

Full wwPDB X-ray Structure Validation Report (i)

Nov 16, 2024 - 05:40 PM EST

PDB ID	:	3MVK
Title	:	The Crystal Structure of FucU from Bifidobacterium longum to 1.65A
Authors	:	Stein, A.J.; Xu, X.; Cui, H.; Savchenko, A.; Joachimiak, A.; Midwest Center
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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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY \, DIFFRACTION$

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.



Matria	Whole archive	Similar resolution
Metric	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R_{free}	164625	2328 (1.66-1.66)
Clashscore	180529	2515(1.66-1.66)
Ramachandran outliers	177936	2475 (1.66-1.66)
Sidechain outliers	177891	2475 (1.66-1.66)
RSRZ outliers	164620	2328 (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 <=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	А	148	% • 85%	9%		5%	
1	В	148	% 8 3%	11%		5%	
1	С	148	7%	15%		5%	
1	D	148	3%	5	%	5%	
1	Е	148	^{2%} 88%	7	%	• 59	%



Mol	Chain	Length	Quality of chain		
1	F	148	84%	9% • 5%	
1	G	148	88%	8% ••	
1	Н	148	% 	5% • 5%	
1	Ι	148	4% 86%	8% • 5%	
1	J	148	86%	9% • 5%	2

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	С	151	-	-	Х	-
3	PGE	J	150	-	-	Х	-
4	GOL	В	152	-	-	Х	-
4	GOL	Е	153	-	-	Х	-



3MVK

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.

Mol	Chain	Residues		Atoms				ZeroOcc	AltConf	Trace	
1	Δ	140	Total	С	Ν	0	\mathbf{S}	Se	0	9	Ο
	Л	140	1054	679	171	198	3	3	0	2	0
1	B	140	Total	С	Ν	Ο	\mathbf{S}	Se	0	1	Ο
1	D	140	1053	676	171	200	3	3	0	I	0
1	C	1/1	Total	С	Ν	Ο	\mathbf{S}	Se	0	1	Ο
1	U	141	1064	685	172	201	3	3	0	I	0
1	П	140	Total	С	Ν	Ο	\mathbf{S}	Se	0	1	Ο
1	D	140	1055	681	172	196	3	3	0	I	0
1	E	1/1	Total	С	Ν	Ο	\mathbf{S}	Se	0	1	Ο
1		141	1061	684	172	199	3	3	0	I	0
1	F	140	Total	С	Ν	Ο	\mathbf{S}	Se	0	1	0
1	1	140	1049	674	171	198	3	3	0	1	0
1	G	1/13	Total	С	Ν	Ο	\mathbf{S}	Se	0	2	Ο
1	ŭ	140	1068	687	173	202	3	3	0	2	0
1	н	1/1	Total	С	Ν	Ο	\mathbf{S}	Se	0	2	Ο
1	11	141	1063	685	172	200	3	3	0	2	0
1	Т	1/1	Total	С	Ν	0	\mathbf{S}	Se	0	9	0
		1,41	1059	683	171	199	3	3	0	<u> </u>	0
1	T	1/1	Total	С	N	0	S	Se	0	1	0
	J	1,71	1064	686	173	199	3	3	0	T	0

• Molecule 1 is a protein called protein FucU.

• Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	2	Total Na 2 2	0	0
2	В	2	Total Na 2 2	0	0
2	С	1	Total Na 1 1	0	0
2	D	1	Total Na 1 1	0	0



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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	Е	2	Total Na 2 2	0	0
2	F	2	Total Na 2 2	0	0
2	G	1	Total Na 1 1	0	0
2	Н	2	Total Na 2 2	0	0
2	Ι	1	Total Na 1 1	0	0
2	J	1	Total Na 1 1	0	0



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	1	Total C O 10 6 4	0	0
3	В	1	Total C O 10 6 4	0	0
3	С	1	Total C O 10 6 4	0	0
3	С	1	Total C O 10 6 4	0	0
3	Ε	1	Total C O 10 6 4	0	0



