Full wwPDB X-ray Structure Validation Report (i)

Oct 6, 2016 – 05:56 PM EDT

PDB ID	:	5AA1
Title	:	Crystal structure of MltF from Pseudomonas aeruginosa in complex with NAG-anhNAM-pentapeptide
Authors	:	Dominguez-Gil, T.; Acebron, I.; Hermoso, J.A.
Deposited on	:	2015-07-23
Resolution	:	2.89 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

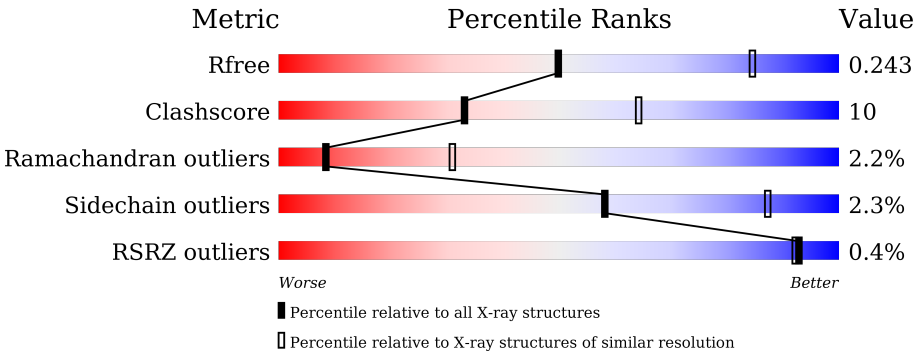
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027939
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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 >=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 <=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	60% 22% • 16%
1	B	499	66% 16% • 17%
1	C	499	% 65% 17% • 16%
1	D	499	63% 18% •• 16%
2	E	6	17% 17% 83%

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	FGA	E	3	-	-	X	-
2	API	E	4	-	-	X	-
3	CL	B	1460	-	-	-	X
3	CL	C	1460	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 13551 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.

- Molecule 1 is a protein called MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	418	Total	C	N	O	S	0	1	0
			3360	2118	597	636	9			
1	B	413	Total	C	N	O	S	0	0	0
			3313	2089	591	624	9			
1	C	419	Total	C	N	O	S	0	0	0
			3360	2119	598	634	9			
1	D	417	Total	C	N	O	S	0	0	0
			3342	2108	595	630	9			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	EXPRESSION TAG	UNP Q9HXN1
A	-7	ALA	-	EXPRESSION TAG	UNP Q9HXN1
A	-6	PRO	-	EXPRESSION TAG	UNP Q9HXN1
A	-5	SER	-	EXPRESSION TAG	UNP Q9HXN1
A	-4	ARG	-	EXPRESSION TAG	UNP Q9HXN1
A	-3	LEU	-	EXPRESSION TAG	UNP Q9HXN1
A	-2	CYS	-	EXPRESSION TAG	UNP Q9HXN1
A	-1	VAL	-	EXPRESSION TAG	UNP Q9HXN1
A	0	TYR	-	EXPRESSION TAG	UNP Q9HXN1
A	1	CYS	-	EXPRESSION TAG	UNP Q9HXN1
A	2	ALA	-	EXPRESSION TAG	UNP Q9HXN1
A	3	ASP	-	EXPRESSION TAG	UNP Q9HXN1
A	4	VAL	-	EXPRESSION TAG	UNP Q9HXN1
A	5	CYS	-	EXPRESSION TAG	UNP Q9HXN1
A	6	PRO	-	EXPRESSION TAG	UNP Q9HXN1
A	7	ASP	-	EXPRESSION TAG	UNP Q9HXN1
A	281	THR	ALA	CONFLICT	UNP Q9HXN1
A	302	LYS	LEU	CONFLICT	UNP Q9HXN1
B	-8	MET	-	EXPRESSION TAG	UNP Q9HXN1
B	-7	ALA	-	EXPRESSION TAG	UNP Q9HXN1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	PRO	-	EXPRESSION TAG	UNP Q9HXN1
B	-5	SER	-	EXPRESSION TAG	UNP Q9HXN1
B	-4	ARG	-	EXPRESSION TAG	UNP Q9HXN1
B	-3	LEU	-	EXPRESSION TAG	UNP Q9HXN1
B	-2	CYS	-	EXPRESSION TAG	UNP Q9HXN1
B	-1	VAL	-	EXPRESSION TAG	UNP Q9HXN1
B	0	TYR	-	EXPRESSION TAG	UNP Q9HXN1
B	1	CYS	-	EXPRESSION TAG	UNP Q9HXN1
B	2	ALA	-	EXPRESSION TAG	UNP Q9HXN1
B	3	ASP	-	EXPRESSION TAG	UNP Q9HXN1
B	4	VAL	-	EXPRESSION TAG	UNP Q9HXN1
B	5	CYS	-	EXPRESSION TAG	UNP Q9HXN1
B	6	PRO	-	EXPRESSION TAG	UNP Q9HXN1
B	7	ASP	-	EXPRESSION TAG	UNP Q9HXN1
B	281	THR	ALA	CONFLICT	UNP Q9HXN1
B	302	LYS	LEU	CONFLICT	UNP Q9HXN1
C	-8	MET	-	EXPRESSION TAG	UNP Q9HXN1
C	-7	ALA	-	EXPRESSION TAG	UNP Q9HXN1
C	-6	PRO	-	EXPRESSION TAG	UNP Q9HXN1
C	-5	SER	-	EXPRESSION TAG	UNP Q9HXN1
C	-4	ARG	-	EXPRESSION TAG	UNP Q9HXN1
C	-3	LEU	-	EXPRESSION TAG	UNP Q9HXN1
C	-2	CYS	-	EXPRESSION TAG	UNP Q9HXN1
C	-1	VAL	-	EXPRESSION TAG	UNP Q9HXN1
C	0	TYR	-	EXPRESSION TAG	UNP Q9HXN1
C	1	CYS	-	EXPRESSION TAG	UNP Q9HXN1
C	2	ALA	-	EXPRESSION TAG	UNP Q9HXN1
C	3	ASP	-	EXPRESSION TAG	UNP Q9HXN1
C	4	VAL	-	EXPRESSION TAG	UNP Q9HXN1
C	5	CYS	-	EXPRESSION TAG	UNP Q9HXN1
C	6	PRO	-	EXPRESSION TAG	UNP Q9HXN1
C	7	ASP	-	EXPRESSION TAG	UNP Q9HXN1
C	281	THR	ALA	CONFLICT	UNP Q9HXN1
C	302	LYS	LEU	CONFLICT	UNP Q9HXN1
D	-8	MET	-	EXPRESSION TAG	UNP Q9HXN1
D	-7	ALA	-	EXPRESSION TAG	UNP Q9HXN1
D	-6	PRO	-	EXPRESSION TAG	UNP Q9HXN1
D	-5	SER	-	EXPRESSION TAG	UNP Q9HXN1
D	-4	ARG	-	EXPRESSION TAG	UNP Q9HXN1
D	-3	LEU	-	EXPRESSION TAG	UNP Q9HXN1
D	-2	CYS	-	EXPRESSION TAG	UNP Q9HXN1
D	-1	VAL	-	EXPRESSION TAG	UNP Q9HXN1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	TYR	-	EXPRESSION TAG	UNP Q9HXN1
D	1	CYS	-	EXPRESSION TAG	UNP Q9HXN1
D	2	ALA	-	EXPRESSION TAG	UNP Q9HXN1
D	3	ASP	-	EXPRESSION TAG	UNP Q9HXN1
D	4	VAL	-	EXPRESSION TAG	UNP Q9HXN1
D	5	CYS	-	EXPRESSION TAG	UNP Q9HXN1
D	6	PRO	-	EXPRESSION TAG	UNP Q9HXN1
D	7	ASP	-	EXPRESSION TAG	UNP Q9HXN1
D	281	THR	ALA	CONFLICT	UNP Q9HXN1
D	302	LYS	LEU	CONFLICT	UNP Q9HXN1

