

wwPDB X-ray Structure Validation Summary Report (i)

Jan 17, 2023 – 10:55 AM EST

PDB ID	:	2GB3
Title	:	Crystal structure of Aspartate aminotransferase (tm1698) from Thermotoga
		maritima at 2.50 A resolution
Authors	:	Joint Center for Structural Genomics (JCSG)
Deposited on	:	2006-03-09
Resolution	:	2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
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)	:	2.31.2

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 2.50 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	Similar resolution		
	$(\# { m Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$		
R_{free}	130704	4661 (2.50-2.50)		
Clashscore	141614	5346 (2.50-2.50)		
Ramachandran outliers	138981	$5231 \ (2.50-2.50)$		
Sidechain outliers	138945	5233 (2.50-2.50)		
RSRZ outliers	127900	4559 (2.50-2.50)		

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		
		10.0	3%		_
1	А	409	87%	7% • 5	%
			4%		
1	В	409	88%	8% •	•
			2%		
1	С	409	88%	8%	•
			5%		
1	D	409	87%	8% 5	%
			4%		
1	E	409	89%	7%	•



Mol	Chain	Length	Quality of chain		
			3%		
1	F	409	86%	9%	5%



2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18415 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			Ato	ms				ZeroOcc	AltConf	Trace
1	Δ	280	Total	С	Ν	0	Р	S	Se	0	0 2	0
1	A	369	3047	1968	513	551	1	5	9	0	5	0
1	р	204	Total	С	Ν	0	Р	S	Se	0	1	0
1	I D	394	3070	1985	514	556	1	5	9	0	L	0
1	1 C	391	Total	С	Ν	0	Р	S	Se	0	1	0
1			3047	1969	508	556	1	5	8	0	T	0
1	л	390	Total	С	Ν	0	Р	S	Se	0	0	0
1	D		3012	1943	495	562	1	4	7	0	0	0
1	F	202	Total	С	Ν	0	Р	S	Se	0	0	0
	393	3031	1959	502	557	1	5	7	0	0	0	
1	1 E	280	Total	С	Ν	0	Р	S	Se	0	0	0
	389	3018	1953	504	547	1	5	8	U	0	0	

• Molecule 1 is a protein called aspartate aminotransferase.

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Actual Comment	
А	-11	MSE	-	expression tag	GB 4982275
А	-10	GLY	-	expression tag	GB 4982275
А	-9	SER	-	expression tag	GB 4982275
А	-8	ASP	-	expression tag	GB 4982275
А	-7	LYS	-	expression tag	GB 4982275
А	-6	ILE	-	expression tag	GB 4982275
А	-5	HIS	-	expression tag	GB 4982275
А	-4	HIS	-	expression tag	GB 4982275
А	-3	HIS	-	expression tag	GB 4982275
А	-2	HIS	-	expression tag	GB 4982275
А	-1	HIS	-	expression tag	GB 4982275
А	0	HIS	-	expression tag	GB 4982275
А	1	MSE	MET	modified residue	GB 4982275
А	25	MSE	MET	modified residue	GB 4982275
А	145	MSE	MET	modified residue	GB 4982275
А	184	MSE	MET	modified residue	GB 4982275
А	232	LLP	LYS	modified residue	GB 4982275



