



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:30 AM UTC

PDB ID : 5AA1 / pdb_00005aa1
Title : Crystal structure of MltF from Pseudomonas aeruginosa in complex with NA
G-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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

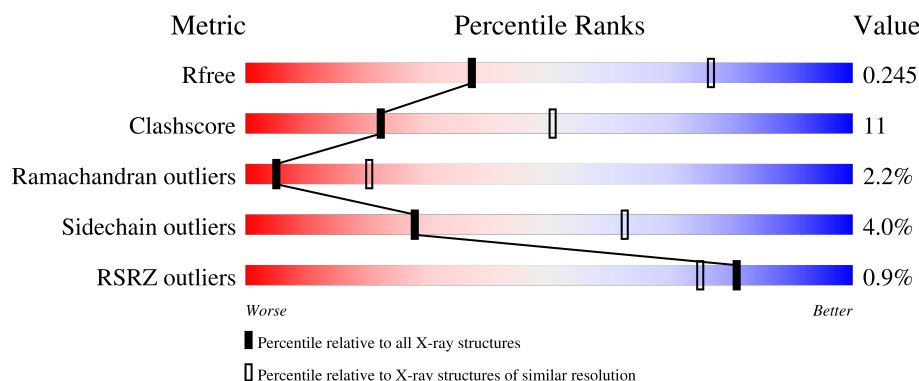
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.89 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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 $\leq 5\%$. 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	59% 23% • 16%
1	B	499	65% 15% • 17%
1	C	499	% 63% 19% • 16%
1	D	499	% 61% 20% •• 16%
2	E	6	17% 17% 50% 33%

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	-

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 Q9HYN1
A	-7	ALA	-	expression tag	UNP Q9HYN1
A	-6	PRO	-	expression tag	UNP Q9HYN1
A	-5	SER	-	expression tag	UNP Q9HYN1
A	-4	ARG	-	expression tag	UNP Q9HYN1
A	-3	LEU	-	expression tag	UNP Q9HYN1
A	-2	CYS	-	expression tag	UNP Q9HYN1
A	-1	VAL	-	expression tag	UNP Q9HYN1
A	0	TYR	-	expression tag	UNP Q9HYN1
A	1	CYS	-	expression tag	UNP Q9HYN1
A	2	ALA	-	expression tag	UNP Q9HYN1
A	3	ASP	-	expression tag	UNP Q9HYN1
A	4	VAL	-	expression tag	UNP Q9HYN1
A	5	CYS	-	expression tag	UNP Q9HYN1
A	6	PRO	-	expression tag	UNP Q9HYN1
A	7	ASP	-	expression tag	UNP Q9HYN1
A	281	THR	ALA	conflict	UNP Q9HYN1
A	302	LYS	LEU	conflict	UNP Q9HYN1
B	-8	MET	-	expression tag	UNP Q9HYN1
B	-7	ALA	-	expression tag	UNP Q9HYN1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	PRO	-	expression tag	UNP Q9HYN1
B	-5	SER	-	expression tag	UNP Q9HYN1
B	-4	ARG	-	expression tag	UNP Q9HYN1
B	-3	LEU	-	expression tag	UNP Q9HYN1
B	-2	CYS	-	expression tag	UNP Q9HYN1
B	-1	VAL	-	expression tag	UNP Q9HYN1
B	0	TYR	-	expression tag	UNP Q9HYN1
B	1	CYS	-	expression tag	UNP Q9HYN1
B	2	ALA	-	expression tag	UNP Q9HYN1
B	3	ASP	-	expression tag	UNP Q9HYN1
B	4	VAL	-	expression tag	UNP Q9HYN1
B	5	CYS	-	expression tag	UNP Q9HYN1
B	6	PRO	-	expression tag	UNP Q9HYN1
B	7	ASP	-	expression tag	UNP Q9HYN1
B	281	THR	ALA	conflict	UNP Q9HYN1
B	302	LYS	LEU	conflict	UNP Q9HYN1
C	-8	MET	-	expression tag	UNP Q9HYN1
C	-7	ALA	-	expression tag	UNP Q9HYN1
C	-6	PRO	-	expression tag	UNP Q9HYN1
C	-5	SER	-	expression tag	UNP Q9HYN1
C	-4	ARG	-	expression tag	UNP Q9HYN1
C	-3	LEU	-	expression tag	UNP Q9HYN1
C	-2	CYS	-	expression tag	UNP Q9HYN1
C	-1	VAL	-	expression tag	UNP Q9HYN1
C	0	TYR	-	expression tag	UNP Q9HYN1
C	1	CYS	-	expression tag	UNP Q9HYN1
C	2	ALA	-	expression tag	UNP Q9HYN1
C	3	ASP	-	expression tag	UNP Q9HYN1
C	4	VAL	-	expression tag	UNP Q9HYN1
C	5	CYS	-	expression tag	UNP Q9HYN1
C	6	PRO	-	expression tag	UNP Q9HYN1
C	7	ASP	-	expression tag	UNP Q9HYN1
C	281	THR	ALA	conflict	UNP Q9HYN1
C	302	LYS	LEU	conflict	UNP Q9HYN1
D	-8	MET	-	expression tag	UNP Q9HYN1
D	-7	ALA	-	expression tag	UNP Q9HYN1
D	-6	PRO	-	expression tag	UNP Q9HYN1
D	-5	SER	-	expression tag	UNP Q9HYN1
D	-4	ARG	-	expression tag	UNP Q9HYN1
D	-3	LEU	-	expression tag	UNP Q9HYN1
D	-2	CYS	-	expression tag	UNP Q9HYN1
D	-1	VAL	-	expression tag	UNP Q9HYN1

