



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:14 PM GMT

PDB ID : 3T88
Title : Crystal structure of Escherichia coli MenB in complex with substrate analogue, OSB-NCoA
Authors : Li, H-J.; Li, X.; Liu, N.; Zhang, H.; Truglio, J.; Mishra, S.; Kisker, C.; Garcia-Diaz, M.; Tonge, P.
Deposited on : 2011-08-01
Resolution : 2.00 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

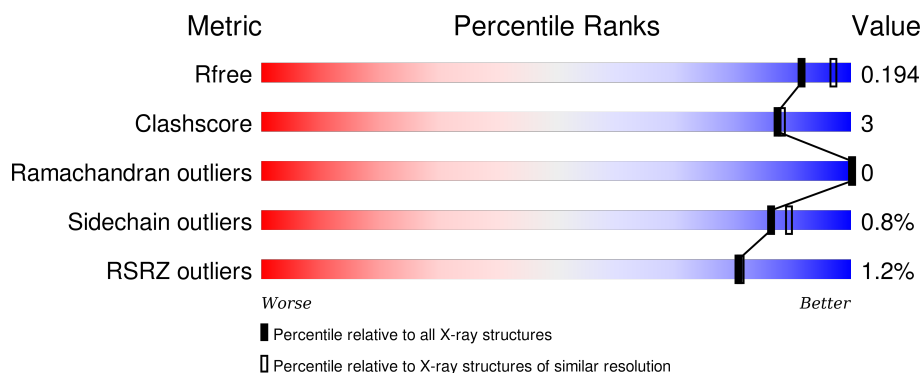
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 ≥ 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	289	<div> <div>2%</div> <div>92%</div> <div>5%</div> <div>.</div> </div>
1	B	289	<div> <div>2%</div> <div>94%</div> <div>.</div> <div>.</div> </div>
1	C	289	<div> <div>%</div> <div>94%</div> <div>.</div> <div>.</div> </div>
1	D	289	<div> <div>%</div> <div>90%</div> <div>8%</div> <div>.</div> </div>
1	E	289	<div> <div>%</div> <div>91%</div> <div>6%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	289	 % 91% 6%

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
3	CL	C	501	-	-	-	X
3	CL	D	601	-	-	-	X
4	PGE	A	302	-	-	-	X
4	PGE	B	402	-	-	-	X
4	PGE	C	502	-	-	-	X
4	PGE	D	602	-	-	-	X
4	PGE	E	702	-	-	-	X
5	GOL	A	303	-	-	-	X
5	GOL	B	403	-	-	-	X
5	GOL	C	503	-	-	-	X
5	GOL	D	603	-	-	-	X
5	GOL	E	703	-	-	-	X
5	GOL	F	803	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14295 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 1,4-Dihydroxy-2-naphthoyl-CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	1	0
			2171	1357	389	406	19			
1	B	281	Total	C	N	O	S	0	2	0
			2167	1356	388	404	19			
1	C	281	Total	C	N	O	S	0	3	0
			2174	1362	389	404	19			
1	D	281	Total	C	N	O	S	0	3	0
			2175	1365	390	401	19			
1	E	281	Total	C	N	O	S	0	1	0
			2157	1350	386	402	19			
1	F	281	Total	C	N	O	S	0	2	0
			2160	1354	386	401	19			

There are 24 discrepancies between the modelled and reference sequences:

