WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Sep 20, 2023 – 05:20 AM EDT

PDB ID	:	5K0P
Title	:	Crystal structure of the archaeosine synthase QueF-Like in the apo form
Authors	:	Mei, X.; Swairjo, M.A.
Deposited on	:	2016-05-17
Resolution	:	1.94 Å(reported)

The following versions of software and data (see references (i)) 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	:	2.35.1
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)	:	2.35.1

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 1.94 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	Percentile Ranks	Value
Rfree		0.242
Clashscore		6
Ramachandran outliers		0.2%
Sidechain outliers		3.5%
RSRZ outliers		3.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
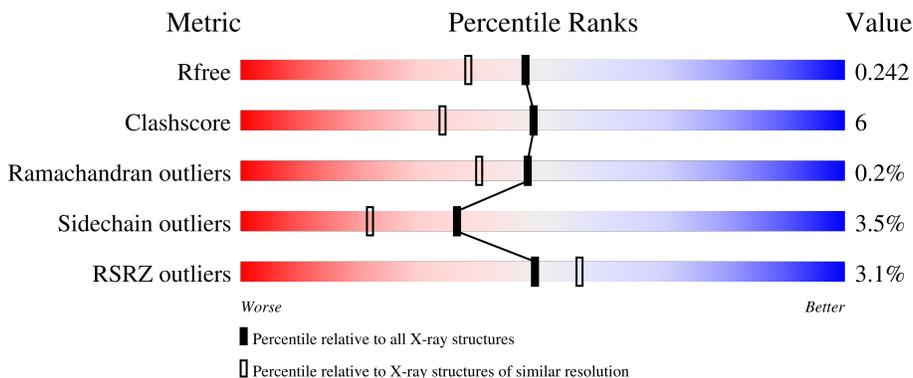
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	4310 (1.96-1.92)
Clashscore	141614	1023 (1.94-1.94)
Ramachandran outliers	138981	1007 (1.94-1.94)
Sidechain outliers	138945	1007 (1.94-1.94)
RSRZ outliers	127900	4250 (1.96-1.92)

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 <=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	109	3% — 78% — 15% — •• 6%
1	B	109	3% — 80% — 11% — • 8%
1	C	109	3% — 73% — 17% — • 7%
1	D	109	2% — 83% — 8% — • 7%
1	E	109	2% — 72% — 17% — • 8%
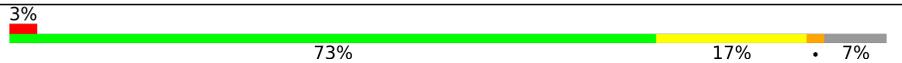
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	109	4% 81% 10% · 7%
1	G	109	4% 76% 14% ·· 7%
1	H	109	5% 72% 17% · 9%
1	I	109	2% 81% 10% · 6%
1	J	109	3% 76% 13% · 8%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 8452 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 Archeaosine synthase QueF-Like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	103	Total	C	N	O	S	0	2	0
			817	528	134	153	2			
1	B	100	Total	C	N	O	S	0	1	0
			781	502	127	150	2			
1	C	101	Total	C	N	O	S	0	2	0
			794	512	129	151	2			
1	D	101	Total	C	N	O	S	0	6	0
			827	532	131	162	2			
1	E	100	Total	C	N	O	S	0	2	0
			787	505	128	152	2			
1	F	101	Total	C	N	O	S	0	1	0
			788	507	128	151	2			
1	G	101	Total	C	N	O	S	0	1	0
			790	508	131	149	2			
1	H	99	Total	C	N	O	S	0	1	0
			776	498	129	147	2			
1	I	102	Total	C	N	O	S	0	3	0
			808	519	131	156	2			
1	J	100	Total	C	N	O	S	0	0	0
			775	498	127	148	2			

- Molecule 2 is THIOCYANATE ION (three-letter code: SCN) (formula: CNS).

