



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:26 AM UTC

PDB ID : 3MVK / pdb_00003mvk
Title : The Crystal Structure of FucU from Bifidobacterium longum to 1.65Å
Authors : Stein, A.J.; Xu, X.; Cui, H.; Savchenko, A.; Joachimiak, A.; Midwest Center
for Structural Genomics (MCSG)
Deposited on : 2010-05-04
Resolution : 1.65 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

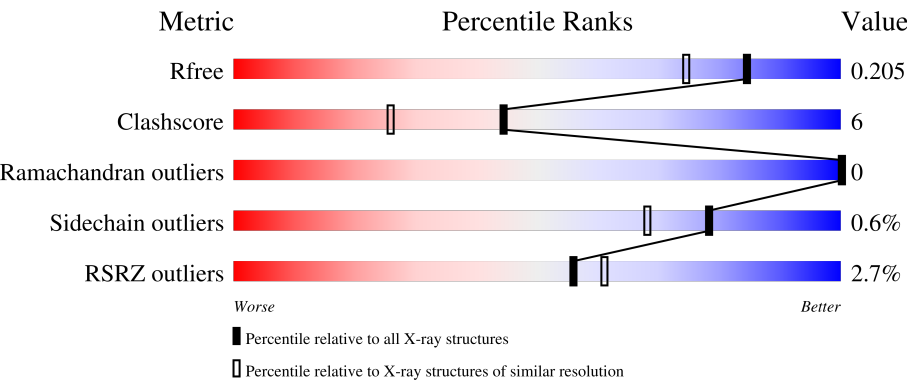
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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}	180053	2563 (1.66-1.66)
Clashscore	190562	2662 (1.66-1.66)
Ramachandran outliers	187476	2621 (1.66-1.66)
Sidechain outliers	187428	2621 (1.66-1.66)
RSRZ outliers	180081	2564 (1.66-1.66)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	148	0% 85%9%• 5%
1	B	148	0% 83%11%• 5%
1	C	148	7% 78%16%• 5%
1	D	148	4% 89%5%• 5%
1	E	148	2% 87%7%• 5%

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Mol	Chain	Length	Quality of chain
1	F	148	
1	G	148	
1	H	148	
1	I	148	
1	J	148	

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	PGE	C	151	-	-	X	-
3	PGE	J	150	-	-	X	-
4	GOL	B	152	-	-	X	-
4	GOL	E	153	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12068 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 protein FucU.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	140	Total	C	N	O	S	Se	0	2	0
			1054	679	171	198	3	3			
1	B	140	Total	C	N	O	S	Se	0	1	0
			1053	676	171	200	3	3			
1	C	141	Total	C	N	O	S	Se	0	1	0
			1064	685	172	201	3	3			
1	D	140	Total	C	N	O	S	Se	0	1	0
			1055	681	172	196	3	3			
1	E	141	Total	C	N	O	S	Se	0	1	0
			1061	684	172	199	3	3			
1	F	140	Total	C	N	O	S	Se	0	1	0
			1049	674	171	198	3	3			
1	G	143	Total	C	N	O	S	Se	0	2	0
			1068	687	173	202	3	3			
1	H	141	Total	C	N	O	S	Se	0	2	0
			1063	685	172	200	3	3			
1	I	141	Total	C	N	O	S	Se	0	2	0
			1059	683	171	199	3	3			
1	J	141	Total	C	N	O	S	Se	0	1	0
			1064	686	173	199	3	3			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

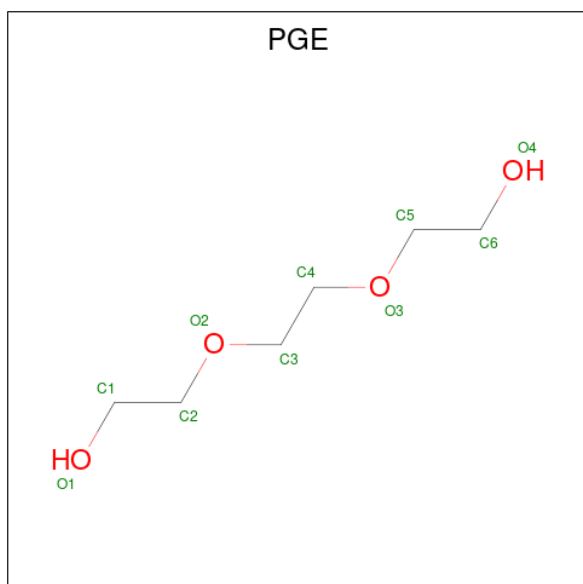
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Na	0	0
			2	2		
2	B	2	Total	Na	0	0
			2	2		
2	C	1	Total	Na	0	0
			1	1		
2	D	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	E	2	Total	Na	0	0
			2	2		
2	F	2	Total	Na	0	0
			2	2		
2	G	1	Total	Na	0	0
			1	1		
2	H	2	Total	Na	0	0
			2	2		
2	I	1	Total	Na	0	0
			1	1		
2	J	1	Total	Na	0	0
			1	1		

