



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:46 PM UTC

PDB ID : 3WX9 / pdb_00003wx9
Title : Crystal structure of Pyrococcus horikoshii kynurenine aminotransferase in complex with PMP, GLA, 4AD, 2OG, GLU and KYA
Authors : Okada, K.; Angkawidjaja, C.; Koga, Y.; Kanaya, S.
Deposited on : 2014-07-28
Resolution : 1.58 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

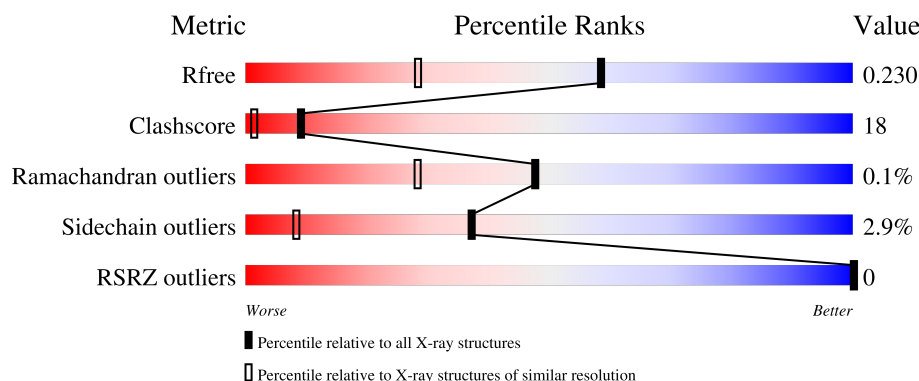
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.58 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	1094 (1.58-1.58)
Clashscore	190562	1105 (1.58-1.58)
Ramachandran outliers	187476	1082 (1.58-1.58)
Sidechain outliers	187428	1081 (1.58-1.58)
RSRZ outliers	180081	1094 (1.58-1.58)

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	448	
1	C	448	

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
3	AKG	A	502	-	X	X	-
3	AKG	C	502	-	X	X	-
4	G9A	A	503	-	-	X	-
4	G9A	C	503	-	-	X	-
5	3EE	A	504	-	-	X	-
5	3EE	C	504	-	-	X	-
6	GLU	A	505	-	-	X	-
7	KYA	C	505	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7447 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 Putative uncharacterized protein PH0207.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	S	0	0	0
			3247	2093	536	602	16			
1	C	404	Total	C	N	O	S	0	0	0
			3247	2093	536	602	16			

There are 40 discrepancies between the modelled and reference sequences:

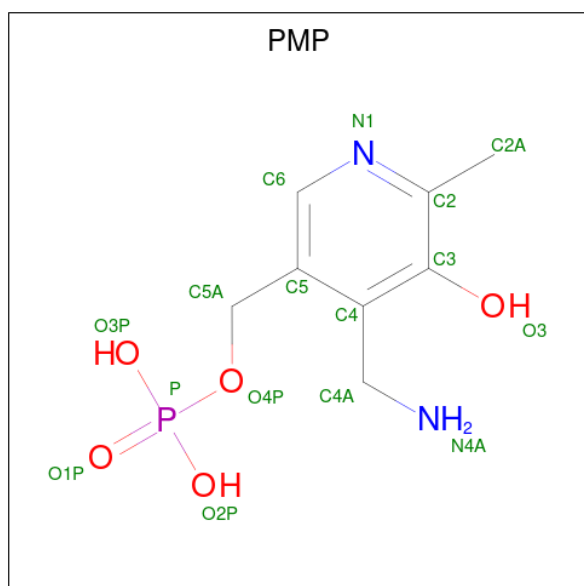
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP O57946
A	-18	GLY	-	expression tag	UNP O57946
A	-17	SER	-	expression tag	UNP O57946
A	-16	SER	-	expression tag	UNP O57946
A	-15	HIS	-	expression tag	UNP O57946
A	-14	HIS	-	expression tag	UNP O57946
A	-13	HIS	-	expression tag	UNP O57946
A	-12	HIS	-	expression tag	UNP O57946
A	-11	HIS	-	expression tag	UNP O57946
A	-10	HIS	-	expression tag	UNP O57946
A	-9	SER	-	expression tag	UNP O57946
A	-8	SER	-	expression tag	UNP O57946
A	-7	GLY	-	expression tag	UNP O57946
A	-6	LEU	-	expression tag	UNP O57946
A	-5	VAL	-	expression tag	UNP O57946
A	-4	PRO	-	expression tag	UNP O57946
A	-3	ARG	-	expression tag	UNP O57946
A	-2	GLY	-	expression tag	UNP O57946
A	-1	SER	-	expression tag	UNP O57946
A	0	HIS	-	expression tag	UNP O57946
C	-19	MET	-	expression tag	UNP O57946
C	-18	GLY	-	expression tag	UNP O57946
C	-17	SER	-	expression tag	UNP O57946
C	-16	SER	-	expression tag	UNP O57946
C	-15	HIS	-	expression tag	UNP O57946

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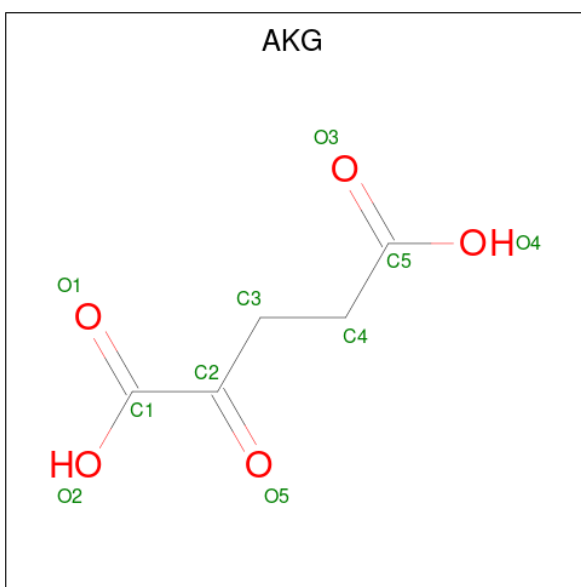
Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	HIS	-	expression tag	UNP O57946
C	-13	HIS	-	expression tag	UNP O57946
C	-12	HIS	-	expression tag	UNP O57946
C	-11	HIS	-	expression tag	UNP O57946
C	-10	HIS	-	expression tag	UNP O57946
C	-9	SER	-	expression tag	UNP O57946
C	-8	SER	-	expression tag	UNP O57946
C	-7	GLY	-	expression tag	UNP O57946
C	-6	LEU	-	expression tag	UNP O57946
C	-5	VAL	-	expression tag	UNP O57946
C	-4	PRO	-	expression tag	UNP O57946
C	-3	ARG	-	expression tag	UNP O57946
C	-2	GLY	-	expression tag	UNP O57946
C	-1	SER	-	expression tag	UNP O57946
C	0	HIS	-	expression tag	UNP O57946

- Molecule 2 is 4'-DEOXY-4'-AMINOPYRIDOXAL-5'-PHOSPHATE (CCD ID: PMP) (formula: $C_8H_{13}N_2O_5P$).