SCN
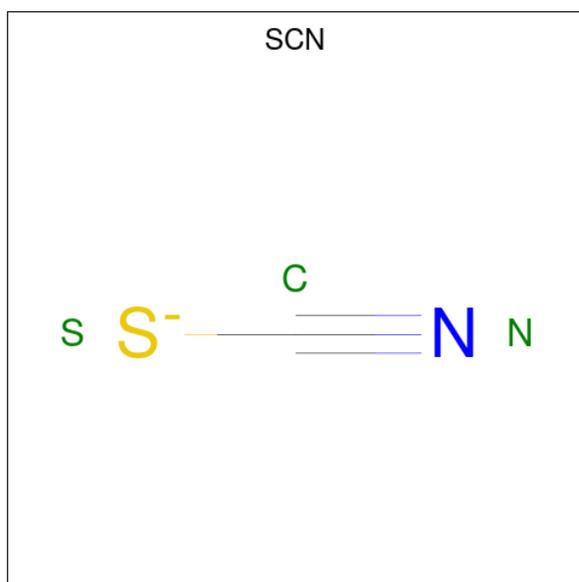
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 3	C 1	N 1	S 1	0	0
2	B	1	Total 3	C 1	N 1	S 1	0	0
2	C	1	Total 3	C 1	N 1	S 1	0	0
2	D	1	Total 3	C 1	N 1	S 1	0	0
2	E	1	Total 3	C 1	N 1	S 1	0	0
2	F	1	Total 3	C 1	N 1	S 1	0	0
2	G	1	Total 3	C 1	N 1	S 1	0	0
2	H	1	Total 3	C 1	N 1	S 1	0	0
2	I	1	Total 3	C 1	N 1	S 1	0	0
2	J	1	Total 3	C 1	N 1	S 1	0	0

- Molecule 3 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).
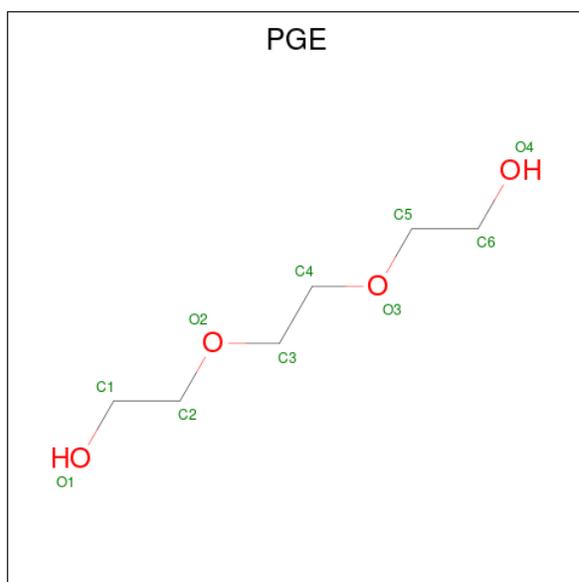
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total 10	C 6	O 4	0	0
3	D	1	Total 10	C 6	O 4	0	0
3	F	1	Total 10	C 6	O 4	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).
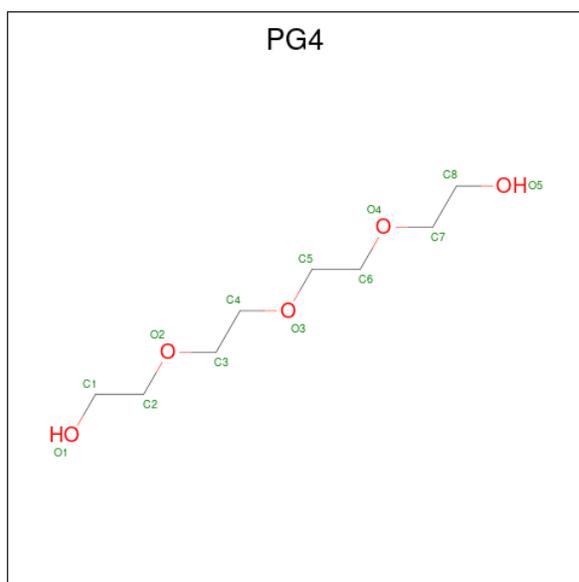
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	I	1	Total 13	C 8	O 5	0	0

• Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	60	Total 60 / O 60	0	0
5	B	50	Total 50 / O 50	0	0
5	C	55	Total 55 / O 55	0	0
5	D	48	Total 48 / O 48	0	0
5	E	37	Total 37 / O 37	0	0
5	F	43	Total 43 / O 43	0	0
5	G	34	Total 34 / O 34	0	0
5	H	45	Total 45 / O 45	0	0
5	I	39	Total 39 / O 39	0	0
5	J	25	Total 25 / O 25	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: Archeaosine synthase QueF-Like

Chain A:

- Molecule 1: Archeaosine synthase QueF-Like

Chain B:

- Molecule 1: Archeaosine synthase QueF-Like

Chain C:

- Molecule 1: Archeaosine synthase QueF-Like

Chain D:

- Molecule 1: Archeaosine synthase QueF-Like

Chain E:

- Molecule 1: Archeaosine synthase QueF-Like

Chain F:

4%

81% 10% · 7%

MET LEU LYS VAL SER K6 R12 R16 G17 E18 S29 R39 E46 E63 N78 P79 V95 E96 V97 G103 V104 P105 P106 VAL TYR ILE

• Molecule 1: Archeaosine synthase QueF-Like

Chain G:

4%

76% 14% ·· 7%

MET LEU LYS VAL SER K6 R12 E18 I23 V27 E35 Y36 I37 G40 E46 D53 R56 L70 N78 P79 P80 E96 S101 V104 P105 P106 VAL TYR ILE

• Molecule 1: Archeaosine synthase QueF-Like

Chain H:

5%

72% 17% · 9%

MET LEU LYS VAL SER K6 S7 P8 S9 L10 V11 R12 E18 P22 K25 R39 G40 I45 E46 E47 F48 K49 K50 L61 H62 E63 E64 D68 L69 L70 A75 N78 P79 P80 V97 E100 S101 G102 G103 V104 PRO PRO VAL TYR ILE

• Molecule 1: Archeaosine synthase QueF-Like

Chain I:

2%

81% 10% · 6%

MET LEU LYS VAL SER K6 R12 R16 E31 G40 K49 K50 R56 E63 V67 E71 V77 N78 P79 E96 V97 V107 TYR ILE

• Molecule 1: Archeaosine synthase QueF-Like

Chain J:

3%

76% 13% · 8%
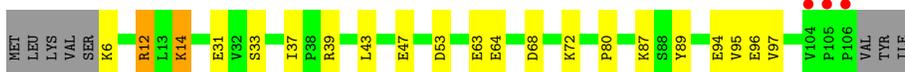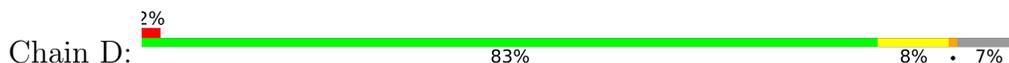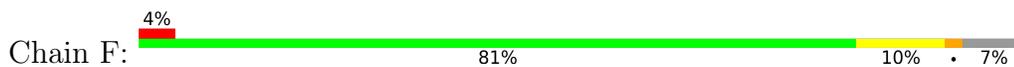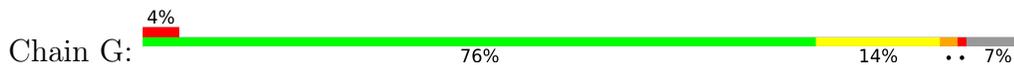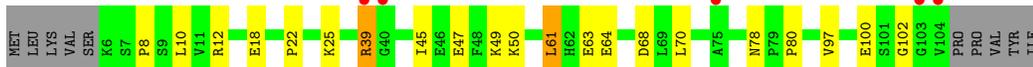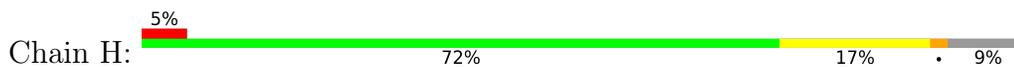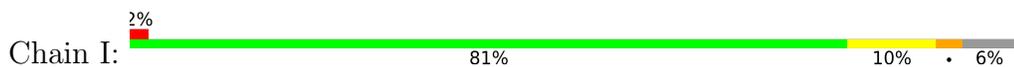
MET LEU LYS VAL SER K6 R12 E35 Y36 I37 P38 R39 G40 A41 E46 R56 E63 V67 E71 V77 N78 P79 K87 E96 V97 V104 P105 PRO VAL TYR ILE
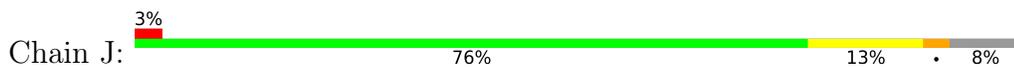
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	62.21Å 125.00Å 74.40Å 90.00° 112.27° 90.00°	Depositor
Resolution (Å)	69.00 – 1.94 28.46 – 1.94	Depositor EDS
% Data completeness (in resolution range)	99.0 (69.00-1.94) 99.1 (28.46-1.94)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.32 (at 1.93Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.155 , 0.238 0.167 , 0.242	Depositor DCC
R_{free} test set	3886 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	26.7	Xtriage
Anisotropy	0.274	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 39.6	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8452	wwPDB-VP
Average B, all atoms (Å^2)	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.96% 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: SCN, PG4, PGE

