



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2026 – 06:19 PM UTC

PDB ID : 4YFA / pdb_00004yfa
Title : Structure of N-acylhomoserine lactone acylase MacQ in complex with decanoic acid
Authors : Yasutake, Y.; Kusada, H.; Kimura, N.
Deposited on : 2015-02-25
Resolution : 2.20 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

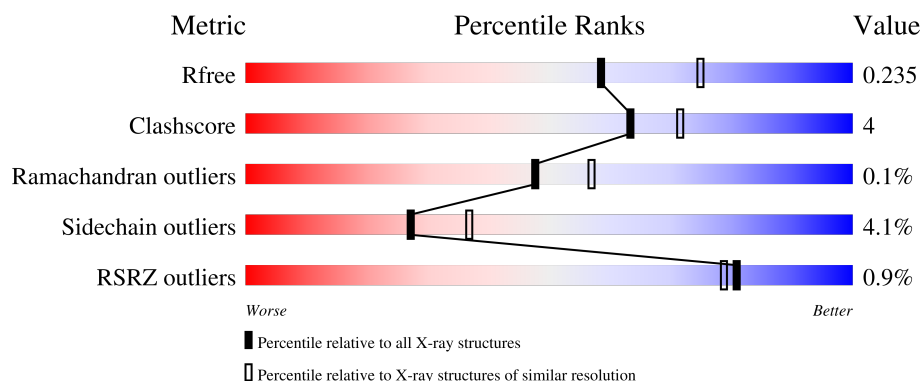
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	178	% 87% 7% 6%
1	D	178	% 88% 6% 6%
1	G	178	% 85% 8% 6%
1	J	178	% 88% 6% 6%
2	B	27	4% 48% 11% 41%

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Mol	Chain	Length	Quality of chain
2	E	27	
2	H	27	
2	K	27	
3	C	581	
3	F	581	
3	I	581	
3	L	581	

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	DKA	I	601	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23903 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 Protein related to penicillin acylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	167	Total	C	N	O	S	0	0	0
			1289	802	243	238	6			
1	D	168	Total	C	N	O	S	0	0	0
			1295	805	244	240	6			
1	G	167	Total	C	N	O	S	0	0	0
			1289	802	243	238	6			
1	J	167	Total	C	N	O	S	0	0	0
			1289	802	243	238	6			

- Molecule 2 is a protein called Protein related to penicillin acylase.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	16	Total	C	N	O	0	0	0
			119	73	23	23			
2	E	15	Total	C	N	O	0	0	0
			110	68	22	20			
2	H	16	Total	C	N	O	0	0	0
			119	73	23	23			
2	K	16	Total	C	N	O	0	0	0
			119	73	23	23			

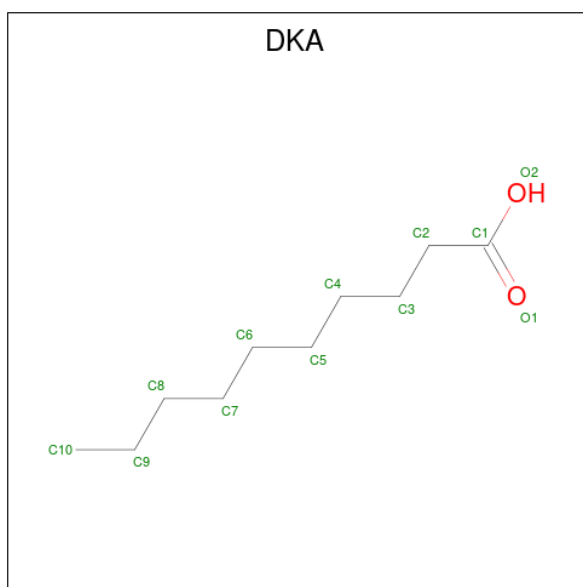
- Molecule 3 is a protein called Protein related to penicillin acylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	574	Total	C	N	O	S	0	0	0
			4344	2734	762	829	19			
3	F	574	Total	C	N	O	S	0	0	0
			4344	2734	762	829	19			
3	I	574	Total	C	N	O	S	0	0	0
			4344	2734	762	829	19			
3	L	575	Total	C	N	O	S	0	0	0
			4353	2739	763	832	19			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	574	LEU	-	expression tag	UNP A0A0A1VBK6
C	575	GLU	-	expression tag	UNP A0A0A1VBK6
C	576	HIS	-	expression tag	UNP A0A0A1VBK6
C	577	HIS	-	expression tag	UNP A0A0A1VBK6
C	578	HIS	-	expression tag	UNP A0A0A1VBK6
C	579	HIS	-	expression tag	UNP A0A0A1VBK6
C	580	HIS	-	expression tag	UNP A0A0A1VBK6
C	581	HIS	-	expression tag	UNP A0A0A1VBK6
F	574	LEU	-	expression tag	UNP A0A0A1VBK6
F	575	GLU	-	expression tag	UNP A0A0A1VBK6
F	576	HIS	-	expression tag	UNP A0A0A1VBK6
F	577	HIS	-	expression tag	UNP A0A0A1VBK6
F	578	HIS	-	expression tag	UNP A0A0A1VBK6
F	579	HIS	-	expression tag	UNP A0A0A1VBK6
F	580	HIS	-	expression tag	UNP A0A0A1VBK6
F	581	HIS	-	expression tag	UNP A0A0A1VBK6
I	574	LEU	-	expression tag	UNP A0A0A1VBK6
I	575	GLU	-	expression tag	UNP A0A0A1VBK6
I	576	HIS	-	expression tag	UNP A0A0A1VBK6
I	577	HIS	-	expression tag	UNP A0A0A1VBK6
I	578	HIS	-	expression tag	UNP A0A0A1VBK6
I	579	HIS	-	expression tag	UNP A0A0A1VBK6
I	580	HIS	-	expression tag	UNP A0A0A1VBK6
I	581	HIS	-	expression tag	UNP A0A0A1VBK6
L	574	LEU	-	expression tag	UNP A0A0A1VBK6
L	575	GLU	-	expression tag	UNP A0A0A1VBK6
L	576	HIS	-	expression tag	UNP A0A0A1VBK6
L	577	HIS	-	expression tag	UNP A0A0A1VBK6
L	578	HIS	-	expression tag	UNP A0A0A1VBK6
L	579	HIS	-	expression tag	UNP A0A0A1VBK6
L	580	HIS	-	expression tag	UNP A0A0A1VBK6
L	581	HIS	-	expression tag	UNP A0A0A1VBK6