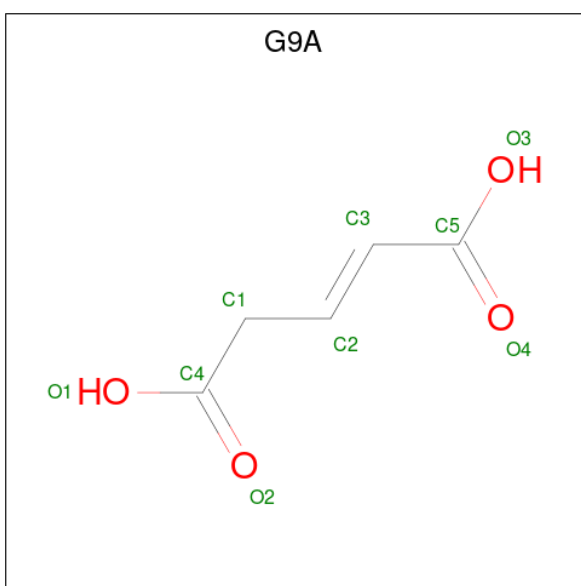
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	C	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

- Molecule 3 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: $C_5H_6O_5$).



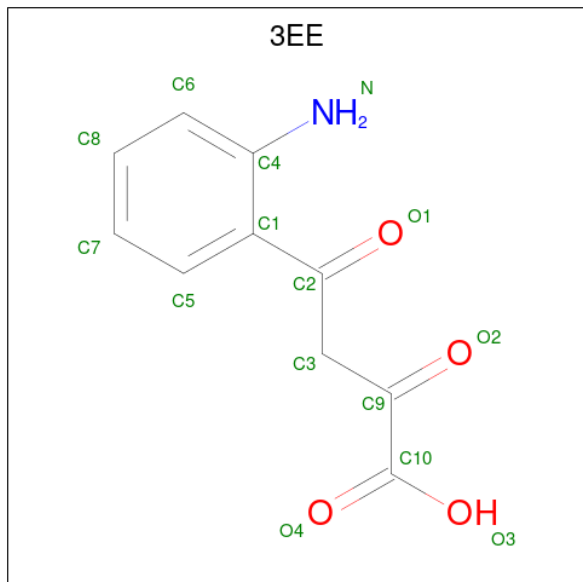
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	C	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is (2E)-pent-2-enedioic acid (CCD ID: G9A) (formula: $C_5H_6O_4$).



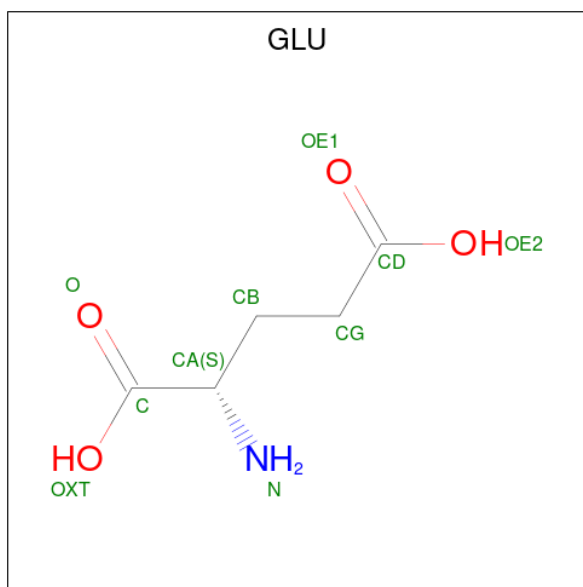
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			9	5	4		
4	C	1	Total	C	O	0	0
			9	5	4		

- Molecule 5 is 4-(2-aminophenyl)-2,4-dioxobutanoic acid (CCD ID: 3EE) (formula: $C_{10}H_9NO_4$).



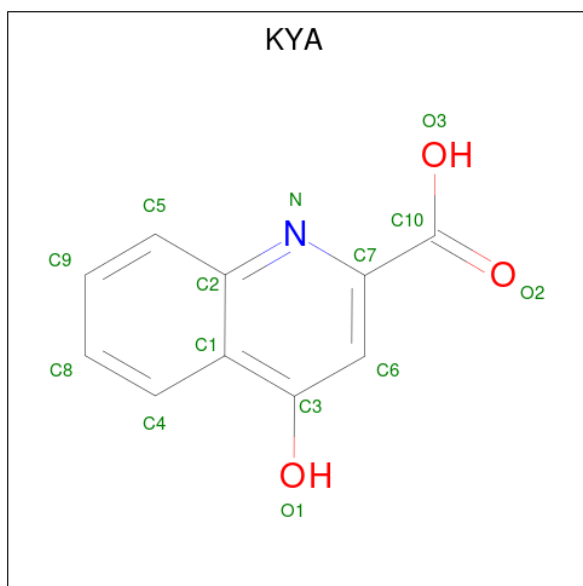
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			15	10	1	4		
5	C	1	Total	C	N	O	0	0
			15	10	1	4		

- Molecule 6 is GLUTAMIC ACID (CCD ID: GLU) (formula: $C_5H_9NO_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			10	5	1	4		

- Molecule 7 is 4-hydroxyquinoline-2-carboxylic acid (CCD ID: KYA) (formula: $C_{10}H_7NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	C	1	Total	C	N	O	0	0
			14	10	1	3		

- Molecule 8 is water.

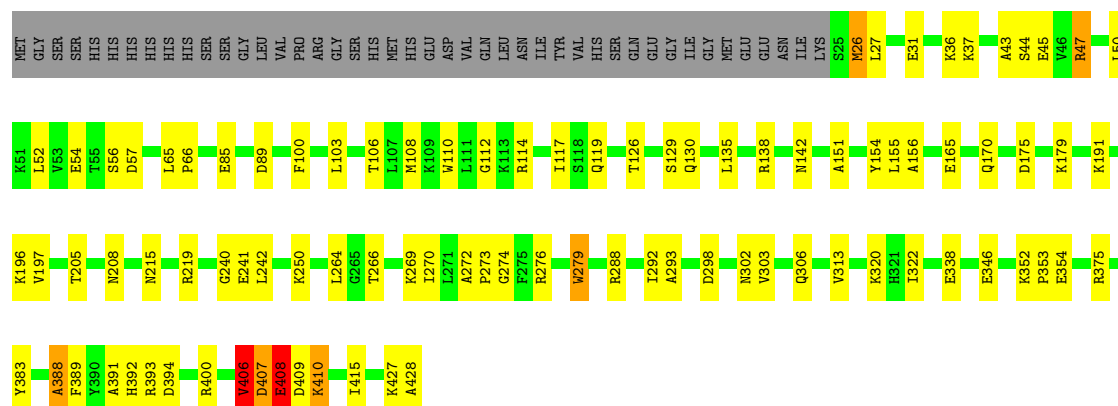
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	409	Total	O	0	0
			409	409		
8	C	420	Total	O	0	0
			420	420		

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.

