



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 28, 2019 – 05:59 PM EST

PDB ID : 5PZZ  
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-(5-bromo-1,3-thiazol-2-yl)-3-(3,4-dichlorophenyl)sulfonylurea  
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 : 2017-04-28  
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](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

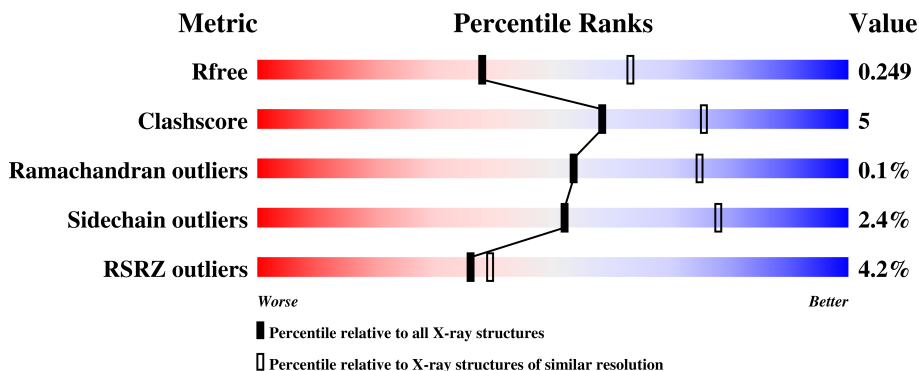
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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.



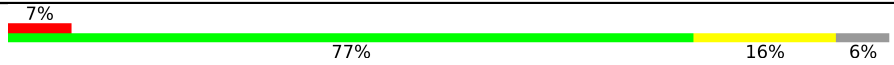

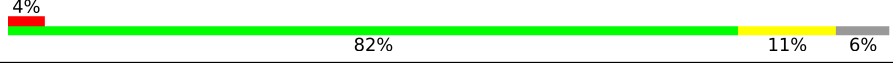
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	111664	4155 (2.50-2.50)
Clashscore	122126	4827 (2.50-2.50)
Ramachandran outliers	120053	4735 (2.50-2.50)
Sidechain outliers	120020	4737 (2.50-2.50)
RSRZ outliers	108989	4058 (2.50-2.50)

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 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% 84% 10% 6%
1	B	338	 4% 79% 14% 6%
1	C	338	 1% 79% 14% 6%
1	D	338	 2% 78% 15% 6%
1	E	338	 9% 79% 14% 6%

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Mol	Chain	Length	Quality of chain
1	F	338	 <p>7% 77% 16% 6%</p>
1	G	338	 <p>% 78% 15% 6%</p>
1	H	338	 <p>4% 82% 11% 6%</p>

## 2 Entry composition [i](#)

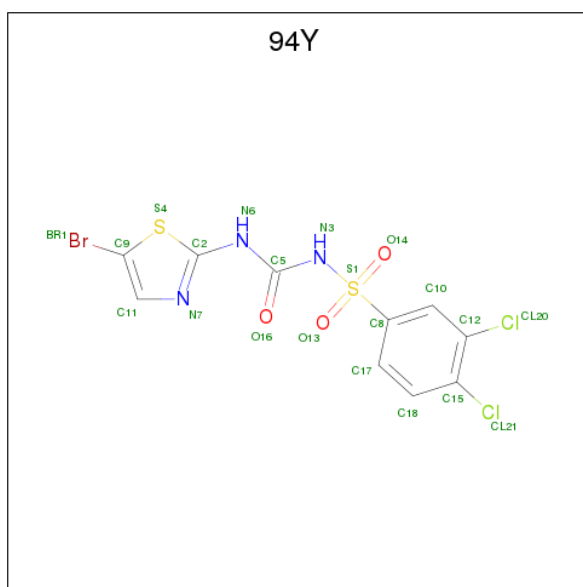
There are 3 unique types of molecules in this entry. The entry contains 19898 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	2431	1548	409	457	17	0	1	0
1	C	317	2425	1545	406	457	17	0	0	0
1	D	317	2431	1548	409	457	17	0	1	0
1	E	319	2447	1559	412	459	17	0	1	0
1	F	317	2430	1547	409	457	17	0	1	0
1	G	317	2430	1547	409	457	17	0	1	0
1	H	317	2425	1545	406	457	17	0	0	0

- Molecule 2 is N-[(5-bromo-1,3-thiazol-2-yl)carbamoyl]-3,4-dichlorobenzene-1-sulfonamide (three-letter code: 94Y) (formula: C<sub>10</sub>H<sub>6</sub>BrCl<sub>2</sub>N<sub>3</sub>O<sub>3</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	Br	C	Cl	N	O	S		
2	A	1	Total	Br	C	Cl	N	O	S	1	0
21	1	10	2	3	3	2					
2	B	1	Total	Br	C	Cl	N	O	S	1	0
21	1	10	2	3	3	2					
2	C	1	Total	Br	C	Cl	N	O	S	1	0
21	1	10	2	3	3	2					
2	D	1	Total	Br	C	Cl	N	O	S	1	0
21	1	10	2	3	3	2					
2	E	1	Total	Br	C	Cl	N	O	S	1	0
21	1	10	2	3	3	2					
2	F	1	Total	Br	C	Cl	N	O	S	1	0
21	1	10	2	3	3	2					
2	G	1	Total	Br	C	Cl	N	O	S	1	0
21	1	10	2	3	3	2					
2	H	1	Total	Br	C	Cl	N	O	S	1	0
21	1	10	2	3	3	2					

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
33	33					
3	B	33	Total	O	0	0
33	33					
3	C	50	Total	O	0	0
50	50					
3	D	42	Total	O	0	0
42	42					

