



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 20, 2016 – 04:08 AM EDT

PDB ID : 5EJ9  
Title : EcMenD-ThDP-Mn<sup>2+</sup> complex soaked with 2-ketoglutarate for 2 min and isochorismate for 13 min  
Authors : Song, H.G.; Dong, C.; Chen, Y.Z.; Sun, Y.R.; Guo, Z.H.  
Deposited on : 2015-11-01  
Resolution : 1.72 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027790  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027790

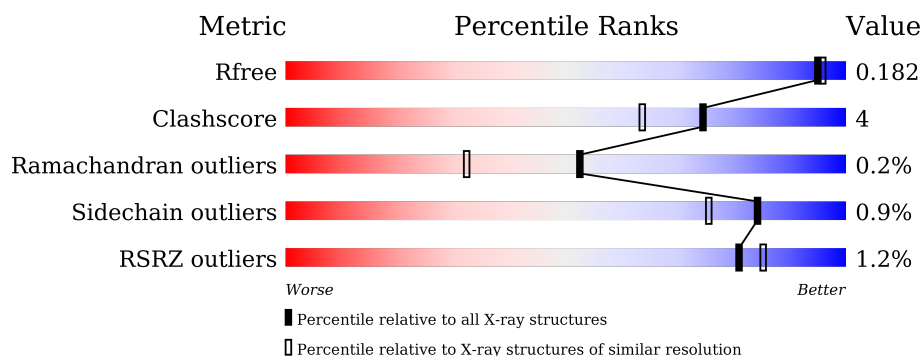
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.72 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3998 (1.74-1.70)
Clashscore	102246	4425 (1.74-1.70)
Ramachandran outliers	100387	4360 (1.74-1.70)
Sidechain outliers	100360	4360 (1.74-1.70)
RSRZ outliers	91569	4010 (1.74-1.70)

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. 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	556	<div> <div></div> <div>91% 9%</div> </div>
1	B	556	<div> <div></div> <div>93% 6%</div> </div>
1	C	556	<div> <div></div> <div>91% 9%</div> </div>
1	D	556	<div> <div>2%</div> <div>92% 8%</div> </div>
1	E	556	<div> <div></div> <div>92% 8%</div> </div>
1	F	556	<div> <div></div> <div>94% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	556	<div> <div>%</div> <div> </div> <div>93%7%</div> </div>
1	H	556	<div> <div>%</div> <div> </div> <div>91%8%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	603	-	-	-	X
5	FMT	E	604	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 40605 atoms, of which 208 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 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	556	Total	C	N	O	S	0	7	0
			4373	2772	790	796	15			
1	B	556	Total	C	N	O	S	0	3	0
			4329	2748	777	790	14			
1	C	556	Total	C	N	O	S	0	6	0
			4352	2762	786	790	14			
1	D	556	Total	C	N	O	S	0	3	0
			4308	2736	773	785	14			
1	E	556	Total	C	N	O	S	0	6	0
			4356	2763	784	794	15			
1	F	556	Total	C	N	O	S	0	4	0
			4337	2754	780	789	14			
1	G	556	Total	C	N	O	S	0	5	0
			4344	2755	784	791	14			
1	H	556	Total	C	N	O	S	0	3	0
			4313	2740	773	786	14			

- Molecule 2 is THIAMINE DIPHOSPHATE (three-letter code: TPP) (formula: C<sub>12</sub>H<sub>19</sub>N<sub>4</sub>O<sub>7</sub>P<sub>2</sub>S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total 42	C 12	H 16	N 4	O 7	P 2	S 1	0	0
2	B	1	Total 42	C 12	H 16	N 4	O 7	P 2	S 1	0	0
2	C	1	Total 42	C 12	H 16	N 4	O 7	P 2	S 1	0	0
2	D	1	Total 42	C 12	H 16	N 4	O 7	P 2	S 1	0	0
2	E	1	Total 42	C 12	H 16	N 4	O 7	P 2	S 1	0	0
2	F	1	Total 42	C 12	H 16	N 4	O 7	P 2	S 1	0	0
2	G	1	Total 42	C 12	H 16	N 4	O 7	P 2	S 1	0	0
2	H	1	Total 42	C 12	H 16	N 4	O 7	P 2	S 1	0	0

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

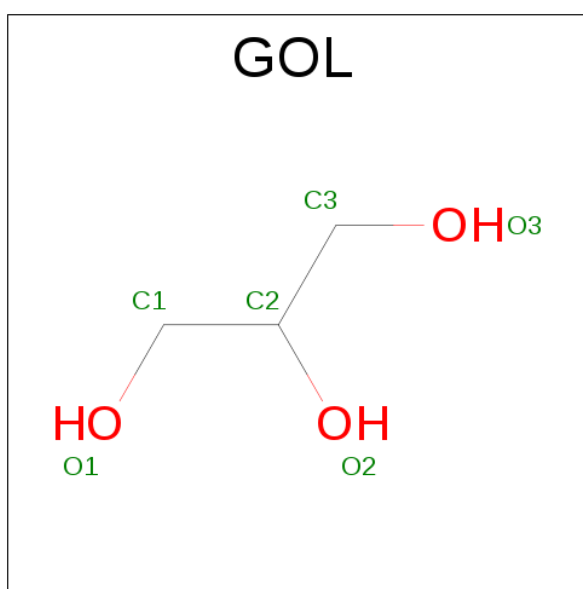
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Mn 1 1	0	0
3	D	1	Total Mn 1 1	0	0
3	E	1	Total Mn 1 1	0	0
3	H	1	Total Mn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Mn 1	0	0
3	C	1	Total 1	Mn 1	0	0
3	A	1	Total 1	Mn 1	0	0
3	F	1	Total 1	Mn 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



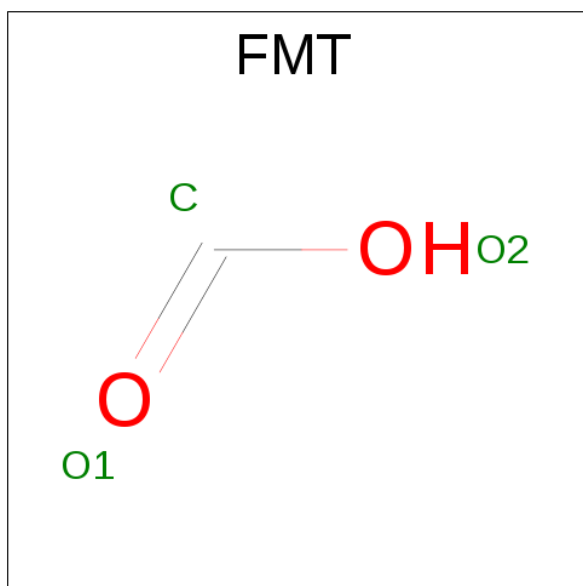
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total 14	C 3	H 8	O 3	0	0
4	B	1	Total 14	C 3	H 8	O 3	0	0
4	C	1	Total 14	C 3	H 8	O 3	0	0
4	D	1	Total 14	C 3	H 8	O 3	0	0
4	E	1	Total 14	C 3	H 8	O 3	0	0
4	F	1	Total 14	C 3	H 8	O 3	0	0
4	G	1	Total 14	C 3	H 8	O 3	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	H	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			5	1	2	2		
5	B	1	Total	C	H	O	0	0
			5	1	2	2		
5	C	1	Total	C	H	O	0	0
			5	1	2	2		
5	D	1	Total	C	H	O	0	0
			5	1	2	2		
5	E	1	Total	C	H	O	0	0
			5	1	2	2		
5	F	1	Total	C	H	O	0	0
			5	1	2	2		
5	G	1	Total	C	H	O	0	0
			5	1	2	2		
5	H	1	Total	C	H	O	0	0
			5	1	2	2		

- Molecule 6 is water.