- Molecule 2 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
2	E	6	Total	C	N	O	0	0	0
			42	24	6	12			

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Cl	0	0
			2	2		
3	A	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		

- Molecule 4 is water.

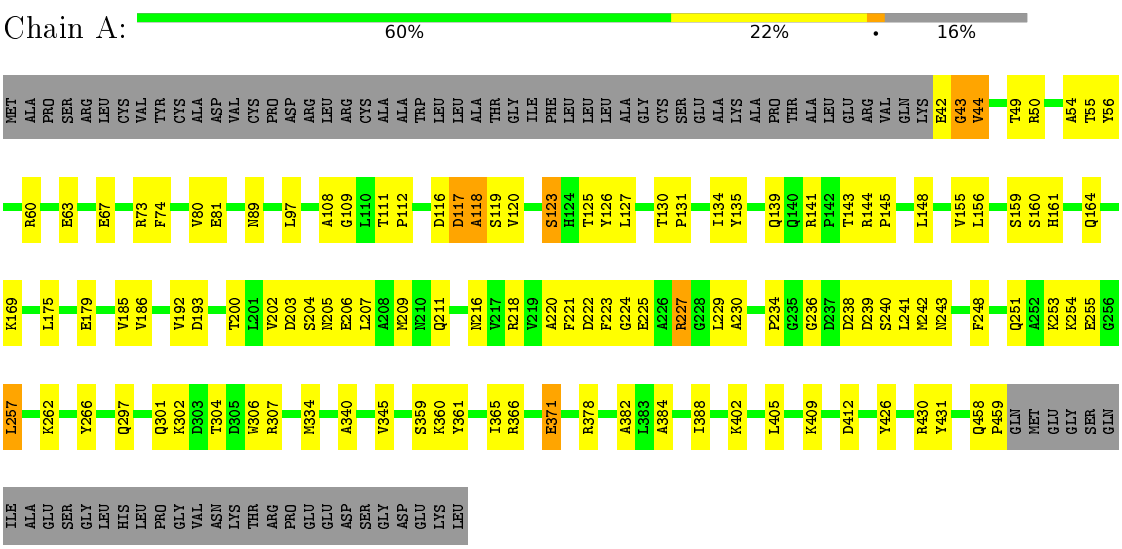
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	52	Total	O	0	0
			52	52		
4	B	28	Total	O	0	0
			28	28		
4	C	35	Total	O	0	0
			35	35		
4	D	14	Total	O	0	0
			14	14		

3 Residue-property plots (i)

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.

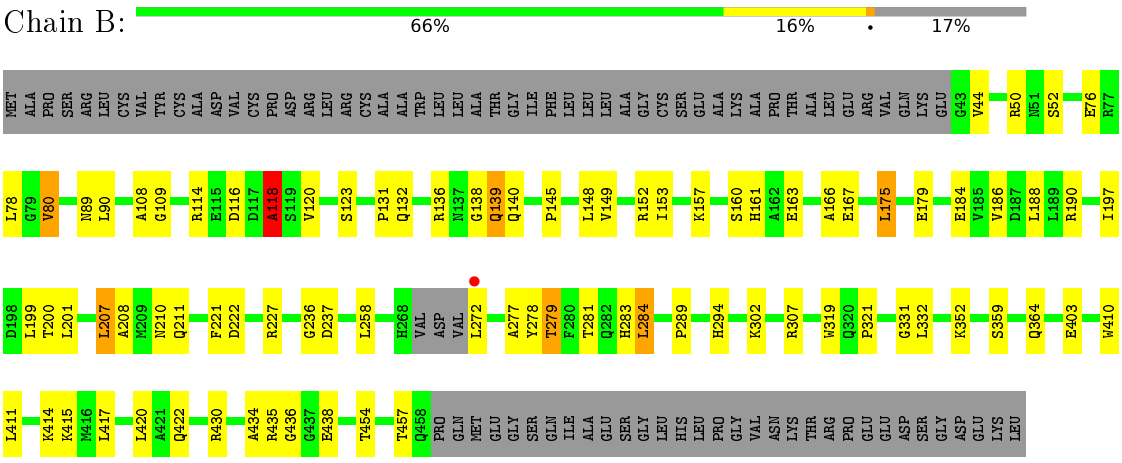
- Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

