



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 6, 2016 – 06:16 PM EDT

PDB ID : 5AA2  
Title : Crystal structure of MltF from *Pseudomonas aeruginosa* in complex with NAM-pentapeptide.  
Authors : Dominguez-Gil, T.; Acebron, I.; Hermoso, J.A.  
Deposited on : 2015-07-23  
Resolution : 2.80 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20027939  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20027939

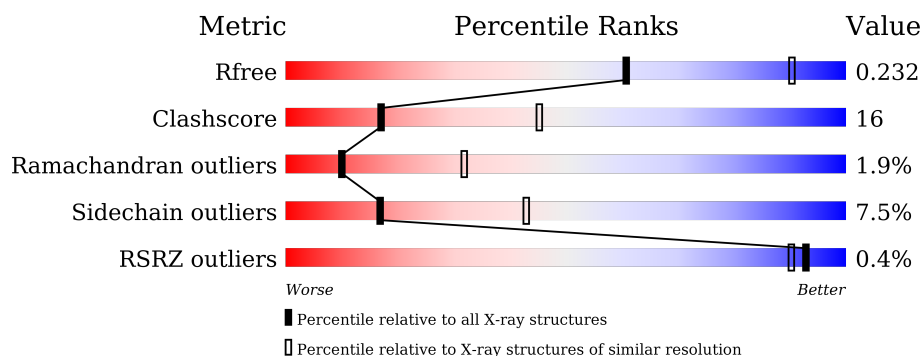
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	499	<div> <div>17%</div> <div>60% 22% 16%</div> </div>
1	C	499	<div> <div>%</div> <div>63% 20% 16%</div> </div>
2	B	499	<div> <div></div> <div>58% 21% 17%</div> </div>
3	D	499	<div> <div></div> <div>53% 28% 17%</div> </div>
4	E	6	<div> <div>17%</div> <div>100%</div> </div>

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
4	API	E	4	-	-	X	-
4	DAL	E	5	-	-	X	-
4	DAL	E	6	-	-	X	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13519 atoms, of which 37 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 MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	1	0
			3371	2126	599	637	9			
1	C	418	Total	C	N	O	S	0	0	0
			3353	2114	597	633	9			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	EXPRESSION TAG	UNP Q9HYN1
A	-20	ALA	-	EXPRESSION TAG	UNP Q9HYN1
A	-19	PRO	-	EXPRESSION TAG	UNP Q9HYN1
A	-18	SER	-	EXPRESSION TAG	UNP Q9HYN1
A	-17	ARG	-	EXPRESSION TAG	UNP Q9HYN1
A	-16	LEU	-	EXPRESSION TAG	UNP Q9HYN1
A	-15	CYS	-	EXPRESSION TAG	UNP Q9HYN1
A	-14	VAL	-	EXPRESSION TAG	UNP Q9HYN1
A	-13	TYR	-	EXPRESSION TAG	UNP Q9HYN1
A	-12	CYS	-	EXPRESSION TAG	UNP Q9HYN1
A	-11	ALA	-	EXPRESSION TAG	UNP Q9HYN1
A	-10	ASP	-	EXPRESSION TAG	UNP Q9HYN1
A	-9	VAL	-	EXPRESSION TAG	UNP Q9HYN1
A	-8	CYS	-	EXPRESSION TAG	UNP Q9HYN1
A	-7	PRO	-	EXPRESSION TAG	UNP Q9HYN1
A	-6	ASP	-	EXPRESSION TAG	UNP Q9HYN1
A	268	THR	ALA	CONFLICT	UNP Q9HYN1
A	289	LYS	LEU	CONFLICT	UNP Q9HYN1
A	446	SER	PRO	CONFLICT	UNP Q9HYN1
C	-21	MET	-	EXPRESSION TAG	UNP Q9HYN1
C	-20	ALA	-	EXPRESSION TAG	UNP Q9HYN1
C	-19	PRO	-	EXPRESSION TAG	UNP Q9HYN1
C	-18	SER	-	EXPRESSION TAG	UNP Q9HYN1
C	-17	ARG	-	EXPRESSION TAG	UNP Q9HYN1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	-16	LEU	-	EXPRESSION TAG	UNP Q9HYN1
C	-15	CYS	-	EXPRESSION TAG	UNP Q9HYN1
C	-14	VAL	-	EXPRESSION TAG	UNP Q9HYN1
C	-13	TYR	-	EXPRESSION TAG	UNP Q9HYN1
C	-12	CYS	-	EXPRESSION TAG	UNP Q9HYN1
C	-11	ALA	-	EXPRESSION TAG	UNP Q9HYN1
C	-10	ASP	-	EXPRESSION TAG	UNP Q9HYN1
C	-9	VAL	-	EXPRESSION TAG	UNP Q9HYN1
C	-8	CYS	-	EXPRESSION TAG	UNP Q9HYN1
C	-7	PRO	-	EXPRESSION TAG	UNP Q9HYN1
C	-6	ASP	-	EXPRESSION TAG	UNP Q9HYN1
C	268	THR	ALA	CONFLICT	UNP Q9HYN1
C	289	LYS	LEU	CONFLICT	UNP Q9HYN1
C	446	SER	PRO	CONFLICT	UNP Q9HYN1

- Molecule 2 is a protein called MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	413	Total	C	N	O	S	0	0	0
			3309	2087	591	622	9			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	MET	-	EXPRESSION TAG	UNP Q9HYN1
B	-20	ALA	-	EXPRESSION TAG	UNP Q9HYN1
B	-19	PRO	-	EXPRESSION TAG	UNP Q9HYN1
B	-18	SER	-	EXPRESSION TAG	UNP Q9HYN1
B	-17	ARG	-	EXPRESSION TAG	UNP Q9HYN1
B	-16	LEU	-	EXPRESSION TAG	UNP Q9HYN1
B	-15	CYS	-	EXPRESSION TAG	UNP Q9HYN1
B	-14	VAL	-	EXPRESSION TAG	UNP Q9HYN1
B	-13	TYR	-	EXPRESSION TAG	UNP Q9HYN1
B	-12	CYS	-	EXPRESSION TAG	UNP Q9HYN1
B	-11	ALA	-	EXPRESSION TAG	UNP Q9HYN1
B	-10	ASP	-	EXPRESSION TAG	UNP Q9HYN1
B	-9	VAL	-	EXPRESSION TAG	UNP Q9HYN1
B	-8	CYS	-	EXPRESSION TAG	UNP Q9HYN1
B	-7	PRO	-	EXPRESSION TAG	UNP Q9HYN1
B	-6	ASP	-	EXPRESSION TAG	UNP Q9HYN1
B	161	PRO	GLU	CONFLICT	UNP Q9HYN1

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
B	268	THR	ALA	CONFLICT	UNP Q9HYN1
B	289	LYS	LEU	CONFLICT	UNP Q9HYN1

- Molecule 3 is a protein called MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	416	Total	C	N	O	S	0	0	0
			3334	2102	594	629	9			

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-21	MET	-	EXPRESSION TAG	UNP Q9HYN1
D	-20	ALA	-	EXPRESSION TAG	UNP Q9HYN1
D	-19	PRO	-	EXPRESSION TAG	UNP Q9HYN1
D	-18	SER	-	EXPRESSION TAG	UNP Q9HYN1
D	-17	ARG	-	EXPRESSION TAG	UNP Q9HYN1
D	-16	LEU	-	EXPRESSION TAG	UNP Q9HYN1
D	-15	CYS	-	EXPRESSION TAG	UNP Q9HYN1
D	-14	VAL	-	EXPRESSION TAG	UNP Q9HYN1
D	-13	TYR	-	EXPRESSION TAG	UNP Q9HYN1
D	-12	CYS	-	EXPRESSION TAG	UNP Q9HYN1
D	-11	ALA	-	EXPRESSION TAG	UNP Q9HYN1
D	-10	ASP	-	EXPRESSION TAG	UNP Q9HYN1
D	-9	VAL	-	EXPRESSION TAG	UNP Q9HYN1
D	-8	CYS	-	EXPRESSION TAG	UNP Q9HYN1
D	-7	PRO	-	EXPRESSION TAG	UNP Q9HYN1
D	-6	ASP	-	EXPRESSION TAG	UNP Q9HYN1
D	102	ASP	GLU	CONFLICT	UNP Q9HYN1
D	268	THR	ALA	CONFLICT	UNP Q9HYN1
D	289	LYS	LEU	CONFLICT	UNP Q9HYN1