- Molecule 3 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



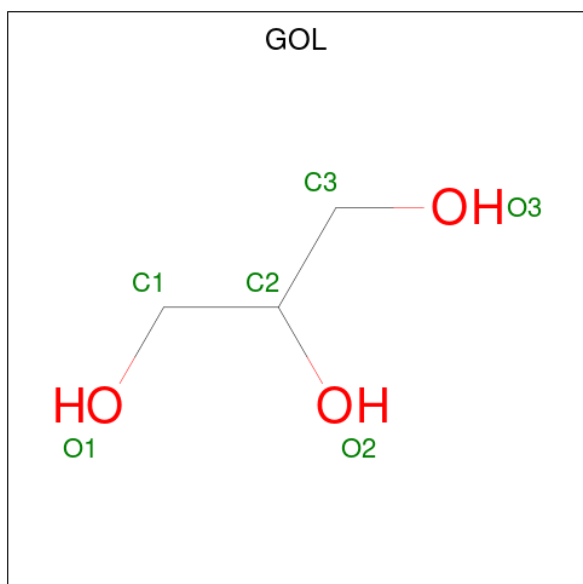
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	6	4		
3	B	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		
3	C	1	Total	C	O	0	0
			10	6	4		
3	E	1	Total	C	O	0	0
			10	6	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			10	6	4		
3	F	1	Total	C	O	0	0
			10	6	4		
3	G	1	Total	C	O	0	0
			10	6	4		
3	H	1	Total	C	O	0	0
			10	6	4		
3	J	1	Total	C	O	0	0
			10	6	4		
3	J	1	Total	C	O	0	0
			10	6	4		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			6	3	3		

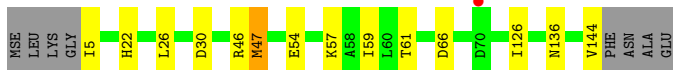
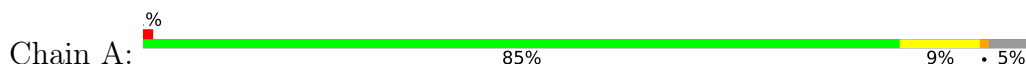
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	137	Total	O	0	0
			137	137		
5	B	139	Total	O	0	0
			139	139		
5	C	116	Total	O	0	0
			116	116		
5	D	121	Total	O	0	0
			121	121		
5	E	136	Total	O	0	0
			136	136		
5	F	120	Total	O	0	0
			120	120		
5	G	156	Total	O	0	0
			156	156		
5	H	138	Total	O	0	0
			138	138		
5	I	121	Total	O	0	0
			121	121		
5	J	133	Total	O	0	0
			133	133		

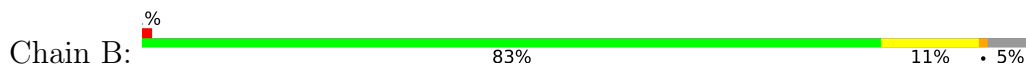
3 Residue-property plots [i](#)

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.

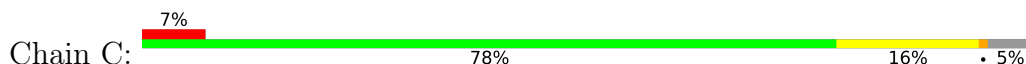
- Molecule 1: protein FucU



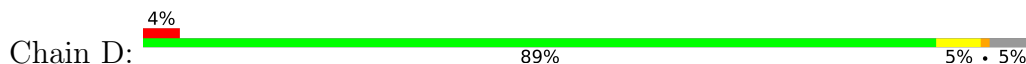
- Molecule 1: protein FucU



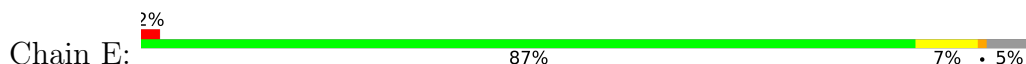
- Molecule 1: protein FucU



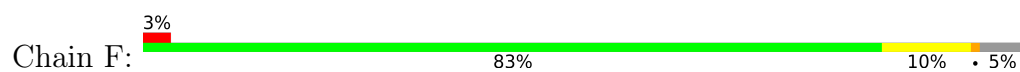
- Molecule 1: protein FucU



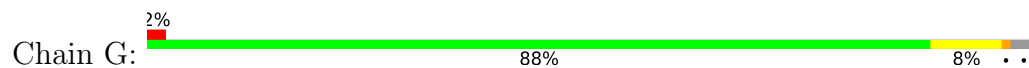
- Molecule 1: protein FucU



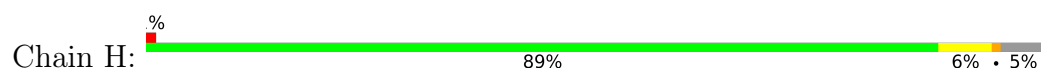
- Molecule 1: protein FucU



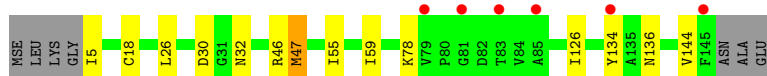
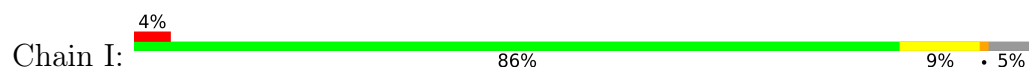
- Molecule 1: protein FucU