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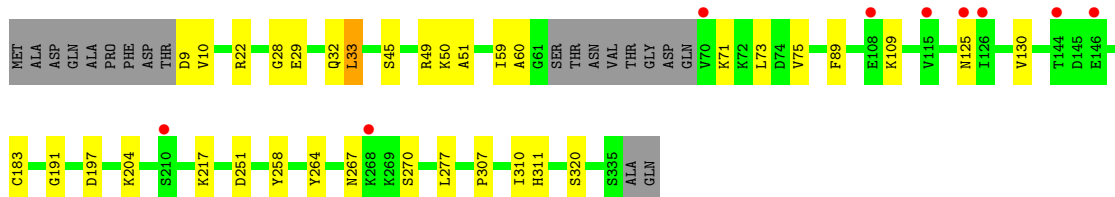
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
3	E	18	Total 18	O 18	0	0
3	F	14	Total 14	O 14	0	0
3	G	42	Total 42	O 42	0	0
3	H	33	Total 33	O 33	0	0

### 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.

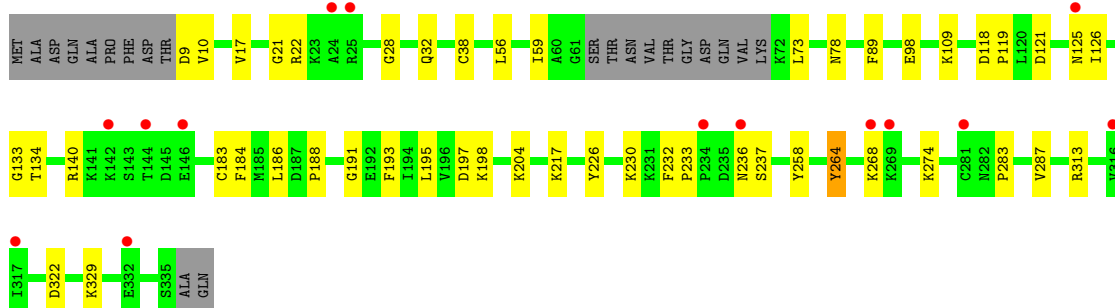
- Molecule 1: Fructose-1,6-bisphosphatase 1

Chain A: 




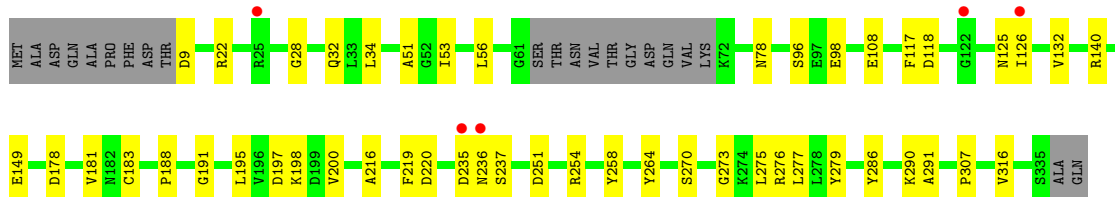
- Molecule 1: Fructose-1,6-bisphosphatase 1

Chain B: 




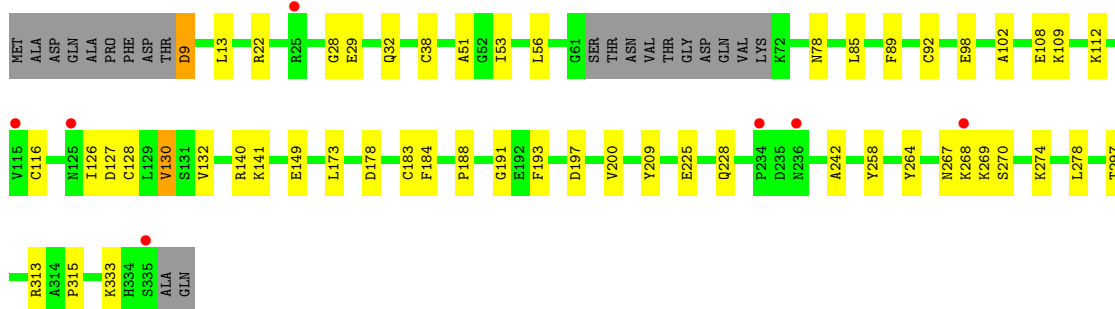
- Molecule 1: Fructose-1,6-bisphosphatase 1

Chain C: 

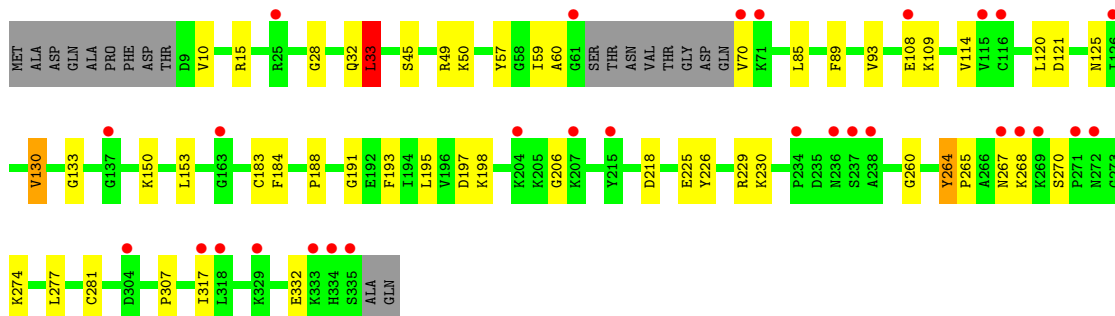
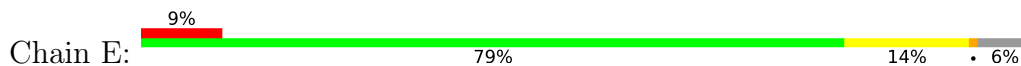


