



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:32 AM UTC

PDB ID : 4EGR / pdb_00004egr
Title : 2.50 angstrom resolution structure of 3-phosphoshikimate 1-carboxyvinyltransferase (AroA) from Coxiella burnetii in complex with phosphoenolpyruvate
Authors : Krishna, S.N.; Light, S.H.; Minasov, G.; Shuvalova, L.; Kwon, K.; Anderson, W.F.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2012-03-31
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

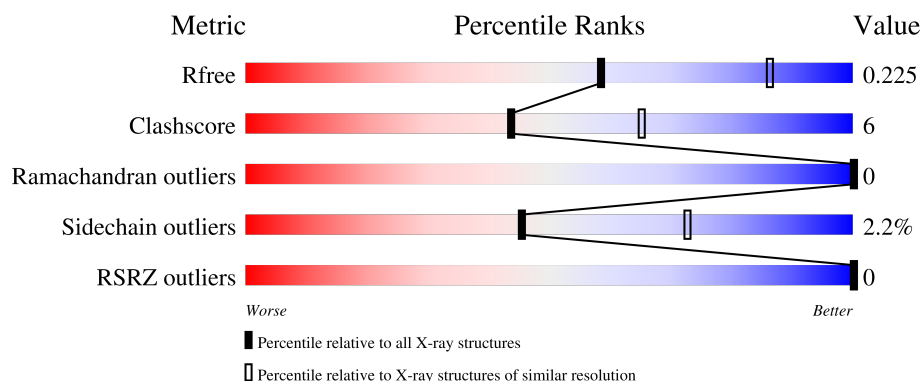
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	441	 83% 14% ..
1	B	441	 86% 11% .
1	C	441	 83% 14% .
1	D	441	 85% 13% .
1	E	441	 85% 13% .

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Mol	Chain	Length	Quality of chain
1	F	441	 83% 14% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19919 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 3-phosphoshikimate 1-carboxyvinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	1	0
			3217	2017	569	611	20			
1	B	434	Total	C	N	O	S	0	5	0
			3234	2028	570	616	20			
1	C	434	Total	C	N	O	S	0	5	0
			3234	2028	570	616	20			
1	D	434	Total	C	N	O	S	0	5	0
			3234	2028	570	616	20			
1	E	434	Total	C	N	O	S	0	5	0
			3234	2028	570	616	20			
1	F	434	Total	C	N	O	S	0	5	0
			3234	2028	570	616	20			

There are 18 discrepancies between the modelled and reference sequences:

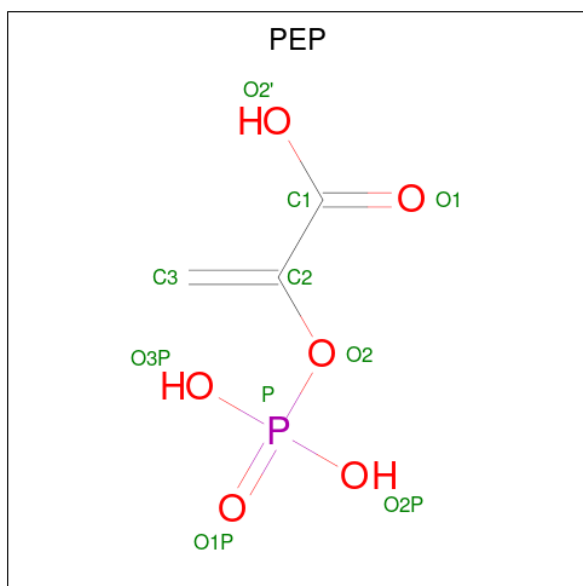
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q83E11
A	-1	ASN	-	expression tag	UNP Q83E11
A	0	ALA	-	expression tag	UNP Q83E11
B	-2	SER	-	expression tag	UNP Q83E11
B	-1	ASN	-	expression tag	UNP Q83E11
B	0	ALA	-	expression tag	UNP Q83E11
C	-2	SER	-	expression tag	UNP Q83E11
C	-1	ASN	-	expression tag	UNP Q83E11
C	0	ALA	-	expression tag	UNP Q83E11
D	-2	SER	-	expression tag	UNP Q83E11
D	-1	ASN	-	expression tag	UNP Q83E11
D	0	ALA	-	expression tag	UNP Q83E11
E	-2	SER	-	expression tag	UNP Q83E11
E	-1	ASN	-	expression tag	UNP Q83E11
E	0	ALA	-	expression tag	UNP Q83E11
F	-2	SER	-	expression tag	UNP Q83E11
F	-1	ASN	-	expression tag	UNP Q83E11

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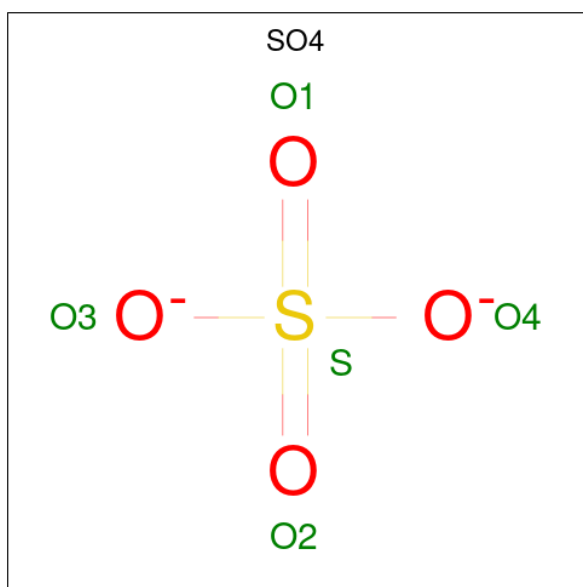
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	ALA	-	expression tag	UNP Q83E11

- Molecule 2 is PHOSPHOENOLPYRUVATE (CCD ID: PEP) (formula: $C_3H_5O_6P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			10	3	6	1		
2	B	1	Total	C	O	P	0	0
			10	3	6	1		
2	C	1	Total	C	O	P	0	0
			10	3	6	1		
2	D	1	Total	C	O	P	0	0
			10	3	6	1		
2	E	1	Total	C	O	P	0	0
			10	3	6	1		
2	F	1	Total	C	O	P	0	0
			10	3	6	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		
3	F	1	Total	O	S	0	0
			5	4	1		

