

Full wwPDB X-ray Structure Validation Report (i)

Jun 17, 2024 – 05:23 PM EDT

PDB ID	:	3K12
Title	:	Crystal structure of an uncharacterized protein A6V7T0 from Pseudomonas
Authors	:	aeruginosa Ho, M.; Ramagopal, U.A.; Toro, R.; Burley, S.K.; Almo, S.C.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on Resolution		2009-09-25 1.49 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:

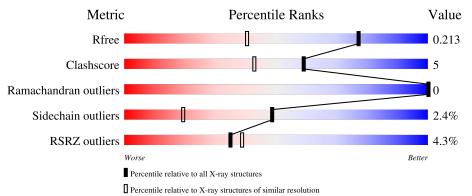
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 1.49 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R_{free}	130704	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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		100	2%	
1	A	122	85%	8% • 6%
1	В	122	88%	5% • 7%
1	С	122	2%	
1	U	122	<u> </u>	11% • 6%
1	D	122	86%	11% ••
1	Е	100	3%	
	Ľ	122	86%	7% • 6%



Mol	Chain	Length	Quality of chain		
			6%		
1	F	122	89%	••	7%

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
2	GOL	С	1	-	-	Х	-
2	GOL	Е	1	-	-	Х	-



2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 6232 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	А	115	Total	С	Ν	0	S	Se	0	7	0
	Л	115	965	600	184	178	1	2	0	1	0
1	В	114	Total	С	Ν	Ο	\mathbf{S}	Se	0	1	0
	D	114	920	572	175	170	1	2	0	1	0
1	C	115	Total	С	Ν	Ο	\mathbf{S}	Se	0	2	0
	U	110	933	579	176	175	1	2	0	2	0
1	D	120	Total	С	Ν	Ο	\mathbf{S}	Se	0	2	0
1	D	120	981	608	191	179	1	2	0	0 2	0
1	Е	115	Total	С	Ν	Ο	\mathbf{S}	Se	0	1	0
1		115	929	577	176	173	1	2	0	1	0
1	F	114	Total	С	Ν	Ο	\mathbf{S}	Se	0	3	0
		114	933	580	179	171	1	2		5	0

• Molecule 1 is a protein called uncharacterized protein A6V7T0.

There are 48 discrepancies between the modelled and reference sequences:

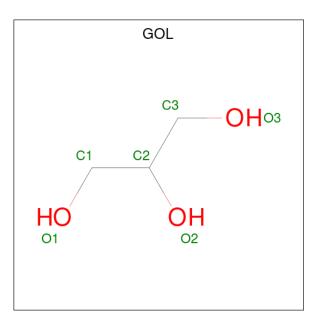
Residue	Modelled	Actual	Comment	Reference
118	GLU	-	expression tag	UNP Q9I3E9
119	GLY	-	expression tag	UNP Q9I3E9
120	HIS	-	expression tag	UNP Q9I3E9
121	HIS	-	expression tag	UNP Q9I3E9
122	HIS	-	expression tag	UNP Q9I3E9
123	HIS	-	expression tag	UNP Q9I3E9
124	HIS	-	expression tag	UNP Q9I3E9
125	HIS	-	expression tag	UNP Q9I3E9
118	GLU	-	expression tag	UNP Q9I3E9
119	GLY	-	expression tag	UNP Q9I3E9
120	HIS	-	expression tag	UNP Q9I3E9
121	HIS	-	expression tag	UNP Q9I3E9
122	HIS	-	expression tag	UNP Q9I3E9
123	HIS	-	expression tag	UNP Q9I3E9
124	HIS	-	expression tag	UNP Q9I3E9
125	HIS	-	expression tag	UNP Q9I3E9
118	GLU	-	expression tag	UNP Q9I3E9
	$\begin{array}{c} 118 \\ 119 \\ 120 \\ 121 \\ 122 \\ 123 \\ 124 \\ 125 \\ 118 \\ 119 \\ 120 \\ 121 \\ 122 \\ 123 \\ 124 \\ 125 \\ \end{array}$	118 GLU 119 GLY 120 HIS 121 HIS 122 HIS 123 HIS 124 HIS 125 HIS 119 GLU 119 GLY 120 HIS 121 HIS 124 HIS 125 HIS 118 GLU 119 GLY 120 HIS 121 HIS 122 HIS 123 HIS 123 HIS 124 HIS 125 HIS 124 HIS 125 HIS	118 GLU - 119 GLY - 120 HIS - 121 HIS - 121 HIS - 122 HIS - 123 HIS - 124 HIS - 125 HIS - 118 GLU - 119 GLY - 120 HIS - 121 HIS - 123 HIS - 124 HIS - 125 HIS - 120 HIS - 121 HIS - 122 HIS - 123 HIS - 124 HIS - 125 HIS -	118GLU-expression tag119GLY-expression tag120HIS-expression tag121HIS-expression tag122HIS-expression tag123HIS-expression tag124HIS-expression tag125HIS-expression tag118GLU-expression tag119GLY-expression tag120HIS-expression tag121HIS-expression tag122HIS-expression tag123HIS-expression tag123HIS-expression tag124HIS-expression tag125HIS-expression tag124HIS-expression tag125HIS-expression tag125HIS-expression tag