- Molecule 1: Fructose-1,6-bisphosphatase 1

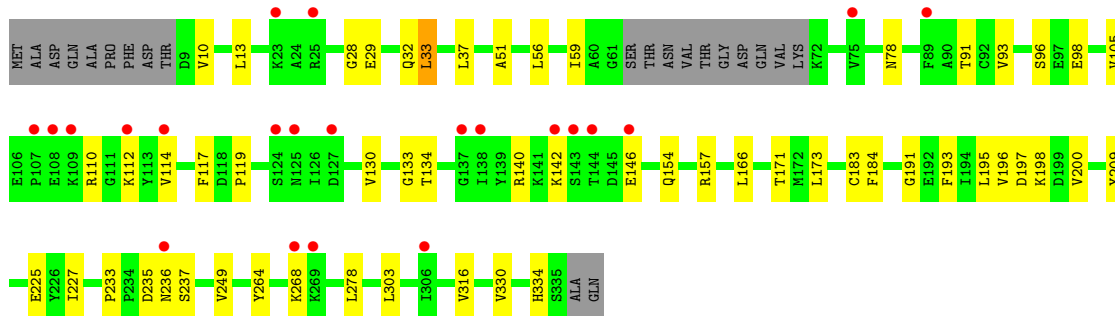
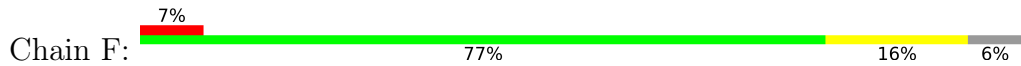
Chain D: 



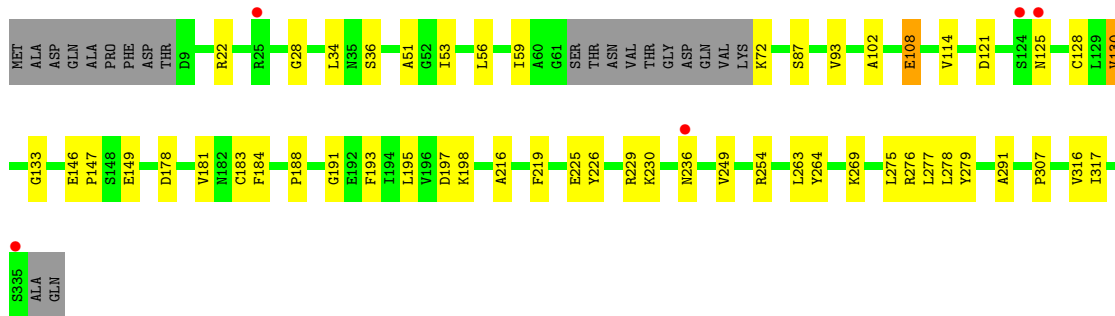
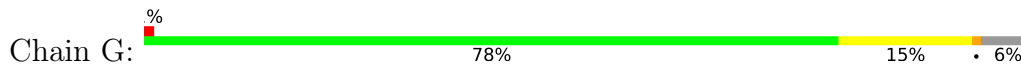
• Molecule 1: Fructose-1,6-bisphosphatase 1



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




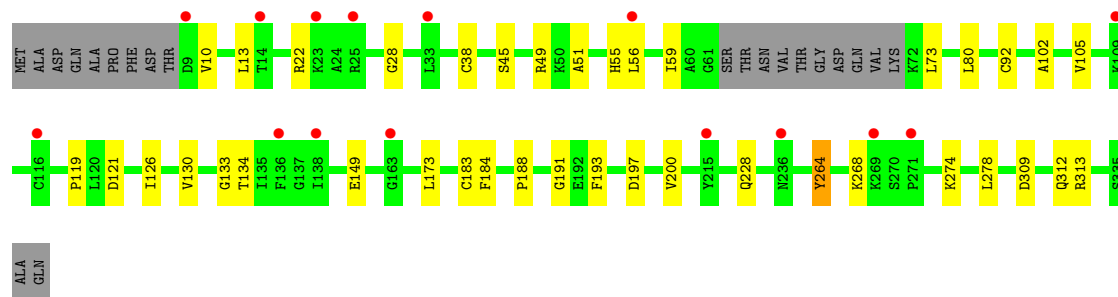
• Molecule 1: Fructose-1,6-bisphosphatase 1





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

Chain H: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	66.00Å 283.85Å 83.48Å 90.00° 97.75° 90.00°	Depositor
Resolution (Å)	24.46 – 2.50 24.46 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (24.46-2.50) 99.6 (24.46-2.50)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.40 (at 2.50Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.183 , 0.249 0.184 , 0.249	Depositor DCC
$R_{free}$ test set	5193 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	46.4	Xtrriage
Anisotropy	0.550	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 62.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19898	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.23% 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 94Y

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	0.43	0/2495	0.65	1/3368 (0.0%)
1	B	0.41	0/2479	0.63	0/3347
1	C	0.45	0/2468	0.65	0/3333
1	D	0.49	0/2479	0.65	0/3347
1	E	0.39	0/2495	0.60	1/3368 (0.0%)
1	F	0.40	0/2479	0.61	1/3347 (0.0%)
1	G	0.45	0/2479	0.62	0/3347
1	H	0.43	0/2468	0.61	0/3333
All	All	0.43	0/19842	0.63	3/26790 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	LEU	CA-CB-CG	7.16	131.76	115.30
1	F	33	LEU	CA-CB-CG	6.58	130.42	115.30
1	E	33	LEU	CA-CB-CG	5.16	127.16	115.30

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	2446	0	2496	25	0
1	B	2431	0	2478	30	0
1	C	2425	0	2469	31	0
1	D	2431	0	2478	34	0
1	E	2447	0	2500	34	0
1	F	2430	0	2474	31	0
1	G	2430	0	2474	31	0
1	H	2425	0	2469	24	0
2	A	21	0	0	1	0
2	B	21	0	0	3	0
2	C	21	0	0	2	0
2	D	21	0	0	2	0
2	E	21	0	0	1	0
2	F	21	0	0	2	0
2	G	21	0	0	1	0
2	H	21	0	0	1	0
3	A	33	0	0	4	0
3	B	33	0	0	1	0
3	C	50	0	0	2	0
3	D	42	0	0	0	0
3	E	18	0	0	2	0
3	F	14	0	0	0	0
3	G	42	0	0	1	0
3	H	33	0	0	0	0
All	All	19898	0	19838	207	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 5.

