Full wwPDB X-ray Structure Validation Report ⓘ

Sep 13, 2020 – 01:43 PM BST

PDB ID	:	3WX9
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 following versions of software and data (see references ⓘ) were used in the production of this report:

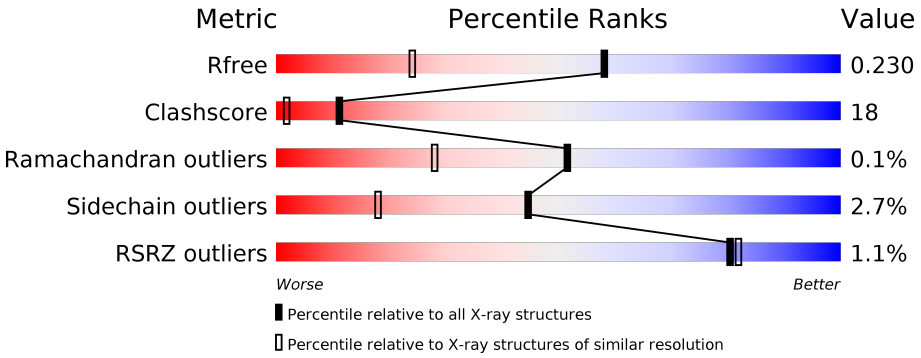
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.14.4.dev1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.14.4.dev1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	5534 (1.60-1.56)
Clashscore	141614	5861 (1.60-1.56)
Ramachandran outliers	138981	5708 (1.60-1.56)
Sidechain outliers	138945	5703 (1.60-1.56)
RSRZ outliers	127900	5431 (1.60-1.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria 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 <=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	% 73% 16% • 10%
1	C	448	% 73% 15% •• 10%

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	-
3	AKG	C	502	-	-	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 (i)

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:

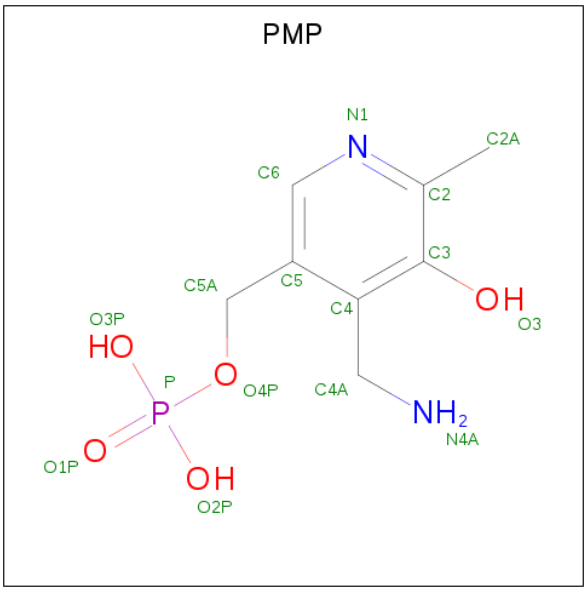
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP O57946
A	-18	GLY	-	EXPRESSION TAG	UNP O57946
A	-17	SER	-	EXPRESSION TAG	UNP O57946
A	-16	SER	-	EXPRESSION TAG	UNP O57946
A	-15	HIS	-	EXPRESSION TAG	UNP O57946
A	-14	HIS	-	EXPRESSION TAG	UNP O57946
A	-13	HIS	-	EXPRESSION TAG	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

Continued on next page...

Continued from previous page...

