



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2020 – 03:39 AM BST

PDB ID : 3VYL  
Title : Structure of L-ribulose 3-epimerase  
Authors : Uechi, K.; Sakuraba, H.; Takata, G.  
Deposited on : 2012-09-27  
Resolution : 2.70 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

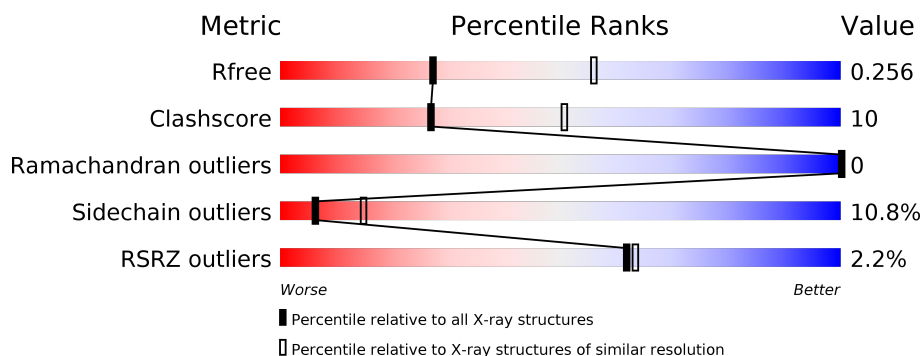
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	297	<div> <div>77%</div> <div>18%</div> <div>5%</div> </div>
1	B	297	<div> <div>82%</div> <div>15%</div> <div>.</div> </div>
1	C	297	<div> <div>80%</div> <div>16%</div> <div>.</div> </div>
1	D	297	<div> <div>80%</div> <div>16%</div> <div>.</div> </div>
1	E	297	<div> <div>%</div> <div>76%</div> <div>20%</div> <div>.</div> </div>
1	F	297	<div> <div>2%</div> <div>76%</div> <div>20%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	297	<div><div></div><div>8%</div><div></div><div>72%</div><div>24%</div><div></div><div></div></div>
1	H	297	<div><div></div><div>6%</div><div></div><div>74%</div><div>22%</div><div></div><div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18302 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 L-ribulose 3-epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2242	1407	402	430	3			
1	B	297	Total	C	N	O	S	0	0	0
			2242	1407	402	430	3			
1	C	297	Total	C	N	O	S	0	0	0
			2242	1407	402	430	3			
1	D	297	Total	C	N	O	S	0	0	0
			2242	1407	402	430	3			
1	E	297	Total	C	N	O	S	0	0	0
			2242	1407	402	430	3			
1	F	297	Total	C	N	O	S	0	0	0
			2242	1407	402	430	3			
1	G	297	Total	C	N	O	S	0	0	0
			2242	1407	402	430	3			
1	H	297	Total	C	N	O	S	0	0	0
			2242	1407	402	430	3			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

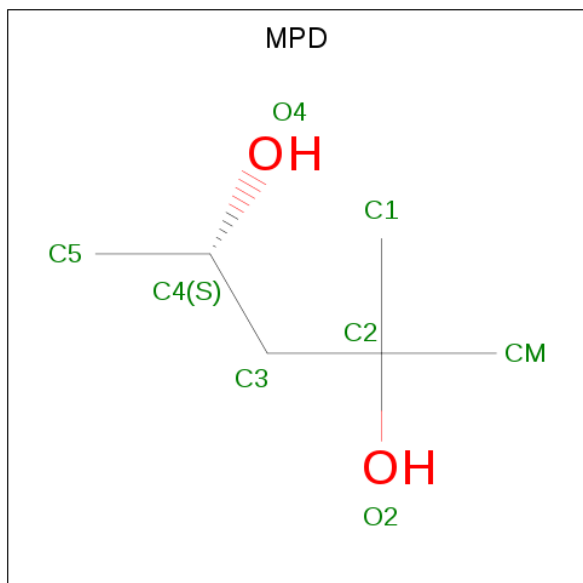
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Mn	0	0
			1	1		
2	D	1	Total	Mn	0	0
			1	1		
2	E	1	Total	Mn	0	0
			1	1		
2	H	1	Total	Mn	0	0
			1	1		
2	B	1	Total	Mn	0	0
			1	1		
2	C	1	Total	Mn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mn	0	0
			1	1		
2	F	1	Total	Mn	0	0
			1	1		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			8	6	2		
3	B	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		
3	E	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	58	Total	O	0	0
			58	58		
4	B	60	Total	O	0	0
			60	60		
4	C	64	Total	O	0	0
			64	64		

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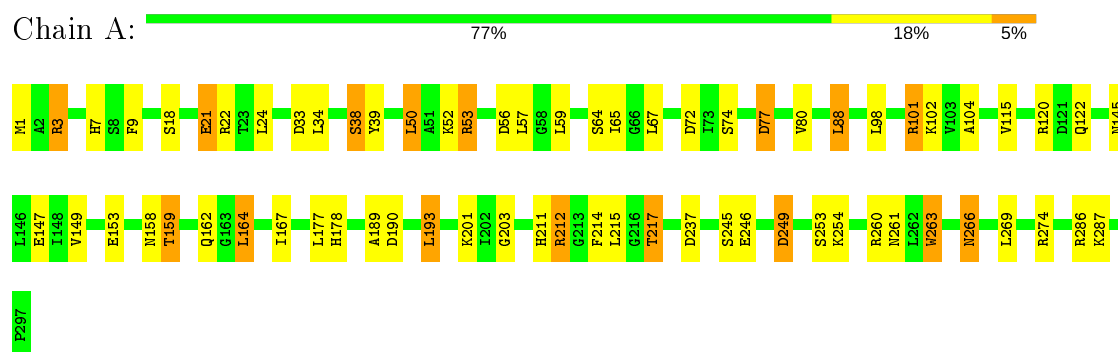
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	72	Total 72	O 72	0	0
4	E	29	Total 29	O 29	0	0
4	F	11	Total 11	O 11	0	0
4	G	11	Total 11	O 11	0	0
4	H	21	Total 21	O 21	0	0

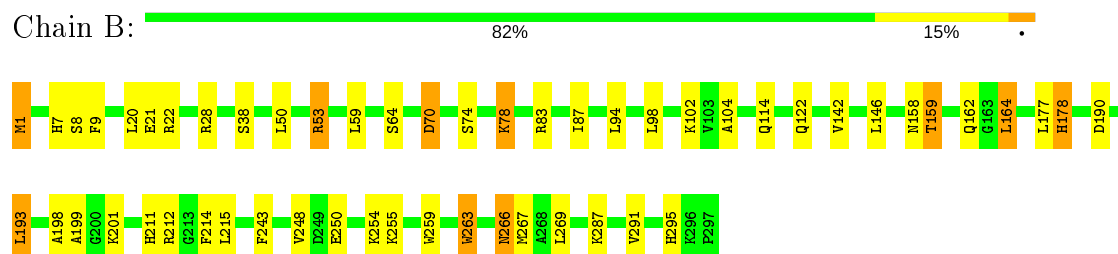
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