All (207) 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:C:251:ASP:OD1	1:C:254:ARG:NH2	2.12	0.82
1:H:183:CYS:HB2	1:H:197:ASP:HB2	1.63	0.81
1:F:142:LYS:HD2	1:F:154:GLN:HG2	1.67	0.74
1:F:110:ARG:NH1	1:F:146:GLU:OE2	2.20	0.72
1:B:191:GLY:HA3	1:D:191:GLY:HA3	1.72	0.71
1:C:275:LEU:HD12	1:C:316:VAL:HG11	1.73	0.70
1:G:102:ALA:HB3	1:G:149:GLU:HG2	1.73	0.70
1:A:9:ASP:N	3:A:502:HOH:O	2.23	0.70
1:D:108:GLU:OE1	1:D:108:GLU:N	2.26	0.69
1:F:32:GLN:OE1	1:H:22:ARG:NH1	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:183:CYS:HB2	1:G:197:ASP:HB2	1.77	0.67
1:D:102:ALA:HB3	1:D:149:GLU:HG2	1.77	0.66
1:B:118:ASP:OD1	3:B:501:HOH:O	2.13	0.66
1:E:150:LYS:HD3	1:E:153:LEU:HD12	1.78	0.65
1:E:191:GLY:HA3	1:G:191:GLY:HA3	1.80	0.64
1:B:195:LEU:HD21	1:B:198:LYS:HG2	1.80	0.62
1:A:32:GLN:OE1	1:C:22:ARG:NH1	2.32	0.62
1:D:89:PHE:HE1	1:D:109:LYS:HG2	1.64	0.62
1:G:53:ILE:HG13	1:G:56:LEU:HD12	1.83	0.60
1:G:181:VAL:HG21	1:G:291:ALA:HB2	1.81	0.60
1:B:32:GLN:OE1	1:D:22:ARG:NH1	2.32	0.60
1:F:28:GLY:HA2	2:F:401:94Y:C5	2.32	0.60
1:F:29:GLU:OE1	1:F:112:LYS:HG2	2.00	0.60
1:A:191:GLY:HA3	1:C:191:GLY:HA3	1.84	0.59
1:C:183:CYS:HB2	1:C:197:ASP:HB2	1.84	0.59
1:B:183:CYS:HB2	1:B:197:ASP:HB2	1.84	0.59
1:D:274:LYS:O	1:D:313:ARG:NH1	2.33	0.59
1:G:225:GLU:OE2	1:G:229:ARG:NH2	2.36	0.59
1:B:109:LYS:NZ	1:D:9:ASP:OD2	2.36	0.58
1:F:233:PRO:HG2	1:F:237:SER:O	2.03	0.58
1:C:118:ASP:OD1	3:C:501:HOH:O	2.16	0.58
1:G:275:LEU:HD12	1:G:316:VAL:HG11	1.84	0.58
1:A:51:ALA:HA	1:B:188:PRO:HD2	1.85	0.58
1:E:183:CYS:HB2	1:E:197:ASP:HB2	1.84	0.58
1:F:184:PHE:HB3	1:F:193:PHE:HB3	1.86	0.58
1:E:15:ARG:NH2	1:G:36:SER:OG	2.29	0.58
1:B:9:ASP:OD2	1:D:109:LYS:NZ	2.32	0.57
1:E:93:VAL:HB	1:E:114:VAL:HG13	1.85	0.57
1:D:225:GLU:OE2	1:D:333:LYS:NZ	2.38	0.56
1:E:188:PRO:HD2	1:F:51:ALA:HA	1.87	0.56
1:F:119:PRO:HA	1:F:134:THR:HG23	1.87	0.56
1:B:89:PHE:CD2	1:B:109:LYS:HA	2.40	0.56
1:H:45:SER:O	1:H:49:ARG:HD3	2.06	0.56
1:B:121:ASP:N	1:B:133:GLY:O	2.36	0.55
1:D:13:LEU:HD22	1:D:173:LEU:HD22	1.87	0.55
1:G:195:LEU:HD21	1:G:198:LYS:HG2	1.89	0.55
1:A:50:LYS:NZ	3:A:503:HOH:O	2.39	0.55
1:F:225:GLU:OE1	1:F:334:HIS:NE2	2.40	0.55
1:D:184:PHE:HB3	1:D:193:PHE:HB3	1.90	0.54
1:D:116:CYS:SG	1:D:278:LEU:HD23	2.47	0.54
1:B:274:LYS:O	1:B:313:ARG:NH1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:GLY:HA2	2:C:401:94Y:O16	2.08	0.53
1:D:209:TYR:CZ	1:D:242:ALA:HB2	2.43	0.53
1:D:78:ASN:HB2	1:D:98:GLU:HG3	1.91	0.53
1:H:28:GLY:HA2	2:H:401:94Y:C5	2.39	0.53
1:G:51:ALA:HA	1:H:188:PRO:HD2	1.91	0.53
1:C:53:ILE:HA	1:C:56:LEU:HD23	1.91	0.52
1:H:102:ALA:HB3	1:H:149:GLU:HG2	1.90	0.52
1:D:183:CYS:HB2	1:D:197:ASP:HB2	1.90	0.52
1:G:277:LEU:HD23	1:G:307:PRO:HB3	1.92	0.52
1:E:267:ASN:OD1	1:E:270:SER:N	2.41	0.52
1:D:29:GLU:OE2	1:D:112:LYS:HE3	2.09	0.52
1:F:197:ASP:HB3	1:F:200:VAL:HG23	1.91	0.52
1:A:277:LEU:HD23	1:A:307:PRO:HB3	1.93	0.51
1:E:225:GLU:O	1:E:229:ARG:HG3	2.09	0.51
1:A:22:ARG:NH1	1:C:32:GLN:OE1	2.43	0.51
1:G:28:GLY:HA2	2:G:401:94Y:C5	2.40	0.51
1:H:264:TYR:CE1	1:H:274:LYS:HB2	2.45	0.51
1:C:270:SER:HB3	1:C:273:GLY:O	2.10	0.50
1:A:29:GLU:HG2	1:C:22:ARG:HH12	1.76	0.50
1:B:204:LYS:NZ	1:B:322:ASP:OD2	2.37	0.50
1:C:28:GLY:HA2	2:C:401:94Y:C5	2.41	0.50
1:F:330:VAL:O	1:F:334:HIS:HD2	1.95	0.49
1:C:51:ALA:HA	1:D:188:PRO:HD2	1.93	0.49
1:E:195:LEU:HD21	1:E:198:LYS:HG2	1.94	0.49
1:A:251:ASP:OD2	3:A:501:HOH:O	2.20	0.49
1:G:276:ARG:HG3	1:G:279:TYR:CE1	2.48	0.49
1:F:28:GLY:HA2	2:F:401:94Y:O16	2.12	0.49
1:H:13:LEU:HD22	1:H:173:LEU:HD22	1.95	0.49
1:E:277:LEU:HA	1:E:281:CYS:HB2	1.95	0.48
1:C:126:ILE:HD12	1:C:132:VAL:HG11	1.94	0.48
1:C:108:GLU:OE1	1:C:108:GLU:N	2.28	0.48
1:C:216:ALA:HA	1:C:219:PHE:CD2	2.47	0.48
1:B:264:TYR:CE1	1:B:274:LYS:HB2	2.49	0.48
1:F:195:LEU:HD21	1:F:198:LYS:HG2	1.95	0.48
1:H:119:PRO:HA	1:H:134:THR:HG23	1.95	0.48
1:C:181:VAL:HB	1:C:200:VAL:HG22	1.94	0.48
1:C:286:TYR:CZ	1:C:290:LYS:HE3	2.49	0.48
1:A:71:LYS:HD3	1:A:75:VAL:HG12	1.96	0.47
1:B:73:LEU:HD23	1:B:126:ILE:HD13	1.95	0.47
1:H:184:PHE:HB3	1:H:193:PHE:HB3	1.96	0.47
1:B:17:VAL:HG13	2:B:401:94Y:CL20	2.51	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:53:ILE:HD12	1:D:56:LEU:HD12	1.96	0.47
1:G:146:GLU:HG3	1:G:147:PRO:HD2	1.97	0.47
1:E:10:VAL:HG11	1:F:59:ILE:HA	1.96	0.47
1:A:183:CYS:HB2	1:A:197:ASP:HB2	1.95	0.47
1:E:60:ALA:HB2	1:H:80:LEU:CD2	2.44	0.47
1:E:277:LEU:HD23	1:E:307:PRO:HB3	1.97	0.47
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.80	0.47
1:B:119:PRO:HA	1:B:134:THR:HG23	1.97	0.47
1:B:233:PRO:HG2	1:B:237:SER:O	2.14	0.47
1:G:128:CYS:SG	1:G:130:VAL:HB	2.55	0.47
1:G:275:LEU:HD12	1:G:316:VAL:CG1	2.45	0.47
1:A:258:TYR:HE2	1:B:125:ASN:HD22	1.62	0.46
1:F:93:VAL:HB	1:F:114:VAL:HG13	1.97	0.46
1:C:258:TYR:OH	1:D:127:ASP:HB2	2.16	0.46
1:E:218:ASP:O	1:E:267:ASN:HB2	2.16	0.46
1:C:96:SER:HA	1:C:117:PHE:O	2.16	0.46