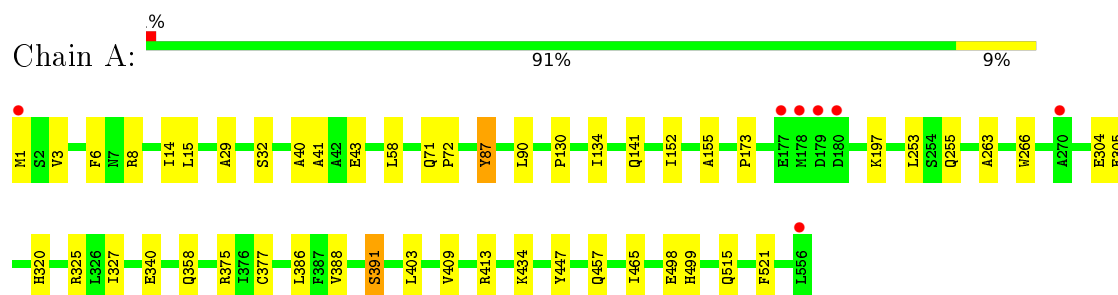
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	737	Total O 737 737	0	0
6	B	669	Total O 669 669	0	0
6	C	676	Total O 676 676	0	0
6	D	592	Total O 592 592	0	0
6	E	712	Total O 712 712	0	0
6	F	682	Total O 682 682	0	0
6	G	714	Total O 714 714	0	0
6	H	615	Total O 615 615	0	0



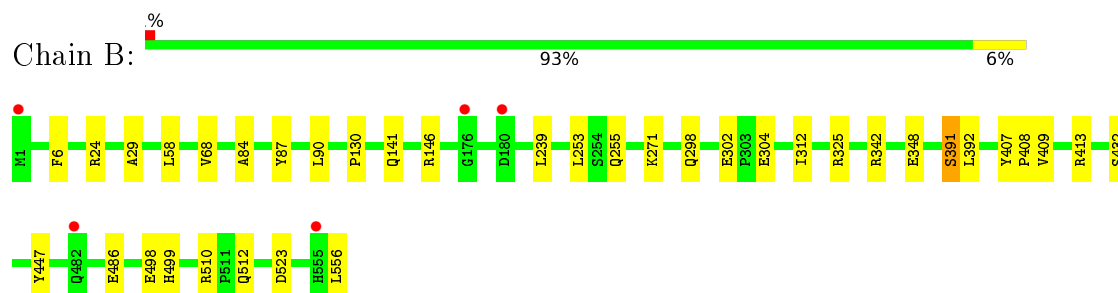
### 3 Residue-property plots

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

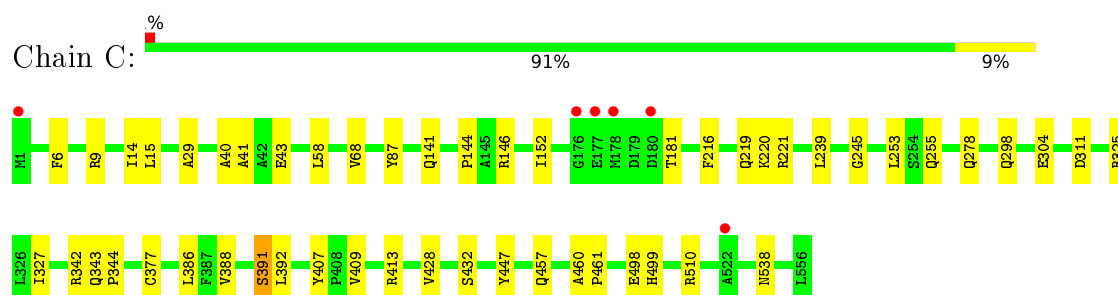
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



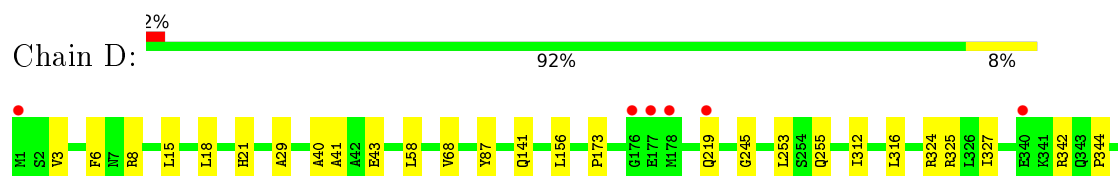
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

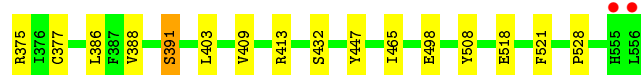


- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase

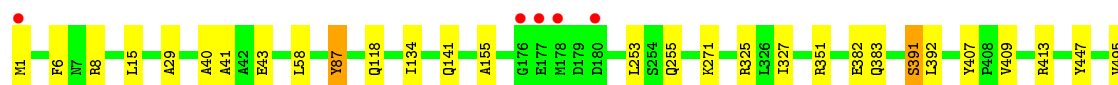
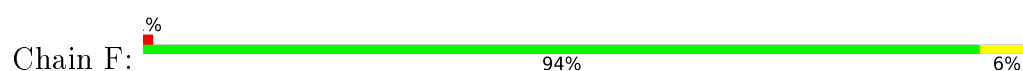




- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



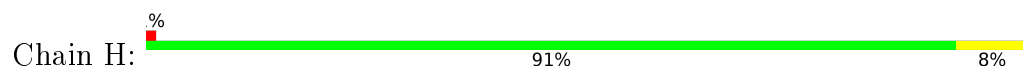
- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



- Molecule 1: 2-succinyl-5-enolpyruvyl-6-hydroxy-3-cyclohexene-1-carboxylate synthase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.72Å 90.72Å 169.47Å 76.06° 83.35° 64.38°	Depositor
Resolution (Å)	39.96 – 1.72 39.96 – 1.72	Depositor EDS
% Data completeness (in resolution range)	96.5 (39.96-1.72) 88.1 (39.96-1.72)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.36 (at 1.72Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, $R_{free}$	0.151 , 0.182 0.151 , 0.182	Depositor DCC
$R_{free}$ test set	23507 reflections (4.92%)	DCC
Wilson B-factor (Å <sup>2</sup> )	14.4	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 54.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.036 for -h,-k,-k+l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	40605	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: GOL, FMT, MN, TPP

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	0.34	0/4482	0.52	0/6116
1	B	0.34	0/4438	0.51	0/6059
1	C	0.34	0/4461	0.51	0/6089
1	D	0.32	0/4417	0.50	0/6034
1	E	0.35	0/4465	0.53	0/6094
1	F	0.34	0/4446	0.51	0/6068
1	G	0.34	0/4453	0.51	0/6078
1	H	0.32	0/4422	0.51	0/6039
All	All	0.34	0/35584	0.51	0/48577

There are no bond length outliers.

There are no bond angle outliers.