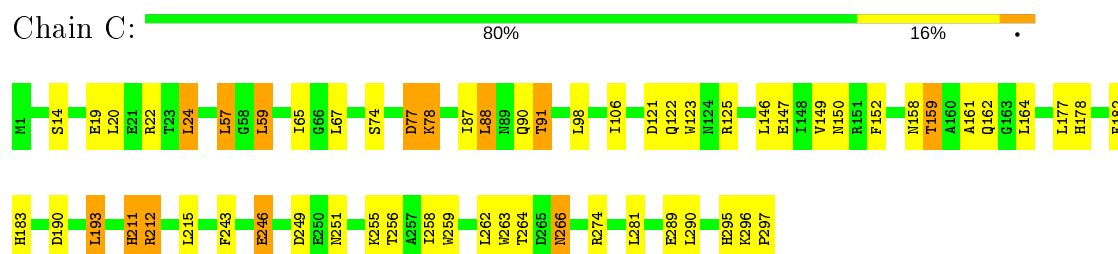
- Molecule 1: L-ribulose 3-epimerase



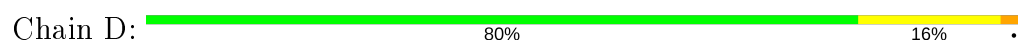
- Molecule 1: L-ribulose 3-epimerase

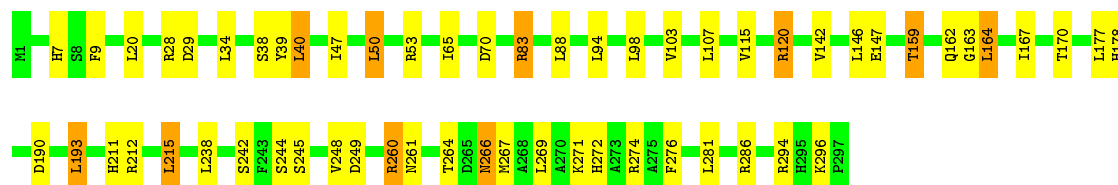


- Molecule 1: L-ribulose 3-epimerase

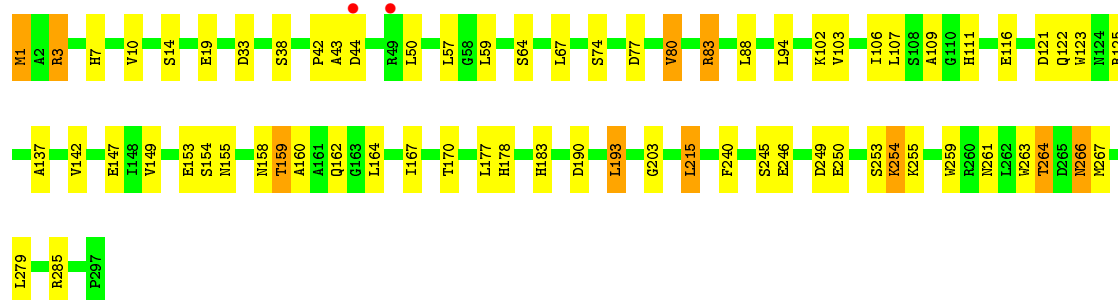
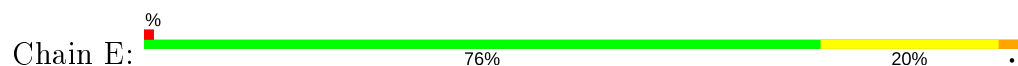


- Molecule 1: L-ribulose 3-epimerase

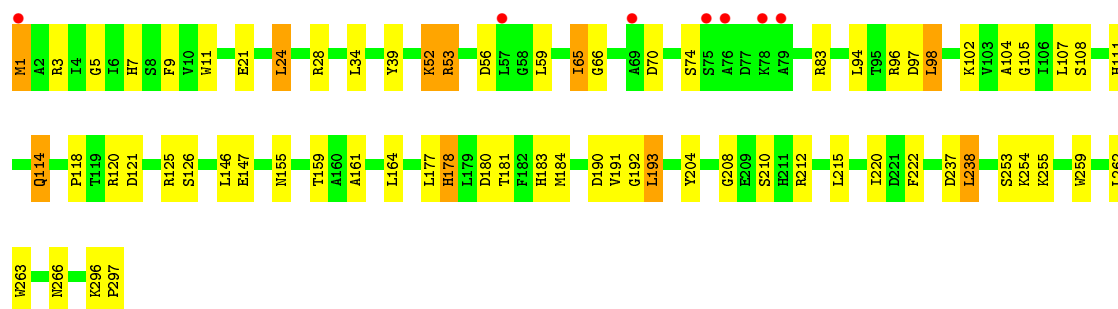
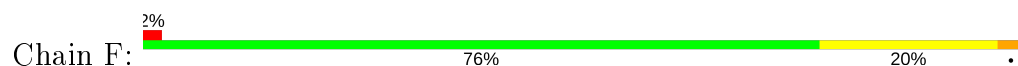




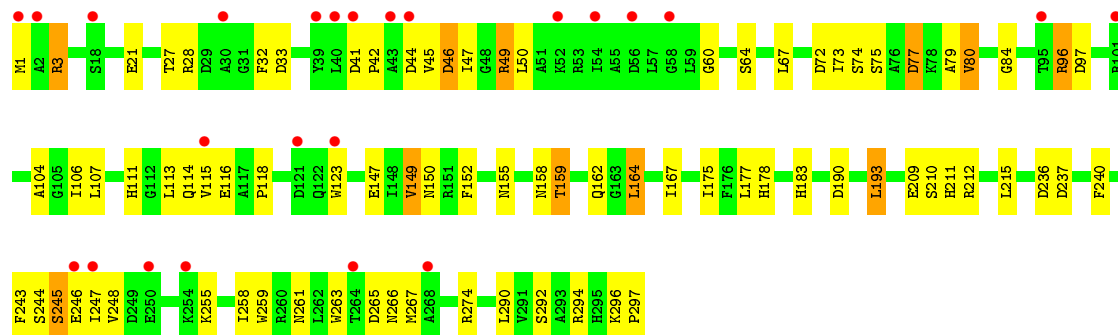
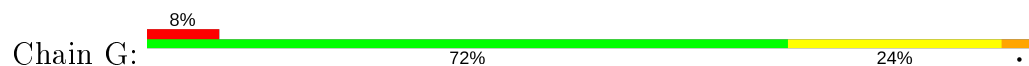
- Molecule 1: L-ribulose 3-epimerase



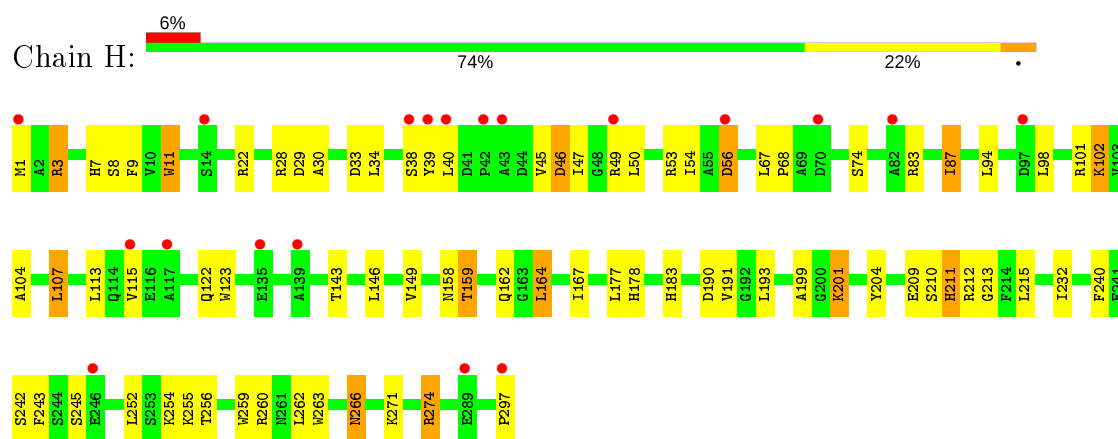
- Molecule 1: L-ribulose 3-epimerase



- Molecule 1: L-ribulose 3-epimerase



- Molecule 1: L-ribulose 3-epimerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	202.51Å 206.23Å 121.97Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.48 – 2.70 34.48 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (34.48-2.70) 99.6 (34.48-2.70)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	12.16 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.209 , 0.264 0.202 , 0.256	Depositor DCC
$R_{free}$ test set	3536 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	45.4	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 48.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.004 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	18302	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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: MPD, MN