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	1.14	1/835 (0.1%)	1.08	3/1132 (0.3%)
1	B	1.22	2/797 (0.3%)	1.14	6/1079 (0.6%)
1	C	1.23	1/814 (0.1%)	1.08	2/1102 (0.2%)
1	D	1.16	2/851 (0.2%)	1.06	0/1153
1	E	1.05	0/803	1.18	5/1088 (0.5%)
1	F	1.11	1/805 (0.1%)	1.23	6/1091 (0.5%)
1	G	1.13	3/807 (0.4%)	1.18	7/1093 (0.6%)
1	H	1.23	3/791 (0.4%)	1.20	7/1069 (0.7%)
1	I	1.08	0/828	1.05	1/1124 (0.1%)
1	J	1.06	1/788 (0.1%)	1.16	2/1067 (0.2%)
All	All	1.14	14/8119 (0.2%)	1.14	39/10998 (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	H	0	1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	18	GLU	CD-OE2	-7.43	1.17	1.25
1	H	64	GLU	CD-OE1	7.28	1.33	1.25
1	B	46	GLU	CD-OE1	6.99	1.33	1.25
1	G	46	GLU	CD-OE1	6.86	1.33	1.25
1	C	64	GLU	CD-OE2	-6.30	1.18	1.25
1	G	18	GLU	CD-OE2	-6.11	1.19	1.25
1	B	59	GLU	CD-OE2	5.75	1.31	1.25
1	D	94[A]	GLU	CD-OE2	-5.44	1.19	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	94[B]	GLU	CD-OE2	-5.44	1.19	1.25
1	G	18	GLU	CB-CG	-5.25	1.42	1.52
1	J	46	GLU	CD-OE1	5.11	1.31	1.25
1	A	71	GLU	CG-CD	5.09	1.59	1.51
1	F	46	GLU	CD-OE1	5.07	1.31	1.25
1	H	102	GLY	N-CA	5.05	1.53	1.46