Chain A:



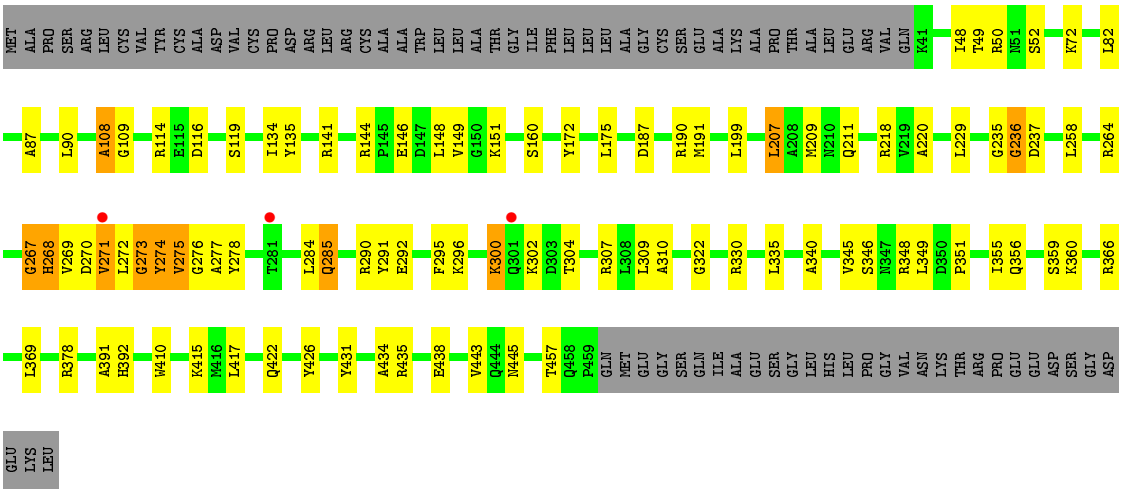
- Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

Chain B:



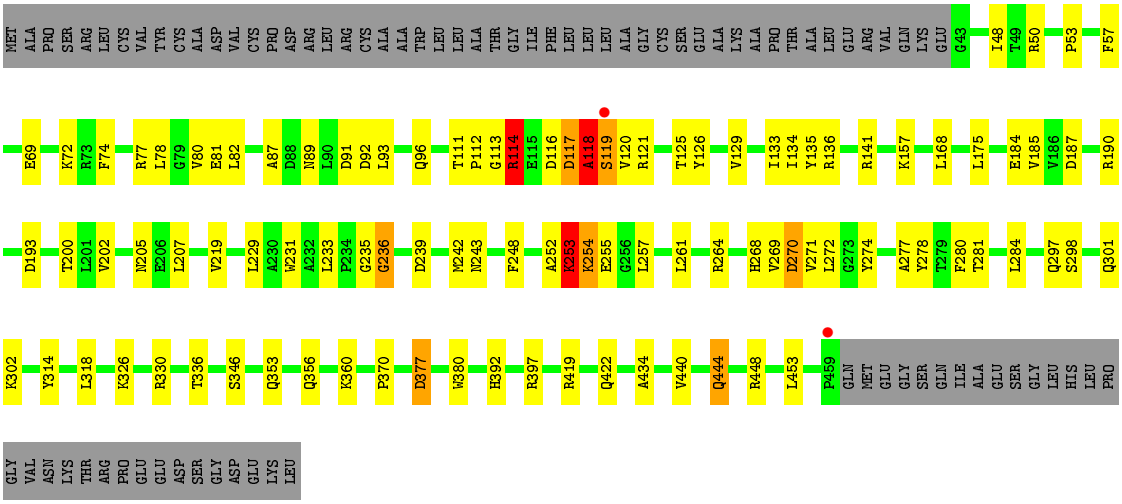
- Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

Chain C:



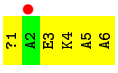
• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

Chain D:



• Molecule 2: N-ACETYLGLUCOSAMINE-1,6-ANHYDRO-N-ACETYLMURAMIC ACID L-A LA-D-GLU-M-DAP-D-ALA-D-ALA

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	65.85Å 135.75Å 138.03Å 90.00° 92.01° 90.00°	Depositor
Resolution (Å)	47.25 – 2.89 47.25 – 2.89	Depositor EDS
% Data completeness (in resolution range)	91.7 (47.25-2.89) 91.7 (47.25-2.89)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 2.91Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.168 , 0.243 0.169 , 0.243	Depositor DCC
R_{free} test set	2022 reflections (4.06%)	DCC
Wilson B-factor (Å^2)	61.3	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 45.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.001 for -h,l,k 0.014 for -h,-l,-k 0.034 for h,-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	13551	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DAL, AH0, API, FGA, 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	0.49	0/3431	0.66	2/4639 (0.0%)
1	B	0.44	0/3382	0.66	2/4569 (0.0%)
1	C	0.48	0/3431	0.66	0/4638
1	D	0.42	0/3413	0.63	3/4615 (0.1%)
2	E	0.85	0/4	0.70	0/4
All	All	0.46	0/13661	0.65	7/18465 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	2
All	All	0	4

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	118	ALA	N-CA-C	5.78	126.60	111.00
1	D	114	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	257	LEU	CA-CB-CG	5.62	128.23	115.30
1	A	43	GLY	C-N-CA	5.55	135.57	121.70
1	D	253	LYS	C-N-CA	5.36	135.09	121.70
1	B	123	SER	C-N-CA	5.11	134.46	121.70
1	B	118	ALA	C-N-CA	5.05	134.33	121.70

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	140	GLN	Peptide
1	C	273	GLY	Peptide
1	D	253	LYS	Peptide
1	D	270	ASP	Peptide

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	3360	0	3300	84	0
1	B	3313	0	3259	50	0
1	C	3360	0	3308	59	0
1	D	3342	0	3289	81	0
2	E	42	0	35	18	0
3	A	1	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	1	0
4	A	52	0	0	5	1
4	B	28	0	0	2	0
4	C	35	0	0	0	1
4	D	14	0	0	3	0
All	All	13551	0	13191	274	1

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 10.