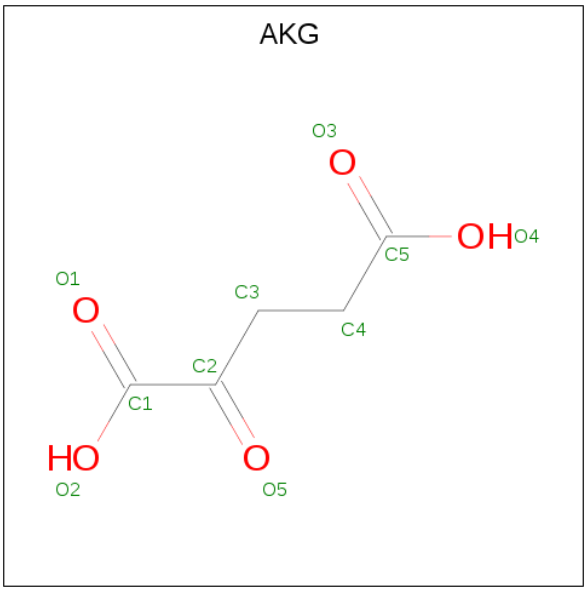
Chain	Residue	Modelled	Actual	Comment	Reference
C	-14	HIS	-	EXPRESSION TAG	UNP O57946
C	-13	HIS	-	EXPRESSION TAG	UNP O57946
C	-12	HIS	-	EXPRESSION TAG	UNP O57946
C	-11	HIS	-	EXPRESSION TAG	UNP O57946
C	-10	HIS	-	EXPRESSION TAG	UNP O57946
C	-9	SER	-	EXPRESSION TAG	UNP O57946
C	-8	SER	-	EXPRESSION TAG	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 (three-letter code: PMP) (formula: $C_8H_{13}N_2O_5P$).



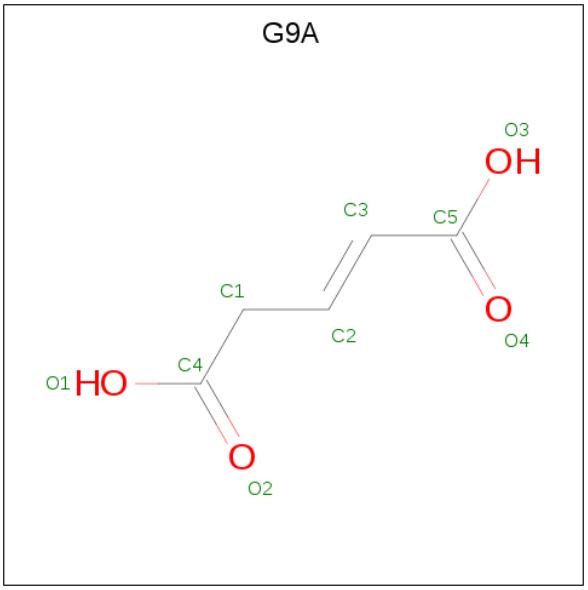
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	2	5	1		
2	C	1	Total	C	N	O	P	0	0
			16	8	2	5	1		

- Molecule 3 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $C_5H_6O_5$).



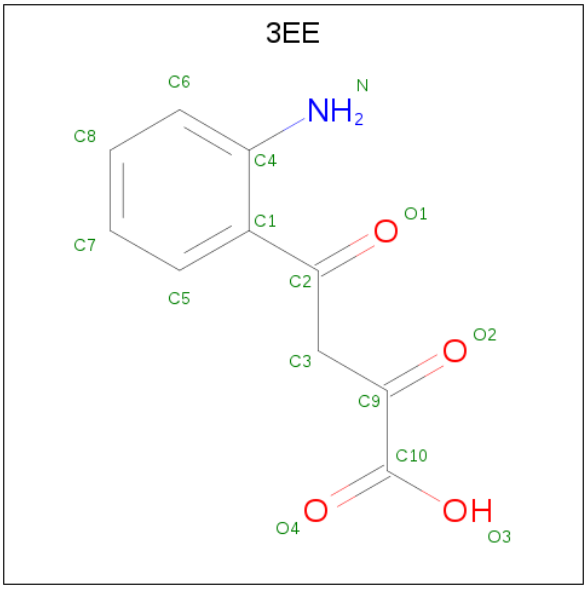
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 10 5 5	0	0
3	C	1	Total C O 10 5 5	0	0

- Molecule 4 is (2E)-pent-2-enedioic acid (three-letter code: G9A) (formula: $C_5H_6O_4$).