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	0.67	2/2278 (0.1%)	0.66	0/3082
1	B	0.68	2/2278 (0.1%)	0.66	0/3082
1	C	0.66	1/2278 (0.0%)	0.67	0/3082
1	D	0.72	0/2278	0.65	0/3082
1	E	0.69	1/2278 (0.0%)	0.64	0/3082
1	F	0.65	3/2278 (0.1%)	0.65	0/3082
1	G	0.68	2/2278 (0.1%)	0.67	0/3082
1	H	0.67	2/2278 (0.1%)	0.64	1/3082 (0.0%)
All	All	0.68	13/18224 (0.1%)	0.66	1/24656 (0.0%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	259	TRP	CD2-CE2	5.42	1.47	1.41
1	F	259	TRP	CD2-CE2	5.40	1.47	1.41
1	A	263	TRP	CD2-CE2	5.37	1.47	1.41
1	H	123	TRP	CD2-CE2	5.32	1.47	1.41
1	A	153	GLU	CD-OE1	-5.31	1.19	1.25
1	G	263	TRP	CD2-CE2	5.28	1.47	1.41
1	B	263	TRP	CD2-CE2	5.27	1.47	1.41
1	H	259	TRP	CD2-CE2	5.26	1.47	1.41
1	F	11	TRP	CD2-CE2	5.22	1.47	1.41
1	F	263	TRP	CD2-CE2	5.21	1.47	1.41
1	C	123	TRP	CD2-CE2	5.08	1.47	1.41
1	G	123	TRP	CD2-CE2	5.06	1.47	1.41
1	B	259	TRP	CD2-CE2	5.01	1.47	1.41

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	11	TRP	N-CA-C	5.38	125.53	111.00

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	2242	0	2229	64	0
1	B	2242	0	2229	32	0
1	C	2242	0	2229	44	0
1	D	2242	0	2229	34	0
1	E	2242	0	2229	48	0
1	F	2242	0	2229	50	0
1	G	2242	0	2229	63	0
1	H	2242	0	2229	45	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	8	0	14	0	0
3	B	8	0	14	1	0
3	D	8	0	14	1	0
3	E	8	0	14	1	0
4	A	58	0	0	0	0
4	B	60	0	0	1	0
4	C	64	0	0	1	0
4	D	72	0	0	0	0
4	E	29	0	0	1	0
4	F	11	0	0	0	0
4	G	11	0	0	0	0
4	H	21	0	0	0	0
All	All	18302	0	17888	367	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 10.