All (274) 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:114:ARG:HD3	1:D:117:ASP:HB3	1.40	1.02
1:D:118:ALA:HA	1:D:119:SER:HB3	1.53	0.88
1:A:185:VAL:HG11	1:A:206:GLU:HG2	1.60	0.84
1:B:50:ARG:NH1	1:B:184:GLU:OE2	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:ARG:HD3	1:D:117:ASP:CB	2.08	0.83
1:D:252:ALA:HA	1:D:255:GLU:HG2	1.62	0.82
1:B:131:PRO:HG2	1:B:227:ARG:HH11	1.44	0.81
1:D:239:ASP:O	1:D:243:ASN:ND2	2.15	0.79
1:A:225:GLU:O	1:A:227:ARG:NH1	2.18	0.77
1:C:144:ARG:HD2	1:C:146:GLU:HG2	1.66	0.76
1:B:161:HIS:HB3	1:B:201:LEU:HG	1.68	0.76
1:A:117:ASP:O	1:A:119:SER:N	2.20	0.74
1:B:118:ALA:HA	1:B:120:VAL:H	1.52	0.74
1:A:111:THR:N	2:E:3:FGA:OXT	2.20	0.74
1:A:42:GLU:HG3	1:A:43:GLY:H	1.53	0.74
4:A:2021:HOH:O	2:E:4:API:N6	2.20	0.73
1:D:114:ARG:HH21	1:D:120:VAL:C	1.93	0.72
1:D:114:ARG:NH1	1:D:116:ASP:O	2.23	0.71
1:A:60:ARG:NH2	4:A:2004:HOH:O	2.14	0.71
1:D:50:ARG:NH1	1:D:184:GLU:OE2	2.24	0.70
1:A:203:ASP:HB2	2:E:5:DAL:HB2	1.71	0.70
1:D:136:ARG:NH1	1:D:193:ASP:O	2.24	0.70
1:A:141:ARG:NH1	1:A:220:ALA:O	2.25	0.70
1:D:187:ASP:OD1	1:D:190:ARG:NH1	2.23	0.70
1:C:304:THR:HG22	1:C:366:ARG:HH22	1.56	0.69
1:D:253:LYS:H	1:D:254:LYS:HB2	1.57	0.68
1:B:114:ARG:NH1	1:B:116:ASP:OD1	2.25	0.68
1:B:131:PRO:HG2	1:B:227:ARG:NH1	2.07	0.68
1:D:301:GLN:NE2	1:D:356:GLN:OE1	2.26	0.68
1:D:92:ASP:OD2	1:D:96:GLN:NE2	2.27	0.68
1:C:48:ILE:HD11	1:C:87:ALA:HB2	1.77	0.67
1:D:78:LEU:HB3	1:D:80:VAL:HG22	1.77	0.67
1:D:207:LEU:HD21	1:D:219:VAL:HG22	1.77	0.66
1:C:435:ARG:HG2	1:C:438:GLU:HG2	1.76	0.66
1:D:298:SER:O	1:D:302:LYS:NZ	2.28	0.66
1:A:159:SER:HA	2:E:3:FGA:HB2	1.78	0.66
1:A:160:SER:HB3	2:E:3:FGA:HA	1.76	0.66
1:D:253:LYS:HB2	1:D:254:LYS:HG3	1.77	0.65
1:A:205:ASN:HD21	2:E:6:DAL:H2	1.44	0.65
1:A:44:VAL:H	1:A:80:VAL:HB	1.62	0.65
1:B:319:TRP:HA	1:B:332:LEU:HD11	1.79	0.64
1:A:304:THR:HG22	1:A:366:ARG:HH22	1.63	0.64
1:A:54:ALA:HB1	2:E:6:DAL:HA	1.79	0.64
1:B:207:LEU:O	1:B:210:ASN:N	2.27	0.63
1:A:304:THR:CG2	1:A:366:ARG:HH22	2.11	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:LYS:HZ1	1:C:360:LYS:HG3	1.65	0.61
1:D:253:LYS:N	1:D:254:LYS:HB2	2.16	0.61
1:B:138:GLY:HA3	1:B:139:GLN:HB2	1.81	0.61
1:C:269:VAL:HG23	1:C:270:ASP:H	1.67	0.60
1:C:273:GLY:HA3	1:C:445:ASN:ND2	2.16	0.60
1:A:125:THR:O	1:A:253:LYS:NZ	2.33	0.60
1:D:114:ARG:CD	1:D:117:ASP:HB3	2.24	0.60
1:D:119:SER:OG	1:D:120:VAL:N	2.31	0.59
1:C:135:TYR:CE1	1:C:218:ARG:HB2	2.37	0.59
1:D:346:SER:N	1:D:353:GLN:OE1	2.35	0.59
1:A:161:HIS:ND1	2:E:4:API:H6	2.18	0.59
1:D:69:GLU:OE2	1:D:264:ARG:NH1	2.35	0.59
1:A:109:GLY:HA3	2:E:5:DAL:C	2.33	0.59
1:B:114:ARG:NH2	1:B:116:ASP:OD2	2.36	0.58
1:D:253:LYS:HG2	1:D:254:LYS:HE2	1.84	0.58
1:B:132:GLN:HA	1:B:222:ASP:H	1.68	0.58
1:C:146:GLU:HB3	1:C:172:TYR:CZ	2.38	0.58
1:D:114:ARG:NH2	1:D:120:VAL:O	2.37	0.58
1:C:351:PRO:O	1:C:355:ILE:HG13	2.04	0.58
1:A:139:GLN:HG3	4:A:2024:HOH:O	2.04	0.57
1:B:403:GLU:OE2	1:D:136:ARG:NH2	2.38	0.57
1:C:330:ARG:HD2	1:C:349:LEU:HD11	1.85	0.57
1:A:74:PHE:HB2	1:A:248:PHE:CE2	2.39	0.57
1:C:141:ARG:NH1	1:C:220:ALA:O	2.37	0.56
1:A:156:LEU:HD13	2:E:4:API:H51	1.87	0.56
1:C:272:LEU:HD23	1:C:275:VAL:HA	1.87	0.56
1:A:116:ASP:O	1:A:118:ALA:N	2.31	0.56
1:C:272:LEU:HB3	1:C:273:GLY:HA2	1.86	0.56
1:D:116:ASP:O	1:D:118:ALA:N	2.37	0.56
1:D:118:ALA:CA	1:D:119:SER:HB3	2.30	0.56
1:A:185:VAL:HG11	1:A:202:VAL:HG21	1.88	0.56
1:D:184:GLU:H	1:D:187:ASP:HB2	1.71	0.56
1:B:278:TYR:O	1:B:279:THR:HB	2.05	0.55
1:A:251:GLN:O	1:A:255:GLU:HB3	2.06	0.55
1:A:42:GLU:HG3	1:A:43:GLY:N	2.20	0.55
1:B:208:ALA:HB2	1:B:211:GLN:HB3	1.88	0.54
1:D:301:GLN:HE22	1:D:356:GLN:CD	2.09	0.54
1:D:77:ARG:HD3	1:D:248:PHE:HD1	1.71	0.54
1:A:202:VAL:HA	2:E:4:API:HN62	1.73	0.54
1:C:292:GLU:OE2	1:C:296:LYS:NZ	2.40	0.54
1:A:131:PRO:HG2	1:A:164:GLN:HE22	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:ASP:HA	4:B:2008:HOH:O	2.07	0.54
1:C:72:LYS:HA	1:C:82:LEU:HD22	1.89	0.54
1:A:224:GLY:HA3	1:A:227:ARG:HH22	1.72	0.53
1:A:123:SER:HA	1:A:242:MET:HE1	1.90	0.53
1:A:143:THR:O	1:A:144:ARG:HD2	2.08	0.53