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	4373	0	4321	42	0
1	B	4329	0	4258	29	0
1	C	4352	0	4294	44	0
1	D	4308	0	4230	38	0
1	E	4356	0	4292	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	4337	0	4278	30	0
1	G	4344	0	4283	26	0
1	H	4313	0	4241	37	0
2	A	26	16	16	0	0
2	B	26	16	16	1	0
2	C	26	16	16	2	0
2	D	26	16	16	1	0
2	E	26	16	16	1	0
2	F	26	16	16	1	0
2	G	26	16	16	0	0
2	H	26	16	16	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	6	8	8	0	0
4	B	6	8	8	0	0
4	C	6	8	8	0	0
4	D	6	8	8	0	0
4	E	6	8	8	0	0
4	F	6	8	8	0	0
4	G	6	8	8	0	0
4	H	6	8	8	0	0
5	A	3	2	1	1	0
5	B	3	2	1	0	0
5	C	3	2	1	0	0
5	D	3	2	1	0	0
5	E	3	2	1	2	0
5	F	3	2	1	0	0
5	G	3	2	1	1	0
5	H	3	2	1	0	0
6	A	737	0	0	12	0
6	B	669	0	0	12	0
6	C	676	0	0	13	0
6	D	592	0	0	5	0
6	E	712	0	0	11	0
6	F	682	0	0	8	4
6	G	714	0	0	8	4

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	615	0	0	13	0
All	All	40397	208	34397	281	4

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 4.