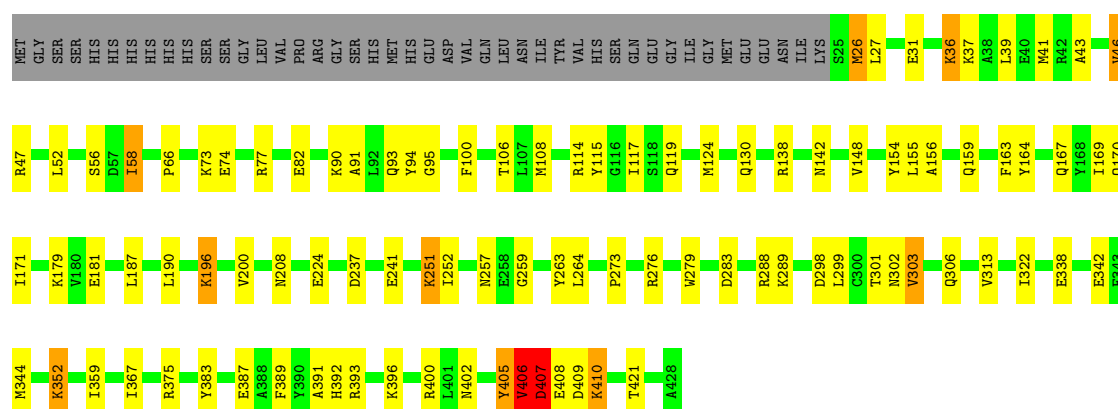
• Molecule 1: Putative uncharacterized protein PH0207

Chain A: 



• Molecule 1: Putative uncharacterized protein PH0207

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	85.77 Å 71.00 Å 136.70 Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	50.00 – 1.58 50.00 – 1.58	Depositor EDS
% Data completeness (in resolution range)	96.6 (50.00-1.58) 96.7 (50.00-1.58)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 1.57 Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.180 , 0.230 0.183 , 0.230	Depositor DCC
R_{free} test set	5458 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.480 for -h,-k,l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7447	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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: 3EE, KYA, PMP, AKG, G9A

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	1.59	19/3313 (0.6%)	1.41	17/4463 (0.4%)
1	C	1.58	22/3313 (0.7%)	1.42	15/4463 (0.3%)
All	All	1.59	41/6626 (0.6%)	1.41	32/8926 (0.4%)

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	3

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	322	ILE	CA-CB	-13.33	1.47	1.54
1	A	66	PRO	CA-C	8.82	1.63	1.52
1	C	407	ASP	CA-C	8.11	1.58	1.52
1	C	171	ILE	CA-C	7.94	1.60	1.52
1	C	387	GLU	N-CA	7.31	1.55	1.46
1	C	322	ILE	CA-CB	-7.16	1.50	1.54
1	A	313	VAL	C-O	6.68	1.31	1.24
1	A	409	ASP	C-O	6.66	1.32	1.24
1	A	298	ASP	C-O	-6.62	1.15	1.23
1	A	197	VAL	N-CA	6.50	1.54	1.46
1	C	58	ILE	CA-CB	6.42	1.60	1.54
1	A	130	GLN	N-CA	-6.29	1.38	1.46
1	A	205	THR	C-O	6.23	1.30	1.24
1	A	103	LEU	CA-CB	6.17	1.63	1.53
1	A	126	THR	C-O	-6.15	1.16	1.23
1	C	66	PRO	CA-C	6.15	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	112	GLY	N-CA	5.96	1.53	1.45
1	C	313	VAL	C-O	5.87	1.30	1.24
1	A	155	LEU	C-O	-5.81	1.17	1.24
1	A	135	LEU	N-CA	5.77	1.53	1.46
1	C	367	ILE	C-O	-5.74	1.17	1.24
1	C	82	GLU	C-O	-5.73	1.17	1.24
1	C	298	ASP	C-O	-5.73	1.17	1.24
1	C	252	ILE	C-O	5.65	1.30	1.24
1	C	124	MET	SD-CE	-5.62	1.65	1.79
1	A	354	GLU	C-N	5.61	1.39	1.33
1	C	187	LEU	N-CA	5.57	1.53	1.46
1	C	352	LYS	CA-CB	5.52	1.60	1.53
1	A	388	ALA	N-CA	5.45	1.53	1.46
1	C	402	ASN	CA-C	5.36	1.59	1.52
1	A	272	ALA	CA-CB	5.25	1.61	1.53
1	C	359	ILE	C-O	5.25	1.29	1.24
1	C	95	GLY	N-CA	5.24	1.49	1.44
1	C	252	ILE	N-CA	5.16	1.52	1.46
1	A	279	TRP	N-CA	5.15	1.52	1.45
1	A	117	ILE	CA-CB	5.13	1.60	1.54
1	C	338	GLU	C-O	5.12	1.30	1.24
1	C	410	LYS	N-CA	-5.08	1.39	1.46
1	A	353	PRO	N-CA	-5.08	1.41	1.47
1	C	130	GLN	N-CA	-5.02	1.40	1.46
1	C	117	ILE	CA-CB	5.02	1.59	1.54