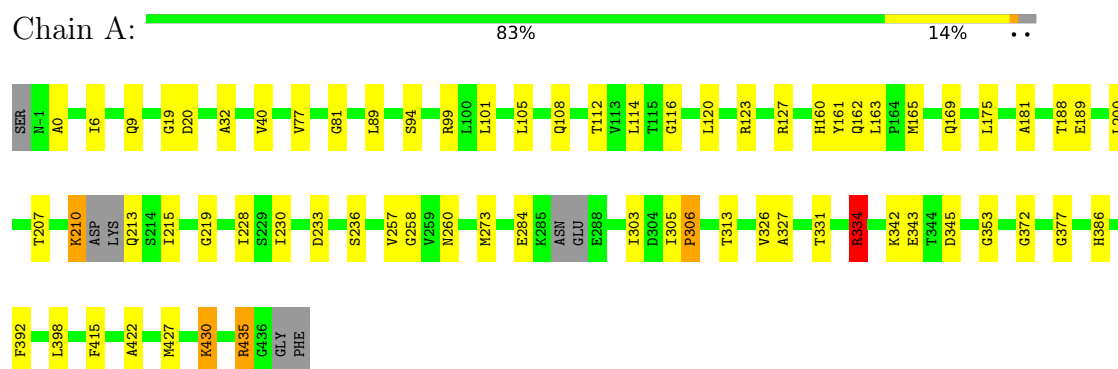
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total 73	O 73	0	0
4	B	77	Total 77	O 77	0	0
4	C	74	Total 74	O 74	0	0
4	D	66	Total 66	O 66	0	0
4	E	62	Total 62	O 62	0	0
4	F	60	Total 60	O 60	0	0

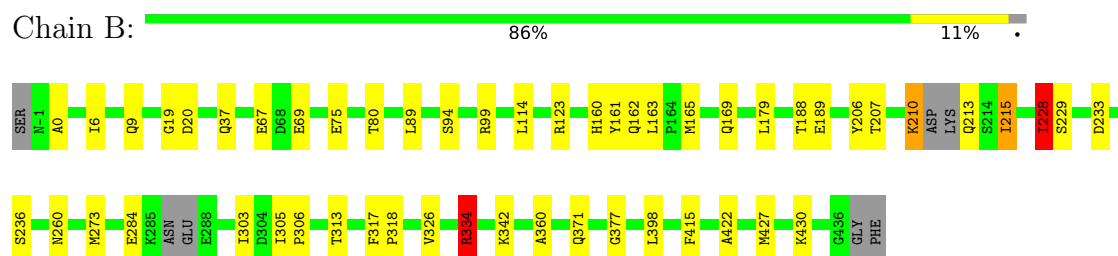
3 Residue-property plots

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

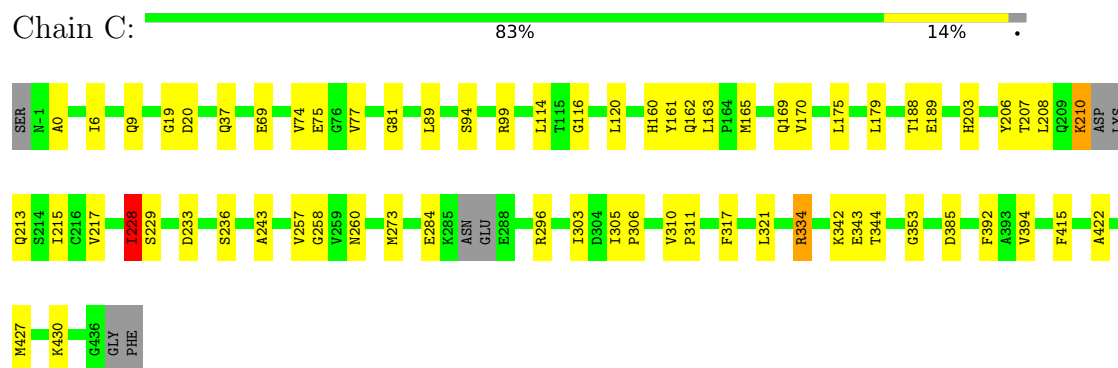
- Molecule 1: 3-phosphoshikimate 1-carboxyvinyltransferase



- Molecule 1: 3-phosphoshikimate 1-carboxyvinyltransferase

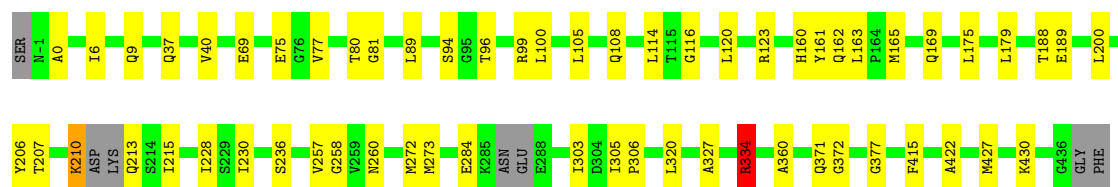


- Molecule 1: 3-phosphoshikimate 1-carboxyvinyltransferase



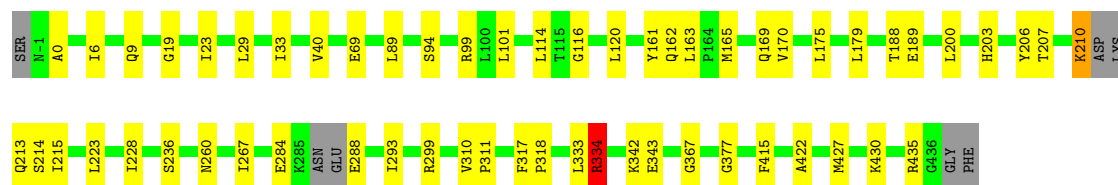
- Molecule 1: 3-phosphoshikimate 1-carboxyvinyltransferase

Chain D:  85% 13% .



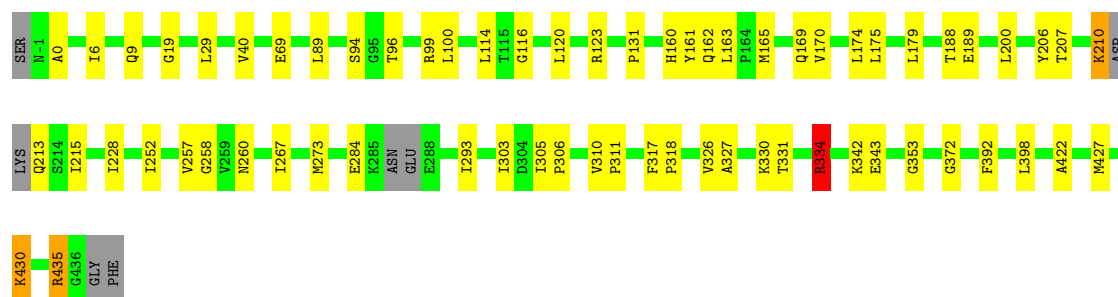
- Molecule 1: 3-phosphoshikimate 1-carboxyvinyltransferase

Chain E:  85% 13% .