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

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	В	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	F	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
4	G	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0



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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	Н	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{C} \\ 6 & 3 & 3 \end{array}$) 3	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	А	137	Total O 137 137	0	0
5	В	139	Total O 139 139	0	0
5	С	116	Total O 116 116	0	0
5	D	121	Total O 121 121	0	0
5	Е	136	Total O 136 136	0	0
5	F	120	Total O 120 120	0	0
5	G	156	Total O 156 156	0	0
5	Н	138	Total O 138 138	0	0
5	Ι	121	Total O 121 121	0	0
5	J	133	Total O 133 133	0	0



3 Residue-property plots (i)

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



• Molecule 1: protein FucU









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	66.05Å 83.86Å 144.81Å	Depositor
a, b, c, α , β , γ	90.00° 95.11° 90.00°	Depositor
Bosolution (Å)	40.72 - 1.65	Depositor
Resolution (A)	40.72 - 1.65	EDS
% Data completeness	99.8 (40.72-1.65)	Depositor
(in resolution range)	99.8 (40.72 - 1.65)	EDS
R _{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$2.14 (at 1.65 \text{\AA})$	Xtriage
Refinement program	REFMAC	Depositor
P. P.	0.182 , 0.205	Depositor
n, n_{free}	0.181 , 0.205	DCC
R_{free} test set	9475 reflections (5.02%)	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.

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.



¹Intensities estimated from amplitudes.

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: NA, GOL, PGE

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	
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.54	0/1078	0.68	1/1462~(0.1%)
1	В	0.56	0/1074	0.67	1/1456~(0.1%)
1	С	0.55	0/1086	0.66	1/1472~(0.1%)
1	D	0.52	0/1076	0.65	1/1454~(0.1%)
1	Е	0.57	0/1083	0.63	1/1468~(0.1%)
1	F	0.53	0/1070	0.64	1/1451~(0.1%)
1	G	0.55	0/1093	0.65	1/1483~(0.1%)
1	Н	0.57	0/1088	0.63	1/1475~(0.1%)
1	Ι	0.55	0/1084	0.65	1/1471~(0.1%)
1	J	0.58	0/1086	0.66	1/1471~(0.1%)
All	All	0.55	0/10818	0.65	10/14663~(0.1%)

There are no bond length outliers.

All	(10)	bond	angle	outliers	are	listed	below:
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Mol	Chain	Res	Type	Atoms		$Observed(^{o})$	$Ideal(^{o})$
1	В	47	MSE	CG-SE-CE	-9.48	78.03	98.90
1	D	47	MSE	CG-SE-CE	-9.34	78.35	98.90
1	А	47	MSE	CG-SE-CE	-9.16	78.75	98.90
1	J	47	MSE	CG-SE-CE	-8.97	79.16	98.90
1	G	47	MSE	CG-SE-CE	-8.69	79.79	98.90
1	С	47	MSE	CG-SE-CE	-8.63	79.90	98.90
1	F	47	MSE	CG-SE-CE	-8.26	80.72	98.90
1	Ι	47	MSE	CG-SE-CE	-8.20	80.86	98.90
1	Н	47	MSE	CG-SE-CE	-7.61	82.16	98.90
1	Е	47	MSE	CG-SE-CE	-5.51	86.77	98.90