All (281) 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:H:255:GLN:HE21	1:H:409:VAL:H	1.21	0.89
1:D:255:GLN:HE21	1:D:409:VAL:H	1.19	0.88
1:B:146[B]:ARG:HH11	1:B:146[B]:ARG:HG2	1.41	0.86
1:B:255:GLN:HE21	1:B:409:VAL:H	1.23	0.85
1:A:15[A]:LEU:HD12	1:A:40:ALA:HB3	1.57	0.85
1:E:15[A]:LEU:HD12	1:E:40:ALA:HB3	1.57	0.85
1:E:255:GLN:HE21	1:E:409:VAL:H	1.24	0.84
1:G:255:GLN:HE21	1:G:409:VAL:H	1.25	0.83
1:F:255:GLN:HE21	1:F:409:VAL:H	1.24	0.82
1:A:255:GLN:HE21	1:A:409:VAL:H	1.25	0.82
1:C:255:GLN:HE21	1:C:409:VAL:H	1.25	0.81
1:B:298:GLN:NE2	6:B:701:HOH:O	2.15	0.79
1:H:15[A]:LEU:HD12	1:H:40:ALA:HB3	1.64	0.78
1:A:515:GLN:NE2	6:A:701:HOH:O	2.16	0.77
1:H:236:LYS:NZ	6:H:701:HOH:O	2.19	0.74
1:C:15[A]:LEU:HD12	1:C:40:ALA:HB3	1.70	0.74
1:D:15[A]:LEU:HD12	1:D:40:ALA:HB3	1.68	0.73
1:A:197:LYS:NZ	6:A:702:HOH:O	2.16	0.72
1:A:15[A]:LEU:HD12	1:A:40:ALA:CB	2.21	0.71
1:A:434:LYS:NZ	6:A:709:HOH:O	2.23	0.70
1:F:271:LYS:NZ	1:F:556:LEU:OXT	2.24	0.70
1:C:9:ARG:NH1	1:C:181:THR:O	2.25	0.69
1:C:538:ASN:ND2	6:C:704:HOH:O	2.22	0.69
1:B:271:LYS:NZ	1:B:556:LEU:OXT	2.27	0.68
1:E:15[A]:LEU:HD12	1:E:40:ALA:CB	2.24	0.67
1:F:15[A]:LEU:HD12	1:F:40:ALA:HB3	1.75	0.67
1:D:255:GLN:NE2	1:D:409:VAL:H	1.93	0.67
1:E:518:GLU:OE1	6:E:701:HOH:O	2.13	0.67
1:B:24:ARG:NH1	6:B:706:HOH:O	2.23	0.67
1:B:6:PHE:CE1	1:B:141:GLN:HG2	2.30	0.67
1:F:1:MET:N	6:F:705:HOH:O	2.28	0.67
1:E:6:PHE:CE1	1:E:141:GLN:HG2	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:383:GLN:NE2	6:H:708:HOH:O	2.30	0.65
1:H:15[A]:LEU:HD12	1:H:40:ALA:CB	2.26	0.64
1:A:375:ARG:HD3	6:A:871:HOH:O	1.97	0.64
1:G:304:GLU:OE1	6:G:701:HOH:O	2.14	0.64
1:D:6:PHE:CE1	1:D:141:GLN:HG2	2.34	0.63
1:F:6:PHE:CE1	1:F:141:GLN:HG2	2.33	0.63
1:G:311:ASP:OD2	6:G:702:HOH:O	2.15	0.63
1:F:498:GLU:HG3	1:F:508:TYR:CD2	2.34	0.62
1:A:6:PHE:CE1	1:A:141:GLN:HG2	2.35	0.62
1:D:15[A]:LEU:HD12	1:D:40:ALA:CB	2.29	0.61
1:H:6:PHE:CE1	1:H:141:GLN:HG2	2.35	0.61
1:C:311:ASP:OD2	6:C:701:HOH:O	2.16	0.61
1:C:15[A]:LEU:HD12	1:C:40:ALA:CB	2.31	0.61
1:E:15[B]:LEU:CD2	1:E:41:ALA:HB2	2.31	0.60
1:E:528:PRO:O	6:E:702:HOH:O	2.16	0.60
1:A:305:GLU:HG2	6:A:1203:HOH:O	2.02	0.60
1:G:456:ARG:NH2	6:G:713:HOH:O	2.34	0.60
1:G:377:CYS:HB2	6:G:1045:HOH:O	2.01	0.60
1:B:512:GLN:NE2	6:B:713:HOH:O	2.35	0.60
1:C:6:PHE:CE1	1:C:141:GLN:HG2	2.37	0.59
1:B:146[B]:ARG:HG2	6:B:1083:HOH:O	2.01	0.59
1:B:255:GLN:NE2	1:B:409:VAL:H	1.98	0.59
1:E:15[B]:LEU:HD21	1:E:41:ALA:HB2	1.85	0.59
1:F:43:GLU:OE1	6:F:701:HOH:O	2.17	0.59
1:E:32:SER:HB3	5:E:604:FMT:H	1.83	0.58
1:E:15[A]:LEU:HD13	1:E:41:ALA:N	2.18	0.58
1:E:15[A]:LEU:CD1	1:E:40:ALA:HB3	2.32	0.58
1:E:340:GLU:OE1	6:E:703:HOH:O	2.17	0.58
1:C:239:LEU:HG	6:C:790:HOH:O	2.03	0.57
1:F:15[B]:LEU:HD23	1:F:41:ALA:HA	1.86	0.57
1:D:21:HIS:HB2	1:D:156:LEU:HD23	1.87	0.57
1:H:255:GLN:NE2	1:H:409:VAL:H	1.98	0.56
1:C:219[A]:GLN:NE2	6:C:710:HOH:O	2.29	0.56
1:C:298[B]:GLN:NE2	6:C:713:HOH:O	2.39	0.56
1:D:18:LEU:HD22	1:D:156:LEU:HD21	1.88	0.56
1:D:15[B]:LEU:HD21	1:D:41:ALA:HB2	1.88	0.56
1:D:68:VAL:HG21	1:D:428:VAL:HG13	1.87	0.56
1:C:220:LYS:HE2	1:C:220:LYS:HA	1.87	0.56
1:A:15[B]:LEU:HD21	1:A:41:ALA:HB2	1.88	0.55
1:G:219[B]:GLN:OE1	6:G:704:HOH:O	2.18	0.55
1:A:320:HIS:HB2	1:C:146[B]:ARG:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:375:ARG:HD3	6:E:1032:HOH:O	2.07	0.55
1:E:465:ILE:HD11	1:E:521:PHE:HZ	1.72	0.55
1:A:1:MET:N	6:A:712:HOH:O	2.32	0.55
2:C:601:TPP:H2	6:D:707:HOH:O	2.07	0.55
1:H:146[A]:ARG:NH1	6:H:712:HOH:O	2.35	0.55
1:G:6:PHE:CE1	1:G:141:GLN:HG2	2.42	0.54
1:A:32:SER:H	5:A:604:FMT:C	2.20	0.54
1:H:3:VAL:HB	1:H:173:PRO:HD2	1.90	0.54
1:C:278:GLN:HG2	6:C:1263:HOH:O	2.08	0.54
1:F:495:VAL:HG22	1:F:496:HIS:N	2.23	0.54
1:A:15[A]:LEU:CD1	1:A:40:ALA:HB3	2.32	0.54
1:D:15[A]:LEU:CD1	1:D:40:ALA:HB3	2.37	0.54
1:H:253:LEU:HD11	1:H:413:ARG:HG3	1.89	0.54
1:B:523:ASP:HB3	6:B:719:HOH:O	2.08	0.53
1:C:68:VAL:HG11	1:C:432:SER:HB3	1.90	0.53
1:F:15[B]:LEU:HD21	1:F:41:ALA:HB2	1.91	0.53
1:G:255:GLN:NE2	1:G:409:VAL:H	2.02	0.53
1:B:302:GLU:OE2	6:B:702:HOH:O	2.19	0.53
1:A:15[A]:LEU:HD13	1:A:41:ALA:N	2.24	0.53
1:B:146[B]:ARG:CG	1:B:146[B]:ARG:HH11	2.18	0.52
1:F:15[A]:LEU:HD12	1:F:40:ALA:CB	2.38	0.52
1:H:15[A]:LEU:CD1	1:H:40:ALA:HB3	2.36	0.52
1:G:68:VAL:HG11	1:G:432:SER:HB3	1.92	0.52
1:E:347:VAL:O	6:E:704:HOH:O	2.19	0.52
1:G:498:GLU:HG2	1:G:499:HIS:N	2.24	0.52
1:F:495:VAL:HG22	1:F:496:HIS:O	2.09	0.51
1:C:43:GLU:OE1	6:C:702:HOH:O	2.19	0.51
1:D:219:GLN:NE2	1:D:342:ARG:HD2	2.25	0.51
1:D:375:ARG:HD3	6:D:922:HOH:O	2.11	0.51
1:A:29:ALA:HB2	1:A:58:LEU:HD22	1.93	0.51
1:A:304:GLU:OE1	6:A:704:HOH:O	2.19	0.51
1:E:32:SER:H	5:E:604:FMT:C	2.24	0.51
1:B:312:ILE:HG23	6:B:1156:HOH:O	2.09	0.51
1:H:15[B]:LEU:HD21	1:H:41:ALA:HB2	1.93	0.50
1:A:255:GLN:NE2	1:A:409:VAL:H	2.03	0.50
1:C:221:ARG:NH2	6:C:714:HOH:O	2.39	0.50
1:H:15[B]:LEU:HD23	1:H:41:ALA:HA	1.93	0.50
1:E:196:ASP:OD2	6:E:705:HOH:O	2.19	0.50
1:D:342:ARG:HD3	6:D:822:HOH:O	2.12	0.50
1:F:255:GLN:NE2	1:F:409:VAL:H	2.01	0.50
1:D:3:VAL:HB	1:D:173:PRO:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:GLU:OE1	6:A:705:HOH:O	2.20	0.50
1:D:18:LEU:CD2	1:D:156:LEU:HD21	2.42	0.50
1:H:169:PRO:HD2	6:H:1062:HOH:O	2.12	0.50
1:B:239:LEU:HG	6:B:743:HOH:O	2.12	0.49
1:E:3:VAL:HB	1:E:173:PRO:HD2	1.93	0.49
1:G:219[A]:GLN:HG2	1:G:340:GLU:OE2	2.12	0.49
1:B:342:ARG:HD3	6:B:745:HOH:O	2.11	0.49
1:B:253:LEU:HD11	1:B:413:ARG:HG3	1.94	0.49
1:G:129:HIS:HD2	6:G:1175:HOH:O	1.95	0.49
1:C:327:ILE:N	1:C:327:ILE:HD12	2.28	0.48
1:C:377:CYS:HB2	6:C:843:HOH:O	2.13	0.48
1:D:324:ARG:NH2	6:D:721:HOH:O	2.44	0.48
1:A:377[A]:CYS:SG	1:A:403:LEU:HA	2.52	0.48
1:D:253:LEU:HD11	1:D:413:ARG:HG3	1.95	0.48
1:A:15[B]:LEU:CD2	1:A:41:ALA:HB2	2.44	0.48
1:D:498:GLU:HG3	1:D:508:TYR:CD2	2.48	0.48
1:A:3:VAL:HB	1:A:173:PRO:HD2	1.94	0.48
1:H:377:CYS:HB2	6:H:771:HOH:O	2.14	0.48
1:A:253:LEU:HD11	1:A:413:ARG:HG3	1.96	0.48
1:A:465:ILE:HD11	1:A:521:PHE:HZ	1.78	0.48
1:C:15[A]:LEU:HD13	1:C:41:ALA:N	2.29	0.48
1:D:8:ARG:NH2	1:D:43:GLU:OE2	2.40	0.48
1:E:253:LEU:HD11	1:E:413:ARG:HG3	1.96	0.48
1:G:253:LEU:HD11	1:G:413:ARG:HG3	1.95	0.48
1:C:144:PRO:HB2	1:C:146[A]:ARG:HG2	1.96	0.48
1:F:15[B]:LEU:HD23	1:F:41:ALA:CA	2.44	0.48