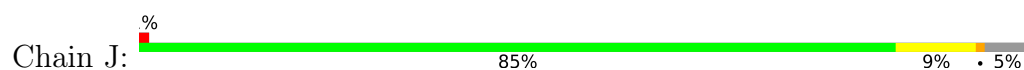
- Molecule 1: protein FucU



- Molecule 1: protein FucU



- Molecule 1: protein FucU



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	66.05Å 83.86Å 144.81Å 90.00° 95.11° 90.00°	Depositor
Resolution (Å)	40.72 – 1.65 40.72 – 1.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (40.72-1.65) 99.8 (40.72-1.65)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 1.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.182 , 0.205 0.181 , 0.205	Depositor DCC
R_{free} test set	9500 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	20.2	Xtriage
Anisotropy	0.025	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	12068	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.02% 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, 0.333 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: PGE, GOL, NA

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	0.70	0/1078	0.84	1/1462 (0.1%)
1	B	0.67	0/1074	0.83	1/1456 (0.1%)
1	C	0.68	0/1086	0.85	1/1472 (0.1%)
1	D	0.65	0/1076	0.81	1/1454 (0.1%)
1	E	0.67	0/1083	0.79	1/1468 (0.1%)
1	F	0.64	0/1070	0.85	1/1451 (0.1%)
1	G	0.66	0/1093	0.82	1/1483 (0.1%)
1	H	0.67	0/1088	0.80	1/1475 (0.1%)
1	I	0.65	0/1084	0.82	1/1471 (0.1%)
1	J	0.70	0/1086	0.81	1/1471 (0.1%)
All	All	0.67	0/10818	0.82	10/14663 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	MSE	CG-SE-CE	-9.49	78.03	98.92
1	D	47	MSE	CG-SE-CE	-9.35	78.35	98.92
1	A	47	MSE	CG-SE-CE	-9.17	78.75	98.92
1	J	47	MSE	CG-SE-CE	-8.98	79.16	98.92
1	G	47	MSE	CG-SE-CE	-8.70	79.79	98.92
1	C	47	MSE	CG-SE-CE	-8.64	79.90	98.92
1	F	47	MSE	CG-SE-CE	-8.27	80.72	98.92
1	I	47	MSE	CG-SE-CE	-8.21	80.86	98.92
1	H	47	MSE	CG-SE-CE	-7.62	82.16	98.92
1	E	47	MSE	CG-SE-CE	-5.53	86.77	98.92

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	1054	0	1057	12	0
1	B	1053	0	1050	20	0
1	C	1064	0	1059	27	0
1	D	1055	0	1056	7	0
1	E	1061	0	1057	15	0
1	F	1049	0	1046	15	0
1	G	1068	0	1054	13	0
1	H	1063	0	1060	9	0
1	I	1059	0	1048	13	0
1	J	1064	0	1066	19	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	1	0	0	0	0
2	H	2	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	10	0	14	0	0
3	B	10	0	14	0	0
3	C	20	0	28	7	0
3	E	20	0	28	2	0
3	F	10	0	14	0	0
3	G	10	0	14	0	0
3	H	10	0	14	0	0
3	J	20	0	28	9	0
4	A	6	0	8	0	0
4	B	6	0	7	5	0
4	E	6	0	7	4	0
4	F	6	0	8	1	0
4	G	6	0	8	0	0
4	H	6	0	8	1	0
5	A	137	0	0	1	0
5	B	139	0	0	3	0
5	C	116	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	121	0	0	2	0
5	E	136	0	0	0	0
5	F	120	0	0	2	0
5	G	156	0	0	1	0
5	H	138	0	0	0	0
5	I	121	0	0	0	0
5	J	133	0	0	0	0
All	All	12068	0	10753	128	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 6.

