W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 22, 2021 – 03:04 PM GMT

PDB ID : 6YY1
Title : Arabidopsis aspartate transcarbamoylase in apo state
Authors : Ramon Maiques, S.; Del Cano Ochoa, F.; Bellin, L.; Mohlmann, T.
Deposited on : 2020-05-04
Resolution : 3.06 Å(reported)

The following versions of software and data (see references (1)) were used in the production of this report:

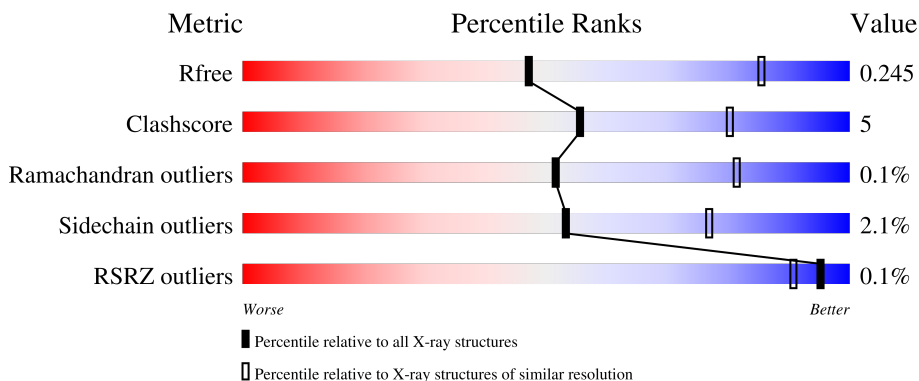|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.17.1.dev1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17.1.dev1

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 3.06 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	Percentile Ranks	Value
Rfree		0.245
Clashscore		5
Ramachandran outliers		0.1%
Sidechain outliers		2.1%
RSRZ outliers		0.1%

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	A	332	78% 13% 8%
1	B	332	79% 12% · 8%
1	C	332	80% 10% · 8%
1	D	332	85% 9% 6%
1	E	332	83% 11% 5%

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Mol	Chain	Length	Quality of chain
1	F	332	

79%   11%   ·   8%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 29112 atoms, of which 14578 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 PYRB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	305	Total 4789	C 1513	H 2402	N 403	O 460	S 11	0	0	0
1	B	304	Total 4794	C 1512	H 2407	N 404	O 459	S 12	0	0	0
1	C	304	Total 4788	C 1514	H 2398	N 406	O 458	S 12	0	1	0
1	D	312	Total 4926	C 1556	H 2474	N 416	O 468	S 12	0	0	0
1	E	314	Total 4945	C 1563	H 2481	N 417	O 472	S 12	0	1	0
1	F	304	Total 4787	C 1512	H 2400	N 403	O 460	S 12	0	1	0

