.46
1:G:28:GLY:HA2	2:G:401:967:C6	2.45	0.46
1:H:157:ARG:HD2	3:H:542:HOH:O	2.15	0.46
1:C:216:ALA:HA	1:C:219:PHE:CD2	2.51	0.46
1:E:28:GLY:HA2	2:E:401:967:C6	2.46	0.46
1:E:277:LEU:HA	1:E:281:CYS:HB2	1.99	0.45
1:D:142:LYS:HA	1:D:142:LYS:HD3	1.75	0.45
1:H:13:LEU:HD21	1:H:173:LEU:HD22	1.99	0.45
1:D:45:SER:O	1:D:49:ARG:HD3	2.17	0.45
1:B:184:PHE:HB3	1:B:193:PHE:HB3	1.98	0.45
1:E:51:ALA:HA	1:F:188:PRO:HD2	1.99	0.45
1:A:55:HIS:HA	1:A:59:ILE:HG22	1.99	0.44
1:G:195:LEU:HD21	1:G:198:LYS:HG2	1.99	0.44
1:F:28:GLY:HA2	2:F:401:967:C6	2.47	0.44
1:C:228:GLN:NE2	3:C:511:HOH:O	2.49	0.44
1:C:106:GLU:OE2	1:C:109:LYS:HE2	2.18	0.44
1:D:112:LYS:HB2	1:D:140[B]:ARG:CZ	2.47	0.44
1:C:157:ARG:NH2	3:C:504:HOH:O	2.37	0.43
1:H:100:LYS:HE2	3:H:566:HOH:O	2.18	0.43
1:D:13:LEU:HD21	1:D:173:LEU:HD22	1.99	0.43
1:B:266:ALA:HB2	1:B:315:PRO:HG3	2.00	0.43
1:A:258:TYR:OH	1:B:127:ASP:HB2	2.19	0.43
1:B:32:GLN:OE1	1:D:22:ARG:NH1	2.44	0.43
1:G:270:SER:HB3	1:G:273:GLY:O	2.19	0.43
1:H:264:TYR:OH	1:H:274:LYS:HD3	2.19	0.43
1:D:121:ASP:N	1:D:133:GLY:O	2.48	0.43
1:C:264:TYR:CZ	1:C:274:LYS:HG2	2.55	0.42
1:C:53:ILE:HA	1:C:56:LEU:HD23	2.00	0.42
1:G:28:GLY:HA2	2:G:401:967:O17	2.19	0.42
1:F:28:GLY:HA2	2:F:401:967:O17	2.18	0.42
1:C:118:ASP:OD2	3:C:501:HOH:O	2.21	0.42
1:E:106:GLU:OE2	1:E:109:LYS:HE2	2.20	0.42
1:E:121:ASP:N	1:E:133:GLY:O	2.51	0.42
1:E:258:TYR:OH	1:F:127:ASP:HB2	2.18	0.42
1:B:13:LEU:HD21	1:B:173:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:212:ASN:HB2	1:C:244:TYR:CE2	2.55	0.42
1:G:276:ARG:HG3	1:G:279:TYR:CE1	2.55	0.42
1:C:78:ASN:HB2	1:C:98:GLU:HG3	2.01	0.42
1:B:73:LEU:HD12	1:B:73:LEU:HA	1.89	0.42
1:G:198:LYS:HB3	3:G:597:HOH:O	2.19	0.42
1:A:198:LYS:NZ	3:A:512:HOH:O	2.48	0.41
1:A:28:GLY:HA2	2:A:401:967:C6	2.50	0.41
1:E:183:CYS:HB2	1:E:197:ASP:HB2	2.01	0.41
1:F:45:SER:O	1:F:49:ARG:HD3	2.20	0.41
1:A:89:PHE:CE1	1:A:109:LYS:HG2	2.56	0.41
2:E:401:967:O17	2:E:401:967:S5	2.78	0.41
1:G:322:ASP:OD1	3:G:502:HOH:O	2.22	0.41
1:G:73:LEU:HD23	1:G:126:ILE:HD13	2.02	0.41
1:A:120:LEU:HD12	1:A:120:LEU:HA	1.94	0.41
2:A:401:967:O17	2:A:401:967:S5	2.79	0.41
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.96	0.41
1:D:184:PHE:HB3	1:D:193:PHE:HB3	2.03	0.41
2:D:401:967:O17	2:D:401:967:S5	2.78	0.41
1:E:103:ILE:HD12	1:E:103:ILE:N	2.35	0.41
2:F:401:967:O17	2:F:401:967:S5	2.79	0.41
1:A:222:ALA:HB1	1:A:331:TYR:HA	2.02	0.41
1:C:72:LYS:HG3	1:C:74:ASP:OD1	2.20	0.41
1:B:226:TYR:CE1	1:B:230:LYS:HE3	2.55	0.41
1:D:28:GLY:HA2	2:D:401:967:C6	2.50	0.41
1:H:120:LEU:HA	1:H:120:LEU:HD12	1.90	0.41
1:B:328:LEU:HA	1:B:328:LEU:HD23	1.89	0.41
1:F:306:ILE:O	3:F:503:HOH:O	2.22	0.41
1:G:106:GLU:OE2	1:G:109:LYS:HE2	2.20	0.41
1:G:120:LEU:HA	1:G:120:LEU:HD12	1.86	0.41
1:G:188:PRO:HD2	1:H:51:ALA:HA	2.02	0.41
1:A:82:MET:HE3	1:A:103:ILE:HD13	2.03	0.40
2:H:401:967:O17	2:H:401:967:S5	2.79	0.40
2:C:401:967:O17	2:C:401:967:S5	2.79	0.40
1:E:125:ASN:HA	1:F:258:TYR:OH	2.21	0.40
2:G:401:967:S5	2:G:401:967:O17	2.79	0.40
1:G:277:LEU:HD23	1:G:307:PRO:HB3	2.04	0.40
1:H:72[B]:LYS:NZ	1:H:72[B]:LYS:HB2	2.37	0.40
1:B:45:SER:O	1:B:49:ARG:HD3	2.22	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:A:332:GLU:OE2	1:E:140[A]:ARG:NE[1_554]	2.19	0.01