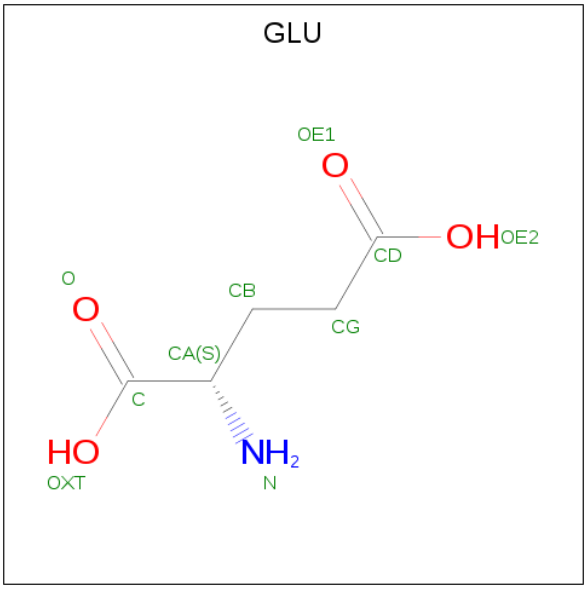
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 9 5 4	0	0
4	C	1	Total C O 9 5 4	0	0

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



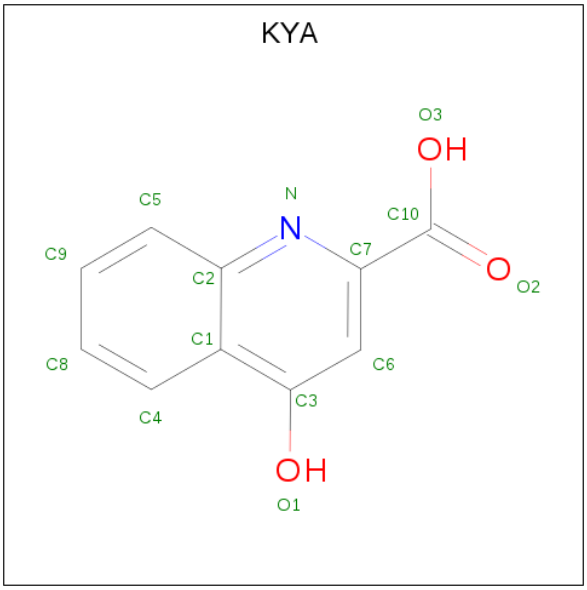
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			15	10	1	4		
5	C	1	Total	C	N	O	0	0
			15	10	1	4		

- Molecule 6 is GLUTAMIC ACID (three-letter code: 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 (three-letter code: 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.

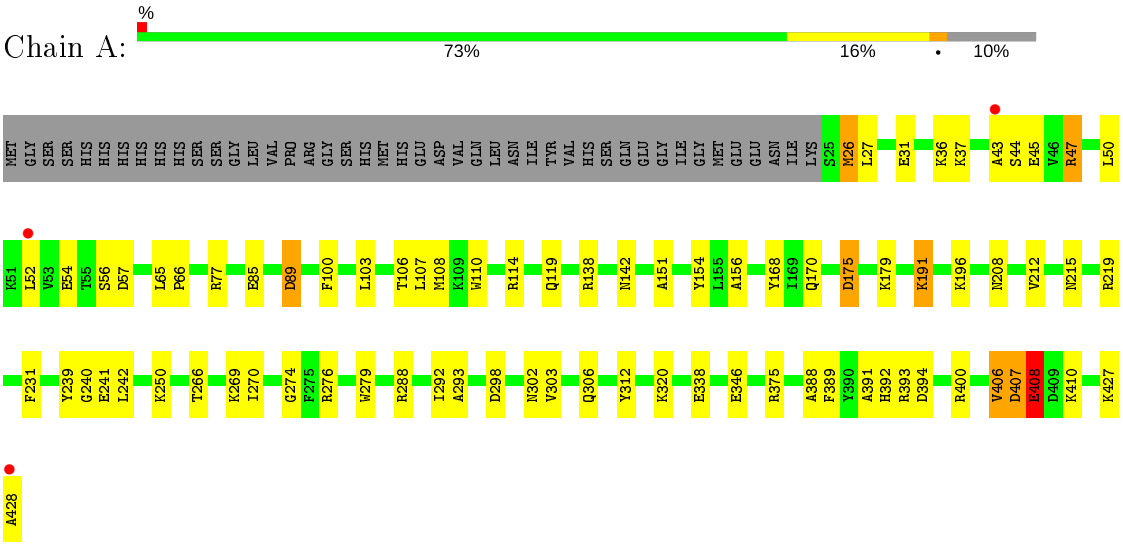
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	409	Total	O	0	0
			409	409		
8	C	420	Total	O	0	0
			420	420		

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.