- Molecule 4 is a protein called N-ACETYLGLUCOSAMINE-1,6-ANHYDRO-N-ACETYLMURAMIC ACID L-ALA-D-GLU-M-DAP-D-ALA-D-ALA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	6	Total	C	H	N	O	0	0	0
			79	24	37	6	12			

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Cl 1	0	0
5	C	1	Total 1	Cl 1	0	0

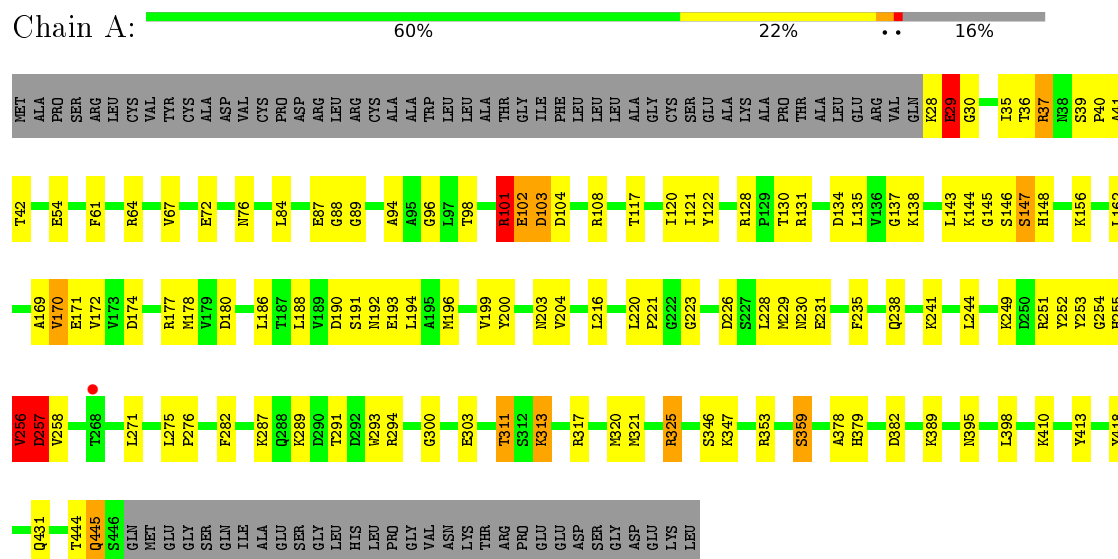
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	25	Total 25	O 25	0	0
6	B	15	Total 15	O 15	0	0
6	C	24	Total 24	O 24	0	0
6	D	7	Total 7	O 7	0	0

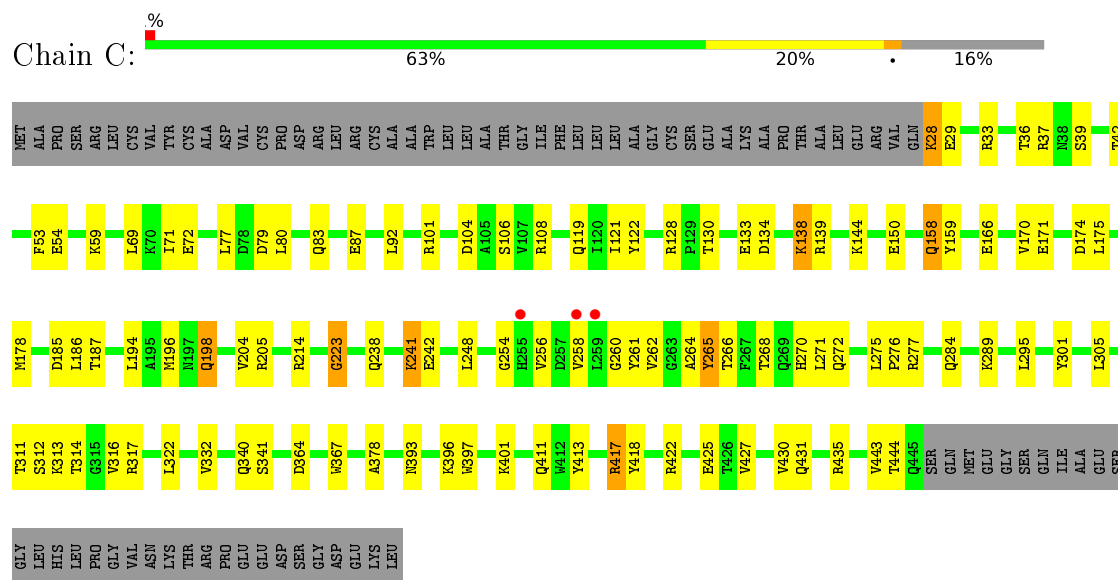
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