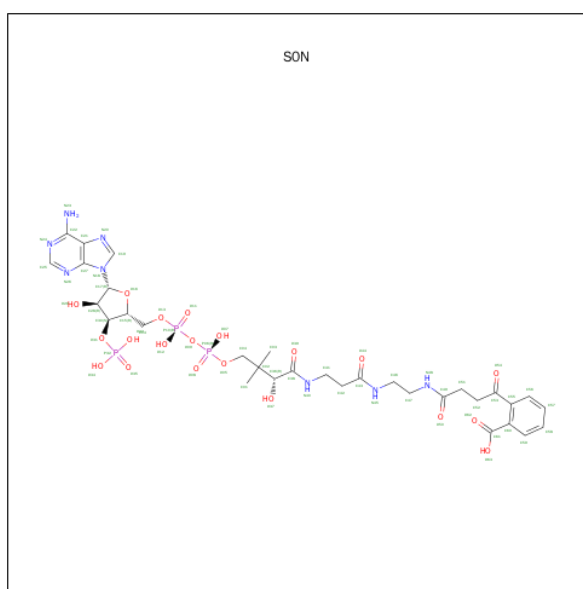
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	EXPRESSION TAG	UNP P0ABU0
A	-2	SER	-	EXPRESSION TAG	UNP P0ABU0
A	-1	HIS	-	EXPRESSION TAG	UNP P0ABU0
A	0	MET	-	EXPRESSION TAG	UNP P0ABU0
B	-3	GLY	-	EXPRESSION TAG	UNP P0ABU0
B	-2	SER	-	EXPRESSION TAG	UNP P0ABU0
B	-1	HIS	-	EXPRESSION TAG	UNP P0ABU0
B	0	MET	-	EXPRESSION TAG	UNP P0ABU0
C	-3	GLY	-	EXPRESSION TAG	UNP P0ABU0
C	-2	SER	-	EXPRESSION TAG	UNP P0ABU0
C	-1	HIS	-	EXPRESSION TAG	UNP P0ABU0
C	0	MET	-	EXPRESSION TAG	UNP P0ABU0
D	-3	GLY	-	EXPRESSION TAG	UNP P0ABU0
D	-2	SER	-	EXPRESSION TAG	UNP P0ABU0
D	-1	HIS	-	EXPRESSION TAG	UNP P0ABU0
D	0	MET	-	EXPRESSION TAG	UNP P0ABU0
E	-3	GLY	-	EXPRESSION TAG	UNP P0ABU0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-2	SER	-	EXPRESSION TAG	UNP P0ABU0
E	-1	HIS	-	EXPRESSION TAG	UNP P0ABU0
E	0	MET	-	EXPRESSION TAG	UNP P0ABU0
F	-3	GLY	-	EXPRESSION TAG	UNP P0ABU0
F	-2	SER	-	EXPRESSION TAG	UNP P0ABU0
F	-1	HIS	-	EXPRESSION TAG	UNP P0ABU0
F	0	MET	-	EXPRESSION TAG	UNP P0ABU0

- Molecule 2 is O-SUCCINYLBENZOYL-N-COENZYME A (three-letter code: SON) (formula: $C_{32}H_{45}N_8O_{20}P_3$).

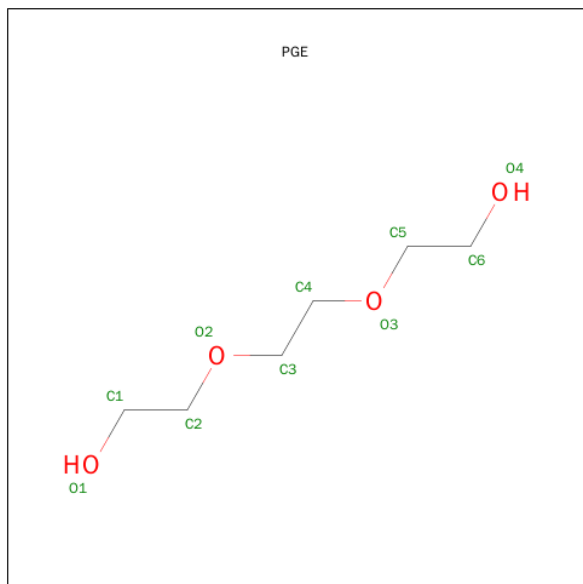


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			63	32	8	20	3		
2	B	1	Total	C	N	O	P	0	0
			63	32	8	20	3		
2	C	1	Total	C	N	O	P	0	0
			63	32	8	20	3		
2	D	1	Total	C	N	O	P	0	0
			63	32	8	20	3		
2	E	1	Total	C	N	O	P	0	0
			63	32	8	20	3		
2	F	1	Total	C	N	O	P	0	0
			63	32	8	20	3		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 6 4	0	0
4	B	1	Total C O 10 6 4	0	0
4	C	1	Total C O 10 6 4	0	0
4	D	1	Total C O 10 6 4	0	0
4	E	1	Total C O 10 6 4	0	0
4	F	1	Total C O 10 6 4	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	135	Total	O	0	0
			135	135		
6	B	137	Total	O	0	0
			137	137		
6	C	133	Total	O	0	0
			133	133		
6	D	150	Total	O	0	0
			150	150		
6	E	130	Total	O	0	0
			130	130		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	126	Total 126	O 126	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 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: 1,4-Dihydroxy-2-naphthoyl-CoA synthase



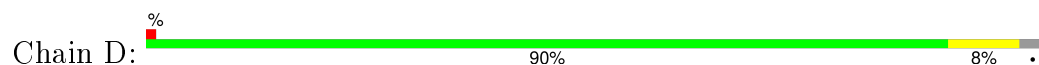
- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase



- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase



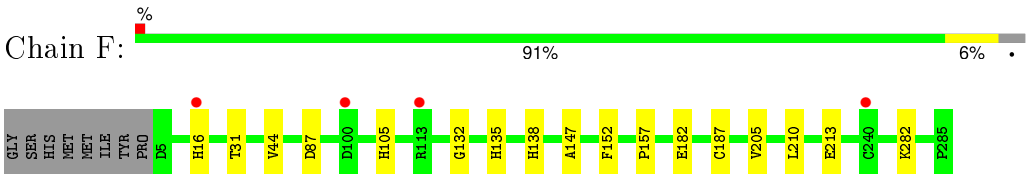
- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase



- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase



- Molecule 1: 1,4-Dihydroxy-2-naphthoyl-CoA synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	140.49Å 141.79Å 89.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.80 – 2.00 44.80 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.80-2.00) 99.6 (44.80-2.00)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.155 , 0.195 0.156 , 0.194	Depositor DCC
R_{free} test set	6053 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	21.4	Xtriage
Anisotropy	0.446	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 50.1	EDS
Estimated twinning fraction	0.014 for k,h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 120514 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	14295	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PGE, S0N, CL

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	0.36	0/2216	0.50	0/2988
1	B	0.36	0/2215	0.53	0/2988
1	C	0.36	0/2225	0.52	0/3001
1	D	0.37	0/2226	0.54	0/3002
1	E	0.35	0/2202	0.51	0/2970
1	F	0.34	0/2208	0.50	0/2980
All	All	0.36	0/13292	0.52	0/17929

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	2171	0	2108	11	0
1	B	2167	0	2104	6	0
1	C	2174	0	2122	6	0
1	D	2175	0	2120	15	0
1	E	2157	0	2087	11	0
1	F	2160	0	2088	10	0
2	A	63	0	40	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	63	0	40	2	0
2	C	63	0	40	2	0
2	D	63	0	40	4	0
2	E	63	0	40	3	0
2	F	63	0	40	3	0
3	A	1	0	0	1	0
3	B	1	0	0	1	0
3	C	1	0	0	1	0
3	D	1	0	0	1	0
3	E	1	0	0	1	0
3	F	1	0	0	1	0
4	A	10	0	14	3	0
4	B	10	0	14	1	0
4	C	10	0	14	0	0
4	D	10	0	14	0	0
4	E	10	0	14	0	0
4	F	10	0	14	1	0
5	A	6	0	8	1	0
5	B	6	0	8	0	0
5	C	6	0	8	0	0
5	D	6	0	8	0	0
5	E	6	0	8	0	0
5	F	6	0	8	0	0
6	A	135	0	0	0	0
6	B	137	0	0	1	0
6	C	133	0	0	1	0
6	D	150	0	0	0	0
6	E	130	0	0	1	0
6	F	126	0	0	0	0
All	All	14295	0	13001	68	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 3.