1:A:327:ILE:HD12	1:A:327:ILE:N	2.29	0.47
1:C:253:LEU:HD11	1:C:413:ARG:HG3	1.95	0.47
1:G:32:SER:H	5:G:604:FMT:C	2.27	0.47
1:B:29:ALA:HB2	1:B:58:LEU:HD22	1.94	0.47
1:C:15[B]:LEU:HD21	1:C:41:ALA:HB2	1.96	0.47
1:E:498:GLU:HG3	1:E:508:TYR:CD2	2.49	0.47
1:F:556:LEU:O	6:F:702:HOH:O	2.20	0.47
1:F:382:GLU:HG2	1:F:383:GLN:HG2	1.97	0.47
1:H:40:ALA:HB2	6:H:762:HOH:O	2.15	0.47
1:G:216:PHE:O	1:G:219[B]:GLN:HG3	2.14	0.47
1:B:68:VAL:HG11	1:B:432:SER:HB3	1.96	0.47
1:H:293:ARG:NH2	1:H:550:LEU:HD11	2.30	0.47
1:G:278:GLN:HG2	6:G:1292:HOH:O	2.14	0.47
1:E:311:ASP:HB2	6:E:1279:HOH:O	2.14	0.47
2:E:601:TPP:H2	6:F:703:HOH:O	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:GLN:HG2	1:B:407:TYR:O	2.14	0.47
1:E:312:ILE:HG13	1:E:316:LEU:HD11	1.96	0.47
1:D:255:GLN:HE21	1:D:409:VAL:N	2.00	0.47
1:D:392:LEU:HB2	2:D:602:TPP:O2B	2.15	0.47
1:G:278:GLN:HG2	6:G:1244:HOH:O	2.14	0.47
1:H:342:ARG:HD3	6:H:716:HOH:O	2.15	0.46
1:D:15[B]:LEU:HD23	1:D:41:ALA:HA	1.96	0.46
1:C:40:ALA:HB2	6:C:796:HOH:O	2.15	0.46
1:C:15[A]:LEU:CD1	1:C:40:ALA:HB3	2.42	0.46
1:B:498:GLU:HG2	1:B:499:HIS:N	2.31	0.46
1:F:118:GLN:OE1	6:F:703:HOH:O	2.21	0.46
1:C:392:LEU:HB2	2:C:601:TPP:O1B	2.16	0.46
1:H:15[A]:LEU:HD13	1:H:41:ALA:N	2.31	0.46
1:C:15[B]:LEU:CD2	1:C:41:ALA:HB2	2.46	0.46
1:C:342:ARG:HD3	6:C:914:HOH:O	2.15	0.45
1:A:358:GLN:HG3	6:A:1336:HOH:O	2.16	0.45
1:A:498:GLU:HG2	1:A:499:HIS:N	2.31	0.45
1:G:327:ILE:HD12	1:G:327:ILE:N	2.30	0.45
1:G:29:ALA:HB2	1:G:58:LEU:HD22	1.98	0.45
1:H:327:ILE:HD12	1:H:327:ILE:N	2.31	0.45
1:C:255:GLN:NE2	1:C:409:VAL:H	2.04	0.45
1:E:43:GLU:OE1	6:E:706:HOH:O	2.21	0.45
1:H:460:ALA:HB1	1:H:461:PRO:HD2	1.99	0.45
1:H:392:LEU:HB2	2:H:602:TPP:O1B	2.17	0.45
1:F:392:LEU:HB2	2:F:602:TPP:O1B	2.16	0.45
1:H:236:LYS:HD3	6:H:1003:HOH:O	2.16	0.45
1:C:29:ALA:HB2	1:C:58:LEU:HD22	1.99	0.45
1:F:255:GLN:HG2	1:F:407:TYR:O	2.17	0.45
1:H:134:ILE:HD11	1:H:155:ALA:HB2	1.99	0.45
1:A:134:ILE:HD11	1:A:155:ALA:HB2	1.98	0.45
1:D:68:VAL:HG11	1:D:432:SER:HB3	1.97	0.44
1:A:15[B]:LEU:HD22	1:A:41:ALA:N	2.32	0.44
1:F:8:ARG:NH2	1:F:43:GLU:OE2	2.47	0.44
1:E:255:GLN:NE2	1:E:409:VAL:H	2.03	0.44
1:A:457:GLN:HG3	6:A:723:HOH:O	2.18	0.44
1:D:382:GLU:HG3	1:D:383:GLN:HG2	1.99	0.44
1:H:129:HIS:HD2	6:H:1124:HOH:O	2.01	0.44
1:C:14:ILE:HG12	1:C:152:ILE:HD11	1.98	0.44
1:B:304:GLU:OE1	6:B:705:HOH:O	2.21	0.44
1:C:386:LEU:HG	1:C:388[A]:VAL:HG23	2.00	0.44
1:C:15[B]:LEU:HD23	1:C:41:ALA:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15[A]:LEU:HD13	1:D:41:ALA:N	2.32	0.43
1:F:29:ALA:HB2	1:F:58:LEU:HD22	1.98	0.43
1:D:327:ILE:HD12	1:D:327:ILE:N	2.32	0.43
1:A:14:ILE:HA	1:A:152:ILE:CD1	2.47	0.43
1:B:392:LEU:HB2	2:B:602:TPP:O2B	2.17	0.43
1:E:15[B]:LEU:HD22	1:E:41:ALA:N	2.32	0.43
1:B:348:GLU:OE2	6:B:703:HOH:O	2.20	0.43
1:F:15[A]:LEU:HD13	1:F:41:ALA:N	2.32	0.43
1:G:347:VAL:HG23	1:G:348:GLU:HG2	1.99	0.43
1:D:245:GLY:O	1:D:344:PRO:HA	2.18	0.43
1:F:15[B]:LEU:CD2	1:F:41:ALA:HB2	2.48	0.43
1:H:498:GLU:HG2	1:H:499:HIS:N	2.32	0.43
1:C:460:ALA:HB1	1:C:461:PRO:HD2	1.99	0.43
1:E:347:VAL:HG23	1:E:348:GLU:HG2	2.01	0.43
1:F:253:LEU:HD11	1:F:413:ARG:HG3	1.99	0.43
1:F:351:ARG:HD2	6:F:1079:HOH:O	2.18	0.43
1:G:144:PRO:HB2	1:G:146[A]:ARG:HG2	2.00	0.43
1:H:68:VAL:HG11	1:H:432:SER:HB3	2.00	0.43
1:A:71[B]:GLN:HB3	1:A:72:PRO:HD2	2.00	0.43
1:C:245:GLY:O	1:C:344:PRO:HA	2.19	0.43
1:H:375:ARG:HD3	6:H:993:HOH:O	2.19	0.43
1:D:15[B]:LEU:CD2	1:D:41:ALA:HB2	2.48	0.43
1:F:134:ILE:HD11	1:F:155:ALA:HB2	2.01	0.43
1:H:255:GLN:HG2	1:H:407:TYR:O	2.19	0.43
1:C:14:ILE:HA	1:C:152:ILE:HD13	2.00	0.42
1:C:498:GLU:OE1	1:C:510:ARG:NH2	2.51	0.42
1:H:14:ILE:HG12	1:H:152:ILE:HD11	2.01	0.42
1:C:457:GLN:HG3	6:C:728:HOH:O	2.19	0.42
1:D:456:ARG:NH1	6:D:703:HOH:O	2.26	0.42
1:A:340:GLU:OE1	6:A:706:HOH:O	2.21	0.42
1:D:255:GLN:HG2	1:D:407:TYR:O	2.20	0.42
1:E:134:ILE:HD11	1:E:155:ALA:HB2	2.01	0.42
1:E:327:ILE:HD12	1:E:327:ILE:N	2.34	0.42
1:B:486:GLU:OE1	6:B:704:HOH:O	2.21	0.42
1:C:14:ILE:HA	1:C:152:ILE:CD1	2.50	0.42
1:F:523:ASP:HB3	6:F:830:HOH:O	2.20	0.42
1:C:216:PHE:O	1:C:219[B]:GLN:HG3	2.20	0.42
1:D:68:VAL:CG2	1:D:428:VAL:HG13	2.50	0.42
1:H:263:ALA:HA	1:H:266:TRP:NE1	2.34	0.42
1:A:197:LYS:NZ	6:A:743:HOH:O	2.52	0.42
1:G:9:ARG:HD2	1:G:182:GLY:C	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:210:LYS:NZ	6:H:724:HOH:O	2.49	0.42
1:C:304:GLU:OE1	6:C:703:HOH:O	2.22	0.42
1:E:29:ALA:HB2	1:E:58:LEU:HD22	2.01	0.42
1:H:97:GLY:HA2	1:H:161:ALA:HB1	2.01	0.42
1:B:407:TYR:HA	1:B:408:PRO:HD3	1.94	0.42
1:A:87:TYR:HB3	1:B:84:ALA:HB1	2.02	0.42
1:D:407:TYR:HA	1:D:408:PRO:HD3	1.91	0.42
1:B:498:GLU:OE1	1:B:510:ARG:NH2	2.53	0.41
1:D:419:ASP:HB3	1:D:447:TYR:CZ	2.55	0.41
1:E:377[A]:CYS:SG	1:E:403:LEU:HA	2.60	0.41
1:H:217:TRP:CE3	1:H:220:LYS:HG3	2.55	0.41
1:E:386:LEU:HG	1:E:388[A]:VAL:HG23	2.00	0.41
1:C:68:VAL:HG21	1:C:428:VAL:HG13	2.03	0.41
1:A:15[B]:LEU:CD2	1:A:41:ALA:CA	2.99	0.41
1:A:386:LEU:HG	1:A:388[A]:VAL:HG23	2.03	0.41
1:A:8:ARG:NH1	1:A:43:GLU:OE2	2.53	0.41
1:B:90:LEU:HD21	1:B:130:PRO:HG3	2.03	0.41
1:F:327:ILE:N	1:F:327:ILE:HD12	2.36	0.41
1:G:14:ILE:HA	1:G:152:ILE:CD1	2.50	0.41
1:E:84:ALA:HB1	1:F:87:TYR:HB3	2.03	0.41
1:A:263:ALA:HA	1:A:266:TRP:NE1	2.36	0.41
1:E:358:GLN:HG2	6:E:1340:HOH:O	2.20	0.41
1:D:312:ILE:HG13	1:D:316:LEU:HD11	2.03	0.41
1:E:197:LYS:NZ	6:E:709:HOH:O	2.26	0.41
1:A:15[B]:LEU:HD23	1:A:41:ALA:HA	2.03	0.41
1:D:403:LEU:HA	1:D:404:PRO:HD3	1.92	0.41
1:H:177:GLU:O	6:H:702:HOH:O	2.22	0.41
1:C:343:GLN:HA	1:C:344:PRO:HD3	1.96	0.40
1:C:498:GLU:HG2	1:C:499:HIS:N	2.35	0.40
1:G:386:LEU:HG	1:G:388[A]:VAL:HG23	2.01	0.40
1:C:255:GLN:HG2	1:C:407:TYR:O	2.22	0.40
1:D:21:HIS:CB	1:D:156:LEU:HD23	2.50	0.40
1:D:15[B]:LEU:CD2	1:D:41:ALA:CA	3.00	0.40
1:E:358:GLN:HG2	6:E:1244:HOH:O	2.21	0.40
1:G:83:VAL:HG13	1:G:104:THR:HG21	2.03	0.40
1:B:146[B]:ARG:NH1	1:B:146[B]:ARG:CG	2.82	0.40
1:F:538:ASN:ND2	6:F:737:HOH:O	2.55	0.40
1:G:343:GLN:HA	1:G:344:PRO:HD3	1.98	0.40
1:A:14:ILE:HG12	1:A:152:ILE:HD11	2.02	0.40
1:A:90:LEU:HD21	1:A:130:PRO:HG3	2.03	0.40
1:H:346:CYS:HB2	6:H:935:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:29:ALA:HB2	1:D:58:LEU:HD22	2.02	0.40
1:E:68:VAL:HG11	1:E:432:SER:HB3	2.04	0.40
1:H:498:GLU:OE1	1:H:510:ARG:NH2	2.55	0.40