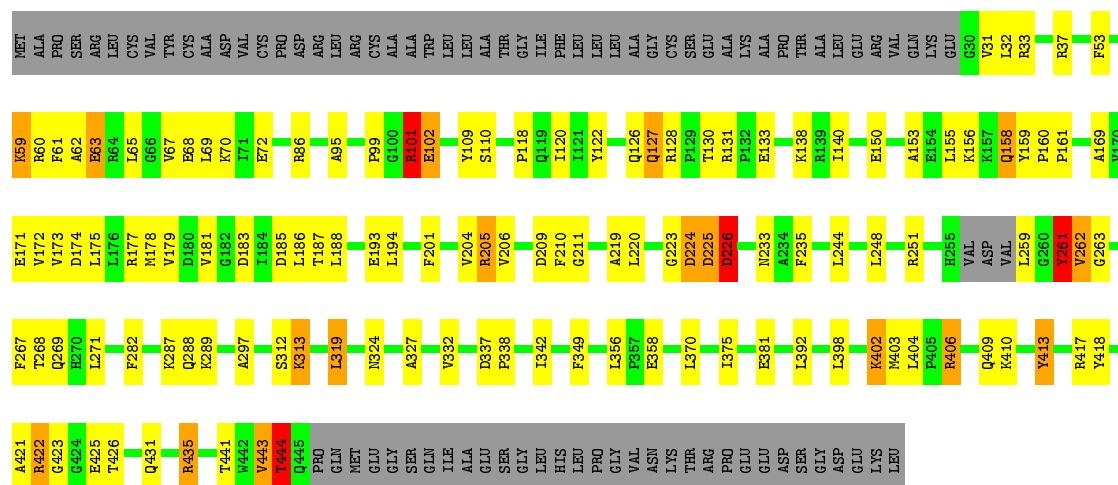


#### • Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F



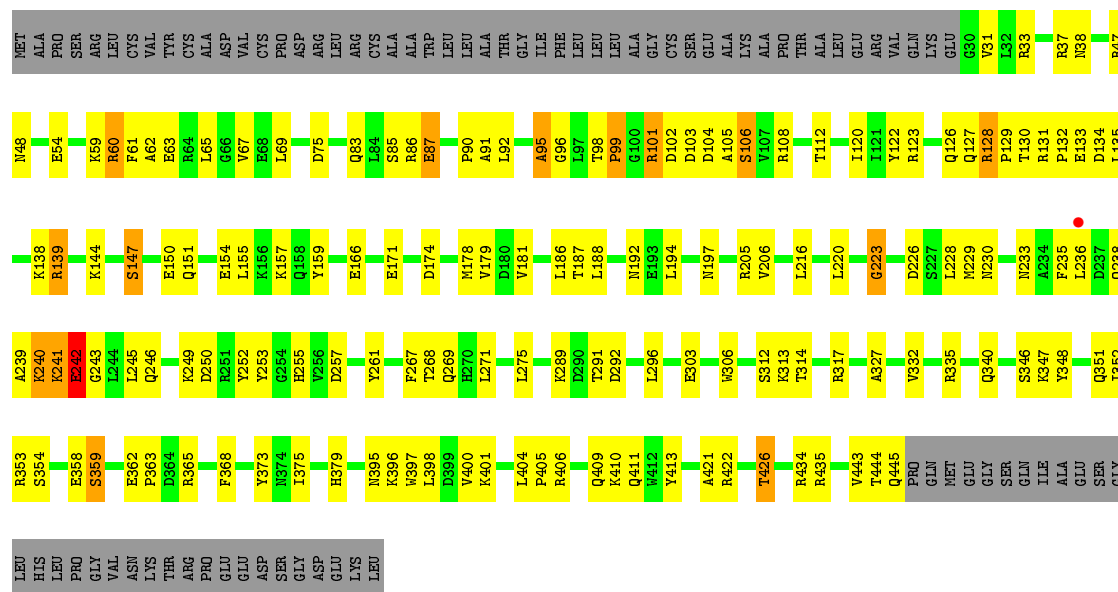
#### • Molecule 2: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

Chain B:  58% 21% 17%



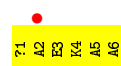
• Molecule 3: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

Chain D:  53% 28% 17%



• Molecule 4: N-ACETYLGLUCOSAMINE-1,6-ANHYDRO-N-ACETYLMURAMIC ACID L-A LA-D-GLU-M-DAP-D-ALA-D-ALA

Chain E:  17% 100%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.58Å 135.65Å 137.46Å 90.00° 92.06° 90.00°	Depositor
Resolution (Å)	48.26 – 2.80 48.26 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.26-2.80) 93.8 (48.26-2.80)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, $R_{free}$	0.167 , 0.235 0.166 , 0.232	Depositor DCC
$R_{free}$ test set	2949 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.2	Xtriage
Anisotropy	0.069	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 39.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.001 for -h,l,k 0.015 for -h,-l,-k 0.032 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13519	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: DAL, AH0, API, DGL, CL

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	0.47	0/3442	0.61	1/4652 (0.0%)
1	C	0.43	0/3423	0.58	0/4626
2	B	0.41	0/3378	0.57	0/4564
3	D	0.36	0/3404	0.53	0/4602
4	E	0.94	0/4	0.83	0/4
All	All	0.42	0/13651	0.57	1/18448 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	37	ARG	NE-CZ-NH2	-6.53	117.03	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	3371	0	3314	132	0
1	C	3353	0	3301	67	0
2	B	3309	0	3254	113	0
3	D	3334	0	3280	124	0
4	E	42	37	33	31	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	1	0	0	0	0
5	C	1	0	0	0	0
6	A	25	0	0	6	0
6	B	15	0	0	1	0
6	C	24	0	0	2	0
6	D	7	0	0	0	0
All	All	13482	37	13182	434	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 16.