There are 138 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	MET	-	initiating methionine	UNP A0A178VJE3
A	60	GLY	-	expression tag	UNP A0A178VJE3
A	61	SER	-	expression tag	UNP A0A178VJE3
A	62	SER	-	expression tag	UNP A0A178VJE3
A	63	HIS	-	expression tag	UNP A0A178VJE3
A	64	HIS	-	expression tag	UNP A0A178VJE3
A	65	HIS	-	expression tag	UNP A0A178VJE3
A	66	HIS	-	expression tag	UNP A0A178VJE3
A	67	HIS	-	expression tag	UNP A0A178VJE3
A	68	HIS	-	expression tag	UNP A0A178VJE3
A	69	SER	-	expression tag	UNP A0A178VJE3
A	70	SER	-	expression tag	UNP A0A178VJE3
A	71	GLY	-	expression tag	UNP A0A178VJE3
A	72	LEU	-	expression tag	UNP A0A178VJE3
A	73	GLU	-	expression tag	UNP A0A178VJE3
A	74	VAL	-	expression tag	UNP A0A178VJE3
A	75	LEU	-	expression tag	UNP A0A178VJE3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	76	PHE	-	expression tag	UNP A0A178VJE3
A	77	GLN	-	expression tag	UNP A0A178VJE3
A	78	GLY	-	expression tag	UNP A0A178VJE3
A	79	PRO	-	expression tag	UNP A0A178VJE3
A	80	HIS	-	expression tag	UNP A0A178VJE3
A	81	MET	-	expression tag	UNP A0A178VJE3
B	59	MET	-	initiating methionine	UNP A0A178VJE3
B	60	GLY	-	expression tag	UNP A0A178VJE3
B	61	SER	-	expression tag	UNP A0A178VJE3
B	62	SER	-	expression tag	UNP A0A178VJE3
B	63	HIS	-	expression tag	UNP A0A178VJE3
B	64	HIS	-	expression tag	UNP A0A178VJE3
B	65	HIS	-	expression tag	UNP A0A178VJE3
B	66	HIS	-	expression tag	UNP A0A178VJE3
B	67	HIS	-	expression tag	UNP A0A178VJE3
B	68	HIS	-	expression tag	UNP A0A178VJE3
B	69	SER	-	expression tag	UNP A0A178VJE3
B	70	SER	-	expression tag	UNP A0A178VJE3
B	71	GLY	-	expression tag	UNP A0A178VJE3
B	72	LEU	-	expression tag	UNP A0A178VJE3
B	73	GLU	-	expression tag	UNP A0A178VJE3
B	74	VAL	-	expression tag	UNP A0A178VJE3
B	75	LEU	-	expression tag	UNP A0A178VJE3
B	76	PHE	-	expression tag	UNP A0A178VJE3
B	77	GLN	-	expression tag	UNP A0A178VJE3
B	78	GLY	-	expression tag	UNP A0A178VJE3
B	79	PRO	-	expression tag	UNP A0A178VJE3
B	80	HIS	-	expression tag	UNP A0A178VJE3
B	81	MET	-	expression tag	UNP A0A178VJE3
C	59	MET	-	initiating methionine	UNP A0A178VJE3
C	60	GLY	-	expression tag	UNP A0A178VJE3
C	61	SER	-	expression tag	UNP A0A178VJE3
C	62	SER	-	expression tag	UNP A0A178VJE3
C	63	HIS	-	expression tag	UNP A0A178VJE3
C	64	HIS	-	expression tag	UNP A0A178VJE3
C	65	HIS	-	expression tag	UNP A0A178VJE3
C	66	HIS	-	expression tag	UNP A0A178VJE3
C	67	HIS	-	expression tag	UNP A0A178VJE3
C	68	HIS	-	expression tag	UNP A0A178VJE3
C	69	SER	-	expression tag	UNP A0A178VJE3
C	70	SER	-	expression tag	UNP A0A178VJE3
C	71	GLY	-	expression tag	UNP A0A178VJE3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	72	LEU	-	expression tag	UNP A0A178VJE3
C	73	GLU	-	expression tag	UNP A0A178VJE3
C	74	VAL	-	expression tag	UNP A0A178VJE3
C	75	LEU	-	expression tag	UNP A0A178VJE3
C	76	PHE	-	expression tag	UNP A0A178VJE3
C	77	GLN	-	expression tag	UNP A0A178VJE3
C	78	GLY	-	expression tag	UNP A0A178VJE3
C	79	PRO	-	expression tag	UNP A0A178VJE3
C	80	HIS	-	expression tag	UNP A0A178VJE3
C	81	MET	-	expression tag	UNP A0A178VJE3
D	59	MET	-	initiating methionine	UNP A0A178VJE3
D	60	GLY	-	expression tag	UNP A0A178VJE3
D	61	SER	-	expression tag	UNP A0A178VJE3
D	62	SER	-	expression tag	UNP A0A178VJE3
D	63	HIS	-	expression tag	UNP A0A178VJE3
D	64	HIS	-	expression tag	UNP A0A178VJE3
D	65	HIS	-	expression tag	UNP A0A178VJE3
D	66	HIS	-	expression tag	UNP A0A178VJE3
D	67	HIS	-	expression tag	UNP A0A178VJE3
D	68	HIS	-	expression tag	UNP A0A178VJE3
D	69	SER	-	expression tag	UNP A0A178VJE3
D	70	SER	-	expression tag	UNP A0A178VJE3
D	71	GLY	-	expression tag	UNP A0A178VJE3
D	72	LEU	-	expression tag	UNP A0A178VJE3
D	73	GLU	-	expression tag	UNP A0A178VJE3
D	74	VAL	-	expression tag	UNP A0A178VJE3
D	75	LEU	-	expression tag	UNP A0A178VJE3
D	76	PHE	-	expression tag	UNP A0A178VJE3
D	77	GLN	-	expression tag	UNP A0A178VJE3
D	78	GLY	-	expression tag	UNP A0A178VJE3
D	79	PRO	-	expression tag	UNP A0A178VJE3
D	80	HIS	-	expression tag	UNP A0A178VJE3
D	81	MET	-	expression tag	UNP A0A178VJE3
E	59	MET	-	initiating methionine	UNP A0A178VJE3
E	60	GLY	-	expression tag	UNP A0A178VJE3
E	61	SER	-	expression tag	UNP A0A178VJE3
E	62	SER	-	expression tag	UNP A0A178VJE3
E	63	HIS	-	expression tag	UNP A0A178VJE3
E	64	HIS	-	expression tag	UNP A0A178VJE3
E	65	HIS	-	expression tag	UNP A0A178VJE3
E	66	HIS	-	expression tag	UNP A0A178VJE3
E	67	HIS	-	expression tag	UNP A0A178VJE3