Chain	Residue	Modelled	Actual	Comment	Reference
С	119	GLY	-	expression tag	UNP Q9I3E9
С	120	HIS	-	expression tag	UNP Q9I3E9
С	121	HIS	_	expression tag	UNP Q9I3E9
С	122	HIS	_	expression tag	UNP Q9I3E9
С	123	HIS	-	expression tag	UNP Q9I3E9
С	124	HIS	_	expression tag	UNP Q9I3E9
С	125	HIS	_	expression tag	UNP Q9I3E9
D	118	GLU	_	expression tag	UNP Q9I3E9
D	119	GLY	_	expression tag	UNP Q9I3E9
D	120	HIS	_	expression tag	UNP Q9I3E9
D	121	HIS	-	expression tag	UNP Q9I3E9
D	122	HIS	-	expression tag	UNP Q9I3E9
D	123	HIS	-	expression tag	UNP Q9I3E9
D	124	HIS	_	expression tag	UNP Q9I3E9
D	125	HIS	-	expression tag	UNP Q9I3E9
Е	118	GLU	_	expression tag	UNP Q9I3E9
Е	119	GLY	-	expression tag	UNP Q9I3E9
Е	120	HIS	-	expression tag	UNP Q9I3E9
Е	121	HIS	_	expression tag	UNP Q9I3E9
Е	122	HIS	_	expression tag	UNP Q9I3E9
Е	123	HIS	_	expression tag	UNP Q9I3E9
Ε	124	HIS	_	expression tag	UNP Q9I3E9
Ε	125	HIS	_	expression tag	UNP Q9I3E9
F	118	GLU	-	expression tag	UNP Q9I3E9
F	119	GLY	-	expression tag	UNP Q9I3E9
F	120	HIS	-	expression tag	UNP Q9I3E9
F	121	HIS	-	expression tag	UNP Q9I3E9
F	122	HIS	_	expression tag	UNP Q9I3E9
F	123	HIS	-	expression tag	UNP Q9I3E9
F	124	HIS	-	expression tag	UNP Q9I3E9
F	125	HIS	-	expression tag	UNP Q9I3E9

• Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).





Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	С	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0
2	Е	1	$\begin{array}{ccc} \text{Total} & \text{C} & \text{O} \\ 6 & 3 & 3 \end{array}$	0	0

• Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	А	116	Total O 116 116	0	0
3	В	90	Total O 90 90	0	0
3	С	83	Total O 83 83	0	0
3	D	89	Total O 89 89	0	0
3	Е	114	Total O 114 114	0	0
3	F	67	$\begin{array}{cc} \text{Total} & \text{O} \\ 67 & 67 \end{array}$	0	0



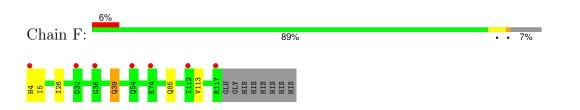
3 Residue-property plots (i)

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.