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	406	VAL	N-CA-C	-8.96	95.42	108.23
1	C	409	ASP	N-CA-C	-8.34	104.25	114.75
1	C	344	MET	CA-C-N	-7.72	112.72	120.98
1	C	344	MET	C-N-CA	-7.72	112.72	120.98
1	A	298	ASP	O-C-N	-7.34	115.57	123.42
1	A	409	ASP	N-CA-C	-7.26	104.95	114.31
1	A	298	ASP	N-CA-C	-7.07	97.97	108.79
1	A	406	VAL	N-CA-C	-6.90	98.23	108.99
1	A	383	TYR	CA-C-N	-6.68	116.90	123.04
1	A	383	TYR	C-N-CA	-6.68	116.90	123.04
1	A	410	LYS	N-CA-C	-6.59	104.71	112.89
1	A	165	GLU	CA-C-N	-6.51	113.96	120.21
1	A	165	GLU	C-N-CA	-6.51	113.96	120.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	ASP	CA-C-O	6.05	125.48	118.77
1	C	74	GLU	N-CA-C	6.04	117.86	111.28
1	A	298	ASP	CB-CA-C	6.00	121.78	110.62
1	C	273	PRO	CB-CA-C	-5.84	103.15	111.68
1	A	415	ILE	N-CA-C	-5.70	104.96	110.72
1	C	383	TYR	CA-C-N	-5.52	117.28	123.02
1	C	383	TYR	C-N-CA	-5.52	117.28	123.02
1	A	129	SER	N-CA-C	5.30	117.80	111.71
1	C	264	LEU	CA-C-N	-5.27	117.78	122.47
1	C	264	LEU	C-N-CA	-5.27	117.78	122.47
1	C	171	ILE	CA-C-N	-5.22	114.40	119.78
1	C	171	ILE	C-N-CA	-5.22	114.40	119.78
1	A	273	PRO	CB-CA-C	-5.22	104.06	111.68
1	C	410	LYS	N-CA-C	-5.20	106.44	112.89
1	A	264	LEU	CA-C-N	-5.11	117.92	122.47
1	A	264	LEU	C-N-CA	-5.11	117.92	122.47
1	C	303	VAL	N-CA-CB	5.10	120.00	110.77
1	A	352	LYS	O-C-N	-5.03	116.78	121.36
1	C	298	ASP	N-CA-C	5.02	121.78	113.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	405	TYR	Peptide
1	C	406	VAL	Peptide
1	C	407	ASP	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3247	0	3306	111	0
1	C	3247	0	3307	128	0
2	A	16	0	9	0	0
2	C	16	0	9	0	0
3	A	10	0	4	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	10	0	4	13	0
4	A	9	0	4	17	0
4	C	9	0	4	18	0
5	A	15	0	8	13	0
5	C	15	0	8	13	0
6	A	10	0	5	7	0
7	C	14	0	5	16	0
8	A	409	0	0	32	0
8	C	420	0	0	36	0
All	All	7447	0	6673	243	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 18.