All (367) 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:78:LYS:CD	1:C:78:LYS:H	1.50	1.18
1:G:3:ARG:HH21	1:G:60:GLY:CA	1.56	1.17
1:C:78:LYS:N	1:C:78:LYS:HD2	1.51	1.15
1:D:39:TYR:O	1:D:40:LEU:HD13	1.48	1.10
1:F:53:ARG:HG3	1:F:53:ARG:HH11	1.00	1.09
1:E:1:MET:O	1:E:1:MET:HG2	1.54	1.05
1:A:101:ARG:HH11	1:A:101:ARG:HG3	1.21	1.04
1:B:78:LYS:HE3	1:B:78:LYS:H	1.22	1.03
1:G:45:VAL:HG12	1:G:46:ASP:H	1.22	1.01
1:G:3:ARG:NH2	1:G:60:GLY:CA	2.24	1.00
1:H:211:HIS:O	1:H:212:ARG:HB2	1.61	0.99
1:H:190:ASP:HB3	1:H:193:LEU:HB2	1.45	0.97
1:H:159:THR:HG22	1:H:162:GLN:H	1.30	0.95
1:G:149:VAL:HG12	1:G:183:HIS:CD2	2.01	0.95
1:A:1:MET:HG2	1:A:1:MET:O	1.66	0.94
1:E:102:LYS:HE2	1:E:203:GLY:O	1.67	0.94
1:C:78:LYS:HD2	1:C:78:LYS:H	0.77	0.94
1:A:212:ARG:CG	1:A:212:ARG:HH11	1.80	0.93
1:F:53:ARG:HG3	1:F:53:ARG:NH1	1.79	0.93
1:A:53:ARG:HH11	1:A:53:ARG:HG3	1.34	0.93
1:G:45:VAL:CG1	1:G:46:ASP:H	1.82	0.93
1:D:7:HIS:HD2	1:D:9:PHE:H	1.18	0.92
1:C:212:ARG:HG3	4:C:1113:HOH:O	1.69	0.91
1:G:45:VAL:HG12	1:G:46:ASP:N	1.81	0.91
1:G:3:ARG:HH21	1:G:60:GLY:HA2	1.32	0.90
1:H:242:SER:O	1:H:243:PHE:HD1	1.53	0.89
4:B:1106:HOH:O	1:D:159:THR:HG21	1.73	0.88
1:D:190:ASP:HB3	1:D:193:LEU:HB2	1.55	0.88
1:F:238:LEU:O	1:F:238:LEU:HD12	1.74	0.88
1:B:159:THR:HG22	1:B:162:GLN:H	1.39	0.88
1:G:3:ARG:HH21	1:G:60:GLY:HA3	1.38	0.87
1:H:7:HIS:HD2	1:H:9:PHE:H	1.21	0.86
1:D:120:ARG:HG3	1:D:120:ARG:HH21	1.40	0.86
1:A:212:ARG:HG2	1:A:212:ARG:HH11	1.42	0.84
1:D:286:ARG:HG2	1:D:286:ARG:HH11	1.42	0.84
1:H:242:SER:O	1:H:243:PHE:CD1	2.30	0.84
1:F:190:ASP:HB3	1:F:193:LEU:HB2	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:ILE:O	1:C:91:THR:HG23	1.80	0.81
1:A:3:ARG:HD2	1:A:33:ASP:OD1	1.80	0.81
1:A:211:HIS:CE1	1:A:217:THR:HG22	2.16	0.80
1:F:238:LEU:O	1:F:238:LEU:CD1	2.30	0.80
1:D:39:TYR:O	1:D:40:LEU:CD1	2.29	0.80
1:E:1:MET:CG	1:E:1:MET:O	2.30	0.80
1:E:3:ARG:HH11	1:E:3:ARG:HG2	1.46	0.80
1:A:266:ASN:H	1:A:266:ASN:HD22	1.27	0.79
1:D:164:LEU:HD13	1:D:177:LEU:HD11	1.65	0.79
1:H:211:HIS:HD2	1:H:213:GLY:H	1.29	0.78
1:G:190:ASP:HB3	1:G:193:LEU:HB2	1.65	0.78
1:B:266:ASN:H	1:B:266:ASN:HD22	1.32	0.77
1:A:53:ARG:NH1	1:A:53:ARG:HG3	1.95	0.77
1:F:111:HIS:O	1:F:255:LYS:HE3	1.85	0.77
1:A:159:THR:HG22	1:A:162:GLN:H	1.49	0.76
1:E:279:LEU:HD23	3:E:1002:MPD:HM2	1.67	0.76
1:C:190:ASP:HB3	1:C:193:LEU:HB2	1.67	0.76
1:F:7:HIS:HD2	1:F:9:PHE:H	1.33	0.76
1:G:243:PHE:HB3	1:G:248:VAL:HG21	1.68	0.76
1:E:159:THR:HG22	1:E:162:GLN:H	1.50	0.76
1:G:64:SER:HA	1:G:104:ALA:O	1.85	0.76
1:A:266:ASN:HD22	1:A:266:ASN:N	1.86	0.73
1:A:190:ASP:HB3	1:A:193:LEU:HB2	1.69	0.73
1:E:3:ARG:HB3	1:E:33:ASP:HB2	1.69	0.73
1:E:83:ARG:HH11	1:E:83:ARG:CG	2.02	0.73
1:C:159:THR:HG22	1:C:162:GLN:H	1.53	0.73
1:F:120:ARG:HG3	1:H:297:PRO:O	1.89	0.72
1:A:145:ASN:HD22	1:A:203:GLY:HA3	1.54	0.71
1:F:238:LEU:H	1:F:238:LEU:HD12	1.55	0.71
1:G:111:HIS:O	1:G:255:LYS:NZ	2.24	0.71
1:F:159:THR:HG22	1:F:161:ALA:H	1.54	0.71
1:A:77:ASP:CG	1:A:80:VAL:HG23	2.11	0.70
1:B:266:ASN:N	1:B:266:ASN:HD22	1.88	0.70
1:H:3:ARG:HB3	1:H:33:ASP:HB2	1.74	0.70
1:C:77:ASP:OD1	1:C:77:ASP:C	2.29	0.70
1:A:101:ARG:HH12	1:A:102:LYS:HE2	1.57	0.69
1:G:77:ASP:C	1:G:77:ASP:OD1	2.29	0.69
1:G:3:ARG:NH2	1:G:60:GLY:N	2.39	0.69
1:G:150:ASN:OD1	1:G:150:ASN:C	2.30	0.69
1:H:209:GLU:HG3	1:H:210:SER:N	2.07	0.69
1:D:159:THR:HG22	1:D:162:GLN:H	1.58	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:1123:HOH:O	1:G:159:THR:HG21	1.92	0.68
1:A:77:ASP:OD1	1:A:77:ASP:C	2.30	0.68
1:B:70:ASP:OD1	1:B:70:ASP:C	2.30	0.68
1:H:164:LEU:HD13	1:H:177:LEU:HD11	1.76	0.67
1:H:74:SER:HB3	1:H:122:GLN:HG3	1.75	0.67
1:C:14:SER:HB3	1:C:19:GLU:HG2	1.77	0.67
1:G:77:ASP:OD1	1:G:80:VAL:HG22	1.95	0.67
1:A:246:GLU:OE2	1:A:246:GLU:HA	1.94	0.66
1:A:145:ASN:ND2	1:A:203:GLY:HA3	2.10	0.66
1:G:77:ASP:O	1:G:80:VAL:HG23	1.95	0.66
1:G:106:ILE:HD12	1:G:111:HIS:CD2	2.31	0.66
1:G:3:ARG:HB3	1:G:237:ASP:OD1	1.97	0.65
1:G:67:LEU:CD1	1:G:73:ILE:HG23	2.26	0.65
1:A:263:TRP:CZ3	1:A:266:ASN:HB3	2.31	0.65
1:G:67:LEU:HD13	1:G:73:ILE:HG23	1.78	0.65
1:H:46:ASP:OD2	1:H:46:ASP:N	2.29	0.65
1:B:7:HIS:HD2	1:B:9:PHE:H	1.45	0.65
1:F:114:GLN:HE21	1:F:114:GLN:HA	1.61	0.64
1:G:77:ASP:OD1	1:G:79:ALA:N	2.29	0.64
1:B:263:TRP:CZ3	1:B:266:ASN:HB3	2.33	0.64
1:A:212:ARG:HG2	1:A:212:ARG:NH1	2.13	0.64
1:A:38:SER:O	1:A:65:ILE:HG22	1.98	0.64
1:A:7:HIS:HD2	1:A:9:PHE:H	1.44	0.64
1:A:245:SER:HB3	1:A:261:ASN:HD21	1.63	0.63
1:A:266:ASN:ND2	1:A:266:ASN:H	1.95	0.63
1:A:101:ARG:NH1	1:A:101:ARG:HG3	1.98	0.63
1:E:14:SER:HB3	1:E:19:GLU:HG2	1.80	0.63
1:F:181:THR:HG21	1:F:222:PHE:HE2	1.64	0.63
1:G:42:PRO:HB3	1:G:47:ILE:HD11	1.81	0.62
1:H:211:HIS:CD2	1:H:213:GLY:H	2.14	0.62
1:A:211:HIS:HE1	1:A:217:THR:HG22	1.60	0.62
1:F:181:THR:HG21	1:F:222:PHE:CE2	2.34	0.62
1:E:77:ASP:HB3	1:E:80:VAL:HG13	1.82	0.61
1:B:190:ASP:HB3	1:B:193:LEU:HB2	1.81	0.61
1:A:212:ARG:HG3	1:A:212:ARG:HH11	1.64	0.61
1:D:120:ARG:HG3	1:D:120:ARG:NH2	2.10	0.61
1:F:53:ARG:CG	1:F:53:ARG:HH11	1.91	0.61
1:D:245:SER:HB2	1:D:261:ASN:HD21	1.66	0.61
1:H:53:ARG:HA	1:H:56:ASP:HB2	1.80	0.61
1:B:50:LEU:HD23	1:B:98:LEU:HD11	1.83	0.61
1:F:147:GLU:HA	1:F:178:HIS:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:236:ASP:OD1	1:G:237:ASP:N	2.30	0.60
1:H:242:SER:C	1:H:243:PHE:CD1	2.75	0.60
1:G:77:ASP:O	1:G:80:VAL:CG2	2.50	0.60
1:E:154:SER:OG	1:E:155:ASN:N	2.31	0.60
1:C:266:ASN:HD22	1:C:266:ASN:N	2.00	0.60
1:F:238:LEU:CD1	1:F:238:LEU:C	2.70	0.60
1:C:78:LYS:N	1:C:78:LYS:CD	2.30	0.59
1:B:1:MET:SD	3:B:1002:MPD:H12	2.42	0.59
1:B:266:ASN:ND2	1:B:266:ASN:H	2.00	0.59
1:F:114:GLN:HG2	1:F:155:ASN:ND2	2.17	0.59