All (4) 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)
6:F:762:HOH:O	6:G:1286:HOH:O[1_465]	2.05	0.15
6:F:1296:HOH:O	6:G:1286:HOH:O[1_465]	2.08	0.12
6:F:760:HOH:O	6:G:1286:HOH:O[1_465]	2.13	0.07
6:F:759:HOH:O	6:G:1286:HOH:O[1_465]	2.14	0.06

## 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	561/556 (101%)	550 (98%)	10 (2%)	1 (0%)	52	32
1	B	557/556 (100%)	546 (98%)	10 (2%)	1 (0%)	52	32
1	C	560/556 (101%)	549 (98%)	10 (2%)	1 (0%)	52	32
1	D	557/556 (100%)	546 (98%)	10 (2%)	1 (0%)	52	32
1	E	560/556 (101%)	548 (98%)	11 (2%)	1 (0%)	52	32
1	F	558/556 (100%)	547 (98%)	10 (2%)	1 (0%)	52	32
1	G	559/556 (100%)	548 (98%)	10 (2%)	1 (0%)	52	32
1	H	557/556 (100%)	544 (98%)	12 (2%)	1 (0%)	52	32
All	All	4469/4448 (100%)	4378 (98%)	83 (2%)	8 (0%)	52	32

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	391	SER
1	B	391	SER
1	C	391	SER
1	F	391	SER
1	G	391	SER
1	H	391	SER
1	D	391	SER
1	E	391	SER

### 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	455/452 (101%)	451 (99%)	4 (1%)	84	75
1	B	446/452 (99%)	442 (99%)	4 (1%)	84	75
1	C	450/452 (100%)	446 (99%)	4 (1%)	84	75
1	D	443/452 (98%)	439 (99%)	4 (1%)	84	75
1	E	451/452 (100%)	447 (99%)	4 (1%)	84	75
1	F	448/452 (99%)	444 (99%)	4 (1%)	84	75
1	G	450/452 (100%)	446 (99%)	4 (1%)	84	75
1	H	444/452 (98%)	440 (99%)	4 (1%)	84	75
All	All	3587/3616 (99%)	3555 (99%)	32 (1%)	84	75

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	87	TYR
1	A	325	ARG
1	A	391	SER
1	A	447	TYR
1	B	87	TYR
1	B	325	ARG
1	B	391	SER
1	B	447	TYR

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Mol	Chain	Res	Type
1	C	87	TYR
1	C	325	ARG
1	C	391	SER
1	C	447	TYR
1	D	87	TYR
1	D	325	ARG
1	D	391	SER
1	D	447	TYR
1	E	87	TYR
1	E	325	ARG
1	E	391	SER
1	E	447	TYR
1	F	87	TYR
1	F	325	ARG
1	F	391	SER
1	F	447	TYR
1	G	87	TYR
1	G	325	ARG
1	G	391	SER
1	G	447	TYR
1	H	87	TYR
1	H	325	ARG
1	H	391	SER
1	H	447	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	129	HIS
1	A	255	GLN
1	B	255	GLN
1	B	278	GLN
1	B	298	GLN
1	C	255	GLN
1	D	219	GLN
1	D	255	GLN
1	D	278	GLN
1	E	255	GLN
1	F	255	GLN
1	G	129	HIS
1	G	255	GLN
1	H	129	HIS