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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 (CCD ID: CL) (formula: Cl).

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

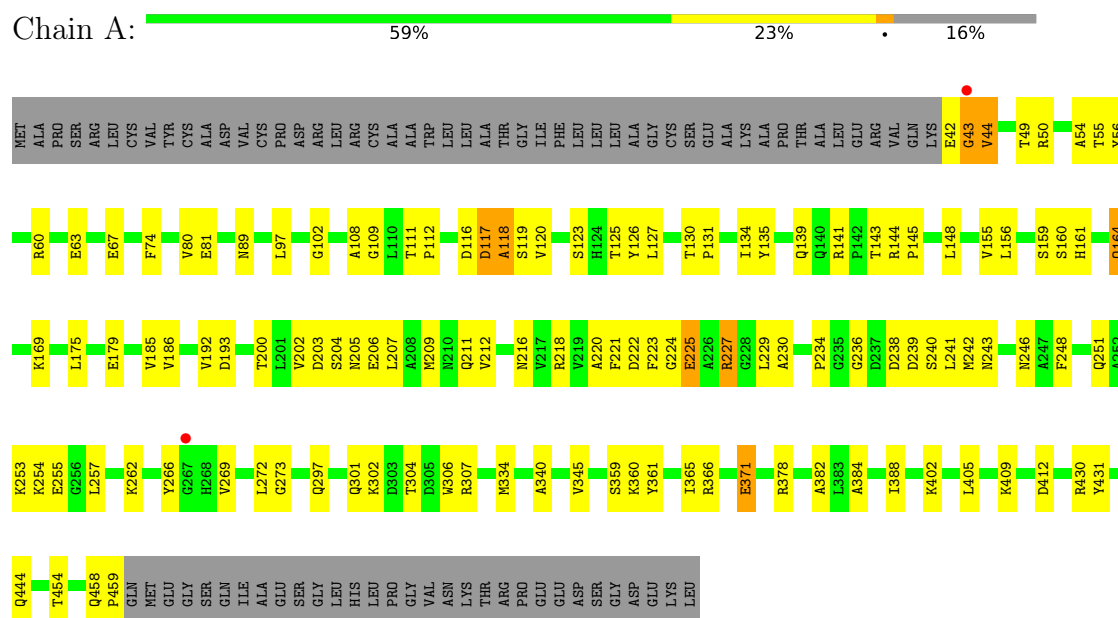
- Molecule 4 is water.