All (68) 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:F:205:VAL:HG11	1:F:213:GLU:HG3	1.66	0.76
5:A:303:GOL:H31	1:C:188:ARG:HH22	1.63	0.64
1:A:54:LYS:HD2	4:A:302:PGE:H4	1.81	0.62
2:E:700:S0N:O62	2:E:700:S0N:H51	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:GLY:HA3	2:D:600:S0N:H47A	1.83	0.61
1:D:132:GLY:HA2	3:D:601:CL:CL	2.39	0.60
2:A:300:S0N:O62	2:A:300:S0N:H51	2.02	0.59
1:D:89:LYS:HE2	2:D:600:S0N:N26	2.18	0.57
1:A:132:GLY:HA2	3:A:301:CL:CL	2.41	0.57
1:A:54:LYS:HD2	4:A:302:PGE:H52	1.87	0.56
1:D:157:PRO:HD2	1:D:187:CYS:SG	2.46	0.56
1:F:157:PRO:HD2	1:F:187:CYS:SG	2.46	0.56
2:B:400:S0N:O63	2:B:400:S0N:H51	2.06	0.55
1:E:157:PRO:HD2	1:E:187:CYS:SG	2.48	0.53
1:D:256:LEU:HA	1:D:259:MET:HE2	1.91	0.53
1:E:132:GLY:HA2	3:E:701:CL:CL	2.45	0.53
1:B:109:LEU:O	1:B:113[B]:ARG:HG3	2.09	0.53
1:F:132:GLY:HA2	3:F:801:CL:CL	2.46	0.52
1:C:132:GLY:HA2	3:C:501:CL:CL	2.47	0.52
2:F:800:S0N:O62	2:F:800:S0N:H51	2.10	0.52
1:A:89:LYS:HE2	2:A:300:S0N:N26	2.24	0.52
1:B:54:LYS:HD2	4:B:402:PGE:H42	1.92	0.52
1:E:276:PRO:HG3	6:E:378:HOH:O	2.10	0.51
1:A:10:TYR:CD1	1:A:212:LYS:HE2	2.45	0.51
1:E:219:ARG:O	1:E:223:GLN:HG2	2.11	0.51
2:C:500:S0N:H52A	2:C:500:S0N:C61	2.40	0.51
1:B:267:ARG:HD3	6:B:1256:HOH:O	2.09	0.51
1:D:155:THR:OG1	2:D:600:S0N:H47	2.11	0.51
2:C:500:S0N:H51	2:C:500:S0N:O63	2.12	0.50
1:B:132:GLY:HA2	3:B:401:CL:CL	2.49	0.48
1:A:105:HIS:CE1	4:A:302:PGE:H3	2.47	0.48
1:A:262:GLU:OE1	1:D:226:PRO:HD2	2.14	0.48
1:F:105:HIS:CE1	4:F:802:PGE:H4	2.50	0.47
1:D:179:LYS:HA	1:D:179:LYS:HD2	1.65	0.46
1:B:132:GLY:HA3	2:B:400:S0N:H47A	1.98	0.46
1:E:16:HIS:NE2	1:E:31:THR:HG22	2.31	0.45
1:A:157:PRO:HD2	1:A:187:CYS:SG	2.56	0.45
1:A:219:ARG:O	1:A:223:GLN:HG2	2.17	0.45
1:E:205:VAL:HG11	1:E:213:GLU:HG3	1.98	0.45
1:F:147:ALA:HB2	1:F:210:LEU:HD22	1.97	0.45
2:F:800:S0N:C51	2:F:800:S0N:O62	2.65	0.45
1:C:54:LYS:O	1:C:58:GLN:HG3	2.17	0.44
2:E:700:S0N:O62	2:E:700:S0N:C51	2.64	0.44
1:F:135:HIS:CD2	1:F:152:PHE:HB3	2.52	0.44
1:F:87:ASP:HA	2:F:800:S0N:N24	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:157:PRO:HD2	1:C:187:CYS:SG	2.58	0.44
1:E:202:ASN:ND2	1:F:182:GLU:HB2	2.33	0.43
2:D:600:S0N:H51	2:D:600:S0N:O62	2.17	0.43
1:C:8:MET:HE2	6:C:1549:HOH:O	2.17	0.43
1:A:277:ASP:O	1:A:280:LYS:HD3	2.18	0.43
1:D:205:VAL:HG11	1:D:213:GLU:HG3	2.01	0.43
1:D:256:LEU:HD23	1:D:259:MET:CE	2.48	0.42
1:E:40:ASN:C	1:E:42:PRO:HD3	2.40	0.42
1:B:219:ARG:O	1:B:223:GLN:HG2	2.19	0.42
1:C:93:ASP:OD1	1:D:267:ARG:NH2	2.32	0.42
2:A:300:S0N:H52A	2:A:300:S0N:C61	2.49	0.42
1:D:26[B]:ARG:HB2	1:D:38:THR:HB	2.00	0.42
1:D:219:ARG:O	1:D:223:GLN:HG2	2.20	0.42
1:A:135:HIS:NE2	1:A:200:LEU:HD21	2.36	0.41
1:E:10:TYR:CD1	1:E:212:LYS:HE2	2.55	0.41
2:A:300:S0N:O62	2:A:300:S0N:C51	2.67	0.41
2:A:300:S0N:C52	2:A:300:S0N:C61	2.99	0.41
1:F:16:HIS:CE1	1:F:31:THR:CG2	3.03	0.41
1:F:282:LYS:HB2	1:F:282:LYS:HE2	1.81	0.41
1:D:9:LEU:HB3	1:D:216:ARG:HG3	2.02	0.40
1:D:136:VAL:O	1:D:140:MET:HG2	2.22	0.40
1:E:44:VAL:HA	2:E:700:S0N:O16	2.21	0.40
1:E:41:ARG:N	1:E:42:PRO:HD3	2.37	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	280/289 (97%)	276 (99%)	4 (1%)	0	100	100
1	B	281/289 (97%)	277 (99%)	4 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	282/289 (98%)	278 (99%)	4 (1%)	0	100	100
1	D	282/289 (98%)	278 (99%)	4 (1%)	0	100	100
1	E	280/289 (97%)	274 (98%)	6 (2%)	0	100	100
1	F	281/289 (97%)	276 (98%)	5 (2%)	0	100	100
All	All	1686/1734 (97%)	1659 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	221/232 (95%)	219 (99%)	2 (1%)	84	88
1	B	220/232 (95%)	218 (99%)	2 (1%)	84	88
1	C	222/232 (96%)	221 (100%)	1 (0%)	92	94
1	D	219/232 (94%)	217 (99%)	2 (1%)	84	88
1	E	218/232 (94%)	216 (99%)	2 (1%)	84	88
1	F	217/232 (94%)	215 (99%)	2 (1%)	84	88
All	All	1317/1392 (95%)	1306 (99%)	11 (1%)	86	89