- Molecule 4 is DECANOIC ACID (CCD ID: DKA) (formula: $C_{10}H_{20}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			12	10	2		
4	F	1	Total	C	O	0	0
			11	10	1		
4	I	1	Total	C	O	0	0
			12	10	2		
4	L	1	Total	C	O	0	0
			11	10	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	38	Total	O	0	0
			38	38		
5	B	2	Total	O	0	0
			2	2		
5	C	160	Total	O	0	0
			160	160		
5	D	64	Total	O	0	0
			64	64		
5	E	3	Total	O	0	0
			3	3		
5	F	144	Total	O	0	0
			144	144		
5	G	59	Total	O	0	0
			59	59		
5	H	6	Total	O	0	0
			6	6		

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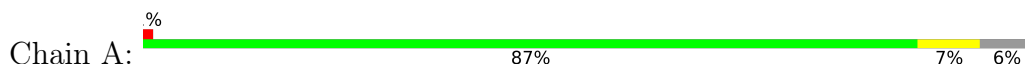
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	196	Total 196	O 196	0	0
5	J	65	Total 65	O 65	0	0
5	K	1	Total 1	O 1	0	0
5	L	105	Total 105	O 105	0	0

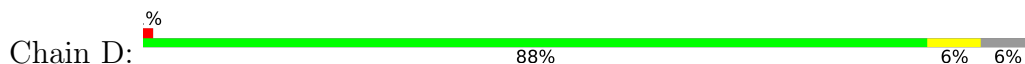
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

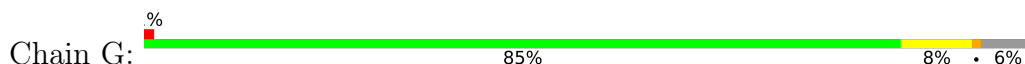
- Molecule 1: Protein related to penicillin acylase



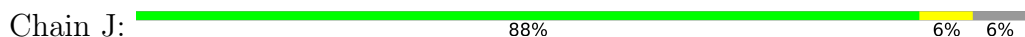
- Molecule 1: Protein related to penicillin acylase



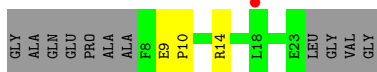
- Molecule 1: Protein related to penicillin acylase



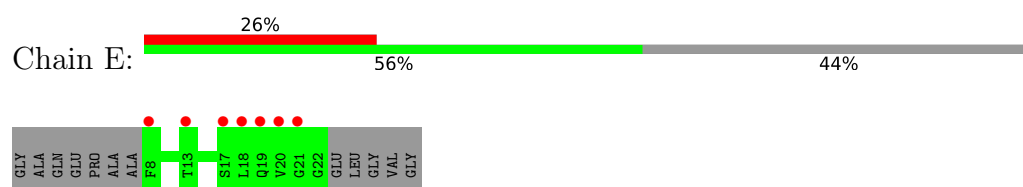
- Molecule 1: Protein related to penicillin acylase



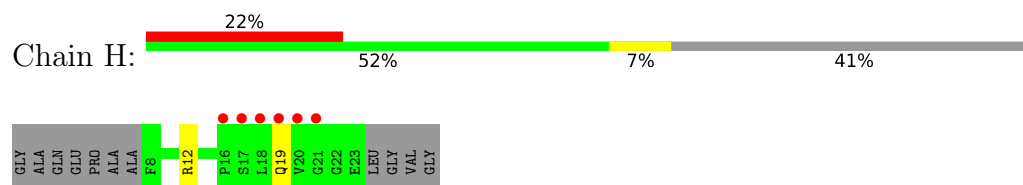
- Molecule 2: Protein related to penicillin acylase



- Molecule 2: Protein related to penicillin acylase



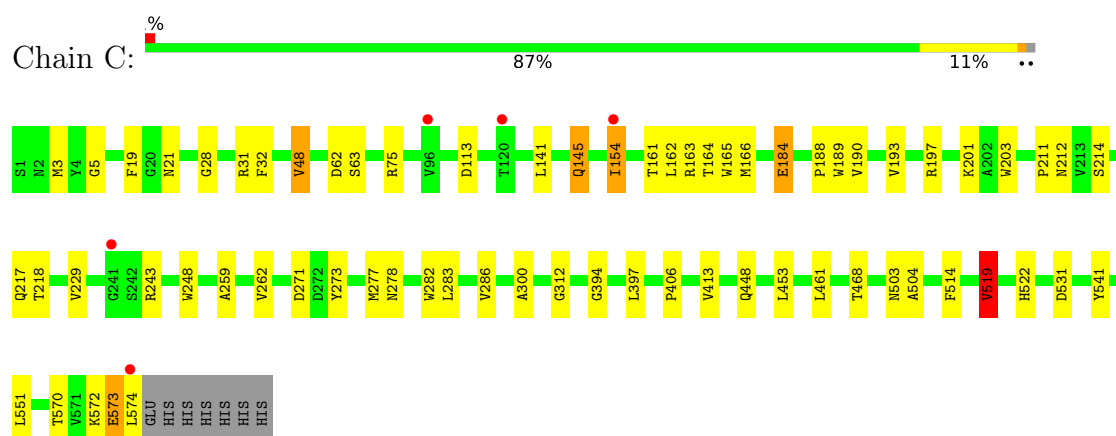
- Molecule 2: Protein related to penicillin acylase