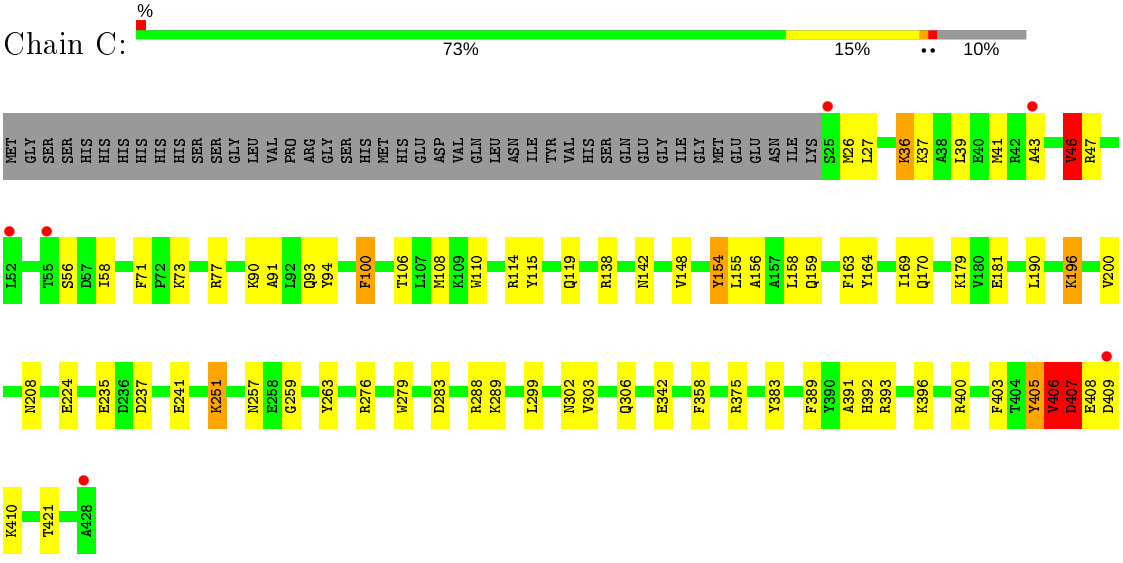
- Molecule 1: Putative uncharacterized protein PH0207

Chain A:



- Molecule 1: Putative uncharacterized protein PH0207

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	85.77Å 71.00Å 136.70Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	50.00 – 1.58 27.35 – 1.58	Depositor EDS
% Data completeness (in resolution range)	96.6 (50.00-1.58) 96.5 (27.35-1.58)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 1.57Å)	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 (5.00%)	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)	0.38 , 43.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AKG, KYA, PMP, 3EE, 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	1.33	4/3313 (0.1%)	1.20	9/4463 (0.2%)
1	C	1.36	6/3313 (0.2%)	1.21	7/4463 (0.2%)
All	All	1.34	10/6626 (0.2%)	1.20	16/8926 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	46	VAL	CB-CG1	-5.77	1.40	1.52
1	A	312	TYR	CE1-CZ	5.74	1.46	1.38
1	A	212	VAL	CB-CG2	5.62	1.64	1.52
1	C	403	PHE	CE1-CZ	5.28	1.47	1.37
1	C	110	TRP	CB-CG	5.17	1.59	1.50
1	C	358	PHE	CE1-CZ	5.15	1.47	1.37
1	C	383	TYR	CE2-CZ	5.10	1.45	1.38
1	C	71	PHE	CE2-CZ	5.10	1.47	1.37
1	A	66	PRO	CA-C	5.09	1.63	1.52
1	A	239	TYR	CG-CD1	5.08	1.45	1.39