1:A:43:GLY:HA3	1:A:44:VAL:HB	1.89	0.53
1:D:253:LYS:HZ2	1:D:253:LYS:N	2.07	0.53
1:D:280:PHE:O	1:D:284:LEU:HD12	2.09	0.53
1:C:274:TYR:O	1:C:275:VAL:HB	2.09	0.53
1:C:50:ARG:HG3	1:C:108:ALA:HB1	1.91	0.53
1:C:148:LEU:HD22	1:C:199:LEU:HD13	1.91	0.53
1:A:169:LYS:HE3	1:A:175:LEU:O	2.09	0.52
1:B:278:TYR:HA	1:B:281:THR:HG22	1.91	0.52
1:B:149:VAL:HG22	1:B:175:LEU:HB2	1.91	0.52
1:B:307:ARG:CZ	1:B:454:THR:HG22	2.40	0.52
1:D:233:LEU:HD13	1:D:242:MET:HE1	1.92	0.52
1:C:273:GLY:O	1:C:274:TYR:HB3	2.10	0.52
1:A:371[A]:GLU:HA	1:A:378:ARG:HH12	1.75	0.51
1:B:138:GLY:CA	1:B:139:GLN:HB2	2.40	0.51
1:D:264:ARG:HG2	4:D:2008:HOH:O	2.10	0.51
1:B:364:GLN:NE2	4:B:2015:HOH:O	2.24	0.51
1:C:335:LEU:O	1:C:348:ARG:NH1	2.43	0.51
1:B:302:LYS:HB2	1:B:302:LYS:NZ	2.25	0.51
1:D:91:ASP:OD2	1:D:157:LYS:NZ	2.44	0.51
1:B:190:ARG:NH1	1:B:422:GLN:HG2	2.26	0.51
1:A:116:ASP:C	1:A:118:ALA:H	2.12	0.50
1:C:369:LEU:O	1:C:378:ARG:NH2	2.44	0.50
1:B:221:PHE:HA	1:B:222:ASP:HB2	1.93	0.50
1:D:121:ARG:NE	1:D:236:GLY:HA2	2.27	0.50
1:A:160:SER:H	2:E:3:FGA:CG	2.24	0.50
1:C:269:VAL:HG23	1:C:270:ASP:N	2.26	0.50
1:D:257:LEU:O	1:D:261:LEU:HB2	2.12	0.49
1:D:280:PHE:CD2	1:D:284:LEU:HD11	2.46	0.49
1:D:377:ASP:HA	1:D:380:TRP:CD1	2.47	0.49
1:D:48:ILE:HD11	1:D:87:ALA:HB2	1.93	0.49
1:A:361:TYR:O	1:A:365:ILE:HG13	2.12	0.49
1:A:185:VAL:CG1	1:A:206:GLU:HG2	2.38	0.49
1:B:148:LEU:HD22	1:B:199:LEU:HD13	1.95	0.49
1:A:202:VAL:HA	2:E:4:API:N6	2.28	0.49
1:A:49:THR:OG1	1:A:50:ARG:N	2.45	0.49
1:D:370:PRO:HG2	1:D:397:ARG:HH12	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:TRP:CE2	1:A:307:ARG:HG3	2.48	0.49
1:A:371[A]:GLU:HG2	1:A:371[A]:GLU:O	2.12	0.49
1:D:392:HIS:CE1	1:D:434:ALA:HB2	2.47	0.49
1:A:302:LYS:HZ2	1:A:302:LYS:HB2	1.78	0.48
1:A:134:ILE:HD12	1:A:207:LEU:HD13	1.94	0.48
1:A:221:PHE:HD2	1:A:222:ASP:O	1.96	0.48
1:D:330:ARG:NH2	3:D:1460:CL:CL	2.84	0.48
1:A:135:TYR:CE1	1:A:218:ARG:HB2	2.48	0.48
1:A:302:LYS:HE2	1:A:360:LYS:N	2.28	0.48
1:C:187:ASP:O	1:C:191:MET:HG3	2.13	0.48
1:C:307:ARG:HH11	1:C:457:THR:HB	1.78	0.48
1:A:192:VAL:HG21	1:A:200:THR:HG22	1.96	0.48
1:C:392:HIS:CD2	1:C:434:ALA:HB2	2.48	0.47
1:A:112:PRO:HG3	1:A:230:ALA:HB3	1.96	0.47
1:B:136:ARG:O	1:B:138:GLY:N	2.47	0.47
1:D:184:GLU:HG3	1:D:185:VAL:H	1.79	0.47
1:B:435:ARG:HG2	1:B:438:GLU:HG2	1.96	0.47
1:D:278:TYR:HB3	4:D:2011:HOH:O	2.13	0.47
1:D:314:TYR:CZ	1:D:318:LEU:HD23	2.49	0.47
1:C:415:LYS:HE3	1:C:415:LYS:HB2	1.58	0.47
1:D:119:SER:N	1:D:235:GLY:HA3	2.29	0.47
1:A:44:VAL:HA	1:A:81:GLU:O	2.15	0.47
4:A:2011:HOH:O	2:E:1:AH0:HB1	2.14	0.47
1:C:276:GLY:C	1:C:278:TYR:H	2.18	0.47
1:D:377:ASP:OD1	1:D:377:ASP:N	2.46	0.47
1:B:410:TRP:O	1:B:414:LYS:HB3	2.14	0.47
1:A:458:GLN:HB3	1:A:459:PRO:HA	1.96	0.47
1:B:284:LEU:O	1:B:289:PRO:HD3	2.15	0.46
1:B:294:HIS:ND1	1:B:352:LYS:HG3	2.30	0.46
1:D:297:GLN:O	1:D:301:GLN:HB3	2.16	0.46
1:D:440:VAL:O	1:D:444:GLN:HG2	2.15	0.46
1:C:272:LEU:HB3	1:C:273:GLY:CA	2.46	0.46
1:A:251:GLN:HA	1:A:254:LYS:HB3	1.97	0.46
1:C:309:LEU:HD22	1:C:359:SER:OG	2.15	0.46
1:A:144:ARG:HB3	1:A:145:PRO:HD2	1.98	0.46
1:A:366:ARG:HG3	1:A:382:ALA:HB2	1.98	0.46
1:D:185:VAL:HG13	1:D:202:VAL:HG11	1.97	0.46
1:D:129:VAL:HG12	1:D:205:ASN:HB3	1.98	0.46
1:D:253:LYS:HA	1:D:253:LYS:HD3	1.80	0.46
1:A:262:LYS:O	1:A:266:TYR:HB2	2.16	0.46
1:D:277:ALA:O	1:D:281:THR:HG23	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:HIS:O	1:B:284:LEU:HB2	2.16	0.45
1:D:81:GLU:HG2	1:D:82:LEU:N	2.31	0.45
1:C:295:PHE:CZ	1:C:310:ALA:HA	2.51	0.45
1:A:239:ASP:O	1:A:243:ASN:ND2	2.36	0.45
1:A:209:MET:HB2	1:A:266:TYR:CE1	2.51	0.45
1:A:405:LEU:HB3	1:A:412:ASP:OD2	2.16	0.45
1:D:53:PRO:HA	1:D:57:PHE:CE1	2.52	0.45
1:D:112:PRO:HA	1:D:113:GLY:HA3	1.50	0.45
1:B:90:LEU:HA	1:B:90:LEU:HD23	1.72	0.45
1:D:253:LYS:HB2	1:D:254:LYS:CG	2.43	0.45
1:C:273:GLY:O	1:C:274:TYR:CB	2.64	0.45
1:D:168:LEU:HD23	1:D:175:LEU:HD22	1.99	0.45
1:A:50:ARG:NH1	2:E:4:API:C3	2.80	0.45
1:B:152:ARG:HD3	1:B:197:ILE:HG22	1.98	0.45
1:A:67:GLU:OE2	1:A:126:TYR:OH	2.31	0.45
1:C:149:VAL:HG13	1:C:175:LEU:HA	1.99	0.45