All (434) 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)
2:B:101:ARG:HA	2:B:102:GLU:HB2	1.21	1.14
2:B:60:ARG:HD2	2:B:244:LEU:HD21	1.35	1.04
2:B:101:ARG:HA	2:B:102:GLU:CB	1.94	0.98
1:C:144:LYS:HA	1:C:166:GLU:HB2	1.47	0.96
2:B:225:ASP:HA	2:B:226:ASP:HB2	1.44	0.96
3:D:241:LYS:N	3:D:242:GLU:HB2	1.80	0.96
2:B:101:ARG:CA	2:B:102:GLU:HB2	1.99	0.91
1:A:29:GLU:HG2	1:A:30:GLY:H	1.36	0.91
2:B:101:ARG:HH11	2:B:101:ARG:HG3	1.38	0.88
2:B:268:THR:HA	2:B:271:LEU:HB3	1.52	0.87
3:D:104:ASP:O	3:D:106:SER:N	2.05	0.87
2:B:225:ASP:HA	2:B:226:ASP:CB	2.04	0.87
3:D:268:THR:HA	3:D:271:LEU:HB2	1.54	0.87
1:A:37:ARG:HH22	4:E:4:API:C1	1.88	0.86
1:A:172:VAL:HG21	4:E:4:API:H41	1.57	0.85
1:A:98:THR:O	4:E:2:ALA:HB3	1.76	0.84
1:A:249:LYS:O	1:A:253[B]:TYR:HB2	1.76	0.83
3:D:241:LYS:HB2	3:D:242:GLU:CG	2.08	0.83
1:A:196:MET:HB2	1:A:253[A]:TYR:CE1	2.14	0.82
3:D:197:ASN:OD1	3:D:422:ARG:NH2	2.13	0.81
3:D:101:ARG:HE	3:D:101:ARG:HA	1.46	0.81
1:C:289:LYS:NZ	1:C:289:LYS:HB2	1.96	0.80
3:D:242:GLU:HB3	3:D:243:GLY:HA2	1.61	0.80
1:A:102:GLU:HA	1:A:103:ASP:O	1.82	0.80
2:B:422:ARG:HG2	2:B:425:GLU:HG2	1.64	0.79
3:D:192:ASN:HB2	3:D:253:TYR:HE2	1.48	0.78
2:B:268:THR:HA	2:B:271:LEU:CB	2.12	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:220:LEU:HD13	3:D:229:MET:HE1	1.64	0.77
1:A:29:GLU:CG	1:A:30:GLY:H	1.97	0.77
2:B:31:VAL:HA	2:B:67:VAL:CG2	2.14	0.77
1:A:172:VAL:HG21	4:E:4:API:C4	2.14	0.77
2:B:261:TYR:O	2:B:263:GLY:N	2.17	0.76
2:B:313:LYS:H	2:B:313:LYS:HE2	1.48	0.76
1:A:226:ASP:O	1:A:230:ASN:ND2	2.18	0.75
2:B:289:LYS:HB2	2:B:289:LYS:NZ	2.01	0.75
3:D:242:GLU:CB	3:D:243:GLY:HA2	2.15	0.73
3:D:261:TYR:CE1	3:D:435:ARG:HG2	2.23	0.73
1:A:120:ILE:HD13	1:A:188:LEU:HD13	1.69	0.72
3:D:246:GLN:HE22	3:D:249:LYS:HE2	1.52	0.72
2:B:225:ASP:CA	2:B:226:ASP:HB2	2.19	0.72
3:D:101:ARG:HG3	3:D:102:ASP:O	1.88	0.72
3:D:154:GLU:O	3:D:157:LYS:HG2	1.88	0.71
2:B:102:GLU:OE1	2:B:102:GLU:HA	1.89	0.71
2:B:60:ARG:HA	2:B:63:GLU:HG2	1.72	0.71
3:D:108:ARG:NH2	3:D:223:GLY:HA2	2.06	0.71
1:A:444:THR:HG22	1:A:445:GLN:H	1.55	0.70
1:A:192:ASN:HD21	4:E:5:DAL:HB3	1.56	0.70
2:B:101:ARG:HH11	2:B:101:ARG:CG	2.04	0.70
1:A:98:THR:HB	4:E:2:ALA:CB	2.22	0.70
3:D:192:ASN:HB2	3:D:253:TYR:CE2	2.27	0.69
1:A:96:GLY:HA3	4:E:5:DAL:C	2.22	0.69
2:B:224:ASP:O	2:B:226:ASP:HB2	1.92	0.69
3:D:397:TRP:O	3:D:401:LYS:HB3	1.92	0.69
3:D:91:ALA:HB1	3:D:228:LEU:CD2	2.23	0.69
3:D:271:LEU:HD23	3:D:275:LEU:HD22	1.73	0.69
3:D:91:ALA:HB1	3:D:228:LEU:HD21	1.75	0.68
1:A:84:LEU:O	1:A:221:PRO:HG3	1.94	0.68
1:A:172:VAL:CG2	4:E:4:API:H41	2.22	0.68
2:B:443:VAL:HG12	2:B:443:VAL:O	1.94	0.67
2:B:158:GLN:HG2	2:B:159:TYR:CD1	2.29	0.67
1:A:256:VAL:HG11	1:A:313:LYS:NZ	2.09	0.67
3:D:241:LYS:H	3:D:242:GLU:HB2	1.59	0.67
3:D:226:ASP:O	3:D:230:ASN:HB2	1.95	0.66
1:A:54:GLU:HG2	4:E:6:DAL:HB2	1.76	0.66
2:B:251:ARG:HG2	2:B:251:ARG:HH11	1.61	0.66
1:C:122:TYR:CZ	1:C:128:ARG:HG3	2.31	0.66
3:D:327:ALA:HB1	3:D:332:VAL:HG22	1.77	0.66
1:A:311:THR:CG2	1:A:317:ARG:HE	2.09	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:VAL:O	2:B:205:ARG:HD3	1.96	0.65
2:B:61:PHE:HB2	2:B:235:PHE:CE2	2.31	0.65
3:D:220:LEU:HD22	3:D:229:MET:HE1	1.78	0.65
2:B:177:ARG:NH1	2:B:409:GLN:HG2	2.11	0.65
1:C:427:VAL:O	1:C:431:GLN:HG2	1.98	0.64
1:A:122:TYR:CE1	1:A:128:ARG:HG3	2.33	0.63
3:D:241:LYS:HB2	3:D:242:GLU:CB	2.27	0.63
3:D:239:ALA:C	3:D:240:LYS:HZ1	2.02	0.63
3:D:102:ASP:C	3:D:104:ASP:H	2.02	0.63
1:C:101:ARG:HH11	1:C:101:ARG:HG2	1.63	0.62
1:A:37:ARG:HD2	1:A:171:GLU:OE2	1.98	0.62
1:A:30:GLY:HA2	1:A:67:VAL:HG12	1.81	0.62
3:D:312:SER:OG	3:D:314:THR:OG1	2.17	0.62
1:A:147:SER:HB3	4:E:3:DGL:N	2.15	0.61
1:A:231:GLU:HG2	6:A:2004:HOH:O	1.99	0.61
1:A:311:THR:HG23	1:A:317:ARG:HG3	1.82	0.61
3:D:229:MET:SD	3:D:233:ASN:ND2	2.73	0.61
3:D:240:LYS:HE3	3:D:245:LEU:HD11	1.82	0.61
1:A:98:THR:HB	4:E:2:ALA:HB1	1.82	0.61
2:B:131:ARG:HB2	2:B:133:GLU:HG2	1.82	0.61
1:A:122:TYR:CZ	1:A:128:ARG:HG3	2.35	0.61
1:C:261:TYR:CE1	1:C:435:ARG:HD3	2.36	0.61
3:D:60:ARG:NH1	3:D:63:GLU:OE1	2.33	0.61
1:A:196:MET:HB2	1:A:253[A]:TYR:CD1	2.35	0.60
2:B:185:ASP:O	2:B:186:LEU:HD23	2.00	0.60
2:B:31:VAL:HA	2:B:67:VAL:HG22	1.81	0.60
3:D:133:GLU:HG3	3:D:159:TYR:CZ	2.35	0.60
1:A:54:GLU:HG2	4:E:6:DAL:CB	2.31	0.60
2:B:313:LYS:H	2:B:313:LYS:CE	2.12	0.60
1:C:289:LYS:HZ2	1:C:289:LYS:HB2	1.66	0.60
1:C:28:LYS:HZ3	1:C:28:LYS:N	1.98	0.60
2:B:289:LYS:HB2	2:B:289:LYS:HZ2	1.65	0.60
2:B:60:ARG:HA	2:B:63:GLU:CG	2.32	0.60
2:B:319:LEU:HD12	2:B:319:LEU:O	2.02	0.59
2:B:60:ARG:CD	2:B:244:LEU:HD21	2.23	0.59
1:C:79:ASP:O	1:C:83:GLN:HG2	2.01	0.59
1:C:378:ALA:HB1	1:C:418:TYR:CE2	2.37	0.59
3:D:220:LEU:HD22	3:D:229:MET:CE	2.32	0.59
1:A:98:THR:OG1	6:A:2007:HOH:O	2.16	0.59
1:C:80:LEU:HD23	1:C:80:LEU:C	2.23	0.59
3:D:132:PRO:O	3:D:135:LEU:HG	2.03	0.59