- Molecule 1: 3-phosphoshikimate 1-carboxyvinyltransferase

Chain F:  83% 14% ..



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	162.36Å 94.05Å 230.51Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	29.75 – 2.50 29.75 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.6 (29.75-2.50) 98.7 (29.75-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.177 , 0.223 0.180 , 0.225	Depositor DCC
R_{free} test set	5942 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	56.1	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 27.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.436 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.419 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.427 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.419 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.457 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	19919	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.81% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, PEP

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	0.97	1/3265 (0.0%)	1.10	18/4424 (0.4%)
1	B	0.99	0/3291	1.10	15/4460 (0.3%)
1	C	0.97	1/3291 (0.0%)	1.09	13/4460 (0.3%)
1	D	0.96	1/3291 (0.0%)	1.07	11/4460 (0.2%)
1	E	0.98	2/3291 (0.1%)	1.08	11/4460 (0.2%)
1	F	0.96	0/3291	1.09	13/4460 (0.3%)
All	All	0.97	5/19720 (0.0%)	1.09	81/26724 (0.3%)

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	C	0	1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	299	ARG	CA-C	-5.56	1.45	1.52
1	D	160	HIS	CE1-NE2	5.52	1.38	1.32
1	C	203	HIS	CG-CD2	5.41	1.41	1.35
1	A	386	HIS	CG-CD2	5.12	1.41	1.35
1	E	203	HIS	CG-CD2	5.06	1.41	1.35

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	334	ARG	NE-CZ-NH2	-9.39	110.74	119.20
1	C	334	ARG	CD-NE-CZ	9.29	137.41	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	ILE	N-CA-C	-8.93	101.87	109.19
1	C	228	ILE	CB-CA-C	-7.93	98.60	110.82
1	D	334	ARG	NE-CZ-NH2	7.49	125.94	119.20
1	A	94	SER	N-CA-C	7.46	120.43	108.41
1	C	94	SER	N-CA-C	7.37	120.81	108.20
1	B	228	ILE	CB-CA-C	-7.25	99.66	110.82
1	F	6	ILE	N-CA-CB	7.21	117.80	111.67
1	E	94	SER	N-CA-C	7.12	120.53	107.99
1	B	19	GLY	N-CA-C	7.10	120.14	112.33
1	F	94	SER	N-CA-C	6.96	120.69	107.75
1	B	94	SER	N-CA-C	6.95	120.09	108.20
1	A	334	ARG	NE-CZ-NH2	6.94	125.45	119.20
1	B	334	ARG	NE-CZ-NH2	6.93	125.44	119.20
1	A	19	GLY	N-CA-C	6.92	119.94	112.33
1	F	334	ARG	NE-CZ-NH2	6.76	125.28	119.20
1	D	160	HIS	N-CA-C	-6.71	98.75	109.76
1	C	19	GLY	N-CA-C	6.69	119.69	112.33
1	E	334	ARG	NE-CZ-NH2	6.69	125.22	119.20
1	E	19	GLY	N-CA-C	6.60	119.59	112.33
1	B	377	GLY	N-CA-C	-6.60	104.09	112.54
1	A	6	ILE	N-CA-C	-6.56	101.60	109.01
1	D	377	GLY	N-CA-C	-6.55	104.15	112.54
1	C	6	ILE	N-CA-CB	6.46	117.16	111.67
1	C	334	ARG	CG-CD-NE	-6.45	97.82	112.00
1	D	94	SER	N-CA-C	6.42	119.28	107.99
1	D	123	ARG	CA-C-N	6.34	126.10	119.76
1	D	123	ARG	C-N-CA	6.34	126.10	119.76
1	E	6	ILE	N-CA-CB	6.33	117.05	111.67
1	D	6	ILE	N-CA-CB	6.29	117.02	111.67
1	F	19	GLY	N-CA-C	6.28	119.24	112.33
1	A	377	GLY	N-CA-C	-6.15	104.67	112.54
1	F	6	ILE	N-CA-C	-6.12	101.10	108.45
1	B	123	ARG	CA-C-N	5.98	125.74	119.76
1	B	123	ARG	C-N-CA	5.98	125.74	119.76
1	A	0	ALA	N-CA-C	5.97	117.75	110.41
1	A	284	GLU	N-CA-C	5.92	119.13	109.06
1	D	0	ALA	N-CA-C	5.88	117.65	110.41
1	E	0	ALA	N-CA-C	5.76	117.50	110.41
1	F	0	ALA	N-CA-C	5.75	117.48	110.41
1	C	284	GLU	N-CA-C	5.66	118.68	109.06
1	A	260	ASN	CA-C-N	5.62	125.98	119.47
1	A	260	ASN	C-N-CA	5.62	125.98	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	284	GLU	N-CA-C	5.61	118.59	109.06
1	B	0	ALA	N-CA-C	5.58	117.27	110.41
1	B	284	GLU	N-CA-C	5.58	118.54	109.06
1	B	160	HIS	N-CA-C	-5.54	100.67	109.76
1	F	160	HIS	N-CA-C	-5.52	100.70	109.76
1	C	260	ASN	CA-C-N	5.34	126.52	119.84
1	C	260	ASN	C-N-CA	5.34	126.52	119.84
1	E	284	GLU	N-CA-C	5.34	118.13	109.06
1	A	127	ARG	CA-C-N	-5.31	117.51	122.66
1	A	127	ARG	C-N-CA	-5.31	117.51	122.66
1	A	160	HIS	N-CA-C	-5.30	101.06	109.76
1	C	74	VAL	N-CA-C	5.30	115.72	107.99
1	B	260	ASN	CA-C-N	5.29	125.60	119.47
1	B	260	ASN	C-N-CA	5.29	125.60	119.47
1	C	160	HIS	N-CA-C	-5.25	101.15	109.76
1	E	435	ARG	N-CA-CB	-5.21	102.27	111.39
1	A	123	ARG	CA-C-N	5.19	125.11	119.76
1	A	123	ARG	C-N-CA	5.19	125.11	119.76
1	E	260	ASN	CA-C-N	5.19	125.49	119.47
1	E	260	ASN	C-N-CA	5.19	125.49	119.47
1	E	377	GLY	N-CA-C	-5.17	105.92	112.54
1	C	0	ALA	N-CA-C	5.15	116.74	110.41
1	B	215	ILE	CB-CA-C	-5.14	102.59	110.50
1	D	284	GLU	N-CA-C	5.13	117.78	109.06
1	A	230	ILE	CA-C-O	5.12	122.52	119.19
1	A	435	ARG	N-CA-CB	-5.08	102.50	111.39
1	F	260	ASN	CA-C-N	5.06	125.34	119.47
1	F	260	ASN	C-N-CA	5.06	125.34	119.47
1	E	6	ILE	N-CA-C	-5.03	102.41	108.45
1	B	67	GLU	N-CA-C	5.02	117.14	111.11
1	F	435	ARG	N-CA-CB	-5.02	102.60	111.39
1	A	306	PRO	CA-C-N	5.01	125.03	119.32
1	A	306	PRO	C-N-CA	5.01	125.03	119.32
1	F	123	ARG	CA-C-N	5.01	124.77	119.76
1	F	123	ARG	C-N-CA	5.01	124.77	119.76
1	D	260	ASN	CA-C-N	5.01	125.28	119.47
1	D	260	ASN	C-N-CA	5.01	125.28	119.47