1:B:157:LYS:HG3	1:B:179:GLU:OE2	2.16	0.45
1:C:50:ARG:NH1	1:C:108:ALA:O	2.50	0.45
1:D:302:LYS:HE2	1:D:360:LYS:N	2.32	0.45
1:A:156:LEU:N	2:E:4:API:O4	2.46	0.45
1:A:430:ARG:HD3	1:A:431:TYR:CE2	2.52	0.44
1:B:153:ILE:HG12	1:B:199:LEU:HB2	2.00	0.44
1:B:221:PHE:CA	1:B:222:ASP:HB2	2.47	0.44
1:A:340:ALA:HB1	1:A:345:VAL:HB	2.00	0.44
1:B:44:VAL:HA	1:B:80:VAL:HG12	1.99	0.44
1:C:340:ALA:HB1	1:C:345:VAL:HB	1.99	0.44
1:A:409:LYS:HA	1:A:409:LYS:HD3	1.83	0.44
1:D:133:ILE:HD13	1:D:133:ILE:HA	1.78	0.44
1:A:193:ASP:OD1	1:A:216:ASN:HB2	2.18	0.44
1:D:269:VAL:HG12	4:D:2009:HOH:O	2.16	0.44
1:A:160:SER:H	2:E:3:FGA:HG3	1.82	0.44
1:C:114:ARG:HD3	1:C:116:ASP:OD2	2.18	0.43
1:D:119:SER:O	1:D:235:GLY:N	2.47	0.43
1:A:238:ASP:OD2	1:A:240:SER:OG	2.35	0.43
1:A:302:LYS:HB2	1:A:302:LYS:NZ	2.32	0.43
1:C:285:GLN:HB2	1:D:281:THR:OG1	2.18	0.43
1:C:322:GLY:HA2	1:C:349:LEU:HD23	2.00	0.43
1:D:135:TYR:CZ	1:D:141:ARG:HB2	2.53	0.43
1:A:127:LEU:HD23	1:A:229:LEU:HD12	2.00	0.43
1:A:207:LEU:HD21	1:A:211:GLN:OE1	2.17	0.43
1:C:271:VAL:HA	1:C:272:LEU:HA	1.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:LEU:HD13	1:B:200:THR:OG1	2.19	0.43
1:D:134:ILE:HB	1:D:200:THR:HG22	2.00	0.43
1:C:190:ARG:NH1	1:C:422:GLN:HG2	2.33	0.43
1:A:56:TYR:CE1	1:A:63:GLU:HG2	2.54	0.43
1:D:268:HIS:HB2	1:D:326:LYS:HD3	2.00	0.43
1:B:258:LEU:HD12	1:B:258:LEU:HA	1.77	0.43
1:B:417:LEU:HD23	1:B:420:LEU:HD12	2.01	0.43
1:C:264:ARG:O	1:C:264:ARG:HG3	2.18	0.42
1:C:391:ALA:HB1	1:C:431:TYR:CE2	2.54	0.42
1:B:321:PRO:O	1:B:331:GLY:HA2	2.20	0.42
1:D:72:LYS:HE2	1:D:72:LYS:HB2	1.94	0.42
1:D:74:PHE:HD1	1:D:248:PHE:CG	2.37	0.42
1:C:290:ARG:HD2	1:C:291:TYR:CZ	2.54	0.42
1:A:155:VAL:O	1:A:179:GLU:HA	2.20	0.42
1:C:134:ILE:CD1	1:C:207:LEU:HD13	2.49	0.42
1:C:258:LEU:HA	1:C:258:LEU:HD23	1.83	0.42
1:C:417:LEU:HD23	1:C:417:LEU:HA	1.79	0.42
1:D:111:THR:HG22	1:D:112:PRO:O	2.20	0.42
1:A:145:PRO:O	1:A:148:LEU:HD13	2.20	0.42
1:B:207:LEU:HD12	1:B:207:LEU:HA	1.82	0.42
1:C:267:GLY:HA2	1:C:268:HIS:HA	1.88	0.42
1:B:302:LYS:HB2	1:B:302:LYS:HZ2	1.84	0.41
1:C:410:TRP:CZ2	1:C:443:VAL:HG11	2.54	0.41
1:D:453:LEU:HD23	1:D:453:LEU:HA	1.73	0.41
1:A:384:ALA:O	1:A:388:ILE:HG22	2.20	0.41
1:B:163:GLU:O	1:B:166:ALA:HB3	2.20	0.41
1:B:302:LYS:HZ1	1:B:359:SER:HB3	1.85	0.41
1:B:417:LEU:O	1:B:436:GLY:HA3	2.20	0.41
1:C:109:GLY:HA2	1:C:229:LEU:HD13	2.00	0.41
1:D:419:ARG:HA	1:D:422:GLN:HG3	2.01	0.41
1:A:297:GLN:HE21	1:A:301:GLN:HE22	1.68	0.41
1:D:114:ARG:HH12	1:D:118:ALA:HB2	1.86	0.41
1:D:274:TYR:CE1	1:D:448:ARG:HG2	2.55	0.41
1:A:242:MET:HE2	1:A:242:MET:O	2.20	0.41
1:C:302:LYS:NZ	1:C:360:LYS:HA	2.35	0.41
1:A:50:ARG:HE	1:A:55:THR:HG21	1.84	0.41
1:A:55:THR:OG1	1:A:56:TYR:N	2.52	0.41
1:D:135:TYR:CE2	1:D:141:ARG:HB2	2.56	0.41
1:B:332:LEU:HD12	1:B:332:LEU:HA	1.75	0.41
1:C:302:LYS:HA	1:C:302:LYS:HD3	1.69	0.41
1:D:126:TYR:HE2	1:D:231:TRP:CD1	2.37	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:LYS:HE2	1:A:359:SER:C	2.40	0.41
1:C:300:LYS:HE3	1:C:300:LYS:HB2	1.75	0.41
1:B:78:LEU:HB3	1:B:80:VAL:HG23	2.02	0.41
1:C:307:ARG:NH1	1:C:457:THR:HB	2.36	0.41
1:A:203:ASP:HB2	2:E:5:DAL:CB	2.47	0.41
1:A:131:PRO:HB2	1:A:223:PHE:O	2.21	0.41
1:B:411:LEU:O	1:B:415:LYS:HE3	2.20	0.41
1:D:48:ILE:HG12	1:D:93:LEU:HD12	2.02	0.41
1:A:50:ARG:HG3	1:A:108:ALA:HB1	2.03	0.40
1:A:241:LEU:HB3	4:A:2027:HOH:O	2.20	0.40
1:B:138:GLY:HA3	1:B:139:GLN:CB	2.49	0.40
1:D:280:PHE:CE2	1:D:284:LEU:HD11	2.56	0.40
1:C:151:LYS:HG3	1:C:199:LEU:HD11	2.02	0.40
1:C:209:MET:O	1:C:209:MET:HG2	2.20	0.40
1:C:284:LEU:HD12	1:C:284:LEU:HA	1.92	0.40
1:C:49:THR:OG1	1:C:50:ARG:N	2.50	0.40
1:C:90:LEU:HD23	1:C:90:LEU:HA	1.78	0.40
1:A:130:THR:O	1:A:204:SER:HB3	2.21	0.40
1:A:97:LEU:O	1:A:234:PRO:HG3	2.22	0.40
1:B:434:ALA:O	1:B:436:GLY:N	2.55	0.40
1:C:235:GLY:HA2	1:C:236:GLY:HA3	1.63	0.40
1:D:121:ARG:CZ	1:D:236:GLY:HA2	2.52	0.40
1:D:125:THR:HA	1:D:229:LEU:O	2.21	0.40
1:D:261:LEU:HA	1:D:261:LEU:HD12	1.88	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:2016:HOH:O	4:C:2025:HOH:O[1_455]	2.16	0.04