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	HIS
1	A	280	LYS
1	B	31	THR
1	B	138	HIS
1	C	138	HIS
1	D	138	HIS
1	D	280	LYS
1	E	31	THR
1	E	138	HIS

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Mol	Chain	Res	Type
1	F	44	VAL
1	F	138	HIS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	GLN
1	C	223	GLN
1	F	16	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 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	S0N	A	300	-	53,66,66	2.44	14 (26%)	68,97,97	2.40	12 (17%)
4	PGE	A	302	-	9,9,9	0.42	0	8,8,8	0.40	0
5	GOL	A	303	-	5,5,5	0.23	0	5,5,5	0.56	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	S0N	B	400	-	53,66,66	2.20	14 (26%)	68,97,97	2.29	18 (26%)
4	PGE	B	402	-	9,9,9	0.43	0	8,8,8	0.30	0
5	GOL	B	403	-	5,5,5	0.35	0	5,5,5	0.27	0
2	S0N	C	500	-	53,66,66	2.32	15 (28%)	68,97,97	2.49	10 (14%)
4	PGE	C	502	-	9,9,9	0.45	0	8,8,8	0.25	0
5	GOL	C	503	-	5,5,5	0.25	0	5,5,5	0.30	0
2	S0N	D	600	-	53,66,66	2.37	13 (24%)	68,97,97	2.36	11 (16%)
4	PGE	D	602	-	9,9,9	0.45	0	8,8,8	0.32	0
5	GOL	D	603	-	5,5,5	0.29	0	5,5,5	0.28	0
2	S0N	E	700	-	53,66,66	2.23	14 (26%)	68,97,97	2.26	9 (13%)
4	PGE	E	702	-	9,9,9	0.45	0	8,8,8	0.46	0
5	GOL	E	703	-	5,5,5	0.20	0	5,5,5	0.46	0
2	S0N	F	800	-	53,66,66	2.25	13 (24%)	68,97,97	2.34	11 (16%)
4	PGE	F	802	-	9,9,9	0.48	0	8,8,8	0.35	0
5	GOL	F	803	-	5,5,5	0.22	0	5,5,5	0.52	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	S0N	A	300	-	-	0/56/80/80	0/4/4/4
4	PGE	A	302	-	-	0/7/7/7	0/0/0/0
5	GOL	A	303	-	-	0/4/4/4	0/0/0/0
2	S0N	B	400	-	-	0/56/80/80	0/4/4/4
4	PGE	B	402	-	-	0/7/7/7	0/0/0/0
5	GOL	B	403	-	-	0/4/4/4	0/0/0/0
2	S0N	C	500	-	-	0/56/80/80	0/4/4/4
4	PGE	C	502	-	-	0/7/7/7	0/0/0/0
5	GOL	C	503	-	-	0/4/4/4	0/0/0/0
2	S0N	D	600	-	-	0/56/80/80	0/4/4/4
4	PGE	D	602	-	-	0/7/7/7	0/0/0/0
5	GOL	D	603	-	-	0/4/4/4	0/0/0/0
2	S0N	E	700	-	-	0/56/80/80	0/4/4/4
4	PGE	E	702	-	-	0/7/7/7	0/0/0/0
5	GOL	E	703	-	-	0/4/4/4	0/0/0/0
2	S0N	F	800	-	-	0/56/80/80	0/4/4/4
4	PGE	F	802	-	-	0/7/7/7	0/0/0/0
5	GOL	F	803	-	-	0/4/4/4	0/0/0/0