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		

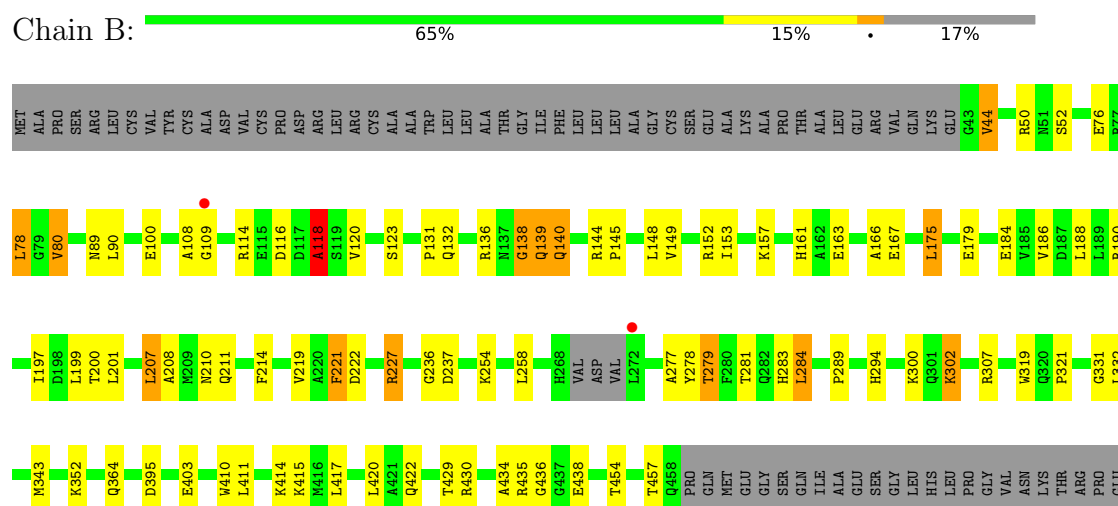
3 Residue-property plots

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: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