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	312	TYR	CB-CG-CD2	-5.97	117.42	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	100	PHE	CB-CG-CD2	-5.95	116.63	120.80
1	C	407	ASP	CB-CG-OD1	5.94	123.65	118.30
1	A	107	LEU	CB-CG-CD1	-5.90	100.97	111.00
1	A	103	LEU	CB-CG-CD2	-5.88	101.01	111.00
1	C	406	VAL	N-CA-C	-5.77	95.42	111.00
1	A	298	ASP	CB-CA-C	5.69	121.78	110.40
1	C	154	TYR	CZ-CE2-CD2	-5.64	114.72	119.80
1	A	191	LYS	CD-CE-NZ	-5.52	99.00	111.70
1	C	158	LEU	CB-CG-CD1	-5.37	101.87	111.00
1	C	409	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	175	ASP	CB-CG-OD1	5.26	123.04	118.30
1	C	235	GLU	OE1-CD-OE2	5.12	129.44	123.30
1	A	89	ASP	CB-CG-OD1	5.08	122.88	118.30
1	A	231	PHE	CB-CG-CD2	-5.04	117.27	120.80
1	A	168	TYR	CB-CG-CD2	-5.01	118.00	121.00

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

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	122	0
2	A	16	0	9	0	0
2	C	16	0	9	0	0
3	A	10	0	4	16	0
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

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	15	0	8	13	0
6	A	10	0	5	8	0
7	C	14	0	5	16	0
8	A	409	0	0	32	0
8	C	420	0	0	34	0
All	All	7447	0	6673	238	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 (238) 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:C9	5:C:504:3EE:H4	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:HG2	1:C:408:GLU:O	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:208:ASN:HD21	4:C:503:G9A:H5	0.96	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: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:400:ARG:HH12	4:C:503:G9A:H3	1.18	1.00
1:C:46:VAL:CG1	7:C:505:KYA:C6	2.39	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:HG3	1:A:408:GLU:O	1.65	0.96
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C3	5:C:504:3EE:H4	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
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:159:GLN:NE2	7:C:505:KYA:H8	2.05	0.72
1:A:241:GLU:H	3:A:502:AKG:C5	2.03	0.72
1:A:36:LYS:CE	8:A:963:HOH:O	2.37	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
8:A:950:HOH:O	1:C:26:MET:HE3	1.91	0.69
1:C:299:LEU:HD23	8:C:977:HOH:O	1.91	0.69
1:C:241:GLU:N	3:C:502:AKG:O3	2.25	0.69
1:C:36:LYS:CE	8:C:972:HOH:O	2.36	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: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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:ILE:HD11	1:C:190:LEU:HD11	1.80	0.61
5:C:504:3EE:O2	5:C:504:3EE:N	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:47:ARG:NH1	8:A:1005:HOH:O	2.34	0.59
1:A:320:LYS:CE	8:A:898:HOH:O	2.50	0.58
1:A:56:SER:HB2	8:A:980:HOH:O	2.01	0.58
1:C:288:ARG:NH1	8:C:785:HOH:O	2.36	0.58
1:C:405:TYR:CD2	1:C:405:TYR:O	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:A:44:SER:HG	6:A:505:GLU:HB2	1.69	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:393:ARG:HH22	6:A:505:GLU:CD	2.11	0.54
1:A:138:ARG:HD3	1:C:163:PHE:CE1	2.42	0.54
1:A:138:ARG:HG3	1:C:163:PHE:CZ	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
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:302:ASN:HA	1:C:276:ARG:HG2	1.92	0.50
1:A:240:GLY:N	3:A:502:AKG:O3	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:TYR:CE1	4:A:503:G9A:H5	2.45	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:407:ASP:N	1:A:407:ASP:OD1	2.45	0.49
1:A:47:ARG:O	1:A:47:ARG:NH2	2.43	0.49
1:C:400:ARG:HH12	4:C:503:G9A:C2	2.25	0.49
1:C:90:LYS:CE	8:C:856:HOH:O	2.56	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:108:MET:HB3	1:C:119:GLN:HE22	1.77	0.48
1:C:46:VAL:CG1	7:C:505:KYA:C10	2.90	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:C:115:TYR:OH	3:C:502:AKG:C5	2.63	0.47
1:A:26:MET:HG3	1:C:259:GLY:HA3	1.96	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:C3	5:C:504:3EE:N	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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:263:TYR:HH	3:C:502:AKG:H42	1.83	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:CG	1:C:405:TYR:O	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: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:C:196:LYS:HG2	1:C:196:LYS:HZ2	1.45	0.42
1:A:276:ARG:CG	1:C:302:ASN:HA	2.49	0.42
1:C:389:PHE:CE1	8:C:755:HOH:O	2.55	0.42
5:A:504:3EE:O4	5:A:504:3EE:C5	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:HA	1:C:289:LYS:HD3	1.84	0.41
1:A:279:TRP:HZ2	8:A:878:HOH:O	2.03	0.41
1:A:302:ASN:HA	1:C:276:ARG:CG	2.51	0.41
1:A:170:GLN:HE22	1:A:392:HIS:H	1.63	0.41
1:C:392:HIS:HD2	8:C:768:HOH:O	2.02	0.41
1:C:251:LYS:NZ	3:C:502:AKG:O4	2.53	0.41
1:A:274:GLY:HA2	1:C:303:VAL:HG12	2.02	0.41
1:A:85:GLU:HG3	1:C:77:ARG:HH12	1.85	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:148:VAL:HB	1:C:200:VAL:HG22	2.03	0.40
5:C:504:3EE:H1	8:C:1017:HOH:O	2.21	0.40
1:C:56:SER:OG	1:C:58:ILE:HD12	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