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	334	ARG	Sidechain

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	3217	0	3308	42	0
1	B	3234	0	3328	27	0
1	C	3234	0	3328	41	0
1	D	3234	0	3328	42	0
1	E	3234	0	3328	42	0
1	F	3234	0	3328	47	0
2	A	10	0	2	1	0
2	B	10	0	2	1	0
2	C	10	0	2	1	0
2	D	10	0	2	1	0
2	E	10	0	2	1	0
2	F	10	0	2	1	0
3	A	10	0	0	0	0
3	B	10	0	0	0	0
3	C	10	0	0	0	0
3	D	10	0	0	0	0
3	E	10	0	0	0	0
3	F	10	0	0	0	0
4	A	73	0	0	0	0
4	B	77	0	0	1	0
4	C	74	0	0	1	0
4	D	66	0	0	0	0
4	E	62	0	0	0	0
4	F	60	0	0	0	0
All	All	19919	0	19960	240	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 6.

All (240) 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:F:175:LEU:HD21	1:F:215:ILE:HD11	1.43	0.99
1:A:175:LEU:HD21	1:A:215:ILE:HD11	1.45	0.96
1:E:175:LEU:HD21	1:E:215:ILE:HD11	1.48	0.94
1:B:334:ARG:HH21	1:B:334:ARG:HG3	1.30	0.93
1:E:334:ARG:HH21	1:E:334:ARG:HG3	1.33	0.93
1:F:175:LEU:HD21	1:F:215:ILE:CD1	1.99	0.93
1:D:334:ARG:HH21	1:D:334:ARG:HG3	1.33	0.92
1:F:334:ARG:HH21	1:F:334:ARG:HG3	1.33	0.92
1:C:175:LEU:HD21	1:C:215:ILE:HD11	1.51	0.90
1:B:210:LYS:C	1:B:210:LYS:HE3	2.01	0.85
1:E:163:LEU:HD12	1:E:189:GLU:HG2	1.57	0.85
1:C:163:LEU:HD12	1:C:189:GLU:HG2	1.59	0.84
1:A:175:LEU:HD21	1:A:215:ILE:CD1	2.08	0.83
1:A:163:LEU:HD12	1:A:189:GLU:HG2	1.58	0.83
1:C:175:LEU:HD21	1:C:215:ILE:CD1	2.08	0.83
1:C:210:LYS:NZ	1:C:210:LYS:O	2.12	0.83
1:B:163:LEU:HD12	1:B:189:GLU:HG2	1.59	0.82
1:F:163:LEU:HD12	1:F:189:GLU:HG2	1.60	0.82
1:F:210:LYS:HE3	1:F:210:LYS:C	2.05	0.81
1:D:210:LYS:O	1:D:210:LYS:NZ	2.11	0.81
1:D:163:LEU:HD12	1:D:189:GLU:HG2	1.62	0.80
1:E:175:LEU:HD21	1:E:215:ILE:CD1	2.12	0.79
1:A:210:LYS:HE3	1:A:210:LYS:C	2.08	0.79
1:F:200:LEU:HD21	1:F:228:ILE:HD11	1.64	0.79
1:D:210:LYS:HZ2	1:D:210:LYS:C	1.91	0.77
1:A:334:ARG:HH21	1:A:334:ARG:HG3	1.50	0.76
1:D:200:LEU:HD21	1:D:228:ILE:HD11	1.67	0.75
1:E:210:LYS:C	1:E:210:LYS:HE3	2.11	0.74
1:A:200:LEU:HD21	1:A:228:ILE:HD11	1.72	0.71
1:D:200:LEU:HD21	1:D:228:ILE:CD1	2.20	0.70
1:C:210:LYS:HZ2	1:C:210:LYS:C	1.99	0.70
1:A:200:LEU:HD21	1:A:228:ILE:CD1	2.22	0.68
1:A:200:LEU:CD2	1:A:228:ILE:CD1	2.72	0.68
1:D:175:LEU:HD21	1:D:215:ILE:HD11	1.76	0.68
1:A:99:ARG:HD2	1:A:169:GLN:OE1	1.94	0.68
1:E:334:ARG:HG3	1:E:334:ARG:NH2	2.08	0.67
1:F:40:VAL:HG22	1:F:228:ILE:CG2	2.24	0.66
1:B:334:ARG:HG3	1:B:334:ARG:NH2	2.05	0.66
1:E:213:GLN:O	1:E:213:GLN:HG2	1.96	0.66
1:E:89:LEU:HD12	1:E:114:LEU:HD21	1.77	0.65
1:E:200:LEU:HD21	1:E:228:ILE:CD1	2.26	0.65
1:B:162:GLN:HG2	1:B:188:THR:HB	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:200:LEU:CD2	1:D:228:ILE:CD1	2.75	0.64
1:F:99:ARG:HD2	1:F:169:GLN:OE1	1.97	0.64
1:F:334:ARG:HG3	1:F:334:ARG:NH2	2.07	0.64
1:C:228:ILE:CG2	1:C:229:SER:N	2.58	0.64
1:C:296:ARG:HD3	4:C:642:HOH:O	1.97	0.63
1:D:334:ARG:HG3	1:D:334:ARG:NH2	2.07	0.63
1:D:175:LEU:HD21	1:D:215:ILE:CD1	2.29	0.62
1:F:422:ALA:HB1	1:F:427:MET:HG3	1.82	0.62
1:E:422:ALA:HB1	1:E:427:MET:HG3	1.81	0.62
1:A:430:LYS:NZ	1:B:80:THR:O	2.33	0.61
1:A:162:GLN:HG2	1:A:188:THR:HB	1.81	0.61
1:D:99:ARG:HD2	1:D:169:GLN:OE1	2.01	0.61
1:A:213:GLN:HG2	1:A:213:GLN:O	2.00	0.61
1:D:175:LEU:HD11	1:D:215:ILE:HD11	1.81	0.61
1:A:422:ALA:HB1	1:A:427:MET:HG3	1.83	0.60
1:C:175:LEU:HD11	1:C:215:ILE:HD11	1.83	0.60
1:C:213:GLN:O	1:C:213:GLN:HG2	2.01	0.59
1:E:162:GLN:HG2	1:E:188:THR:HB	1.83	0.59
1:D:162:GLN:HG2	1:D:188:THR:HB	1.84	0.59
1:F:213:GLN:HG2	1:F:213:GLN:O	2.02	0.59
1:D:80:THR:O	1:F:430:LYS:NZ	2.35	0.59
1:F:89:LEU:HD12	1:F:114:LEU:HD21	1.84	0.59
1:D:213:GLN:O	1:D:213:GLN:HG2	2.01	0.59
1:E:99:ARG:HD2	1:E:169:GLN:OE1	2.02	0.59
1:F:40:VAL:HG22	1:F:228:ILE:HG22	1.85	0.59
2:B:503:PEP:O2P	2:B:503:PEP:H32	2.02	0.58
1:F:162:GLN:HG2	1:F:188:THR:HB	1.84	0.58
1:F:200:LEU:HD21	1:F:228:ILE:CD1	2.33	0.58
1:C:99:ARG:HD2	1:C:169:GLN:OE1	2.03	0.58
1:F:200:LEU:CD2	1:F:228:ILE:CD1	2.82	0.57
1:E:40:VAL:HG22	1:E:228:ILE:CG2	2.33	0.57
1:F:89:LEU:HB2	1:F:114:LEU:HD23	1.86	0.57
1:E:200:LEU:CD2	1:E:228:ILE:CD1	2.83	0.57