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	417/499 (84%)	387 (93%)	22 (5%)	8 (2%)	10 35
1	B	409/499 (82%)	370 (90%)	27 (7%)	12 (3%)	6 23
1	C	417/499 (84%)	389 (93%)	20 (5%)	8 (2%)	10 35
1	D	415/499 (83%)	375 (90%)	32 (8%)	8 (2%)	10 35
2	E	1/6 (17%)	1 (100%)	0	0	100 100
All	All	1659/2002 (83%)	1522 (92%)	101 (6%)	36 (2%)	8 31

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	VAL
1	A	118	ALA
1	A	120	VAL
1	B	118	ALA
1	B	277	ALA
1	C	275	VAL
1	C	300	LYS
1	D	118	ALA
1	D	119	SER
1	D	270	ASP
1	D	271	VAL
1	A	117	ASP
1	B	109	GLY
1	B	207	LEU
1	B	284	LEU
1	B	457	THR
1	C	271	VAL
1	C	274	TYR
1	C	277	ALA
1	D	254	LYS
1	A	89	ASN
1	A	236	GLY
1	B	108	ALA
1	D	114	ARG
1	D	236	GLY
1	A	334	MET
1	B	89	ASN
1	B	236	GLY
1	B	279	THR

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Mol	Chain	Res	Type
1	D	117	ASP
1	A	123	SER
1	C	108	ALA
1	C	236	GLY
1	B	139	GLN
1	C	267	GLY
1	B	145	PRO