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%)	47 25
1	C	402/448 (90%)	388 (96%)	14 (4%)	0	100 100
All	All	804/896 (90%)	783 (97%)	20 (2%)	1 (0%)	51 28

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	408	GLU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	349/388 (90%)	339 (97%)	10 (3%)	42	16
1	C	349/388 (90%)	340 (97%)	9 (3%)	46	19
All	All	698/776 (90%)	679 (97%)	19 (3%)	44	18

All (19) 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	77	ARG
1	A	346	GLU
1	A	406	VAL
1	A	407	ASP
1	A	408	GLU
1	C	27	LEU
1	C	36	LYS
1	C	46	VAL
1	C	181	GLU
1	C	196	LYS
1	C	251	LYS
1	C	257	ASN
1	C	396	LYS
1	C	407	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	295	GLN
1	C	306	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

There are no monosaccharides in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
5	3EE	C	504	-	12,15,15	1.52	1 (8%)	14,20,20	0.71	0
5	3EE	A	504	-	12,15,15	1.60	1 (8%)	14,20,20	1.82	5 (35%)
6	GLU	A	505	-	2,9,9	1.55	0	2,11,11	0.36	0
7	KYA	C	505	-	12,15,15	1.81	3 (25%)	16,21,21	2.08	4 (25%)
2	PMP	C	501	1	16,16,16	0.93	1 (6%)	21,23,23	1.00	2 (9%)
4	G9A	A	503	-	2,8,8	0.46	0	1,9,9	1.54	0
4	G9A	C	503	-	2,8,8	0.44	0	1,9,9	1.51	0
3	AKG	C	502	-	3,9,9	2.64	2 (66%)	4,11,11	2.00	2 (50%)
2	PMP	A	501	1	16,16,16	1.62	3 (18%)	21,23,23	1.51	4 (19%)
3	AKG	A	502	-	3,9,9	1.94	1 (33%)	4,11,11	2.14	2 (50%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	3EE	C	504	-	-	3/8/12/12	0/1/1/1
5	3EE	A	504	-	-	7/8/12/12	0/1/1/1
6	GLU	A	505	-	-	2/3/9/9	-
7	KYA	C	505	-	-	0/0/4/4	0/2/2/2
2	PMP	C	501	1	-	3/8/8/8	0/1/1/1
4	G9A	A	503	-	-	0/2/6/6	-
4	G9A	C	503	-	-	1/2/6/6	-
3	AKG	C	502	-	-	3/3/9/9	-
2	PMP	A	501	1	-	3/8/8/8	0/1/1/1
3	AKG	A	502	-	-	3/3/9/9	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	504	3EE	C1-C4	5.28	1.49	1.41
5	C	504	3EE	C1-C4	5.03	1.48	1.41
3	C	502	AKG	O5-C2	-3.66	1.16	1.22
7	C	505	KYA	C1-C2	3.63	1.48	1.42
2	A	501	PMP	O4P-C5A	-3.53	1.31	1.45
7	C	505	KYA	C3-C1	3.21	1.48	1.42
2	A	501	PMP	P-O2P	-3.09	1.42	1.54
3	A	502	AKG	C3-C2	-2.93	1.46	1.51
3	C	502	AKG	C3-C2	-2.68	1.47	1.51
2	A	501	PMP	C3-C2	-2.64	1.38	1.40
2	C	501	PMP	C2-N1	2.46	1.38	1.33
7	C	505	KYA	C7-N	2.08	1.36	1.33