Chain	Besidue	Modelled	Actual	Comment	Reference
Δ	256	MSE	MET	modified residue	GB 4982275
Δ	335	MSE	MET	modified residue	GB 4982275
	3/1	MSE	MET	modified residue	GB 4982275
	347	MSE	MET	modified residue	CB 4982275
	384	MSE	MET	modified residue	GD 4982275
	280	MSE	MET	modified residue	GD 4982275
A D	11	MSE		avanagion tog	GD 4982275
D	-11	M5E CLV	-	expression tag	GD 4982273
	-10	GLI	-	expression tag	GD 4962275
B	-9	SER ACD	-	expression tag	GB 4982275
B	-8	ASP	-	expression tag	GB 4982275
B	-7		-	expression tag	GB 4982275
В	-6	ILE	-	expression tag	GB 4982275
B	-5	HIS	-	expression tag	GB 4982275
B	-4	HIS	-	expression tag	GB 4982275
В	-3	HIS	-	expression tag	GB 4982275
В	-2	HIS	-	expression tag	GB 4982275
В	-1	HIS	-	expression tag	GB 4982275
В	0	HIS	-	expression tag	GB 4982275
В	1	MSE	MET	modified residue	GB 4982275
В	25	MSE	MET	modified residue	GB 4982275
В	145	MSE	MET	modified residue	GB 4982275
В	184	MSE	MET	modified residue	GB 4982275
В	232	LLP	LYS	modified residue	GB 4982275
В	256	MSE	MET	modified residue	GB 4982275
В	335	MSE	MET	modified residue	GB 4982275
В	341	MSE	MET	modified residue	GB 4982275
В	347	MSE	MET	modified residue	GB 4982275
В	384	MSE	MET	modified residue	GB 4982275
В	389	MSE	MET	modified residue	GB 4982275
С	-11	MSE	-	expression tag	GB 4982275
С	-10	GLY	_	expression tag	GB 4982275
С	-9	SER	_	expression tag	GB 4982275
С	-8	ASP	-	expression tag	GB 4982275
С	-7	LYS	-	expression tag	GB 4982275
С	-6	ILE	-	expression tag	GB 4982275
C	-5	HIS	_	expression tag	GB 4982275
С	-4	HIS	_	expression tag	GB 4982275
C	-3	HIS	_	expression tag	GB 4982275
C	-2	HIS	-	expression tag	GB 4982275
C	-1	HIS	_	expression tag	GB 4982275
C	0	HIS	_	expression tag	GB 4982275
C	1	MSE	MET	modified residue	GB 4982275
. ~					



	Desidere	Madallad	Asteral	Comment	Defense
Chain	Residue	Modelled	Actual	Comment	Reference
C	25	MSE	MET	modified residue	GB 4982275
C	145	MSE	MET	modified residue	GB 4982275
С	184	MSE	MET	modified residue	GB 4982275
C	232	LLP	LYS	modified residue	GB 4982275
C	256	MSE	MET	modified residue	GB 4982275
С	335	MSE	MET	modified residue	GB 4982275
C	341	MSE	MET	modified residue	GB 4982275
С	347	MSE	MET	modified residue	GB 4982275
С	384	MSE	MET	modified residue	GB 4982275
С	389	MSE	MET	modified residue	GB 4982275
D	-11	MSE	-	expression tag	GB 4982275
D	-10	GLY	-	expression tag	GB 4982275
D	-9	SER	-	expression tag	GB 4982275
D	-8	ASP	-	expression tag	GB 4982275
D	-7	LYS	-	expression tag	GB 4982275
D	-6	ILE	-	expression tag	GB 4982275
D	-5	HIS	-	expression tag	GB 4982275
D	-4	HIS	-	expression tag	GB 4982275
D	-3	HIS	-	expression tag	GB 4982275
D	-2	HIS	-	expression tag	GB 4982275
D	-1	HIS	-	expression tag	GB 4982275
D	0	HIS	-	expression tag	GB 4982275
D	1	MSE	MET	modified residue	GB 4982275
D	25	MSE	MET	modified residue	GB 4982275
D	145	MSE	MET	modified residue	GB 4982275
D	184	MSE	MET	modified residue	GB 4982275
D	232	LLP	LYS	modified residue	GB 4982275
D	256	MSE	MET	modified residue	GB 4982275
D	335	MSE	MET	modified residue	GB 4982275
D	341	MSE	MET	modified residue	GB 4982275
D	347	MSE	MET	modified residue	GB 4982275
D	384	MSE	MET	modified residue	GB 4982275
D	389	MSE	MET	modified residue	GB 4982275
Е	-11	MSE	_	expression tag	GB 4982275
Е	-10	GLY	_	expression tag	GB 4982275
Е	-9	SER	_	expression tag	GB 4982275
Е	-8	ASP	-	expression tag	GB 4982275
Е	-7	LYS	_	expression tag	GB 4982275
Е	-6	ILE	-	expression tag	GB 4982275
Е	-5	HIS	-	expression tag	GB 4982275
E	-4	HIS	-	expression tag	GB 4982275
E	-3	HIS	-	expression tag	GB 4982275