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	39	ARG	NE-CZ-NH2	-10.37	115.12	120.30
1	H	12	ARG	NE-CZ-NH1	10.01	125.30	120.30
1	F	39	ARG	NE-CZ-NH1	9.88	125.24	120.30
1	E	12	ARG	NE-CZ-NH2	9.73	125.17	120.30
1	E	39	ARG	NE-CZ-NH1	9.00	124.80	120.30
1	E	39	ARG	NE-CZ-NH2	-8.33	116.13	120.30
1	E	12	ARG	NE-CZ-NH1	-7.31	116.64	120.30
1	G	12[A]	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	G	12[B]	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	C	12	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	B	12	ARG	NE-CZ-NH2	-6.63	116.98	120.30
1	B	12	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	H	64	GLU	CG-CD-OE2	-6.33	105.64	118.30
1	C	53	ASP	CB-CG-OD1	6.31	123.97	118.30
1	G	12[A]	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	G	12[B]	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	H	12	ARG	NE-CZ-NH2	-6.27	117.17	120.30
1	F	12	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	B	71[A]	GLU	OE1-CD-OE2	-6.09	116.00	123.30
1	B	71[B]	GLU	OE1-CD-OE2	-6.09	116.00	123.30
1	G	18	GLU	CB-CA-C	-6.03	98.34	110.40
1	J	12	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	H	18	GLU	CB-CA-C	-5.93	98.53	110.40
1	H	68	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	59	GLU	OE1-CD-OE2	5.85	130.32	123.30
1	H	64	GLU	CG-CD-OE1	5.84	129.98	118.30
1	G	56	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	F	63	GLU	CB-CA-C	-5.53	99.34	110.40
1	A	50	LYS	CD-CE-NZ	5.51	124.37	111.70
1	A	39	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	I	12	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	B	58	ARG	NE-CZ-NH2	-5.35	117.62	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	18	GLU	CB-CA-C	-5.35	99.69	110.40
1	F	18	GLU	CB-CA-C	-5.32	99.75	110.40
1	G	56	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	J	56	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	35	GLU	CB-CA-C	5.14	120.69	110.40
1	F	16	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	H	61	LEU	CA-CB-CG	5.01	126.82	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	100	GLU	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	817	0	852	12	0
1	B	781	0	810	7	0
1	C	794	0	830	14	0
1	D	827	0	847	8	0
1	E	787	0	814	12	0
1	F	788	0	817	5	0
1	G	790	0	824	11	0
1	H	776	0	810	15	0
1	I	808	0	836	11	0
1	J	775	0	804	13	0
2	A	3	0	0	0	0
2	B	3	0	0	0	0
2	C	3	0	0	0	0
2	D	3	0	0	0	0
2	E	3	0	0	0	0
2	F	3	0	0	0	0
2	G	3	0	0	0	0
2	H	3	0	0	1	0
2	I	3	0	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	3	0	0	0	0
3	C	10	0	14	0	0
3	D	10	0	14	2	0
3	F	10	0	14	0	0
4	I	13	0	18	4	0
5	A	60	0	0	3	0
5	B	50	0	0	3	0
5	C	55	0	0	0	0
5	D	48	0	0	2	0
5	E	37	0	0	2	0
5	F	43	0	0	0	0
5	G	34	0	0	1	0
5	H	45	0	0	6	0
5	I	39	0	0	3	0
5	J	25	0	0	2	0
All	All	8452	0	8304	98	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 (98) 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:A:56:ARG:NH2	5:A:301:HOH:O	2.14	0.80
1:D:89[B]:TYR:CE2	3:D:201:PGE:H42	2.18	0.77
1:H:39[B]:ARG:CZ	5:H:302:HOH:O	2.32	0.76
1:A:79:PRO:HG2	1:A:82:VAL:CG2	2.19	0.72
1:H:47:GLU:HG3	5:H:339:HOH:O	1.91	0.70
1:E:39:ARG:HD2	5:E:312:HOH:O	1.91	0.70
1:H:8:PRO:C	5:H:306:HOH:O	2.30	0.68
1:I:96:GLU:OE1	5:I:301:HOH:O	2.11	0.68
1:J:39:ARG:HG3	5:J:324:HOH:O	1.96	0.64
1:F:95:VAL:HG21	1:H:45:ILE:HD13	1.80	0.64
1:A:16:ARG:NH2	5:A:303:HOH:O	2.32	0.62
1:A:12[B]:ARG:NH2	1:D:96:GLU:OE1	2.32	0.62
1:H:63:GLU:HA	1:H:97:VAL:HG11	1.80	0.62
1:H:39[B]:ARG:NH2	5:H:302:HOH:O	2.33	0.62
1:A:31:GLU:OE1	5:A:302:HOH:O	2.16	0.61
1:I:12:ARG:NH1	1:J:96:GLU:OE1	2.34	0.60
1:C:14[A]:LYS:NZ	1:C:33:SER:OG	2.20	0.60
1:B:96:GLU:OE1	1:C:12:ARG:NH1	2.35	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:16:ARG:HD2	1:I:16:ARG:HD3	1.84	0.59
1:I:63:GLU:HA	1:I:97:VAL:HG11	1.85	0.58
1:E:16:ARG:NH1	5:E:302:HOH:O	2.36	0.57
1:B:63:GLU:HG3	5:B:338:HOH:O	2.04	0.57
1:H:8:PRO:HB2	5:H:306:HOH:O	2.04	0.57