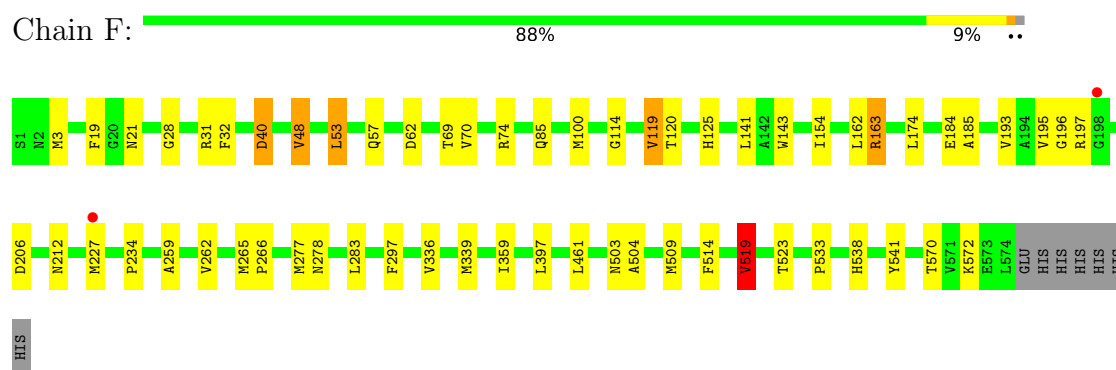
- Molecule 2: Protein related to penicillin acylase



- Molecule 3: Protein related to penicillin acylase

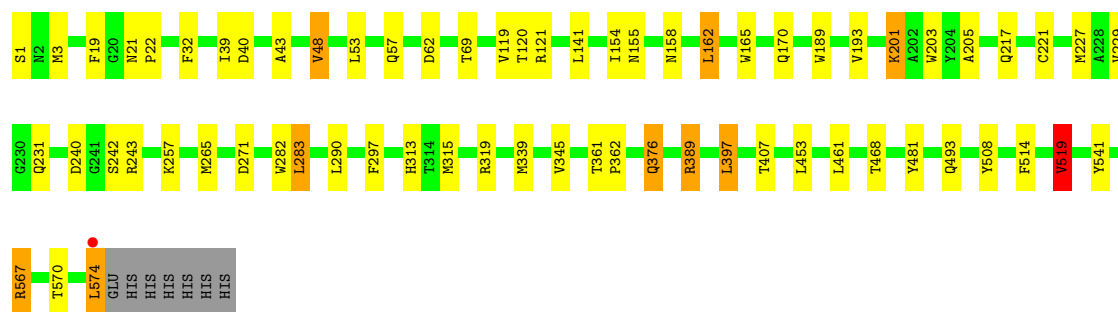


- Molecule 3: Protein related to penicillin acylase

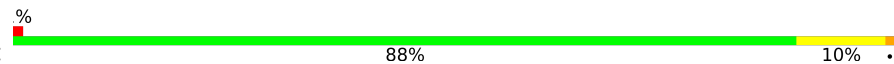


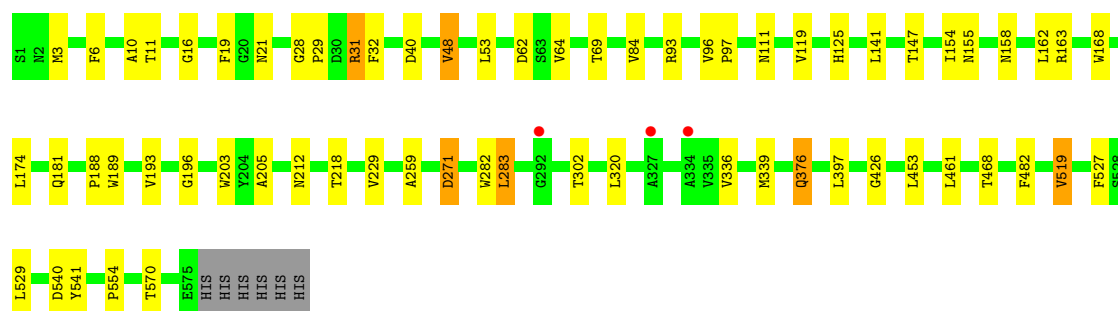
- Molecule 3: Protein related to penicillin acylase

Chain I:  87% 10% ..