1:E:89:PHE:CD2	1:E:109:LYS:HA	2.50	0.46
1:D:112:LYS:HB2	1:D:140[B]:ARG:NH1	2.31	0.46
1:D:297:THR:HB	1:D:315:PRO:HG2	1.98	0.46
1:F:13:LEU:HD22	1:F:173:LEU:HD22	1.96	0.46
1:H:309:ASP:HB3	1:H:312:GLN:HB3	1.98	0.46
1:E:59:ILE:HA	1:F:10:VAL:HG11	1.98	0.45
1:D:126:ILE:HD12	1:D:132:VAL:HG11	1.97	0.45
1:G:125:ASN:O	1:G:130:VAL:HG12	2.16	0.45
1:H:268:LYS:HE2	1:H:268:LYS:HB3	1.72	0.45
1:B:28:GLY:HA2	2:B:401:94Y:C5	2.46	0.45
1:E:125:ASN:O	1:E:130:VAL:HG12	2.16	0.45
1:E:277:LEU:N	3:E:503:HOH:O	2.48	0.45
1:F:166:LEU:O	1:F:171:THR:HA	2.16	0.45
1:E:15:ARG:NH1	1:G:87:SER:OG	2.45	0.45
1:D:102:ALA:CB	1:D:149:GLU:HG2	2.46	0.45
1:C:276:ARG:HG3	1:C:279:TYR:CE1	2.51	0.45
1:H:274:LYS:HA	1:H:313:ARG:HD3	1.99	0.45
1:C:181:VAL:HG21	1:C:291:ALA:HB2	1.99	0.45
1:D:28:GLY:HA2	2:D:401:94Y:O16	2.17	0.45
1:F:209:TYR:CD2	1:F:227:ILE:HD12	2.51	0.45
1:A:89:PHE:HD1	1:A:109:LYS:HA	1.82	0.45
1:E:32:GLN:OE1	1:G:22:ARG:NH1	2.47	0.45
1:A:10:VAL:HG11	1:B:59:ILE:HA	1.98	0.44
1:E:28:GLY:HA2	2:E:401:94Y:C5	2.47	0.44
1:B:78:ASN:HB2	1:B:98:GLU:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:91:THR:OG1	1:F:105:VAL:HG21	2.17	0.44
1:G:184:PHE:HB3	1:G:193:PHE:HB3	1.99	0.44
1:A:125:ASN:OD1	1:B:258:TYR:HE2	2.00	0.44
1:A:45:SER:O	1:A:49:ARG:HD3	2.18	0.44
1:E:33:LEU:HD13	1:E:85:LEU:HD22	2.00	0.44
1:D:28:GLY:HA2	2:D:401:94Y:C5	2.48	0.44
1:A:59:ILE:HA	1:B:10:VAL:HG11	1.99	0.44
1:F:96:SER:HB2	1:F:117:PHE:CZ	2.53	0.43
1:F:78:ASN:HB2	1:F:98:GLU:HG3	1.99	0.43
1:G:34:LEU:HA	1:G:34:LEU:HD23	1.82	0.43
1:G:93:VAL:HB	1:G:114:VAL:HG22	2.00	0.43
1:G:188:PRO:HD2	1:H:51:ALA:HA	2.00	0.43
1:B:22:ARG:NH1	1:D:32:GLN:OE1	2.51	0.43
1:E:121:ASP:N	1:E:133:GLY:O	2.50	0.43
1:H:121:ASP:N	1:H:133:GLY:O	2.46	0.43
1:C:195:LEU:HD21	1:C:198:LYS:HG2	2.00	0.43
1:D:128:CYS:SG	1:D:130:VAL:HB	2.59	0.43
1:E:184:PHE:HB3	1:E:193:PHE:HB3	2.00	0.43
1:E:120:LEU:HD12	1:E:120:LEU:HA	1.89	0.43
1:B:184:PHE:HB3	1:B:193:PHE:HB3	2.01	0.43
1:D:268:LYS:HE2	1:D:268:LYS:HB3	1.60	0.43
1:B:283:PRO:O	1:B:287:VAL:HG23	2.19	0.43
1:E:264:TYR:CE1	1:E:274:LYS:HB2	2.54	0.43
1:H:278:LEU:HA	1:H:278:LEU:HD23	1.81	0.43
1:F:157:ARG:HG2	1:F:303:LEU:O	2.18	0.43
1:F:183:CYS:HB2	1:F:197:ASP:HB2	2.01	0.42
1:H:197:ASP:HB3	1:H:200:VAL:CG1	2.49	0.42
1:B:21:GLY:HA2	2:B:401:94Y:C17	2.49	0.42
1:A:267:ASN:OD1	1:A:270:SER:N	2.52	0.42
1:A:60:ALA:HB3	3:A:509:HOH:O	2.20	0.42
1:C:149:GLU:OE1	3:C:502:HOH:O	2.21	0.42
1:G:121:ASP:OD2	3:G:501:HOH:O	2.21	0.42
1:H:73:LEU:HD23	1:H:126:ILE:HD13	2.00	0.42
1:A:204:LYS:O	1:A:320:SER:HB3	2.19	0.42
1:G:133:GLY:HA3	1:G:249:VAL:HG21	2.02	0.42
1:H:92:CYS:HA	1:H:105:VAL:HB	2.02	0.42
1:A:217:LYS:HA	1:B:232:PHE:CE2	2.55	0.41
1:F:37:LEU:HA	1:F:37:LEU:HD12	1.82	0.41
1:A:28:GLY:HA2	2:A:401:94Y:C5	2.50	0.41
1:G:102:ALA:CB	1:G:149:GLU:HG2	2.46	0.41
1:G:263:LEU:HG	1:G:317:ILE:HG23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:LEU:HB2	1:B:193:PHE:CE1	2.55	0.41
1:C:277:LEU:HD23	1:C:307:PRO:HB3	2.02	0.41
1:C:125:ASN:OD1	1:D:258:TYR:HE2	2.03	0.41
1:E:206:GLY:HA3	1:E:260:GLY:N	2.35	0.41
1:D:267:ASN:OD1	1:D:270:SER:N	2.54	0.41
1:D:85:LEU:HA	1:D:85:LEU:HD23	1.88	0.41
1:G:216:ALA:HA	1:G:219:PHE:CD2	2.55	0.41
1:F:191:GLY:HA3	1:H:191:GLY:HA3	2.02	0.41
1:G:108:GLU:H	1:G:108:GLU:HG2	1.47	0.41
1:C:78:ASN:HB2	1:C:98:GLU:HG3	2.03	0.41
1:C:188:PRO:HD2	1:D:51:ALA:HA	2.01	0.41
1:E:50:LYS:NZ	3:E:506:HOH:O	2.53	0.41
1:F:133:GLY:HA3	1:F:249:VAL:HG21	2.02	0.41
1:E:57:TYR:CZ	1:F:196:VAL:HG12	2.55	0.41
1:B:226:TYR:CE1	1:B:230:LYS:HE3	2.56	0.41
1:E:226:TYR:CE1	1:E:230:LYS:HE3	2.56	0.41
1:E:265:PRO:HB3	1:E:317:ILE:HD11	2.02	0.41
1:E:45:SER:O	1:E:49:ARG:HD3	2.20	0.41
1:G:226:TYR:CE1	1:G:230:LYS:HE3	2.55	0.41
1:C:235:ASP:O	1:C:237:SER:N	2.54	0.41
1:E:89:PHE:HA	1:E:109:LYS:O	2.20	0.41
1:H:197:ASP:HB3	1:H:200:VAL:HG11	2.03	0.41
1:C:34:LEU:HD23	1:C:34:LEU:HA	1.94	0.41
1:E:226:TYR:CZ	1:E:230:LYS:HE3	2.56	0.41
1:G:59:ILE:HA	1:H:10:VAL:HG11	2.03	0.41
1:A:89:PHE:CD1	1:A:109:LYS:HA	2.56	0.40
1:A:310:ILE:HG13	1:A:311:HIS:CD2	2.56	0.40
1:C:286:TYR:OH	1:C:290:LYS:HE3	2.21	0.40
1:D:269:LYS:HE2	1:D:269:LYS:HB3	1.91	0.40
1:D:92:CYS:SG	1:D:141:LYS:HD3	2.61	0.40
1:F:278:LEU:HD23	1:F:278:LEU:HA	1.87	0.40
1:H:55:HIS:HA	1:H:59:ILE:HG22	2.04	0.40
1:F:235:ASP:O	1:F:237:SER:N	2.55	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	316/338 (94%)	308 (98%)	8 (2%)	0	100	100
1	B	314/338 (93%)	306 (98%)	8 (2%)	0	100	100
1	C	313/338 (93%)	305 (97%)	7 (2%)	1 (0%)	43	64
1	D	314/338 (93%)	308 (98%)	6 (2%)	0	100	100
1	E	316/338 (94%)	306 (97%)	10 (3%)	0	100	100
1	F	314/338 (93%)	304 (97%)	9 (3%)	1 (0%)	43	64
1	G	314/338 (93%)	304 (97%)	9 (3%)	1 (0%)	43	64
1	H	313/338 (93%)	305 (97%)	8 (3%)	0	100	100
All	All	2514/2704 (93%)	2446 (97%)	65 (3%)	3 (0%)	53	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	236	ASN
1	F	236	ASN
1	G	236	ASN