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	А	1054	0	1057	12	0
1	В	1053	0	1050	20	0
1	С	1064	0	1059	26	0
1	D	1055	0	1056	7	0
1	Е	1061	0	1057	14	0
1	F	1049	0	1046	14	0
1	G	1068	0	1054	13	0
1	Н	1063	0	1060	8	0
1	Ι	1059	0	1048	12	0
1	J	1064	0	1066	18	0
2	А	2	0	0	0	0
2	В	2	0	0	0	0
2	С	1	0	0	0	0
2	D	1	0	0	0	0
2	Е	2	0	0	0	0
2	F	2	0	0	0	0
2	G	1	0	0	0	0
2	Н	2	0	0	0	0
2	Ι	1	0	0	0	0
2	J	1	0	0	0	0
3	А	10	0	14	0	0
3	В	10	0	14	0	0
3	С	20	0	28	7	0
3	Е	20	0	28	2	0
3	F	10	0	14	0	0
3	G	10	0	14	0	0
3	Н	10	0	14	0	0
3	J	20	0	28	9	0
4	А	6	0	8	0	0
4	В	6	0	7	5	0
4	Е	6	0	7	4	0
4	F	6	0	8	1	0
4	G	6	0	8	0	0
4	Н	6	0	8	1	0
5	А	137	0	0	1	0
5	В	139	0	0	3	0
5	С	116	0	0	3	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	121	0	0	2	0
5	Ε	136	0	0	0	0
5	F	120	0	0	2	0
5	G	156	0	0	1	0
5	Н	138	0	0	0	0
5	Ι	121	0	0	0	0
5	J	133	0	0	0	0
All	All	12068	0	10753	122	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 (122) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	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



		Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	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: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:A:57:LYS:O	1:A:61:THR:HG23	2.02	0.59
1:B:133:GLN:NE2	4:B:152:GOL:H32	2.13	0.58
1:A:46:ARG:C	1:A:47:MSE:HG2	2.24	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: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:I:46:ARG:C	1:I:47:MSE:HG2	2.25	0.56
1:H:133:GLN:HE21	4:H:152:GOL:C3	2.18	0.56
1:B:46:ARG:C	1:B:47:MSE:HG2	2.27	0.55
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
1:D:46:ARG:C	1:D:47:MSE:HG2	2.26	0.54
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:C:46:ARG:C	1:C:47:MSE:HG2	2.29	0.53



	• • • • • • • •	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:J:25:GLN:HB2	3:J:150:PGE:H22	1.91	0.52
1:J:46:ARG:C	1:J:47:MSE:HG2	2.28	0.52
1:C:123:TYR:N	3:C:151:PGE:H6	2.24	0.52
1:E:26:LEU:C	1:E:26:LEU:HD12	2.30	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: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: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:G:46:ARG:C	1:G:47:MSE:HG2	2.34	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: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: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:H:46:ARG:C	1:H:47:MSE:HG2	2.37	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:G:26:LEU:C	1:G:26:LEU:HD12	2.37	0.44
1:E:113:PHE:CE2	3:E:151:PGE:H52	2.53	0.44
1:E:133:GLN:NE2	4:E:153:GOL:H32	2.32	0.43
1:F:46:ARG:C	1:F:47:MSE:HG2	2.39	0.43
1:A:26:LEU:C	1:A:26:LEU:HD12	2.39	0.43
1:B:54:GLU:OE1	5:B:1303:HOH:O	2.21	0.43



Atom-1	Atom-2	Interatomic	Clash
		distance (A)	overlap (A)
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: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: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: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: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	Perce	ntiles
1	А	140/148~(95%)	140 (100%)	0	0	100	100
1	В	139/148~(94%)	138 (99%)	1 (1%)	0	100	100
1	С	140/148~(95%)	137~(98%)	3(2%)	0	100	100
1	D	137/148~(93%)	136 (99%)	1 (1%)	0	100	100
1	Е	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	Н	141/148~(95%)	140 (99%)	1 (1%)	0	100	100
1	Ι	141/148~(95%)	141 (100%)	0	0	100	100



001000	Contributed from precious page									
Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	\mathbf{ntiles}			
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 (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	А	110/113~(97%)	110 (100%)	0	100 100
1	В	110/113~(97%)	110 (100%)	0	100 100
1	С	111/113~(98%)	109 (98%)	2(2%)	54 32
1	D	109/113~(96%)	109 (100%)	0	100 100
1	Ε	110/113~(97%)	110 (100%)	0	100 100
1	F	109/113~(96%)	107~(98%)	2(2%)	54 32
1	G	110/113~(97%)	110 (100%)	0	100 100
1	Η	111/113~(98%)	111 (100%)	0	100 100
1	Ι	109/113~(96%)	108 (99%)	1 (1%)	75 63
1	J	111/113~(98%)	111 (100%)	0	100 100
All	All	1100/1130~(97%)	1095 (100%)	5 (0%)	86 80