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:SER:HA	4:E:3:DGL:OXT	2.03	0.59
1:A:254:GLY:O	1:A:256:VAL:HG22	2.01	0.59
2:B:128:ARG:HH12	2:B:130:THR:HG22	1.68	0.59
1:A:117:THR:O	1:A:191:SER:HB3	2.02	0.58
1:A:102:GLU:N	1:A:103:ASP:HB2	2.18	0.58
2:B:59:LYS:HA	2:B:69:LEU:HD22	1.85	0.58
1:C:174:ASP:O	1:C:178:MET:HG3	2.03	0.58
1:C:443:VAL:HG23	1:C:443:VAL:O	2.03	0.58
3:D:242:GLU:HB3	3:D:243:GLY:CA	2.32	0.58
1:A:256:VAL:HG11	1:A:313:LYS:HZ3	1.68	0.58
1:A:192:ASN:ND2	4:E:5:DAL:HB3	2.19	0.58
1:C:261:TYR:CD1	1:C:435:ARG:HD3	2.38	0.58
3:D:296:LEU:HD13	3:D:346:SER:OG	2.03	0.58
1:A:325:ARG:CG	1:A:325:ARG:HH11	2.17	0.57
3:D:150:GLU:O	3:D:154:GLU:HG2	2.04	0.57
3:D:122:TYR:CE1	3:D:205:ARG:HB2	2.39	0.57
3:D:240:LYS:HB3	3:D:245:LEU:HG	1.86	0.57
1:A:289:LYS:HE3	1:A:346:SER:C	2.25	0.57
2:B:99:PRO:HB3	2:B:109:TYR:CG	2.39	0.57
1:A:29:GLU:CG	1:A:30:GLY:N	2.67	0.57
3:D:241:LYS:HB2	3:D:242:GLU:HG3	1.85	0.57
3:D:267:PHE:O	3:D:268:THR:OG1	2.21	0.57
3:D:96:GLY:HA2	3:D:216:LEU:HD13	1.87	0.57
3:D:268:THR:HA	3:D:271:LEU:CB	2.30	0.56
2:B:313:LYS:CD	2:B:313:LYS:H	2.17	0.56
1:C:378:ALA:HB1	1:C:418:TYR:CD2	2.39	0.56
2:B:402:LYS:HD2	2:B:402:LYS:N	2.20	0.56
1:C:393:ASN:ND2	1:C:396:LYS:HG2	2.19	0.56
1:A:220:LEU:HD22	1:A:229:MET:HE2	1.86	0.56
1:C:92:LEU:C	1:C:92:LEU:HD12	2.25	0.56
3:D:238:GLN:O	3:D:242:GLU:HG3	2.05	0.56
3:D:220:LEU:HD22	3:D:229:MET:HB2	1.87	0.56
2:B:233:ASN:OD1	6:B:2008:HOH:O	2.18	0.56
1:A:54:GLU:CG	4:E:6:DAL:HB2	2.36	0.56
1:C:122:TYR:CE1	1:C:128:ARG:HG3	2.41	0.56
1:C:289:LYS:HZ3	1:C:289:LYS:HB2	1.70	0.56
1:A:121:ILE:CG2	1:A:204:VAL:HG13	2.36	0.55
3:D:246:GLN:NE2	3:D:249:LYS:HE2	2.20	0.55
2:B:194:LEU:CD2	2:B:206:VAL:HG22	2.37	0.55
2:B:183:ASP:O	3:D:411:GLN:HG2	2.06	0.55
4:E:1:AH0:HB3	4:E:2:ALA:HA	1.87	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ARG:O	1:A:251:ARG:HG3	2.07	0.55
3:D:104:ASP:O	3:D:106:SER:OG	2.22	0.55
1:A:253[A]:TYR:OH	4:E:6:DAL:OXT	2.10	0.55
1:A:102:GLU:H	1:A:103:ASP:HB2	1.72	0.55
1:A:169:ALA:CB	1:C:139:ARG:HD2	2.37	0.55
2:B:251:ARG:NH1	2:B:251:ARG:HG2	2.21	0.55
1:C:134:ASP:O	1:C:138:LYS:HE2	2.06	0.54
1:A:37:ARG:NH2	4:E:4:API:C1	2.64	0.54
2:B:118:PRO:HB2	2:B:210:PHE:O	2.08	0.54
3:D:289:LYS:HE3	3:D:347:LYS:N	2.23	0.54
3:D:240:LYS:CE	3:D:245:LEU:HD11	2.38	0.54
1:A:193:GLU:HG3	4:E:4:API:H31	1.89	0.54
1:C:223:GLY:HA3	6:C:2009:HOH:O	2.07	0.54
2:B:128:ARG:NH1	2:B:130:THR:HG22	2.23	0.54
1:C:443:VAL:O	1:C:444:THR:HG23	2.07	0.54
1:A:291:THR:CG2	1:A:353:ARG:HH22	2.21	0.54
1:C:170:VAL:HG21	1:C:175:LEU:HD21	1.90	0.54
3:D:108:ARG:HH21	3:D:223:GLY:HA2	1.73	0.54
1:A:148:HIS:CE1	4:E:4:API:H52	2.43	0.54
1:C:271:LEU:CD1	1:C:275:LEU:HD23	2.38	0.54
2:B:267:PHE:O	2:B:268:THR:OG1	2.21	0.53
3:D:240:LYS:HE3	3:D:245:LEU:CD1	2.38	0.53
3:D:75:ASP:O	3:D:410:LYS:NZ	2.24	0.53
1:A:138:LYS:HD2	1:A:138:LYS:N	2.23	0.53
1:C:238:GLN:O	1:C:242:GLU:HB2	2.08	0.53
1:C:417:ARG:HD2	1:C:418:TYR:CE2	2.44	0.53
3:D:134:ASP:O	3:D:138:LYS:NZ	2.32	0.53
3:D:249:LYS:O	3:D:253:TYR:HB2	2.08	0.53
1:A:289:LYS:HE3	1:A:347:LYS:N	2.22	0.53
1:C:264:ALA:O	1:C:268:THR:HG23	2.08	0.53
3:D:102:ASP:O	3:D:104:ASP:N	2.38	0.53
1:A:172:VAL:CG2	4:E:4:API:C4	2.84	0.53
1:A:300:GLY:HA3	1:A:320:MET:HE2	1.90	0.53
2:B:262:VAL:HG23	2:B:263:GLY:N	2.24	0.53
1:C:122:TYR:CE1	1:C:205:ARG:HB2	2.44	0.53
1:A:42:THR:O	1:A:54:GLU:HB2	2.09	0.53
1:A:137:GLY:C	1:A:138:LYS:HD2	2.30	0.52
2:B:381:GLU:HA	2:B:381:GLU:OE1	2.10	0.52
1:A:300:GLY:HA3	1:A:320:MET:CE	2.40	0.52
2:B:175:LEU:HD13	2:B:187:THR:OG1	2.10	0.52
2:B:289:LYS:HB2	2:B:289:LYS:HZ3	1.74	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:144:LYS:HE2	3:D:166:GLU:HB2	1.91	0.52
3:D:239:ALA:CA	3:D:240:LYS:HZ1	2.22	0.52
1:A:311:THR:HG23	1:A:317:ARG:HE	1.73	0.52
2:B:337:ASP:OD1	2:B:338:PRO:HD2	2.09	0.52
2:B:60:ARG:HD2	2:B:244:LEU:CD2	2.25	0.52
1:C:316:VAL:HA	1:C:322:LEU:O	2.10	0.52
3:D:131:ARG:HD2	3:D:133:GLU:OE1	2.10	0.52
1:A:144:LYS:HD2	1:A:145:GLY:N	2.25	0.52
3:D:359:SER:HB2	3:D:395:ASN:ND2	2.25	0.52
3:D:255:HIS:ND1	3:D:313:LYS:HE2	2.25	0.52
3:D:138:LYS:HD2	3:D:186:LEU:HD11	1.92	0.51
1:A:120:ILE:CD1	1:A:188:LEU:HD13	2.38	0.51
1:A:54:GLU:OE1	1:A:94:ALA:HB1	2.11	0.51
2:B:282:PHE:CZ	2:B:297:ALA:HA	2.45	0.51
1:A:135:LEU:CD2	1:A:186:LEU:HD13	2.39	0.51
1:A:291:THR:CG2	1:A:353:ARG:NH2	2.73	0.51
2:B:37:ARG:HD2	2:B:171:GLU:OE2	2.10	0.51
2:B:31:VAL:HG22	2:B:68:GLU:HB3	1.92	0.51
3:D:317:ARG:HB3	3:D:335:ARG:HH21	1.76	0.51
2:B:375:ILE:HB	2:B:426:THR:OG1	2.11	0.51
2:B:158:GLN:HG2	2:B:159:TYR:HD1	1.74	0.51
3:D:362:GLU:HB3	3:D:363:PRO:HA	1.93	0.51
1:A:101:ARG:O	1:A:102:GLU:HG3	2.11	0.51
1:A:200:TYR:OH	1:A:257:ASP:HB2	2.11	0.51
2:B:443:VAL:O	2:B:444:THR:HG23	2.11	0.51
1:C:271:LEU:HD12	1:C:275:LEU:HD23	1.92	0.51
3:D:275:LEU:HB2	3:D:306:TRP:CZ3	2.46	0.50
1:A:174:ASP:O	1:A:178:MET:HG3	2.10	0.50
1:C:133:GLU:HG3	1:C:159:TYR:CD2	2.46	0.50
1:A:378:ALA:HB1	1:A:418:TYR:CE2	2.47	0.50
2:B:126:GLN:O	2:B:127:GLN:HB2	2.12	0.50
2:B:122:TYR:CE1	2:B:205:ARG:HB3	2.46	0.50
1:A:347:LYS:HE3	2:B:358:GLU:OE2	2.10	0.50
3:D:379:HIS:CE1	3:D:421:ALA:HB2	2.46	0.50
1:A:325:ARG:NH1	1:A:325:ARG:HG3	2.27	0.50
2:B:169:ALA:CB	3:D:139:ARG:HD3	2.42	0.50
3:D:104:ASP:C	3:D:106:SER:H	2.06	0.50
2:B:223:GLY:O	2:B:224:ASP:HB2	2.11	0.50
1:A:220:LEU:HD13	1:A:229:MET:CE	2.41	0.49
1:A:98:THR:HB	4:E:2:ALA:HB3	1.94	0.49
2:B:101:ARG:HA	2:B:102:GLU:CG	2.42	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ARG:HH11	1:A:325:ARG:CB	2.25	0.49
1:C:194:LEU:O	1:C:198:GLN:HB2	2.12	0.49
1:C:275:LEU:HD12	1:C:275:LEU:O	2.12	0.49
3:D:375:ILE:HB	3:D:426:THR:OG1	2.11	0.49
3:D:268:THR:HA	3:D:271:LEU:HD12	1.93	0.49
3:D:347:LYS:O	3:D:351:GLN:HB2	2.12	0.49
3:D:54:GLU:HG3	3:D:95:ALA:HA	1.95	0.49
1:A:444:THR:HG22	1:A:445:GLN:N	2.25	0.49
1:C:108:ARG:HD2	6:C:2010:HOH:O	2.11	0.49
3:D:252:TYR:C	3:D:253:TYR:HD1	2.16	0.49
1:A:143:LEU:HB2	4:E:4:API:O3	2.13	0.49
2:B:244:LEU:HD12	2:B:244:LEU:O	2.13	0.49
1:A:170:VAL:HG22	1:A:174:ASP:CB	2.43	0.49
2:B:403:MET:O	2:B:406:ARG:HB2	2.13	0.49
2:B:33:ARG:HD2	2:B:72:GLU:OE2	2.13	0.49
3:D:404:LEU:HB2	3:D:405:PRO:HD3	1.95	0.49
2:B:120:ILE:HD13	2:B:188:LEU:HD13	1.95	0.48
1:A:177:ARG:HD3	6:A:2011:HOH:O	2.14	0.48
2:B:268:THR:OG1	2:B:269:GLN:N	2.46	0.48
1:C:37:ARG:NH1	1:C:171:GLU:OE2	2.45	0.48
3:D:147:SER:O	3:D:151:GLN:HG3	2.14	0.48
2:B:268:THR:HA	2:B:271:LEU:HB2	1.95	0.48
3:D:83:GLN:O	3:D:90:PRO:HD2	2.14	0.48
1:A:143:LEU:HD13	4:E:4:API:O3	2.13	0.48
2:B:289:LYS:CB	2:B:289:LYS:NZ	2.71	0.48
3:D:220:LEU:CD1	3:D:229:MET:HE1	2.41	0.48
1:C:289:LYS:NZ	1:C:289:LYS:CB	2.73	0.48
1:A:325:ARG:CG	1:A:325:ARG:NH1	2.77	0.48
1:C:104:ASP:OD2	1:C:106:SER:HB2	2.13	0.48
1:C:138:LYS:HG3	1:C:186:LEU:HD11	1.96	0.48
3:D:133:GLU:HG3	3:D:159:TYR:CE2	2.49	0.48
3:D:410:LYS:HA	3:D:413:TYR:CE2	2.49	0.48
2:B:133:GLU:HB3	2:B:159:TYR:HE2	1.77	0.47
3:D:120:ILE:HD13	3:D:188:LEU:HD13	1.95	0.47
2:B:53:PHE:CE2	2:B:248:LEU:HB3	2.50	0.47
2:B:404:LEU:O	2:B:423:GLY:HA3	2.14	0.47
1:C:397:TRP:CZ2	1:C:430:VAL:HG11	2.49	0.47
1:A:359:SER:HB2	1:A:395:ASN:OD1	2.14	0.47
3:D:220:LEU:HD13	3:D:229:MET:CE	2.40	0.47
3:D:240:LYS:HB3	3:D:240:LYS:HE3	1.68	0.47
4:E:5:DAL:O	4:E:6:DAL:HB3	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:LYS:HE3	1:A:162:LEU:O	2.15	0.47
2:B:31:VAL:CG1	2:B:32:LEU:N	2.76	0.47