All (128) 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:25:GLN:H	3:C:151:PGE:H62	1.05	1.12
1:B:133:GLN:HE21	4:B:152:GOL:C3	1.80	0.95
1:J:123:TYR:HB2	3:J:150:PGE:H3	1.47	0.94
1:B:32:ASN:HD21	1:E:144:VAL:H	1.18	0.91
1:H:32:ASN:HD21	1:I:144:VAL:H	1.13	0.91
1:B:133:GLN:HE21	4:B:152:GOL:H32	1.35	0.89
1:C:144:VAL:H	1:F:32:ASN:HD21	1.15	0.88
1:G:32:ASN:HD21	1:J:144:VAL:H	1.22	0.88
1:F:99:HIS:HE1	5:F:224:HOH:O	1.57	0.87
1:C:25:GLN:HE21	1:C:140:GLN:HE21	1.22	0.85
1:A:144:VAL:H	1:I:32:ASN:HD21	1.25	0.84
1:B:144:VAL:H	1:C:32:ASN:HD21	1.24	0.82
1:C:25:GLN:N	3:C:151:PGE:H62	1.90	0.81
1:D:32:ASN:HD21	1:F:144:VAL:H	1.31	0.77
1:E:133:GLN:HE21	4:E:153:GOL:C3	2.00	0.75
1:C:25:GLN:H	3:C:151:PGE:C6	1.94	0.74
1:A:144:VAL:H	1:I:32:ASN:ND2	1.85	0.74
1:C:8:ILE:HD11	1:C:58:ALA:CB	2.18	0.73
1:A:5:ILE:HD11	1:E:5:ILE:HD11	1.71	0.70
1:C:12:GLU:HG3	5:C:405:HOH:O	1.90	0.70
1:I:30:ASP:H	1:I:136:ASN:ND2	1.90	0.70
1:J:121:ASN:O	3:J:150:PGE:H2	1.92	0.70
1:B:144:VAL:H	1:C:32:ASN:ND2	1.90	0.69
1:F:12:GLU:HG3	5:F:1307:HOH:O	1.92	0.69
1:C:30:ASP:H	1:C:136:ASN:ND2	1.90	0.69
1:A:30:ASP:H	1:A:136:ASN:ND2	1.90	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:VAL:H	1:F:32:ASN:ND2	1.90	0.68
1:J:121:ASN:O	3:J:150:PGE:H42	1.93	0.68
1:C:24:ASP:OD1	3:C:151:PGE:H5	1.94	0.67
1:B:32:ASN:ND2	1:E:144:VAL:H	1.90	0.67
1:C:81:GLY:HA3	5:C:1305:HOH:O	1.96	0.65
1:D:32:ASN:ND2	1:F:144:VAL:H	1.95	0.65
1:C:99:HIS:HE1	5:C:162:HOH:O	1.80	0.65
1:G:99:HIS:HE1	5:G:291:HOH:O	1.78	0.64
1:C:25:GLN:HE21	1:C:140:GLN:NE2	1.93	0.64
5:D:645:HOH:O	1:I:18[A]:CYS:SG	2.40	0.64
1:C:47:MSE:HG3	1:C:126:ILE:HG23	1.81	0.63
1:D:30:ASP:H	1:D:136:ASN:ND2	1.95	0.63
1:G:30:ASP:H	1:G:136:ASN:ND2	1.96	0.63
1:B:32:ASN:HD21	1:E:144:VAL:N	1.94	0.62
1:G:32:ASN:ND2	1:J:144:VAL:H	1.97	0.62
1:H:32:ASN:ND2	1:I:144:VAL:H	1.93	0.61
1:J:30:ASP:H	1:J:136:ASN:ND2	1.98	0.61
1:A:46:ARG:C	1:A:47:MSE:HG2	2.24	0.61
1:I:46:ARG:C	1:I:47:MSE:HG2	2.25	0.61
1:C:8:ILE:HD11	1:C:58:ALA:HB2	1.82	0.61
1:B:5:ILE:HD11	1:G:5:ILE:HD11	1.82	0.60
1:I:47:MSE:HG3	1:I:126:ILE:HG23	1.84	0.60
1:B:12:GLU:HG3	5:B:620:HOH:O	2.00	0.60
1:D:46:ARG:C	1:D:47:MSE:HG2	2.26	0.60
1:A:57:LYS:O	1:A:61:THR:HG23	2.02	0.59
1:B:46:ARG:C	1:B:47:MSE:HG2	2.27	0.59
1:B:133:GLN:NE2	4:B:152:GOL:H32	2.13	0.58
1:C:46:ARG:C	1:C:47:MSE:HG2	2.29	0.58
1:C:144:VAL:N	1:F:32:ASN:HD21	1.95	0.58
1:B:47:MSE:HG3	1:B:126:ILE:HG23	1.86	0.57
1:G:37:SER:HB2	3:J:150:PGE:H52	1.86	0.57
1:E:133:GLN:HE21	4:E:153:GOL:H32	1.69	0.57
1:J:46:ARG:C	1:J:47:MSE:HG2	2.28	0.57
1:E:26:LEU:C	1:E:26:LEU:HD12	2.30	0.56
1:J:47:MSE:HG3	1:J:126:ILE:HG23	1.86	0.56
1:B:22:HIS:HE1	1:B:66:ASP:OD1	1.88	0.56
1:F:22:HIS:HE1	1:F:66:ASP:OD1	1.86	0.56
1:C:121:ASN:O	3:C:151:PGE:H42	2.05	0.56
1:H:133:GLN:HE21	4:H:152:GOL:C3	2.18	0.56
1:A:22:HIS:HE1	1:A:66:ASP:OD1	1.90	0.55
1:B:57:LYS:O	1:B:61:THR:HG23	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:ASP:H	1:A:136:ASN:HD22	1.52	0.54
1:C:24:ASP:HA	3:C:151:PGE:H5	1.90	0.53
1:J:25:GLN:HB2	3:J:150:PGE:H22	1.91	0.52
1:C:123:TYR:N	3:C:151:PGE:H6	2.24	0.52
1:G:46:ARG:C	1:G:47:MSE:HG2	2.34	0.52
1:A:47:MSE:HG3	1:A:126:ILE:HG23	1.93	0.51
1:F:5:ILE:HG13	1:F:5:ILE:O	2.10	0.51
1:E:57:LYS:O	1:E:61:THR:HG23	2.10	0.51
1:D:57:LYS:O	1:D:61:THR:HG23	2.12	0.50