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	С	8	ILE
1	С	101	GLU
1	F	5	ILE
1	F	14	LEU
1	Ι	5	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:



\mathbf{Mol}	Chain	\mathbf{Res}	Type
1	А	22	HIS
1	А	136	ASN
1	В	22	HIS
1	В	32	ASN
1	В	133	GLN
1	С	32	ASN
1	С	99	HIS
1	С	136	ASN
1	С	140	GLN
1	D	32	ASN
1	D	99	HIS
1	D	118	GLN
1	D	136	ASN
1	Е	133	GLN
1	F	22	HIS
1	F	32	ASN
1	F	99	HIS
1	F	133	GLN
1	G	32	ASN
1	G	99	HIS
1	G	136	ASN
1	Н	32	ASN
1	Н	118	GLN
1	Ι	32	ASN
1	Ι	118	GLN
1	Ι	136	ASN
1	J	136	ASN

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).

Mal	Type	Chain	Dog	Tink	B	ond leng	gths	E	ond ang	gles
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
3	PGE	С	151	-	9,9,9	0.40	0	8,8,8	0.47	0
3	PGE	J	151	-	9,9,9	0.44	0	8,8,8	0.39	0
3	PGE	Е	152	-	9,9,9	0.47	0	8,8,8	0.28	0
4	GOL	В	152	2	5,5,5	0.35	0	$5,\!5,\!5$	0.68	0
4	GOL	Н	152	2	$5,\!5,\!5$	0.50	0	$5,\!5,\!5$	1.44	2 (40%)
4	GOL	F	152	2	$5,\!5,\!5$	0.42	0	$5,\!5,\!5$	0.64	0
3	PGE	С	150	-	9,9,9	0.47	0	8,8,8	0.29	0
3	PGE	А	151	-	9,9,9	0.50	0	8,8,8	0.16	0
3	PGE	J	150	-	9,9,9	0.62	0	8,8,8	0.90	0
4	GOL	A	152	2	$5,\!5,\!5$	0.40	0	$5,\!5,\!5$	0.80	0
3	PGE	Е	151	-	9,9,9	0.48	0	8,8,8	0.22	0
3	PGE	G	150	-	9,9,9	0.43	0	8,8,8	0.34	0
4	GOL	E	153	2	$5,\!5,\!5$	0.41	0	$5,\!5,\!5$	0.94	0
4	GOL	G	151	-	$5,\!5,\!5$	0.37	0	$5,\!5,\!5$	0.46	0
3	PGE	Н	151	-	9,9,9	0.55	0	8,8,8	0.34	0
3	PGE	В	151	-	9,9,9	0.44	0	8,8,8	0.40	0
3	PGE	F	151	-	9,9,9	0.47	0	8,8,8	0.27	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	С	151	-	-	5/7/7/7	-
3	PGE	J	151	-	-	6/7/7/7	-
3	PGE	Е	152	-	-	4/7/7/7	-
4	GOL	В	152	2	-	2/4/4/4	-
4	GOL	Н	152	2	-	2/4/4/4	-
4	GOL	F	152	2	-	2/4/4/4	-



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PGE	С	150	-	-	3/7/7/7	-
3	PGE	А	151	-	-	3/7/7/7	-
3	PGE	J	150	-	-	4/7/7/7	-
4	GOL	А	152	2	-	3/4/4/4	-
3	PGE	Е	151	-	-	2/7/7/7	-
3	PGE	G	150	-	-	2/7/7/7	-
4	GOL	Е	153	2	-	2/4/4/4	-
4	GOL	G	151	-	-	0/4/4/4	-
3	PGE	Н	151	-	-	5/7/7/7	-
3	PGE	В	151	-	-	4/7/7/7	-
3	PGE	F	151	-	-	4/7/7/7	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	Н	152	GOL	O3-C3-C2	-2.31	99.97	110.38
4	Н	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	А	152	GOL	O1-C1-C2-O2
4	А	152	GOL	O1-C1-C2-C3
4	Е	153	GOL	O1-C1-C2-O2
4	Е	153	GOL	O1-C1-C2-C3
4	Н	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	Н	152	GOL	O2-C2-C3-O3
3	С	151	PGE	O3-C5-C6-O4
3	Н	151	PGE	O3-C5-C6-O4
3	J	151	PGE	O1-C1-C2-O2
3	J	151	PGE	O3-C5-C6-O4
3	Н	151	PGE	C1-C2-O2-C3
4	А	152	GOL	C1-C2-C3-O3
4	В	152	GOL	O1-C1-C2-C3