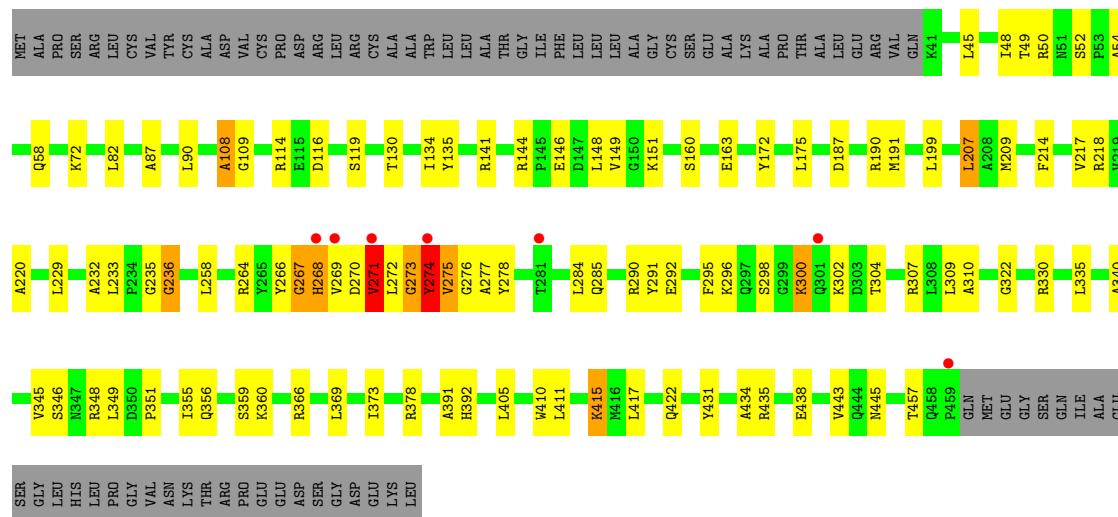


• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F

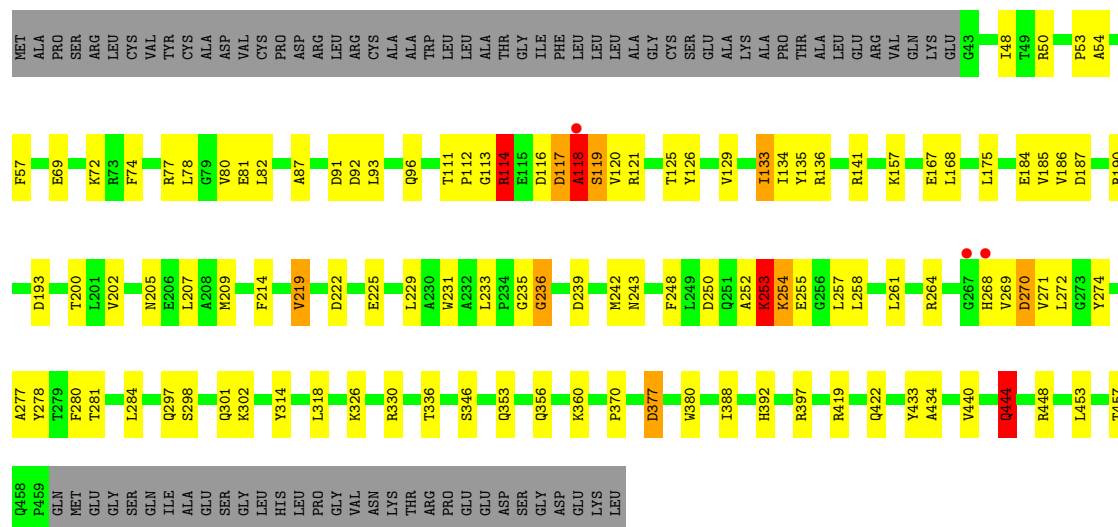


GLU
ASP
SER
GLY
ASP
GLU
LYS
LEU

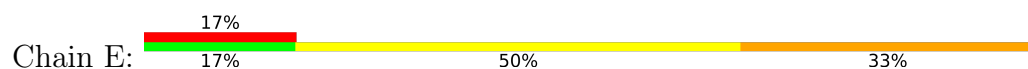
• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F



• Molecule 1: MEMBRANE-BOUND LYTIC MUREIN TRANSGLYCOSYLASE F



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



AH01
A2
E3
K4
A5
A6

4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.91Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.168 , 0.243 0.174 , 0.245	Depositor DCC
R_{free} test set	2025 reflections (4.06%)	wwPDB-VP
Wilson B-factor (Å ²)	61.3	Xtriage
Anisotropy	0.186	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.64	0/3431	0.95	6/4639 (0.1%)
1	B	0.57	0/3382	0.97	15/4569 (0.3%)
1	C	0.62	0/3431	0.94	6/4638 (0.1%)
1	D	0.54	0/3413	0.93	11/4615 (0.2%)
2	E	0.80	0/4	1.07	0/4
All	All	0.59	0/13661	0.95	38/18465 (0.2%)