• Molecule 3: Protein related to penicillin acylase

Chain L:  88% 10% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	85.41Å 89.85Å 122.71Å 103.26° 104.84° 106.05°	Depositor
Resolution (Å)	38.94 – 2.20 38.94 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (38.94-2.20) 98.0 (38.94-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.193 , 0.235 0.194 , 0.235	Depositor DCC
R_{free} test set	8025 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	39.8	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for -h,-k,h+k+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23903	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.42% 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: DKA

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	0.67	0/1320	0.85	0/1788
1	D	0.69	0/1326	0.82	0/1796
1	G	0.69	0/1320	0.86	2/1788 (0.1%)
1	J	0.70	0/1320	0.84	0/1788
2	B	0.52	0/121	0.76	0/162
2	E	0.59	0/112	0.62	0/150
2	H	0.50	0/121	0.73	0/162
2	K	0.49	0/121	0.74	0/162
3	C	0.68	0/4458	0.82	4/6082 (0.1%)
3	F	0.67	0/4458	0.83	2/6082 (0.0%)
3	I	0.68	0/4458	0.84	1/6082 (0.0%)
3	L	0.66	0/4467	0.85	2/6094 (0.0%)
All	All	0.67	0/23602	0.83	11/32136 (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
3	C	0	1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	519	VAL	CB-CA-C	-7.62	98.94	111.51
3	I	519	VAL	CB-CA-C	-6.47	100.67	111.29
1	G	145	GLN	N-CA-C	6.02	113.64	108.22
3	L	482	PHE	N-CA-C	-5.90	105.74	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	519	VAL	CB-CA-C	-5.55	102.19	111.29
3	F	262	VAL	N-CA-C	5.26	116.61	110.62
3	L	529	LEU	N-CA-C	5.25	117.00	111.28
3	C	28	GLY	CA-C-N	5.18	124.79	119.56
3	C	28	GLY	C-N-CA	5.18	124.79	119.56
3	C	262	VAL	N-CA-C	5.11	115.83	110.62
1	G	47	ASN	N-CA-C	5.00	118.41	111.71