All (243) 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:C:208:ASN:ND2	4:C:503:G9A:H5	1.39	1.36
1:A:65:LEU:CD2	5:A:504:3EE:H6	1.64	1.28
1:A:175:ASP:HB3	8:A:903:HOH:O	1.38	1.21
5:C:504:3EE:H4	5:C:504:3EE:C9	1.56	1.19
1:C:288:ARG:HD2	8:C:785:HOH:O	1.42	1.18
1:A:65:LEU:HD21	5:A:504:3EE:H6	1.26	1.12
1:C:47:ARG:HD3	8:C:993:HOH:O	1.47	1.12
1:C:408:GLU:O	1:C:408:GLU:HG2	1.50	1.10
1:A:241:GLU:HG2	3:A:502:AKG:H42	1.14	1.09
4:C:503:G9A:H4	5:C:504:3EE:H9	1.12	1.08
1:A:250:LYS:HE3	8:A:964:HOH:O	1.55	1.03
1:C:46:VAL:HG11	7:C:505:KYA:C6	1.88	1.03
1:C:208:ASN:HD21	4:C:503:G9A:H5	0.96	1.03
1:C:208:ASN:HD21	4:C:503:G9A:C3	1.72	1.02
4:C:503:G9A:C2	5:C:504:3EE:H9	1.90	1.01
3:A:502:AKG:H32	8:A:880:HOH:O	1.60	1.01
1:C:46:VAL:CG1	7:C:505:KYA:C6	2.39	1.00
1:C:400:ARG:HH12	4:C:503:G9A:H3	1.18	1.00
1:C:170:GLN:NE2	1:C:392:HIS:H	1.58	0.99
1:A:241:GLU:CG	3:A:502:AKG:H42	1.92	0.98
4:C:503:G9A:H4	5:C:504:3EE:C5	1.93	0.98
1:A:241:GLU:HG2	3:A:502:AKG:C4	1.93	0.97
1:C:400:ARG:NH1	4:C:503:G9A:H3	1.79	0.97
1:A:408:GLU:O	1:A:408:GLU:HG3	1.65	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:SER:OG	6:A:505:GLU:HB2	1.65	0.96
1:A:400:ARG:HH12	4:A:503:G9A:H3	1.27	0.96
1:A:65:LEU:HD23	5:A:504:3EE:H6	1.47	0.94
1:A:400:ARG:NH1	4:A:503:G9A:H3	1.84	0.92
1:A:65:LEU:CD2	5:A:504:3EE:C6	2.48	0.92
1:A:65:LEU:HD23	5:A:504:3EE:C6	2.00	0.92
1:A:36:LYS:H	1:C:142:ASN:HD21	1.17	0.90
5:C:504:3EE:C9	5:C:504:3EE:N	2.35	0.89
1:A:142:ASN:HD21	1:C:36:LYS:H	1.13	0.89
1:C:46:VAL:HG11	7:C:505:KYA:H6	1.54	0.89
4:C:503:G9A:O4	5:C:504:3EE:C5	2.21	0.89
1:A:241:GLU:CG	3:A:502:AKG:C4	2.51	0.88
4:A:503:G9A:O3	5:A:504:3EE:C7	2.20	0.88
4:A:503:G9A:O3	5:A:504:3EE:C5	2.23	0.86
1:A:36:LYS:HD2	8:A:624:HOH:O	1.77	0.83
1:A:170:GLN:NE2	1:A:392:HIS:H	1.77	0.82
1:C:237:ASP:O	3:C:502:AKG:H31	1.79	0.82
1:C:237:ASP:OD2	3:C:502:AKG:H42	1.78	0.81
1:C:224:GLU:HG2	8:C:1000:HOH:O	1.80	0.81
1:C:342:GLU:HG2	8:C:686:HOH:O	1.79	0.81
1:C:400:ARG:HH12	4:C:503:G9A:C1	1.93	0.81
1:C:36:LYS:HE2	8:C:972:HOH:O	1.81	0.80
1:A:26:MET:HG2	1:C:283:ASP:OD1	1.80	0.80
1:C:46:VAL:HG13	7:C:505:KYA:C6	2.10	0.80
1:A:400:ARG:HH12	4:A:503:G9A:C1	1.93	0.79
4:C:503:G9A:O4	5:C:504:3EE:C7	2.30	0.79
1:A:36:LYS:HE3	8:A:963:HOH:O	1.81	0.79
5:C:504:3EE:H4	5:C:504:3EE:C3	1.96	0.78
1:C:159:GLN:HE22	7:C:505:KYA:H8	1.47	0.78
1:C:408:GLU:O	1:C:408:GLU:CG	2.28	0.77
8:A:950:HOH:O	1:C:26:MET:HE3	1.83	0.77
1:C:100:PHE:H	1:C:306:GLN:HE22	1.31	0.77
1:A:100:PHE:H	1:A:306:GLN:HE22	1.31	0.77
1:A:196:LYS:HE2	8:A:659:HOH:O	1.84	0.77
1:C:389:PHE:HE1	8:C:755:HOH:O	1.68	0.76
5:C:504:3EE:C7	8:C:659:HOH:O	2.35	0.75
1:C:208:ASN:ND2	4:C:503:G9A:C3	2.34	0.75
1:C:155:LEU:HD21	7:C:505:KYA:C4	2.17	0.74
4:C:503:G9A:H2	8:C:755:HOH:O	1.87	0.74
1:C:169:ILE:CD1	1:C:190:LEU:HD11	2.17	0.74
1:C:46:VAL:CG1	7:C:505:KYA:C7	2.66	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:503:G9A:C1	8:A:798:HOH:O	2.35	0.74
1:A:389:PHE:HE1	8:A:798:HOH:O	1.70	0.73
1:A:393:ARG:NH2	6:A:505:GLU:OE2	2.21	0.73
1:C:407:ASP:HB2	8:C:995:HOH:O	1.87	0.73
8:A:950:HOH:O	1:C:26:MET:CE	2.37	0.72
1:C:159:GLN:NE2	7:C:505:KYA:H8	2.05	0.72
1:A:36:LYS:CE	8:A:963:HOH:O	2.37	0.72
1:A:241:GLU:H	3:A:502:AKG:C5	2.03	0.72
5:C:504:3EE:H8	8:C:659:HOH:O	1.90	0.72
4:C:503:G9A:C1	8:C:755:HOH:O	2.38	0.71
1:C:90:LYS:HE3	8:C:856:HOH:O	1.89	0.71
1:A:44:SER:OG	6:A:505:GLU:CB	2.40	0.70
1:C:46:VAL:HG11	7:C:505:KYA:C7	2.22	0.69
1:C:299:LEU:HD23	8:C:977:HOH:O	1.91	0.69
1:C:36:LYS:CE	8:C:972:HOH:O	2.36	0.69
1:C:241:GLU:N	3:C:502:AKG:O3	2.25	0.69
1:C:241:GLU:HG2	3:C:502:AKG:O3	1.93	0.69
1:C:106:THR:HG23	8:C:669:HOH:O	1.94	0.68
1:C:170:GLN:HE21	1:C:392:HIS:H	1.41	0.68
1:C:299:LEU:CD2	8:C:977:HOH:O	2.41	0.68
4:A:503:G9A:H2	8:A:798:HOH:O	1.91	0.68
1:A:196:LYS:HD2	8:A:811:HOH:O	1.93	0.68
1:A:288:ARG:NH2	1:C:43:ALA:HB2	2.10	0.67
1:C:179:LYS:NZ	8:C:800:HOH:O	2.27	0.66
1:C:100:PHE:H	1:C:306:GLN:NE2	1.92	0.66
1:A:241:GLU:HB2	3:A:502:AKG:H41	1.77	0.66
1:A:31:GLU:HG3	8:A:753:HOH:O	1.95	0.66
1:A:100:PHE:H	1:A:306:GLN:NE2	1.92	0.66
1:A:44:SER:HB2	6:A:505:GLU:HG2	1.78	0.66
1:C:36:LYS:HE3	1:C:36:LYS:HA	1.77	0.66
1:C:208:ASN:HD22	4:C:503:G9A:H5	1.55	0.65
1:C:47:ARG:HD2	8:C:901:HOH:O	1.94	0.65
1:C:352:LYS:NZ	8:C:984:HOH:O	2.30	0.65
1:A:138:ARG:HG3	1:C:163:PHE:CE1	2.31	0.65
1:C:170:GLN:HE22	1:C:392:HIS:H	1.42	0.65
1:A:241:GLU:CG	3:A:502:AKG:H41	2.27	0.64
1:A:303:VAL:HG23	8:A:657:HOH:O	1.98	0.64
1:A:320:LYS:HE2	8:A:898:HOH:O	1.97	0.63
1:C:237:ASP:OD2	3:C:502:AKG:C4	2.46	0.63
1:C:93:GLN:O	1:C:303:VAL:HG11	1.98	0.62
1:C:405:TYR:O	1:C:406:VAL:CG1	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:ASN:HD21	4:A:503:G9A:C2	2.12	0.62
1:A:241:GLU:CB	3:A:502:AKG:C4	2.77	0.62
1:C:46:VAL:HG11	7:C:505:KYA:C10	2.30	0.61
1:A:270:ILE:HG21	3:A:502:AKG:H41	1.82	0.61
1:A:400:ARG:HH12	4:A:503:G9A:C2	2.13	0.61
1:C:169:ILE:HD11	1:C:190:LEU:HD11	1.80	0.61
5:C:504:3EE:N	5:C:504:3EE:O2	2.32	0.61
1:A:270:ILE:HD13	3:A:502:AKG:H31	1.83	0.61
1:A:154:TYR:HE1	4:A:503:G9A:H5	1.66	0.61
1:A:241:GLU:HB2	3:A:502:AKG:C4	2.30	0.60
1:A:44:SER:CB	6:A:505:GLU:HG2	2.31	0.60
1:A:406:VAL:HG22	1:A:410:LYS:HB2	1.84	0.60
1:A:26:MET:HE2	1:C:283:ASP:HA	1.83	0.59
1:A:393:ARG:HH22	6:A:505:GLU:CD	2.11	0.59
1:A:47:ARG:NH1	8:A:1005:HOH:O	2.34	0.59