All (83) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	S0N	O39-C38	-2.62	1.18	1.23
2	B	400	S0N	O39-C38	-2.36	1.18	1.23
2	A	300	S0N	O39-C38	-2.27	1.19	1.23
2	C	500	S0N	O39-C38	-2.20	1.19	1.23
2	F	800	S0N	O39-C38	-2.10	1.19	1.23
2	E	700	S0N	O39-C38	-2.05	1.19	1.23
2	C	500	S0N	C56-C55	2.01	1.43	1.39
2	F	800	S0N	O29-C28	2.04	1.47	1.43
2	C	500	S0N	C58-C59	2.08	1.43	1.38
2	E	700	S0N	C58-C59	2.16	1.43	1.38
2	A	300	S0N	O29-C28	2.21	1.48	1.43
2	B	400	S0N	C55-C53	2.36	1.53	1.48
2	A	300	S0N	C41-C42	2.51	1.59	1.51
2	B	400	S0N	C51-C49	2.54	1.56	1.51
2	B	400	S0N	C42-C43	2.66	1.56	1.51
2	E	700	S0N	C52-C51	2.66	1.59	1.52
2	C	500	S0N	C42-C43	2.71	1.56	1.51
2	A	300	S0N	C55-C53	2.72	1.54	1.48
2	B	400	S0N	C57-C58	2.77	1.45	1.38
2	D	600	S0N	C57-C58	2.77	1.45	1.38
2	E	700	S0N	C57-C58	2.84	1.45	1.38
2	F	800	S0N	C55-C60	2.85	1.45	1.40
2	D	600	S0N	C55-C53	2.85	1.54	1.48
2	E	700	S0N	C19-N20	2.86	1.40	1.34
2	F	800	S0N	C57-C58	2.89	1.45	1.38
2	D	600	S0N	C51-C49	2.91	1.57	1.51
2	C	500	S0N	C55-C60	2.93	1.45	1.40
2	C	500	S0N	C57-C58	2.95	1.45	1.38
2	A	300	S0N	C57-C58	2.96	1.45	1.38
2	E	700	S0N	C42-C43	3.03	1.57	1.51
2	D	600	S0N	C19-N20	3.12	1.40	1.34
2	D	600	S0N	C55-C60	3.15	1.46	1.40
2	C	500	S0N	C19-N20	3.17	1.40	1.34
2	F	800	S0N	C19-N20	3.18	1.40	1.34
2	C	500	S0N	C51-C49	3.19	1.57	1.51
2	A	300	S0N	C19-N20	3.20	1.40	1.34
2	B	400	S0N	C19-N20	3.21	1.40	1.34
2	A	300	S0N	C55-C60	3.21	1.46	1.40
2	F	800	S0N	C55-C53	3.26	1.55	1.48
2	E	700	S0N	C55-C60	3.28	1.46	1.40
2	B	400	S0N	C55-C60	3.47	1.46	1.40
2	D	600	S0N	C22-N23	3.54	1.45	1.34
2	C	500	S0N	C22-N23	3.61	1.46	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	300	S0N	C22-N23	3.69	1.46	1.34
2	B	400	S0N	C22-N23	3.72	1.46	1.34
2	F	800	S0N	C22-N23	3.74	1.46	1.34
2	E	700	S0N	C22-N23	3.83	1.46	1.34
2	C	500	S0N	C52-C53	3.87	1.57	1.51
2	E	700	S0N	C52-C53	3.88	1.57	1.51
2	B	400	S0N	C38-N40	3.92	1.41	1.33
2	E	700	S0N	C43-N45	4.03	1.43	1.33
2	B	400	S0N	C52-C53	4.13	1.57	1.51
2	F	800	S0N	C38-N40	4.29	1.42	1.33
2	A	300	S0N	C52-C53	4.31	1.57	1.51
2	B	400	S0N	C49-N48	4.37	1.43	1.33
2	F	800	S0N	C52-C53	4.40	1.58	1.51
2	E	700	S0N	C49-N48	4.68	1.44	1.33
2	D	600	S0N	C52-C53	4.76	1.58	1.51
2	D	600	S0N	O16-C17	4.82	1.47	1.41
2	D	600	S0N	C49-N48	4.82	1.44	1.33
2	B	400	S0N	O16-C17	4.93	1.47	1.41
2	F	800	S0N	C43-N45	5.15	1.45	1.33
2	F	800	S0N	O16-C17	5.17	1.47	1.41
2	C	500	S0N	O16-C17	5.19	1.47	1.41
2	A	300	S0N	O16-C17	5.29	1.47	1.41
2	C	500	S0N	C49-N48	5.39	1.46	1.33
2	E	700	S0N	O16-C17	5.45	1.48	1.41
2	C	500	S0N	C43-N45	5.60	1.46	1.33
2	F	800	S0N	C49-N48	5.65	1.46	1.33
2	B	400	S0N	C43-N45	5.83	1.47	1.33
2	D	600	S0N	C25-N26	5.92	1.42	1.32
2	C	500	S0N	C25-N26	5.94	1.42	1.32
2	B	400	S0N	C25-N26	5.94	1.42	1.32
2	C	500	S0N	C38-N40	5.96	1.46	1.33
2	A	300	S0N	C38-N40	5.97	1.46	1.33
2	E	700	S0N	C38-N40	6.00	1.46	1.33
2	E	700	S0N	C25-N26	6.04	1.42	1.32
2	F	800	S0N	C25-N26	6.06	1.42	1.32
2	A	300	S0N	C25-N26	6.10	1.43	1.32
2	D	600	S0N	C43-N45	6.33	1.48	1.33
2	A	300	S0N	C43-N45	6.42	1.48	1.33
2	A	300	S0N	C49-N48	6.54	1.49	1.33
2	D	600	S0N	C38-N40	6.89	1.48	1.33