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Chain	Residue	Modelled	Actual	Comment	Reference
E	68	HIS	-	expression tag	UNP A0A178VJE3
E	69	SER	-	expression tag	UNP A0A178VJE3
E	70	SER	-	expression tag	UNP A0A178VJE3
E	71	GLY	-	expression tag	UNP A0A178VJE3
E	72	LEU	-	expression tag	UNP A0A178VJE3
E	73	GLU	-	expression tag	UNP A0A178VJE3
E	74	VAL	-	expression tag	UNP A0A178VJE3
E	75	LEU	-	expression tag	UNP A0A178VJE3
E	76	PHE	-	expression tag	UNP A0A178VJE3
E	77	GLN	-	expression tag	UNP A0A178VJE3
E	78	GLY	-	expression tag	UNP A0A178VJE3
E	79	PRO	-	expression tag	UNP A0A178VJE3
E	80	HIS	-	expression tag	UNP A0A178VJE3
E	81	MET	-	expression tag	UNP A0A178VJE3
F	59	MET	-	initiating methionine	UNP A0A178VJE3
F	60	GLY	-	expression tag	UNP A0A178VJE3
F	61	SER	-	expression tag	UNP A0A178VJE3
F	62	SER	-	expression tag	UNP A0A178VJE3
F	63	HIS	-	expression tag	UNP A0A178VJE3
F	64	HIS	-	expression tag	UNP A0A178VJE3
F	65	HIS	-	expression tag	UNP A0A178VJE3
F	66	HIS	-	expression tag	UNP A0A178VJE3
F	67	HIS	-	expression tag	UNP A0A178VJE3
F	68	HIS	-	expression tag	UNP A0A178VJE3
F	69	SER	-	expression tag	UNP A0A178VJE3
F	70	SER	-	expression tag	UNP A0A178VJE3
F	71	GLY	-	expression tag	UNP A0A178VJE3
F	72	LEU	-	expression tag	UNP A0A178VJE3
F	73	GLU	-	expression tag	UNP A0A178VJE3
F	74	VAL	-	expression tag	UNP A0A178VJE3
F	75	LEU	-	expression tag	UNP A0A178VJE3
F	76	PHE	-	expression tag	UNP A0A178VJE3
F	77	GLN	-	expression tag	UNP A0A178VJE3
F	78	GLY	-	expression tag	UNP A0A178VJE3
F	79	PRO	-	expression tag	UNP A0A178VJE3
F	80	HIS	-	expression tag	UNP A0A178VJE3
F	81	MET	-	expression tag	UNP A0A178VJE3