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	573	GLU	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	1289	0	1228	10	0
1	D	1295	0	1233	7	0
1	G	1289	0	1228	9	0
1	J	1289	0	1228	10	0
2	B	119	0	114	1	0
2	E	110	0	108	0	0
2	H	119	0	114	1	0
2	K	119	0	114	0	0
3	C	4344	0	4155	47	0
3	F	4344	0	4154	39	0
3	I	4344	0	4155	46	0
3	L	4353	0	4160	35	0
4	C	12	0	19	4	0
4	F	11	0	19	3	0
4	I	12	0	19	7	0
4	L	11	0	19	3	0
5	A	38	0	0	0	0
5	B	2	0	0	0	0
5	C	160	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	64	0	0	1	0
5	E	3	0	0	0	0
5	F	144	0	0	2	0
5	G	59	0	0	1	0
5	H	6	0	0	0	0
5	I	196	0	0	1	0
5	J	65	0	0	0	0
5	K	1	0	0	0	0
5	L	105	0	0	2	0
All	All	23903	0	22067	182	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (182) 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)
3:F:70:VAL:HG23	4:F:601:DKA:H22	1.56	0.85
3:I:567:ARG:HH21	3:I:567:ARG:HG3	1.41	0.85
3:F:163:ARG:HG2	3:F:163:ARG:HH21	1.41	0.83
3:L:32:PHE:HB3	3:L:48:VAL:HG21	1.64	0.80
3:L:32:PHE:HB3	3:L:48:VAL:CG2	2.13	0.79
3:I:389:ARG:HH11	3:I:389:ARG:HG3	1.46	0.78
3:C:32:PHE:HB3	3:C:48:VAL:CG2	2.13	0.78
3:F:100:MET:HE1	3:F:143:TRP:CH2	2.22	0.74
3:C:145:GLN:H	3:C:145:GLN:CD	1.96	0.73
3:C:164:THR:OG1	3:C:184:GLU:HG2	1.89	0.73
2:H:12:ARG:NH1	1:J:176:GLN:OE1	2.22	0.73
3:C:32:PHE:HB3	3:C:48:VAL:HG22	1.71	0.71
3:L:69:THR:HA	4:L:601:DKA:H21	1.76	0.68
3:I:165:TRP:CH2	4:I:601:DKA:H91	2.29	0.67
3:L:32:PHE:HZ	4:L:601:DKA:H61	1.61	0.65
3:L:62:ASP:HA	3:L:519:VAL:CG2	2.26	0.65
3:I:32:PHE:CD1	3:I:48:VAL:HG13	2.31	0.65
3:L:31:ARG:HD3	5:L:736:HOH:O	1.97	0.64
3:F:514:PHE:CE2	3:F:519:VAL:HG13	2.32	0.64
3:I:567:ARG:HH21	3:I:567:ARG:CG	2.10	0.63
3:L:376:GLN:HG2	3:L:453:LEU:HD12	1.80	0.63
3:L:336:VAL:HA	3:L:339:MET:HG2	1.81	0.62
3:C:32:PHE:HB3	3:C:48:VAL:HG21	1.82	0.62
1:G:88:PHE:CZ	3:I:121:ARG:HG3	2.35	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:165:TRP:HH2	4:I:601:DKA:H91	1.63	0.62
3:L:32:PHE:CZ	4:L:601:DKA:H61	2.36	0.60
3:F:197:ARG:HG3	3:F:514:PHE:HB3	1.84	0.60
1:A:160:ASN:HD21	3:C:161:THR:CG2	2.15	0.59
3:L:3:MET:HE3	3:L:193:VAL:HG23	1.84	0.59
3:I:62:ASP:HA	3:I:519:VAL:HG22	1.84	0.59
1:G:12:THR:HA	3:I:574:LEU:HB3	1.85	0.59
3:F:100:MET:HE1	3:F:143:TRP:CZ2	2.37	0.59
3:C:154:ILE:HG12	3:C:211:PRO:HD3	1.85	0.59
3:C:19:PHE:CZ	3:C:21:ASN:HB2	2.38	0.58
3:C:165:TRP:HZ2	4:C:601:DKA:H71	1.67	0.58
3:F:74:ARG:HH21	3:F:234:PRO:HG2	1.69	0.58
3:F:100:MET:HE1	3:F:143:TRP:HH2	1.69	0.57
3:I:514:PHE:CE1	3:I:519:VAL:HG13	2.39	0.57
1:D:115:GLU:HG3	5:D:242:HOH:O	2.03	0.57
3:I:389:ARG:HH11	3:I:389:ARG:CG	2.17	0.57
3:F:32:PHE:CD1	3:F:48:VAL:CG1	2.88	0.57
3:L:271:ASP:OD1	3:L:271:ASP:N	2.33	0.56
3:F:62:ASP:HA	3:F:519:VAL:HG22	1.86	0.56
3:L:62:ASP:HA	3:L:519:VAL:HG21	1.87	0.56
3:F:19:PHE:CZ	3:F:21:ASN:HB2	2.41	0.55
3:L:19:PHE:CZ	3:L:21:ASN:HB2	2.41	0.55
3:C:62:ASP:O	3:C:197:ARG:NH1	2.41	0.53
1:A:160:ASN:HD21	3:C:161:THR:HG21	1.73	0.53
1:J:106:GLN:HG3	1:J:153:TRP:CH2	2.44	0.53
3:C:62:ASP:HA	3:C:519:VAL:CG2	2.38	0.53
3:I:165:TRP:HH2	4:I:601:DKA:C10	2.22	0.53
3:L:32:PHE:HB3	3:L:48:VAL:HG22	1.88	0.53
3:I:19:PHE:CZ	3:I:21:ASN:HB2	2.43	0.53
1:A:16:GLU:HG2	1:A:18:ARG:CD	2.39	0.52
3:F:32:PHE:CD1	3:F:48:VAL:HG13	2.44	0.52
3:I:69:THR:HA	4:I:601:DKA:O1	2.09	0.52
3:C:514:PHE:CE2	3:C:519:VAL:HG13	2.45	0.52
3:F:28:GLY:O	3:F:31:ARG:HG2	2.10	0.52
3:C:75:ARG:HD2	3:C:188:PRO:O	2.10	0.52
3:I:3:MET:HE3	3:I:193:VAL:HG23	1.93	0.51
3:I:62:ASP:HA	3:I:519:VAL:CG2	2.40	0.51
1:A:58:TYR:CE2	1:A:155:ARG:HG2	2.45	0.51
3:C:145:GLN:CD	3:C:145:GLN:N	2.65	0.51
3:L:283:LEU:HB2	5:L:780:HOH:O	2.10	0.51
1:D:84:ILE:HD11	3:F:119:VAL:HG21	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:165:TRP:HH2	4:I:601:DKA:C9	2.23	0.51
3:C:154:ILE:HG23	3:C:248:TRP:HZ3	1.75	0.51
3:I:203:TRP:CZ2	3:I:205:ALA:HB2	2.46	0.50
1:D:84:ILE:HD11	3:F:119:VAL:CG2	2.41	0.50
1:A:106:GLN:HG3	1:A:153:TRP:CH2	2.47	0.50
3:F:339:MET:HE3	5:F:827:HOH:O	2.11	0.49
3:L:155:ASN:HA	3:L:158:ASN:HB3	1.94	0.49
1:A:16:GLU:HG2	1:A:18:ARG:HD3	1.93	0.49
3:C:154:ILE:HG23	3:C:248:TRP:CZ3	2.48	0.49
3:F:212:ASN:HB2	3:F:259:ALA:C	2.37	0.49
3:F:3:MET:HE3	3:F:193:VAL:HG23	1.95	0.49
3:I:315:MET:HB3	3:I:339:MET:HE2	1.95	0.49
3:L:28:GLY:O	3:L:31:ARG:HB3	2.13	0.48
3:L:31:ARG:HG3	3:L:527:PHE:CZ	2.49	0.48
1:G:31:ASN:HB2	5:G:248:HOH:O	2.12	0.47
3:C:165:TRP:CZ2	4:C:601:DKA:H71	2.47	0.47
3:C:201:LYS:HD3	3:C:271:ASP:HB3	1.96	0.47
3:I:1:SER:HG	4:I:601:DKA:C1	2.28	0.47
1:J:155:ARG:HD3	1:J:155:ARG:C	2.40	0.47
3:F:174:LEU:HB2	3:F:196:GLY:HA3	1.96	0.47
3:I:282:TRP:CD2	3:I:283:LEU:HD13	2.49	0.47
3:C:573:GLU:HG2	3:C:574:LEU:N	2.30	0.47
3:C:212:ASN:HB2	3:C:259:ALA:C	2.40	0.46
3:F:336:VAL:HA	3:F:339:MET:HG2	1.96	0.46