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	600	S0N	N26-C25-N24	-12.45	119.36	128.89
2	C	500	S0N	N26-C25-N24	-12.32	119.46	128.89
2	F	800	S0N	N26-C25-N24	-11.77	119.88	128.89
2	E	700	S0N	N26-C25-N24	-11.68	119.95	128.89
2	B	400	S0N	N26-C25-N24	-11.38	120.18	128.89
2	A	300	S0N	N26-C25-N24	-11.32	120.23	128.89
2	A	300	S0N	C41-C42-C43	-10.15	95.58	112.31
2	C	500	S0N	C41-C42-C43	-9.19	97.17	112.31
2	E	700	S0N	C41-C42-C43	-8.74	97.91	112.31
2	C	500	S0N	C51-C52-C53	-8.38	100.47	112.72
2	F	800	S0N	C41-C42-C43	-8.32	98.60	112.31
2	D	600	S0N	C52-C51-C49	-6.89	100.13	112.66
2	D	600	S0N	C41-C42-C43	-6.82	101.06	112.31
2	B	400	S0N	C41-C42-C43	-6.37	101.81	112.31
2	F	800	S0N	O05-C04-C02	-5.54	101.64	110.55
2	A	300	S0N	O05-C04-C02	-5.22	102.16	110.55
2	A	300	S0N	C52-C51-C49	-5.16	103.28	112.66
2	E	700	S0N	C52-C51-C49	-5.15	103.31	112.66
2	B	400	S0N	O05-C04-C02	-4.67	103.04	110.55
2	F	800	S0N	C52-C51-C49	-4.59	104.31	112.66
2	F	800	S0N	C03-C02-C04	-4.31	102.92	108.50
2	B	400	S0N	C52-C51-C49	-3.85	105.66	112.66
2	D	600	S0N	P10-O09-P06	-3.82	121.99	132.73
2	A	300	S0N	C03-C02-C04	-3.47	104.01	108.50
2	D	600	S0N	C46-C47-N48	-3.45	98.24	111.51
2	C	500	S0N	C03-C02-C04	-3.44	104.04	108.50
2	E	700	S0N	P10-O09-P06	-3.28	123.51	132.73
2	F	800	S0N	P10-O09-P06	-3.28	123.51	132.73
2	A	300	S0N	P10-O09-P06	-3.25	123.59	132.73
2	C	500	S0N	O05-C04-C02	-3.24	105.34	110.55
2	F	800	S0N	O16-C17-N18	-2.97	101.88	108.10
2	B	400	S0N	C03-C02-C04	-2.91	104.73	108.50
2	C	500	S0N	C52-C51-C49	-2.87	107.45	112.66
2	D	600	S0N	C51-C52-C53	-2.86	108.53	112.72
2	D	600	S0N	O05-C04-C02	-2.82	106.02	110.55
2	F	800	S0N	C15-O16-C17	-2.80	106.64	109.72
2	C	500	S0N	P10-O09-P06	-2.78	124.93	132.73
2	D	600	S0N	C15-O16-C17	-2.67	106.79	109.72
2	B	400	S0N	P10-O09-P06	-2.65	125.30	132.73
2	B	400	S0N	O37-C36-C38	-2.64	104.32	110.38
2	B	400	S0N	C47-C46-N45	-2.53	101.80	111.51
2	B	400	S0N	C51-C52-C53	-2.51	109.05	112.72
2	E	700	S0N	C46-C47-N48	-2.44	102.15	111.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	S0N	C15-O16-C17	-2.41	107.07	109.72
2	A	300	S0N	C15-O16-C17	-2.41	107.07	109.72
2	B	400	S0N	C59-C60-C61	-2.32	116.66	120.23
2	E	700	S0N	C15-O16-C17	-2.29	107.20	109.72
2	D	600	S0N	C17-N18-C27	-2.29	123.49	126.94
2	B	400	S0N	O39-C38-N40	-2.23	118.60	123.08
2	D	600	S0N	C59-C60-C61	-2.23	116.80	120.23
2	B	400	S0N	C46-C47-N48	-2.20	103.04	111.51
2	A	300	S0N	C59-C60-C61	-2.14	116.94	120.23
2	A	300	S0N	C17-N18-C27	-2.13	123.73	126.94
2	A	300	S0N	C01-C02-C04	-2.05	105.84	108.50
2	B	400	S0N	C41-N40-C38	-2.04	118.49	122.53
2	B	400	S0N	C15-O16-C17	-2.04	107.48	109.72
2	C	500	S0N	C28-C17-N18	2.02	117.38	114.29
2	F	800	S0N	C59-C60-C55	2.03	120.36	118.03
2	F	800	S0N	O13-C14-C15	2.07	116.74	109.12
2	E	700	S0N	C59-C60-C55	2.23	120.58	118.03
2	B	400	S0N	C28-C17-N18	2.27	117.77	114.29
2	B	400	S0N	C01-C02-C04	2.46	111.69	108.50
2	B	400	S0N	C01-C02-C36	2.52	113.94	109.34
2	A	300	S0N	C28-C17-N18	2.61	118.27	114.29
2	A	300	S0N	C01-C02-C36	2.73	114.32	109.34
2	E	700	S0N	C01-C02-C36	2.73	114.33	109.34
2	F	800	S0N	C28-C17-N18	2.95	118.81	114.29
2	E	700	S0N	C03-C02-C36	3.89	116.44	109.34
2	D	600	S0N	C01-C02-C36	3.94	116.53	109.34
2	B	400	S0N	O09-P06-O05	4.03	113.63	102.94
2	C	500	S0N	C01-C02-C36	4.75	118.02	109.34