3:D:354:SER:HA	3:D:365:ARG:HH21	1.80	0.47
1:A:289:LYS:HE3	1:A:347:LYS:HA	1.97	0.47
3:D:61:PHE:HD1	3:D:235:PHE:CG	2.33	0.47
3:D:268:THR:HG22	3:D:271:LEU:HD12	1.97	0.47
3:D:348:TYR:O	3:D:352:ILE:HG13	2.13	0.47
1:A:108:ARG:NH2	1:A:223:GLY:HA2	2.30	0.47
2:B:210:PHE:HA	2:B:211:GLY:HA2	1.54	0.47
2:B:312:SER:HA	2:B:313:LYS:HE2	1.97	0.46
2:B:327:ALA:HB1	2:B:332:VAL:CG1	2.45	0.46
1:A:271:LEU:O	1:A:276:PRO:HD3	2.14	0.46
1:C:443:VAL:CG2	1:C:443:VAL:O	2.62	0.46
3:D:241:LYS:CA	3:D:242:GLU:HB2	2.44	0.46
1:A:148:HIS:HD2	1:A:188:LEU:HG	1.79	0.46
1:C:332:VAL:HG13	1:C:340:GLN:HB3	1.98	0.46
1:A:192:ASN:ND2	4:E:6:DAL:OXT	2.48	0.46
1:A:172:VAL:HG21	4:E:4:API:H42	1.96	0.46
3:D:127:GLN:O	3:D:129:PRO:HD3	2.16	0.46
2:B:174:ASP:O	2:B:178:MET:HG3	2.16	0.46
3:D:174:ASP:O	3:D:178:MET:HG3	2.15	0.46
3:D:239:ALA:HB3	3:D:240:LYS:HZ1	1.79	0.46
1:A:88:GLY:HA2	1:A:89:GLY:HA3	1.57	0.46
2:B:349:PHE:CE1	2:B:370:LEU:HD23	2.51	0.46
3:D:37:ARG:HG2	3:D:95:ALA:HB1	1.97	0.46
1:A:291:THR:HG21	1:A:353:ARG:NH2	2.30	0.46
2:B:194:LEU:HD21	2:B:206:VAL:HG22	1.97	0.46
1:C:277:ARG:HH11	1:C:277:ARG:HG2	1.81	0.45
3:D:102:ASP:C	3:D:104:ASP:N	2.68	0.45
1:A:180:ASP:OD1	1:A:203:ASN:HB2	2.17	0.45
1:A:379:HIS:O	1:A:382:ASP:HB2	2.15	0.45
1:C:241:LYS:HA	1:C:241:LYS:HD2	1.48	0.45
2:B:443:VAL:CG1	2:B:443:VAL:O	2.63	0.45
2:B:338:PRO:O	2:B:342:ILE:HG13	2.16	0.45
1:C:77:LEU:HA	1:C:77:LEU:HD23	1.80	0.45
1:A:255:HIS:O	1:A:256:VAL:HG13	2.16	0.45
3:D:239:ALA:HB3	3:D:240:LYS:NZ	2.32	0.45
2:B:219:ALA:C	2:B:220:LEU:HD12	2.37	0.45
1:A:64:ARG:NH1	6:A:2004:HOH:O	2.50	0.45
1:C:36:THR:OG1	1:C:37:ARG:N	2.50	0.45
1:A:289:LYS:HB2	1:A:289:LYS:HZ3	1.82	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:LYS:HB3	1:A:28:LYS:HE3	1.66	0.45
1:A:216:LEU:HD13	4:E:5:DAL:O	2.16	0.45
2:B:313:LYS:N	2:B:313:LYS:HE2	2.25	0.44
2:B:251:ARG:O	2:B:251:ARG:HG2	2.17	0.44
3:D:289:LYS:HZ3	3:D:289:LYS:HB2	1.83	0.44
3:D:59:LYS:O	3:D:63:GLU:HG2	2.17	0.44
1:C:185:ASP:O	1:C:186:LEU:HD23	2.17	0.44
3:D:92:LEU:C	3:D:92:LEU:HD12	2.37	0.44
2:B:59:LYS:O	2:B:62:ALA:HB3	2.18	0.44
3:D:122:TYR:CZ	3:D:128:ARG:HB2	2.53	0.44
2:B:402:LYS:HE3	2:B:402:LYS:HA	2.00	0.44
1:A:220:LEU:HD13	1:A:229:MET:HE2	1.99	0.44
2:B:159:TYR:N	2:B:159:TYR:CD1	2.85	0.44
3:D:62:ALA:HB1	3:D:67:VAL:O	2.18	0.44
4:E:4:API:HN21	4:E:5:DAL:HA	1.83	0.44
1:C:295:LEU:HA	1:C:295:LEU:HD12	1.79	0.44
3:D:268:THR:CA	3:D:271:LEU:HB2	2.38	0.44
1:A:325:ARG:HG3	1:A:325:ARG:HH11	1.82	0.44
1:A:196:MET:CE	1:A:252:TYR:HB3	2.48	0.44
1:A:238:GLN:HA	1:A:241:LYS:HG2	1.99	0.44
1:A:256:VAL:HG11	1:A:313:LYS:HZ1	1.83	0.44
1:C:311:THR:CG2	1:C:312:SER:N	2.81	0.44
1:C:254:GLY:HA3	1:C:313:LYS:NZ	2.33	0.44
1:C:401:LYS:NZ	1:C:401:LYS:HB3	2.33	0.44
1:A:293:TRP:CE2	1:A:294:ARG:HG3	2.53	0.43
1:C:28:LYS:HA	1:C:29:GLU:HA	1.72	0.43
1:A:291:THR:HG22	1:A:353:ARG:HH22	1.82	0.43
2:B:101:ARG:CG	2:B:101:ARG:NH1	2.74	0.43
2:B:259:LEU:HD22	2:B:261:TYR:OH	2.18	0.43
1:C:277:ARG:NH1	1:C:277:ARG:HG2	2.34	0.43
3:D:271:LEU:CD2	3:D:275:LEU:HD22	2.44	0.43
3:D:86:ARG:HG2	3:D:87:GLU:OE1	2.18	0.43
2:B:392:LEU:HA	2:B:392:LEU:HD23	1.75	0.43
2:B:101:ARG:NH1	2:B:101:ARG:HG3	2.16	0.43
2:B:410:LYS:HA	2:B:413:TYR:CE2	2.52	0.43
1:C:301:TYR:CD1	1:C:305:LEU:HA	2.53	0.43
1:A:135:LEU:HD23	1:A:186:LEU:HD13	2.01	0.43
1:A:144:LYS:HD2	1:A:145:GLY:H	1.83	0.43
2:B:133:GLU:HA	2:B:159:TYR:CD2	2.53	0.43
3:D:31:VAL:HA	3:D:67:VAL:HG12	2.01	0.43
2:B:172:VAL:HG11	2:B:193:GLU:HB3	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:262:VAL:CG2	2:B:263:GLY:N	2.81	0.43
3:D:317:ARG:HB3	3:D:335:ARG:NH2	2.34	0.43
1:A:170:VAL:HG22	1:A:174:ASP:HB3	2.00	0.43
1:A:35:ILE:HA	1:A:72:GLU:O	2.19	0.43
3:D:406:ARG:HA	3:D:409:GLN:HG3	2.01	0.43
1:A:148:HIS:CD2	1:A:188:LEU:HG	2.54	0.43
2:B:133:GLU:HB3	2:B:159:TYR:CE2	2.54	0.43
1:A:311:THR:HG21	1:A:317:ARG:HE	1.82	0.42
2:B:127:GLN:O	2:B:128:ARG:HB3	2.19	0.42
1:C:425:GLU:OE1	1:C:425:GLU:HA	2.19	0.42
1:C:59:LYS:HA	1:C:69:LEU:HD22	1.99	0.42
3:D:303:GLU:OE2	3:D:373:TYR:HE1	2.02	0.42
1:A:289:LYS:HE3	1:A:347:LYS:CA	2.49	0.42
2:B:288:GLN:O	2:B:288:GLN:HG2	2.20	0.42
1:A:169:ALA:HB2	1:C:139:ARG:HD2	2.01	0.42
1:A:41:ALA:O	4:E:6:DAL:HA	2.19	0.42
3:D:122:TYR:CE2	3:D:128:ARG:HB2	2.54	0.42
3:D:194:LEU:HD22	3:D:206:VAL:HG22	2.00	0.42
1:C:101:ARG:NH1	1:C:101:ARG:HG2	2.31	0.42
1:A:257:ASP:HB3	1:A:258:VAL:H	1.48	0.42
2:B:375:ILE:HD11	2:B:421:ALA:HB1	2.01	0.42
3:D:236:LEU:C	3:D:240:LYS:HZ3	2.23	0.42
1:A:300:GLY:CA	1:A:320:MET:HE2	2.49	0.42
2:B:175:LEU:HD23	2:B:178:MET:CE	2.50	0.42
2:B:327:ALA:O	2:B:332:VAL:HB	2.19	0.42
1:C:314:THR:OG1	1:C:316:VAL:HG22	2.20	0.42
3:D:236:LEU:HA	3:D:240:LYS:HZ3	1.85	0.42
3:D:291:THR:CG2	3:D:292:ASP:N	2.83	0.42
3:D:396:LYS:HA	3:D:396:LYS:HD3	1.91	0.42
1:A:275:LEU:N	1:A:276:PRO:CD	2.83	0.41
1:A:275:LEU:HB3	1:A:276:PRO:HD3	2.02	0.41
2:B:150:GLU:HA	2:B:153:ALA:HB3	2.02	0.41
1:C:33:ARG:NE	1:C:72:GLU:OE2	2.43	0.41
3:D:47:ARG:HB3	3:D:47:ARG:HE	1.46	0.41
1:A:300:GLY:CA	1:A:320:MET:CE	2.98	0.41
2:B:267:PHE:O	2:B:268:THR:CB	2.66	0.41
3:D:123:ARG:O	3:D:126:GLN:HB2	2.20	0.41
3:D:267:PHE:O	3:D:269:GLN:N	2.51	0.41
1:C:121:ILE:HB	1:C:187:THR:HG22	2.01	0.41
1:A:135:LEU:HD23	1:A:186:LEU:CD1	2.51	0.41
1:A:282:PHE:HE1	1:A:320:MET:CE	2.34	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:413:TYR:C	2:B:413:TYR:CD1	2.94	0.41
1:C:275:LEU:N	1:C:276:PRO:CD	2.84	0.41
3:D:368:PHE:CZ	3:D:400:VAL:HG21	2.56	0.41
1:A:190:ASP:OD2	6:A:2007:HOH:O	2.22	0.41
1:C:364:ASP:HA	1:C:367:TRP:CD1	2.55	0.41
1:A:117:THR:O	1:A:191:SER:N	2.51	0.41
1:A:61:PHE:HB2	1:A:235:PHE:CE2	2.55	0.41
2:B:417:ARG:HD2	2:B:418:TYR:CE2	2.55	0.41
1:C:53:PHE:CE2	1:C:248:LEU:HB3	2.55	0.41
1:A:410:LYS:HA	1:A:413:TYR:CE2	2.56	0.41
2:B:261:TYR:O	2:B:435:ARG:NH1	2.43	0.41
3:D:241:LYS:HB2	3:D:242:GLU:CA	2.51	0.41
3:D:241:LYS:HB2	3:D:242:GLU:HG2	1.97	0.41
3:D:291:THR:HG22	3:D:292:ASP:N	2.34	0.41
3:D:332:VAL:HB	3:D:340:GLN:HB3	2.02	0.41
1:A:244:LEU:O	1:A:244:LEU:HD22	2.20	0.41
2:B:140:ILE:HG12	2:B:186:LEU:HB2	2.03	0.41
2:B:175:LEU:HD23	2:B:178:MET:HE3	2.03	0.41
3:D:353:ARG:HG2	3:D:353:ARG:O	2.21	0.41
1:A:228:LEU:HB3	6:A:2008:HOH:O	2.20	0.41
1:A:36:THR:OG1	1:A:37:ARG:N	2.54	0.41
2:B:160:PRO:N	2:B:161:PRO:CD	2.84	0.41
3:D:358:GLU:HG2	3:D:358:GLU:O	2.19	0.41
3:D:98:THR:HA	3:D:99:PRO:HD2	1.93	0.41
1:A:147:SER:CB	4:E:2:ALA:HB1	2.50	0.41
1:A:256:VAL:HB	1:A:257:ASP:H	1.45	0.40
1:A:291:THR:HG22	1:A:353:ARG:NH2	2.36	0.40
2:B:313:LYS:CD	2:B:313:LYS:N	2.83	0.40
1:C:42:THR:HG22	1:C:54:GLU:HG3	2.03	0.40
3:D:159:TYR:N	3:D:159:TYR:CD1	2.89	0.40
2:B:177:ARG:HA	2:B:201:PHE:CE1	2.56	0.40
1:A:303:GLU:OE1	1:A:321:MET:HB2	2.20	0.40
1:A:410:LYS:HA	1:A:413:TYR:CZ	2.57	0.40
3:D:179:VAL:HG21	3:D:187:THR:HG22	2.03	0.40
1:A:131:ARG:O	1:A:134:ASP:HB2	2.21	0.40
2:B:356:LEU:HA	2:B:356:LEU:HD23	1.89	0.40
1:C:266:THR:HG22	1:C:270:HIS:CE1	2.56	0.40
1:C:422:ARG:HG2	1:C:425:GLU:HG2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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	418/499 (84%)	390 (93%)	22 (5%)	6 (1%)	14	42
1	C	416/499 (83%)	385 (92%)	25 (6%)	6 (1%)	14	42
2	B	409/499 (82%)	374 (91%)	23 (6%)	12 (3%)	6	19
3	D	414/499 (83%)	379 (92%)	27 (6%)	8 (2%)	10	32
4	E	1/6 (17%)	1 (100%)	0	0	100	100
All	All	1658/2002 (83%)	1529 (92%)	97 (6%)	32 (2%)	10	32