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Mol	Chain	Res	Type
1	H	255	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 32 ligands modelled in this entry, 8 are monoatomic - leaving 24 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$
2	TPP	A	601	3	20,27,27	1.51	3 (15%)	27,40,40	1.55	6 (22%)
4	GOL	A	603	-	5,5,5	0.36	0	5,5,5	0.43	0
5	FMT	A	604	-	2,2,2	0.57	0	1,1,1	0.35	0
5	FMT	B	601	-	2,2,2	0.65	0	1,1,1	0.54	0
2	TPP	B	602	3	20,27,27	1.50	4 (20%)	27,40,40	1.62	8 (29%)
4	GOL	B	604	-	5,5,5	0.32	0	5,5,5	0.59	0
2	TPP	C	601	3	20,27,27	1.57	3 (15%)	27,40,40	1.55	7 (25%)
4	GOL	C	603	-	5,5,5	0.41	0	5,5,5	0.40	0
5	FMT	C	604	-	2,2,2	0.72	0	1,1,1	0.58	0
5	FMT	D	601	-	2,2,2	0.72	0	1,1,1	0.62	0
2	TPP	D	602	3	20,27,27	1.52	4 (20%)	27,40,40	1.73	8 (29%)
4	GOL	D	604	-	5,5,5	0.35	0	5,5,5	0.30	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	TPP	E	601	3	20,27,27	1.53	4 (20%)	27,40,40	1.63	7 (25%)
4	GOL	E	603	-	5,5,5	0.37	0	5,5,5	0.44	0
5	FMT	E	604	-	2,2,2	0.68	0	1,1,1	0.42	0
5	FMT	F	601	-	2,2,2	0.68	0	1,1,1	0.62	0
2	TPP	F	602	3	20,27,27	1.47	2 (10%)	27,40,40	1.68	8 (29%)
4	GOL	F	604	-	5,5,5	0.31	0	5,5,5	0.51	0
2	TPP	G	601	3	20,27,27	1.56	3 (15%)	27,40,40	1.65	7 (25%)
4	GOL	G	603	-	5,5,5	0.38	0	5,5,5	0.49	0
5	FMT	G	604	-	2,2,2	0.73	0	1,1,1	0.63	0
5	FMT	H	601	-	2,2,2	0.73	0	1,1,1	0.57	0
2	TPP	H	602	3	20,27,27	1.44	3 (15%)	27,40,40	1.61	8 (29%)
4	GOL	H	604	-	5,5,5	0.34	0	5,5,5	0.28	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
2	TPP	A	601	3	-	0/16/17/17	0/2/2/2
4	GOL	A	603	-	-	0/4/4/4	0/0/0/0
5	FMT	A	604	-	-	0/0/0/0	0/0/0/0
5	FMT	B	601	-	-	0/0/0/0	0/0/0/0
2	TPP	B	602	3	-	0/16/17/17	0/2/2/2
4	GOL	B	604	-	-	0/4/4/4	0/0/0/0
2	TPP	C	601	3	-	0/16/17/17	0/2/2/2
4	GOL	C	603	-	-	0/4/4/4	0/0/0/0
5	FMT	C	604	-	-	0/0/0/0	0/0/0/0
5	FMT	D	601	-	-	0/0/0/0	0/0/0/0
2	TPP	D	602	3	-	0/16/17/17	0/2/2/2
4	GOL	D	604	-	-	0/4/4/4	0/0/0/0
2	TPP	E	601	3	-	0/16/17/17	0/2/2/2
4	GOL	E	603	-	-	0/4/4/4	0/0/0/0
5	FMT	E	604	-	-	0/0/0/0	0/0/0/0
5	FMT	F	601	-	-	0/0/0/0	0/0/0/0
2	TPP	F	602	3	-	0/16/17/17	0/2/2/2
4	GOL	F	604	-	-	0/4/4/4	0/0/0/0
2	TPP	G	601	3	-	0/16/17/17	0/2/2/2
4	GOL	G	603	-	-	0/4/4/4	0/0/0/0
5	FMT	G	604	-	-	0/0/0/0	0/0/0/0
5	FMT	H	601	-	-	0/0/0/0	0/0/0/0
2	TPP	H	602	3	-	0/16/17/17	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	H	604	-	-	0/4/4/4	0/0/0/0

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	TPP	C4-N3	-4.65	1.35	1.39
2	A	601	TPP	C4-N3	-4.62	1.35	1.39
2	E	601	TPP	C4-N3	-4.29	1.36	1.39
2	D	602	TPP	C4-N3	-4.16	1.36	1.39
2	G	601	TPP	C4-N3	-4.10	1.36	1.39
2	F	602	TPP	C4-N3	-4.03	1.36	1.39
2	B	602	TPP	C4-N3	-3.99	1.36	1.39
2	H	602	TPP	C4-N3	-3.88	1.36	1.39
2	D	602	TPP	C5'-C4'	-2.09	1.39	1.42
2	A	601	TPP	C6'-N1'	2.00	1.38	1.34
2	E	601	TPP	C6'-N1'	2.03	1.38	1.34
2	D	602	TPP	C4'-N3'	2.05	1.38	1.35
2	B	602	TPP	C6'-N1'	2.07	1.38	1.34
2	C	601	TPP	C4'-N3'	2.10	1.38	1.35
2	H	602	TPP	C2'-N1'	2.13	1.38	1.34
2	E	601	TPP	C2'-N3'	2.14	1.38	1.34
2	G	601	TPP	C6'-N1'	2.15	1.38	1.34
2	H	602	TPP	C2'-N3'	2.16	1.38	1.34
2	D	602	TPP	C2'-N3'	2.18	1.38	1.34
2	B	602	TPP	C4'-N3'	2.19	1.38	1.35
2	F	602	TPP	C2'-N1'	2.37	1.38	1.34
2	B	602	TPP	C2'-N1'	2.45	1.38	1.34
2	C	601	TPP	C2'-N1'	2.57	1.38	1.34
2	E	601	TPP	C2'-N1'	2.62	1.38	1.34
2	A	601	TPP	C2'-N1'	2.62	1.38	1.34
2	G	601	TPP	C2'-N1'	2.73	1.39	1.34

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	602	TPP	N1'-C2'-N3'	-3.48	118.97	125.50
2	H	602	TPP	N1'-C2'-N3'	-3.23	119.44	125.50
2	G	601	TPP	N1'-C2'-N3'	-3.23	119.45	125.50
2	A	601	TPP	N1'-C2'-N3'	-3.15	119.59	125.50
2	E	601	TPP	C6-C5-S1	-3.10	115.90	120.24
2	B	602	TPP	N1'-C2'-N3'	-3.09	119.70	125.50
2	E	601	TPP	N1'-C2'-N3'	-3.00	119.88	125.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	TPP	N1'-C2'-N3'	-2.96	119.95	125.50
2	F	602	TPP	N1'-C2'-N3'	-2.91	120.03	125.50
2	A	601	TPP	C6-C5-S1	-2.85	116.25	120.24
2	C	601	TPP	CM4-C4-C5	-2.58	123.45	128.91
2	D	602	TPP	CM4-C4-C5	-2.57	123.47	128.91
2	C	601	TPP	C5'-C6'-N1'	-2.52	119.46	123.86
2	B	602	TPP	CM4-C4-C5	-2.51	123.59	128.91
2	G	601	TPP	CM4-C4-C5	-2.45	123.73	128.91
2	F	602	TPP	CM4-C4-C5	-2.41	123.81	128.91
2	H	602	TPP	C6-C5-S1	-2.35	116.95	120.24
2	D	602	TPP	C6-C5-S1	-2.28	117.04	120.24
2	E	601	TPP	CM4-C4-C5	-2.23	124.19	128.91
2	B	602	TPP	C6-C5-S1	-2.23	117.12	120.24
2	F	602	TPP	C6-C5-S1	-2.15	117.23	120.24
2	G	601	TPP	C6-C5-S1	-2.14	117.25	120.24
2	H	602	TPP	C5'-C6'-N1'	-2.06	120.26	123.86
2	D	602	TPP	C5'-C6'-N1'	-2.01	120.35	123.86
2	F	602	TPP	C6'-N1'-C2'	2.00	119.72	115.92
2	D	602	TPP	O2A-PA-O3A	2.00	113.84	105.27
2	G	601	TPP	C6-C5-C4	2.03	129.62	127.34
2	H	602	TPP	C6'-C5'-C4'	2.04	118.53	115.65
2	A	601	TPP	C6'-N1'-C2'	2.08	119.88	115.92
2	B	602	TPP	C6'-C5'-C4'	2.11	118.63	115.65
2	H	602	TPP	CM4-C4-N3	2.14	125.06	122.43
2	H	602	TPP	C6-C5-C4	2.17	129.77	127.34
2	G	601	TPP	C6'-C5'-C4'	2.18	118.72	115.65
2	A	601	TPP	CM4-C4-N3	2.22	125.15	122.43
2	B	602	TPP	C6-C5-C4	2.23	129.84	127.34
2	B	602	TPP	C6'-N1'-C2'	2.25	120.19	115.92
2	E	601	TPP	O2A-PA-O3A	2.26	114.96	105.27
2	A	601	TPP	C6-C5-C4	2.29	129.91	127.34
2	F	602	TPP	O2A-PA-O3A	2.38	115.46	105.27
2	C	601	TPP	C6'-C5'-C4'	2.39	119.03	115.65
2	E	601	TPP	C6-C5-C4	2.46	130.10	127.34
2	H	602	TPP	C6'-N1'-C2'	2.51	120.68	115.92
2	F	602	TPP	C6'-C5'-C4'	2.51	119.19	115.65
2	B	602	TPP	CM4-C4-N3	2.57	125.58	122.43
2	C	601	TPP	C6'-N1'-C2'	2.57	120.81	115.92
2	D	602	TPP	C6'-N1'-C2'	2.62	120.90	115.92
2	E	601	TPP	CM4-C4-N3	2.63	125.66	122.43
2	G	601	TPP	CM4-C4-N3	2.66	125.69	122.43
2	F	602	TPP	CM4-C4-N3	2.84	125.91	122.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	TPP	CM4-C4-N3	2.97	126.07	122.43
2	D	602	TPP	CM4-C4-N3	3.12	126.26	122.43
2	E	601	TPP	CM2-C2'-N1'	3.57	121.46	117.05
2	C	601	TPP	CM2-C2'-N1'	3.59	121.47	117.05
2	A	601	TPP	CM2-C2'-N1'	3.59	121.48	117.05
2	D	602	TPP	CM2-C2'-N1'	3.94	121.91	117.05
2	B	602	TPP	CM2-C2'-N1'	3.94	121.91	117.05
2	F	602	TPP	CM2-C2'-N1'	3.97	121.94	117.05
2	G	601	TPP	CM2-C2'-N1'	4.14	122.16	117.05
2	H	602	TPP	CM2-C2'-N1'	4.33	122.39	117.05