1:F:133:GLN:HE21	4:F:152:GOL:H31	1.76	0.49
1:H:47:MSE:HG3	1:H:126:ILE:HG23	1.93	0.49
1:G:32:ASN:HD21	1:J:144:VAL:N	2.02	0.49
1:G:47:MSE:HG3	1:G:126:ILE:HG23	1.94	0.49
1:J:123:TYR:CB	3:J:150:PGE:H3	2.31	0.49
1:G:26:LEU:C	1:G:26:LEU:HD12	2.37	0.49
1:A:54:GLU:HG3	5:A:156:HOH:O	2.12	0.49
1:F:11:PRO:HG3	1:H:18[B]:CYS:SG	2.53	0.49
1:H:46:ARG:C	1:H:47:MSE:HG2	2.37	0.49
1:J:24:ASP:OD1	3:J:150:PGE:H32	2.12	0.49
1:C:15:LYS:O	1:C:19:GLU:HG3	2.13	0.48
1:A:26:LEU:C	1:A:26:LEU:HD12	2.39	0.48
1:J:30:ASP:H	1:J:136:ASN:HD22	1.60	0.48
1:B:133:GLN:HE21	4:B:152:GOL:H31	1.74	0.48
1:F:46:ARG:C	1:F:47:MSE:HG2	2.39	0.48
1:B:79:VAL:CG2	1:B:82:ASP:HB2	2.44	0.47
1:G:30:ASP:H	1:G:136:ASN:HD22	1.61	0.47
1:D:47:MSE:HG3	1:D:126:ILE:HG23	1.96	0.47
1:C:15:LYS:NZ	1:C:19:GLU:OE2	2.36	0.47
1:E:133:GLN:NE2	4:E:153:GOL:C3	2.75	0.47
1:I:55:ILE:O	1:I:59[A]:ILE:HG12	2.15	0.47
1:E:78:LYS:HA	1:E:134:TYR:CE1	2.50	0.47
1:B:133:GLN:NE2	4:B:152:GOL:C3	2.64	0.45
1:F:47:MSE:HG3	1:F:126:ILE:HG23	1.97	0.45
1:C:78:LYS:HA	1:C:134:TYR:CE1	2.52	0.45
1:G:78:LYS:HA	1:G:134:TYR:CE1	2.52	0.45
1:B:144:VAL:HG22	1:C:32:ASN:ND2	2.32	0.44
1:J:25:GLN:H	3:J:150:PGE:H22	1.82	0.44
1:D:57:LYS:HD2	5:D:959:HOH:O	2.17	0.44
1:E:47:MSE:HG3	1:E:126:ILE:HG23	1.99	0.44
1:J:26:LEU:HD12	1:J:26:LEU:C	2.42	0.44
1:E:113:PHE:CE2	3:E:151:PGE:H52	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:GLN:NE2	4:E:153:GOL:H32	2.32	0.43
1:B:54:GLU:OE1	5:B:1303:HOH:O	2.21	0.43
1:A:59[A]:ILE:HD11	1:A:126:ILE:CD1	2.49	0.43
1:J:25:GLN:H	3:J:150:PGE:C2	2.32	0.42
5:B:1087:HOH:O	1:G:18[B]:CYS:SG	2.60	0.42
1:C:79:VAL:HG23	1:C:82:ASP:HB2	2.01	0.42
1:H:26:LEU:C	1:H:26:LEU:HD12	2.45	0.42
1:F:78:LYS:HA	1:F:134:TYR:CE1	2.53	0.42
1:B:77:GLU:HG3	1:B:109:SER:HB2	2.01	0.42
1:E:46:ARG:C	1:E:47:MSE:HG2	2.44	0.42
1:E:113:PHE:HE2	3:E:151:PGE:H52	1.84	0.42
1:J:78:LYS:HA	1:J:134:TYR:CE1	2.55	0.42
1:I:30:ASP:H	1:I:136:ASN:HD22	1.67	0.42
1:H:29:ALA:HB1	1:H:33:PHE:HB3	2.02	0.41
1:F:26:LEU:HD12	1:F:26:LEU:C	2.45	0.41
1:I:78:LYS:HA	1:I:134:TYR:CE1	2.54	0.41
1:J:33:PHE:HB2	1:J:136:ASN:HD21	1.85	0.41
1:I:26:LEU:HD12	1:I:26:LEU:C	2.47	0.40
1:I:47:MSE:HG3	1:I:126:ILE:CG2	2.51	0.40
1:H:19:GLU:HB2	1:J:36:GLU:HG3	2.04	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	140/148 (95%)	140 (100%)	0	0	100	100
1	B	139/148 (94%)	138 (99%)	1 (1%)	0	100	100
1	C	140/148 (95%)	137 (98%)	3 (2%)	0	100	100
1	D	137/148 (93%)	136 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	140/148 (95%)	139 (99%)	1 (1%)	0	100	100
1	F	139/148 (94%)	138 (99%)	1 (1%)	0	100	100
1	G	143/148 (97%)	142 (99%)	1 (1%)	0	100	100
1	H	141/148 (95%)	140 (99%)	1 (1%)	0	100	100
1	I	141/148 (95%)	141 (100%)	0	0	100	100
1	J	140/148 (95%)	140 (100%)	0	0	100	100
All	All	1400/1480 (95%)	1391 (99%)	9 (1%)	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	110/113 (97%)	110 (100%)	0	100	100
1	B	110/113 (97%)	110 (100%)	0	100	100
1	C	111/113 (98%)	108 (97%)	3 (3%)	39	16
1	D	109/113 (96%)	109 (100%)	0	100	100
1	E	110/113 (97%)	110 (100%)	0	100	100
1	F	109/113 (96%)	106 (97%)	3 (3%)	38	15
1	G	110/113 (97%)	110 (100%)	0	100	100
1	H	111/113 (98%)	111 (100%)	0	100	100
1	I	109/113 (96%)	108 (99%)	1 (1%)	70	56
1	J	111/113 (98%)	111 (100%)	0	100	100
All	All	1100/1130 (97%)	1093 (99%)	7 (1%)	78	68