1:A:164:LEU:HD13	1:A:177:LEU:HD11	1.84	0.59
1:A:53:ARG:HH11	1:A:53:ARG:CG	2.09	0.59
1:B:164:LEU:HD13	1:B:177:LEU:HD11	1.85	0.59
1:A:9:PHE:CZ	1:A:38:SER:HB3	2.37	0.58
1:B:78:LYS:CE	1:B:78:LYS:H	2.07	0.58
1:G:3:ARG:NH2	1:G:60:GLY:HA2	2.01	0.58
1:E:3:ARG:NH1	1:E:3:ARG:HG2	2.16	0.58
1:G:64:SER:CA	1:G:104:ALA:O	2.52	0.58
1:D:47:ILE:HG23	1:D:98:LEU:HD13	1.86	0.58
1:F:7:HIS:CD2	1:F:9:PHE:H	2.17	0.58
1:A:249:ASP:OD2	1:A:249:ASP:C	2.42	0.57
1:D:163:GLY:O	1:D:167:ILE:HG13	2.05	0.57
1:E:7:HIS:O	1:E:10:VAL:HG13	2.04	0.57
1:A:120:ARG:HH11	1:C:296:LYS:HD2	1.70	0.57
1:H:50:LEU:O	1:H:54:ILE:HG12	2.05	0.57
1:C:74:SER:HB2	1:C:122:GLN:HG3	1.86	0.57
1:D:286:ARG:HG2	1:D:286:ARG:NH1	2.09	0.57
1:B:83:ARG:O	1:B:87:ILE:HG13	2.04	0.56
1:C:266:ASN:ND2	1:C:266:ASN:H	2.04	0.56
1:A:167:ILE:HG21	1:A:201:LYS:HE3	1.86	0.56
1:F:94:LEU:HG	1:F:98:LEU:HD22	1.87	0.56
1:E:83:ARG:HH11	1:E:83:ARG:HG3	1.70	0.56
1:H:7:HIS:CD2	1:H:9:PHE:H	2.13	0.56
1:B:162:GLN:HB3	1:D:294:ARG:O	2.05	0.56
1:E:38:SER:HA	1:E:64:SER:O	2.05	0.56
1:E:147:GLU:HA	1:E:178:HIS:O	2.06	0.55
1:E:121:ASP:O	1:E:125:ARG:HB2	2.05	0.55
1:C:24:LEU:HB3	1:C:57:LEU:HD23	1.88	0.55
1:E:250:GLU:HG2	1:E:254:LYS:NZ	2.21	0.55
1:H:209:GLU:HG3	1:H:210:SER:H	1.70	0.55
1:A:189:ALA:HB2	1:C:290:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:111:HIS:NE2	1:E:153:GLU:OE2	2.27	0.55
1:E:266:ASN:HD22	1:E:267:MET:N	2.05	0.55
1:A:1:MET:CG	1:A:1:MET:O	2.46	0.55
1:D:266:ASN:HD22	1:D:267:MET:N	2.04	0.54
1:E:190:ASP:HB3	1:E:193:LEU:HB2	1.89	0.54
1:G:164:LEU:HD13	1:G:177:LEU:HD11	1.88	0.54
1:G:77:ASP:CG	1:G:80:VAL:HG22	2.27	0.54
1:G:159:THR:HG22	1:G:162:GLN:H	1.72	0.54
1:G:45:VAL:CG1	1:G:46:ASP:N	2.46	0.54
1:A:149:VAL:O	1:A:158:ASN:HA	2.09	0.53
1:F:3:ARG:HB3	1:F:237:ASP:OD1	2.08	0.53
1:F:96:ARG:NH1	1:F:97:ASP:OD1	2.40	0.53
1:D:103:VAL:HG23	1:D:142:VAL:HG11	1.89	0.53
1:B:78:LYS:HE3	1:B:78:LYS:N	2.06	0.53
1:C:150:ASN:HD22	1:C:152:PHE:H	1.57	0.53
1:D:164:LEU:CD1	1:D:177:LEU:HD11	2.38	0.53
1:H:263:TRP:CZ3	1:H:266:ASN:HB3	2.44	0.53
1:G:118:PRO:HD3	1:G:155:ASN:HD22	1.72	0.53
1:C:57:LEU:HB3	1:C:59:LEU:HD22	1.91	0.52
1:D:266:ASN:HD22	1:D:267:MET:H	1.57	0.52
1:C:121:ASP:HB3	1:C:125:ARG:HH12	1.74	0.52
1:C:295:HIS:CD2	1:D:260:ARG:HE	2.27	0.52
1:F:238:LEU:O	1:F:238:LEU:HD13	2.09	0.52
1:G:41:ASP:OD1	1:G:42:PRO:HD2	2.10	0.52
1:C:263:TRP:CZ3	1:C:266:ASN:HB3	2.43	0.52
1:E:137:ALA:HB1	1:E:142:VAL:HG12	1.90	0.52
1:F:159:THR:HG22	1:F:161:ALA:N	2.21	0.52
1:F:266:ASN:HD22	1:F:266:ASN:H	1.58	0.52
1:E:246:GLU:HG3	1:E:264:THR:HA	1.91	0.52
1:F:5:GLY:HA3	1:F:34:LEU:HD23	1.91	0.52
1:F:53:ARG:CG	1:F:53:ARG:NH1	2.60	0.52
1:F:104:ALA:HB1	1:F:178:HIS:CD2	2.45	0.51
1:E:123:TRP:NE1	1:G:296:LYS:HE3	2.26	0.51
1:F:266:ASN:H	1:F:266:ASN:ND2	2.07	0.51
1:F:238:LEU:HD12	1:F:238:LEU:N	2.14	0.51
1:G:147:GLU:HA	1:G:178:HIS:HB3	1.93	0.51
1:A:77:ASP:OD1	1:A:80:VAL:HG23	2.11	0.51
1:H:8:SER:O	1:H:11:TRP:N	2.42	0.51
1:C:182:PHE:CD1	1:C:212:ARG:HD2	2.45	0.51
1:F:114:GLN:NE2	1:F:114:GLN:HA	2.26	0.51
1:F:181:THR:HG22	1:F:208:GLY:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:GLU:HA	1:F:24:LEU:HD22	1.93	0.51
1:H:102:LYS:HB3	1:H:143:THR:OG1	2.11	0.51
1:E:83:ARG:HG2	1:E:83:ARG:HH11	1.75	0.51
1:H:9:PHE:CZ	1:H:38:SER:OG	2.64	0.51
1:F:52:LYS:HE2	1:F:56:ASP:OD2	2.11	0.50
1:G:72:ASP:OD1	1:G:74:SER:OG	2.29	0.50
1:A:74:SER:HB2	1:A:122:GLN:CG	2.40	0.50
1:C:67:LEU:HD21	1:C:88:LEU:HD13	1.94	0.50
1:B:266:ASN:ND2	1:B:266:ASN:N	2.59	0.50
1:B:70:ASP:OD1	1:B:70:ASP:O	2.30	0.50
1:H:209:GLU:CG	1:H:210:SER:N	2.75	0.50
1:E:3:ARG:HB3	1:E:33:ASP:CB	2.38	0.50
1:C:121:ASP:HB3	1:C:125:ARG:NH1	2.27	0.49
1:G:77:ASP:O	1:G:77:ASP:OD1	2.30	0.49
1:C:256:THR:OG1	1:C:258:ILE:CD1	2.61	0.49
1:B:287:LYS:O	1:B:291:VAL:HG23	2.13	0.49
1:E:245:SER:OG	1:E:261:ASN:HB3	2.12	0.49
1:G:244:SER:HB3	1:G:247:ILE:HB	1.93	0.49
1:B:21:GLU:OE2	1:B:53:ARG:NH1	2.46	0.49
1:A:21:GLU:HG2	1:A:53:ARG:HH12	1.78	0.49
1:G:159:THR:O	1:G:162:GLN:HB2	2.13	0.49
1:E:263:TRP:CZ3	1:E:266:ASN:HB3	2.48	0.48
1:E:43:ALA:O	1:E:44:ASP:HB2	2.12	0.48
1:H:94:LEU:O	1:H:98:LEU:HB2	2.13	0.48
1:A:64:SER:HA	1:A:104:ALA:O	2.14	0.48
1:A:260:ARG:HH11	1:B:295:HIS:CD2	2.30	0.48
1:C:296:LYS:HG2	1:C:297:PRO:HD2	1.95	0.48
1:G:3:ARG:NH2	1:G:60:GLY:HA3	2.09	0.48
1:A:38:SER:HA	1:A:64:SER:O	2.14	0.48
1:A:3:ARG:CD	1:A:33:ASP:OD1	2.59	0.48
1:C:266:ASN:HD22	1:C:266:ASN:H	1.58	0.47
1:E:83:ARG:CG	1:E:83:ARG:NH1	2.69	0.47
1:E:164:LEU:HD13	1:E:177:LEU:HD11	1.96	0.47
1:H:74:SER:HB3	1:H:122:GLN:CG	2.43	0.47
1:C:149:VAL:HG12	1:C:183:HIS:CD2	2.49	0.47
1:D:94:LEU:O	1:D:98:LEU:HB2	2.14	0.47
1:E:123:TRP:CE2	1:G:296:LYS:HE3	2.49	0.47
1:D:167:ILE:O	1:D:170:THR:OG1	2.30	0.47
1:E:103:VAL:HG12	1:E:107:LEU:HD21	1.97	0.47
1:C:147:GLU:HA	1:C:178:HIS:O	2.14	0.47
1:C:149:VAL:O	1:C:158:ASN:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:149:VAL:O	1:H:158:ASN:HA	2.13	0.47
1:B:9:PHE:HB3	1:B:248:VAL:HG12	1.96	0.47
1:E:77:ASP:HB3	1:E:80:VAL:CG1	2.45	0.47
1:F:70:ASP:HB3	1:F:83:ARG:HE	1.80	0.47
1:D:70:ASP:HB2	1:D:83:ARG:HH21	1.80	0.47
1:E:167:ILE:O	1:E:170:THR:OG1	2.28	0.47
1:G:73:ILE:HG22	1:G:84:GLY:HA3	1.97	0.47
1:H:167:ILE:HG21	1:H:201:LYS:HE2	1.96	0.47
1:A:72:ASP:C	1:A:72:ASP:OD1	2.52	0.47
1:C:212:ARG:HG2	1:C:243:PHE:HD2	1.79	0.47
1:E:249:ASP:O	1:E:253:SER:HB3	2.14	0.47
1:F:184:MET:HB3	1:F:191:VAL:HG12	1.95	0.47
1:G:149:VAL:O	1:G:158:ASN:HA	2.14	0.47
1:C:164:LEU:HD13	1:C:177:LEU:HD11	1.97	0.46
1:H:240:PHE:CZ	1:H:242:SER:HB2	2.50	0.46
1:A:38:SER:OG	1:A:39:TYR:N	2.48	0.46
1:E:74:SER:HB2	1:E:122:GLN:HG2	1.97	0.46
1:F:105:GLY:H	1:F:178:HIS:HD2	1.63	0.46