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	256	VAL
2	B	102	GLU
2	B	262	VAL
3	D	105	ALA
1	A	29	GLU
1	A	104	ASP
1	A	257	ASP
2	B	95	ALA
2	B	101	ARG
2	B	127	GLN
2	B	158	GLN
2	B	226	ASP
2	B	261	TYR
2	B	444	THR
1	C	158	GLN
3	D	223	GLY
3	D	242	GLU
1	C	223	GLY
1	C	260	GLY
1	C	265	TYR
3	D	65	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	D	257	ASP
1	A	101	ARG
1	A	103	ASP
2	B	110	SER
2	B	224	ASP
1	C	258	VAL
3	D	95	ALA
1	C	198	GLN
2	B	443	VAL
3	D	99	PRO
3	D	443	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	351/414 (85%)	328 (93%)	23 (7%)	21	51
1	C	349/414 (84%)	326 (93%)	23 (7%)	21	51
2	B	343/414 (83%)	313 (91%)	30 (9%)	13	35
3	D	347/414 (84%)	319 (92%)	28 (8%)	15	39
All	All	1390/1656 (84%)	1286 (92%)	104 (8%)	17	43

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	39	SER
1	A	40	PRO
1	A	76	ASN
1	A	87	GLU
1	A	101	ARG
1	A	102	GLU
1	A	130	THR
1	A	147	SER
1	A	170	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	194	LEU
1	A	199	VAL
1	A	256	VAL
1	A	257	ASP
1	A	287	LYS
1	A	311	THR
1	A	313	LYS
1	A	325	ARG
1	A	359	SER
1	A	389	LYS
1	A	398	LEU
1	A	431	GLN
1	A	445	GLN
2	B	59	LYS
2	B	63	GLU
2	B	65	LEU
2	B	70	LYS
2	B	86	ARG
2	B	101	ARG
2	B	138	LYS
2	B	155	LEU
2	B	156	LYS
2	B	173	VAL
2	B	179	VAL
2	B	181	VAL
2	B	205	ARG
2	B	209	ASP
2	B	225	ASP
2	B	226	ASP
2	B	261	TYR
2	B	287	LYS
2	B	313	LYS
2	B	319	LEU
2	B	324	ASN
2	B	398	LEU
2	B	402	LYS
2	B	406	ARG
2	B	413	TYR
2	B	422	ARG
2	B	431	GLN
2	B	435	ARG
2	B	441	THR