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	505	KYA	C7-N-C2	5.22	121.94	118.06
5	A	504	3EE	C6-C4-C1	-4.16	114.06	118.10
2	A	501	PMP	O2P-P-O4P	3.96	117.27	106.73
7	C	505	KYA	O1-C3-C1	3.85	121.12	116.31
7	C	505	KYA	C1-C2-N	-3.15	119.47	122.81
3	C	502	AKG	C3-C4-C5	-2.89	107.83	112.67
3	A	502	AKG	C3-C4-C5	2.83	117.42	112.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	PMP	C5A-C5-C6	-2.79	114.78	119.37
3	C	502	AKG	C4-C3-C2	-2.62	107.50	113.14
3	A	502	AKG	O5-C2-C3	-2.57	115.98	120.38
5	A	504	3EE	C7-C8-C6	2.44	123.90	120.19
2	C	501	PMP	C6-C5-C4	2.32	119.76	118.12
2	A	501	PMP	C3-C4-C5	-2.31	116.51	118.72
7	C	505	KYA	C6-C3-C1	-2.28	117.81	120.52
2	C	501	PMP	C5-C6-N1	-2.24	120.08	123.82
5	A	504	3EE	C8-C7-C5	-2.15	116.91	120.19
5	A	504	3EE	C3-C2-C1	-2.11	115.23	119.01
5	A	504	3EE	O1-C2-C3	2.07	122.89	120.56
2	A	501	PMP	C4A-C4-C5	2.04	124.43	120.19

There are no chirality outliers.

All (25) torsion outliers are listed below:

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

There are no ring outliers.

8 monomers are involved in 106 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	504	3EE	13	0
5	A	504	3EE	13	0
6	A	505	GLU	8	0
7	C	505	KYA	16	0
4	A	503	G9A	17	0
4	C	503	G9A	18	0
3	C	502	AKG	13	0
3	A	502	AKG	16	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	404/448 (90%)	-0.40	3 (0%)	87 88	15, 21, 41, 59	0
1	C	404/448 (90%)	-0.38	6 (1%)	73 75	14, 21, 41, 59	0
All	All	808/896 (90%)	-0.39	9 (1%)	80 82	14, 21, 41, 59	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	428	ALA	5.0
1	C	428	ALA	4.9
1	C	43	ALA	3.7
1	C	55	THR	3.3
1	A	43	ALA	2.6
1	A	52	LEU	2.5
1	C	52	LEU	2.3
1	C	409	ASP	2.2
1	C	25	SER	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 monosaccharides 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	G9A	C	503	9/9	0.64	0.26	24,37,44,47	0
5	3EE	C	504	15/15	0.67	0.29	34,41,44,48	0
4	G9A	A	503	9/9	0.68	0.24	20,34,43,44	0
5	3EE	A	504	15/15	0.70	0.23	30,38,46,48	0
7	KYA	C	505	14/14	0.74	0.25	35,40,43,50	0
6	GLU	A	505	10/10	0.83	0.22	34,38,43,45	0
3	AKG	A	502	10/10	0.94	0.23	19,35,41,45	0
3	AKG	C	502	10/10	0.95	0.24	24,37,42,46	0
2	PMP	A	501	16/16	0.96	0.08	15,19,24,32	0
2	PMP	C	501	16/16	0.97	0.08	16,18,23,27	0

6.5 Other polymers (i)

There are no such residues in this entry.