Chain	Residue	Modelled	Actual	Comment	Reference
Е	-2	HIS	-	expression tag	GB 4982275
Е	-1	HIS	-	expression tag	GB 4982275
Е	0	HIS	-	expression tag	GB 4982275
Е	1	MSE	MET	modified residue	GB 4982275
Е	25	MSE	MET	modified residue	GB 4982275
Е	145	MSE	MET	modified residue	GB 4982275
Е	184	MSE	MET	modified residue	GB 4982275
Е	232	LLP	LYS	modified residue	GB 4982275
Е	256	MSE	MET	modified residue	GB 4982275
Е	335	MSE	MET	modified residue	GB 4982275
Е	341	MSE	MET	modified residue	GB 4982275
Е	347	MSE	MET	modified residue	GB 4982275
Е	384	MSE	MET	modified residue	GB 4982275
Е	389	MSE	MET	modified residue	GB 4982275
F	-11	MSE	-	expression tag	GB 4982275
F	-10	GLY	-	expression tag	GB 4982275
F	-9	SER	-	expression tag	GB 4982275
F	-8	ASP	-	expression tag	GB 4982275
F	-7	LYS	-	expression tag	GB 4982275
F	-6	ILE	-	expression tag	GB 4982275
F	-5	HIS	-	expression tag	GB 4982275
F	-4	HIS	-	expression tag	GB 4982275
F	-3	HIS	-	expression tag	GB 4982275
F	-2	HIS	-	expression tag	GB 4982275
F	-1	HIS	-	expression tag	GB 4982275
F	0	HIS	-	expression tag	GB 4982275
F	1	MSE	MET	modified residue	GB 4982275
F	25	MSE	MET	modified residue	GB 4982275
F	145	MSE	MET	modified residue	GB 4982275
F	184	MSE	MET	modified residue	GB 4982275
F	232	LLP	LYS	modified residue	GB 4982275
F	256	MSE	MET	modified residue	GB 4982275
F	335	MSE	MET	modified residue	GB 4982275
F	341	MSE	MET	modified residue	GB 4982275
F	347	MSE	MET	modified residue	GB 4982275
F	384	MSE	MET	modified residue	GB 4982275
F	389	MSE	MET	modified residue	GB 4982275

• Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	А	33	Total O 33 33	0	0
			Co	ntinued on r	pert nage



Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	В	38	Total O 38 38	0	0
2	С	31	Total O 31 31	0	0
2	D	18	Total O 18 18	0	0
2	Е	28	TotalO2828	0	0
2	F	42	$\begin{array}{cc} \text{Total} & \text{O} \\ 42 & 42 \end{array}$	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.



• Molecule 1: aspartate aminotransferase







• Molecule 1: aspartate aminotransferase

C	Ch	ai	n	F:	39	6											8	6%										•	9%)	5'	%			
MSE	GLY	SER	LYS	ILE	SIH	SIH	SIH	MSE	ASP	V3	V8	E12	E13	S14	K28	133	Y63	AG7	E101	L118	1139	E161	P174	Y179	M184 P185	D201	S205	E206	L217	S218 T240	CT 7T	K223	V226	V230	
K232		A236	A239	R240	T246	1252		Q QZW	R262	L263	E269	E296	T297	V298	L302	E329	A332	N340	M347	R366	■ 1380	M384	L387	M389	F390 C391 SFR	SER	ILE SER	CYS							