1:B:63:GLU:HA	1:B:97:VAL:HG11	1.85	0.56
1:A:79:PRO:HG2	1:A:82:VAL:HG23	1.88	0.56
1:A:12[A]:ARG:NH2	1:A:35:GLU:OE1	2.39	0.55
1:C:14[A]:LYS:NZ	1:C:31:GLU:OE1	2.40	0.55
1:G:37:ILE:O	1:G:80:PRO:HD2	2.08	0.54
1:J:87:LYS:HG2	1:J:96:GLU:HG2	1.90	0.54
1:J:37:ILE:O	1:J:79:PRO:HB3	2.09	0.53
1:G:78:ASN:N	1:G:79:PRO:HD3	2.24	0.52
1:J:63:GLU:HA	1:J:97:VAL:HG11	1.92	0.51
1:J:41:ALA:HB3	1:J:77:VAL:HG22	1.91	0.51
1:I:16:ARG:HH12	4:I:201:PG4:H72	1.75	0.51
1:G:96:GLU:HB2	1:J:12:ARG:HB2	1.93	0.51
1:F:63:GLU:HA	1:F:97:VAL:HG11	1.92	0.51
1:I:77:VAL:HG23	1:I:79:PRO:HG3	1.93	0.50
1:C:89:TYR:CE2	1:C:94:GLU:HG2	2.47	0.50
1:B:47:GLU:CG	5:B:339:HOH:O	2.60	0.50
1:F:95:VAL:HG21	1:H:45:ILE:CD1	2.43	0.49
1:G:27:VAL:HG11	1:H:49:LYS:HE2	1.94	0.49
1:A:63:GLU:HA	1:A:97:VAL:HG11	1.94	0.49
1:I:16:ARG:NH1	4:I:201:PG4:H72	2.28	0.49
1:A:96:GLU:OE1	1:E:12:ARG:NH2	2.44	0.48
1:C:63:GLU:HA	1:C:97:VAL:HG11	1.94	0.48
1:D:77:VAL:HG23	1:D:79:PRO:HG3	1.95	0.48
1:G:12[B]:ARG:NH1	1:G:35:GLU:OE1	2.46	0.48
1:D:24:SER:OG	1:D:26:THR:HB	2.14	0.48
2:I:202:SCN:C	5:I:310:HOH:O	2.60	0.47
1:C:43:LEU:HD11	1:C:47[C]:GLU:HG2	1.95	0.47
1:C:14[A]:LYS:HE2	1:C:31:GLU:HG2	1.97	0.47
1:E:55:TYR:OH	1:E:72:LYS:HE2	2.15	0.47
1:G:53:ASP:O	1:G:56:ARG:HB2	2.14	0.47
1:J:77:VAL:HG13	1:J:79:PRO:HG3	1.96	0.47
1:I:67:VAL:O	1:I:71:GLU:HG3	2.15	0.46
1:C:68:ASP:OD2	1:C:72:LYS:HE2	2.16	0.46
1:E:37:ILE:O	1:E:80:PRO:HD2	2.16	0.46
1:F:104:VAL:HG22	1:F:106:PRO:HD2	1.98	0.46
1:J:41:ALA:HA	5:J:310:HOH:O	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:70:LEU:HD21	1:G:101:SER:HB2	1.98	0.46
1:D:64[A]:GLU:OE1	5:D:301:HOH:O	2.20	0.46
1:E:20:VAL:O	1:E:59:GLU:HA	2.16	0.45
1:J:104:VAL:O	1:J:105:PRO:O	2.34	0.45
1:C:96:GLU:OE1	1:G:12[A]:ARG:NH2	2.43	0.45
1:E:104:VAL:CG1	1:E:105:PRO:HD2	2.47	0.45
1:B:63:GLU:CG	5:B:338:HOH:O	2.62	0.45
1:D:64[B]:GLU:HG2	5:D:314:HOH:O	2.17	0.45
1:F:78:ASN:N	1:F:79:PRO:HD3	2.32	0.45
1:H:22:PRO:HD2	2:H:201:SCN:S	2.58	0.44
1:C:39:ARG:HB2	1:C:80:PRO:HD3	2.00	0.44
1:H:39[B]:ARG:NE	1:H:78:ASN:O	2.51	0.44
1:I:16:ARG:HH12	4:I:201:PG4:C7	2.31	0.44
1:G:56:ARG:HD2	5:G:313:HOH:O	2.18	0.43
1:E:14:LYS:HE3	1:E:31:GLU:CD	2.39	0.43
1:H:10:LEU:N	5:H:306:HOH:O	2.51	0.43
4:I:201:PG4:H12	5:I:316:HOH:O	2.18	0.43
1:C:14[A]:LYS:HE3	1:C:14[A]:LYS:HB2	1.50	0.43
1:A:37:ILE:O	1:A:80:PRO:HD2	2.19	0.43
1:D:89[B]:TYR:CZ	3:D:201:PGE:H42	2.54	0.43
1:G:105:PRO:HB3	1:G:106:PRO:HD2	2.01	0.43
1:H:39[B]:ARG:NH2	1:H:80:PRO:HD3	2.34	0.43
1:H:39[A]:ARG:CG	1:H:39[A]:ARG:HH21	2.31	0.42
1:B:87:LYS:HG2	1:B:96:GLU:HG2	2.01	0.42
1:J:41:ALA:CB	1:J:77:VAL:HG22	2.50	0.42
1:E:63:GLU:HA	1:E:97:VAL:HG11	2.01	0.42
1:A:12[A]:ARG:HG2	1:A:35:GLU:HB2	2.02	0.42
1:E:56:ARG:NH1	1:I:56:ARG:NH2	2.67	0.41
1:I:16:ARG:NH1	1:I:31:GLU:HB2	2.35	0.41
1:C:87:LYS:HG2	1:C:96:GLU:HG2	2.01	0.41
1:G:105:PRO:CB	1:G:106:PRO:HD2	2.50	0.41
1:J:67:VAL:O	1:J:71:GLU:HG2	2.21	0.41
1:B:37:ILE:O	1:B:80:PRO:HD2	2.21	0.41
1:C:37:ILE:O	1:C:80:PRO:HD2	2.21	0.41
1:A:12[B]:ARG:HB2	1:D:96:GLU:HB2	2.03	0.40
1:J:12:ARG:HG2	1:J:35:GLU:HB3	2.03	0.40
1:E:78:ASN:N	1:E:79:PRO:HD3	2.36	0.40
1:C:87:LYS:HA	1:C:95:VAL:O	2.21	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	103/109 (94%)	99 (96%)	3 (3%)	1 (1%)	15	6
1	B	99/109 (91%)	96 (97%)	3 (3%)	0	100	100
1	C	101/109 (93%)	98 (97%)	3 (3%)	0	100	100
1	D	105/109 (96%)	101 (96%)	4 (4%)	0	100	100
1	E	100/109 (92%)	97 (97%)	3 (3%)	0	100	100
1	F	100/109 (92%)	97 (97%)	3 (3%)	0	100	100
1	G	100/109 (92%)	95 (95%)	4 (4%)	1 (1%)	15	6
1	H	98/109 (90%)	95 (97%)	3 (3%)	0	100	100
1	I	103/109 (94%)	101 (98%)	2 (2%)	0	100	100
1	J	98/109 (90%)	92 (94%)	6 (6%)	0	100	100
All	All	1007/1090 (92%)	971 (96%)	34 (3%)	2 (0%)	47	39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	VAL
1	G	40	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	93/97 (96%)	89 (96%)	4 (4%)	29	14