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	604	FMT	1	0
2	B	602	TPP	1	0
2	C	601	TPP	2	0
2	D	602	TPP	1	0
2	E	601	TPP	1	0
5	E	604	FMT	2	0
2	F	602	TPP	1	0
5	G	604	FMT	1	0
2	H	602	TPP	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	556/556 (100%)	-0.31	7 (1%) 79 83	9, 14, 27, 44	0
1	B	556/556 (100%)	-0.28	5 (0%) 85 89	9, 15, 26, 43	0
1	C	556/556 (100%)	-0.28	6 (1%) 82 86	10, 15, 28, 43	0
1	D	556/556 (100%)	-0.14	11 (1%) 68 73	10, 18, 34, 57	0
1	E	556/556 (100%)	-0.25	6 (1%) 82 86	9, 14, 28, 47	0
1	F	556/556 (100%)	-0.24	7 (1%) 79 83	9, 15, 25, 43	0
1	G	556/556 (100%)	-0.27	5 (0%) 85 89	10, 15, 28, 43	0
1	H	556/556 (100%)	-0.21	5 (0%) 85 89	10, 17, 31, 45	0
All	All	4448/4448 (100%)	-0.25	52 (1%) 81 85	9, 15, 29, 57	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	347	VAL	5.1
1	E	556	LEU	4.5
1	E	176	GLY	4.0
1	D	556	LEU	3.9
1	F	1	MET	3.8
1	A	1	MET	3.7
1	B	176	GLY	3.6
1	B	180	ASP	3.5
1	D	555	HIS	3.3
1	C	1	MET	3.2
1	A	556	LEU	3.1
1	C	178	MET	3.1
1	F	176	GLY	3.0
1	A	178	MET	3.0
1	D	347	VAL	3.0
1	D	1	MET	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	1	MET	2.9
1	G	178	MET	2.9
1	F	555	HIS	2.9
1	E	1	MET	2.9
1	C	522	ALA	2.8
1	D	178	MET	2.8
1	E	177	GLU	2.8
1	A	180	ASP	2.8
1	H	556	LEU	2.8
1	F	178	MET	2.8
1	H	555	HIS	2.8
1	E	178	MET	2.7
1	G	556	LEU	2.6
1	F	556	LEU	2.6
1	A	177	GLU	2.5
1	F	180	ASP	2.5
1	E	555	HIS	2.5
1	H	178	MET	2.5
1	B	555	HIS	2.4
1	D	519	THR	2.4
1	D	522	ALA	2.4
1	G	176	GLY	2.4
1	F	177	GLU	2.3
1	B	1	MET	2.3
1	C	180	ASP	2.3
1	D	219	GLN	2.2
1	C	176	GLY	2.2
1	B	482	GLN	2.2
1	D	340	GLU	2.2
1	D	176	GLY	2.2
1	H	277	GLN	2.1
1	D	177	GLU	2.1
1	A	179	ASP	2.1
1	C	177	GLU	2.0
1	A	270	ALA	2.0
1	G	555	HIS	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	A	603	6/6	0.96	0.11	2.35	16,23,28,28	0
4	GOL	F	604	6/6	0.96	0.09	1.89	15,23,29,29	0
5	FMT	G	604	3/3	0.98	0.10	1.76	21,22,26,30	0
4	GOL	C	603	6/6	0.94	0.11	1.71	18,29,34,35	0
5	FMT	H	601	3/3	0.96	0.08	1.04	20,22,26,27	0
4	GOL	E	603	6/6	0.97	0.10	0.86	12,22,28,28	0
5	FMT	F	601	3/3	0.98	0.09	0.77	20,22,26,27	0
4	GOL	H	604	6/6	0.95	0.08	0.62	17,28,34,34	0
3	MN	C	602	1/1	1.00	0.07	0.34	20,20,20,20	0
5	FMT	A	604	3/3	0.95	0.10	0.30	20,21,24,25	0
4	GOL	G	603	6/6	0.96	0.09	0.13	16,28,35,35	0
4	GOL	D	604	6/6	0.95	0.08	-0.15	20,29,35,37	0
2	TPP	D	602	26/26	0.97	0.07	-0.27	12,17,22,25	0
5	FMT	E	604	3/3	0.97	0.09	-0.27	17,20,24,25	0
2	TPP	A	601	26/26	0.98	0.07	-0.54	9,15,22,30	0
2	TPP	F	602	26/26	0.98	0.07	-0.70	10,16,21,25	0
2	TPP	G	601	26/26	0.98	0.06	-0.74	8,15,21,23	0
4	GOL	B	604	6/6	0.96	0.07	-0.85	17,23,28,28	0
2	TPP	H	602	26/26	0.98	0.07	-0.85	10,16,22,22	0
2	TPP	B	602	26/26	0.98	0.07	-0.96	10,15,23,28	0
3	MN	G	602	1/1	1.00	0.05	-0.96	20,20,20,20	0
5	FMT	B	601	3/3	0.98	0.06	-1.04	19,19,23,25	0
2	TPP	C	601	26/26	0.98	0.06	-1.13	10,14,21,25	0
2	TPP	E	601	26/26	0.99	0.06	-1.20	9,14,19,27	0
5	FMT	C	604	3/3	0.98	0.06	-1.24	18,19,22,25	0
5	FMT	D	601	3/3	0.99	0.06	-1.74	20,21,24,25	0
3	MN	H	603	1/1	0.99	0.06	-1.83	21,21,21,21	0
3	MN	A	602	1/1	1.00	0.05	-2.29	19,19,19,19	0
3	MN	F	603	1/1	0.99	0.04	-2.45	20,20,20,20	0
3	MN	B	603	1/1	1.00	0.03	-2.64	20,20,20,20	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MN	D	603	1/1	0.99	0.05	-2.68	22,22,22,22	0
3	MN	E	602	1/1	1.00	0.05	-2.74	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.