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

GOL

C3

OH O3

C1   C2

HO   OH

O1   O2

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 14	C 3	H 8	O 3	0	0
2	B	1	Total 14	C 3	H 8	O 3	0	0

• Molecule 3 is water.

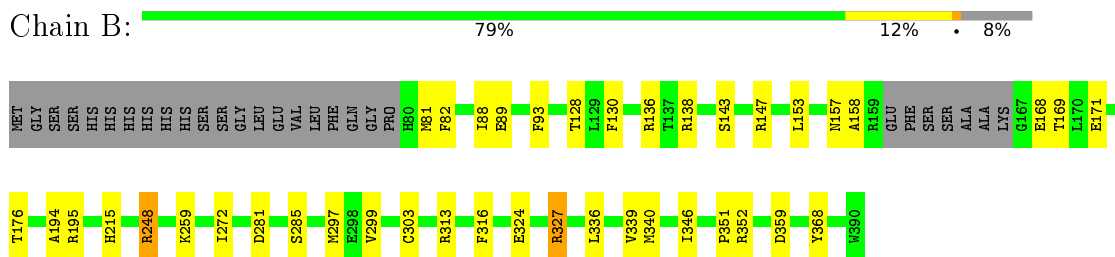| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	19	Total 19	O 19	0	0
3	B	8	Total 8	O 8	0	0
3	C	9	Total 9	O 9	0	0
3	D	7	Total 7	O 7	0	0
3	E	8	Total 8	O 8	0	0
3	F	4	Total 4	O 4	0	0

3 Residue-property plots ⓘ

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.
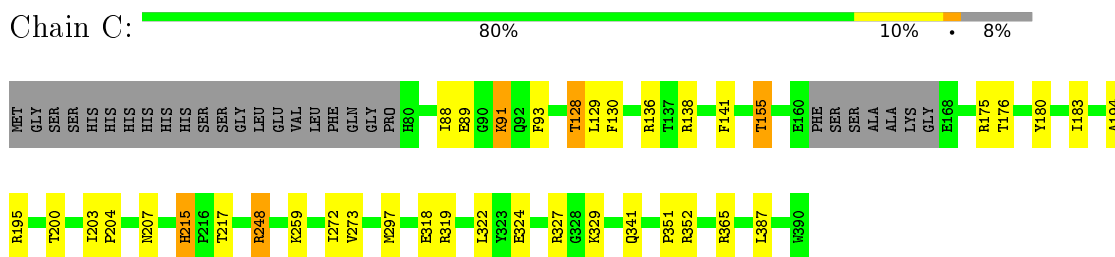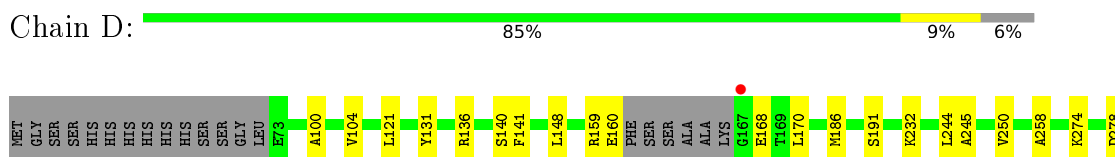
- Molecule 1: PYRB

Chain A:

- Molecule 1: PYRB

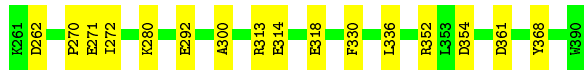Chain B:

- Molecule 1: PYRB

Chain C:

- Molecule 1: PYRB

Chain D:

I279 V288 R310 R352 L353 D354 G375 R379 K384 V388 G389 W390
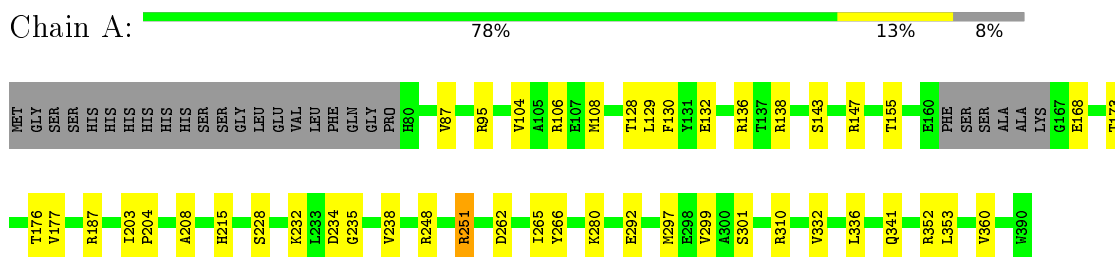
• Molecule 1: PYRB

Chain E:

83%   11%   5%

MET GLY SER HIS HIS HIS HIS HIS HIS SER SER G71 E89 G90 K91 K113 T128 L129 R136 L139 E151 T155 R159 E160 PHE SER SER ALA ALA LYS G167 E168 T169 T176 M186 F189 R195 L221 I230 L233 D234 G235 F260

K261 D262 P270 E271 I272 K280 E292 A300 R313 E314 E318 F330 L336 R352 L353 D354 D361 Y368 W390

• Molecule 1: PYRB

Chain F:

79%   11% • 8%

MET GLY SER HIS HIS HIS HIS HIS SER SER GLY LEU GLU VAL LEU PHE GLN GLY PRO H80 D94 M97 T128 L129 F130 R136 T137 R138 T155 E156 E160 PHE SER SER ALA ALA LYS GLY E168 T169 I174 M186 S191 A194 R195 A201 N202

I203 P204 N207 H215 S228 G235 N246 G247 R248 D262 I265 I272 V273 M297 E324 R327 G328 I331 M340 I346 M347 H348 P349 L350 P351 R352 E355 D359 W390
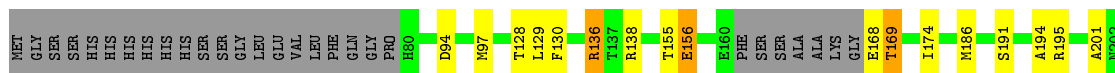
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	103.69Å 109.57Å 208.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.85 – 3.06 92.85 – 3.06	Depositor EDS
% Data completeness (in resolution range)	99.3 (92.85-3.06) 93.8 (92.85-3.06)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 3.07Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.190 , 0.245 0.190 , 0.245	Depositor DCC
R_{free} test set	2241 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	61.2	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 28.4	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	29112	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.65	0/2422	0.70	0/3261
1	B	0.57	0/2422	0.63	0/3260
1	C	0.59	1/2426 (0.0%)	0.65	2/3268 (0.1%)
1	D	0.54	0/2490	0.63	0/3352
1	E	0.62	1/2502 (0.0%)	0.67	0/3369
1	F	0.51	0/2425	0.60	1/3266 (0.0%)
All	All	0.58	2/14687 (0.0%)	0.65	3/19776 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	155	THR	CB-CG2	-5.42	1.34	1.52
1	E	151	GLU	CG-CD	5.37	1.60	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	136	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	C	128	THR	CB-CA-C	-5.42	96.95	111.60
1	C	319	ARG	NE-CZ-NH1	5.23	122.91	120.30