1:B:161:TYR:HE1	1:B:163:LEU:HD23	1.70	0.56
1:A:40:VAL:HG22	1:A:228:ILE:CG2	2.35	0.56
1:B:213:GLN:O	1:B:213:GLN:HG2	2.03	0.56
1:B:228:ILE:CG2	1:B:229:SER:N	2.66	0.56
1:C:210:LYS:NZ	1:C:210:LYS:C	2.62	0.56
1:E:200:LEU:HD21	1:E:228:ILE:HD13	1.88	0.56
1:B:99:ARG:HD2	1:B:169:GLN:OE1	2.06	0.56
1:B:89:LEU:HB2	1:B:114:LEU:HD23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:ILE:C	1:E:215:ILE:HD12	2.31	0.56
1:C:162:GLN:HG2	1:C:188:THR:HB	1.86	0.56
1:C:422:ALA:HB1	1:C:427:MET:HG3	1.87	0.56
2:D:503:PEP:O3P	2:D:503:PEP:H32	2.06	0.55
1:D:75:GLU:OE2	1:F:435:ARG:NH1	2.39	0.55
1:C:179:LEU:HD22	1:C:206:TYR:CZ	2.41	0.55
1:E:40:VAL:HG22	1:E:228:ILE:HG22	1.88	0.54
1:B:422:ALA:HB1	1:B:427:MET:HG3	1.88	0.54
1:F:200:LEU:CD2	1:F:228:ILE:HD11	2.35	0.54
1:D:89:LEU:HB2	1:D:114:LEU:HD23	1.88	0.54
1:A:326:VAL:HG11	1:A:398:LEU:HD23	1.89	0.54
1:F:116:GLY:HA3	1:F:120:LEU:HD23	1.90	0.54
2:C:503:PEP:O3P	2:C:503:PEP:H32	2.08	0.54
1:F:215:ILE:HD12	1:F:215:ILE:C	2.33	0.54
1:B:179:LEU:HD22	1:B:206:TYR:CZ	2.43	0.54
1:D:210:LYS:C	1:D:210:LYS:CE	2.81	0.54
1:C:210:LYS:C	1:C:210:LYS:CE	2.81	0.53
1:F:257:VAL:HG12	1:F:258:GLY:O	2.09	0.53
1:E:89:LEU:HB2	1:E:114:LEU:HD23	1.91	0.53
1:D:40:VAL:HG13	1:D:228:ILE:HG23	1.92	0.52
1:D:210:LYS:NZ	1:D:210:LYS:C	2.62	0.52
1:D:273:MET:HG3	1:D:303:ILE:HD13	1.90	0.52
1:B:326:VAL:HG11	1:B:398:LEU:HD23	1.92	0.52
1:B:273:MET:HG3	1:B:303:ILE:HD13	1.91	0.52
1:B:342:LYS:NZ	4:B:677:HOH:O	2.42	0.52
1:D:40:VAL:HG22	1:D:228:ILE:HG22	1.92	0.52
1:A:175:LEU:CD2	1:A:215:ILE:HD11	2.31	0.51
1:D:40:VAL:HG22	1:D:228:ILE:CG2	2.40	0.51
1:A:273:MET:HG3	1:A:303:ILE:HD13	1.91	0.51
1:D:215:ILE:HD12	1:D:215:ILE:C	2.35	0.51
1:E:89:LEU:HD12	1:E:114:LEU:CD2	2.39	0.51
1:C:310:VAL:HB	1:C:311:PRO:HD3	1.93	0.51
1:B:37:GLN:NE2	1:B:75:GLU:OE2	2.43	0.51
1:A:40:VAL:HG22	1:A:228:ILE:HG22	1.92	0.50
2:E:503:PEP:H32	2:E:503:PEP:O1P	2.11	0.50
1:A:89:LEU:HB2	1:A:114:LEU:HD23	1.93	0.50
1:A:435:ARG:NH1	1:B:75:GLU:OE2	2.44	0.50
1:C:175:LEU:CD2	1:C:215:ILE:HD11	2.35	0.50
1:C:89:LEU:HB2	1:C:114:LEU:HD23	1.93	0.50
1:E:116:GLY:HA3	1:E:120:LEU:HD23	1.94	0.50
1:D:422:ALA:HB1	1:D:427:MET:HG3	1.92	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:501:PEP:O3P	2:A:501:PEP:H32	2.11	0.49
1:E:200:LEU:CD2	1:E:228:ILE:HD13	2.43	0.49
1:A:116:GLY:HA3	1:A:120:LEU:HD23	1.95	0.49
1:B:210:LYS:C	1:B:210:LYS:CE	2.80	0.49
1:A:303:ILE:O	1:A:331:THR:HA	2.12	0.49
2:F:503:PEP:O2P	2:F:503:PEP:H32	2.11	0.49
1:C:215:ILE:C	1:C:215:ILE:HD12	2.38	0.49
1:C:116:GLY:HA3	1:C:120:LEU:HD23	1.94	0.49
1:E:33:ILE:HG13	1:E:223:LEU:HD12	1.95	0.48
1:F:131:PRO:HB2	1:F:174:LEU:HD21	1.95	0.48
1:C:228:ILE:HG23	1:C:229:SER:N	2.29	0.48
1:E:179:LEU:HD22	1:E:206:TYR:CZ	2.48	0.48
1:F:326:VAL:HG11	1:F:398:LEU:HD23	1.95	0.48
1:D:161:TYR:HE1	1:D:163:LEU:HD23	1.79	0.48
1:F:40:VAL:HG13	1:F:228:ILE:HG23	1.96	0.47
1:E:161:TYR:HE1	1:E:163:LEU:HD23	1.78	0.47
1:A:40:VAL:HG13	1:A:228:ILE:HG23	1.97	0.47
1:A:353:GLY:HA3	1:A:392:PHE:CZ	2.49	0.47
1:D:200:LEU:CD2	1:D:228:ILE:HD11	2.40	0.47
1:F:179:LEU:HD22	1:F:206:TYR:CZ	2.50	0.47
1:A:334:ARG:HG3	1:A:334:ARG:NH2	2.22	0.47
1:C:210:LYS:C	1:C:210:LYS:HE3	2.40	0.47
1:C:273:MET:HG3	1:C:303:ILE:HD13	1.95	0.47
1:D:327:ALA:O	1:D:372:GLY:HA3	2.15	0.46
1:A:236:SER:HB3	1:A:415:PHE:CE1	2.50	0.46
1:F:89:LEU:HD12	1:F:114:LEU:CD2	2.45	0.46
1:A:161:TYR:HE1	1:A:163:LEU:HD23	1.80	0.46
1:D:96:THR:HG22	1:D:100:LEU:HD22	1.98	0.46
1:D:210:LYS:C	1:D:210:LYS:HE3	2.40	0.46
1:A:215:ILE:HD12	1:A:215:ILE:C	2.40	0.46
1:E:175:LEU:CD2	1:E:215:ILE:HD11	2.35	0.46
1:C:37:GLN:NE2	1:C:75:GLU:OE2	2.45	0.46
1:C:77:VAL:O	1:C:81:GLY:HA3	2.16	0.46
1:A:327:ALA:O	1:A:372:GLY:HA3	2.17	0.45
1:C:344:THR:HG22	1:C:385:ASP:OD2	2.16	0.45
1:F:96:THR:HG22	1:F:100:LEU:HD22	1.99	0.45
1:F:273:MET:HG3	1:F:303:ILE:HD13	1.97	0.45
1:D:77:VAL:O	1:D:81:GLY:HA3	2.16	0.45
1:F:161:TYR:HE1	1:F:163:LEU:HD23	1.81	0.45
1:F:327:ALA:O	1:F:372:GLY:HA3	2.17	0.45