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	444	THR
1	C	28	LYS
1	C	39	SER
1	C	71	ILE
1	C	87	GLU
1	C	119	GLN
1	C	130	THR
1	C	138	LYS
1	C	150	GLU
1	C	158	GLN
1	C	196	MET
1	C	204	VAL
1	C	214	ARG
1	C	241	LYS
1	C	256	VAL
1	C	262	VAL
1	C	265	TYR
1	C	272	GLN
1	C	284	GLN
1	C	317	ARG
1	C	341	SER
1	C	411	GLN
1	C	413	TYR
1	C	417	ARG
3	D	33	ARG
3	D	38	ASN
3	D	48	ASN
3	D	60	ARG
3	D	69	LEU
3	D	85	SER
3	D	87	GLU
3	D	101	ARG
3	D	103	ASP
3	D	106	SER
3	D	112	THR
3	D	128	ARG
3	D	130	THR
3	D	139	ARG
3	D	147	SER
3	D	155	LEU
3	D	171	GLU
3	D	181	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
3	D	240	LYS
3	D	241	LYS
3	D	242	GLU
3	D	250	ASP
3	D	359	SER
3	D	398	LEU
3	D	426	THR
3	D	434	ARG
3	D	444	THR
3	D	445	GLN

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

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 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).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	DGL	E	3	4	5,8,9	1.13	0	3,9,11	0.76	0
4	API	E	4	4	6,11,12	0.95	0	5,13,15	2.22	1 (20%)
4	DAL	E	5	4	1,4,5	0.30	0	1,4,6	0.52	0
4	DAL	E	6	4	0,5,5	0.00	-	2,6,6	0.54	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
4	DGL	E	3	4	-	0/3/8/9	0/0/0/0
4	API	E	4	4	-	0/6/12/14	0/0/0/0
4	DAL	E	5	4	-	0/0/2/4	0/0/0/0
4	DAL	E	6	4	-	0/0/4/4	0/0/0/0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
4	E	4	API	O1-C1-C2	-4.22	114.41	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	3	DGL	2	0
4	E	4	API	12	0
4	E	5	DAL	6	0
4	E	6	DAL	7	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	419/499 (83%)	-0.39	1 (0%) 95 94	24, 45, 86, 156	0
1	C	418/499 (83%)	-0.33	3 (0%) 89 84	29, 50, 92, 149	0
2	B	413/499 (82%)	-0.37	0 100 100	30, 57, 93, 136	0
3	D	416/499 (83%)	-0.18	1 (0%) 95 94	38, 67, 110, 156	0
4	E	1/6 (16%)	7.07	1 (100%) 0 0	163, 163, 163, 163	0
All	All	1667/2002 (83%)	-0.31	6 (0%) 93 90	24, 56, 100, 163	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	E	2	ALA	7.1
1	C	259	LEU	3.4
1	C	258	VAL	2.6
1	A	268	THR	2.4
1	C	255	HIS	2.4
3	D	236	LEU	2.1

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	DAL	E	6	6/6	0.81	0.56	-	109,124,146,163	0
4	DGL	E	3	9/10	0.86	0.37	-	118,144,167,173	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	API	E	4	12/13	0.82	0.62	-	133,186,235,282	0
4	DAL	E	5	5/6	0.82	0.74	-	142,147,175,177	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	CL	C	1446	1/1	0.95	0.11	-1.37	100,100,100,100	0
5	CL	A	1446	1/1	0.95	0.07	-2.60	61,61,61,61	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.