- Chain A: 85% 8% • 6% SIH SIH SIH SIH SIH SIH SIH • Molecule 1: uncharacterized protein A6V7T0 Chain B: 88% 5% • 7% GLU GLY HIS HIS HIS HIS HIS HIS HIS • Molecule 1: uncharacterized protein A6V7T0 Chain C: 81% 11% 6% • Molecule 1: uncharacterized protein A6V7T0 Chain D: 86% 11% • Molecule 1: uncharacterized protein A6V7T0 Chain E: 86% 7% • 6%
- Molecule 1: uncharacterized protein A6V7T0

• Molecule 1: uncharacterized protein A6V7T0







4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants	78.72Å 86.55Å 104.90Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 - 1.49	Depositor
Resolution (A)	37.92 - 1.49	EDS
% Data completeness	99.8 (50.00-1.49)	Depositor
(in resolution range)	99.8 (37.92-1.49)	EDS
R _{merge}	0.09	Depositor
R _{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.95 (at 1.49 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.5.0089	Depositor
D D.	0.188 , 0.214	Depositor
R, R_{free}	0.187 , 0.213	DCC
R_{free} test set	5868 reflections (5.01%)	wwPDB-VP
Wilson B-factor $(Å^2)$	18.0	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$, $B_{sol}(Å^2)$	0.41 , 48.9	EDS
L-test for twinning ²	$ \langle L \rangle = 0.50, \langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6232	wwPDB-VP
Average B, all atoms $(Å^2)$	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.78% 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: GOL

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	Bo	nd angles
	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.60	0/1000	0.78	3/1349~(0.2%)
1	В	0.54	0/937	0.67	0/1266
1	С	0.58	0/953	0.70	0/1288
1	D	0.58	0/1005	0.71	1/1357~(0.1%)
1	Ε	0.58	0/946	0.71	0/1278
1	F	0.54	0/956	0.66	0/1291
All	All	0.57	0/5797	0.71	4/7829~(0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	D	19	LEU	CA-CB-CG	5.59	128.15	115.30
1	А	106	ARG	NE-CZ-NH1	-5.53	117.54	120.30
1	А	95	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	А	37	ASP	CB-CG-OD1	5.05	122.84	118.30

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	965	0	967	5	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	В	920	0	910	6	0
1	С	933	0	918	13	0
1	D	981	0	958	13	0
1	Е	929	0	916	14	0
1	F	933	0	929	5	0
2	С	6	0	8	6	0
2	Ε	6	0	8	6	0
3	А	116	0	0	0	0
3	В	90	0	0	1	0
3	С	83	0	0	1	0
3	D	89	0	0	1	0
3	Ε	114	0	0	2	0
3	F	67	0	0	1	0
All	All	6232	0	5614	53	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 5.

All (53) 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:A:48:ASN:OD1	1:A:51[A]:ARG:NH2	1.94	0.99
1:E:97:CYS:H	2:E:1:GOL:H32	1.27	0.99
1:D:62:GLN:HE22	1:D:118:GLU:H	1.02	0.93
1:C:48[B]:ASN:ND2	3:C:489:HOH:O	2.05	0.88
1:E:85[A]:GLN:HG3	3:E:152:HOH:O	1.78	0.82
1:C:39:GLN:HE21	1:C:39:GLN:H	1.28	0.82
1:B:87:PHE:O	3:B:558:HOH:O	1.99	0.80
2:C:1:GOL:O1	1:D:14:ARG:NH2	2.15	0.80
1:A:39:GLN:H	1:A:39:GLN:HE21	1.27	0.79
1:C:95:ARG:HE	2:C:1:GOL:H11	1.48	0.77
1:F:39:GLN:HE21	1:F:39:GLN:H	1.35	0.75
1:C:97:CYS:HB3	2:C:1:GOL:H2	1.69	0.75
1:B:39:GLN:HE21	1:B:39:GLN:H	1.33	0.74
1:E:39:GLN:HE21	1:E:39:GLN:H	1.32	0.73
1:C:95:ARG:HE	2:C:1:GOL:C1	2.05	0.69
1:D:39:GLN:HE21	1:D:39:GLN:H	1.41	0.67
1:E:97:CYS:N	2:E:1:GOL:H32	2.08	0.62
1:E:97:CYS:H	2:E:1:GOL:C3	2.09	0.62
1:D:39:GLN:O	1:D:43:ARG:HG3	2.00	0.61
1:D:43:ARG:O	1:D:47[B]:GLU:HG3	2.02	0.60