1:F:178:HIS:HA	1:F:204:TYR:O	2.15	0.46
1:C:246:GLU:HG3	1:C:264:THR:HG22	1.98	0.46
1:G:245:SER:HB2	1:G:261:ASN:OD1	2.15	0.46
1:H:104:ALA:O	1:H:107:LEU:HD11	2.16	0.46
1:C:106:ILE:H	1:C:106:ILE:HD12	1.81	0.46
1:C:266:ASN:ND2	1:C:266:ASN:N	2.60	0.46
1:D:238:LEU:O	1:D:238:LEU:HD12	2.15	0.46
1:G:106:ILE:HD12	1:G:111:HIS:CG	2.51	0.46
1:F:254:LYS:HG2	1:F:254:LYS:H	1.50	0.46
1:F:164:LEU:HD13	1:F:177:LEU:HD11	1.97	0.45
1:G:77:ASP:OD1	1:G:79:ALA:HB3	2.16	0.45
1:D:28:ARG:NH1	1:D:29:ASP:OD1	2.48	0.45
1:A:21:GLU:CG	1:A:53:ARG:HH12	2.30	0.45
1:A:72:ASP:OD1	1:A:74:SER:OG	2.30	0.45
1:A:147:GLU:HA	1:A:178:HIS:HB3	1.98	0.45
1:D:40:LEU:HA	1:D:40:LEU:HD12	1.75	0.45
1:H:209:GLU:CG	1:H:210:SER:H	2.29	0.45
1:H:8:SER:O	1:H:11:TRP:HB2	2.17	0.45
1:A:3:ARG:HD2	1:A:3:ARG:HA	1.40	0.45
1:B:263:TRP:CE2	1:B:269:LEU:HD22	2.52	0.45
1:A:212:ARG:NH1	1:A:212:ARG:CG	2.53	0.45
1:F:180:ASP:HB3	1:F:183:HIS:HD2	1.82	0.45
1:G:111:HIS:O	1:G:255:LYS:CE	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:114:GLN:HG2	1:F:155:ASN:CG	2.37	0.44
1:H:30:ALA:HA	1:H:271:LYS:HG2	1.99	0.44
1:B:74:SER:HB2	1:B:122:GLN:HG2	1.99	0.44
1:H:39:TYR:O	1:H:40:LEU:HD12	2.17	0.44
1:C:243:PHE:HB3	1:C:258:ILE:HG12	1.99	0.44
1:A:254:LYS:HD3	1:D:115:VAL:O	2.17	0.44
1:D:215:LEU:O	1:D:272:HIS:HE1	2.01	0.44
1:G:46:ASP:OD2	1:G:49:ARG:HB2	2.17	0.44
1:F:65:ILE:HG13	1:F:66:GLY:N	2.32	0.44
1:H:178:HIS:HA	1:H:204:TYR:O	2.18	0.44
1:E:160:ALA:O	1:E:164:LEU:HB2	2.18	0.44
1:F:74:SER:HB3	1:F:126:SER:HB2	2.00	0.44
1:A:38:SER:O	1:A:39:TYR:HB2	2.18	0.43
1:H:199:ALA:HB1	1:H:232:ILE:HB	2.00	0.43
1:A:74:SER:HB2	1:A:122:GLN:HG3	1.99	0.43
1:C:251:ASN:O	1:C:255:LYS:HD2	2.19	0.43
1:F:121:ASP:O	1:F:125:ARG:HG3	2.18	0.43
1:D:50:LEU:HD13	1:D:98:LEU:HD11	2.01	0.43
1:G:106:ILE:CD1	1:G:111:HIS:CD2	3.00	0.43
1:G:27:THR:HG23	1:G:32:PHE:HB2	2.01	0.43
1:H:274:ARG:HD2	1:H:274:ARG:HA	1.88	0.43
1:A:74:SER:HB2	1:A:122:GLN:HG2	1.99	0.43
1:F:39:TYR:HA	1:F:65:ILE:HD12	1.99	0.43
1:B:64:SER:HA	1:B:104:ALA:O	2.19	0.43
1:C:147:GLU:HB2	1:C:178:HIS:ND1	2.33	0.43
1:B:94:LEU:O	1:B:98:LEU:HB2	2.18	0.43
1:C:67:LEU:HD21	1:C:88:LEU:CD1	2.48	0.43
1:F:210:SER:HB3	1:F:220:ILE:HG13	2.01	0.43
1:H:149:VAL:HA	1:H:183:HIS:CG	2.53	0.43
1:A:3:ARG:HB2	1:A:237:ASP:OD1	2.19	0.43
1:A:3:ARG:HB3	1:A:34:LEU:HB2	2.01	0.43
1:B:158:ASN:HD21	1:C:259:TRP:HD1	1.66	0.43
1:A:266:ASN:ND2	1:A:266:ASN:N	2.56	0.43
1:D:242:SER:HB3	1:D:269:LEU:HD21	2.01	0.43
1:E:250:GLU:HG2	1:E:254:LYS:HZ1	1.83	0.42
1:A:50:LEU:HD13	1:A:98:LEU:HD11	2.01	0.42
1:E:149:VAL:O	1:E:158:ASN:HA	2.19	0.42
1:H:101:ARG:HG3	1:H:102:LYS:HG2	2.00	0.42
1:B:250:GLU:O	1:B:254:LYS:HE3	2.19	0.42
1:E:42:PRO:HG3	1:E:94:LEU:HD22	2.01	0.42
1:H:252:LEU:O	1:H:256:THR:OG1	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:103:VAL:HG23	1:D:142:VAL:CG1	2.49	0.42
1:A:67:LEU:HD21	1:A:88:LEU:HD13	2.01	0.42
1:D:244:SER:O	1:D:248:VAL:HG22	2.20	0.42
1:D:276:PHE:CE1	3:D:1002:MPD:H12	2.53	0.42
1:G:167:ILE:HG12	1:G:175:ILE:HG22	2.02	0.42
1:B:104:ALA:HB1	1:B:178:HIS:CD2	2.55	0.42
1:C:211:HIS:O	1:C:212:ARG:HB2	2.20	0.42
1:A:193:LEU:HD12	1:A:193:LEU:HA	1.85	0.42
1:G:3:ARG:CB	1:G:237:ASP:OD1	2.66	0.42
1:G:290:LEU:HD11	1:H:262:LEU:HG	2.01	0.42
1:B:9:PHE:HB2	1:B:243:PHE:CE1	2.56	0.41
1:E:159:THR:O	1:E:162:GLN:HB2	2.20	0.41
1:E:67:LEU:HB2	1:E:109:ALA:O	2.20	0.41
1:F:118:PRO:CD	1:G:259:TRP:HB3	2.50	0.41
1:E:83:ARG:HG2	1:E:83:ARG:NH1	2.33	0.41
1:E:215:LEU:HD13	1:E:240:PHE:HE1	1.85	0.41
1:G:115:VAL:HG13	1:G:116:GLU:HG2	2.03	0.41
1:A:21:GLU:HG2	1:A:53:ARG:NH1	2.35	0.41
1:G:113:LEU:HD13	1:G:152:PHE:HA	2.01	0.41
1:H:199:ALA:CB	1:H:232:ILE:HB	2.50	0.41
1:H:83:ARG:O	1:H:87:ILE:HG22	2.20	0.41
1:G:215:LEU:HD13	1:G:240:PHE:CE1	2.55	0.41
1:A:245:SER:CB	1:A:261:ASN:HD21	2.30	0.41
1:C:159:THR:CG2	1:C:161:ALA:HB3	2.50	0.41
1:A:214:PHE:CE2	1:A:269:LEU:HA	2.55	0.41
1:C:249:ASP:HB3	1:C:251:ASN:H	1.85	0.41
1:F:296:LYS:HA	1:F:297:PRO:HD3	1.94	0.41
1:E:106:ILE:HD13	1:E:111:HIS:CG	2.56	0.41
1:B:198:ALA:O	1:B:199:ALA:C	2.59	0.40
1:G:42:PRO:C	1:G:44:ASP:N	2.73	0.40
1:H:67:LEU:HA	1:H:68:PRO:HD3	1.97	0.40
1:F:191:VAL:HG23	1:F:192:GLY:N	2.37	0.40
1:G:96:ARG:HG2	1:G:97:ASP:N	2.36	0.40
1:A:274:ARG:HA	1:A:274:ARG:HD2	1.87	0.40
1:C:65:ILE:HD13	1:C:91:THR:HG21	2.03	0.40
1:D:147:GLU:HA	1:D:178:HIS:HB3	2.02	0.40
1:E:123:TRP:CE3	1:G:297:PRO:HD2	2.56	0.40
1:F:1:MET:HB3	1:F:1:MET:HE3	1.69	0.40
1:G:209:GLU:HG3	1:G:210:SER:N	2.35	0.40
1:B:214:PHE:CE1	1:B:269:LEU:HA	2.57	0.40
1:E:149:VAL:HA	1:E:183:HIS:CG	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:75:SER:OG	1:G:80:VAL:HG21	2.22	0.40
1:H:46:ASP:HB2	1:H:49:ARG:HB3	2.03	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	295/297 (99%)	292 (99%)	3 (1%)	0	100	100
1	B	295/297 (99%)	285 (97%)	10 (3%)	0	100	100
1	C	295/297 (99%)	289 (98%)	6 (2%)	0	100	100
1	D	295/297 (99%)	293 (99%)	2 (1%)	0	100	100
1	E	295/297 (99%)	291 (99%)	4 (1%)	0	100	100
1	F	295/297 (99%)	290 (98%)	5 (2%)	0	100	100
1	G	295/297 (99%)	291 (99%)	4 (1%)	0	100	100
1	H	295/297 (99%)	287 (97%)	8 (3%)	0	100	100
All	All	2360/2376 (99%)	2318 (98%)	42 (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	225/225 (100%)	198 (88%)	27 (12%)	5	11
1	B	225/225 (100%)	200 (89%)	25 (11%)	6	14
1	C	225/225 (100%)	202 (90%)	23 (10%)	7	17
1	D	225/225 (100%)	199 (88%)	26 (12%)	5	12
1	E	225/225 (100%)	208 (92%)	17 (8%)	13	30
1	F	225/225 (100%)	205 (91%)	20 (9%)	9	22
1	G	225/225 (100%)	197 (88%)	28 (12%)	4	11
1	H	225/225 (100%)	197 (88%)	28 (12%)	4	11
All	All	1800/1800 (100%)	1606 (89%)	194 (11%)	6	15