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	8	ILE

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Mol	Chain	Res	Type
1	C	98	GLU
1	C	101	GLU
1	F	5	ILE
1	F	14	LEU
1	F	143	VAL
1	I	5	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	HIS
1	A	25	GLN
1	A	118	GLN
1	A	136	ASN
1	B	22	HIS
1	B	25	GLN
1	B	32	ASN
1	B	118	GLN
1	B	133	GLN
1	C	32	ASN
1	C	99	HIS
1	C	136	ASN
1	C	140	GLN
1	D	25	GLN
1	D	32	ASN
1	D	136	ASN
1	E	25	GLN
1	E	118	GLN
1	E	133	GLN
1	F	22	HIS
1	F	25	GLN
1	F	32	ASN
1	F	99	HIS
1	F	118	GLN
1	F	133	GLN
1	G	32	ASN
1	G	99	HIS
1	G	118	GLN
1	G	136	ASN
1	H	25	GLN
1	H	32	ASN
1	H	133	GLN

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Mol	Chain	Res	Type
1	I	25	GLN
1	I	32	ASN
1	I	136	ASN
1	J	25	GLN
1	J	118	GLN
1	J	136	ASN
1	J	140	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 32 ligands modelled in this entry, 15 are monoatomic - leaving 17 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	PGE	G	150	-	9,9,9	0.43	0	8,8,8	0.34	0
3	PGE	E	152	-	9,9,9	0.47	0	8,8,8	0.28	0
3	PGE	J	151	-	9,9,9	0.44	0	8,8,8	0.39	0
4	GOL	E	153	2	5,5,5	0.41	0	5,5,5	0.94	0
3	PGE	J	150	-	9,9,9	0.62	0	8,8,8	0.90	0
3	PGE	A	151	-	9,9,9	0.50	0	8,8,8	0.16	0
3	PGE	H	151	-	9,9,9	0.55	0	8,8,8	0.34	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	152	2	5,5,5	0.40	0	5,5,5	0.80	0
3	PGE	E	151	-	9,9,9	0.48	0	8,8,8	0.22	0
4	GOL	G	151	-	5,5,5	0.37	0	5,5,5	0.46	0
3	PGE	C	150	-	9,9,9	0.47	0	8,8,8	0.29	0
4	GOL	H	152	2	5,5,5	0.50	0	5,5,5	1.44	2 (40%)
3	PGE	F	151	-	9,9,9	0.47	0	8,8,8	0.27	0
4	GOL	F	152	2	5,5,5	0.42	0	5,5,5	0.64	0
3	PGE	B	151	-	9,9,9	0.44	0	8,8,8	0.40	0
4	GOL	B	152	2	5,5,5	0.35	0	5,5,5	0.68	0
3	PGE	C	151	-	9,9,9	0.40	0	8,8,8	0.47	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	PGE	G	150	-	-	2/7/7/7	-
3	PGE	E	152	-	-	4/7/7/7	-
3	PGE	J	151	-	-	6/7/7/7	-
4	GOL	E	153	2	-	2/4/4/4	-
3	PGE	J	150	-	-	4/7/7/7	-
3	PGE	A	151	-	-	3/7/7/7	-
3	PGE	H	151	-	-	5/7/7/7	-
4	GOL	A	152	2	-	3/4/4/4	-
3	PGE	E	151	-	-	2/7/7/7	-
4	GOL	G	151	-	-	0/4/4/4	-
3	PGE	C	150	-	-	3/7/7/7	-
4	GOL	H	152	2	-	2/4/4/4	-
3	PGE	F	151	-	-	4/7/7/7	-
4	GOL	F	152	2	-	2/4/4/4	-
3	PGE	B	151	-	-	4/7/7/7	-
4	GOL	B	152	2	-	2/4/4/4	-
3	PGE	C	151	-	-	5/7/7/7	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	152	GOL	O3-C3-C2	-2.31	99.97	110.38
4	H	152	GOL	O2-C2-C1	2.08	117.81	109.18