Mol	Chain	Res	Type	Atoms
3	G	150	PGE	O3-C5-C6-O4
3	J	150	PGE	O3-C5-C6-O4
3	С	151	PGE	O2-C3-C4-O3
3	Е	152	PGE	O3-C5-C6-O4
4	В	152	GOL	O1-C1-C2-O2
3	А	151	PGE	O1-C1-C2-O2
3	С	151	PGE	O1-C1-C2-O2
3	А	151	PGE	C3-C4-O3-C5
3	Е	152	PGE	C4-C3-O2-C2
3	J	151	PGE	C4-C3-O2-C2
3	В	151	PGE	C4-C3-O2-C2
3	С	151	PGE	C3-C4-O3-C5
3	G	150	PGE	C3-C4-O3-C5
3	F	151	PGE	C4-C3-O2-C2
3	Н	151	PGE	C3-C4-O3-C5
3	Е	152	PGE	O1-C1-C2-O2
3	С	151	PGE	C6-C5-O3-C4
3	J	151	PGE	C6-C5-O3-C4
3	В	151	PGE	C6-C5-O3-C4
3	J	150	PGE	C3-C4-O3-C5
3	J	151	PGE	O2-C3-C4-O3
3	Н	151	PGE	O1-C1-C2-O2
3	F	151	PGE	C6-C5-O3-C4
3	Е	152	PGE	C3-C4-O3-C5
3	Е	151	PGE	C6-C5-O3-C4
3	Е	151	PGE	O1-C1-C2-O2
3	В	151	PGE	O1-C1-C2-O2
4	F	152	GOL	C1-C2-C3-O3
4	F	152	GOL	O2-C2-C3-O3
3	С	150	PGE	O3-C5-C6-O4
3	С	150	PGE	C3-C4-O3-C5
3	F	151	PGE	C3-C4-O3-C5
3	С	150	PGE	O1-C1-C2-O2
3	А	151	PGE	C4-C3-O2-C2
3	J	151	PGE	C3-C4-O3-C5
3	В	151	PGE	C3-C4-O3-C5
3	Н	151	PGE	O2-C3-C4-O3

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There are no ring outliers.

7 monomers are involved in 29 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	С	151	PGE	7	0
4	В	152	GOL	5	0
4	Н	152	GOL	1	0
4	F	152	GOL	1	0
3	J	150	PGE	9	0
3	Е	151	PGE	2	0
4	Е	153	GOL	4	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 (i)