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	75.09Å 214.05 Å 76.84 Å	Deperitor
a, b, c, α , β , γ	90.00° 112.31° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	107.03 - 2.50	Depositor
Resolution (A)	107.03 - 2.50	EDS
% Data completeness	97.5 (107.03-2.50)	Depositor
(in resolution range)	97.8 (107.03-2.50)	EDS
R _{merge}	0.14	Depositor
R _{sym}	0.14	Depositor
$< I/\sigma(I) > 1$	$1.39 (at 2.48 \text{\AA})$	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
D D	0.229 , 0.266	Depositor
Λ, Λ_{free}	0.237 , 0.270	DCC
R_{free} test set	3791 reflections $(5.01%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	36.8	Xtriage
Anisotropy	0.536	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.33 , 66.5	EDS
L-test for $twinning^2$	$< L >=0.47, < L^2>=0.30$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18415	wwPDB-VP
Average B, all atoms $(Å^2)$	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 75.86 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1638e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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: LLP

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).

Mal	Chain	Bond	lengths	Bo	ond angles
MIOI	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.43	0/3083	0.74	1/4163~(0.0%)
1	В	0.42	0/3104	0.75	0/4191
1	С	0.44	0/3077	0.73	0/4157
1	D	0.39	0/3042	0.72	1/4118~(0.0%)
1	Е	0.43	0/3062	0.74	1/4143~(0.0%)
1	F	0.46	0/3048	0.75	0/4119
All	All	0.43	0/18416	0.74	3/24891~(0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	D	240	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	Е	7	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	А	384	MSE	CA-CB-CG	-5.15	104.55	113.30

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	3047	0	3008	21	0
1	В	3070	0	3025	22	0



	<u> </u>	1	1 5			
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	С	3047	0	2997	26	0
1	D	3012	0	2914	22	0
1	Е	3031	0	2938	19	0
1	F	3018	0	2974	29	0
2	А	33	0	0	0	0
2	В	38	0	0	1	0
2	С	31	0	0	0	0
2	D	18	0	0	0	0
2	Е	28	0	0	1	0
2	F	42	0	0	1	0
All	All	18415	0	17856	133	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 4.

The worst 5 of 133 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:D:346:THR:HG21	1:D:379:ALA:O	1.86	0.75
1:D:34:HIS:HB2	1:D:346:THR:HG22	1.70	0.73
1:B:33:ILE:HG21	1:B:347:MSE:HE3	1.71	0.71
1:E:112:ASN:HD22	1:E:113:PRO:HD2	1.54	0.70
1:C:254:HIS:HB3	1:D:8:VAL:HG21	1.77	0.66

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	389/409~(95%)	376 (97%)	10 (3%)	3 (1%)	19	35
1	В	392/409~(96%)	380~(97%)	10 (3%)	2(0%)	29	48



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
1	С	389/409~(95%)	376~(97%)	12 (3%)	1 (0%)	41	61
1	D	387/409~(95%)	373~(96%)	12 (3%)	2~(0%)	29	48
1	Ε	390/409~(95%)	377~(97%)	12 (3%)	1 (0%)	41	61
1	F	386/409~(94%)	372~(96%)	13 (3%)	1 (0%)	41	61
All	All	2333/2454~(95%)	2254 (97%)	69 (3%)	10 (0%)	34	54

 $5~{\rm of}~10$ Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	206	GLU
1	В	206	GLU
1	С	206	GLU
1	Е	206	GLU
1	F	206	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	А	312/343~(91%)	311 (100%)	1 (0%)	92 97
1	В	314/343~(92%)	313~(100%)	1 (0%)	92 97
1	С	312/343~(91%)	312~(100%)	0	100 100
1	D	306/343~(89%)	304 (99%)	2(1%)	84 94
1	Ε	306/343~(89%)	305~(100%)	1 (0%)	92 97
1	F	308/343~(90%)	308 (100%)	0	100 100
All	All	1858/2058~(90%)	1853 (100%)	5 (0%)	92 97

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

Mol	Chain	Res	Type
1	А	265	PRO
1	В	88	VAL



Continued from previous page...