### 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	316/338 (94%)	311 (98%)	5 (2%)	0	100	100
1	B	315/338 (93%)	308 (98%)	7 (2%)	0	100	100
1	C	314/338 (93%)	309 (98%)	5 (2%)	0	100	100
1	D	316/338 (94%)	310 (98%)	6 (2%)	0	100	100
1	E	316/338 (94%)	312 (99%)	4 (1%)	0	100	100
1	F	316/338 (94%)	309 (98%)	7 (2%)	0	100	100
1	G	314/338 (93%)	308 (98%)	6 (2%)	0	100	100
1	H	313/338 (93%)	307 (98%)	6 (2%)	0	100	100
All	All	2520/2704 (93%)	2474 (98%)	46 (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	267/281 (95%)	262 (98%)	5 (2%)	60	74
1	B	266/281 (95%)	260 (98%)	6 (2%)	53	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	265/281 (94%)	260 (98%)	5 (2%)	60	74
1	D	267/281 (95%)	263 (98%)	4 (2%)	67	80
1	E	267/281 (95%)	264 (99%)	3 (1%)	76	87
1	F	267/281 (95%)	263 (98%)	4 (2%)	67	80
1	G	265/281 (94%)	261 (98%)	4 (2%)	67	80
1	H	265/281 (94%)	262 (99%)	3 (1%)	76	87
All	All	2129/2248 (95%)	2095 (98%)	34 (2%)	67	79

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	70	VAL
1	A	72	LYS
1	A	264	TYR
1	A	278	LEU
1	B	33	LEU
1	B	72	LYS
1	B	200	VAL
1	B	264	TYR
1	B	268	LYS
1	B	299	LYS
1	C	38[A]	CYS
1	C	38[B]	CYS
1	C	140	ARG
1	C	264	TYR
1	C	278	LEU
1	D	70	VAL
1	D	72	LYS
1	D	228	GLN
1	D	264	TYR
1	E	72	LYS
1	E	264	TYR
1	E	267	ASN
1	F	33	LEU
1	F	150	LYS
1	F	264	TYR
1	F	268	LYS
1	G	56	LEU
1	G	264	TYR

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Mol	Chain	Res	Type
1	G	278	LEU
1	G	332	GLU
1	H	72[A]	LYS
1	H	72[B]	LYS
1	H	264	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	267	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](#)

8 ligands are modelled in this entry.