Continued from previ Atom-1	Atom-2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:62:GLN:NE2	1:D:118:GLU:H	1.87	0.59
1:E:97:CYS:HB3	2:E:1:GOL:C1	2.33	0.59
1:E:56:VAL:O	1:E:117:ARG:HD2	2.05	0.56
1:A:35[A]:SER:OG	1:E:73:ARG:NH1	2.39	0.56
1:E:97:CYS:HB3	2:E:1:GOL:H12	1.89	0.55
1:F:85[B]:GLN:HG3	3:F:525:HOH:O	2.07	0.55
1:F:39:GLN:H	1:F:39:GLN:NE2	2.02	0.54
1:C:62:GLN:HE22	1:C:118:GLU:H	1.56	0.54
1:C:39:GLN:H	1:C:39:GLN:NE2	2.01	0.53
1:A:17:MSE:HG2	1:A:26:ILE:HG12	1.92	0.52
1:B:56:VAL:O	1:B:117:ARG:HD3	2.09	0.51
1:A:39:GLN:H	1:A:39:GLN:NE2	2.03	0.50
2:C:1:GOL:O1	1:D:14:ARG:CZ	2.63	0.47
1:E:97:CYS:HB3	2:E:1:GOL:H11	1.96	0.47
1:C:26:ILE:HB	1:C:113:VAL:HB	1.96	0.46
1:C:34:PRO:HG2	1:C:106:ARG:HE	1.80	0.46
1:D:121:HIS:HB2	3:D:340:HOH:O	2.16	0.46
1:D:119:GLY:HA3	1:D:121:HIS:CE1	2.51	0.46
1:B:39:GLN:H	1:B:39:GLN:NE2	2.09	0.46
1:B:19:LEU:HD22	1:B:24:VAL:HG22	1.99	0.45
1:C:99:LEU:HD12	1:D:101:GLU:CD	2.36	0.45
1:E:26:ILE:HB	1:E:113:VAL:HB	1.99	0.45
1:E:85[A]:GLN:CG	3:E:152:HOH:O	2.49	0.45
1:E:39:GLN:H	1:E:39:GLN:NE2	2.05	0.45
1:C:4:HIS:CD2	1:C:4:HIS:N	2.84	0.45
1:D:104:ASP:HB3	1:D:107:TRP:CD2	2.52	0.44
1:F:26:ILE:HB	1:F:113:VAL:HB	2.01	0.43
1:D:43:ARG:HG2	1:D:43:ARG:NH2	2.34	0.43
1:D:26:ILE:HB	1:D:113:VAL:HB	2.02	0.41
1:C:95:ARG:NE	2:C:1:GOL:H11	2.26	0.41
1:C:104:ASP:HB3	1:C:107:TRP:CD2	2.55	0.41
1:E:104:ASP:HB3	1:E:107:TRP:CD2	2.55	0.41
1:B:116:ALA:HB3	1:F:5:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.



5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
1	А	120/122~(98%)	119 (99%)	1 (1%)	0	100	100
1	В	113/122~(93%)	112 (99%)	1 (1%)	0	100	100
1	С	115/122~(94%)	112 (97%)	3~(3%)	0	100	100
1	D	120/122~(98%)	117 (98%)	3~(2%)	0	100	100
1	Е	114/122~(93%)	111 (97%)	3~(3%)	0	100	100
1	F	$115/122 \ (94\%)$	113 (98%)	2(2%)	0	100	100
All	All	697/732~(95%)	684 (98%)	13 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	104/101~(103%)	101~(97%)	3~(3%)	42 13
1	В	97/101~(96%)	96~(99%)	1 (1%)	76 57
1	С	99/101~(98%)	95~(96%)	4 (4%)	31 6
1	D	103/101~(102%)	100~(97%)	3~(3%)	42 13
1	Е	98/101~(97%)	97~(99%)	1 (1%)	76 57
1	F	99/101~(98%)	97~(98%)	2(2%)	55 25
All	All	600/606~(99%)	586~(98%)	14~(2%)	49 20