1:A:56:SER:HB2	8:A:980:HOH:O	2.01	0.58
1:A:320:LYS:CE	8:A:898:HOH:O	2.50	0.58
1:C:288:ARG:NH1	8:C:785:HOH:O	2.36	0.58
1:C:405:TYR:O	1:C:405:TYR:CD2	2.57	0.58
1:A:37:LYS:HG2	8:A:871:HOH:O	2.03	0.57
1:C:405:TYR:O	1:C:406:VAL:HG13	2.04	0.57
1:A:208:ASN:HD21	4:A:503:G9A:C3	2.18	0.57
1:C:375:ARG:HG3	8:C:690:HOH:O	2.04	0.57
1:C:393:ARG:HH22	7:C:505:KYA:C10	2.18	0.57
1:C:46:VAL:HG12	8:C:1010:HOH:O	2.05	0.57
1:A:208:ASN:HD21	4:A:503:G9A:C1	2.18	0.57
5:A:504:3EE:H7	1:C:94:TYR:CD2	2.40	0.56
1:C:410:LYS:N	8:C:995:HOH:O	2.27	0.55
1:A:43:ALA:HB2	1:C:288:ARG:NH2	2.21	0.55
1:A:65:LEU:HD21	5:A:504:3EE:C6	2.17	0.54
1:A:138:ARG:HG3	1:C:163:PHE:CZ	2.42	0.54
1:A:138:ARG:HD3	1:C:163:PHE:CE1	2.42	0.54
1:A:241:GLU:CB	3:A:502:AKG:H41	2.37	0.54
4:A:503:G9A:H4	5:A:504:3EE:O1	2.07	0.54
1:C:196:LYS:HE2	8:C:957:HOH:O	2.08	0.53
1:A:242:LEU:HD11	1:A:269:LYS:O	2.08	0.53
1:C:170:GLN:NE2	1:C:392:HIS:N	2.42	0.53
1:A:45:GLU:HB2	8:A:824:HOH:O	2.08	0.53
1:C:91:ALA:O	1:C:303:VAL:HG13	2.09	0.52
1:C:154:TYR:CZ	1:C:156:ALA:HB3	2.45	0.52
1:A:276:ARG:HG2	1:C:302:ASN:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:LYS:NZ	8:A:745:HOH:O	2.41	0.51
1:C:251:LYS:CE	3:C:502:AKG:O4	2.59	0.51
1:A:170:GLN:HE21	1:A:391:ALA:N	2.09	0.50
1:A:154:TYR:CE1	4:A:503:G9A:H5	2.45	0.50
1:A:240:GLY:N	3:A:502:AKG:O3	2.45	0.50
1:A:302:ASN:HA	1:C:276:ARG:HG2	1.92	0.50
1:C:263:TYR:OH	3:C:502:AKG:H42	2.12	0.49
1:A:407:ASP:HB2	1:A:410:LYS:HG2	1.95	0.49
1:A:47:ARG:O	1:A:47:ARG:NH2	2.43	0.49
1:A:407:ASP:N	1:A:407:ASP:OD1	2.45	0.49
1:C:90:LYS:CE	8:C:856:HOH:O	2.56	0.49
1:C:400:ARG:HH12	4:C:503:G9A:C2	2.25	0.49
1:A:241:GLU:CB	3:A:502:AKG:H42	2.39	0.49
1:A:110:TRP:CZ2	1:A:114:ARG:HD3	2.48	0.49
1:C:46:VAL:CG1	7:C:505:KYA:C10	2.90	0.48
1:C:108:MET:HB3	1:C:119:GLN:HE22	1.77	0.48
1:A:208:ASN:ND2	4:A:503:G9A:C3	2.76	0.48
1:C:208:ASN:HD21	4:C:503:G9A:C1	2.26	0.48
1:A:191:LYS:NZ	8:A:969:HOH:O	2.46	0.48
1:A:106:THR:HG23	8:A:684:HOH:O	2.14	0.48
1:C:170:GLN:HE21	1:C:391:ALA:HB3	1.79	0.48
1:A:119:GLN:NE2	8:A:825:HOH:O	2.46	0.48
1:A:108:MET:HB3	1:A:119:GLN:HE22	1.79	0.47
1:A:43:ALA:HB2	1:C:288:ARG:HH21	1.79	0.47
1:C:208:ASN:HD21	4:C:503:G9A:C2	2.25	0.47
1:C:393:ARG:NH2	7:C:505:KYA:C10	2.77	0.47
1:A:26:MET:HG3	1:C:259:GLY:HA3	1.96	0.47
1:C:115:TYR:OH	3:C:502:AKG:C5	2.63	0.47
1:C:393:ARG:HH22	7:C:505:KYA:C7	2.28	0.47
1:C:114:ARG:HG2	1:C:115:TYR:CE1	2.50	0.46
1:C:159:GLN:NE2	7:C:505:KYA:C8	2.77	0.46
1:C:251:LYS:HE3	3:C:502:AKG:O4	2.15	0.46
1:C:138:ARG:HG2	1:C:164:TYR:OH	2.15	0.46
1:A:375:ARG:HG3	8:A:710:HOH:O	2.15	0.45
1:A:170:GLN:NE2	1:A:391:ALA:N	2.64	0.45
5:C:504:3EE:N	5:C:504:3EE:C3	2.67	0.45
1:A:179:LYS:NZ	8:A:764:HOH:O	2.49	0.45
1:A:388:ALA:CB	6:A:505:GLU:HA	2.47	0.45
1:A:89:ASP:OD1	1:C:73:LYS:NZ	2.48	0.45
1:C:36:LYS:HD2	8:C:610:HOH:O	2.16	0.45
1:C:375:ARG:HG2	1:C:421:THR:HG23	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:LEU:O	1:A:54:GLU:HG2	2.17	0.45
1:A:292:ILE:HG21	1:C:41:MET:HB3	1.99	0.45
1:C:405:TYR:C	1:C:406:VAL:HG13	2.42	0.45
1:A:142:ASN:HD21	1:C:36:LYS:N	1.97	0.45
1:A:65:LEU:HD23	5:A:504:3EE:C8	2.43	0.44
1:C:237:ASP:O	3:C:502:AKG:C3	2.57	0.44
1:C:407:ASP:N	8:C:995:HOH:O	2.42	0.44
1:A:138:ARG:HD2	1:A:293:ALA:HB1	1.99	0.44
1:C:303:VAL:HG12	8:C:739:HOH:O	2.18	0.44
1:C:405:TYR:O	1:C:406:VAL:HG12	2.18	0.43
1:A:138:ARG:CZ	1:A:138:ARG:HB2	2.48	0.43
1:C:167:GLN:CD	8:C:941:HOH:O	2.61	0.43
1:C:170:GLN:HE21	1:C:392:HIS:N	2.12	0.43
1:A:406:VAL:CG2	1:A:410:LYS:HB2	2.48	0.43
1:C:36:LYS:HE3	1:C:39:LEU:HD12	2.00	0.43
1:A:427:LYS:O	1:A:428:ALA:O	2.37	0.43
1:C:279:TRP:HZ2	8:C:894:HOH:O	2.01	0.43
1:C:405:TYR:O	1:C:405:TYR:CG	2.68	0.43
1:C:169:ILE:HD12	1:C:190:LEU:HD11	1.97	0.43
5:A:504:3EE:H9	8:A:641:HOH:O	2.17	0.43
3:C:502:AKG:O5	8:C:900:HOH:O	2.21	0.43
1:A:288:ARG:NH2	1:C:43:ALA:CB	2.78	0.43
1:C:37:LYS:HD2	8:C:627:HOH:O	2.18	0.43
1:C:31:GLU:H	1:C:31:GLU:CD	2.27	0.43
1:A:154:TYR:CZ	1:A:156:ALA:HB3	2.54	0.43
4:A:503:G9A:H3	8:A:798:HOH:O	2.12	0.42
1:A:276:ARG:CG	1:C:302:ASN:HA	2.49	0.42
1:C:196:LYS:HZ2	1:C:196:LYS:HG2	1.45	0.42
1:C:389:PHE:CE1	8:C:755:HOH:O	2.55	0.42
5:A:504:3EE:C5	5:A:504:3EE:O4	2.67	0.42
1:A:394:ASP:OD1	1:A:394:ASP:N	2.46	0.42
1:C:410:LYS:HB2	8:C:995:HOH:O	2.19	0.42
1:A:338:GLU:HG3	8:A:742:HOH:O	2.20	0.42
1:A:266:THR:O	3:A:502:AKG:O2	2.38	0.42
1:C:46:VAL:CG1	7:C:505:KYA:H6	2.27	0.42
1:A:389:PHE:CE1	8:A:798:HOH:O	2.57	0.42
1:A:47:ARG:HH22	1:A:50:LEU:HB2	1.85	0.42
1:C:170:GLN:HE21	1:C:391:ALA:N	2.18	0.41
1:C:289:LYS:HD3	1:C:289:LYS:HA	1.84	0.41
1:A:279:TRP:HZ2	8:A:878:HOH:O	2.03	0.41
1:C:263:TYR:HH	3:C:502:AKG:H42	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:GLN:HE22	1:A:392:HIS:H	1.63	0.41
1:A:302:ASN:HA	1:C:276:ARG:CG	2.51	0.41
1:C:251:LYS:NZ	3:C:502:AKG:O4	2.53	0.41
1:C:392:HIS:HD2	8:C:768:HOH:O	2.02	0.41
1:A:85:GLU:HG3	1:C:77:ARG:HH12	1.85	0.41
1:A:274:GLY:HA2	1:C:303:VAL:HG12	2.02	0.41
1:A:276:ARG:HH11	1:A:276:ARG:HD2	1.73	0.41
1:A:215:ASN:O	1:A:219:ARG:HG3	2.21	0.41
1:C:148:VAL:HB	1:C:200:VAL:HG22	2.03	0.40
1:C:56:SER:OG	1:C:58:ILE:HD12	2.21	0.40
5:C:504:3EE:H1	8:C:1017:HOH:O	2.21	0.40
1:A:151:ALA:HB2	1:A:170:GLN:HB3	2.03	0.40
1:A:208:ASN:HD21	4:A:503:G9A:H2	1.85	0.40
1:C:301:THR:O	1:C:302:ASN:C	2.62	0.40