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	A	2387	2402	2402	30	0
1	B	2387	2407	2407	28	0
1	C	2390	2398	2397	30	0
1	D	2452	2474	2474	23	0
1	E	2464	2481	2481	29	0
1	F	2387	2400	2400	30	0
2	A	6	8	8	0	0
2	B	6	8	8	0	0
3	A	19	0	0	1	0
3	B	8	0	0	0	0
3	C	9	0	0	0	0
3	D	7	0	0	0	0
3	E	8	0	0	0	0
3	F	4	0	0	0	0
All	All	14534	14578	14577	148	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.

The worst 5 of 148 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:170:LEU:HD11	1:D:186:MET:HE1	1.47	0.94
1:D:170:LEU:HD11	1:D:186:MET:CE	1.97	0.92
1:C:128:THR:HG22	1:C:128:THR:O	1.80	0.81
1:C:176:THR:HG21	1:D:136:ARG:HG3	1.64	0.79
1:A:176:THR:HG21	1:B:136:ARG:HH11	1.50	0.76

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	301/332 (91%)	289 (96%)	12 (4%)	0	100	100
1	B	300/332 (90%)	289 (96%)	11 (4%)	0	100	100
1	C	301/332 (91%)	294 (98%)	7 (2%)	0	100	100
1	D	308/332 (93%)	299 (97%)	9 (3%)	0	100	100
1	E	310/332 (93%)	296 (96%)	14 (4%)	0	100	100
1	F	301/332 (91%)	288 (96%)	12 (4%)	1 (0%)	41	70
All	All	1821/1992 (91%)	1755 (96%)	65 (4%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	169	THR

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	A	254/280 (91%)	248 (98%)	6 (2%)	49	74
1	B	255/280 (91%)	250 (98%)	5 (2%)	55	78
1	C	254/280 (91%)	248 (98%)	6 (2%)	49	74
1	D	262/280 (94%)	260 (99%)	2 (1%)	81	91
1	E	263/280 (94%)	258 (98%)	5 (2%)	57	79
1	F	255/280 (91%)	247 (97%)	8 (3%)	40	68
All	All	1543/1680 (92%)	1511 (98%)	32 (2%)	53	77

5 of 32 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	246	ASN
1	F	248	ARG
1	C	215	HIS
1	C	91	LYS

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Mol	Chain	Res	Type
1	F	297	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	GOL	B	401	-	5,5,5	1.02	0	5,5,5	1.41	1 (20%)
2	GOL	A	401	-	5,5,5	1.10	1 (20%)	5,5,5	1.00	1 (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 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	B	401	-	-	0/4/4/4	-
2	GOL	A	401	-	-	0/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	GOL	O2-C2	-2.15	1.37	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	401	GOL	C3-C2-C1	-2.73	101.09	111.70
2	A	401	GOL	C3-C2-C1	-2.01	103.90	111.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 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(Å²)	Q<0.9
1	A	305/332 (91%)	-0.08	0	100	100	38, 45, 58, 72	0
1	B	304/332 (91%)	0.01	0	100	100	41, 54, 71, 81	0
1	C	304/332 (91%)	-0.04	0	100	100	44, 57, 68, 80	0
1	D	312/332 (93%)	0.07	1 (0%)	94	85	49, 58, 70, 87	0
1	E	314/332 (94%)	-0.01	0	100	100	35, 52, 68, 90	0
1	F	304/332 (91%)	0.11	1 (0%)	94	85	51, 65, 76, 100	0
All	All	1843/1992 (92%)	0.01	2 (0%)	95	91	35, 56, 71, 100	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	167	GLY	2.1
1	F	265	ILE	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, 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(Å²)	Q<0.9
2	GOL	B	401	6/6	0.85	0.23	59,71,76,77	0
2	GOL	A	401	6/6	0.91	0.24	43,52,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.