1:C:20:ASP:HA	1:C:233:ASP:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:GLY:HA3	1:D:120:LEU:HD23	1.98	0.45
1:D:257:VAL:HG12	1:D:258:GLY:O	2.16	0.45
1:B:179:LEU:HD22	1:B:206:TYR:CE2	2.52	0.45
1:B:360:ALA:HB3	1:B:371:GLN:HB3	1.99	0.45
1:C:208:LEU:HD12	1:C:217:VAL:HG12	1.99	0.44
1:F:179:LEU:HD22	1:F:206:TYR:CE2	2.52	0.44
1:A:210:LYS:C	1:A:210:LYS:CE	2.85	0.44
1:F:353:GLY:HA3	1:F:392:PHE:CZ	2.52	0.44
1:A:257:VAL:HG12	1:A:258:GLY:O	2.17	0.44
1:C:161:TYR:HE1	1:C:163:LEU:HD23	1.82	0.44
1:F:29:LEU:C	1:F:29:LEU:HD23	2.42	0.44
1:D:360:ALA:HB3	1:D:371:GLN:HB3	2.00	0.44
1:C:89:LEU:HD12	1:C:114:LEU:HD21	1.99	0.44
1:C:243:ALA:HB2	1:C:394:VAL:HG13	2.00	0.44
1:F:310:VAL:HB	1:F:311:PRO:HD3	2.00	0.43
1:E:163:LEU:HD21	1:E:170:VAL:HG12	2.00	0.43
1:F:342:LYS:O	1:F:343:GLU:C	2.61	0.43
1:A:305:ILE:HA	1:A:306:PRO:HD3	1.86	0.43
1:A:342:LYS:O	1:A:343:GLU:C	2.61	0.43
1:C:163:LEU:HD21	1:C:170:VAL:HG12	2.00	0.43
1:D:272:MET:HE2	1:D:303:ILE:HD12	2.01	0.43
1:B:236:SER:HB3	1:B:415:PHE:CE1	2.54	0.43
1:B:20:ASP:HA	1:B:233:ASP:HB2	1.99	0.43
1:E:310:VAL:HB	1:E:311:PRO:HD3	2.01	0.43
1:C:342:LYS:O	1:C:343:GLU:C	2.61	0.43
1:E:200:LEU:HD21	1:E:228:ILE:HD11	1.98	0.43
1:A:435:ARG:HD2	1:B:37:GLN:HB2	2.01	0.42
1:E:210:LYS:C	1:E:210:LYS:CE	2.86	0.42
1:F:267:ILE:HD11	1:F:293:ILE:HD13	2.01	0.42
1:D:105:LEU:HA	1:D:108:GLN:HG2	2.01	0.42
1:D:175:LEU:HA	1:D:175:LEU:HD23	1.84	0.42
1:E:236:SER:HB3	1:E:415:PHE:CE1	2.54	0.42
1:E:333:LEU:O	1:E:367:GLY:HA3	2.20	0.42
1:F:317:PHE:O	1:F:318:PRO:C	2.60	0.42
1:A:77:VAL:O	1:A:81:GLY:HA3	2.19	0.42
1:A:101:LEU:HD23	1:A:101:LEU:HA	1.91	0.42
1:D:320:LEU:HD12	1:D:320:LEU:HA	1.90	0.42
1:A:105:LEU:HD13	1:A:112:THR:HG21	2.01	0.42
1:C:228:ILE:HG22	1:C:229:SER:N	2.29	0.42
1:D:37:GLN:HB2	1:F:435:ARG:HD2	2.02	0.42
1:E:23:ILE:HD13	1:E:288:GLU:HG3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:29:LEU:C	1:E:29:LEU:HD23	2.45	0.42
1:E:175:LEU:HD11	1:E:215:ILE:HD11	2.02	0.42
1:E:179:LEU:HD22	1:E:206:TYR:CE2	2.54	0.42
1:F:210:LYS:C	1:F:210:LYS:CE	2.86	0.42
1:C:236:SER:HB3	1:C:415:PHE:CE1	2.55	0.42
1:C:353:GLY:HA3	1:C:392:PHE:CZ	2.55	0.42
1:A:105:LEU:HA	1:A:108:GLN:HG2	2.03	0.41
1:B:317:PHE:O	1:B:318:PRO:C	2.62	0.41
1:C:257:VAL:HG12	1:C:258:GLY:O	2.20	0.41
1:E:89:LEU:HB2	1:E:114:LEU:CD2	2.50	0.41
1:E:267:ILE:HD11	1:E:293:ILE:HD13	2.02	0.41
1:F:305:ILE:HA	1:F:306:PRO:HD3	1.89	0.41
1:E:101:LEU:HD23	1:E:101:LEU:HA	1.90	0.41
1:C:305:ILE:HA	1:C:306:PRO:HD3	1.86	0.41
1:E:163:LEU:CD2	1:E:170:VAL:CG1	2.99	0.41
1:D:305:ILE:HA	1:D:306:PRO:HD3	1.86	0.41
1:D:179:LEU:HD22	1:D:206:TYR:CZ	2.55	0.41
1:F:303:ILE:O	1:F:331:THR:HA	2.20	0.41
1:B:305:ILE:HA	1:B:306:PRO:HD3	1.88	0.41
1:A:181:ALA:O	1:A:219:GLY:HA3	2.20	0.41
1:C:317:PHE:O	1:C:321:LEU:HG	2.21	0.41
1:E:317:PHE:O	1:E:318:PRO:C	2.62	0.41
1:F:163:LEU:CD2	1:F:170:VAL:CG1	2.99	0.41
1:A:32:ALA:O	1:A:77:VAL:HG22	2.21	0.41
1:F:252:ILE:HD13	1:F:252:ILE:HG21	1.89	0.41
1:A:20:ASP:HA	1:A:233:ASP:HB2	2.03	0.40
1:C:163:LEU:CD2	1:C:170:VAL:CG1	3.00	0.40
1:E:342:LYS:O	1:E:343:GLU:C	2.63	0.40
1:F:163:LEU:HD21	1:F:170:VAL:HG12	2.03	0.40
1:A:345:ASP:OD1	1:A:345:ASP:C	2.64	0.40
1:B:69:GLU:OE2	1:F:330:LYS:HD3	2.20	0.40
1:C:179:LEU:HD22	1:C:206:TYR:CE2	2.57	0.40
1:D:236:SER:HB3	1:D:415:PHE:CE1	2.57	0.40
1:E:188:THR:HG23	1:E:214:SER: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	429/441 (97%)	417 (97%)	12 (3%)	0	100	100
1	B	433/441 (98%)	420 (97%)	13 (3%)	0	100	100
1	C	433/441 (98%)	420 (97%)	13 (3%)	0	100	100
1	D	433/441 (98%)	419 (97%)	14 (3%)	0	100	100
1	E	433/441 (98%)	417 (96%)	16 (4%)	0	100	100
1	F	433/441 (98%)	417 (96%)	16 (4%)	0	100	100
All	All	2594/2646 (98%)	2510 (97%)	84 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	347/352 (99%)	340 (98%)	7 (2%)	48	75
1	B	350/352 (99%)	341 (97%)	9 (3%)	40	68
1	C	350/352 (99%)	343 (98%)	7 (2%)	48	75
1	D	350/352 (99%)	342 (98%)	8 (2%)	44	72
1	E	350/352 (99%)	343 (98%)	7 (2%)	48	75
1	F	350/352 (99%)	343 (98%)	7 (2%)	48	75
All	All	2097/2112 (99%)	2052 (98%)	45 (2%)	45	74