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	350/414 (84%)	342 (98%)	8 (2%)	58 87
1	B	344/414 (83%)	335 (97%)	9 (3%)	54 85
1	C	350/414 (84%)	339 (97%)	11 (3%)	47 82
1	D	348/414 (84%)	343 (99%)	5 (1%)	74 93
All	All	1392/1656 (84%)	1359 (98%)	33 (2%)	58 86

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	73	ARG
1	A	186	VAL
1	A	227	ARG
1	A	257	LEU
1	A	371[A]	GLU
1	A	371[B]	GLU
1	A	402	LYS
1	A	426	TYR
1	B	52	SER
1	B	76	GLU
1	B	80	VAL
1	B	160	SER
1	B	167	GLU
1	B	175	LEU

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Mol	Chain	Res	Type
1	B	186	VAL
1	B	272	LEU
1	B	430	ARG
1	C	52	SER
1	C	119	SER
1	C	160	SER
1	C	207	LEU
1	C	211	GLN
1	C	237	ASP
1	C	268	HIS
1	C	285	GLN
1	C	346	SER
1	C	356	GLN
1	C	426	TYR
1	D	89	ASN
1	D	272	LEU
1	D	336	THR
1	D	377	ASP
1	D	444	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	297	GLN
1	C	445	ASN
1	D	243	ASN
1	D	301	GLN
1	D	356	GLN

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	$\#\|Z\| > 2$
2	FGA	E	3	2	5,8,9	0.83	0	3,9,11	1.42	0
2	API	E	4	2	6,11,12	1.15	1 (16%)	5,13,15	1.88	3 (60%)
2	DAL	E	5	2	1,4,5	0.48	0	1,4,6	0.36	0
2	DAL	E	6	2	0,5,5	0.00	-	2,6,6	5.04	1 (50%)

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	FGA	E	3	2	-	0/3/8/9	0/0/0/0
2	API	E	4	2	-	0/6/12/14	0/0/0/0
2	DAL	E	5	2	-	0/0/2/4	0/0/0/0
2	DAL	E	6	2	-	0/0/4/4	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	4	API	C3-C2	-2.10	1.50	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	6	DAL	CB-CA-C	-7.13	99.25	110.93
2	E	4	API	O1-C1-C2	-2.86	118.06	125.72
2	E	4	API	C3-C2-N2	-2.32	104.00	110.54
2	E	4	API	C5-C4-C3	-2.01	103.23	113.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	3	FGA	5	0

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 5 ligands modelled in this entry, 5 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

6.1 Protein, DNA and RNA chains

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	A	418/499 (83%)	-0.35	0 100 100	27, 47, 94, 138	0
1	B	413/499 (82%)	-0.29	1 (0%) 95 95	31, 60, 104, 135	0
1	C	419/499 (83%)	-0.30	3 (0%) 89 88	28, 54, 96, 173	0
1	D	417/499 (83%)	-0.07	2 (0%) 91 90	42, 73, 130, 242	0
2	E	1/6 (16%)	2.38	1 (100%) 0 0	103, 103, 103, 103	1 (100%)
All	All	1668/2002 (83%)	-0.25	7 (0%) 93 92	27, 60, 109, 242	1 (0%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	301	GLN	4.6
1	C	271	VAL	4.2
1	D	459	PRO	3.7
1	D	119	SER	3.0
1	B	272	LEU	2.5
2	E	2	ALA	2.4
1	C	281	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains

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^{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	LLDF	B-factors(Å^2)	Q<0.9
2	API	E	4	12/13	0.89	0.46	-	88,137,141,142	12

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	DAL	E	5	5/6	0.78	0.59	-	118,123,124,127	5
2	DAL	E	6	6/6	0.91	0.45	-	68,85,111,115	6
2	FGA	E	3	9/10	0.80	0.38	-	76,82,90,99	9

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^{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	LLDF	B-factors(Å^2)	Q<0.9
3	CL	B	1460	1/1	0.90	0.57	5.82	120,120,120,120	0
3	CL	C	1460	1/1	0.96	0.21	3.42	58,58,58,58	0
3	CL	B	1459	1/1	0.95	0.13	-1.20	76,76,76,76	0
3	CL	A	1460	1/1	0.91	0.12	-1.69	68,68,68,68	0
3	CL	D	1460	1/1	0.87	0.14	-	92,92,92,92	0

6.5 Other polymers (i)

There are no such residues in this entry.