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	18	SER
1	A	21	GLU
1	A	22	ARG
1	A	24	LEU
1	A	38	SER
1	A	50	LEU
1	A	52	LYS
1	A	53	ARG
1	A	56	ASP
1	A	57	LEU
1	A	59	LEU
1	A	77	ASP
1	A	88	LEU
1	A	101	ARG
1	A	115	VAL
1	A	159	THR
1	A	164	LEU
1	A	193	LEU
1	A	212	ARG
1	A	215	LEU
1	A	217	THR
1	A	249	ASP
1	A	253	SER
1	A	266	ASN
1	A	286	ARG
1	A	287	LYS

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Mol	Chain	Res	Type
1	B	1	MET
1	B	8	SER
1	B	20	LEU
1	B	22	ARG
1	B	28	ARG
1	B	38	SER
1	B	53	ARG
1	B	59	LEU
1	B	70	ASP
1	B	78	LYS
1	B	102	LYS
1	B	114	GLN
1	B	142	VAL
1	B	146	LEU
1	B	159	THR
1	B	164	LEU
1	B	178	HIS
1	B	193	LEU
1	B	201	LYS
1	B	211	HIS
1	B	212	ARG
1	B	215	LEU
1	B	255	LYS
1	B	266	ASN
1	B	267	MET
1	C	20	LEU
1	C	22	ARG
1	C	24	LEU
1	C	57	LEU
1	C	59	LEU
1	C	77	ASP
1	C	78	LYS
1	C	88	LEU
1	C	90	GLN
1	C	91	THR
1	C	98	LEU
1	C	146	LEU
1	C	159	THR
1	C	193	LEU
1	C	211	HIS
1	C	212	ARG
1	C	215	LEU