6.1 Protein, DNA and RNA chains (i)

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^{th} 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>	#RSRZ>2		$\mathbf{OWAB}(\mathrm{\AA}^2)$	Q < 0.9
1	А	137/148~(92%)	-0.27	1 (0%) 84 87		10, 18, 29, 32	2(1%)
1	В	137/148~(92%)	-0.30	1 (0%) 84 87		13,18,30,36	1 (0%)
1	С	138/148~(93%)	0.13	10 (7%) 23 24		13, 20, 35, 40	1 (0%)
1	D	137/148~(92%)	-0.10	4 (2%) 54 57		12, 18, 34, 43	1 (0%)
1	Е	138/148~(93%)	-0.15	3 (2%) 62 66		13, 18, 33, 42	1 (0%)
1	F	137/148~(92%)	-0.15	4 (2%) 54 57		14, 20, 32, 39	1 (0%)
1	G	140/148~(94%)	-0.30	3 (2%) 63 67		12, 18, 29, 43	2(1%)
1	Н	138/148~(93%)	-0.21	2 (1%) 73 77		13, 18, 29, 38	2(1%)
1	Ι	138/148~(93%)	0.12	6 (4%) 40 43		12, 21, 35, 38	2(1%)
1	J	138/148~(93%)	-0.21	1 (0%) 84 87		13, 18, 29, 34	1 (0%)
All	All	1378/1480~(93%)	-0.14	35 (2%) 58 62		10, 19, 32, 43	14 (1%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	С	81	GLY	5.5
1	Е	145	PHE	4.7
1	Н	145	PHE	4.6
1	С	79	VAL	4.4
1	Ι	134	TYR	4.4
1	С	83	THR	4.0
1	С	134	TYR	3.4
1	Ι	83	THR	3.3
1	D	145	PHE	3.2
1	В	144	VAL	3.1
1	G	4	GLY	3.0
1	С	145	PHE	3.0
1	J	145	PHE	2.8



Mol	Chain	Res	Type	RSRZ
1	С	84	VAL	2.7
1	D	80	PRO	2.6
1	Ι	79	VAL	2.5
1	С	133	GLN	2.5
1	Н	144	VAL	2.5
1	С	85	ALA	2.5
1	С	82	ASP	2.4
1	F	144	VAL	2.4
1	Ι	145	PHE	2.3
1	F	105	ASP	2.2
1	Е	103	GLY	2.2
1	Ι	81	GLY	2.2
1	G	5	ILE	2.2
1	D	85	ALA	2.2
1	С	80	PRO	2.2
1	F	5	ILE	2.2
1	Ι	85	ALA	2.2
1	А	70	ASP	2.2
1	D	84	VAL	2.2
1	F	98	GLU	2.1
1	G	3	LYS	2.1
1	Е	144	VAL	2.1

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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
3	PGE	С	151	10/10	0.77	0.18	$38,\!41,\!47,\!48$	0



Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
4	GOL	Н	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	Е	153	6/6	0.83	0.16	34,35,37,39	0
3	PGE	В	151	10/10	0.84	0.17	47,47,49,49	0
3	PGE	Е	152	10/10	0.84	0.16	44,46,48,49	0
3	PGE	Н	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	В	152	6/6	0.86	0.14	34,39,40,41	0
3	PGE	F	151	10/10	0.87	0.15	51,51,53,54	0
3	PGE	Е	151	10/10	0.87	0.13	44,45,45,45	0
3	PGE	С	150	10/10	0.88	0.13	40,41,42,43	0
3	PGE	А	151	10/10	0.88	0.13	48,49,50,51	0
3	PGE	J	151	10/10	0.89	0.14	48,50,52,53	0
4	GOL	А	152	6/6	0.89	0.14	$27,\!33,\!35,\!39$	0
2	NA	F	149	1/1	0.93	0.10	27,27,27,27	0
2	NA	Е	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	Н	150	1/1	0.94	0.08	$25,\!25,\!25,\!25$	0
2	NA	F	150	1/1	0.95	0.07	28,28,28,28	0
2	NA	В	150	1/1	0.96	0.09	26,26,26,26	0
2	NA	А	150	1/1	0.96	0.09	27,27,27,27	0
2	NA	D	149	1/1	0.97	0.05	20,20,20,20	0
2	NA	В	149	1/1	0.97	0.09	22,22,22,22	0
2	NA	G	149	1/1	0.98	0.06	22,22,22,22	0
2	NA	Н	149	1/1	0.98	0.05	23,23,23,23	0
2	NA	С	149	1/1	0.98	0.04	24,24,24,24	0
2	NA	А	149	1/1	0.98	0.09	23,23,23,23	0
2	NA	Е	149	1/1	0.98	0.08	24,24,24,24	0
2	NA	J	149	1/1	0.99	0.03	22,22,22,22	0
2	NA	Ι	149	1/1	0.99	0.04	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.