1:G:110:LEU:HD22	3:I:162:LEU:CD1	2.45	0.46
3:L:282:TRP:CD2	3:L:283:LEU:HD13	2.50	0.46
3:C:163:ARG:NH1	3:C:184:GLU:OE2	2.48	0.46
3:C:165:TRP:CH2	4:C:601:DKA:H92	2.50	0.46
3:I:155:ASN:HA	3:I:158:ASN:HB3	1.97	0.46
3:L:203:TRP:CZ2	3:L:205:ALA:HB2	2.50	0.46
3:C:282:TRP:HB2	3:C:300:ALA:HA	1.97	0.46
3:I:32:PHE:CD1	3:I:48:VAL:CG1	2.99	0.46
3:C:413:VAL:HG22	3:I:231:GLN:OE1	2.15	0.46
3:C:503:ASN:O	3:C:504:ALA:C	2.59	0.46
3:I:53:LEU:HD12	3:I:57:GLN:CD	2.40	0.46
1:J:58:TYR:CE2	1:J:155:ARG:HG2	2.51	0.46
3:C:277:MET:O	3:C:278:ASN:HB2	2.16	0.46
1:G:106:GLN:HG3	1:G:153:TRP:CH2	2.51	0.46
1:D:92:HIS:CE1	3:F:125:HIS:CD2	3.05	0.45
3:F:572:LYS:HE2	3:F:572:LYS:HB3	1.74	0.45
3:I:376:GLN:CG	3:I:453:LEU:HD12	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:154:ILE:CG1	3:C:211:PRO:HD3	2.47	0.45
3:F:70:VAL:H	4:F:601:DKA:H21	1.82	0.45
3:I:22:PRO:HD2	3:I:508:TYR:O	2.17	0.45
3:I:201:LYS:HD2	3:I:271:ASP:HB3	1.99	0.45
3:C:189:TRP:CE3	3:C:190:VAL:HG13	2.52	0.45
3:C:214:SER:OG	3:C:217:GLN:HB2	2.17	0.45
3:I:217:GLN:O	3:I:221:CYS:HB2	2.17	0.44
3:F:53:LEU:HD12	3:F:57:GLN:CD	2.42	0.44
3:F:69:THR:HA	4:F:601:DKA:H21	1.99	0.44
3:I:265:MET:HG2	3:I:297:PHE:HZ	1.83	0.44
3:I:397:LEU:HG	3:I:453:LEU:HD22	2.00	0.44
3:L:188:PRO:HB2	3:L:189:TRP:CD1	2.53	0.44
3:C:63:SER:HA	3:C:197:ARG:NH1	2.32	0.44
3:F:163:ARG:HG2	3:F:163:ARG:NH2	2.18	0.43
3:I:567:ARG:CG	3:I:567:ARG:NH2	2.72	0.43
3:F:265:MET:HG2	3:F:297:PHE:HZ	1.83	0.43
3:F:277:MET:O	3:F:278:ASN:HB2	2.18	0.43
3:I:240:ASP:OD1	3:I:242:SER:HB2	2.19	0.43
3:L:174:LEU:HB2	3:L:196:GLY:HA3	1.99	0.43
3:C:394:GLY:HA2	3:C:453:LEU:O	2.19	0.43
3:F:533:PRO:HA	3:F:538:HIS:CD2	2.53	0.43
1:G:162:ALA:HB3	3:I:189:TRP:CE2	2.54	0.43
3:C:62:ASP:HA	3:C:519:VAL:HG21	2.00	0.43
3:L:168:TRP:HZ2	3:L:181:GLN:HB2	1.84	0.43
3:F:514:PHE:CD2	3:F:519:VAL:HG13	2.54	0.43
1:J:97:GLU:O	1:J:101:ARG:HG3	2.18	0.43
3:C:32:PHE:CD1	3:C:48:VAL:HG13	2.53	0.43
3:C:154:ILE:HG12	3:C:211:PRO:CD	2.49	0.42
3:C:5:GLY:O	3:C:273:TYR:HA	2.19	0.42
3:F:197:ARG:HG3	3:F:514:PHE:CB	2.47	0.42
1:G:58:TYR:CE2	1:G:155:ARG:HG2	2.54	0.42
1:J:20:THR:HG21	3:L:554:PRO:HG2	1.99	0.42
3:I:345:VAL:HG22	3:I:481:TYR:CZ	2.55	0.42
3:I:283:LEU:O	3:I:313:HIS:CE1	2.73	0.42
3:I:361:THR:HA	3:I:362:PRO:HA	1.86	0.42
2:B:9:GLU:HA	2:B:10:PRO:HD2	1.91	0.42
1:A:160:ASN:ND2	3:C:161:THR:HG21	2.35	0.42
3:I:389:ARG:CG	3:I:389:ARG:NH1	2.81	0.42
1:J:54:SER:CB	3:L:29:PRO:HB3	2.50	0.42
3:F:509:MET:O	3:F:523:THR:HA	2.19	0.42
3:I:165:TRP:CZ2	4:I:601:DKA:H91	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:92:HIS:CE1	3:L:125:HIS:CD2	3.08	0.42
3:C:522:HIS:HA	3:C:551:LEU:O	2.20	0.42
3:C:573:GLU:O	3:C:574:LEU:HB2	2.20	0.42
3:L:376:GLN:CG	3:L:453:LEU:HD12	2.49	0.42
1:A:47:ASN:HA	3:C:531:ASP:OD1	2.20	0.41
1:A:110:LEU:HG	3:C:166:MET:SD	2.60	0.41
3:C:193:VAL:HA	3:C:203:TRP:O	2.19	0.41
3:C:163:ARG:H	3:C:163:ARG:HG3	1.66	0.41
3:C:406:PRO:HB3	3:F:114:GLY:HA3	2.02	0.41
3:C:189:TRP:CH2	4:C:601:DKA:H82	2.55	0.41
1:D:30:GLY:HA2	3:F:40:ASP:HB2	2.02	0.41
1:A:76:SER:C	1:A:78:LEU:H	2.29	0.41
3:C:277:MET:HE2	3:C:312:GLY:HA3	2.02	0.41
1:D:87:ASP:O	1:D:91:ARG:HG2	2.20	0.41
3:F:503:ASN:O	3:F:504:ALA:C	2.63	0.41
3:I:283:LEU:HB2	5:I:760:HOH:O	2.19	0.41
3:I:319:ARG:NE	3:I:319:ARG:HA	2.36	0.41
1:D:156:ILE:HG12	3:F:53:LEU:HD22	2.03	0.41
3:I:39:ILE:O	3:I:40:ASP:C	2.64	0.41
3:I:43:ALA:HB2	3:I:170:GLN:HG2	2.03	0.41
3:L:6:PHE:O	3:L:16:GLY:HA3	2.20	0.41
3:L:212:ASN:HB2	3:L:259:ALA:C	2.46	0.41
3:C:3:MET:HE3	3:C:193:VAL:HG23	2.03	0.41
3:F:339:MET:CE	5:F:827:HOH:O	2.67	0.41
1:G:156:ILE:HG12	3:I:53:LEU:HD22	2.03	0.41
3:L:10:ALA:HB1	3:L:320:LEU:HD21	2.03	0.41
3:L:96:VAL:HA	3:L:97:PRO:HD2	1.89	0.41
3:F:184:GLU:O	3:F:185:ALA:C	2.63	0.41
1:J:22:MET:HA	3:L:540:ASP:OD2	2.20	0.41
3:L:62:ASP:HA	3:L:519:VAL:HG22	1.99	0.41
3:F:206:ASP:HB3	3:F:266:PRO:HG2	2.03	0.41
3:I:282:TRP:HD1	3:I:290:LEU:O	2.04	0.40
3:L:84:VAL:HG21	3:L:97:PRO:HB3	2.03	0.40
1:G:56:LEU:HD11	1:G:143:TRP:CB	2.51	0.40
1:J:54:SER:HB3	3:L:29:PRO:HB3	2.03	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	165/178 (93%)	160 (97%)	5 (3%)	0	100	100
1	D	166/178 (93%)	160 (96%)	6 (4%)	0	100	100
1	G	165/178 (93%)	160 (97%)	5 (3%)	0	100	100
1	J	165/178 (93%)	160 (97%)	5 (3%)	0	100	100
2	B	14/27 (52%)	14 (100%)	0	0	100	100
2	E	13/27 (48%)	12 (92%)	1 (8%)	0	100	100
2	H	14/27 (52%)	12 (86%)	1 (7%)	1 (7%)	1	0
2	K	14/27 (52%)	14 (100%)	0	0	100	100
3	C	572/581 (98%)	545 (95%)	27 (5%)	0	100	100
3	F	572/581 (98%)	545 (95%)	26 (4%)	1 (0%)	43	51
3	I	572/581 (98%)	552 (96%)	20 (4%)	0	100	100
3	L	573/581 (99%)	547 (96%)	24 (4%)	2 (0%)	36	42
All	All	3005/3144 (96%)	2881 (96%)	120 (4%)	4 (0%)	48	57