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Mol	Chain	Res	Type
1	C	246	GLU
1	C	262	LEU
1	C	266	ASN
1	C	274	ARG
1	C	281	LEU
1	C	289	GLU
1	D	20	LEU
1	D	34	LEU
1	D	38	SER
1	D	40	LEU
1	D	50	LEU
1	D	53	ARG
1	D	65	ILE
1	D	83	ARG
1	D	88	LEU
1	D	107	LEU
1	D	120	ARG
1	D	146	LEU
1	D	159	THR
1	D	164	LEU
1	D	193	LEU
1	D	211	HIS
1	D	212	ARG
1	D	215	LEU
1	D	249	ASP
1	D	260	ARG
1	D	264	THR
1	D	266	ASN
1	D	271	LYS
1	D	274	ARG
1	D	281	LEU
1	D	296	LYS
1	E	1	MET
1	E	3	ARG
1	E	50	LEU
1	E	57	LEU
1	E	59	LEU
1	E	80	VAL
1	E	83	ARG
1	E	88	LEU
1	E	116	GLU
1	E	159	THR

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Mol	Chain	Res	Type
1	E	193	LEU
1	E	215	LEU
1	E	254	LYS
1	E	255	LYS
1	E	264	THR
1	E	266	ASN
1	E	285	ARG
1	F	1	MET
1	F	24	LEU
1	F	28	ARG
1	F	52	LYS
1	F	53	ARG
1	F	59	LEU
1	F	65	ILE
1	F	98	LEU
1	F	102	LYS
1	F	107	LEU
1	F	108	SER
1	F	114	GLN
1	F	146	LEU
1	F	178	HIS
1	F	193	LEU
1	F	212	ARG
1	F	215	LEU
1	F	238	LEU
1	F	253	SER
1	F	262	LEU
1	G	1	MET
1	G	3	ARG
1	G	21	GLU
1	G	28	ARG
1	G	33	ASP
1	G	46	ASP
1	G	49	ARG
1	G	50	LEU
1	G	77	ASP
1	G	80	VAL
1	G	96	ARG
1	G	107	LEU
1	G	114	GLN
1	G	149	VAL
1	G	159	THR

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Mol	Chain	Res	Type
1	G	164	LEU
1	G	193	LEU
1	G	211	HIS
1	G	212	ARG
1	G	245	SER
1	G	246	GLU
1	G	258	ILE
1	G	265	ASP
1	G	266	ASN
1	G	267	MET
1	G	274	ARG
1	G	292	SER
1	G	294	ARG
1	H	1	MET
1	H	3	ARG
1	H	22	ARG
1	H	28	ARG
1	H	29	ASP
1	H	34	LEU
1	H	45	VAL
1	H	46	ASP
1	H	47	ILE
1	H	56	ASP
1	H	87	ILE
1	H	102	LYS
1	H	107	LEU
1	H	113	LEU
1	H	115	VAL
1	H	146	LEU
1	H	159	THR
1	H	164	LEU
1	H	191	VAL
1	H	201	LYS
1	H	211	HIS
1	H	215	LEU
1	H	245	SER
1	H	254	LYS
1	H	255	LYS
1	H	260	ARG
1	H	266	ASN
1	H	274	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	17	GLN
1	A	145	ASN
1	A	158	ASN
1	A	266	ASN
1	B	7	HIS
1	B	158	ASN
1	B	178	HIS
1	B	266	ASN
1	B	272	HIS
1	B	295	HIS
1	C	150	ASN
1	C	158	ASN
1	C	266	ASN
1	C	295	HIS
1	D	7	HIS
1	D	158	ASN
1	D	266	ASN
1	D	295	HIS
1	E	266	ASN
1	F	7	HIS
1	F	114	GLN
1	F	178	HIS
1	F	266	ASN
1	G	183	HIS
1	G	197	HIS
1	G	251	ASN
1	G	266	ASN
1	G	272	HIS
1	H	7	HIS
1	H	17	GLN
1	H	158	ASN
1	H	211	HIS
1	H	266	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 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	MPD	A	1002	-	7,7,7	0.20	0	9,10,10	0.31	0
3	MPD	D	1002	-	7,7,7	0.27	0	9,10,10	0.54	0
3	MPD	B	1002	-	7,7,7	0.38	0	9,10,10	0.49	0
3	MPD	E	1002	-	7,7,7	0.26	0	9,10,10	0.35	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	A	1002	-	-	4/5/5/5	-
3	MPD	D	1002	-	-	5/5/5/5	-
3	MPD	B	1002	-	-	3/5/5/5	-
3	MPD	E	1002	-	-	0/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	1002	MPD	C2-C3-C4-C5
3	D	1002	MPD	O2-C2-C3-C4
3	B	1002	MPD	O2-C2-C3-C4
3	A	1002	MPD	C2-C3-C4-C5
3	D	1002	MPD	C1-C2-C3-C4
3	D	1002	MPD	CM-C2-C3-C4
3	B	1002	MPD	C1-C2-C3-C4
3	B	1002	MPD	CM-C2-C3-C4
3	A	1002	MPD	CM-C2-C3-C4
3	A	1002	MPD	O2-C2-C3-C4
3	D	1002	MPD	C2-C3-C4-O4
3	A	1002	MPD	C2-C3-C4-O4

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1002	MPD	1	0
3	B	1002	MPD	1	0
3	E	1002	MPD	1	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	297/297 (100%)	-0.32	0 100 100	19, 36, 60, 79	0
1	B	297/297 (100%)	-0.29	0 100 100	18, 36, 60, 87	0
1	C	297/297 (100%)	-0.40	0 100 100	20, 33, 52, 65	0
1	D	297/297 (100%)	-0.50	0 100 100	18, 31, 58, 78	0
1	E	297/297 (100%)	-0.24	2 (0%) 87 89	26, 44, 72, 92	0
1	F	297/297 (100%)	-0.05	7 (2%) 59 60	26, 49, 72, 96	0
1	G	297/297 (100%)	0.55	24 (8%) 12 10	38, 67, 100, 130	0
1	H	297/297 (100%)	0.30	19 (6%) 19 18	36, 59, 99, 123	0
All	All	2376/2376 (100%)	-0.12	52 (2%) 62 63	18, 43, 84, 130	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	39	TYR	6.1
1	G	40	LEU	5.7
1	G	1	MET	5.6
1	H	39	TYR	5.5
1	H	42	PRO	4.6
1	H	43	ALA	4.4
1	G	44	ASP	4.1
1	G	43	ALA	4.1
1	G	101	ARG	4.0
1	G	54	ILE	3.7
1	H	139	ALA	3.5
1	H	82	ALA	3.2
1	H	70	ASP	3.1
1	G	246	GLU	2.9
1	F	76	ALA	2.9
1	G	58	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	H	38	SER	2.9
1	G	18	SER	2.8
1	H	14	SER	2.7
1	G	2	ALA	2.7
1	F	69	ALA	2.7
1	H	297	PRO	2.7
1	H	49	ARG	2.7
1	G	250	GLU	2.6
1	G	30	ALA	2.6
1	G	254	LYS	2.5
1	H	135	GLU	2.5
1	G	41	ASP	2.4
1	G	56	ASP	2.4
1	F	1	MET	2.3
1	G	95	THR	2.3
1	E	44	ASP	2.3
1	G	123	TRP	2.3
1	H	289	GLU	2.3
1	G	115	VAL	2.3
1	G	52	LYS	2.3
1	H	56	ASP	2.2
1	H	40	LEU	2.2
1	H	246	GLU	2.2
1	F	57	LEU	2.1
1	H	97	ASP	2.1
1	H	1	MET	2.1
1	G	247	ILE	2.1
1	H	115	VAL	2.1
1	G	121	ASP	2.1
1	G	268	ALA	2.1
1	H	117	ALA	2.1
1	F	75	SER	2.1
1	F	78	LYS	2.0
1	G	264	THR	2.0
1	F	79	ALA	2.0
1	E	49	ARG	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MPD	B	1002	8/8	0.79	0.25	46,50,53,56	0
3	MPD	D	1002	8/8	0.81	0.25	62,66,76,80	0
3	MPD	A	1002	8/8	0.86	0.23	59,61,67,70	0
3	MPD	E	1002	8/8	0.88	0.21	57,60,64,68	0
2	MN	E	1001	1/1	0.97	0.17	33,33,33,33	0
2	MN	H	1001	1/1	0.98	0.10	43,43,43,43	0
2	MN	G	1001	1/1	0.98	0.14	50,50,50,50	0
2	MN	C	1001	1/1	0.99	0.16	26,26,26,26	0
2	MN	F	1001	1/1	0.99	0.18	41,41,41,41	0
2	MN	A	1001	1/1	0.99	0.15	21,21,21,21	0
2	MN	B	1001	1/1	0.99	0.14	26,26,26,26	0
2	MN	D	1001	1/1	0.99	0.16	22,22,22,22	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.