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLN
1	A	165	MET
1	A	207	THR
1	A	210	LYS
1	A	313	THR
1	A	334	ARG
1	A	430	LYS
1	B	9	GLN
1	B	165	MET
1	B	207	THR
1	B	210	LYS
1	B	215	ILE
1	B	228	ILE
1	B	313	THR
1	B	334	ARG
1	B	430	LYS
1	C	9	GLN
1	C	69	GLU
1	C	165	MET
1	C	207	THR
1	C	210	LYS
1	C	228	ILE
1	C	430	LYS
1	D	9	GLN
1	D	69	GLU
1	D	165	MET
1	D	207	THR
1	D	210	LYS
1	D	230	ILE
1	D	334	ARG
1	D	430	LYS
1	E	9	GLN
1	E	69	GLU
1	E	165	MET
1	E	207	THR
1	E	210	LYS
1	E	334	ARG
1	E	430	LYS
1	F	9	GLN
1	F	69	GLU
1	F	165	MET
1	F	207	THR

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Mol	Chain	Res	Type
1	F	210	LYS
1	F	334	ARG
1	F	430	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	B	39	GLN
1	B	70	ASN
1	B	121	GLN
1	B	209	GLN
1	B	213	GLN
1	C	70	ASN
1	C	209	GLN
1	C	213	GLN
1	D	57	GLN
1	D	70	ASN
1	D	121	GLN
1	D	209	GLN
1	D	213	GLN
1	E	70	ASN
1	E	209	GLN
1	F	25	HIS
1	F	37	GLN
1	F	57	GLN
1	F	70	ASN
1	F	121	GLN
1	F	209	GLN
1	F	213	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