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	19	GLN
3	L	40	ASP
3	F	40	ASP
3	L	426	GLY

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	125/130 (96%)	124 (99%)	1 (1%)	73	85
1	D	126/130 (97%)	122 (97%)	4 (3%)	34	47
1	G	125/130 (96%)	123 (98%)	2 (2%)	55	71
1	J	125/130 (96%)	125 (100%)	0	100	100
2	B	12/17 (71%)	11 (92%)	1 (8%)	10	11
2	E	11/17 (65%)	11 (100%)	0	100	100
2	H	12/17 (71%)	12 (100%)	0	100	100
2	K	12/17 (71%)	12 (100%)	0	100	100
3	C	445/452 (98%)	424 (95%)	21 (5%)	23	31
3	F	445/452 (98%)	427 (96%)	18 (4%)	28	38
3	I	445/452 (98%)	421 (95%)	24 (5%)	20	25
3	L	446/452 (99%)	421 (94%)	25 (6%)	19	24
All	All	2329/2396 (97%)	2233 (96%)	96 (4%)	27	37

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
2	B	14	ARG
3	C	31	ARG
3	C	48	VAL
3	C	113	ASP
3	C	141	LEU
3	C	145	GLN
3	C	154	ILE
3	C	162	LEU
3	C	184	GLU
3	C	218	THR
3	C	229	VAL
3	C	243	ARG
3	C	283	LEU
3	C	286	VAL
3	C	397	LEU
3	C	448	GLN
3	C	461	LEU
3	C	468	THR
3	C	519	VAL

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Mol	Chain	Res	Type
3	C	541	TYR
3	C	570	THR
3	C	572	LYS
1	D	12	THR
1	D	64	ARG
1	D	72	LEU
1	D	176	GLN
3	F	48	VAL
3	F	53	LEU
3	F	85	GLN
3	F	119	VAL
3	F	120	THR
3	F	141	LEU
3	F	154	ILE
3	F	162	LEU
3	F	163	ARG
3	F	195	VAL
3	F	227	MET
3	F	283	LEU
3	F	359	ILE
3	F	397	LEU
3	F	461	LEU
3	F	519	VAL
3	F	541	TYR
3	F	570	THR
1	G	12	THR
1	G	72	LEU
3	I	48	VAL
3	I	119	VAL
3	I	120	THR
3	I	141	LEU
3	I	154	ILE
3	I	162	LEU
3	I	201	LYS
3	I	227	MET
3	I	229	VAL
3	I	243	ARG
3	I	257	LYS
3	I	283	LEU
3	I	376	GLN
3	I	389	ARG
3	I	397	LEU

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Mol	Chain	Res	Type
3	I	407	THR
3	I	461	LEU
3	I	468	THR
3	I	493	GLN
3	I	519	VAL
3	I	541	TYR
3	I	567	ARG
3	I	570	THR
3	I	574	LEU
3	L	11	THR
3	L	31	ARG
3	L	48	VAL
3	L	53	LEU
3	L	64	VAL
3	L	93	ARG
3	L	111	ASN
3	L	119	VAL
3	L	141	LEU
3	L	147	THR
3	L	154	ILE
3	L	162	LEU
3	L	163	ARG
3	L	218	THR
3	L	229	VAL
3	L	271	ASP
3	L	283	LEU
3	L	302	THR
3	L	376	GLN
3	L	397	LEU
3	L	461	LEU
3	L	468	THR
3	L	519	VAL
3	L	541	TYR
3	L	570	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	HIS
1	A	112	GLN
1	A	160	ASN
2	B	19	GLN