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 (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	43	GLY	CA-C-N	7.70	135.57	121.70
1	A	43	GLY	C-N-CA	7.70	135.57	121.70
1	D	253	LYS	CA-C-N	7.44	135.09	121.70
1	D	253	LYS	C-N-CA	7.44	135.09	121.70
1	D	118	ALA	N-CA-C	7.42	126.60	110.80
1	A	102	GLY	CA-C-N	7.26	127.18	120.21
1	A	102	GLY	C-N-CA	7.26	127.18	120.21
1	B	123	SER	CA-C-N	7.09	134.46	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	SER	C-N-CA	7.09	134.46	121.70
1	B	118	ALA	CA-C-N	7.02	134.33	121.70
1	B	118	ALA	C-N-CA	7.02	134.33	121.70
1	D	118	ALA	CA-C-N	6.58	133.54	121.70
1	D	118	ALA	C-N-CA	6.58	133.54	121.70
1	B	221	PHE	CA-C-N	6.56	133.51	121.70
1	B	221	PHE	C-N-CA	6.56	133.51	121.70
1	C	271	VAL	N-CA-C	6.48	122.82	109.34
1	A	444	GLN	N-CA-C	-6.31	104.48	111.36
1	B	221	PHE	N-CA-C	-6.15	99.80	108.96
1	B	138	GLY	CA-C-N	6.06	132.60	121.70
1	B	138	GLY	C-N-CA	6.06	132.60	121.70
1	B	144	ARG	CA-C-N	5.94	127.27	119.84
1	B	144	ARG	C-N-CA	5.94	127.27	119.84
1	D	214	PHE	CA-C-N	5.76	125.44	119.05
1	D	214	PHE	C-N-CA	5.76	125.44	119.05
1	C	373	ILE	CB-CA-C	-5.74	106.13	112.68
1	B	214	PHE	CA-C-N	5.61	126.86	119.84
1	B	214	PHE	C-N-CA	5.61	126.86	119.84
1	B	221	PHE	CA-C-O	-5.24	115.85	121.45
1	D	444	GLN	N-CA-CB	5.21	118.33	110.30
1	D	114	ARG	N-CA-C	5.21	121.90	110.80
1	A	273	GLY	N-CA-C	5.18	118.03	112.33
1	D	433	TYR	N-CA-C	5.14	117.76	110.10
1	C	214	PHE	CA-C-N	5.10	125.18	119.87
1	C	214	PHE	C-N-CA	5.10	125.18	119.87
1	C	373	ILE	N-CA-C	5.06	113.89	106.55
1	C	274	TYR	N-CA-C	-5.06	100.03	110.80
1	B	140	GLN	N-CA-C	5.04	117.55	110.14
1	D	444	GLN	N-CA-C	-5.04	105.88	112.23

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 ⓘ

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	85	0
1	B	3313	0	3259	51	0
1	C	3360	0	3308	62	0
1	D	3342	0	3289	85	0
2	E	42	0	31	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	13187	283	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 11.