There are no symmetry-related clashes.

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	402/448 (90%)	395 (98%)	6 (2%)	1 (0%)	43	26
1	C	402/448 (90%)	388 (96%)	14 (4%)	0	100	100
All	All	804/896 (90%)	783 (97%)	20 (2%)	1 (0%)	48	28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	408	GLU

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	349/388 (90%)	340 (97%)	9 (3%)	40	11
1	C	349/388 (90%)	338 (97%)	11 (3%)	34	7
All	All	698/776 (90%)	678 (97%)	20 (3%)	37	8

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	MET
1	A	27	LEU
1	A	47	ARG
1	A	52	LEU
1	A	57	ASP
1	A	346	GLU
1	A	406	VAL
1	A	407	ASP
1	A	408	GLU
1	C	26	MET
1	C	27	LEU
1	C	36	LYS
1	C	46	VAL
1	C	52	LEU
1	C	181	GLU
1	C	196	LYS
1	C	251	LYS
1	C	257	ASN
1	C	396	LYS
1	C	407	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	GLN
1	A	142	ASN

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Mol	Chain	Res	Type
1	A	167	GLN
1	A	170	GLN
1	A	306	GLN
1	C	119	GLN
1	C	142	ASN
1	C	170	GLN
1	C	306	GLN

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](#)

10 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	$\# Z > 2$
7	KYA	C	505	-	15,15,15	1.65	2 (13%)	20,21,21	1.47	3 (15%)
2	PMP	C	501	-	16,16,16	0.97	1 (6%)	22,23,23	1.02	2 (9%)
4	G9A	A	503	-	8,8,8	0.61	0	8,9,9	1.58	1 (12%)
3	AKG	C	502	-	9,9,9	3.33	5 (55%)	11,11,11	2.48	5 (45%)
3	AKG	A	502	-	9,9,9	3.48	6 (66%)	11,11,11	2.36	5 (45%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	3EE	C	504	-	15,15,15	2.25	4 (26%)	17,20,20	1.03	2 (11%)
2	PMP	A	501	-	16,16,16	1.64	3 (18%)	22,23,23	1.55	4 (18%)
6	GLU	A	505	-	8,9,9	1.67	2 (25%)	8,11,11	0.75	0
5	3EE	A	504	-	15,15,15	2.04	2 (13%)	17,20,20	2.16	7 (41%)
4	G9A	C	503	-	8,8,8	1.60	2 (25%)	8,9,9	1.56	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
7	KYA	C	505	-	-	4/4/4/4	0/2/2/2
2	PMP	C	501	-	-	3/8/8/8	0/1/1/1
4	G9A	A	503	-	-	2/6/6/6	-
3	AKG	C	502	-	-	3/9/9/9	-
3	AKG	A	502	-	-	7/9/9/9	-
5	3EE	C	504	-	-	2/12/12/12	0/1/1/1
2	PMP	A	501	-	-	3/8/8/8	0/1/1/1
6	GLU	A	505	-	-	2/9/9/9	-
5	3EE	A	504	-	-	6/12/12/12	0/1/1/1
4	G9A	C	503	-	-	2/6/6/6	-