Mol	Chain	Res	Type
1	D	338	ASP
1	D	341	MSE
1	Е	112	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	126	ASN
1	Ε	112	ASN
1	F	65	HIS
1	С	126	ASN
1	А	65	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)

6 non-standard protein/DNA/RNA residues 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	Type Chain Res		Tink	Bo	ond leng	ths	Bond angles			
INIOI	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	D	232	1	23,24,25	1.79	4 (17%)	25,32,34	1.69	5 (20%)
1	LLP	F	232	1	23,24,25	1.91	5 (21%)	25,32,34	1.64	4 (16%)
1	LLP	С	232	1	23,24,25	1.85	5 (21%)	25,32,34	1.55	5 (20%)
1	LLP	Е	232	1	23,24,25	1.78	5 (21%)	25,32,34	1.82	4 (16%)
1	LLP	А	232	1	23,24,25	1.81	5 (21%)	25,32,34	1.60	2 (8%)
1	LLP	В	232	1	23,24,25	1.79	6 (26%)	25,32,34	1.84	5 (20%)

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



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	D	232	1	-	6/16/17/19	0/1/1/1
1	LLP	F	232	1	-	5/16/17/19	0/1/1/1
1	LLP	С	232	1	-	5/16/17/19	0/1/1/1
1	LLP	Е	232	1	-	9/16/17/19	0/1/1/1
1	LLP	А	232	1	-	6/16/17/19	0/1/1/1
1	LLP	В	232	1	-	9/16/17/19	0/1/1/1

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

The worst 5 of 30 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\operatorname{Ideal}(\operatorname{\AA})$
1	А	232	LLP	O3-C3	-6.00	1.23	1.37
1	С	232	LLP	O3-C3	-5.84	1.23	1.37
1	D	232	LLP	O3-C3	-5.81	1.23	1.37
1	F	232	LLP	O3-C3	-5.81	1.23	1.37
1	В	232	LLP	O3-C3	-5.79	1.23	1.37

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	Е	232	LLP	OP4-C5'-C5	6.72	122.16	109.35
1	В	232	LLP	OP4-C5'-C5	6.14	121.06	109.35
1	D	232	LLP	OP4-C5'-C5	5.56	119.95	109.35
1	А	232	LLP	OP4-C5'-C5	5.50	119.82	109.35
1	F	232	LLP	OP4-C5'-C5	5.10	119.07	109.35

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	В	232	LLP	C5'-OP4-P-OP2
1	В	232	LLP	C5'-OP4-P-OP3
1	D	232	LLP	C5'-OP4-P-OP2
1	Е	232	LLP	C5'-OP4-P-OP1
1	Е	232	LLP	C5'-OP4-P-OP2

There are no ring outliers.

3 monomers are involved in 3 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	232	LLP	1	0
1	F	232	LLP	1	0
1	В	232	LLP	1	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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 >	>2	$OWAB(Å^2)$	Q<0.9
1	А	379/409~(92%)	0.24	13 (3%) 45	48	26, 30, 32, 39	0
1	В	383/409~(93%)	0.29	15 (3%) 39	42	21, 30, 32, 37	0
1	С	381/409~(93%)	0.33	9 (2%) 59	62	26, 30, 32, 38	0
1	D	379/409~(92%)	0.39	22 (5%) 23	24	27, 30, 32, 35	0
1	Ε	382/409~(93%)	0.29	16 (4%) 36	39	22, 30, 32, 39	0
1	F	379/409~(92%)	0.21	12 (3%) 47	51	27, 30, 32, 37	0
All	All	2283/2454 (93%)	0.29	87 (3%) 40	43	21, 30, 32, 39	0

The worst 5 of 87 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	16	ILE	5.6
1	А	340	ASN	4.9
1	С	212	GLU	4.8
1	Е	191	ALA	4.2
1	Е	16	ILE	4.1

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	LLP	С	232	24/25	0.94	0.15	29,31,33,34	0
1	LLP	F	232	24/25	0.95	0.16	28,32,33,35	0
1	LLP	Е	232	24/25	0.96	0.14	27,30,33,34	0
1	LLP	D	232	24/25	0.96	0.14	28,31,33,33	0



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q<0.9
1	LLP	А	232	24/25	0.97	0.14	29,31,33,34	0
1	LLP	В	232	24/25	0.97	0.14	28,31,33,33	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.