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	89/97 (92%)	87 (98%)	2 (2%)	52	39
1	C	91/97 (94%)	88 (97%)	3 (3%)	38	24
1	D	95/97 (98%)	91 (96%)	4 (4%)	30	14
1	E	90/97 (93%)	87 (97%)	3 (3%)	38	24
1	F	90/97 (93%)	88 (98%)	2 (2%)	52	39
1	G	90/97 (93%)	87 (97%)	3 (3%)	38	24
1	H	88/97 (91%)	82 (93%)	6 (7%)	16	4
1	I	93/97 (96%)	88 (95%)	5 (5%)	22	8
1	J	88/97 (91%)	86 (98%)	2 (2%)	50	38
All	All	907/970 (94%)	873 (96%)	34 (4%)	36	19

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	GLU
1	A	50	LYS
1	A	70	LEU
1	A	108	TYR
1	B	9	SER
1	B	63	GLU
1	C	6	LYS
1	C	14[A]	LYS
1	C	14[B]	LYS
1	D	9[A]	SER
1	D	9[B]	SER
1	D	26	THR
1	D	50	LYS
1	E	6	LYS
1	E	16	ARG
1	E	28	ASP
1	F	29	SER
1	F	104	VAL
1	G	56	ARG
1	G	70	LEU
1	G	104	VAL
1	H	25	LYS
1	H	39[A]	ARG
1	H	39[B]	ARG
1	H	50	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	61	LEU
1	H	70	LEU
1	I	6	LYS
1	I	49	LYS
1	I	50	LYS
1	I	56	ARG
1	I	63	GLU
1	J	71	GLU
1	J	77	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	78	ASN
1	E	78	ASN
1	G	78	ASN

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 ⓘ

14 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
4	PG4	I	201	-	12,12,12	0.77	0	11,11,11	0.92	1 (9%)
2	SCN	G	201	1	1,2,2	0.13	0	0,1,1	-	-
2	SCN	H	201	1	1,2,2	0.47	0	0,1,1	-	-
3	PGE	F	201	-	9,9,9	0.79	0	8,8,8	0.62	0
2	SCN	I	202	1	1,2,2	0.07	0	0,1,1	-	-
2	SCN	A	201	1	1,2,2	0.48	0	0,1,1	-	-
2	SCN	C	202	1	1,2,2	0.33	0	0,1,1	-	-
2	SCN	E	201	1	1,2,2	0.05	0	0,1,1	-	-
3	PGE	C	201	-	9,9,9	0.54	0	8,8,8	0.58	0
2	SCN	D	202	1	1,2,2	0.72	0	0,1,1	-	-
2	SCN	B	201	1	1,2,2	0.42	0	0,1,1	-	-
3	PGE	D	201	-	9,9,9	0.97	0	8,8,8	0.70	0
2	SCN	F	202	1	1,2,2	0.09	0	0,1,1	-	-
2	SCN	J	201	1	1,2,2	0.38	0	0,1,1	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PG4	I	201	-	-	5/10/10/10	-
3	PGE	D	201	-	-	4/7/7/7	-
3	PGE	C	201	-	-	2/7/7/7	-
3	PGE	F	201	-	-	4/7/7/7	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	201	PG4	O4-C7-C8	2.47	120.90	110.07