Mol	Chain	Res	Type
1	А	4	HIS
1	А	39	GLN
1	А	117	ARG
1	В	39	GLN
1	С	4	HIS
1	С	39	GLN
1	С	54	GLN
1	С	117	ARG
1	D	19	LEU
1	D	39	GLN
1	D	50	ASP
1	Е	39	GLN
1	F	4	HIS
1	F	39	GLN

All (14) residues with a non-rotameric sidechain are listed below:

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	4	HIS
1	А	22	ASN
1	А	39	GLN
1	А	81	GLN
1	В	39	GLN
1	В	81	GLN
1	С	4	HIS
1	C C C C	22	ASN
1	С	39	GLN
1	С	54	GLN
1	С	62	GLN
1	С	81	GLN
1	D	39	GLN
1	D	62	GLN
1	D	81	GLN
1	D	121	HIS
1	Е	39	GLN
1	Е	81	GLN
1	F	39	GLN
1	F	81	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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	Mol Type Chain R	Chain Re		Link	B	ond leng	gths	В	ond ang	gles
IVIOI	туре	Chain	Res	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
2	GOL	С	1	-	$5,\!5,\!5$	0.28	0	$5,\!5,\!5$	1.27	1 (20%)
2	GOL	Е	1	-	$5,\!5,\!5$	0.66	0	$5,\!5,\!5$	0.76	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	GOL	С	1	-	-	1/4/4/4	-
2	GOL	Е	1	-	-	3/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	С	1	GOL	O2-C2-C3	2.21	118.33	109.18

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	Ε	1	GOL	C1-C2-C3-O3
2	Ε	1	GOL	O2-C2-C3-O3
2	С	1	GOL	O1-C1-C2-C3
2	Е	1	GOL	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	С	1	GOL	6	0
2	Е	1	GOL	6	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	$\langle RSRZ \rangle$	# RSRZ > 2	$OWAB(Å^2)$	Q<0.9
1	А	113/122~(92%)	0.19	3 (2%) 54 59	11, 16, 25, 38	0
1	В	112/122 (91%)	0.26	5 (4%) 33 36	12, 19, 27, 35	0
1	С	113/122 (92%)	0.29	3 (2%) 54 59	11, 18, 28, 36	0
1	D	118/122~(96%)	0.20	7 (5%) 22 24	11, 17, 29, 43	0
1	Е	113/122 (92%)	0.09	4 (3%) 44 48	11, 16, 25, 37	0
1	F	112/122 (91%)	0.45	7 (6%) 20 21	12, 22, 31, 38	0
All	All	681/732~(93%)	0.25	29 (4%) 35 39	11, 18, 29, 43	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	120	HIS	6.2
1	F	4	HIS	5.9
1	С	4	HIS	5.6
1	А	4	HIS	5.5
1	В	4	HIS	5.3
1	D	121	HIS	5.2
1	Е	4	HIS	5.1
1	D	122	HIS	3.9
1	А	118	GLU	3.9
1	D	4	HIS	3.6
1	D	119	GLY	3.0
1	С	112	ILE	2.9
1	С	118	GLU	2.8
1	F	74	GLU	2.7
1	F	54	GLN	2.7
1	В	114	VAL	2.6
1	F	32	ASP	2.4
1	В	21	GLY	2.4
1	F	117	ARG	2.4



Mol	Chain	Res	Type	RSRZ
1	F	112	ILE	2.3
1	Е	118	GLU	2.3
1	В	66	VAL	2.2
1	Е	112	ILE	2.2
1	F	36	GLY	2.1
1	В	112	ILE	2.0
1	D	112	ILE	2.0
1	Е	66	VAL	2.0
1	А	66	VAL	2.0
1	D	35	SER	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 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
2	GOL	Е	1	6/6	0.66	0.25	$28,\!31,\!33,\!35$	0
2	GOL	С	1	6/6	0.78	0.18	29,32,33,34	0

6.5 Other polymers (i)

There are no such residues in this entry.