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	152	GOL	O1-C1-C2-O2
4	A	152	GOL	O1-C1-C2-C3
4	E	153	GOL	O1-C1-C2-O2
4	E	153	GOL	O1-C1-C2-C3
4	H	152	GOL	C1-C2-C3-O3
3	J	150	PGE	C4-C3-O2-C2
3	F	151	PGE	O2-C3-C4-O3
3	J	150	PGE	O2-C3-C4-O3
4	H	152	GOL	O2-C2-C3-O3
3	C	151	PGE	O3-C5-C6-O4
3	H	151	PGE	O3-C5-C6-O4
3	J	151	PGE	O1-C1-C2-O2
3	J	151	PGE	O3-C5-C6-O4
3	H	151	PGE	C1-C2-O2-C3
4	A	152	GOL	C1-C2-C3-O3
4	B	152	GOL	O1-C1-C2-C3
3	G	150	PGE	O3-C5-C6-O4
3	J	150	PGE	O3-C5-C6-O4
3	C	151	PGE	O2-C3-C4-O3
3	E	152	PGE	O3-C5-C6-O4
4	B	152	GOL	O1-C1-C2-O2
3	A	151	PGE	O1-C1-C2-O2
3	C	151	PGE	O1-C1-C2-O2
3	A	151	PGE	C3-C4-O3-C5
3	E	152	PGE	C4-C3-O2-C2
3	J	151	PGE	C4-C3-O2-C2
3	B	151	PGE	C4-C3-O2-C2
3	C	151	PGE	C3-C4-O3-C5
3	G	150	PGE	C3-C4-O3-C5
3	F	151	PGE	C4-C3-O2-C2
3	H	151	PGE	C3-C4-O3-C5
3	E	152	PGE	O1-C1-C2-O2
3	C	151	PGE	C6-C5-O3-C4
3	J	151	PGE	C6-C5-O3-C4
3	B	151	PGE	C6-C5-O3-C4
3	J	150	PGE	C3-C4-O3-C5

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Mol	Chain	Res	Type	Atoms
3	J	151	PGE	O2-C3-C4-O3
3	H	151	PGE	O1-C1-C2-O2
3	F	151	PGE	C6-C5-O3-C4
3	E	152	PGE	C3-C4-O3-C5
3	E	151	PGE	C6-C5-O3-C4
3	E	151	PGE	O1-C1-C2-O2
3	B	151	PGE	O1-C1-C2-O2
4	F	152	GOL	C1-C2-C3-O3
4	F	152	GOL	O2-C2-C3-O3
3	C	150	PGE	O3-C5-C6-O4
3	C	150	PGE	C3-C4-O3-C5
3	F	151	PGE	C3-C4-O3-C5
3	C	150	PGE	O1-C1-C2-O2
3	A	151	PGE	C4-C3-O2-C2
3	J	151	PGE	C3-C4-O3-C5
3	B	151	PGE	C3-C4-O3-C5
3	H	151	PGE	O2-C3-C4-O3

There are no ring outliers.