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
2	967	A	401	-	18,24,24	1.12	2 (11%)	19,35,35	1.17	2 (10%)
2	967	B	401	-	18,24,24	1.14	1 (5%)	19,35,35	1.16	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	967	C	401	-	18,24,24	1.22	1 (5%)	19,35,35	1.57	3 (15%)
2	967	D	401	-	18,24,24	1.12	1 (5%)	19,35,35	1.20	1 (5%)
2	967	E	401	-	18,24,24	1.08	1 (5%)	19,35,35	1.43	2 (10%)
2	967	F	401	-	18,24,24	1.03	1 (5%)	19,35,35	1.24	2 (10%)
2	967	G	401	-	18,24,24	1.17	1 (5%)	19,35,35	1.28	2 (10%)
2	967	H	401	-	18,24,24	1.19	1 (5%)	19,35,35	1.26	3 (15%)

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
2	967	A	401	-	-	0/7/15/15	0/3/3/3
2	967	B	401	-	-	0/7/15/15	0/3/3/3
2	967	C	401	-	-	0/7/15/15	0/3/3/3
2	967	D	401	-	-	0/7/15/15	0/3/3/3
2	967	E	401	-	-	0/7/15/15	0/3/3/3
2	967	F	401	-	-	0/7/15/15	0/3/3/3
2	967	G	401	-	-	0/7/15/15	0/3/3/3
2	967	H	401	-	-	0/7/15/15	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	401	967	C2-S1	-3.76	1.74	1.77
2	H	401	967	C2-S1	-3.47	1.74	1.77
2	B	401	967	C2-S1	-3.18	1.74	1.77
2	G	401	967	C2-S1	-2.92	1.74	1.77
2	D	401	967	C2-S1	-2.88	1.74	1.77
2	A	401	967	C2-S1	-2.47	1.75	1.77
2	E	401	967	C2-S1	-2.30	1.75	1.77
2	F	401	967	C2-S1	-2.03	1.75	1.77
2	A	401	967	C7-S12	2.11	1.73	1.70

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	401	967	C2-C7-S12	-2.67	111.78	112.53
2	A	401	967	O15-S1-O14	-2.33	116.63	119.56
2	H	401	967	C2-C7-S12	-2.15	111.93	112.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	401	967	C2-S1-N3	2.02	110.74	107.29
2	F	401	967	C2-S1-N3	2.22	111.06	107.29
2	H	401	967	BR18-C11-C13	2.52	128.24	124.38
2	D	401	967	BR18-C11-C13	2.54	128.27	124.38
2	B	401	967	BR18-C11-C13	2.55	128.29	124.38
2	C	401	967	BR18-C11-C13	2.57	128.31	124.38
2	G	401	967	BR18-C11-C13	2.58	128.33	124.38
2	A	401	967	BR18-C11-C13	2.60	128.36	124.38
2	F	401	967	BR18-C11-C13	2.61	128.38	124.38
2	E	401	967	BR18-C11-C13	2.61	128.38	124.38
2	G	401	967	C2-S1-N3	2.62	111.75	107.29
2	C	401	967	C2-S1-N3	3.83	113.82	107.29
2	E	401	967	C2-S1-N3	3.94	114.00	107.29

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	967	3	0
2	B	401	967	2	0
2	C	401	967	2	0
2	D	401	967	3	0
2	E	401	967	2	0
2	F	401	967	3	0
2	G	401	967	3	0
2	H	401	967	3	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