All (283) 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
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:D:114:ARG:HH21	1:D:120:VAL:C	1.93	0.75
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:302:LYS:HB2	1:B:302:LYS:HZ2	1.59	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:C:302:LYS:HZ2	1:C:360:LYS:HA	1.59	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:D:233:LEU:HD22	1:D:242:MET:HE2	1.78	0.64
1:B:207:LEU:O	1:B:210:ASN:N	2.27	0.63
1:A:54:ALA:HA	1:A:209:MET:HE1	1.80	0.63
1:A:304:THR:CG2	1:A:366:ARG:HH22	2.11	0.62
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:C:209:MET:HE3	1:C:266:TYR:CE1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:161:HIS:ND1	2:E:4:API:H6	2.18	0.59
1:D:301:GLN:HE22	1:D:356:GLN:CD	2.09	0.59
1:D:346:SER:N	1:D:353:GLN:OE1	2.35	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:A:116:ASP:C	1:A:118:ALA:H	2.12	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: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
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:43:GLY:HA3	1:A:44:VAL:HB	1.89	0.53
1:A:143:THR:O	1:A:144:ARG:HD2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:54:ALA:HA	1:C:209:MET:HE1	1.89	0.53
1:D:253:LYS:N	1:D:253:LYS:HZ2	2.07	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:C:273:GLY:O	1:C:274:TYR:HB3	2.10	0.52
1:C:276:GLY:C	1:C:278:TYR:H	2.18	0.52
1:A:371[A]:GLU:HA	1:A:378:ARG:HH12	1.75	0.51
1:A:242:MET:HE2	1:A:246:ASN:ND2	2.25	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:D:91:ASP:OD2	1:D:157:LYS:NZ	2.44	0.51
1:D:114:ARG:NH2	1:D:120:VAL:C	2.67	0.51
1:B:190:ARG:NH1	1:B:422:GLN:HG2	2.26	0.51
1:B:343:MET:HE2	1:B:343:MET:HA	1.92	0.51
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:B:302:LYS:HB2	1:B:302:LYS:NZ	2.25	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:54:ALA:HA	1:D:209:MET:HE1	1.93	0.49
1:D:257:LEU:O	1:D:261:LEU:HB2	2.12	0.49
1:D:48:ILE:HD11	1:D:87:ALA:HB2	1.93	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: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:A:202:VAL:HA	2:E:4:API:N6	2.28	0.49
1:B:148:LEU:HD22	1:B:199:LEU:HD13	1.95	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
1:A:306:TRP:CE2	1:A:307:ARG:HG3	2.48	0.49
1:A:371[A]:GLU:O	1:A:371[A]:GLU:HG2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:392:HIS:CE1	1:D:434:ALA:HB2	2.47	0.49
1:A:302:LYS:HB2	1:A:302:LYS:HZ2	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: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:129:VAL:HG12	1:D:205:ASN:HB3	1.98	0.46
1:D:185:VAL:HG13	1:D:202:VAL:HG11	1.97	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
1:A:302:LYS:HE2	1:A:359:SER:C	2.40	0.45
1:B:283:HIS:O	1:B:284:LEU:HB2	2.16	0.45
1:C:295:PHE:CZ	1:C:310:ALA:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:81:GLU:HG2	1:D:82:LEU:N	2.31	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:A:156:LEU:N	2:E:4:API:O4	2.46	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: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:116:ASP:C	1:A:118:ALA:N	2.76	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:D:250:ASP:C	1:D:254:LYS:HE3	2.42	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:232:ALA:C	1:C:233:LEU:HD12	2.44	0.42
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:D:252:ALA:C	1:D:253:LYS:HZ2	2.28	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:HD23	1:C:258:LEU:HA	1.83	0.42
1:C:417:LEU:HA	1:C:417:LEU:HD23	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:395:ASP:CG	1:B:429:THR:HB	2.45	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: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: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:HA	1:B:332:LEU:HD12	1.75	0.41
1:C:302:LYS:HD3	1:C:302:LYS:HA	1.69	0.41
1:D:126:TYR:HE2	1:D:231:TRP:CD1	2.37	0.41
1:C:300:LYS:HE3	1:C:300:LYS:HB2	1.75	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:ASP:HB2	2:E:5:DAL:CB	2.47	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: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:49:THR:OG1	1:C:50:ARG:N	2.50	0.40
1:C:90:LEU:HA	1:C:90:LEU:HD23	1.78	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:A:130:THR:O	1:A:204:SER:HB3	2.21	0.40
1:C:298:SER:C	1:C:300:LYS:H	2.28	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:HD12	1:D:261:LEU:HA	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%)	6	23
1	B	409/499 (82%)	370 (90%)	27 (7%)	12 (3%)	3	15
1	C	417/499 (84%)	389 (93%)	20 (5%)	8 (2%)	6	23
1	D	415/499 (83%)	375 (90%)	32 (8%)	8 (2%)	6	23
2	E	1/6 (17%)	1 (100%)	0	0	100	100
All	All	1659/2002 (83%)	1522 (92%)	101 (6%)	36 (2%)	5	20

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
1	D	117	ASP
1	A	123	SER

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Mol	Chain	Res	Type
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 ⓘ

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%)	338 (97%)	12 (3%)	32	66
1	B	344/414 (83%)	329 (96%)	15 (4%)	25	59
1	C	350/414 (84%)	335 (96%)	15 (4%)	26	60
1	D	348/414 (84%)	333 (96%)	15 (4%)	26	60
All	All	1392/1656 (84%)	1335 (96%)	57 (4%)	28	61

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	GLN
1	A	186	VAL
1	A	212	VAL
1	A	225	GLU
1	A	227	ARG
1	A	257	LEU
1	A	269	VAL
1	A	272	LEU
1	A	371[A]	GLU
1	A	371[B]	GLU
1	A	402	LYS
1	A	454	THR
1	B	44	VAL
1	B	52	SER
1	B	76	GLU
1	B	78	LEU