### 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%)	264 (99%)	3 (1%)	76	91
1	B	265/281 (94%)	256 (97%)	9 (3%)	40	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	264/281 (94%)	259 (98%)	5 (2%)	60	83
1	D	265/281 (94%)	258 (97%)	7 (3%)	49	76
1	E	267/281 (95%)	260 (97%)	7 (3%)	49	76
1	F	265/281 (94%)	257 (97%)	8 (3%)	44	71
1	G	265/281 (94%)	257 (97%)	8 (3%)	44	71
1	H	264/281 (94%)	259 (98%)	5 (2%)	60	83
All	All	2122/2248 (94%)	2070 (98%)	52 (2%)	52	77

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	LEU
1	A	130	VAL
1	A	264	TYR
1	B	38	CYS
1	B	56	LEU
1	B	140[A]	ARG
1	B	140[B]	ARG
1	B	217	LYS
1	B	236	ASN
1	B	264	TYR
1	B	268	LYS
1	B	329	LYS
1	C	9	ASP
1	C	140	ARG
1	C	178	ASP
1	C	220	ASP
1	C	264	TYR
1	D	9	ASP
1	D	38	CYS
1	D	130	VAL
1	D	178	ASP
1	D	200	VAL
1	D	228	GLN
1	D	264	TYR
1	E	33	LEU
1	E	70	VAL
1	E	108	GLU
1	E	130	VAL
1	E	264	TYR