### 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	319/338 (94%)	-0.28	11 (3%) 45 43	20, 34, 68, 87	0
1	B	317/338 (93%)	-0.12	11 (3%) 44 42	19, 35, 73, 124	0
1	C	317/338 (93%)	-0.39	3 (0%) 84 83	18, 29, 53, 82	0
1	D	319/338 (94%)	-0.50	3 (0%) 84 83	16, 27, 52, 66	0
1	E	319/338 (94%)	-0.12	16 (5%) 29 27	22, 41, 80, 110	0
1	F	317/338 (93%)	-0.16	20 (6%) 20 19	20, 38, 77, 132	0
1	G	317/338 (93%)	-0.40	5 (1%) 72 70	20, 30, 55, 89	0
1	H	317/338 (93%)	-0.39	8 (2%) 57 55	18, 30, 57, 83	0
All	All	2542/2704 (94%)	-0.29	77 (3%) 50 48	16, 33, 64, 132	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	70	VAL	5.6
1	A	70	VAL	4.8
1	E	236	ASN	4.5
1	F	144	THR	4.4
1	E	268	LYS	4.1
1	F	268	LYS	4.1
1	H	25	ARG	4.0
1	F	269	LYS	3.9
1	B	268	LYS	3.8
1	B	144	THR	3.8
1	A	268	LYS	3.7
1	F	236	ASN	3.6
1	H	269	LYS	3.5
1	F	271	PRO	3.5
1	F	234	PRO	3.4
1	E	269	LYS	3.3

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	145	ASP	3.2
1	C	236	ASN	3.2
1	G	25	ARG	3.1
1	A	234	PRO	3.1
1	B	269	LYS	3.1
1	F	143	SER	3.0
1	G	236	ASN	3.0
1	F	237	SER	3.0
1	F	229	ARG	3.0
1	E	266	ALA	2.9
1	E	108	GLU	2.9
1	B	267	ASN	2.9
1	E	25	ARG	2.9
1	A	25	ARG	2.9
1	D	236	ASN	2.9
1	E	235	ASP	2.8
1	E	237	SER	2.8
1	H	236	ASN	2.8
1	F	145	ASP	2.7
1	E	271	PRO	2.7
1	C	25	ARG	2.7
1	D	70	VAL	2.7
1	B	271	PRO	2.7
1	A	71	LYS	2.6
1	F	107	PRO	2.6
1	F	267	ASN	2.6
1	B	236	ASN	2.6
1	F	238	ALA	2.6
1	E	234	PRO	2.6
1	G	335	SER	2.5
1	F	235	ASP	2.5
1	F	25	ARG	2.5
1	B	38[A]	CYS	2.4
1	E	267	ASN	2.4
1	F	109	LYS	2.3
1	F	124	SER	2.4
1	E	334	HIS	2.3
1	H	234	PRO	2.3
1	B	234	PRO	2.3
1	H	271	PRO	2.3
1	E	272	ASN	2.3
1	A	142	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	142	LYS	2.2
1	F	270	SER	2.2
1	B	25	ARG	2.2
1	A	144	THR	2.2
1	A	145	ASP	2.2
1	A	233	PRO	2.1
1	E	335	SER	2.1
1	A	269	LYS	2.1
1	A	108	GLU	2.1
1	H	268	LYS	2.1
1	G	332	GLU	2.1
1	C	126	ILE	2.1
1	E	238	ALA	2.1
1	B	136	PHE	2.1
1	H	107	PRO	2.1
1	D	25	ARG	2.0
1	F	106	GLU	2.0
1	H	108	GLU	2.0
1	G	237	SER	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. 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
2	967	F	401	22/22	0.96	0.10	30,41,52,56	1
2	967	E	401	22/22	0.97	0.09	32,39,47,48	1
2	967	D	401	22/22	0.97	0.08	20,33,50,51	1
2	967	B	401	22/22	0.97	0.10	28,37,58,60	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	967	A	401	22/22	0.97	0.10	17,30,54,58	1
2	967	C	401	22/22	0.97	0.10	23,36,46,52	1
2	967	H	401	22/22	0.97	0.10	25,36,57,58	1
2	967	G	401	22/22	0.98	0.10	25,35,46,50	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.