18 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	$\# Z > 2$
3	SO4	B	502	-	4,4,4	0.59	0	6,6,6	0.31	0
2	PEP	E	503	-	9,9,9	1.58	2 (22%)	11,13,13	1.64	2 (18%)
2	PEP	D	503	-	9,9,9	1.59	2 (22%)	11,13,13	1.64	2 (18%)
2	PEP	C	503	-	9,9,9	1.58	2 (22%)	11,13,13	1.65	2 (18%)
3	SO4	A	502	-	4,4,4	0.44	0	6,6,6	0.48	0
3	SO4	B	501	-	4,4,4	0.53	0	6,6,6	0.40	0
3	SO4	E	501	-	4,4,4	0.46	0	6,6,6	0.46	0
3	SO4	A	503	-	4,4,4	0.42	0	6,6,6	0.34	0
3	SO4	E	502	-	4,4,4	0.42	0	6,6,6	0.47	0
3	SO4	D	502	-	4,4,4	0.47	0	6,6,6	0.60	0
2	PEP	B	503	-	9,9,9	1.58	2 (22%)	11,13,13	1.64	2 (18%)
3	SO4	F	502	-	4,4,4	0.64	0	6,6,6	0.42	0
3	SO4	F	501	-	4,4,4	0.52	0	6,6,6	0.47	0
2	PEP	A	501	-	9,9,9	1.58	2 (22%)	11,13,13	1.65	2 (18%)
2	PEP	F	503	-	9,9,9	1.57	2 (22%)	11,13,13	1.64	2 (18%)
3	SO4	D	501	-	4,4,4	0.47	0	6,6,6	0.43	0
3	SO4	C	501	-	4,4,4	0.38	0	6,6,6	0.56	0
3	SO4	C	502	-	4,4,4	0.36	0	6,6,6	0.20	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEP	E	503	-	-	4/9/9/9	-
2	PEP	D	503	-	-	4/9/9/9	-
2	PEP	C	503	-	-	4/9/9/9	-
2	PEP	B	503	-	-	4/9/9/9	-
2	PEP	A	501	-	-	4/9/9/9	-
2	PEP	F	503	-	-	4/9/9/9	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	PEP	C2-C1	-3.02	1.46	1.49
2	D	503	PEP	C2-C1	-3.01	1.46	1.49
2	C	503	PEP	C2-C1	-2.99	1.46	1.49
2	F	503	PEP	C2-C1	-2.98	1.46	1.49
2	B	503	PEP	C2-C1	-2.97	1.46	1.49
2	E	503	PEP	C2-C1	-2.95	1.46	1.49
2	E	503	PEP	O2-C2	2.46	1.45	1.39
2	C	503	PEP	O2-C2	2.46	1.45	1.39
2	F	503	PEP	O2-C2	2.45	1.45	1.39
2	D	503	PEP	O2-C2	2.44	1.45	1.39
2	B	503	PEP	O2-C2	2.43	1.45	1.39
2	A	501	PEP	O2-C2	2.41	1.45	1.39

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	503	PEP	O2'-C1-C2	3.00	119.03	113.91
2	A	501	PEP	O2'-C1-C2	2.99	119.01	113.91
2	D	503	PEP	O2'-C1-C2	2.98	119.00	113.91
2	F	503	PEP	O2'-C1-C2	2.98	118.98	113.91
2	E	503	PEP	O2'-C1-C2	2.97	118.98	113.91
2	B	503	PEP	O2'-C1-C2	2.96	118.96	113.91
2	B	503	PEP	O2-C2-C3	-2.54	119.99	124.85
2	A	501	PEP	O2-C2-C3	-2.54	119.99	124.85
2	F	503	PEP	O2-C2-C3	-2.54	120.00	124.85
2	C	503	PEP	O2-C2-C3	-2.54	120.00	124.85
2	E	503	PEP	O2-C2-C3	-2.53	120.02	124.85
2	D	503	PEP	O2-C2-C3	-2.52	120.03	124.85

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PEP	O1-C1-C2-C3
2	A	501	PEP	O1-C1-C2-O2
2	A	501	PEP	O2'-C1-C2-C3
2	A	501	PEP	O2'-C1-C2-O2
2	B	503	PEP	O1-C1-C2-C3
2	B	503	PEP	O2'-C1-C2-C3
2	C	503	PEP	O1-C1-C2-C3
2	C	503	PEP	O2'-C1-C2-C3
2	C	503	PEP	O2'-C1-C2-O2
2	D	503	PEP	O1-C1-C2-C3
2	D	503	PEP	O2'-C1-C2-C3
2	E	503	PEP	O1-C1-C2-C3
2	E	503	PEP	O1-C1-C2-O2
2	E	503	PEP	O2'-C1-C2-C3
2	E	503	PEP	O2'-C1-C2-O2
2	F	503	PEP	O1-C1-C2-C3
2	F	503	PEP	O1-C1-C2-O2
2	F	503	PEP	O2'-C1-C2-C3
2	F	503	PEP	O2'-C1-C2-O2
2	B	503	PEP	O1-C1-C2-O2
2	C	503	PEP	O1-C1-C2-O2
2	D	503	PEP	O1-C1-C2-O2
2	B	503	PEP	O2'-C1-C2-O2
2	D	503	PEP	O2'-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	503	PEP	1	0
2	D	503	PEP	1	0
2	C	503	PEP	1	0
2	B	503	PEP	1	0
2	A	501	PEP	1	0
2	F	503	PEP	1	0

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 [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	434/441 (98%)	-1.39	0 100 100	25, 53, 85, 126	4 (0%)
1	B	434/441 (98%)	-1.41	0 100 100	27, 53, 86, 125	5 (1%)
1	C	434/441 (98%)	-1.42	0 100 100	25, 53, 82, 129	5 (1%)
1	D	434/441 (98%)	-1.40	0 100 100	26, 53, 87, 123	5 (1%)
1	E	434/441 (98%)	-1.38	0 100 100	26, 53, 86, 132	5 (1%)
1	F	434/441 (98%)	-1.40	0 100 100	26, 53, 85, 131	5 (1%)
All	All	2604/2646 (98%)	-1.40	0 100 100	25, 53, 86, 132	29 (1%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no 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
2	PEP	E	503	10/10	0.98	0.04	52,66,79,93	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PEP	B	503	10/10	0.99	0.04	54,66,81,89	0
2	PEP	C	503	10/10	0.99	0.03	51,63,85,86	0
2	PEP	D	503	10/10	0.99	0.03	50,59,74,86	0
2	PEP	A	501	10/10	0.99	0.03	50,66,82,90	0
2	PEP	F	503	10/10	0.99	0.03	49,66,80,90	0
3	SO4	A	503	5/5	0.99	0.03	65,67,68,80	0
3	SO4	B	502	5/5	0.99	0.05	60,67,72,82	0
3	SO4	C	501	5/5	0.99	0.03	52,57,62,65	0
3	SO4	C	502	5/5	0.99	0.04	62,64,69,80	0
3	SO4	D	502	5/5	0.99	0.03	65,65,71,78	0
3	SO4	E	501	5/5	0.99	0.03	60,63,68,70	0
3	SO4	E	502	5/5	0.99	0.04	62,65,75,84	0
3	SO4	F	502	5/5	0.99	0.04	62,67,74,80	0
3	SO4	A	502	5/5	1.00	0.03	51,56,59,63	0
3	SO4	D	501	5/5	1.00	0.03	55,60,63,72	0
3	SO4	F	501	5/5	1.00	0.02	54,64,65,66	0
3	SO4	B	501	5/5	1.00	0.02	52,56,63,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.