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Mol	Chain	Res	Type
1	E	268	LYS
1	E	332	GLU
1	F	33	LEU
1	F	56	LEU
1	F	130	VAL
1	F	140[A]	ARG
1	F	140[B]	ARG
1	F	264	TYR
1	F	268	LYS
1	F	316	VAL
1	G	72	LYS
1	G	108	GLU
1	G	130	VAL
1	G	178	ASP
1	G	254	ARG
1	G	264	TYR
1	G	269	LYS
1	G	278	LEU
1	H	38	CYS
1	H	56	LEU
1	H	130	VAL
1	H	228	GLN
1	H	264	TYR

Some 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 carbohydrates in this entry.

## 5.6 Ligand geometry

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	94Y	A	401	-	19,22,22	0.78	0	23,32,32	0.86	2 (8%)
2	94Y	B	401	-	19,22,22	0.83	1 (5%)	23,32,32	0.77	1 (4%)
2	94Y	C	401	-	19,22,22	0.99	1 (5%)	23,32,32	0.74	1 (4%)
2	94Y	D	401	-	19,22,22	0.93	1 (5%)	23,32,32	0.77	1 (4%)
2	94Y	E	401	-	19,22,22	0.99	1 (5%)	23,32,32	0.74	1 (4%)
2	94Y	F	401	-	19,22,22	0.60	0	23,32,32	0.65	1 (4%)
2	94Y	G	401	-	19,22,22	0.81	1 (5%)	23,32,32	0.69	1 (4%)
2	94Y	H	401	-	19,22,22	0.87	1 (5%)	23,32,32	0.64	1 (4%)

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. <sup>1,2</sup> means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	94Y	A	401	-	-	0/13/15/15	0/2/2/2
2	94Y	B	401	-	-	0/13/15/15	0/2/2/2
2	94Y	C	401	-	-	0/13/15/15	0/2/2/2
2	94Y	D	401	-	-	0/13/15/15	0/2/2/2
2	94Y	E	401	-	-	0/13/15/15	0/2/2/2
2	94Y	F	401	-	-	0/13/15/15	0/2/2/2
2	94Y	G	401	-	-	0/13/15/15	0/2/2/2
2	94Y	H	401	-	-	0/13/15/15	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	94Y	C5-N3	-2.72	1.33	1.39
2	B	401	94Y	C5-N3	-2.33	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	401	94Y	C2-N6	2.46	1.41	1.36
2	H	401	94Y	C2-N6	2.75	1.41	1.36
2	E	401	94Y	C2-N6	3.15	1.42	1.36
2	C	401	94Y	C2-N6	3.37	1.42	1.36