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	504	3EE	C9-C10	-5.56	1.45	1.53
3	A	502	AKG	O4-C5	-5.55	1.12	1.30
3	C	502	AKG	C2-C1	-5.29	1.45	1.53
3	C	502	AKG	O2-C1	-5.20	1.16	1.30
5	A	504	3EE	C1-C4	5.01	1.49	1.41
3	A	502	AKG	C2-C1	-4.86	1.46	1.53
5	C	504	3EE	C1-C4	4.78	1.48	1.41
5	C	504	3EE	C9-C10	-4.71	1.46	1.53
3	A	502	AKG	O2-C1	-4.46	1.18	1.30
5	C	504	3EE	O4-C10	4.40	1.33	1.22
3	C	502	AKG	O4-C5	-4.03	1.17	1.30
3	A	502	AKG	C3-C2	-3.94	1.46	1.51
7	C	505	KYA	C1-C2	3.81	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	502	AKG	C3-C2	-3.61	1.47	1.51
2	A	501	PMP	O4P-C5A	-3.53	1.31	1.44
4	C	503	G9A	O2-C4	3.45	1.33	1.22
3	C	502	AKG	O5-C2	-3.27	1.16	1.23
2	A	501	PMP	P-O2P	-3.19	1.42	1.54
7	C	505	KYA	C3-C1	3.08	1.48	1.42
3	A	502	AKG	O1-C1	-2.99	1.15	1.22
5	C	504	3EE	O3-C10	-2.98	1.22	1.30
6	A	505	GLU	OE2-CD	-2.97	1.21	1.30
2	A	501	PMP	C3-C2	-2.61	1.38	1.41
2	C	501	PMP	C2-N1	2.61	1.38	1.33
3	A	502	AKG	O3-C5	-2.53	1.13	1.22
4	C	503	G9A	O1-C4	-2.52	1.22	1.30
6	A	505	GLU	CB-CG	-2.10	1.46	1.52

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	502	AKG	O1-C1-C2	-5.34	115.17	121.81
3	A	502	AKG	O5-C2-C1	4.73	126.43	119.67
2	A	501	PMP	O2P-P-O4P	4.07	117.27	106.67
5	A	504	3EE	O3-C10-C9	3.85	124.26	113.59
5	A	504	3EE	C6-C4-C1	-3.83	114.06	118.16
3	C	502	AKG	O2-C1-C2	3.53	123.38	113.59
3	A	502	AKG	O4-C5-C4	3.32	124.49	114.00
7	C	505	KYA	C1-C2-N	-3.15	119.47	122.80
5	A	504	3EE	C7-C8-C6	2.97	123.90	120.24
3	A	502	AKG	O4-C5-O3	-2.95	115.73	123.33
7	C	505	KYA	C7-N-C2	2.90	121.94	117.56
3	C	502	AKG	C4-C3-C2	-2.88	107.50	112.91
5	A	504	3EE	O4-C10-C9	-2.88	118.23	121.81
2	A	501	PMP	C5A-C5-C6	-2.81	114.78	119.36
3	C	502	AKG	C3-C2-C1	2.80	120.61	115.86
7	C	505	KYA	O1-C3-C1	2.75	121.12	116.42
5	A	504	3EE	C8-C7-C5	-2.70	116.91	120.24
5	A	504	3EE	O3-C10-O4	-2.69	117.50	123.90
5	C	504	3EE	O3-C10-C9	2.56	120.67	113.59
4	A	503	G9A	C2-C1-C4	-2.54	109.43	113.83
3	A	502	AKG	O1-C1-C2	2.50	124.91	121.81
4	C	503	G9A	C2-C1-C4	-2.49	109.51	113.83
2	A	501	PMP	C3-C4-C5	-2.45	116.51	118.73
3	A	502	AKG	O5-C2-C3	-2.42	115.98	121.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	501	PMP	C5-C6-N1	-2.30	120.08	123.83
2	C	501	PMP	C6-C5-C4	2.25	119.76	118.06
3	C	502	AKG	C3-C4-C5	-2.20	107.83	113.67
5	A	504	3EE	C3-C2-C1	-2.19	115.23	118.95
2	A	501	PMP	C4A-C4-C5	2.08	124.43	120.27
5	C	504	3EE	O3-C10-O4	-2.02	119.10	123.90

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	PMP	C5A-O4P-P-O1P
2	A	501	PMP	C5A-O4P-P-O2P
2	A	501	PMP	C5A-O4P-P-O3P
2	C	501	PMP	C5A-O4P-P-O1P
2	C	501	PMP	C5A-O4P-P-O2P
2	C	501	PMP	C5A-O4P-P-O3P
3	A	502	AKG	C1-C2-C3-C4
3	A	502	AKG	C2-C3-C4-C5
3	C	502	AKG	C1-C2-C3-C4
5	A	504	3EE	O1-C2-C3-C9
5	A	504	3EE	C1-C2-C3-C9
5	C	504	3EE	C4-C1-C2-O1
5	C	504	3EE	C4-C1-C2-C3
6	A	505	GLU	C-CA-CB-CG
7	C	505	KYA	O2-C10-C7-N
7	C	505	KYA	O3-C10-C7-N
7	C	505	KYA	O2-C10-C7-C6
7	C	505	KYA	O3-C10-C7-C6
4	A	503	G9A	C2-C3-C5-O4
4	A	503	G9A	C2-C3-C5-O3
5	A	504	3EE	C5-C1-C2-C3
3	C	502	AKG	C2-C3-C4-C5
5	A	504	3EE	C5-C1-C2-O1
5	A	504	3EE	C4-C1-C2-C3
5	A	504	3EE	C4-C1-C2-O1
6	A	505	GLU	N-CA-CB-CG
3	A	502	AKG	O5-C2-C3-C4
3	A	502	AKG	O2-C1-C2-O5
4	C	503	G9A	C2-C1-C4-O1
4	C	503	G9A	C4-C1-C2-C3
3	C	502	AKG	O5-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
3	A	502	AKG	O1-C1-C2-O5
3	A	502	AKG	C3-C4-C5-O4
3	A	502	AKG	C3-C4-C5-O3

There are no ring outliers.

8 monomers are involved in 105 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	505	KYA	16	0
4	A	503	G9A	17	0
3	C	502	AKG	13	0
3	A	502	AKG	16	0
5	C	504	3EE	13	0
6	A	505	GLU	7	0
5	A	504	3EE	13	0
4	C	503	G9A	18	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	404/448 (90%)	-0.90	0 100 100	15, 21, 41, 59	0
1	C	404/448 (90%)	-0.89	0 100 100	14, 21, 41, 59	0
All	All	808/896 (90%)	-0.90	0 100 100	14, 21, 41, 59	0

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
6	GLU	A	505	10/10	0.97	0.05	34,38,43,45	0
7	KYA	C	505	14/14	0.97	0.06	35,40,43,50	0
4	G9A	C	503	9/9	0.98	0.06	24,37,44,47	0
5	3EE	C	504	15/15	0.98	0.06	34,41,44,48	0
3	AKG	C	502	10/10	0.98	0.06	24,37,42,46	0
4	G9A	A	503	9/9	0.98	0.06	20,34,43,44	0
5	3EE	A	504	15/15	0.99	0.05	30,38,46,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PMP	A	501	16/16	0.99	0.04	15,19,24,32	0
2	PMP	C	501	16/16	0.99	0.03	16,18,23,27	0
3	AKG	A	502	10/10	0.99	0.06	19,35,41,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.