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	I	201	PG4	O2-C3-C4-O3
3	F	201	PGE	O3-C5-C6-O4
3	D	201	PGE	O3-C5-C6-O4
4	I	201	PG4	C6-C5-O3-C4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	201	PGE	O2-C3-C4-O3
3	C	201	PGE	O2-C3-C4-O3
3	D	201	PGE	O1-C1-C2-O2
4	I	201	PG4	O4-C7-C8-O5
4	I	201	PG4	C8-C7-O4-C6
3	F	201	PGE	C4-C3-O2-C2
3	F	201	PGE	O1-C1-C2-O2
4	I	201	PG4	C3-C4-O3-C5
3	C	201	PGE	C1-C2-O2-C3
3	D	201	PGE	C4-C3-O2-C2
3	F	201	PGE	C3-C4-O3-C5

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	201	PG4	4	0
2	H	201	SCN	1	0
2	I	202	SCN	1	0
3	D	201	PGE	2	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.

W O R L D W I D E
wwPDB
PROTEIN DATA BANK

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	103/109 (94%)	-0.33	3 (2%)	51	59	19, 28, 50, 109	0
1	B	100/109 (91%)	-0.38	3 (3%)	50	57	19, 29, 53, 107	0
1	C	101/109 (92%)	-0.47	3 (2%)	50	57	19, 28, 48, 111	0
1	D	101/109 (92%)	-0.53	2 (1%)	65	71	20, 29, 50, 75	0
1	E	100/109 (91%)	-0.31	2 (2%)	65	71	22, 33, 55, 96	0
1	F	101/109 (92%)	-0.32	4 (3%)	38	45	24, 33, 49, 125	0
1	G	101/109 (92%)	-0.33	4 (3%)	38	45	23, 33, 58, 95	0
1	H	99/109 (90%)	-0.35	5 (5%)	28	35	19, 32, 57, 87	0
1	I	102/109 (93%)	-0.45	2 (1%)	65	71	24, 34, 55, 76	0
1	J	100/109 (91%)	-0.45	3 (3%)	50	57	26, 36, 66, 101	0
All	All	1008/1090 (92%)	-0.39	31 (3%)	49	56	19, 32, 56, 125	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	106	PRO	12.3
1	A	108	TYR	11.1
1	E	105	PRO	8.2
1	C	106	PRO	8.2
1	B	105	PRO	7.8
1	A	107	VAL	6.9
1	F	104	VAL	6.6
1	F	105	PRO	6.2
1	E	104	VAL	5.6
1	G	106	PRO	5.6
1	H	104	VAL	5.0
1	G	105	PRO	4.2
1	F	103	GLY	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	J	105	PRO	3.4
1	B	104	VAL	3.2
1	H	40	GLY	3.1
1	H	103	GLY	3.1
1	A	40	GLY	3.0
1	G	104	VAL	3.0
1	I	107	VAL	2.9
1	C	104	VAL	2.9
1	I	40	GLY	2.8
1	J	104	VAL	2.8
1	J	6	LYS	2.4
1	C	105	PRO	2.4
1	D	106	PRO	2.4
1	D	89[A]	TYR	2.2
1	H	39[A]	ARG	2.1
1	G	23	ILE	2.1
1	B	40	GLY	2.1
1	H	75	ALA	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PGE	C	201	10/10	0.65	0.22	62,73,81,81	0
3	PGE	F	201	10/10	0.71	0.15	54,62,74,77	0
4	PG4	I	201	13/13	0.74	0.15	54,70,77,88	0
3	PGE	D	201	10/10	0.85	0.14	40,42,52,55	0
2	SCN	F	202	3/3	0.87	0.15	67,67,74,79	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
2	SCN	H	201	3/3	0.89	0.13	50,50,54,70	0
2	SCN	B	201	3/3	0.92	0.16	73,73,75,89	0
2	SCN	J	201	3/3	0.95	0.13	66,66,77,85	0
2	SCN	E	201	3/3	0.96	0.13	66,66,77,90	0
2	SCN	I	202	3/3	0.97	0.11	66,66,88,100	0
2	SCN	D	202	3/3	0.97	0.12	51,51,64,72	0
2	SCN	A	201	3/3	0.99	0.08	44,44,57,63	0
2	SCN	G	201	3/3	0.99	0.16	71,71,72,81	0
2	SCN	C	202	3/3	0.99	0.06	40,40,51,69	0

6.5 Other polymers (i)

There are no such residues in this entry.