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	300	S0N	5	0
4	A	302	PGE	3	0
5	A	303	GOL	1	0
2	B	400	S0N	2	0
4	B	402	PGE	1	0
2	C	500	S0N	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	600	S0N	4	0
2	E	700	S0N	3	0
2	F	800	S0N	3	0
4	F	802	PGE	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, 95th 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 ²)	Q<0.9
1	A	281/289 (97%)	-0.18	5 (1%) 71 72	14, 20, 33, 49	0
1	B	281/289 (97%)	-0.12	5 (1%) 71 72	14, 19, 34, 45	0
1	C	281/289 (97%)	-0.19	2 (0%) 89 89	14, 19, 32, 44	0
1	D	281/289 (97%)	-0.21	2 (0%) 89 89	13, 18, 28, 46	0
1	E	281/289 (97%)	-0.03	3 (1%) 82 83	15, 22, 37, 46	0
1	F	281/289 (97%)	-0.12	4 (1%) 78 78	13, 22, 34, 50	0
All	All	1686/1734 (97%)	-0.14	21 (1%) 81 81	13, 20, 34, 50	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	7	ALA	4.3
1	D	113[A]	ARG	3.2
1	B	113[A]	ARG	3.0
1	F	16	HIS	2.9
1	F	113[A]	ARG	2.9
1	C	113[A]	ARG	2.9
1	A	7	ALA	2.8
1	A	113[A]	ARG	2.8
1	D	238	ALA	2.6
1	B	246	LEU	2.6
1	A	246	LEU	2.5
1	B	8	MET	2.4
1	F	100	ASP	2.4
1	E	31	THR	2.2
1	B	31	THR	2.2
1	A	240	CYS	2.1
1	F	240	CYS	2.1
1	C	238	ALA	2.1
1	A	5	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	E	277	ASP	2.0
1	E	113[A]	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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 ²)	Q<0.9
5	GOL	C	503	6/6	0.97	0.26	7.17	27,29,31,34	0
5	GOL	D	603	6/6	0.95	0.21	6.80	24,28,28,33	0
5	GOL	A	303	6/6	0.92	0.20	5.28	27,33,37,37	0
4	PGE	D	602	10/10	0.94	0.13	4.65	22,32,49,52	0
5	GOL	F	803	6/6	0.94	0.15	3.90	31,33,40,41	0
4	PGE	C	502	10/10	0.92	0.13	3.43	25,33,41,53	0
3	CL	C	501	1/1	0.99	0.11	3.25	20,20,20,20	0
3	CL	D	601	1/1	0.99	0.10	3.09	20,20,20,20	0
4	PGE	E	702	10/10	0.93	0.16	3.00	25,34,49,55	0
5	GOL	E	703	6/6	0.96	0.15	2.78	29,35,37,39	0
5	GOL	B	403	6/6	0.96	0.14	2.54	24,26,29,30	0
4	PGE	B	402	10/10	0.92	0.13	2.44	25,33,46,48	0
4	PGE	A	302	10/10	0.94	0.11	2.08	28,35,45,48	0
3	CL	A	301	1/1	0.98	0.11	1.80	22,22,22,22	0
3	CL	F	801	1/1	0.97	0.10	1.15	27,27,27,27	0
4	PGE	F	802	10/10	0.91	0.12	1.05	30,36,45,47	0
2	S0N	F	800	63/63	0.95	0.12	0.52	24,31,41,49	0
2	S0N	E	700	63/63	0.96	0.10	0.18	18,25,33,49	0
2	S0N	D	600	63/63	0.96	0.10	0.17	16,22,34,40	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	S0N	B	400	63/63	0.97	0.09	0.06	18,23,32,33	0
2	S0N	A	300	63/63	0.95	0.09	-0.10	18,27,36,46	0
2	S0N	C	500	63/63	0.97	0.08	-0.27	16,23,32,35	0
3	CL	E	701	1/1	0.98	0.07	-1.19	23,23,23,23	0
3	CL	B	401	1/1	0.99	0.06	-2.05	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.