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Mol	Chain	Res	Type
1	B	80	VAL
1	B	100	GLU
1	B	167	GLU
1	B	175	LEU
1	B	186	VAL
1	B	219	VAL
1	B	227	ARG
1	B	254	LYS
1	B	300	LYS
1	B	302	LYS
1	B	430	ARG
1	C	45	LEU
1	C	52	SER
1	C	58	GLN
1	C	119	SER
1	C	130	THR
1	C	160	SER
1	C	163	GLU
1	C	207	LEU
1	C	217	VAL
1	C	268	HIS
1	C	346	SER
1	C	356	GLN
1	C	405	LEU
1	C	411	LEU
1	C	415	LYS
1	D	114	ARG
1	D	133	ILE
1	D	167	GLU
1	D	186	VAL
1	D	219	VAL
1	D	222	ASP
1	D	225	GLU
1	D	253	LYS
1	D	258	LEU
1	D	272	LEU
1	D	336	THR
1	D	377	ASP
1	D	388	ILE
1	D	444	GLN
1	D	457	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	HIS
1	A	251	GLN
1	A	268	HIS
1	A	294	HIS
1	A	297	GLN
1	B	140	GLN
1	C	297	GLN
1	C	337	ASN
1	D	89	ASN
1	D	137	ASN
1	D	164	GLN
1	D	243	ASN
1	D	301	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	API	E	4	2	9,11,12	1.48	1 (11%)	5,13,15	1.54	1 (20%)
2	FGA	E	3	2	6,8,9	0.97	0	6,9,11	2.06	2 (33%)

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	API	E	4	2	-	6/11/12/14	-
2	FGA	E	3	2	-	3/8/8/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	4	API	O4-C7	-2.74	1.21	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	3	FGA	CG-CB-CA	-3.55	103.86	115.24
2	E	4	API	C5-C4-C3	-2.24	103.23	113.28
2	E	3	FGA	CB-CA-C	-2.10	104.89	110.45

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	4	API	C4-C3-CA-C
2	E	4	API	C4-C3-CA-N
2	E	4	API	C4-C5-C6-C7
2	E	4	API	C4-C5-C6-N6
2	E	3	FGA	CA-CB-CG-CD
2	E	4	API	CA-C3-C4-C5
2	E	3	FGA	N-CA-CB-CG
2	E	3	FGA	C-CA-CB-CG
2	E	4	API	C3-C4-C5-C6

There are no ring outliers.

2 monomers are involved in 12 short contacts:

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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(Å ²)	Q<0.9
1	A	418/499 (83%)	-0.67	2 (0%) 87 83	27, 47, 94, 138	1 (0%)
1	B	413/499 (82%)	-0.52	2 (0%) 87 83	31, 60, 104, 135	0
1	C	419/499 (83%)	-0.59	7 (1%) 69 61	28, 54, 96, 173	0
1	D	417/499 (83%)	-0.34	3 (0%) 84 79	42, 73, 130, 242	0
2	E	1/6 (16%)	2.96	1 (100%) 0 0	84, 84, 84, 84	1 (100%)
All	All	1668/2002 (83%)	-0.53	15 (0%) 81 75	27, 60, 109, 242	2 (0%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	301	GLN	3.8
1	C	269	VAL	3.4
1	D	118	ALA	3.2
1	A	43	GLY	3.1
1	B	272	LEU	3.0
2	E	2	ALA	3.0
1	D	267	GLY	2.8
1	C	459	PRO	2.8
1	C	274	TYR	2.7
1	C	271	VAL	2.5
1	C	268	HIS	2.4
1	C	281	THR	2.3
1	A	267	GLY	2.1
1	D	268	HIS	2.1
1	B	109	GLY	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. 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(Å ²)	Q<0.9
2	FGA	E	3	9/10	0.81	0.21	76,82,90,99	9
2	DAL	E	5	5/6	0.90	0.21	118,123,124,127	5
2	DAL	E	6	6/6	0.92	0.21	68,85,111,115	6
2	API	E	4	12/13	0.95	0.19	88,137,141,142	12

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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(Å ²)	Q<0.9
3	CL	D	1460	1/1	0.85	0.09	92,92,92,92	0
3	CL	B	1460	1/1	0.86	0.36	120,120,120,120	0
3	CL	B	1459	1/1	0.95	0.08	76,76,76,76	0
3	CL	C	1460	1/1	0.96	0.09	58,58,58,58	0
3	CL	A	1460	1/1	0.96	0.16	68,68,68,68	0

6.5 Other polymers [i](#)

There are no such residues in this entry.