7 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	153	GOL	4	0
3	J	150	PGE	9	0
3	E	151	PGE	2	0
4	H	152	GOL	1	0
4	F	152	GOL	1	0
4	B	152	GOL	5	0
3	C	151	PGE	7	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	137/148 (92%)	-0.20	1 (0%) 84 89	10, 18, 29, 32	2 (1%)
1	B	137/148 (92%)	-0.23	1 (0%) 84 89	13, 18, 30, 36	1 (0%)
1	C	138/148 (93%)	0.21	10 (7%) 21 24	13, 20, 35, 40	1 (0%)
1	D	137/148 (92%)	-0.03	6 (4%) 39 42	12, 18, 34, 43	1 (0%)
1	E	138/148 (93%)	-0.08	3 (2%) 62 68	13, 18, 33, 42	1 (0%)
1	F	137/148 (92%)	-0.08	4 (2%) 53 58	14, 20, 32, 39	1 (0%)
1	G	140/148 (94%)	-0.22	3 (2%) 63 69	12, 18, 29, 43	2 (1%)
1	H	138/148 (93%)	-0.13	2 (1%) 73 78	13, 18, 29, 38	2 (1%)
1	I	138/148 (93%)	0.21	6 (4%) 40 43	12, 21, 35, 38	2 (1%)
1	J	138/148 (93%)	-0.14	1 (0%) 84 89	13, 18, 29, 34	1 (0%)
All	All	1378/1480 (93%)	-0.07	37 (2%) 56 61	10, 19, 32, 43	14 (1%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	81	GLY	5.7
1	E	145	PHE	4.9
1	H	145	PHE	4.7
1	C	79	VAL	4.6
1	I	134	TYR	4.5
1	C	83	THR	4.2
1	C	134	TYR	3.5
1	I	83	THR	3.4
1	D	145	PHE	3.3
1	B	144	VAL	3.2
1	G	4	GLY	3.1
1	C	145	PHE	3.1
1	J	145	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	80	PRO	2.8
1	C	84	VAL	2.8
1	I	79	VAL	2.7
1	C	133	GLN	2.6
1	H	144	VAL	2.6
1	C	85	ALA	2.6
1	C	82	ASP	2.5
1	F	144	VAL	2.5
1	I	81	GLY	2.4
1	E	103	GLY	2.4
1	I	145	PHE	2.4
1	C	80	PRO	2.3
1	F	105	ASP	2.3
1	G	5	ILE	2.3
1	A	70	ASP	2.3
1	D	85	ALA	2.3
1	I	85	ALA	2.3
1	F	5	ILE	2.3
1	D	84	VAL	2.3
1	E	144	VAL	2.2
1	G	3	LYS	2.2
1	F	98	GLU	2.1
1	D	79	VAL	2.1
1	D	81	GLY	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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
3	PGE	C	151	10/10	0.77	0.18	38,41,47,48	0
4	GOL	H	152	6/6	0.80	0.16	31,39,39,40	0
4	GOL	F	152	6/6	0.82	0.15	29,36,39,42	0
3	PGE	J	150	10/10	0.82	0.15	33,35,38,40	0
4	GOL	E	153	6/6	0.83	0.16	34,35,37,39	0
3	PGE	B	151	10/10	0.84	0.17	47,47,49,49	0
3	PGE	E	152	10/10	0.84	0.16	44,46,48,49	0
3	PGE	H	151	10/10	0.86	0.15	43,47,49,49	0
3	PGE	G	150	10/10	0.86	0.15	43,44,44,45	0
4	GOL	B	152	6/6	0.86	0.14	34,39,40,41	0
3	PGE	C	150	10/10	0.87	0.13	40,41,42,43	0
3	PGE	F	151	10/10	0.87	0.14	51,51,53,54	0
3	PGE	E	151	10/10	0.87	0.13	44,45,45,45	0
3	PGE	A	151	10/10	0.88	0.13	48,49,50,51	0
4	GOL	A	152	6/6	0.88	0.14	27,33,35,39	0
3	PGE	J	151	10/10	0.89	0.14	48,50,52,53	0
2	NA	F	149	1/1	0.93	0.09	27,27,27,27	0
2	NA	E	150	1/1	0.94	0.08	27,27,27,27	0
4	GOL	G	151	6/6	0.94	0.08	20,25,25,27	0
2	NA	H	150	1/1	0.94	0.09	25,25,25,25	0
2	NA	F	150	1/1	0.95	0.06	28,28,28,28	0
2	NA	B	149	1/1	0.97	0.09	22,22,22,22	0
2	NA	B	150	1/1	0.97	0.08	26,26,26,26	0
2	NA	D	149	1/1	0.97	0.04	20,20,20,20	0
2	NA	A	150	1/1	0.97	0.09	27,27,27,27	0
2	NA	G	149	1/1	0.98	0.06	22,22,22,22	0
2	NA	H	149	1/1	0.98	0.05	23,23,23,23	0
2	NA	A	149	1/1	0.98	0.09	23,23,23,23	0
2	NA	C	149	1/1	0.98	0.04	24,24,24,24	0
2	NA	J	149	1/1	0.99	0.03	22,22,22,22	0
2	NA	E	149	1/1	0.99	0.07	24,24,24,24	0
2	NA	I	149	1/1	0.99	0.04	23,23,23,23	0

6.5 Other polymers

There are no such residues in this entry.