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	94Y	C8-S1-N3	2.14	108.84	105.89
2	H	401	94Y	BR1-C9-C11	2.28	127.87	124.38
2	G	401	94Y	BR1-C9-C11	2.28	127.88	124.38
2	F	401	94Y	BR1-C9-C11	2.33	127.95	124.38
2	C	401	94Y	BR1-C9-C11	2.36	127.99	124.38
2	A	401	94Y	BR1-C9-C11	2.39	128.04	124.38
2	E	401	94Y	BR1-C9-C11	2.40	128.05	124.38
2	B	401	94Y	BR1-C9-C11	2.44	128.12	124.38
2	D	401	94Y	BR1-C9-C11	2.49	128.19	124.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	94Y	1	0
2	B	401	94Y	3	0
2	C	401	94Y	2	0
2	D	401	94Y	2	0
2	E	401	94Y	1	0
2	F	401	94Y	2	0
2	G	401	94Y	1	0
2	H	401	94Y	1	0

## 5.7 Other polymers [i](#)

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	319/338 (94%)	-0.09	9 (2%) 53 56	32, 52, 84, 135	0
1	B	317/338 (93%)	0.17	14 (4%) 34 37	30, 56, 95, 137	0
1	C	317/338 (93%)	-0.18	5 (1%) 72 74	31, 48, 79, 125	0
1	D	317/338 (93%)	-0.16	7 (2%) 62 64	30, 45, 75, 136	0
1	E	319/338 (94%)	0.25	29 (9%) 9 9	42, 63, 101, 150	0
1	F	317/338 (93%)	0.22	22 (6%) 17 17	41, 65, 107, 157	0
1	G	317/338 (93%)	-0.08	5 (1%) 72 74	38, 53, 85, 133	0
1	H	317/338 (93%)	0.04	15 (4%) 31 34	39, 58, 93, 122	0
All	All	2540/2704 (93%)	0.02	106 (4%) 36 39	30, 55, 94, 157	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	70	VAL	12.8
1	B	144	THR	5.5
1	E	238	ALA	5.3
1	B	268	LYS	5.3
1	B	125	ASN	5.1
1	F	268	LYS	5.1
1	F	125	ASN	4.9
1	G	335	SER	4.9
1	F	109	LYS	4.8
1	H	215	TYR	4.6
1	B	269	LYS	4.6
1	C	236	ASN	4.5
1	E	236	ASN	4.2
1	D	125	ASN	4.2
1	F	107	PRO	4.1
1	F	142	LYS	4.0

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	A	70	VAL	3.9
1	D	335	SER	3.8
1	E	317	ILE	3.8
1	B	146	GLU	3.7
1	E	268	LYS	3.6
1	B	142	LYS	3.6
1	H	236	ASN	3.5
1	F	108	GLU	3.5
1	C	126	ILE	3.4
1	F	306	ILE	3.4
1	A	144	THR	3.3
1	F	124	SER	3.3
1	F	25	ARG	3.2
1	H	9	ASP	3.2
1	F	114	VAL	3.1
1	F	144	THR	3.1
1	A	268	LYS	3.0
1	E	272	ASN	3.0
1	E	234	PRO	3.0
1	E	25	ARG	2.9
1	F	143	SER	2.9
1	A	126	ILE	2.9
1	G	125	ASN	2.9
1	A	108	GLU	2.8
1	F	89	PHE	2.8
1	B	234	PRO	2.8
1	F	146	GLU	2.8
1	E	269	LYS	2.7
1	B	332	GLU	2.7
1	F	112	LYS	2.7
1	E	71	LYS	2.7
1	E	116	CYS	2.7
1	E	271	PRO	2.7
1	E	237	SER	2.6
1	E	333	LYS	2.6
1	H	25	ARG	2.6
1	D	236	ASN	2.6
1	G	236	ASN	2.6
1	D	25	ARG	2.6
1	B	317	ILE	2.6
1	E	329	LYS	2.6
1	F	137	GLY	2.6

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>RSRZ</b>
1	B	316	VAL	2.5
1	C	25	ARG	2.5
1	B	25	ARG	2.5
1	D	234	PRO	2.5
1	H	109	LYS	2.5
1	H	269	LYS	2.5
1	E	163	GLY	2.5
1	B	24	ALA	2.5
1	G	25	ARG	2.4
1	H	56	LEU	2.4
1	B	281	CYS	2.4
1	E	215	TYR	2.4
1	F	269	LYS	2.4
1	E	267	ASN	2.4
1	D	115	VAL	2.4
1	A	125	ASN	2.4
1	A	146	GLU	2.4
1	E	335	SER	2.4
1	C	122	GLY	2.3
1	E	204	LYS	2.3
1	F	236	ASN	2.3
1	E	304	ASP	2.3
1	H	23	LYS	2.3
1	H	271	PRO	2.3
1	C	235	ASP	2.3
1	H	163	GLY	2.2
1	B	236	ASN	2.2
1	D	268	LYS	2.2
1	E	115	VAL	2.2
1	E	334	HIS	2.2
1	A	210	SER	2.2
1	E	207	LYS	2.2
1	E	137	GLY	2.2
1	G	124	SER	2.1
1	E	318	LEU	2.1
1	E	108	GLU	2.1
1	H	136	PHE	2.1
1	F	23	LYS	2.1
1	H	14	THR	2.1
1	A	115	VAL	2.1
1	F	75	VAL	2.1
1	E	126	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	138	ILE	2.1
1	E	61	GLY	2.1
1	H	33	LEU	2.1
1	F	127	ASP	2.0
1	F	138	ILE	2.0
1	H	116	CYS	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	94Y	F	401	21/21	0.95	0.11	74,91,99,109	2
2	94Y	B	401	21/21	0.96	0.11	54,68,78,86	2
2	94Y	A	401	21/21	0.96	0.10	44,57,74,78	2
2	94Y	G	401	21/21	0.96	0.12	49,65,72,88	2
2	94Y	E	401	21/21	0.97	0.12	40,62,77,90	2
2	94Y	H	401	21/21	0.97	0.12	64,84,90,112	2
2	94Y	D	401	21/21	0.98	0.11	41,56,70,91	2
2	94Y	C	401	21/21	0.98	0.10	43,61,69,90	2

## 6.5 Other polymers [i](#)

There are no such residues in this entry.