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Mol	Chain	Res	Type
3	C	125	HIS
3	C	287	HIS
3	C	305	GLN
3	C	563	ASN
1	D	65	HIS
1	D	92	HIS
1	D	145	GLN
3	F	125	HIS
3	F	287	HIS
3	F	563	ASN
1	G	160	ASN
3	I	111	ASN
3	I	125	HIS
3	I	287	HIS
3	I	489	ASN
1	J	92	HIS
1	J	106	GLN
3	L	125	HIS
3	L	170	GLN
3	L	235	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	DKA	C	601	-	11,11,11	0.62	0	11,11,11	1.12	1 (9%)
4	DKA	I	601	-	11,11,11	0.64	0	11,11,11	1.06	1 (9%)
4	DKA	F	601	3	9,10,11	0.47	0	8,9,11	0.71	0
4	DKA	L	601	3	9,10,11	0.50	0	8,9,11	1.01	1 (12%)

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	DKA	C	601	-	-	7/9/9/9	-
4	DKA	I	601	-	-	5/9/9/9	-
4	DKA	F	601	3	-	4/8/8/9	-
4	DKA	L	601	3	-	7/8/8/9	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	601	DKA	C3-C2-C1	-2.45	108.13	114.51
4	I	601	DKA	O2-C1-C2	2.07	120.53	114.00
4	L	601	DKA	C4-C3-C2	-2.05	104.02	113.86

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	601	DKA	C1-C2-C3-C4
4	L	601	DKA	O1-C1-C2-C3
4	L	601	DKA	C4-C5-C6-C7
4	L	601	DKA	C7-C8-C9-C10
4	I	601	DKA	C6-C7-C8-C9
4	C	601	DKA	C5-C6-C7-C8
4	C	601	DKA	C4-C5-C6-C7
4	F	601	DKA	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
4	L	601	DKA	C3-C4-C5-C6
4	I	601	DKA	C3-C4-C5-C6
4	C	601	DKA	C2-C3-C4-C5
4	F	601	DKA	C5-C6-C7-C8
4	L	601	DKA	C5-C6-C7-C8
4	I	601	DKA	C5-C6-C7-C8
4	I	601	DKA	C4-C5-C6-C7
4	I	601	DKA	C7-C8-C9-C10
4	C	601	DKA	C6-C7-C8-C9
4	L	601	DKA	C6-C7-C8-C9
4	L	601	DKA	C2-C3-C4-C5
4	C	601	DKA	O2-C1-C2-C3
4	C	601	DKA	O1-C1-C2-C3
4	C	601	DKA	C7-C8-C9-C10
4	F	601	DKA	C7-C8-C9-C10

There are no ring outliers.

4 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	601	DKA	4	0
4	I	601	DKA	7	0
4	F	601	DKA	3	0
4	L	601	DKA	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	167/178 (93%)	-0.01	1 (0%) 85 83	36, 51, 64, 89	0
1	D	168/178 (94%)	-0.33	1 (0%) 85 83	28, 40, 57, 75	0
1	G	167/178 (93%)	-0.40	1 (0%) 85 83	30, 40, 52, 64	0
1	J	167/178 (93%)	-0.25	0 100 100	32, 42, 57, 68	0
2	B	16/27 (59%)	0.93	1 (6%) 26 23	61, 75, 95, 95	0
2	E	15/27 (55%)	1.91	7 (46%) 0 0	73, 77, 94, 95	0
2	H	16/27 (59%)	1.62	6 (37%) 1 0	46, 69, 106, 107	0
2	K	16/27 (59%)	0.94	0 100 100	69, 76, 83, 87	0
3	C	574/581 (98%)	-0.11	5 (0%) 81 79	29, 44, 75, 95	0
3	F	574/581 (98%)	-0.19	2 (0%) 90 88	28, 43, 63, 82	0
3	I	574/581 (98%)	-0.32	1 (0%) 91 90	27, 40, 62, 79	0
3	L	575/581 (98%)	0.10	3 (0%) 87 85	32, 50, 71, 84	0
All	All	3029/3144 (96%)	-0.13	28 (0%) 81 79	27, 44, 70, 107	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	20	VAL	5.3
2	H	21	GLY	4.2
2	E	20	VAL	4.1
2	H	17	SER	3.4
3	C	574	LEU	3.3
2	H	16	PRO	3.0
3	I	574	LEU	2.9
1	D	178	PRO	2.8
2	H	18	LEU	2.7
1	G	12	THR	2.7
2	H	19	GLN	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	13	THR	2.6
2	E	21	GLY	2.6
2	B	18	LEU	2.5
1	A	178	PRO	2.5
3	C	120	THR	2.4
2	E	19	GLN	2.4
2	E	17	SER	2.3
2	E	18	LEU	2.2
3	C	154	ILE	2.2
3	F	227	MET	2.1
3	L	292	GLY	2.1
3	L	327	ALA	2.1
3	C	96	VAL	2.1
3	L	334	ALA	2.1
3	C	241	GLY	2.1
3	F	198	GLY	2.0
2	E	8	PHE	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
4	DKA	L	601	11/12	0.85	0.14	34,40,46,48	0
4	DKA	I	601	12/12	0.89	0.11	41,43,46,48	0
4	DKA	C	601	12/12	0.90	0.11	45,48,52,54	0
4	DKA	F	601	11/12	0.90	0.12	39,41,48,49	0

6.5 Other polymers [i](#)

There are no such residues in this entry.